Electronic Supplementary Information (ESI)

One-pot synthesis of 4-(imidazol-1-yl)indole derivatives through sequential dearomatization and Ag-catalyzed cyclization/Cs_2CO_3-mediated addition/aromatization reaction

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1. General Information.

All one-pot reactions were carried out in an over-dried vial equipped with a magnetic stir bar under nitrogen atmosphere. MeCN was distilled from P_2O_5; THF and dioxane were distilled from sodium; DCE and DMF was distilled from CaH_2. *o*-Alkynylanilines and N-protected o-alkynylanilines[1] were synthesized according to the known literatures. All other reagents were obtained from commercial sources and utilized without further purification, if not stated otherwise. All melting points are uncorrected. The NMR spectra were recorded in $CDCl_3$ on a 400 or 600 M Hz instrument with TMS as internal standard. Recorded shifts were reported in parts per million (δ) downfield from TMS. Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad), coupling constant (*J*, Hz) and integration. TLC was carried out with 0.2 mm thick silica gel plates (GF254). Visualization was accomplished by UV light. The column chromatography was hand packed with silica gel 60 (160-200 mesh). The products were additionally confirmed by HRMS. Mass spectra were obtained using ESI ionization.

2. General Procedure for the One-Pot Synthesis of Products 3.

An oven-dried vial was charged with a magnetic stir bar, *o*-alkynylaniline **1** (0.2 mmol) and MeOH (1 mL). PhIO (0.22 mmol, 1.1 equiv.) was added into the stirred solution at rt. After being stirred for about 10 min, MeOH was removed under reduced pressure. Cs_2CO_3 (0.4 mmol, 2 equiv), MeCN (1 mL), and $AgNO_3$ (0.02 mmol, 10 mol%) was added to the mixture subsequentially under N_2. The mixture was pre-stirred at rt for about 10 min. After that, a solution of imidazole **2** (0.22, 1.1 equiv) in MeCN (1 mL) was added to the mixture under N_2 at rt. The mixture was stirred at rt for about 12 h (monitored by TLC). The solvent was removed in vacuo, and the residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (4:1~1:1, v:v) as eluent to afford product **3**.

3. Procedure for the One-Pot Synthesis of 3a at 3-mmol Scale.

An oven-dried flask was charged with a magnetic stir bar, *o*-alkynylaniline **1a** (3 mmol) and MeOH (15 mL). PhIO (3.3 mmol, 1.1 equiv.) was added to the stirred solution in portions at rt. After being stirred for about 20 min, MeOH was removed under reduced pressure. Cs_2CO_3 (6 mmol, 2 equiv), MeCN (20 mL), and $AgNO_3$ (0.3 mmol, 10 mol%) was added to the mixture subsequentially under N_2. The mixture was pre-stirred at rt for about 20 min. After that, a solution of imidazole **2** (3.3 mmol, 1.1 equiv) in MeCN (10 mL) was added to the mixture under N_2 at rt. The mixture was stirred at rt for about 20 h (monitored by TLC). The solvent was removed in vacuo, and the residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (3:1, v:v) as eluent to afford product **3a** (0.856 g, 67% yield).

4. Procedures for the Derivatizations.

(1) Procedure for the Synthesis of Derivative 7a.

To a stirred solution of **3a** (0.4 mmol) in MeOH (3 mL) was added K_2CO_3 (1.2 mmol, 3.0 equiv). After being stirred for 2 h at 60 °C, MeOH was removed in vacuo, and the reaction mixture was poured into water (20 mL) and extracted with ethyl acetate (20 mL × 3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in vacuo, subsequently. The residue was purified by flash column chromatography on silica gel using petroleum ether/ethyl acetate (2:1, v:v) as eluent to afford derivative **7a** (82% yield).

(2) Procedure for the Synthesis of Derivative 8a.

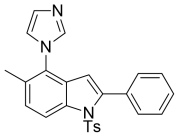
To a stirred solution of **10** (0.2 mmol) and NaH (60%, 8.0 mg, 0.2 mmol, 1.0 equiv) in dry DMF (2 mL), was added CH_3I (0.2 mmol, 1.0 equiv). After stirring for 2 h at rt, the reaction mixture was poured into H_2O (20 mL) and extracted with ethyl acetate (10 mL × 3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in vacuo to give a residue, which was purified by flash column chromatography on silica gel using petroleum ether/ethyl acetate (3:1, v:v) as eluent to afford derivative **8a** (78% yield).

(3) General Procedure for the Synthesis of Derivatives 9.

To a sealing tube equipped with a magnetic stirrer were added **3t** (0.2 mmol), arylboronic acid (0.4 mmol, 2.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 5 mol%) and Na_2CO_3 (0.2 mmol, 1.0 equiv). To this mixture were added a mixed solvent (2.2 mL, toluene:ethanol:water = 5:5:1, v:v:v) under N_2. The mixture stirred at 120 °C for 16 h under N_2. After being cooled to rt, the solvent was removed in vacuo, and the residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (3:1, v:v) as eluent to afford derivative **9**.

5. Characterization Data of Compounds 3

4-(1H-Imidazol-1-yl)-5-methyl-2-phenyl-1-tosyl-1H-indole (3a).

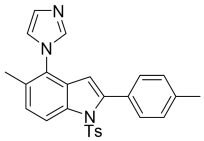


Prepared according to general procedure. The mixture was stirred at rt for about 12 h (monitored by TLC) and the product was isolated in 72% yield after chromatography as white solid (61.2 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.41); mp 195 – 197 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.6 Hz, 1H), 7.54 (s, 1H), 7.45 – 7.32 (m, 5H), 7.31 – 7.25 (m, 3H), 7.19 (s, 1H), 7.06 (d, J = 8.0 Hz, 2H), 7.01 (s, 1H), 6.18 (s, 1H), 2.29 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.96, 143.33, 137.74, 136.96, 134.59, 131.51, 130.37,

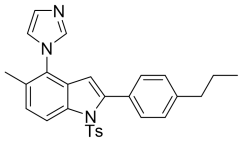
129.83, 129.43, 129.37, 129.00, 128.18, 127.90, 127.49, 127.35, 126.81, 120.53, 116.76, 109.58, 21.56, 16.99.
HRMS (ESI) for $C_{25}H_{22}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 428.1427, found 428.1440.

4-(1H-Imidazol-1-yl)-5-methyl-2-(*p*-tolyl)-1-tosyl-1H-indole (3b)



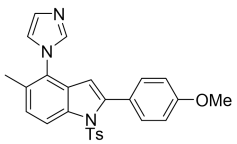
Prepared according to general procedure. The mixture was stirred at rt for about 16 h (monitored by TLC) and the product was isolated in 73% yield after chromatography as white solid (64.8 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.40); mp 166 – 168 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.5 Hz, 1H), 7.55 (s, 1H), 7.34 – 7.27 (m, 5H), 7.21 – 7.16 (m, 3H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.01 (s, 1H), 6.15 (s, 1H), 2.40 (s, 3H), 2.31 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.95, 143.68, 139.15, 137.81, 137.03, 134.70, 130.32, 129.86, 129.46, 129.36, 128.70, 128.38, 128.33, 127.87, 127.23, 126.92, 120.62, 116.90, 109.35, 21.64, 21.48, 17.07.
HRMS (ESI) for $C_{26}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 442.1584, found 442.1601.

4-(1H-Imidazol-1-yl)-5-methyl-2-(4-propylphenyl)-1-tosyl-1H-indole (3c)



Prepared according to general procedure. The mixture was stirred at rt for about 16 h (monitored by TLC) and the product was isolated in 70% yield after chromatography as white solid (65.9 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.39); mp 189 – 191 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.6 Hz, 1H), 7.57 (s, 1H), 7.34 – 7.26 (m, 5H), 7.23 – 7.17 (m, 3H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.03 (s, 1H), 6.15 (s, 1H), 2.64 (t, *J* = 7.7 Hz, 2H), 2.32 (s, 3H), 2.21 (s, 3H), 1.72 – 1.65 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.90, 143.83, 143.65, 137.81, 137.03, 134.73, 130.33, 129.79, 129.42, 129.02, 128.86, 128.33, 127.87, 127.67, 127.19, 126.92, 120.57, 116.84, 109.30, 37.90, 24.41, 21.62, 17.05, 13.89.
HRMS (ESI) for $C_{28}H_{28}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 470.1897, found 470.1890.

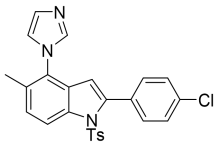
4-(1H-Imidazol-1-yl)-2-(4-methoxyphenyl)-5-methyl-1-tosyl-1H-indole (3d)



Prepared according to general procedure. The mixture was stirred at rt for about 16 h (monitored by TLC) and the product was isolated in 61% yield after chromatography as white solid (55.4 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.28); mp 192 – 194 °C.

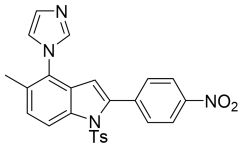
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.6 Hz, 1H), 7.55 (s, 1H), 7.35 – 7.31 (m, 2H), 7.30 – 7.26 (m, 3H), 7.21 (s, 1H), 7.08 (d, *J* = 8.1 Hz, 2H), 7.02 (s, 1H), 6.93 – 6.88 (m, 2H), 6.12 (s, 1H), 3.86 (s, 3H), 2.32 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.44, 145.00, 143.50, 137.94, 137.08, 134.87, 131.91, 129.93, 129.52, 128.49, 127.89, 127.18, 127.00, 123.92, 120.67, 119.52, 117.00, 113.14, 109.07, 55.46, 21.73, 17.16.
HRMS (ESI) for $C_{26}H_{24}N_3O_3S^+$ [M+H]$^+$ m/z: calcd 458.1533, found 458.1551.

2-(4-Chlorophenyl)-4-(1H-imidazol-1-yl)-5-methyl-1-tosyl-1H-indole (3e)



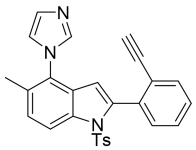
Prepared according to general procedure. The mixture was stirred at rt for about 18 h (monitored by TLC) and the product was isolated in 79% yield after chromatography as white solid (73.2 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.43); mp 176 – 178 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.6 Hz, 1H), 7.55 (s, 1H), 7.38 – 7.26 (m, 7H), 7.21 (s, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 7.02 (s, 1H), 6.18 (s, 1H), 2.32 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (101MHz, $CDCl_3$) δ 145.25, 142.13, 137.85, 137.14, 135.32, 134.57, 131.68, 130.16, 130.07, 129.61, 129.16, 128.21, 128.07, 127.93, 127.74, 126.86, 120.64, 116.95, 110.05, 21.70, 17.10.
HRMS (ESI) for $C_{25}H_{21}ClN_3O_2S^+$ [M+H]$^+$ m/z: calcd 462.1038, found 462.1051.

4-(1H-Imidazol-1-yl)-5-methyl-2-(4-nitrophenyl)-1-tosyl-1H-indole (3f)



Prepared according to general procedure. The mixture was stirred at rt for about 18 h (monitored by TLC) and the product was isolated in 65% yield after chromatography as yellow solid (61 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.32); mp 243 – 245 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 – 8.19 (m, 3H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.56 (s, 1H), 7.36 (d, *J* = 8.6 Hz, 1H), 7.30 – 7.26 (m, 2H), 7.22 (s, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.02 (s, 1H), 6.32 (s, 1H), 2.33 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.97, 145.62, 140.84, 138.11, 137.81, 137.51, 134.13, 131.06, 130.64, 129.78, 129.61, 128.59, 128.40, 128.11, 126.79, 122.93, 120.63, 117.08, 111.86, 21.72, 17.13.
HRMS (ESI) for $C_{25}H_{21}N_4O_4S^+$ [M+H]$^+$ m/z: calcd 473.1278, found 473.1290.

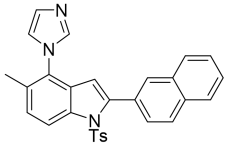
2-(2-Ethynylphenyl)-4-(1H-imidazol-1-yl)-5-methyl-1-tosyl-1H-indole (3g)



Prepared according to general procedure. The mixture was stirred at rt for about 14 h (monitored by TLC) and the product was isolated in 57% yield after chromatography as white solid (51.4 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.26); mp 196 – 198 °C.

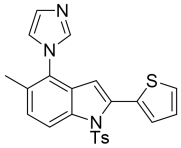
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.7 Hz, 1H), 7.54 (s, 2H), 7.49 – 7.27 (m, 6H), 7.20 – 7.07 (m, 3H), 7.02 (s, 1H), 6.33 (s, 1H), 2.90 (s, 1H), 2.30 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.01, 140.29, 137.91, 136.28, 135.00, 134.42, 132.87, 131.72, 129.63, 129.54, 129.53, 128.96, 128.22, 127.85, 127.82, 127.52, 127.24, 123.10, 120.66, 116.10, 110.33, 82.09, 81.15, 21.72, 17.17.
HRMS (ESI) for $C_{27}H_{22}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 452.1427, found 452.1426.

4-(1H-Imidazol-1-yl)-5-methyl-2-(naphthalen-2-yl)-1-tosyl-1H-indole (3h)



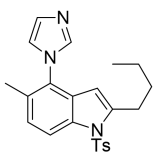
Prepared according to general procedure. The mixture was stirred at rt for about 16 h (monitored by TLC) and the product was isolated in 68% yield after chromatography as white solid (64.6 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.38); mp 194 – 196 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.5 Hz, 1H), 7.88 – 7.81 (m, 4H), 7.62 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.57 (s, 1H), 7.54 – 7.50 (m, 2H), 7.33 – 7.27 (m, 3H), 7.22 (s, 1H), 7.05 (d, *J* = 8.7 Hz, 3H), 6.30 (s, 1H), 2.30 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.08, 143.51, 137.88, 137.23, 134.66, 133.42, 132.59, 130.04, 129.58, 129.51, 129.31, 129.21, 128.44, 128.38, 128.28, 128.07, 127.88, 127.54, 126.98, 126.94, 126.54, 120.63, 116.94, 110.25, 21.67, 17.13 (one peak is missing).
HRMS (ESI) for $C_{29}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 478.1584, found 478.1589.

4-(1H-Imidazol-1-yl)-5-methyl-2-(thiophen-2-yl)-1-tosyl-1H-indole (3i)



Prepared according to general procedure. The mixture was stirred at rt for about 12 h (monitored by TLC) and the product was isolated in 66% yield after chromatography as white solid (57.6 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.34); mp 175 – 177 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.6 Hz, 1H), 7.55 (s, 1H), 7.36 (d, *J* = 5.1 Hz, 1H), 7.34 – 7.29 (m, 3H), 7.28 – 7.26 (m, 1H), 7.20 (s, 1H), 7.10 – 7.05 (m, 3H), 7.02 (s, 1H), 6.26 (s, 1H), 2.30 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.11, 137.80, 137.06, 135.27, 134.81, 131.24, 131.13, 129.86, 129.58, 129.49, 127.89, 127.74, 127.69, 127.67, 127.08, 126.89, 120.60, 116.66, 110.42, 21.64, 17.02.
HRMS (ESI) for $C_{23}H_{20}N_3O_2S_2^+$ $[M+H]^+$ m/z: calcd 434.0991, found 434.0999.

2-Butyl-4-(1H-imidazol-1-yl)-5-methyl-1-tosyl-1H-indole (3j)



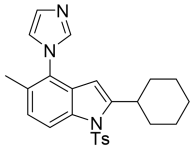
Prepared according to general procedure. The mixture was stirred at rt for about 18 h (monitored

by TLC) and the product was isolated in 64% yield after chromatography as white solid (51.9 mg) (petroleum ether/EtOAc = 3:1, R_f = 0.25); mp 114 – 116 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.56 (s, 1H), 7.26 – 7.16 (m, 4H), 7.02 (s, 1H), 6.00 (s, 1H), 2.91 (t, *J* = 7.7 Hz, 2H), 2.35 (s, 3H), 2.17 (s, 3H), 1.66 – 1.57 (m, 2H), 1.43 – 1.33 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.11, 144.23, 137.91, 136.12, 130.06, 129.47, 129.09, 127.75, 127.50, 126.47, 126.46, 126.36, 120.66, 115.15, 104.82, 30.92, 28.74, 22.58, 21.69, 17.01, 13.94.

HRMS (ESI) for $C_{23}H_{26}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 408.1740, found 408.1750.

2-Cyclohexyl-4-(1H-imidazol-1-yl)-5-methyl-1-tosyl-1H-indole (3k)

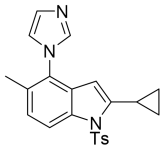


Prepared according to general procedure. The mixture was stirred at rt for about 18 h (monitored by TLC) and the product was isolated in 51% yield after chromatography as white solid (44 mg) (petroleum ether/EtOAc = 3:1, R_f = 0.27); mp 170– 172 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.63 – 7.54 (m, 3H), 7.24 – 7.13 (m, 4H), 7.02 (s, 1H), 6.01 (s, 1H), 3.26 (t, *J* = 11.9 Hz, 1H), 2.35 (s, 3H), 2.16 (s, 3H), 1.98 (d, *J* = 12.6 Hz, 2H), 1.81 – 1.69 (m, 3H), 1.45 – 1.34 (m, 2H), 1.27 – 1.17 (m, 3H). ^{13}C NMR (101MHz, $CDCl_3$) δ 150.19, 145.01, 137.91, 136.14, 136.11, 129.98, 129.41, 129.18, 128.03, 127.59, 126.35, 126.33, 120.68, 115.62, 103.49, 37.48, 34.47, 26.66, 26.13, 21.69, 16.99.

HRMS (ESI) for $C_{25}H_{28}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 434.1897, found 434.1905.

2-cyclopropyl-4-(1H-imidazol-1-yl)-5-methyl-1-tosyl-1H-indole (3l)

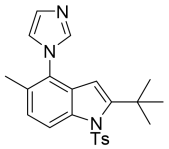


Prepared according to general procedure. The mixture was stirred at rt for about 15 h (monitored by TLC) and the product was isolated in 60% yield after chromatography as white solid (47.2 mg) (petroleum ether/EtOAc = 3:1, R_f = 0.22); mp 145 – 147 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.6 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 2H), 7.56 (s, 1H), 7.26 – 7.22 (m, 3H), 7.20 (d, *J* = 8.6 Hz, 1H), 7.02 (s, 1H), 5.78 (s, 1H), 2.45 – 2.39 (m, 1H), 2.38 (s, 3H), 2.18 (s, 3H), 0.96 – 0.91 (m, 2H), 0.54 – 0.49 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.71, 145.10, 137.87, 136.34, 136.27, 129.90, 129.48, 129.04, 127.58, 127.29, 126.80, 126.43, 120.63, 114.87, 102.26, 21.70, 16.98, 9.39, 8.68.

HRMS (ESI) for $C_{22}H_{22}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 392.1427, found 392.1442.

2-(*tert*-Butyl)-4-(1H-imidazol-1-yl)-5-methyl-1-tosyl-1H-indole (3m)

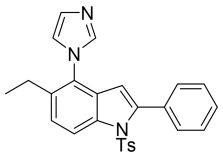


Prepared according to general procedure. The mixture was stirred at rt for about 12 h (monitored by TLC) and the product was isolated in 58% yield after chromatography as white solid (47.3 mg) (petroleum ether/EtOAc = 3:1, R_f = 0.23); mp 171 – 173 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.6 Hz, 1H), 7.55 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.23 (s, 1H), 7.15 (d, *J* = 8.1 Hz, 2H), 7.09 (d, *J* = 8.7 Hz, 1H), 7.02 (s, 1H), 6.19 (s, 1H), 2.31 (s, 3H), 2.11 (s, 3H), 1.50 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.39, 144.50, 137.85, 137.76, 136.79, 129.75, 129.46, 129.21, 127.66, 126.89, 126.66, 126.08, 120.65, 116.33, 106.46, 35.16, 31.26, 21.58, 16.88.

HRMS (ESI) for $C_{23}H_{26}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 408.1740, found 408.1749.

5-Ethyl-4-(1H-imidazol-1-yl)-2-phenyl-1-tosyl-1H-indole (3n)

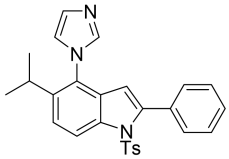


Prepared according to general procedure. The mixture was stirred at rt for about 18 h (monitored by TLC) and the product was isolated in 64% yield after chromatography as white solid (56.6 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.30); mp 134 – 135 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.7 Hz, 1H), 7.53 (s, 1H), 7.48 – 7.26 (m, 8H), 7.18 (s, 1H), 7.11 – 6.97 (m, 3H), 6.13 (s, 1H), 2.49 (q, *J* = 7.6 Hz, 2H), 2.30 (s, 3H), 1.11 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.05, 143.37, 138.16, 136.89, 136.32, 134.92, 131.64, 130.56, 129.55, 129.15, 128.49, 127.63, 127.42, 127.03, 126.02, 125.41, 121.06, 117.25, 109.72, 23.86, 21.72, 15.95.

HRMS (ESI) for $C_{26}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 442.1584, found 442.1595.

4-(1H-Imidazol-1-yl)-5-isopropyl-2-phenyl-1-tosyl-1H-indole (3o)

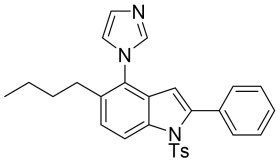


Prepared according to general procedure and isolated, the mixture was stirred at rt for about 16 h (monitored by TLC) in 69% yield after chromatography as white solid (62.5 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.33); mp 203 – 205 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.8 Hz, 1H), 7.58 (s, 1H), 7.45 – 7.39 (m, 2H), 7.38 – 7.34 (m, 4H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.23 (s, 1H), 7.10 (d, *J* = 8.1 Hz, 2H), 7.04 (s, 1H), 6.10 (s, 1H), 2.85 – 2.71 (m, 1H), 2.33 (s, 3H), 1.21 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.99, 143.13, 140.97, 138.30, 136.43, 134.99, 131.56, 130.54, 129.51, 129.48, 129.06, 128.30, 127.54, 127.01, 126.51, 122.95, 121.30, 117.45, 109.65, 27.55, 24.42, 21.67.

HRMS (ESI) for $C_{27}H_{26}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 456.1740, found 456.1751.

5-Butyl-4-(1H-imidazol-1-yl)-2-phenyl-1-tosyl-1H-indole (3p)

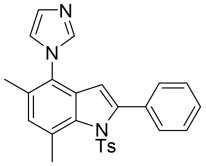


Prepared according to general procedure. The mixture was stirred at rt for about 16 h (monitored by TLC) and the product was isolated in 77% yield after chromatography as white solid (72.6 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.32); mp 156 – 158 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.6 Hz, 1H), 7.53 (s, 1H), 7.41 – 7.31 (m, 6H), 7.30 – 7.26 (m, 2H), 7.18 (s, 1H), 7.06 (d, *J* = 7.9 Hz, 2H), 7.00 (s, 1H), 6.13 (s, 1H), 2.46 (t, *J* = 7.8 Hz, 2H), 2.29 (s, 3H), 1.49 – 1.40 (m, 2H), 1.25 – 1.17 (m, 2H), 0.81 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.97, 143.21, 138.07, 136.76, 134.96, 134.78, 131.56, 130.45, 129.45, 129.39, 129.02, 128.41, 127.51, 126.91, 126.84, 126.51, 121.01, 116.99, 109.64, 33.63, 30.27, 22.47, 21.60, 13.83.

HRMS (ESI) for $C_{28}H_{28}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 470.1897, found 470.1905.

4-(1H-Imidazol-1-yl)-5,7-dimethyl-2-phenyl-1-tosyl-1H-indole (3q)

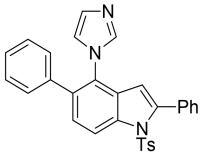


Prepared according to general procedure. The mixture was stirred at rt for about 18 h (monitored by TLC) and the product was isolated in 71% yield after chromatography as white solid (62.4 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.28); mp 180 – 182 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.38 (m, 3H), 7.37 – 7.33 (m, 3H), 7.22 (s, 1H), 7.14 (s, 1H), 6.99 (d, *J* = 8.2 Hz, 2H), 6.97 – 6.90 (m, 3H), 6.07 (s, 1H), 2.86 (s, 3H), 2.33 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.70, 144.82, 139.74, 138.11, 132.59, 132.21, 132.12, 131.78, 131.41, 130.91, 129.63, 129.11, 128.56, 128.02, 127.66, 127.44, 126.08, 120.73, 112.51, 21.70, 21.41, 16.98.

HRMS (ESI) for $C_{26}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 442.1584, found 442.1589.

4-(1H-Imidazol-1-yl)-2,5-diphenyl-1-tosyl-1H-indole (3r)

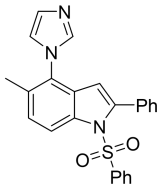


Prepared according to general procedure. The mixture was stirred at rt for about 12 h (monitored by TLC) and the product was isolated in 53% yield after chromatography as white solid (51.5 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.25); mp 208 – 210 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.6 Hz, 1H), 7.56 – 7.31 (m, 10H), 7.29 – 7.24 (m, 3H), 7.17 – 7.05 (m, 5H), 6.38 (s, 1H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.17, 143.63, 137.94, 137.69, 134.85, 133.79, 131.42, 130.55, 129.60, 129.49, 129.32, 129.19, 128.59, 128.51, 128.44, 127.59, 127.44, 126.98, 126.75, 126.69, 116.64, 109.74, 21.66 (one peak is missing).

HRMS (ESI) for $C_{30}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 490.1584, found 490.1584.

4-(1H-Imidazol-1-yl)-5-methyl-2-phenyl-1-(phenylsulfonyl)-1H-indole (3s)

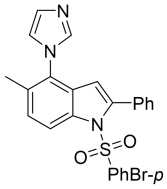


Prepared according to general procedure. The mixture was stirred at rt for about 15 h (monitored by TLC) and the product was isolated in 85% yield after chromatography as white solid (70.5 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.26); mp 225 – 226 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.6 Hz, 1H), 7.54 (s, 1H), 7.48 (d, *J* = 7.3 Hz, 1H), 7.45 – 7.36 (m, 7H), 7.35 – 7.27 (m, 3H), 7.20 (s, 1H), 7.01 (s, 1H), 6.19 (s, 1H), 2.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.45, 137.87, 137.61, 137.10, 133.97, 131.50, 130.50, 130.11, 129.57, 129.21, 128.92, 128.34, 128.09, 127.67, 127.54, 126.92, 120.61, 116.90, 109.81, 17.12.

HRMS (ESI) for $C_{24}H_{20}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 414.1271, found 414.1280.

1-((4-Bromophenyl)sulfonyl)-4-(1H-imidazol-1-yl)-5-methyl-2-phenyl-1H-indole (3t)

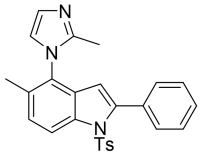


Prepared according to general procedure. The mixture was stirred at rt for about 14 h (monitored by TLC) and the product was isolated in 69% yield after chromatography as white solid (68.3 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.43); mp 138 – 140 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.6 Hz, 1H), 7.57 (s, 1H), 7.53 – 7.28 (m, 9H), 7.26 – 7.19 (m, 2H), 7.04 (s, 1H), 6.24 (s, 1H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.30, 137.83, 136.93, 136.39, 132.26, 131.30, 130.45, 129.64, 129.35, 129.28, 128.42, 128.38, 128.24, 127.75, 127.73, 125.44, 120.59, 116.83, 110.22, 17.13.

HRMS (ESI) for $C_{24}H_{19}BrN_3O_2S^+$ $[M+H]^+$ m/z: calcd 492.0376, found 492.0388.

5-Methyl-4-(2-methyl-1H-imidazol-1-yl)-2-phenyl-1-tosyl-1H-indole (3u)

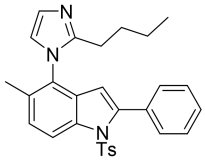


Prepared according to general procedure. The mixture was stirred at rt for about 16 h (monitored by TLC) and the product was isolated in 68% yield after chromatography as white solid (59.8 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.27); mp 173 – 175 °C.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.2 Hz, 1H), 7.61 – 7.32 (m, 6H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.25 (s, 1H), 7.11 – 7.02 (m, 3H), 6.84 (s, 1H), 6.07 (s, 1H), 2.30 (s, 3H), 2.11 (s, 3H), 1.99 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.39, 144.93, 143.84, 137.29, 134.44, 131.58, 131.12, 130.35, 129.29, 129.08, 128.96, 128.18, 128.11, 127.58, 127.27, 126.88, 120.33, 117.29, 109.84, 21.57, 16.77, 12.86.

HRMS (ESI) for $C_{26}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 442.1584, found 442.1596.

4-(2-Butyl-1H-imidazol-1-yl)-5-methyl-2-phenyl-1-tosyl-1H-indole (3v)

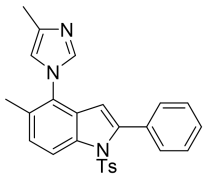


Prepared according to general procedure. The mixture was stirred at rt for about 24 h (monitored by TLC) and the product was isolated in 37% yield after chromatography as white solid (35.9 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.25); mp 100 – 102 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.6 Hz, 1H), 7.41 – 7.33 (m, 5H), 7.28 (d, *J* = 8.5 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.07 – 7.02 (m, 3H), 6.80 (s, 1H), 6.05 (s, 1H), 2.27 (s, 3H), 2.25 – 2.13 (m, 2H), 2.08 (s, 3H), 1.43 – 1.35 (m, 2H), 1.11 – 1.05 (m, 2H), 0.65 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.14, 144.86, 143.82, 137.22, 134.27, 131.57, 131.21, 130.25, 129.24, 129.19, 129.04, 128.14, 128.08, 127.56, 127.27, 126.79, 120.06, 117.29, 110.06, 29.77, 26.40, 22.12, 21.53, 16.74, 13.61.

HRMS (ESI) for $C_{29}H_{30}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 484.2053, found 484.2066.

5-Methyl-4-(4-methyl-1H-imidazol-1-yl)-2-phenyl-1-tosyl-1H-indole (3w)

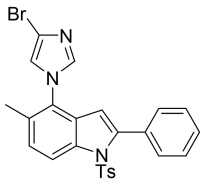


Prepared according to general procedure. The mixture was stirred at rt for about 18 h (monitored by TLC) and the product was isolated in 63% yield after chromatography as white solid (55.5 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.28); mp 176 – 178 °C.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.6 Hz, 1H), 7.43 – 7.40 (m, 4H), 7.39 – 7.36 (m, 2H), 7.29 – 7.26 (m, 3H), 7.08 (d, *J* = 8.1 Hz, 2H), 6.72 (s, 1H), 6.23 (s, 1H), 2.31 (s, 3H), 2.27 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.98, 143.27, 138.46, 137.07, 137.03, 134.70, 131.69, 130.46, 129.85, 129.50, 129.08, 128.31, 128.28, 127.59, 127.42, 126.93, 117.00, 116.67, 109.99, 21.69, 17.19, 13.79.

HRMS (ESI) for $C_{26}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 442.1584, found 442.1599.

4-(4-Bromo-1H-imidazol-1-yl)-5-methyl-2-phenyl-1-tosyl-1H-indole (3x)

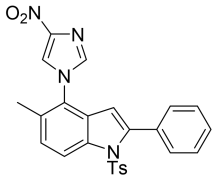


Prepared according to general procedure. The mixture was stirred at rt for about 15 h (monitored by TLC) and the product was isolated in 78% yield after chromatography as white solid (78.8 mg) (petroleum ether/EtOAc = 3:1, R_f = 0.42); mp 190 – 192 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.6 Hz, 1H), 7.49 – 7.32 (m, 7H), 7.31 – 7.27 (m, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 7.01 (s, 1H), 6.20 (s, 1H), 2.31 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (101 MHz,

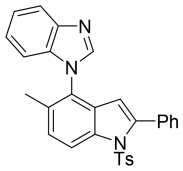
$CDCl_3$) δ 145.12, 143.74, 137.60, 137.04, 134.65, 131.40, 130.47, 129.88, 129.54, 129.21, 128.07, 127.61, 127.41, 127.10, 126.89, 119.74, 117.33, 115.81, 109.19, 21.66, 17.05.
HRMS (ESI) for $C_{25}H_{21}BrN_3O_2S^+$ $[M+H]^+$ m/z: calcd 506.0532, found 506.0547.

5-Methyl-4-(4-nitro-1H-imidazol-1-yl)-2-phenyl-1-tosyl-1H-indole (3y)



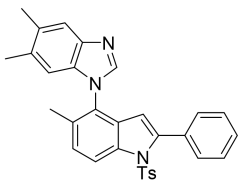
Prepared according to general procedure. The mixture was stirred at rt for about 20 h (monitored by TLC) and the product was isolated in 49% yield after chromatography as yellow solid (46.5 mg), (petroleum ether/EtOAc = 3:1, R_f = 0.32); mp 223 – 225 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.6 Hz, 1H), 7.85 (s, 1H), 7.50 (s, 1H), 7.42 – 7.31 (m, 6H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 6.15 (s, 1H), 2.31 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.49, 145.35, 144.36, 137.09, 136.93, 134.60, 131.07, 130.51, 129.68, 129.63, 129.40, 127.66, 127.49, 126.90, 125.81, 120.57, 118.12, 108.24, 21.67, 17.05 (one peak is missing).
HRMS (ESI) for $C_{25}H_{21}N_4O_4S^+$ $[M+H]^+$ m/z: calcd 473.1278, found 473.1294.

1-(5-Methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-1H-benzo[*d*]imidazole (3z)



Prepared according to general procedure. The mixture was stirred at rt for about 22 h (monitored by TLC) and the product was isolated in 55% yield after chromatography as white solid (52.5 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.24); mp 197 – 199 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.6 Hz, 1H), 7.96 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.40 – 7.37 (m, 3H), 7.35 – 7.29 (m, 5H), 7.28 – 7.25 (m, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.03 (s, 1H), 2.30 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.93, 143.52, 143.14, 143.04, 137.26, 134.33, 134.26, 131.35, 131.20, 130.25, 129.34, 128.94, 128.79, 127.51, 127.41, 126.77, 125.84, 123.49, 122.50, 120.34, 117.33, 110.45, 109.73, 21.52, 17.06.
HRMS (ESI) for $C_{29}H_{24}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 478.1584, found 478.1592.

5,6-Dimethyl-1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-1H-benzo[*d*]imidazole (3aa)



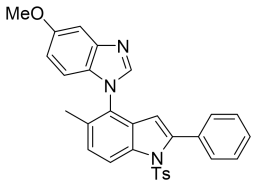
Prepared according to general procedure. The mixture was stirred at rt for about 22 h (monitored by TLC) and the product was isolated in 64% yield after chromatography as white solid (64.4 mg)

(petroleum ether/EtOAc = 1:1, R_f = 0.24); mp 192 – 194 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.6 Hz, 1H), 7.84 (s, 1H), 7.63 (s, 1H), 7.40 – 7.34 (m, 6H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.67 (s, 1H), 6.03 (s, 1H), 2.37 (s, 3H), 2.34 (s, 3H), 2.26 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.00, 143.62, 142.40, 141.91, 137.44, 134.58, 133.04, 132.88, 131.61, 131.58, 131.45, 130.42, 129.45, 129.12, 129.09, 127.58, 127.57, 126.96, 126.33, 120.48, 117.40, 110.62, 110.07, 21.70, 20.58, 20.35, 17.23.

HRMS (ESI) for $C_{31}H_{28}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 506.1897, found 506.1909.

5-Methoxy-1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-1H-benzo[*d*]imidazole (3ab)



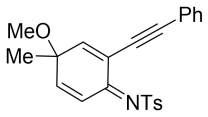
Prepared according to general procedure. The mixture was stirred at rt for about 24 h (monitored by TLC) and the product was isolated in 79% yield after chromatography as white solid (80.7 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.20); mp 178 – 180 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.6 Hz, 1H), 7.84 (s, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.41 – 7.33 (m, 6H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.92 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.33 (d, *J* = 2.3 Hz, 1H), 6.04 (s, 1H), 3.67 (s, 3H), 2.32 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.29, 145.02, 143.63, 142.27, 137.70, 137.39, 135.08, 134.56, 131.47, 131.34, 130.39, 129.44, 129.09, 128.89, 127.63, 127.55, 126.92, 125.98, 120.94, 117.42, 112.03, 109.91, 93.75, 55.75, 21.63, 17.22.

HRMS (ESI) for $C_{30}H_{26}N_3O_3S^+$ $[M+H]^+$ m/z: calcd 508.1689, found 508.1711.

6. Characterization Data of Intermediate 4a

N-(4-Methoxy-4-methyl-2-(phenylethynyl)cyclohexa-2,5-dien-1-ylidene)-4-methylbenzenesulfonamide[2]

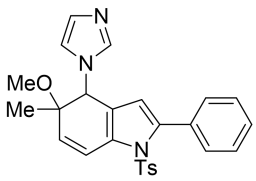


The compound was isolated as an intermediate during the optimization. White solid (petroleum ether/EtOAc = 5:1, R_f = 0.33); mp 148 – 150 °C (Lit. mp 155-156 °C)[2].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.1 Hz, 2H), 7.64 (d, *J* = 10.3 Hz, 1H), 7.36 – 7.28 (m, 7H), 7.02 (d, *J* = 2.6 Hz, 1H), 6.77 (dd, *J* = 10.3, 2.6 Hz, 1H), 3.22 (s, 3H), 2.45 (s, 3H), 1.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.00, 153.28, 151.52, 143.64, 138.76, 131.80, 129.44, 128.94, 128.42, 127.22, 125.26, 123.94, 122.49, 94.34, 83.15, 73.07, 53.99, 26.30, 21.72.

7. Characterization Data of by-Products 5a and 6a

4-(1H-Imidazol-1-yl)-5-methoxy-5-methyl-2-phenyl-1-tosyl-4,5-dihydro-1H-indole (5a)

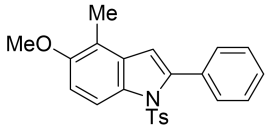


The compound was isolated as a by-product during the optimization. White solid (petroleum ether/EtOAc = 1:5, R_f = 0.31); mp 151 – 153 °C.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (s, 9H), 7.17 (s, 2H), 6.94 (s, 1H), 6.64 (s, 1H), 6.03 (s, 1H), 5.73 (d, *J* = 9.5 Hz, 1H), 5.13 (s, 1H), 3.23 (s, 3H), 2.37 (s, 3H), 0.92 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.29, 139.42, 137.03, 135.24, 131.72, 131.64, 130.37, 129.56, 129.14, 128.79, 128.61, 127.54, 126.80, 123.18, 121.45, 118.60, 115.78, 77.71, 58.69, 51.21, 21.72, 20.02.

HRMS (ESI) for $C_{26}H_{26}N_3O_3S^+$ $[M+H]^+$ m/z: calcd 460.1689, found 460.1697.

5-Methoxy-4-methyl-2-phenyl-1-tosyl-1H-indole (6a)[3]

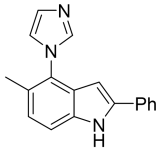


The compound was isolated as a by-product during the optimization. White solid (petroleum ether/EtOAc = 5:1, R_f = 0.34); mp 167 – 169 °C (Lit. mp 167-168 °C).[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 9.0 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.47 – 7.39 (m, 3H), 7.28 (s, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.94 (d, *J* = 9.0 Hz, 1H), 6.55 (s, 1H), 3.88 (s, 3H), 2.28 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.43, 144.44, 142.78, 134.45, 132.80, 132.78, 131.88, 130.25, 129.24, 128.68, 127.61, 126.93, 117.28, 114.54, 112.82, 109.11, 56.46, 21.64, 11.94.

8. Characterization Data of Derivatives 7a-9b

4-(1H-Imidazol-1-yl)-5-methyl-2-phenyl-1H-indole (7a)

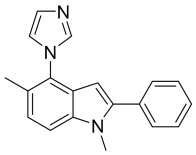


Prepared according to corresponding procedure and the product was isolated in 82% yield after chromatography as white solid (90 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.44); mp 248 – 250 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (s, 1H), 7.74 (s, 1H), 7.65 (d, *J* = 7.4 Hz, 2H), 7.45 – 7.38 (m, 3H), 7.35 – 7.30 (m, 2H), 7.20 (s, 1H), 7.12 (d, *J* = 8.3 Hz, 1H), 6.50 (s, 1H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, d^6-DMSO) δ 139.40, 138.47, 137.01, 132.10, 129.40, 129.01, 128.26, 127.87, 126.75, 125.65, 124.87, 124.05, 121.48, 112.14, 95.87, 17.37.

HRMS (ESI) for $C_{18}H_{16}N_3^+$ $[M+H]^+$ m/z: calcd 274.1339, found 274.1337.

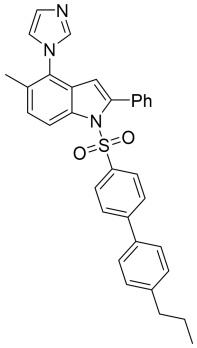
4-(1H-Imidazol-1-yl)-1,5-dimethyl-2-phenyl-1H-indole (8a)



Prepared according to corresponding procedure and the product was isolated in 78% yield after chromatography as white solid (44.8 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.42); mp 180 – 182 °C.

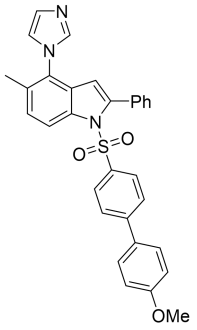
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.48 – 7.44 (m, 4H), 7.43 – 7.40 (m, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.27 (s, 1H), 7.21 – 7.16 (m, 2H), 6.25 (s, 1H), 3.78 (s, 3H), 2.27 (s, 3H).^{13}C NMR (151 MHz, $CDCl_3$) δ 142.99, 138.17, 137.92, 132.15, 129.36, 129.17, 128.71, 128.39, 127.84, 126.00, 124.94, 124.49, 120.83, 110.23, 98.73, 31.61, 17.20.
HRMS (ESI) for $C_{19}H_{18}N_3^+$ $[M+H]^+$ m/z: calcd 288.1495, found 288.1492.

4-(1H-Imidazol-1-yl)-5-methyl-2-phenyl-1-((4'-propyl-[1,1'-biphenyl]-4-yl)sulfonyl)-1H-indole (9a)



Prepared according to corresponing procedure and the product was isolated in 84% yield after chromatography as white solid (89.5 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.36); mp 98 – 100 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.6 Hz, 1H), 7.58 (s, 1H), 7.52 – 7.48 (m, 2H), 7.45 – 7.37 (m, 9H), 7.32 (d, *J* = 8.6 Hz, 1H), 7.26 – 7.20 (m, 3H), 7.03 (s, 1H), 6.22 (s, 1H), 2.61 (t, *J* = 7.7 Hz, 2H), 2.23 (s, 3H), 1.68 – 1.62 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.71, 143.84, 143.45, 137.90, 137.12, 136.05, 135.76, 131.61, 130.56, 130.07, 129.59, 129.33, 129.20, 128.36, 128.13, 127.68, 127.52, 127.48, 127.14, 127.12, 120.63, 116.91, 109.80, 37.75, 24.54, 17.15, 13.89.
HRMS (ESI) for $C_{33}H_{30}N_3O_2S^+$ $[M+H]^+$ m/z: calcd 532.2053, found 532.2035.

4-(1H-Imidazol-1-yl)-1-((4'-methoxy-[1,1'-biphenyl]-4-yl)sulfonyl)-5-methyl-2-phenyl-1H-indole (9b)



Prepared according to corresponding procedure and the product was isolated in 88% yield after chromatography as white solid (91.2 mg) (petroleum ether/EtOAc = 1:1, R_f = 0.30); mp 188 – 190 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.6 Hz, 1H), 7.56 (s, 1H), 7.48 – 7.38 (m, 11H), 7.32 (d, *J* = 8.6 Hz, 1H), 7.21 (s, 1H), 7.02 (s, 1H), 6.94 (d, *J* = 8.3 Hz, 2H), 6.22 (s, 1H), 3.82 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.39, 146.26, 143.40, 137.86, 137.06, 135.32,

131.59, 130.98, 130.52, 130.02, 129.55, 129.16, 128.44, 128.32, 128.09, 127.64, 127.48, 126.68, 120.61, 116.86, 114.59, 109.77, 55.45, 17.11 (one peak is missing).

HRMS (ESI) for $C_{31}H_{26}N_3O_3S^+$ $[M+H]^+$ m/z: calcd 520.1689, found 520.1677.

9. X-Ray Crystallographic Information of Product 3a

Important Crystal Data for 3a (CCDC 2233028).

Bond precision:	C-C = 0.0032 A	Wavelength=0.71073	
Cell:	a=7.6654(6)	b=23.1002(14)	c=12.1164(9)
	alpha=90	beta=98.245(2)	gamma=90
Temperature:	152 K		
	Calculated	Reported	
Volume	2123.3(3)	2123.3(3)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	$C_{25}H_{21}N_3O_2S$	$C_{25}H_{21}N_3O_2S$	
Sum formula	$C_{25}H_{21}N_3O_2S$	$C_{25}H_{21}N_3O_2S$	
Mr	427.51	427.51	
Dx, g cm-3	1.337	1.337	
Z	4	4	
Mu (mm-1)	0.180	0.180	
F000	896.0	896.0	
F000’	896.83		
h,k,lmax	9,30,15	9,29,15	
Nref	4867	4846	
Tmin,Tmax	0.965,0.972	0.686,0.746	
Tmin’	0.965		

Correction method= # Reported T Limits: Tmin=0.686 Tmax=0.746 AbsCorr = NONE

Data completeness= 0.996 Theta(max)= 27.501

R(reflections)= 0.0467(3486) wR2(reflections)=0.1315(4846)

S = 0.968 Npar= 282

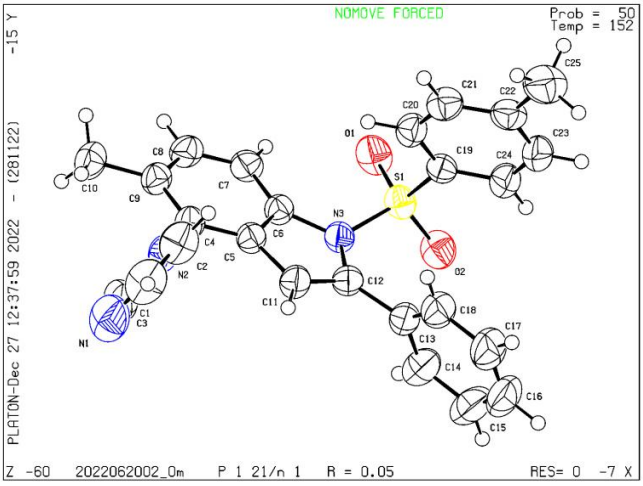


Figure S1. ORTEP drawing of compound **3a**.

10. References

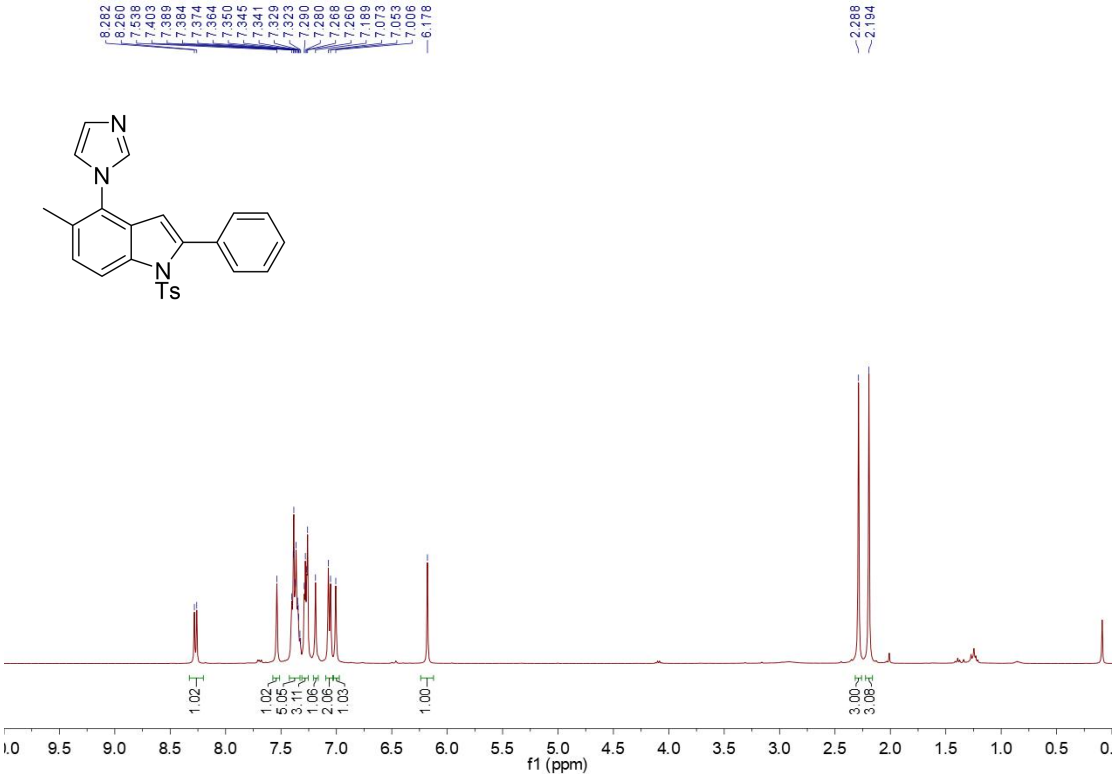
[1] (a) C. N. Voth and G. R. Dake, Nickel-Catalyzed Arylative Additions on 2-Alkynyl-N-Arylsulfonylanilides to Construct Functionalized Indoles. *Eur. J. Org. Chem.,* 2020, 744-748; (b) M. Jash, B. Das and C. Chowdhury, One-Pot Access to Benzo[*a*]carbazoles via Palladium(II)-Catalyzed Hetero- and Carboannulations, *J. Org. Chem.* 2016, **81**, 10987-10999; (c) E. Chong, S. A. Blum, Aminoboration: Addition of B-N σ Bonds across C-C π Bonds, *J. Am. Chem. Soc.,* 2015, **137**, 10144-10147; (d) S. Serra and C. Fuganti, A New Preparative Route to Substituted Carbazoles by Benzannulation, *Synlett,* 2005, 809-812.

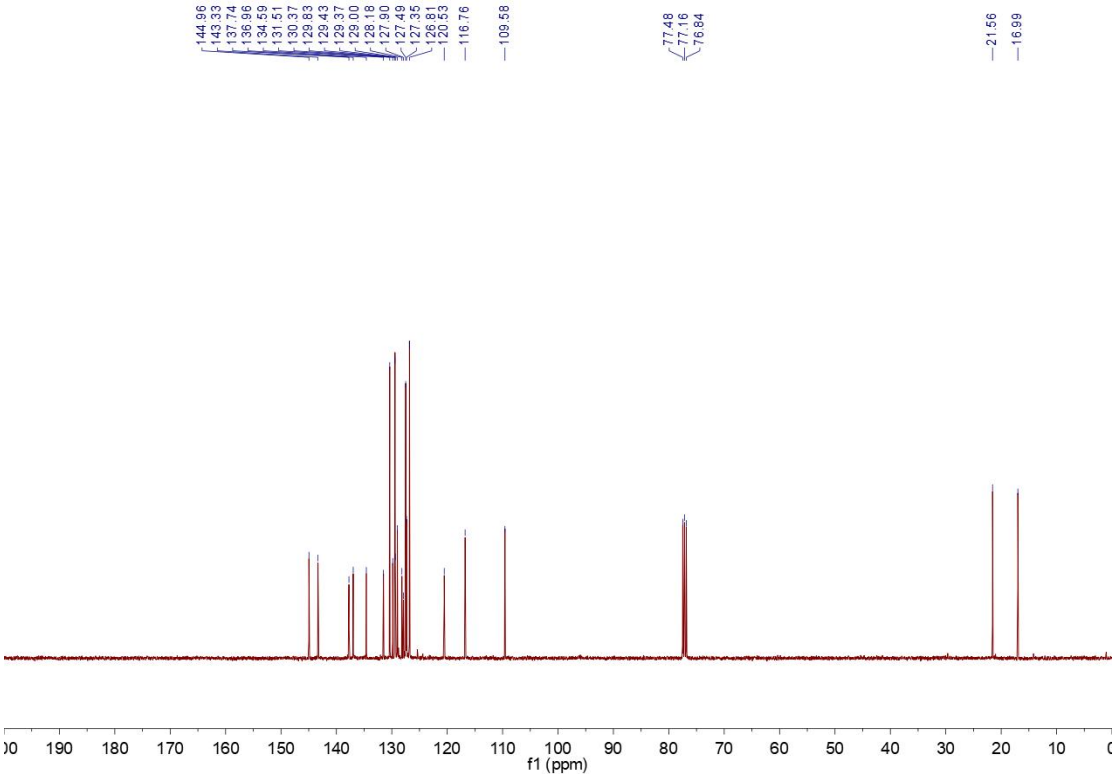
[2] L. F. Wang and R. H. Fan, Divergent Construction of Nitrogen-Containing Polycyclic Compounds with a Dearomatization Strategy, *Org. Lett.,* 2012, **14**, 3596-3599.

[3] L. Li, X. H. Li, W. Y. Wang, Q. Q. He and R. H. Fan, Synthesis of 4-Alkylindoles from 2-Alkynylanilines via Dearomatization- and Aromatization-Triggered Alkyl Migration, *Org. Lett.,* 2021, **23**, 2130-3134.

11. Spectra of the Compounds

3a:





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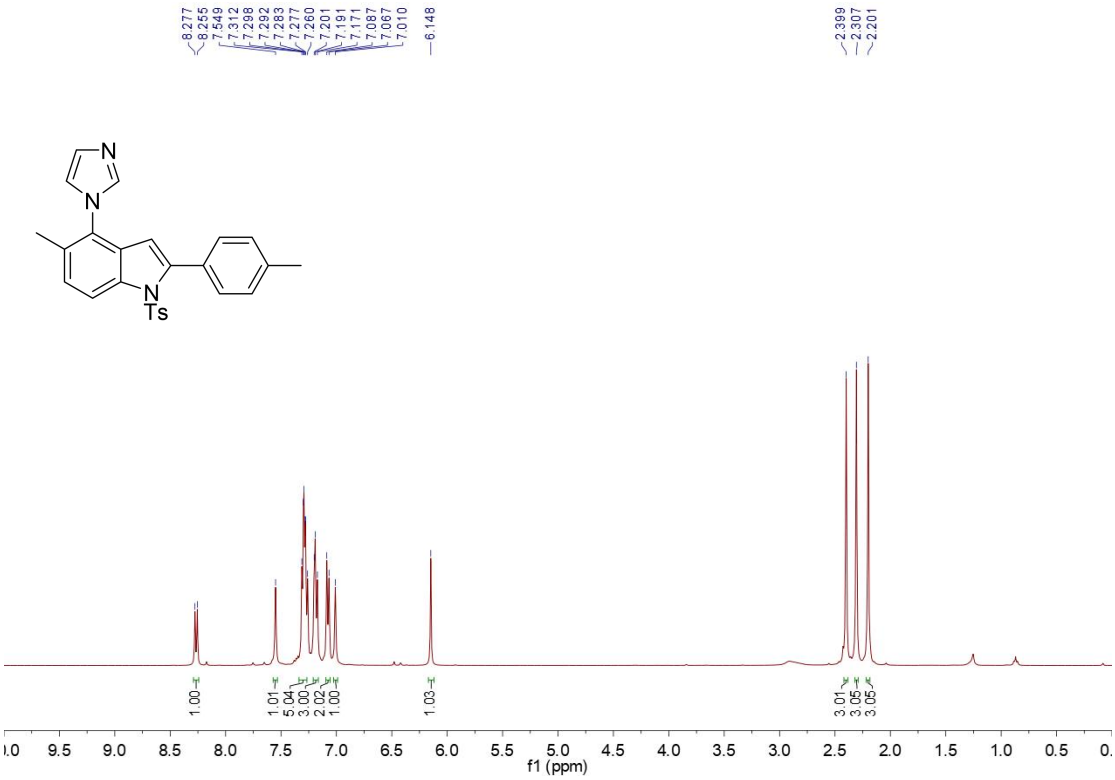
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8.255
7.549
7.312
7.298
7.292
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7.277
7.260
7.201
7.191
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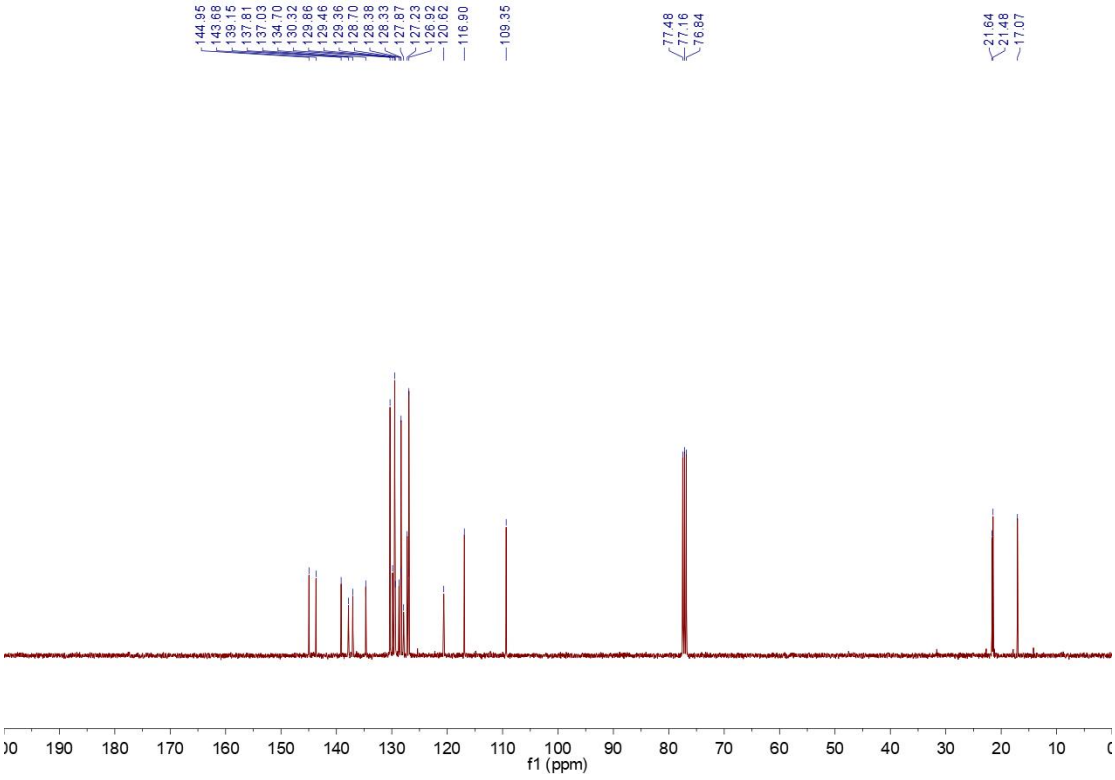
7.087
7.067
7.010
6.148
2.399
2.307
2.201
N
N
N
Ts
1.00
1.01
5.04
3.00
2.02
1.00
1.03
3.01
3.05
3.05
f1 (ppm)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143.68
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129.46
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128.70
128.38
128.33
127.87
127.23
126.92
120.62
116.90
109.35
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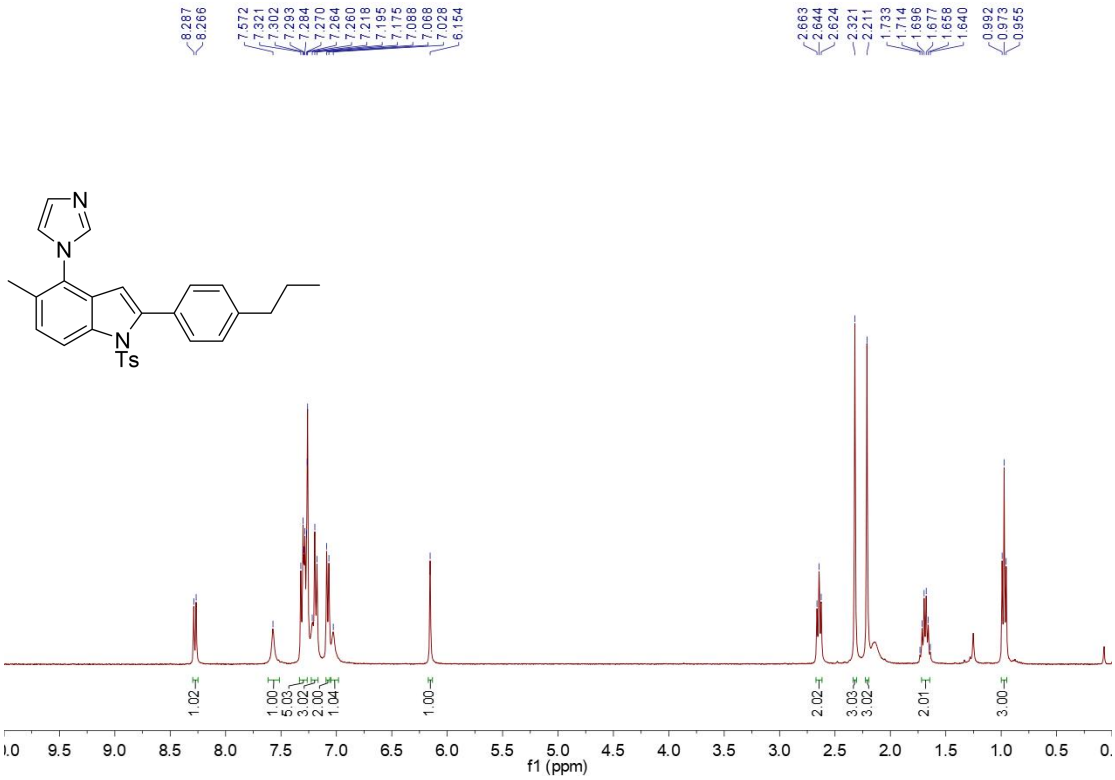
77.16
76.84
21.64
21.48
17.07
f1 (ppm)

3c: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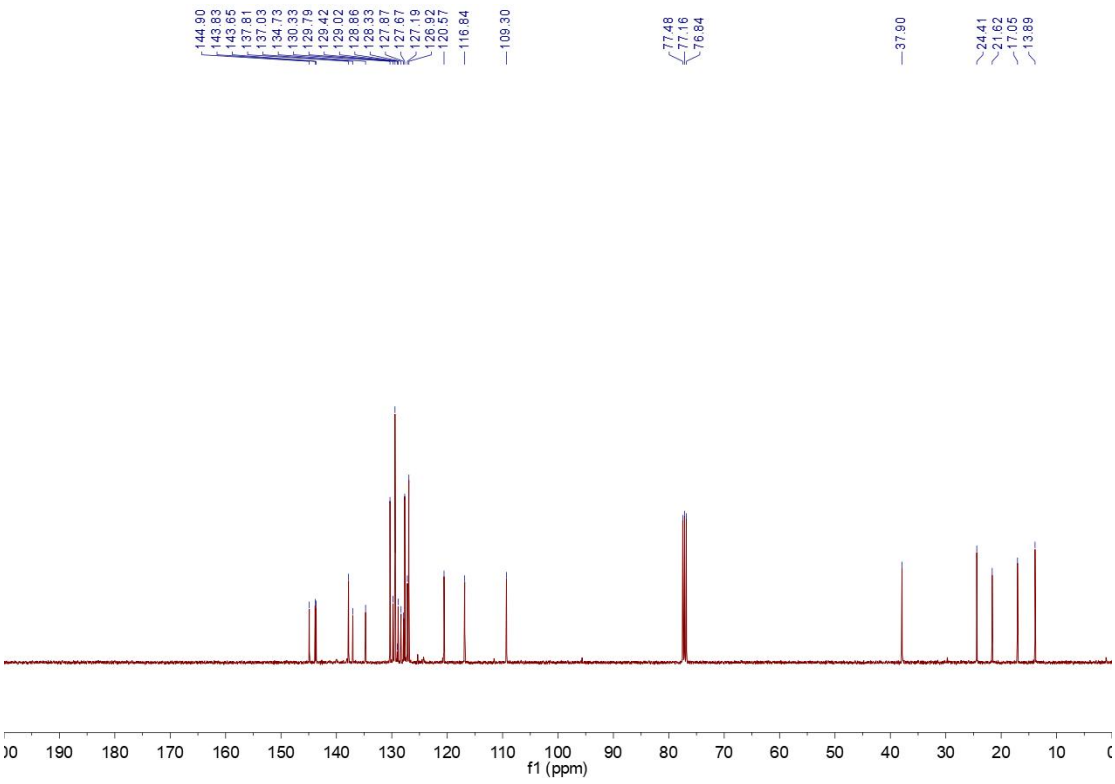
7.175
7.088
7.068
7.028
6.154
2.663
2.644
2.624
2.321
2.211
1.733
1.714
1.696
1.677
1.658
1.640
0.992
0.973
0.955
N
N
N
Ts
1.02
1.00
5.03
3.02
2.00
1.04
1.00
2.02
3.03
3.02
2.01
3.00
f1 (ppm)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143.65
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130.33
129.79
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128.33
127.87
127.67
127.19
126.92
120.57
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109.30
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77.16
76.84
37.90
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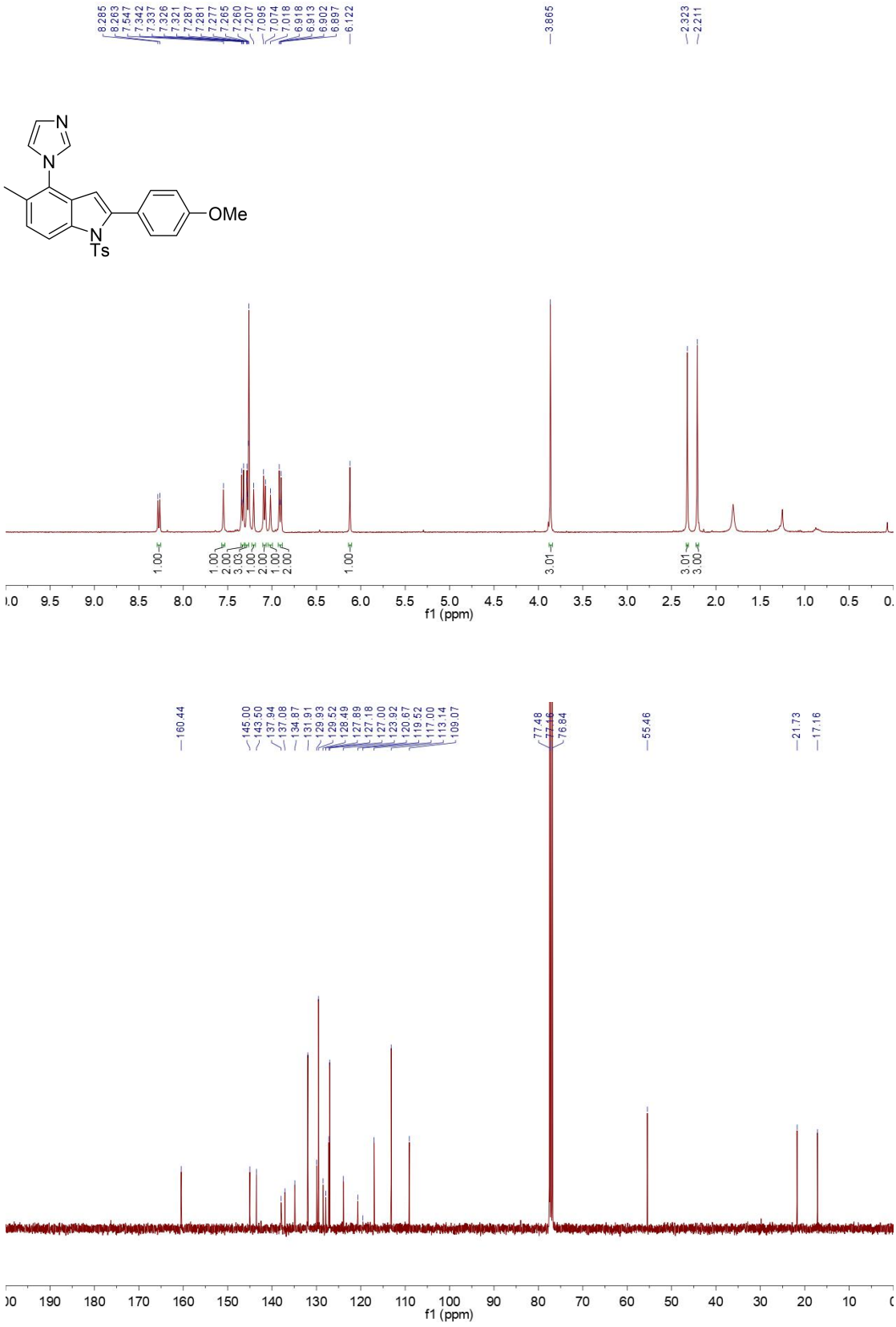
17.05
13.89
f1 (ppm)

3d: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7.095
7.074
7.018
6.918
6.913
6.902
6.897
6.122
3.865
2.323
2.211
N
N
OMe
N
Ts
1.00
2.00
3.03
1.00
2.00
1.00
2.00
1.00
3.01
3.01
3.00
f1 (ppm)
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145.00
143.50
137.94
137.08
134.87
131.91
129.93
129.52
128.49
127.89
127.18
127.00
123.92
120.67
119.52
117.00
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109.07
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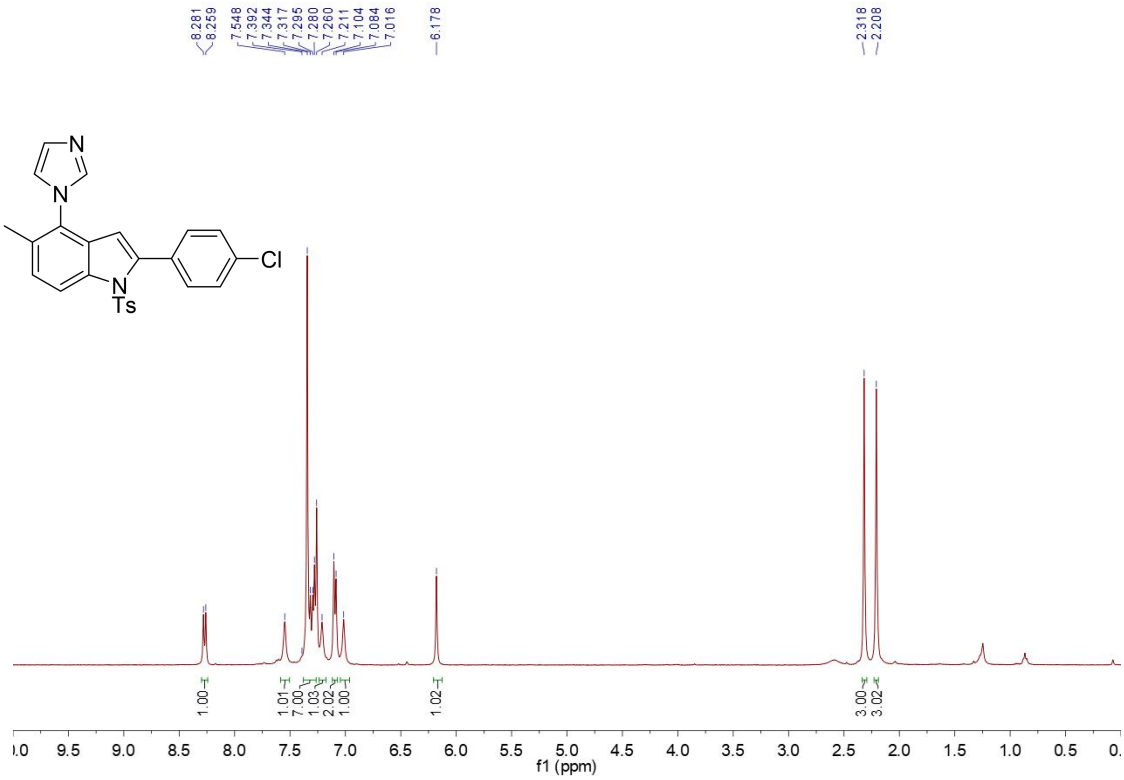
21.73
17.16
f1 (ppm)

3e: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7.084
7.016
6.178
2.318
2.208
N
N
Cl
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Ts
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1.01
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1.03
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1.00
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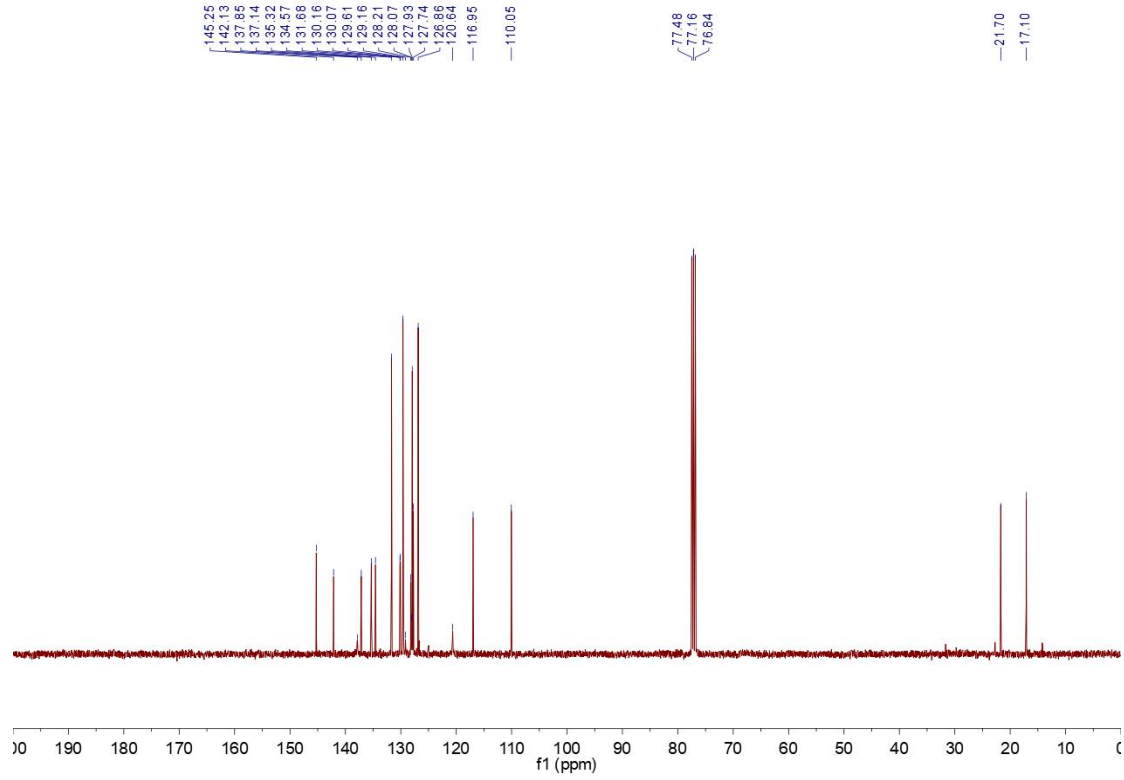
3.00
3.02
f1 (ppm)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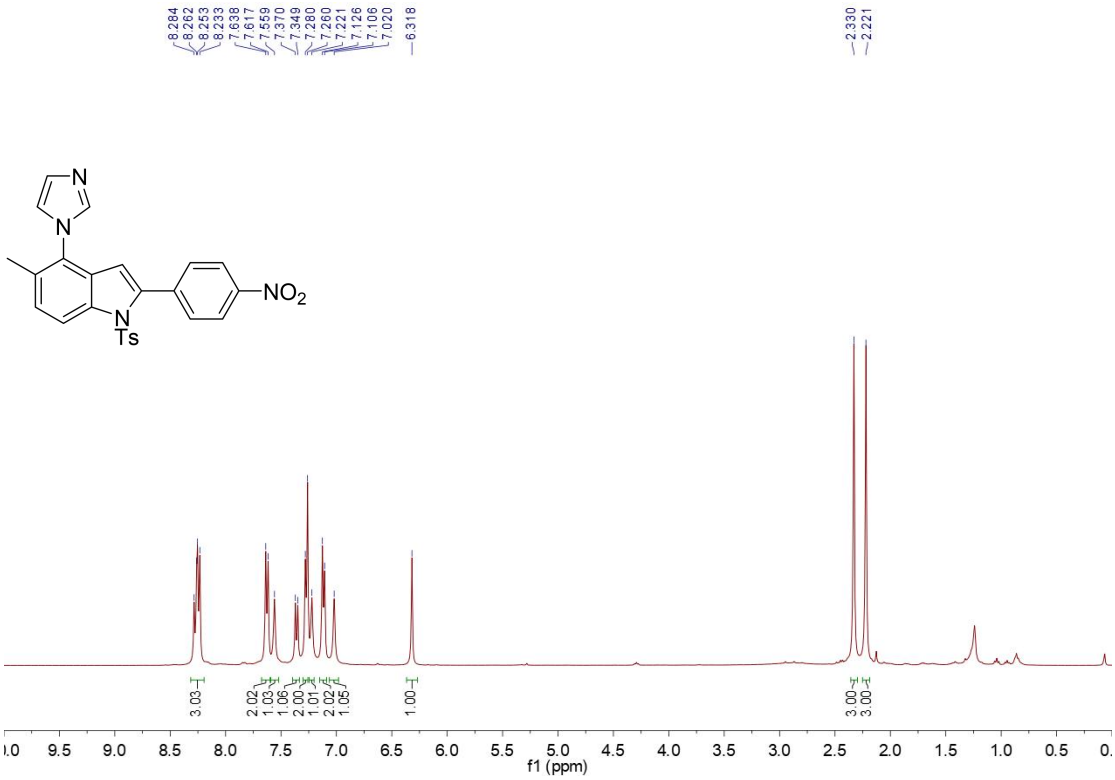
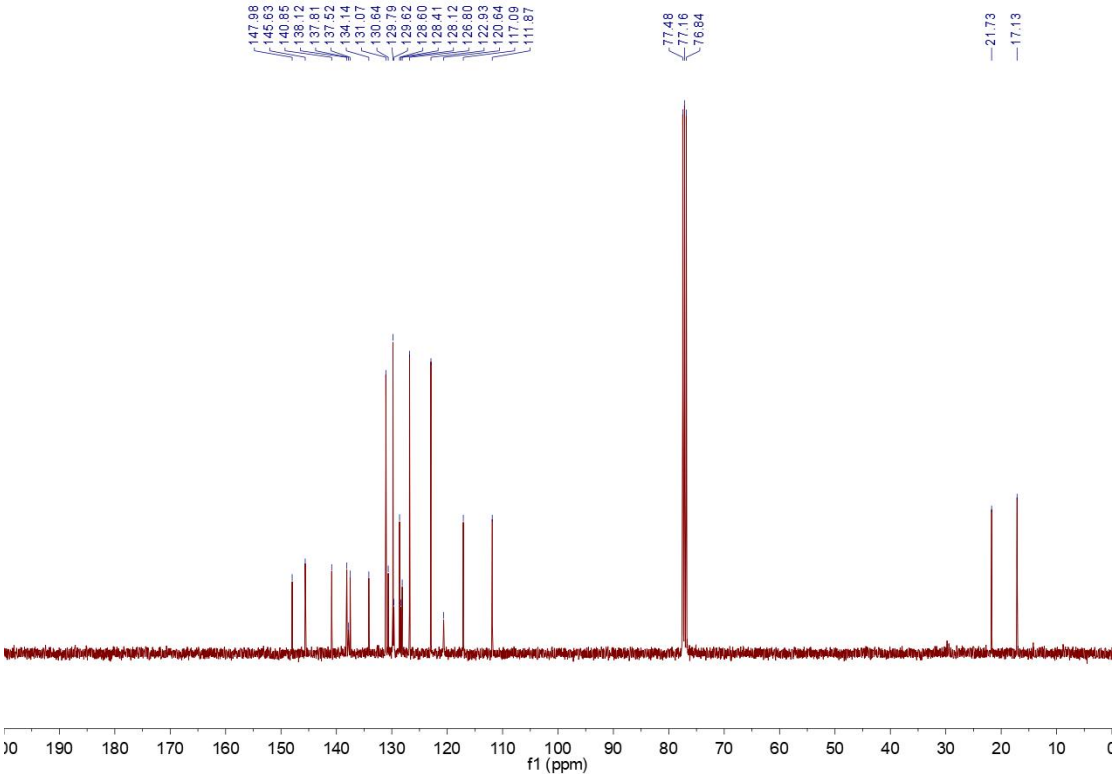
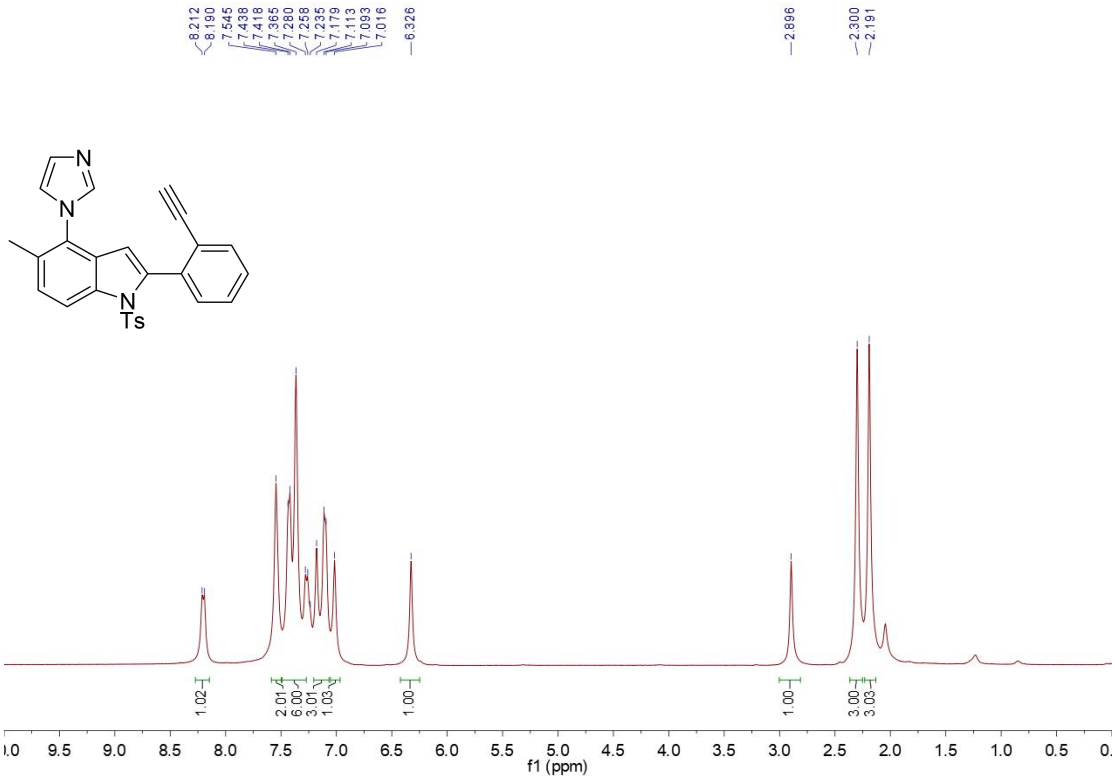
130.16
130.07
129.61
129.16
128.21
128.07
127.93
127.74
126.86
120.64
116.95
110.05
77.48
77.16
76.84
21.70
17.10
f1 (ppm)

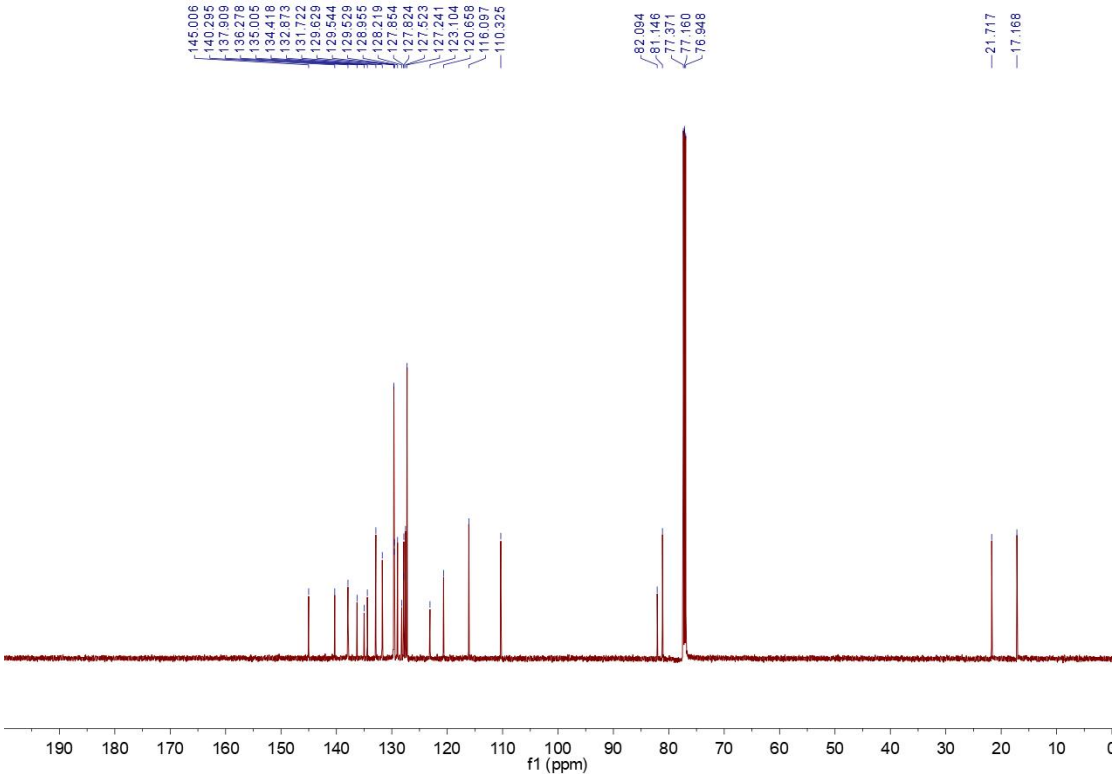
3f:


8.284
8.262
8.253
8.233
7.638
7.617
7.559
7.370
7.349
7.280
7.260
7.221
7.126
7.106
7.020
6.318
2.330
2.221
N
N
NO2
N
Ts
3.03
2.02
1.03
1.06
2.00
1.01
2.02
1.05
1.00
3.00
3.00
f1 (ppm)

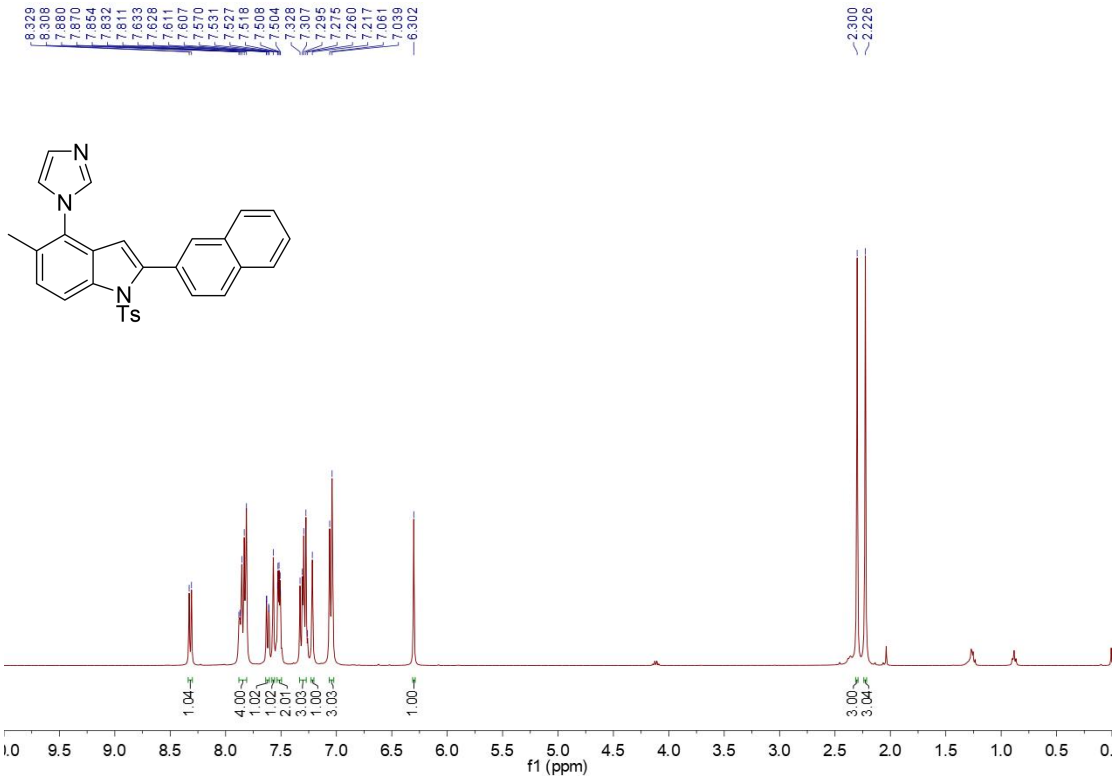

147.98
145.63
140.85
138.12
137.81
137.52
134.14
131.07
130.64
129.79
129.62
128.60
128.41
128.12
126.80
122.93
120.64
117.09
111.87
77.48
77.16
76.84
21.73
17.13
f1 (ppm)

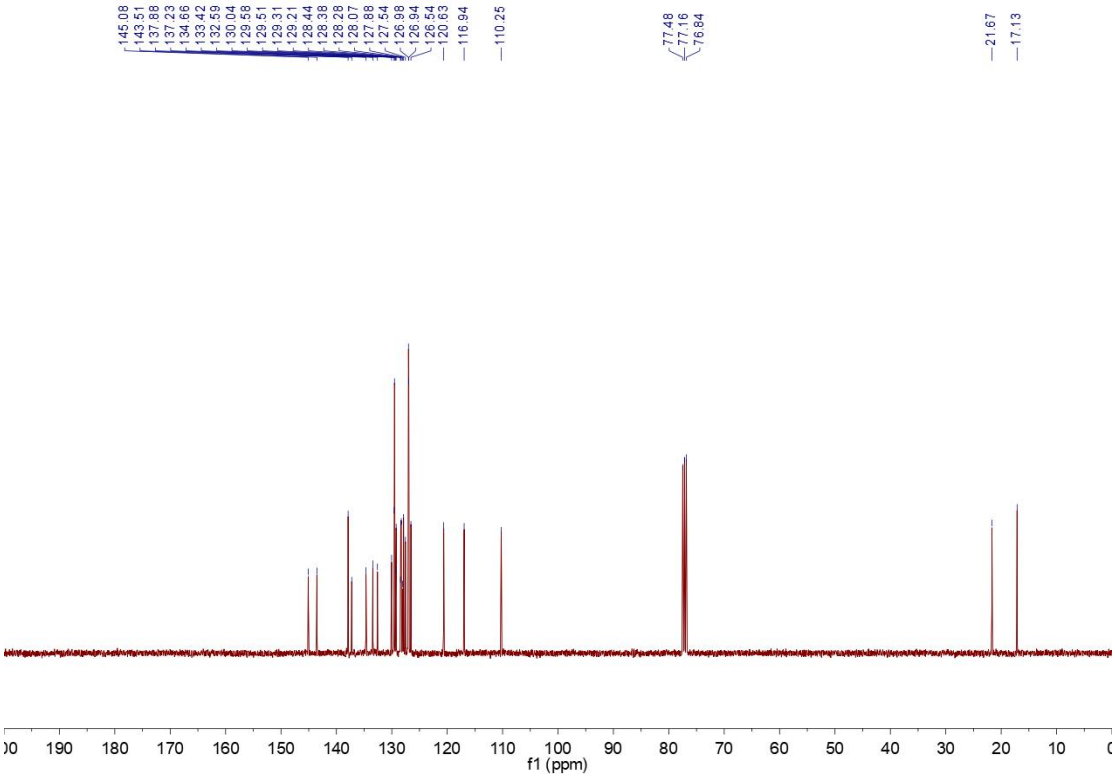
3g:


8.212
8.190
7.545
7.438
7.418
7.365
7.280
7.258
7.235
7.179
7.113
7.093
7.016
6.326
2.896
2.300
2.191
N
N
N
Ts
1.02
2.01
6.00
3.01
1.03
1.00
1.00
3.00
3.03
f1 (ppm)

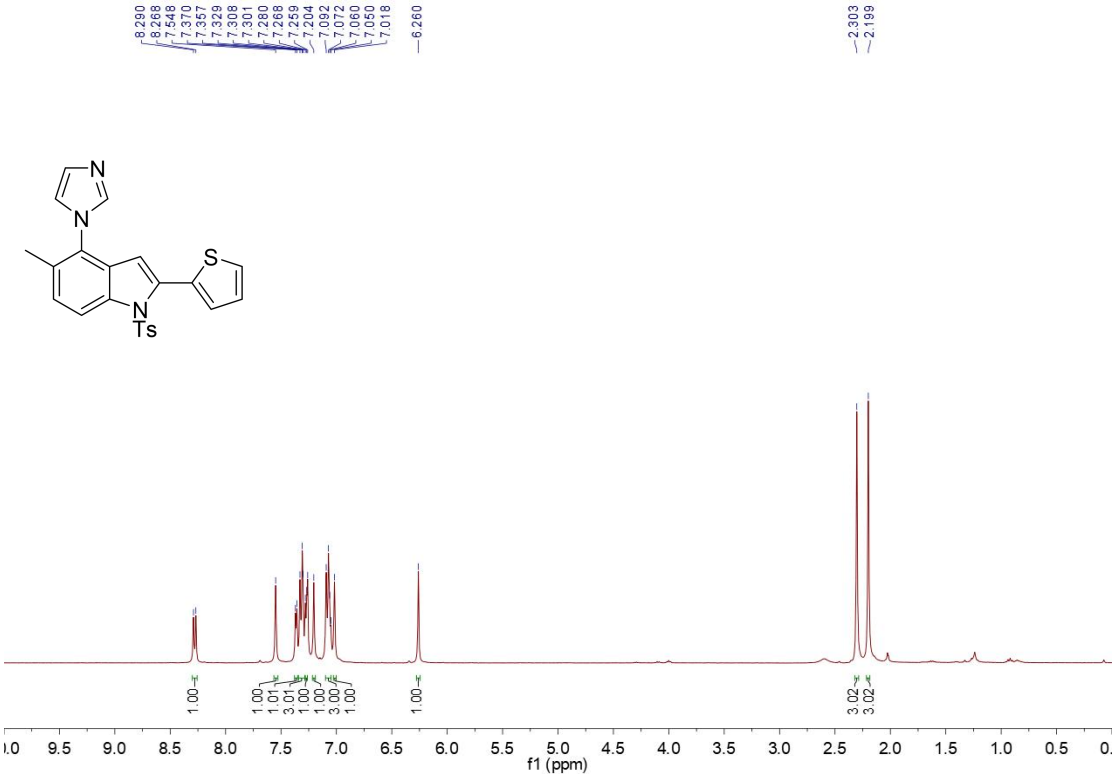

145.006
140.295
137.909
136.278
135.005
134.418
132.873
131.722
129.629
129.544
129.529
128.955
128.219
127.854
127.824
127.523
127.241
123.104
120.658
116.097
110.325
82.094
81.146
77.371
77.160
76.948
21.717
17.168
f1 (ppm)

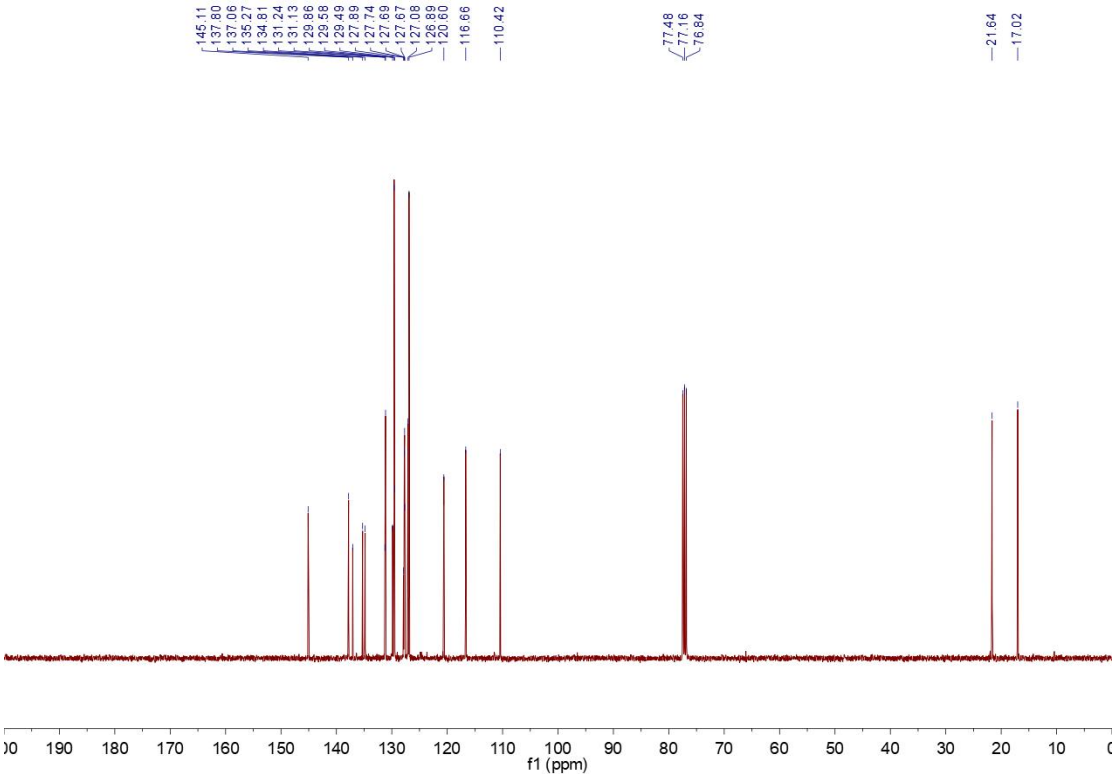
3h:


8.329
8.308
7.880
7.870
7.854
7.832
7.811
7.633
7.628
7.611
7.607
7.570
7.531
7.527
7.518
7.508
7.504
7.328
7.307
7.295
7.275
7.260
7.217
7.061
7.039
6.302
2.300
2.226
N
N
N
Ts
1.04
4.00
1.02
1.02
2.01
3.03
1.00
3.03
1.00
3.00
3.04
f1 (ppm)

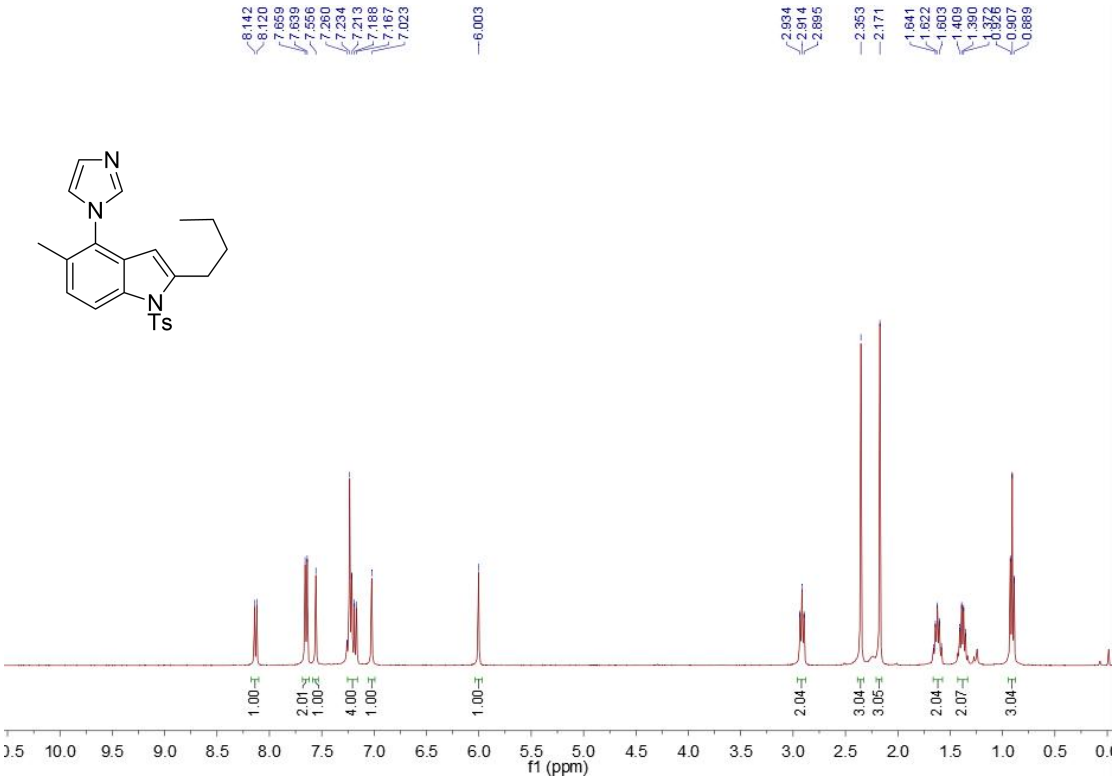

145.08
143.51
137.88
137.23
134.66
133.42
132.59
130.04
129.58
129.51
129.31
129.21
128.44
128.38
128.29
128.07
127.88
127.54
126.98
126.94
126.54
120.63
116.94
110.25
77.48
77.16
76.84
21.67
17.13
f1 (ppm)

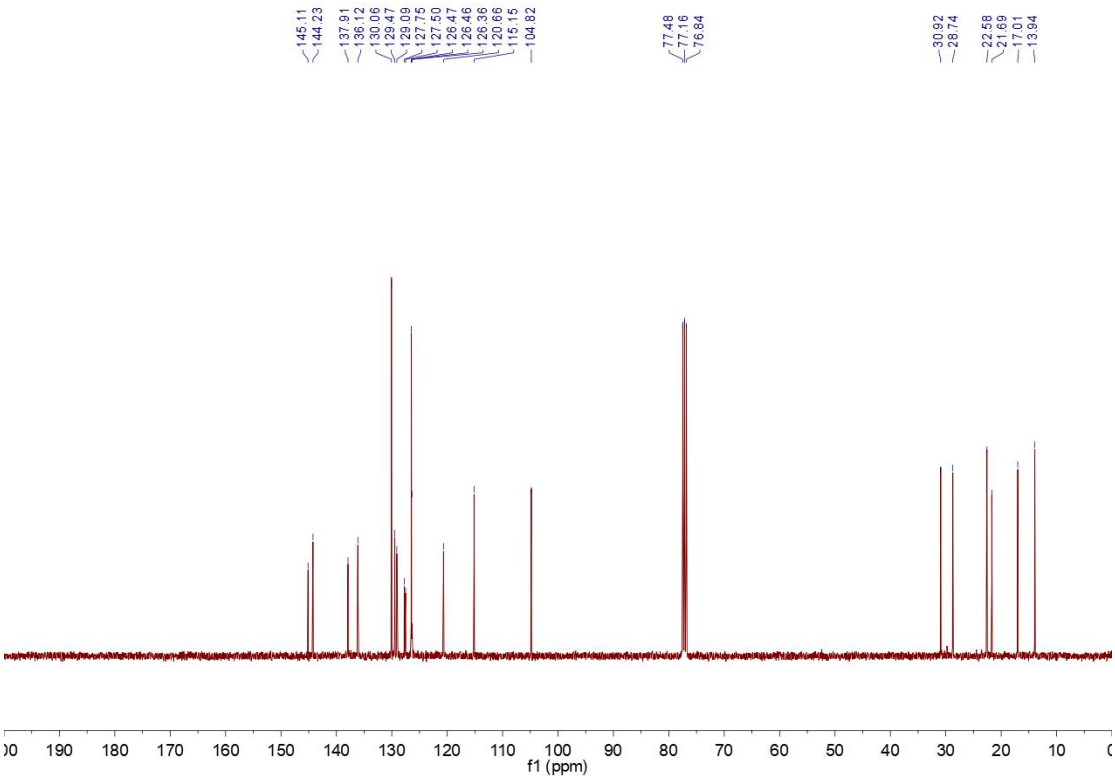
3i:


8.290
8.268
7.548
7.370
7.357
7.329
7.308
7.301
7.280
7.268
7.259
7.204
7.092
7.072
7.060
7.050
7.018
6.260
2.303
2.199
N
N
S
N
Ts
1.00
1.00
1.01
3.01
1.00
1.00
3.00
1.00
1.00
3.02
3.02
f1 (ppm)

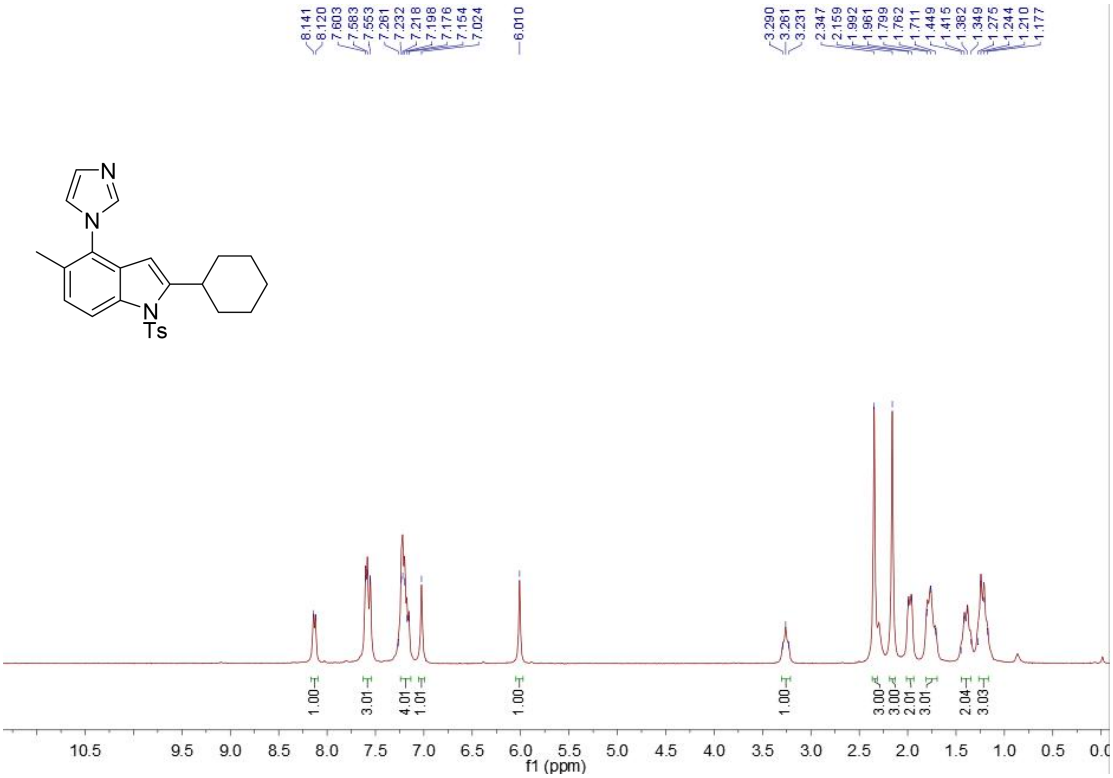

145.11
137.80
137.06
135.27
134.81
131.24
131.13
129.86
129.58
129.49
127.89
127.74
127.69
127.67
127.08
126.89
120.60
116.66
110.42
77.48
77.16
76.84
21.64
17.02
f1 (ppm)

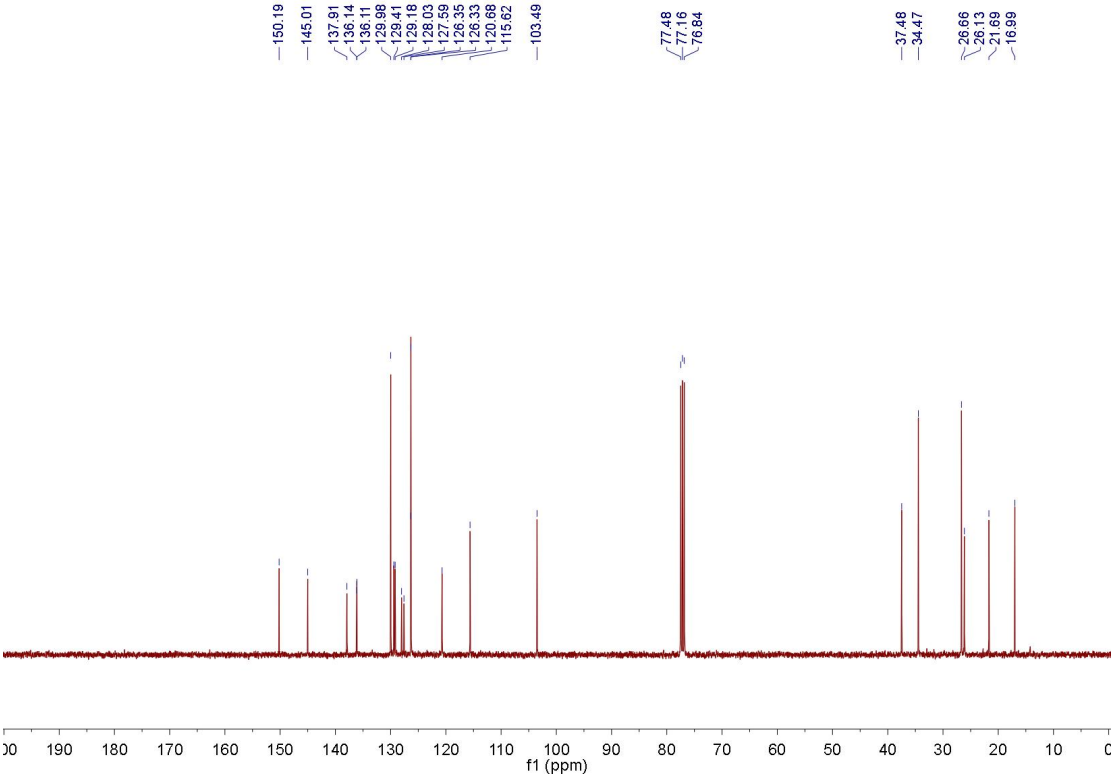
3j:


8.142
8.120
7.659
7.639
7.556
7.260
7.234
7.213
7.188
7.167
7.023
6.003
2.934
2.914
2.895
2.353
2.171
1.641
1.622
1.603
1.409
1.390
0.907
0.889
N
N
N
Ts
1.00
2.01
1.00
4.00
1.00
1.00
2.04
3.04
3.05
2.04
2.07
3.04
f1 (ppm)

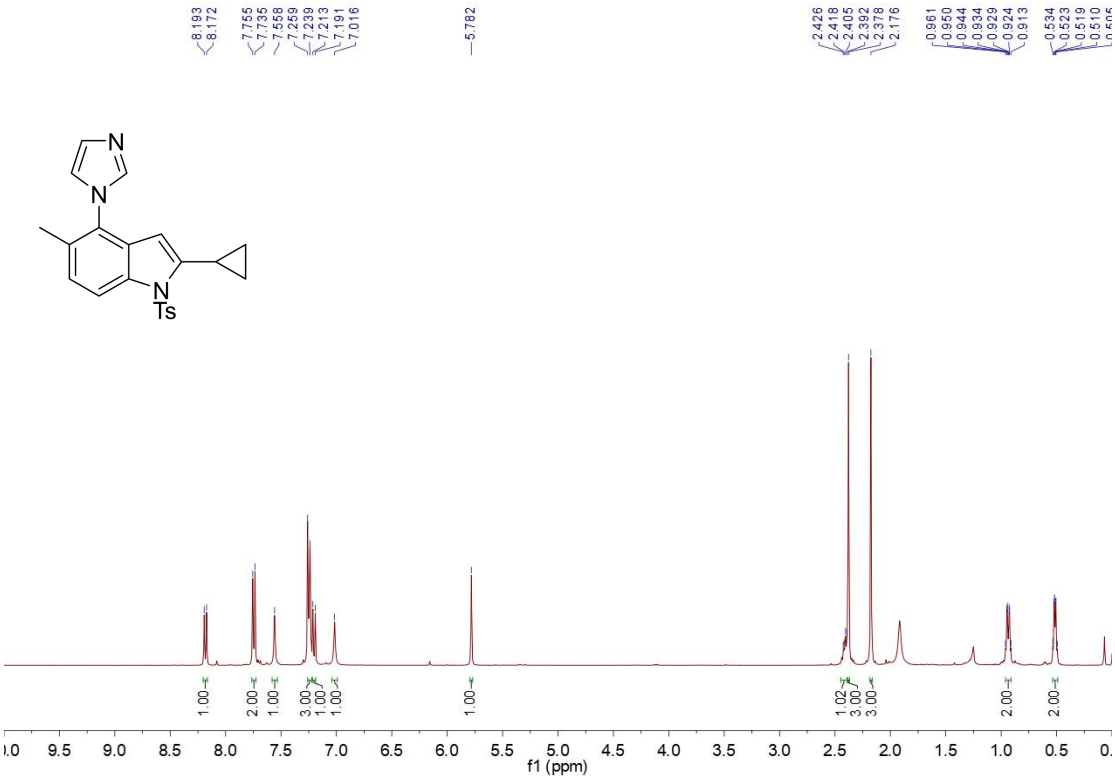

145.11
144.23
137.91
136.12
130.06
129.47
129.09
127.75
127.50
126.47
126.46
126.36
120.66
115.15
104.82
77.48
77.16
76.84
30.92
28.74
22.58
21.69
17.01
13.94
f1 (ppm)

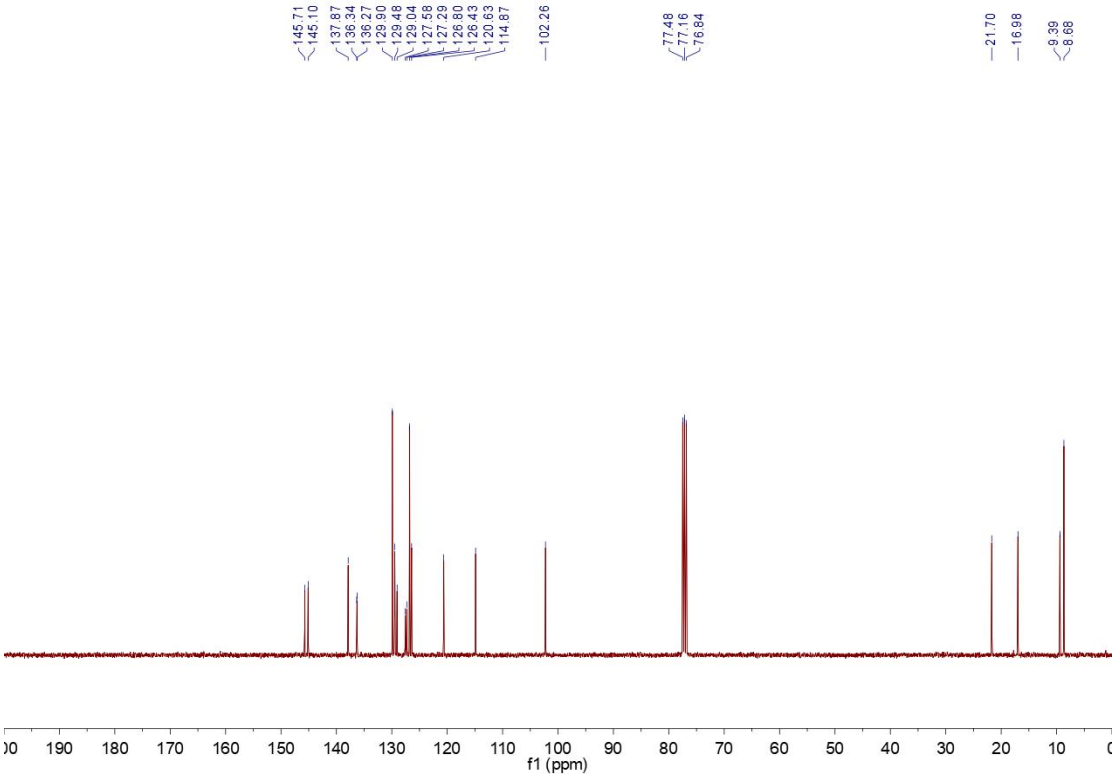
3k:


8.141
8.120
7.603
7.583
7.553
7.261
7.232
7.218
7.198
7.176
7.154
7.024
6.010
3.290
3.261
3.231
2.347
2.159
1.992
1.961
1.799
1.762
1.711
1.449
1.415
1.382
1.349
1.275
1.244
1.210
1.177
N
N
N
Ts
1.00
3.01
4.01
1.01
1.00
1.00
3.00
3.00
2.01
3.01
2.04
3.03
f1 (ppm)

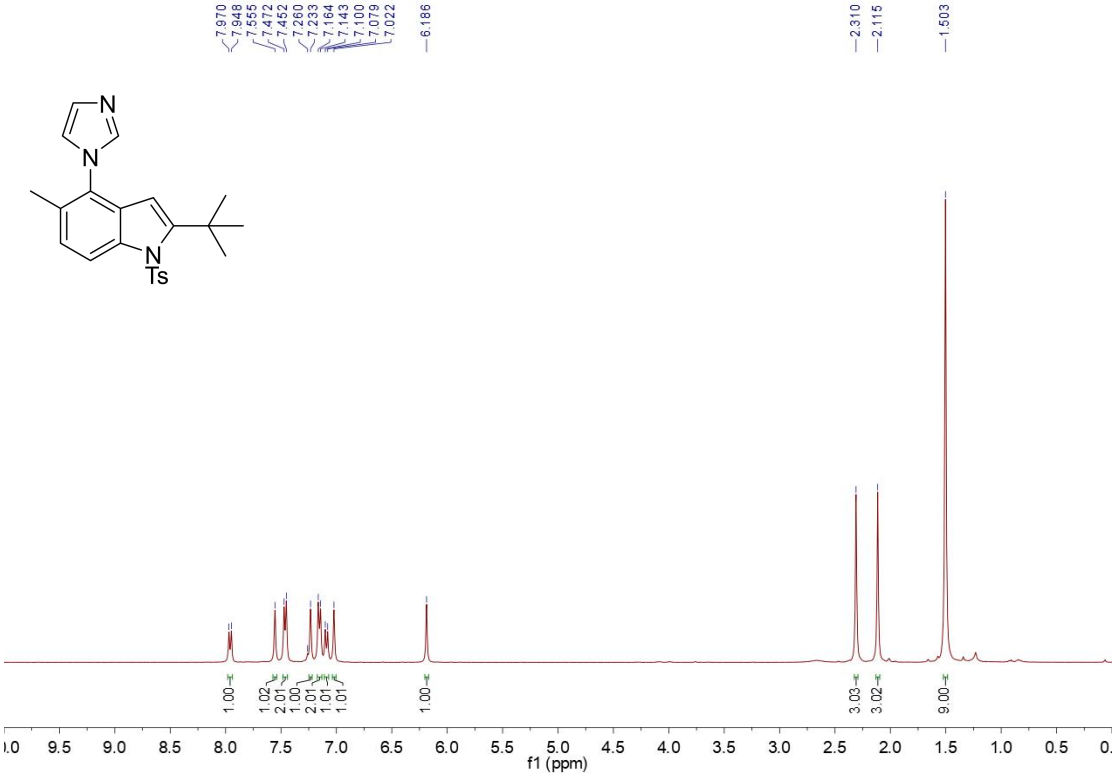

150.19
145.01
137.91
136.14
136.11
129.98
129.41
129.18
128.03
127.59
126.35
126.33
120.68
115.62
103.49
77.48
77.16
76.84
37.48
34.47
26.66
26.13
21.69
16.99
f1 (ppm)

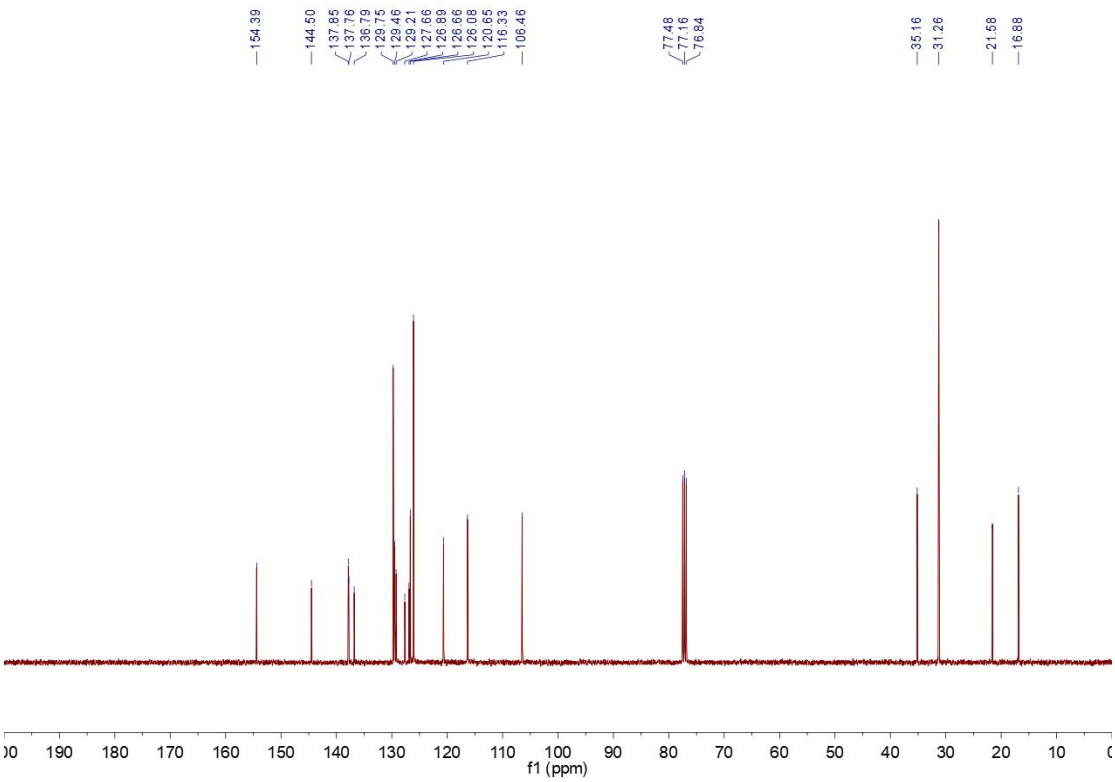
3l:


8.193
8.172
7.755
7.735
7.558
7.259
7.239
7.213
7.191
7.016
5.782
2.426
2.418
2.405
2.392
2.378
2.176
0.961
0.950
0.944
0.934
0.929
0.924
0.913
0.534
0.523
0.519
0.510
N
N
N
Ts
1.00
2.00
1.00
3.00
1.00
1.00
1.00
1.02
3.00
3.00
2.00
2.00
f1 (ppm)

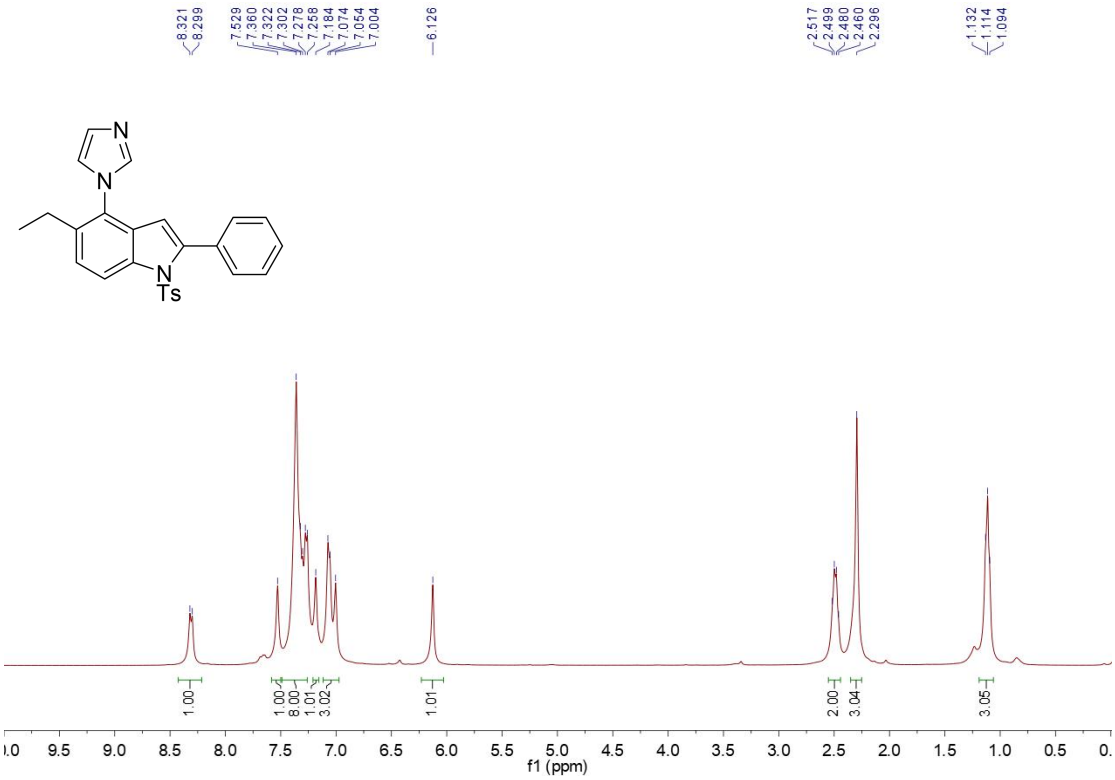

145.71
145.10
137.87
136.34
136.27
129.90
129.48
129.04
127.58
127.29
126.80
126.43
120.63
114.87
102.26
77.48
77.16
76.84
21.70
16.98
9.39
8.68
f1 (ppm)

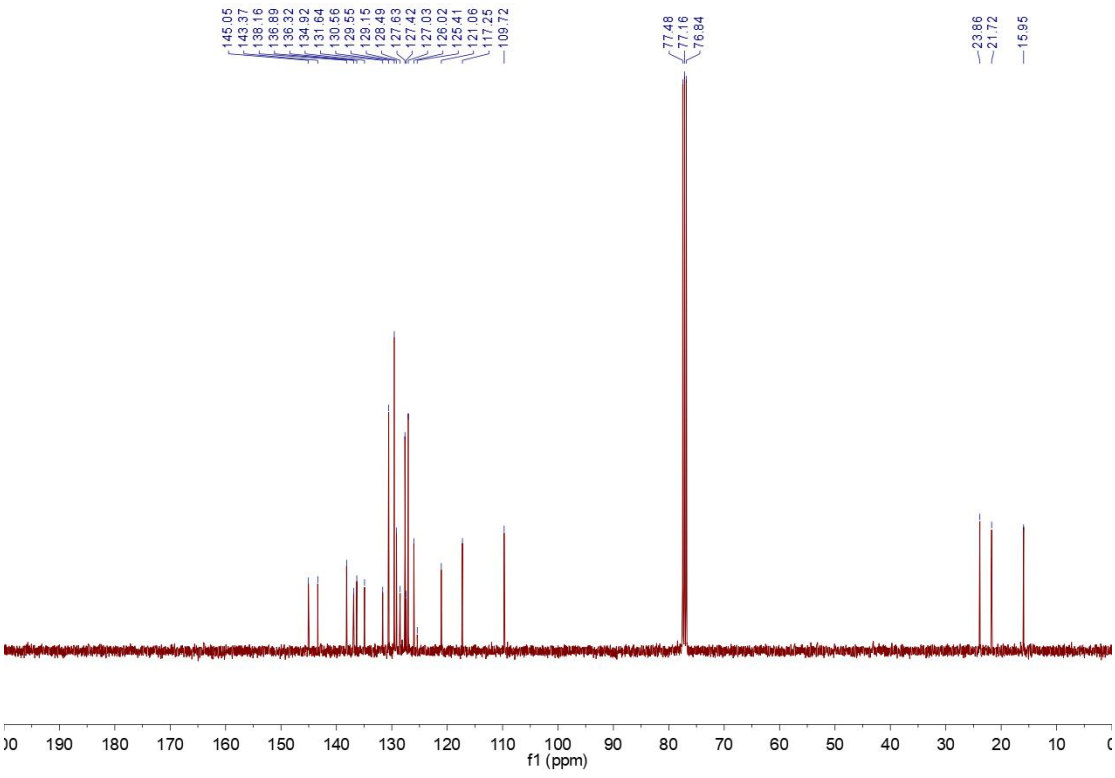
3m:


7.970
7.948
7.555
7.472
7.452
7.260
7.233
7.164
7.143
7.100
7.079
7.022
6.186
2.310
2.115
1.503
N
N
N
Ts
1.00
1.02
2.01
1.00
2.01
1.01
1.01
1.00
3.03
3.02
9.00
f1 (ppm)

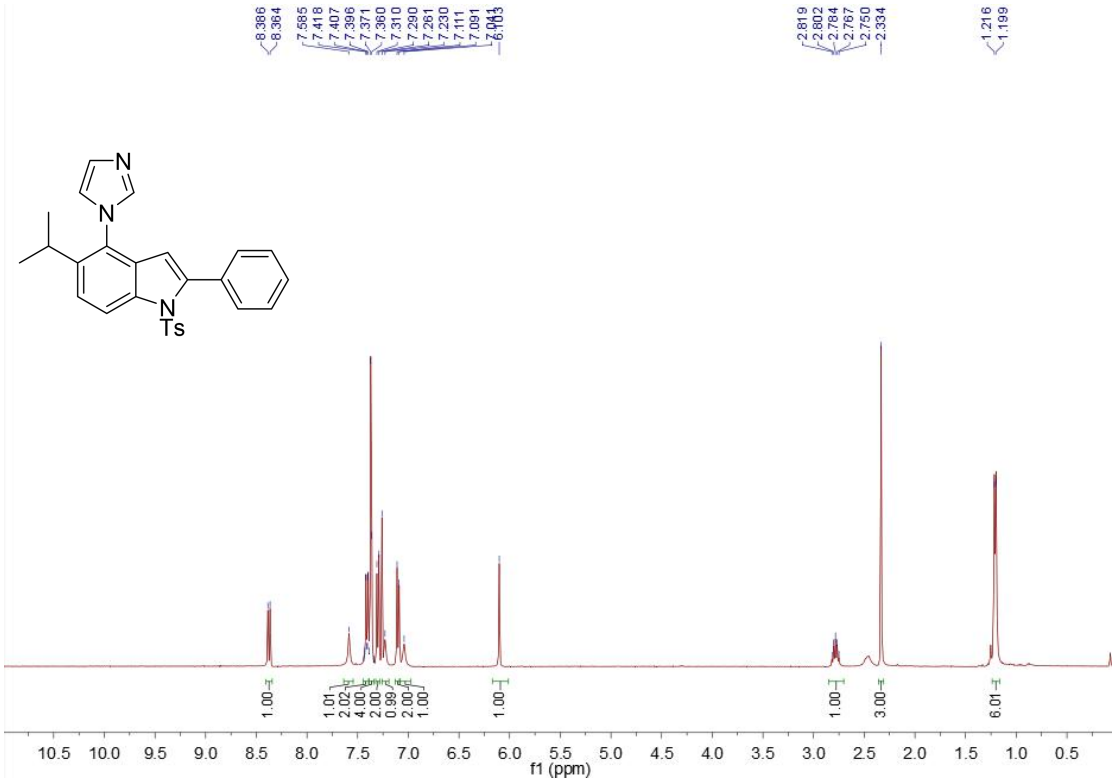

154.39
144.50
137.85
137.76
136.79
129.75
129.46
129.21
127.66
126.89
126.66
126.08
120.65
116.33
106.46
77.48
77.16
76.84
35.16
31.26
21.58
16.88
f1 (ppm)

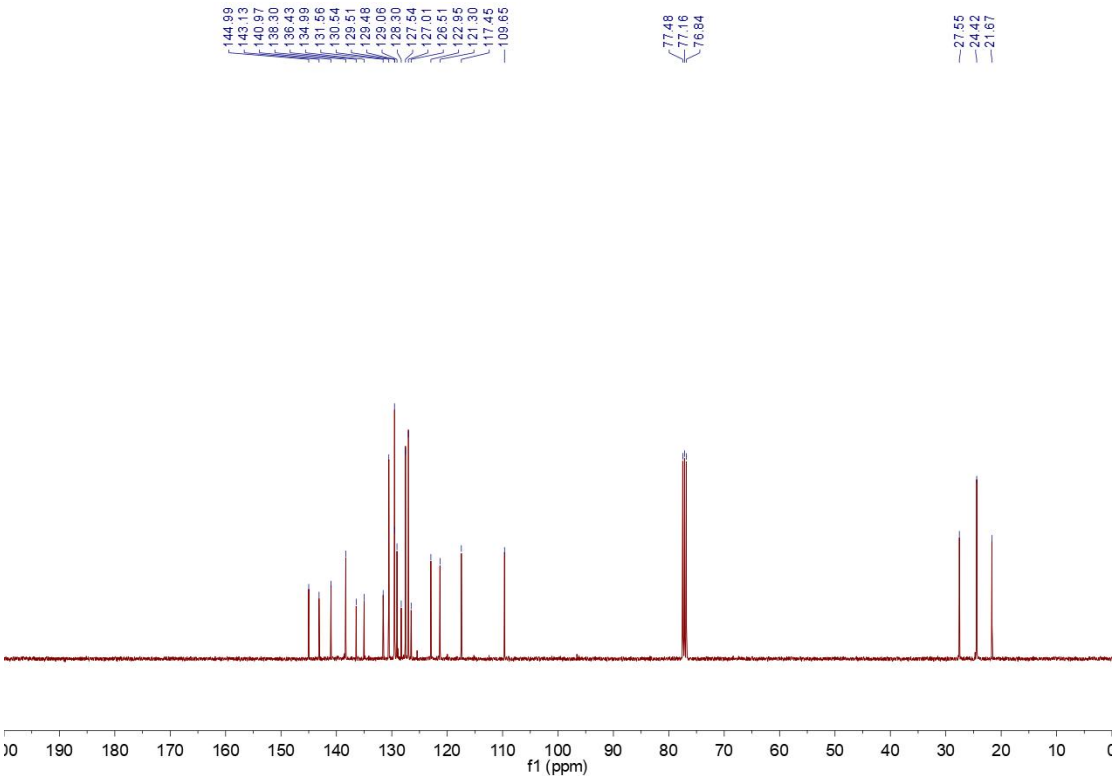
3n:


8.321
8.299
7.529
7.360
7.322
7.302
7.278
7.258
7.184
7.074
7.054
7.004
6.126
2.517
2.499
2.480
2.460
2.296
1.132
1.114
1.094
N
N
N
Ts
1.00
1.00
8.00
1.01
3.02
1.01
2.00
3.04
3.05
f1 (ppm)

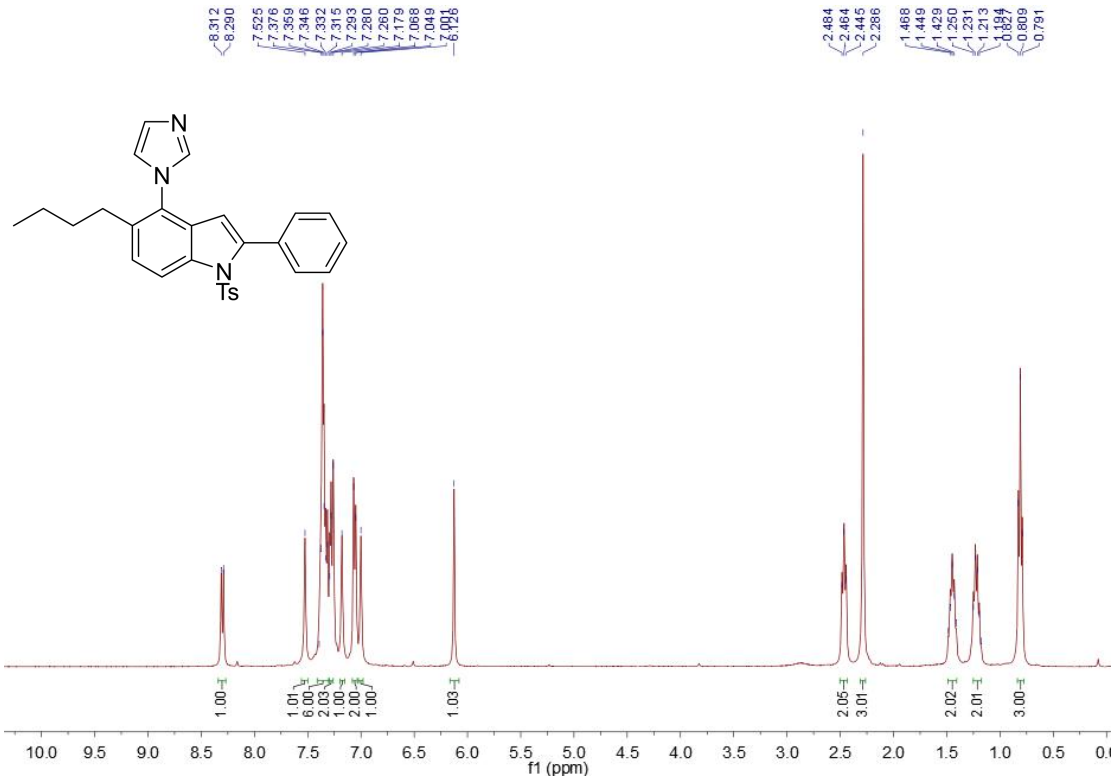

145.05
143.37
138.16
136.89
136.32
134.92
131.64
130.56
129.55
129.15
128.49
127.63
127.42
127.03
126.02
125.41
121.06
117.25
109.72
77.48
77.16
76.84
23.86
21.72
15.95
f1 (ppm)

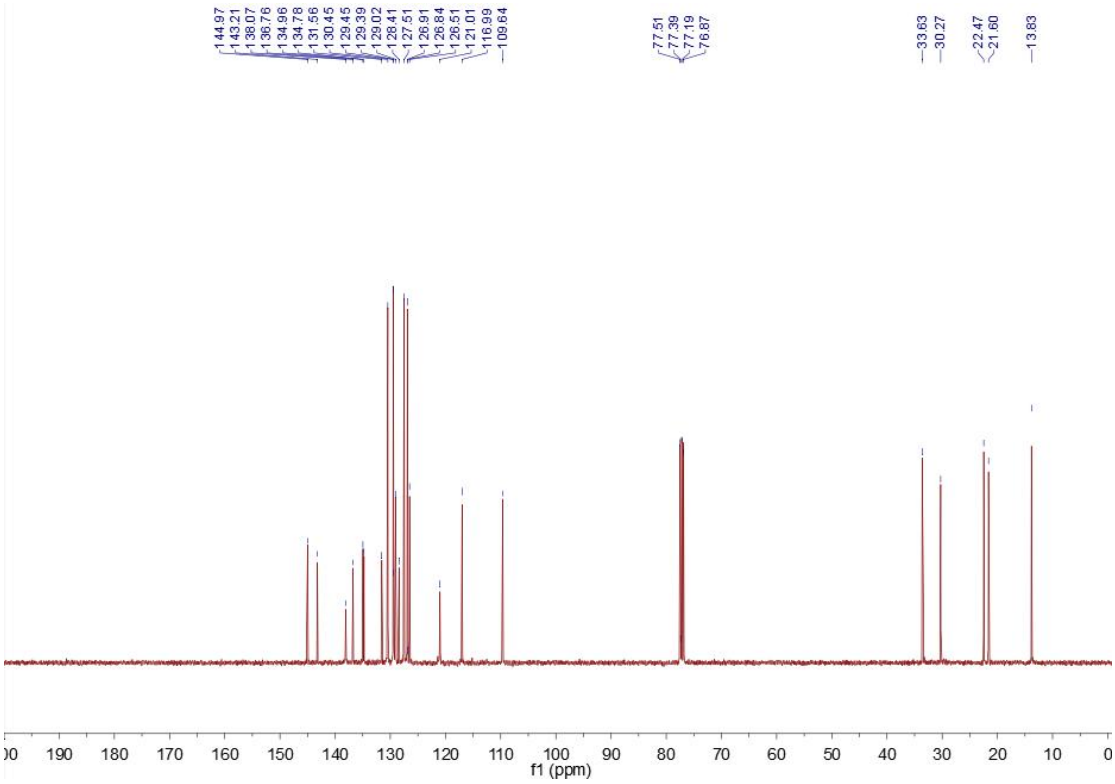
3o:


8.386
8.364
7.585
7.418
7.407
7.396
7.371
7.360
7.310
7.290
7.261
7.230
7.111
7.091
7.041
6.103
2.819
2.802
2.784
2.767
2.750
2.334
1.216
1.199
N
N
N
Ts
1.00
1.01
2.02
4.00
2.00
0.99
2.00
1.00
1.00
1.00
3.00
6.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

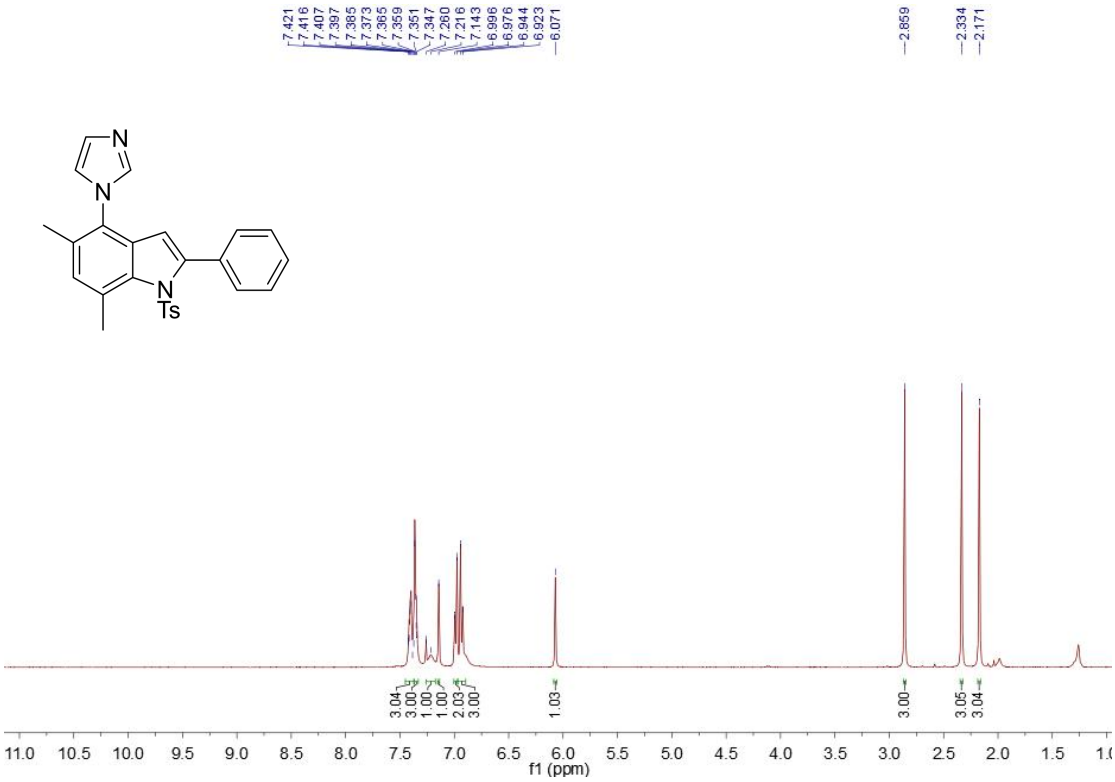

144.99
143.13
140.97
138.30
136.43
134.99
131.56
130.54
129.51
129.48
129.06
128.30
127.54
127.01
126.51
122.95
121.30
117.45
109.65
77.48
77.16
76.84
27.55
24.42
21.67
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

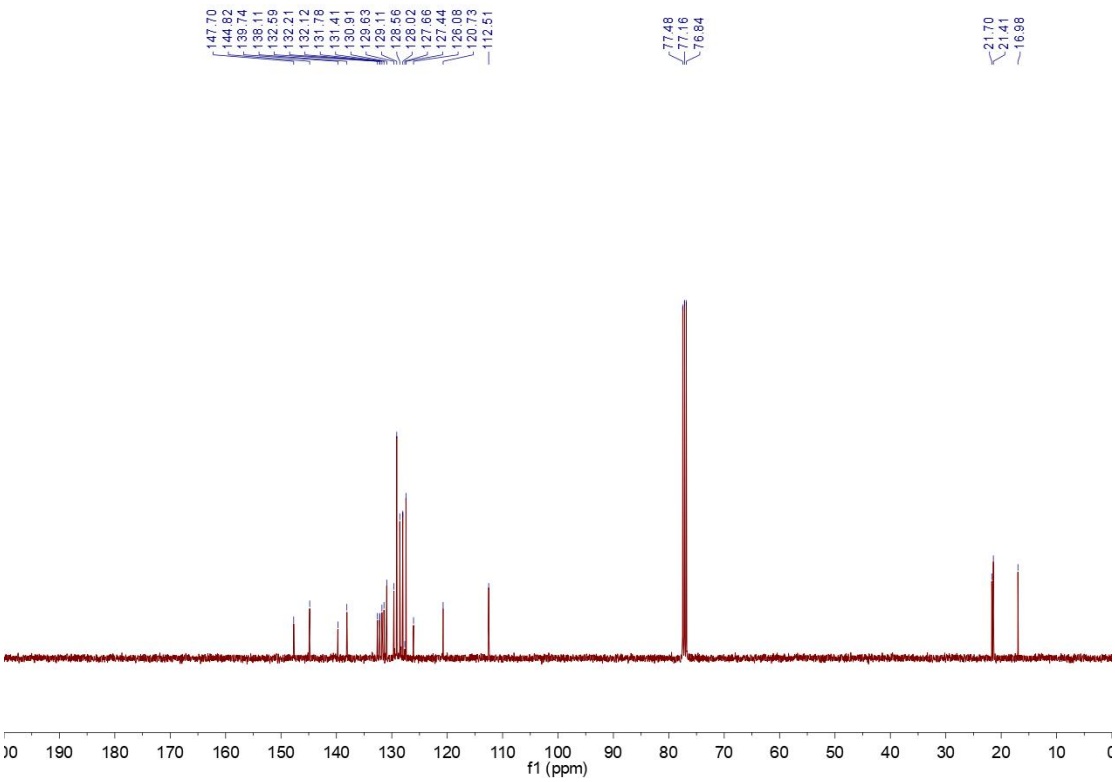
3p:


8.312
8.290
7.525
7.376
7.359
7.346
7.332
7.315
7.293
7.280
7.260
7.179
7.068
7.049
7.001
6.126
2.484
2.464
2.445
2.286
1.468
1.449
1.429
1.250
1.231
1.213
0.809
0.791
N
N
N
Ts
1.00
1.01
6.00
2.03
1.00
2.00
1.00
1.03
2.05
3.01
2.02
2.01
3.00
f1 (ppm)

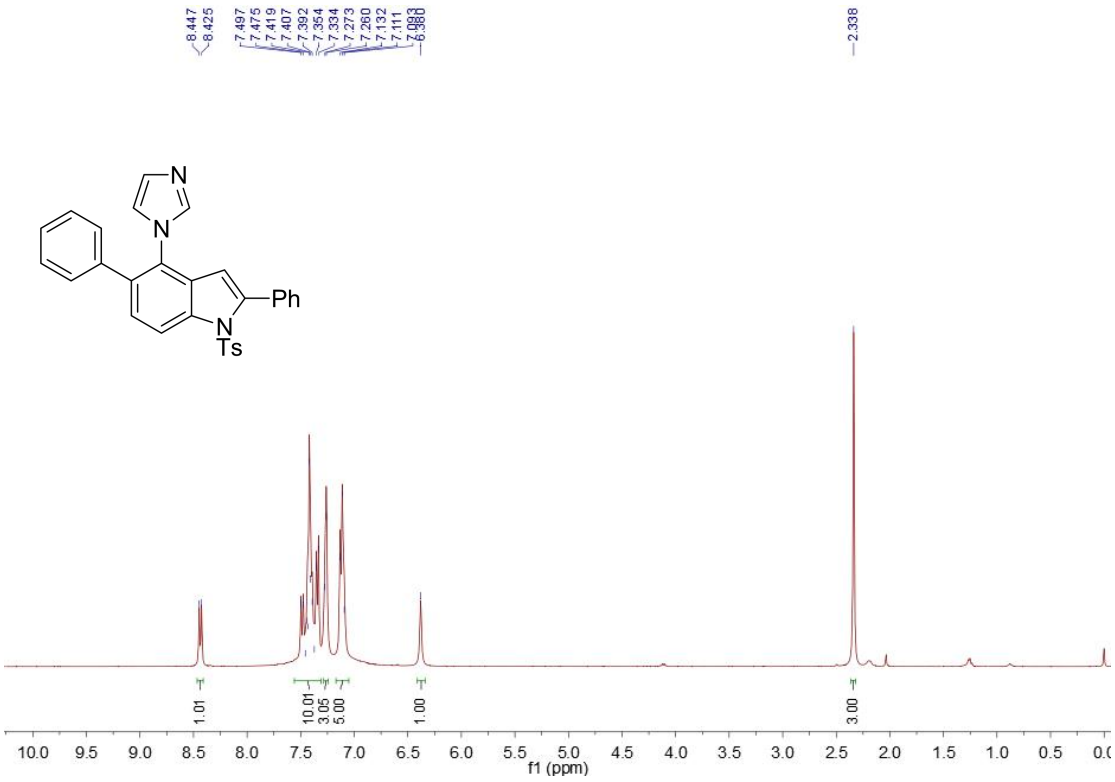

144.97
143.21
138.07
136.76
134.96
134.78
131.56
130.45
129.45
129.39
129.02
128.41
127.51
126.91
126.84
126.51
121.01
116.99
109.64
77.51
77.39
77.19
76.87
33.63
30.27
22.47
21.60
13.83
f1 (ppm)

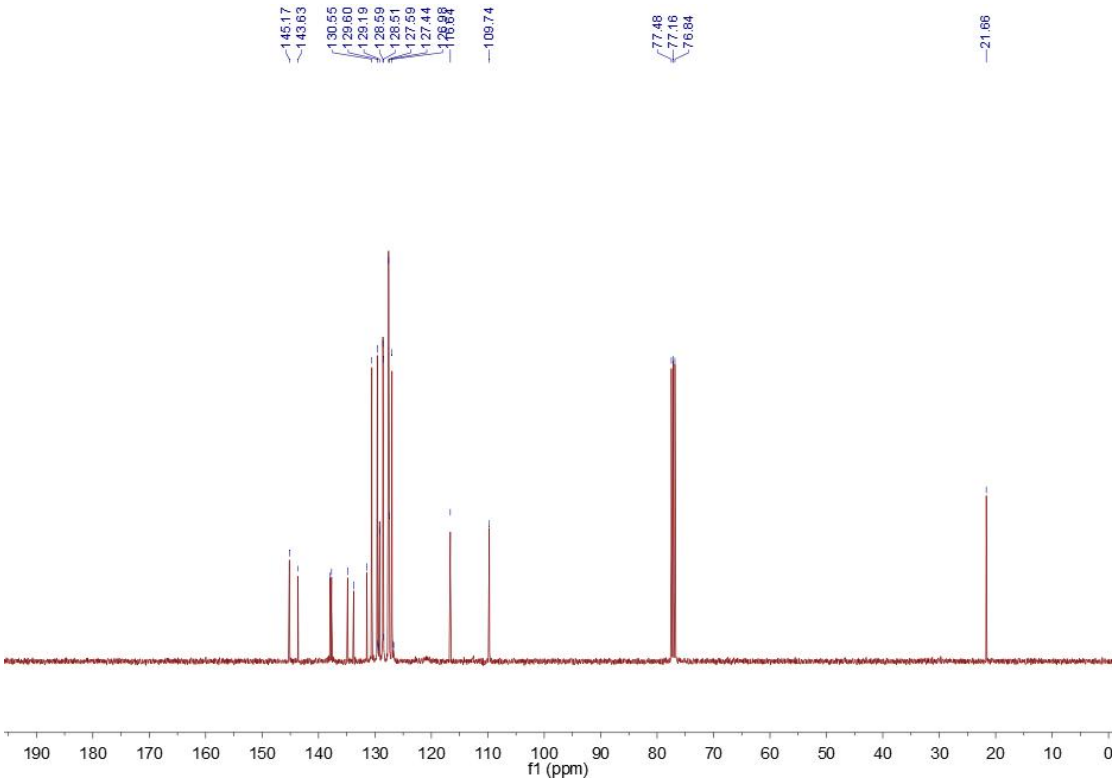
3q:


7.421
7.416
7.407
7.397
7.385
7.373
7.365
7.359
7.351
7.347
7.260
7.216
7.143
6.996
6.976
6.944
6.923
6.071
2.859
2.334
2.171
N
N
N
Ts
3.04
3.00
1.00
1.00
2.03
3.00
1.03
3.00
3.05
3.04
f1 (ppm)

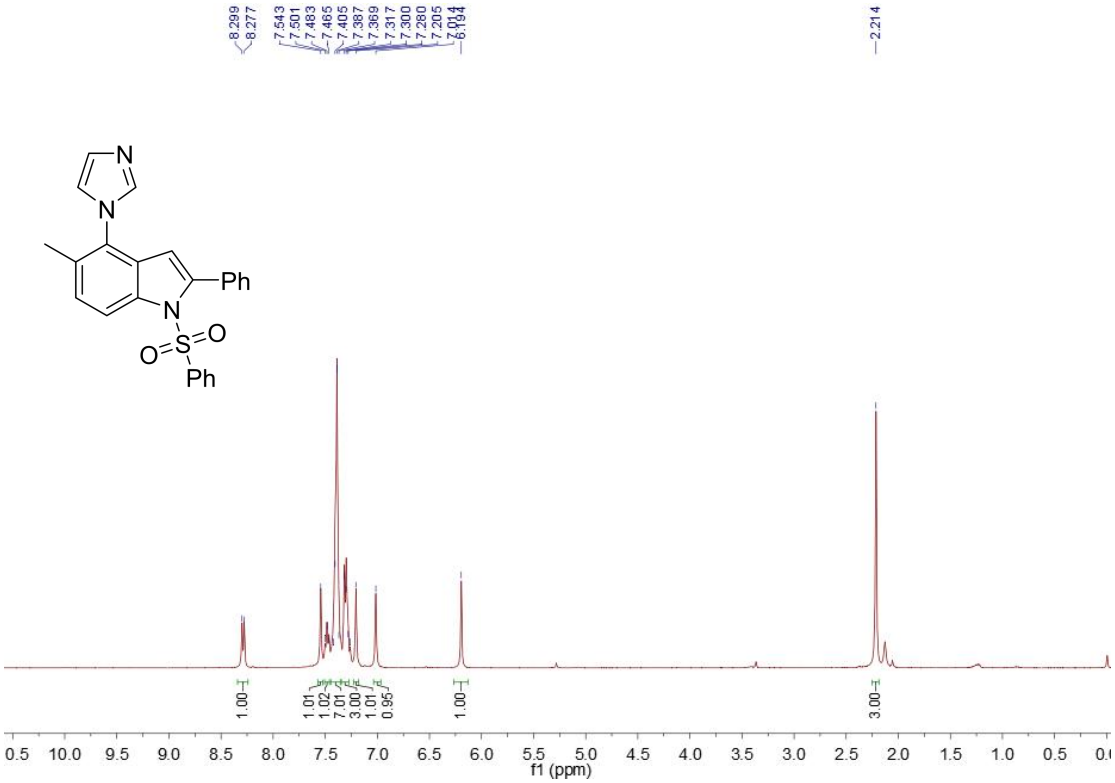

147.70
144.92
139.74
138.11
132.59
132.21
132.12
131.78
131.41
130.91
129.63
129.11
128.56
128.02
127.66
127.44
126.08
120.73
112.51
77.48
77.16
76.84
21.70
21.41
16.98
f1 (ppm)

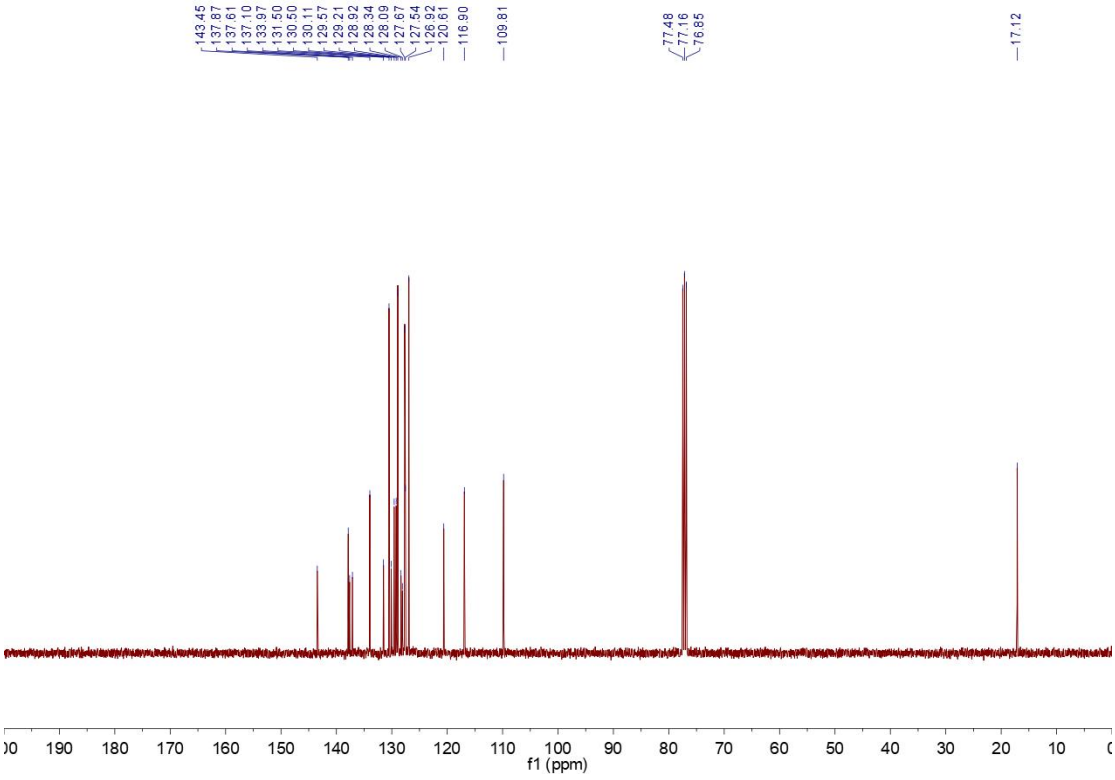
3r:


8.447
8.425
7.497
7.475
7.419
7.407
7.392
7.354
7.334
7.273
7.260
7.132
7.111
2.338
N
N
Ph
N
Ts
1.01
10.01
3.05
5.00
1.00
3.00
f1 (ppm)

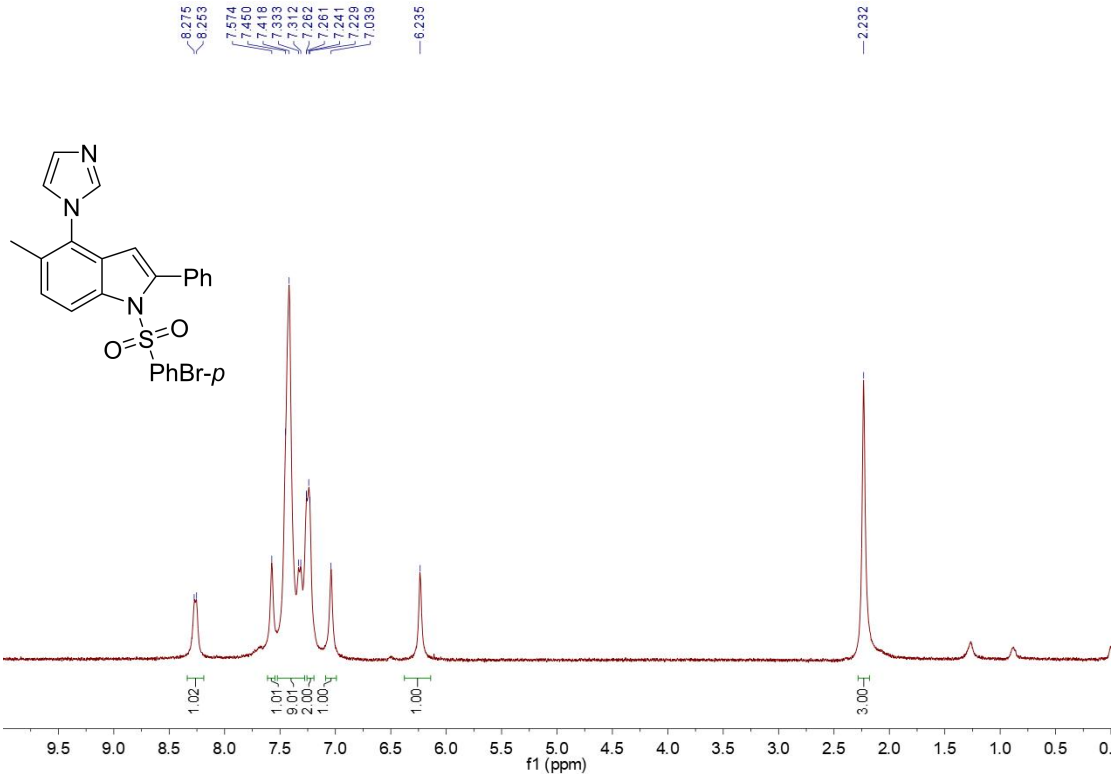

145.17
143.63
130.55
129.60
129.19
128.59
128.51
127.59
127.44
109.74
77.48
77.16
76.84
21.66
f1 (ppm)

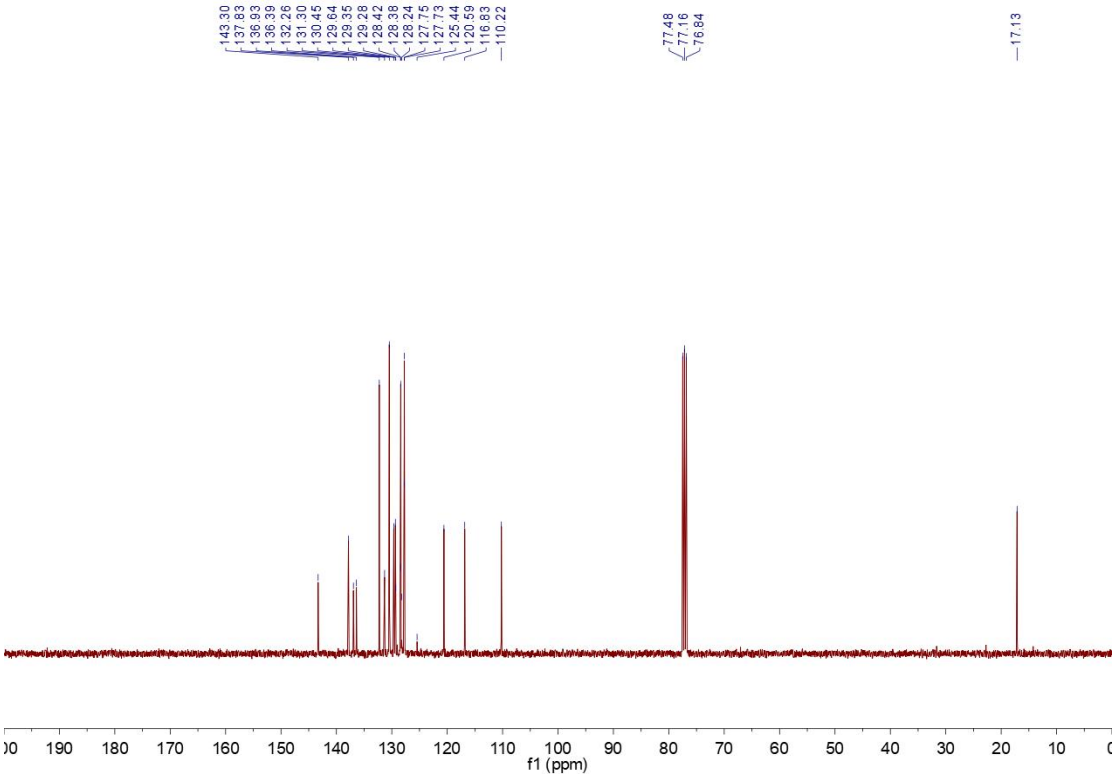
3s:


8.299
8.277
7.543
7.501
7.483
7.465
7.405
7.387
7.369
7.317
7.300
7.280
7.205
7.014
6.994
2.214
N
N
Ph
N
O=S=O
Ph
1.00
1.01
1.02
7.01
3.00
1.01
0.95
1.00
3.00
f1 (ppm)

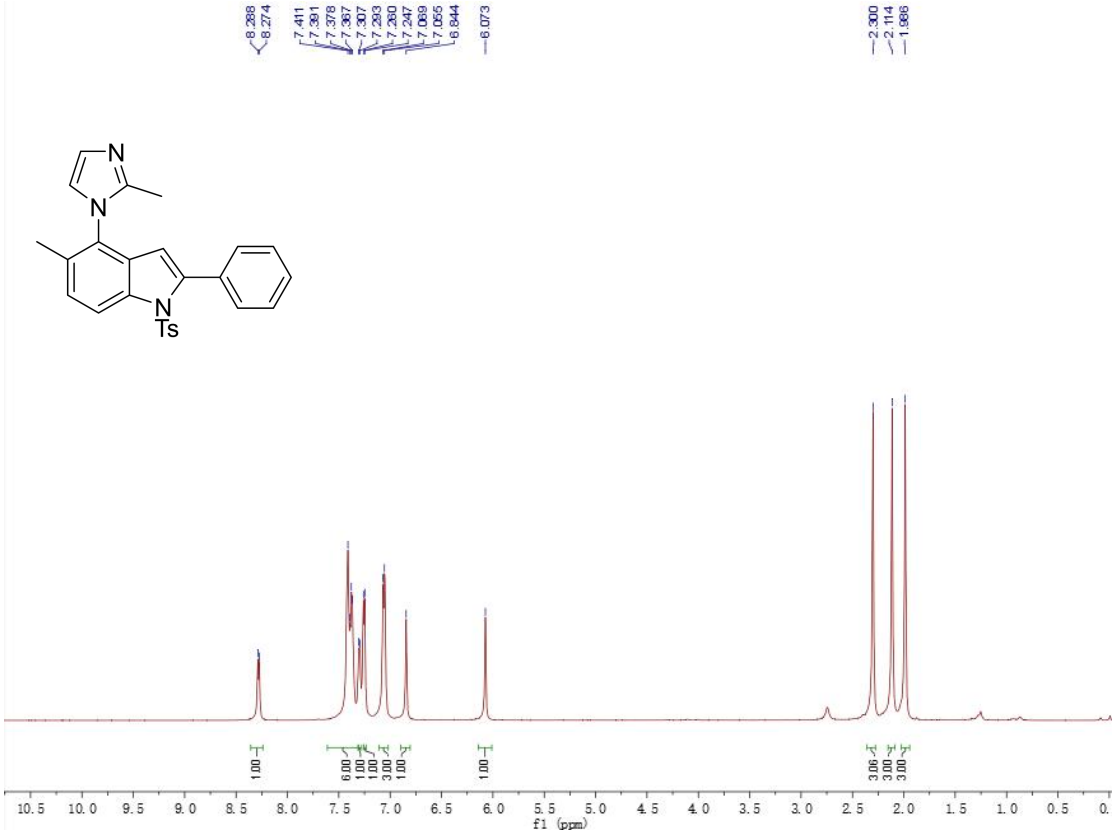

143.45
137.87
137.61
137.10
133.97
131.50
130.50
130.11
129.57
129.21
128.92
128.34
128.09
127.67
127.54
126.92
120.61
116.90
109.81
77.48
77.16
76.85
17.12
f1 (ppm)

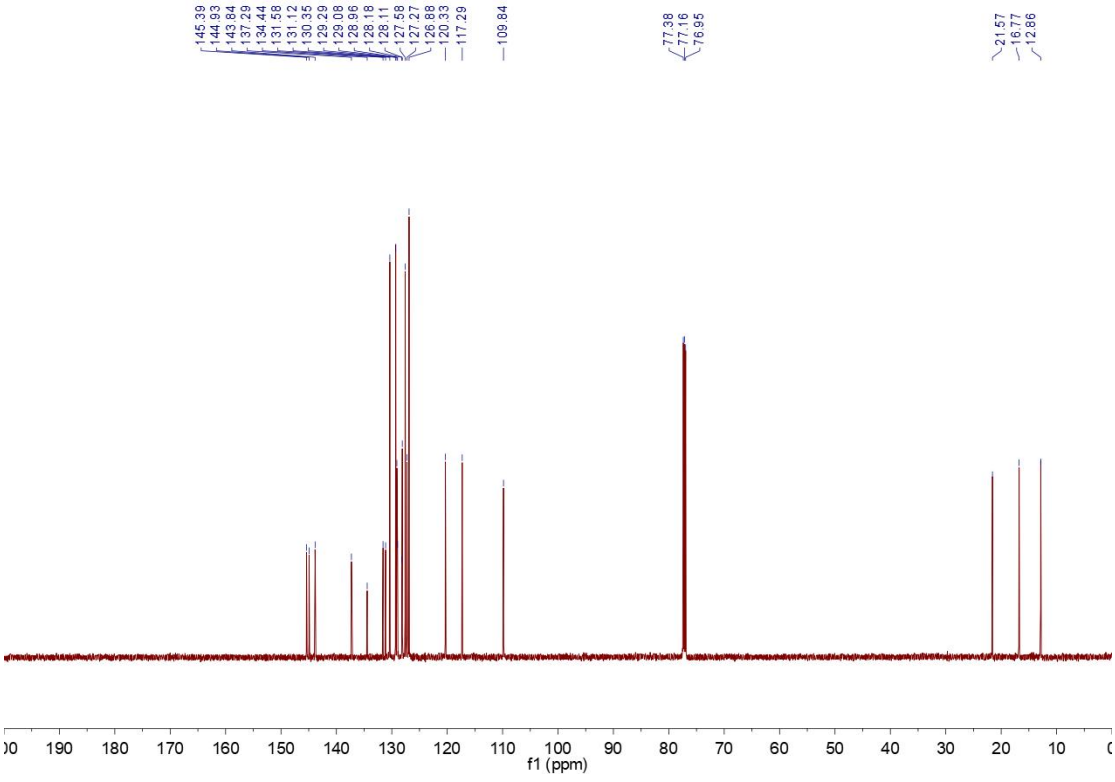
3t:


8.275
8.253
7.574
7.450
7.418
7.333
7.312
7.262
7.261
7.241
7.229
7.039
6.235
2.232
N
N
Ph
N
S
O
O
PhBr-p
1.02
1.01
9.01
2.00
1.00
1.00
3.00
f1 (ppm)

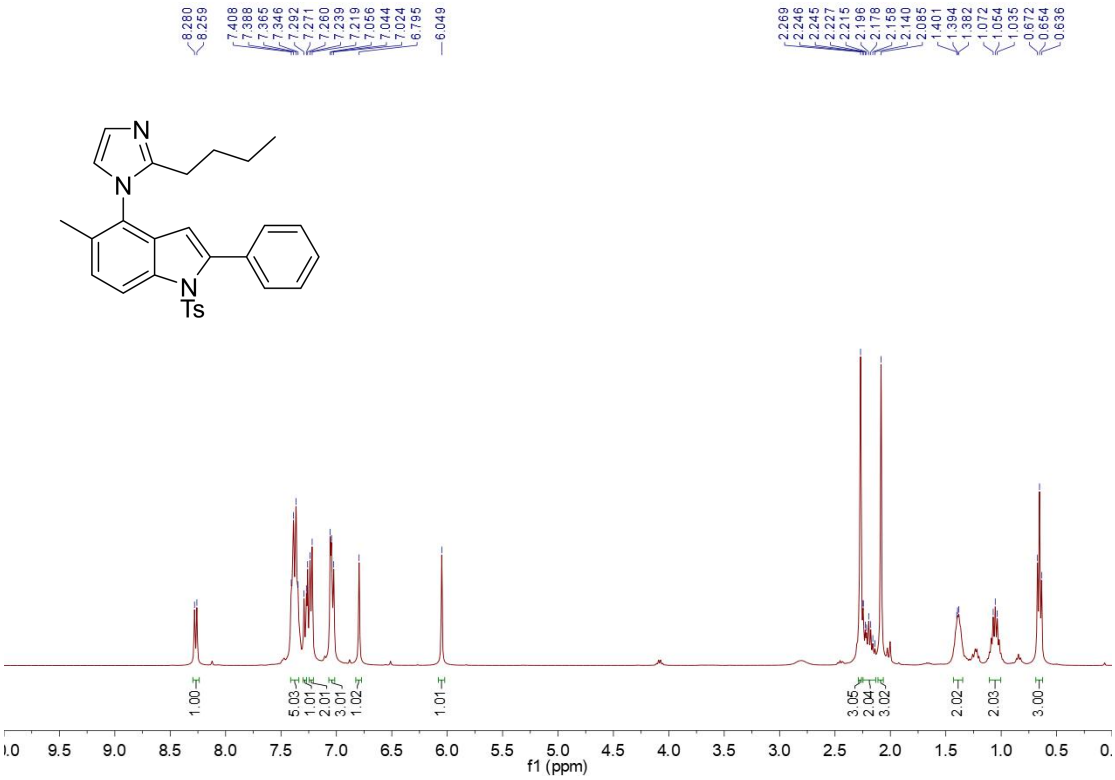

143.30
137.83
136.93
136.39
132.26
131.30
130.45
129.64
129.35
129.28
128.42
128.38
128.24
127.75
127.73
125.44
120.59
116.83
110.22
77.48
77.16
76.84
17.13
f1 (ppm)

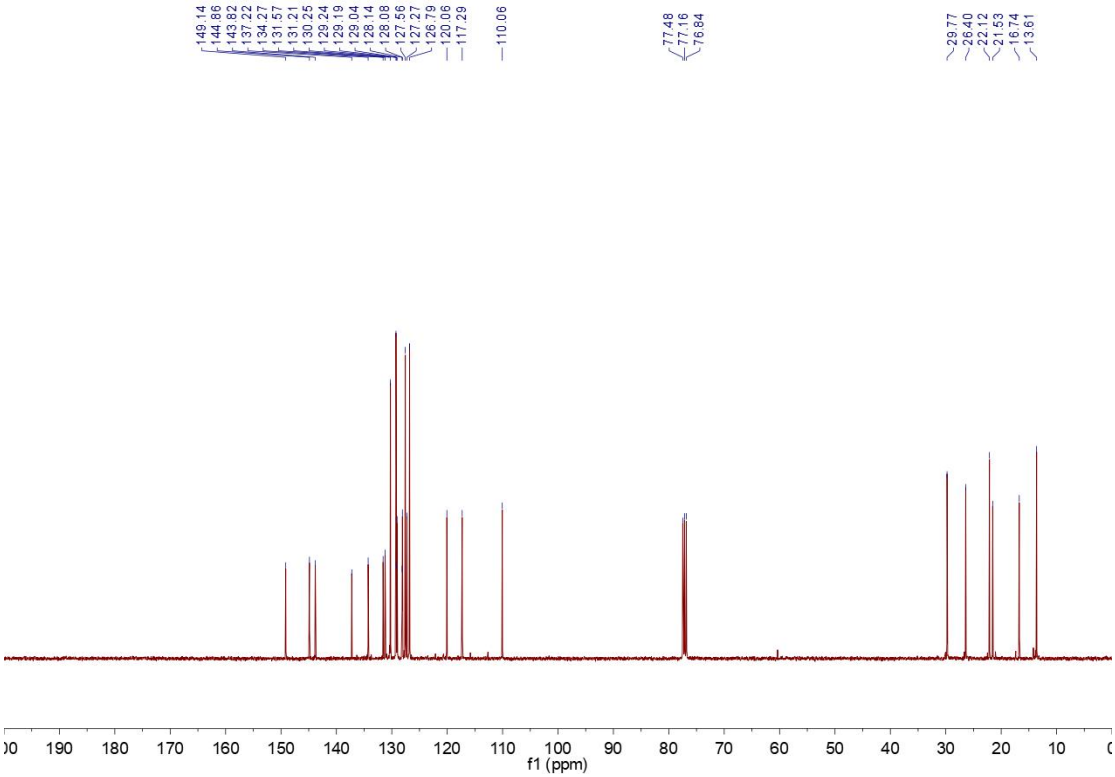
3u:


8.288
8.274
7.411
7.391
7.378
7.367
7.307
7.293
7.260
7.247
7.069
7.055
6.844
6.073
2.300
2.114
1.986
N
N
Ts
1.00
6.00
1.00
1.00
3.00
1.00
1.00
3.06
3.00
3.00
f1 (ppm)

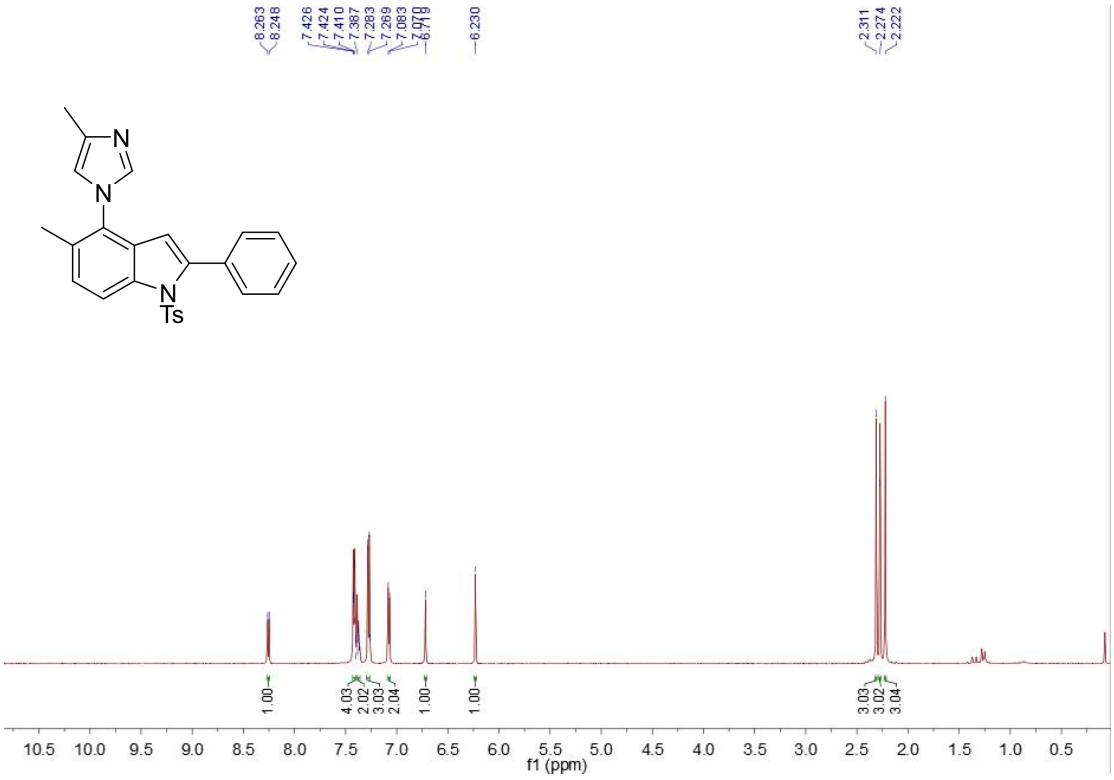

145.39
144.93
143.84
137.29
134.44
131.58
131.12
130.35
129.29
129.08
128.96
128.18
128.11
127.58
127.27
126.88
120.33
117.29
109.84
77.38
77.16
76.95
21.57
16.77
12.86
f1 (ppm)

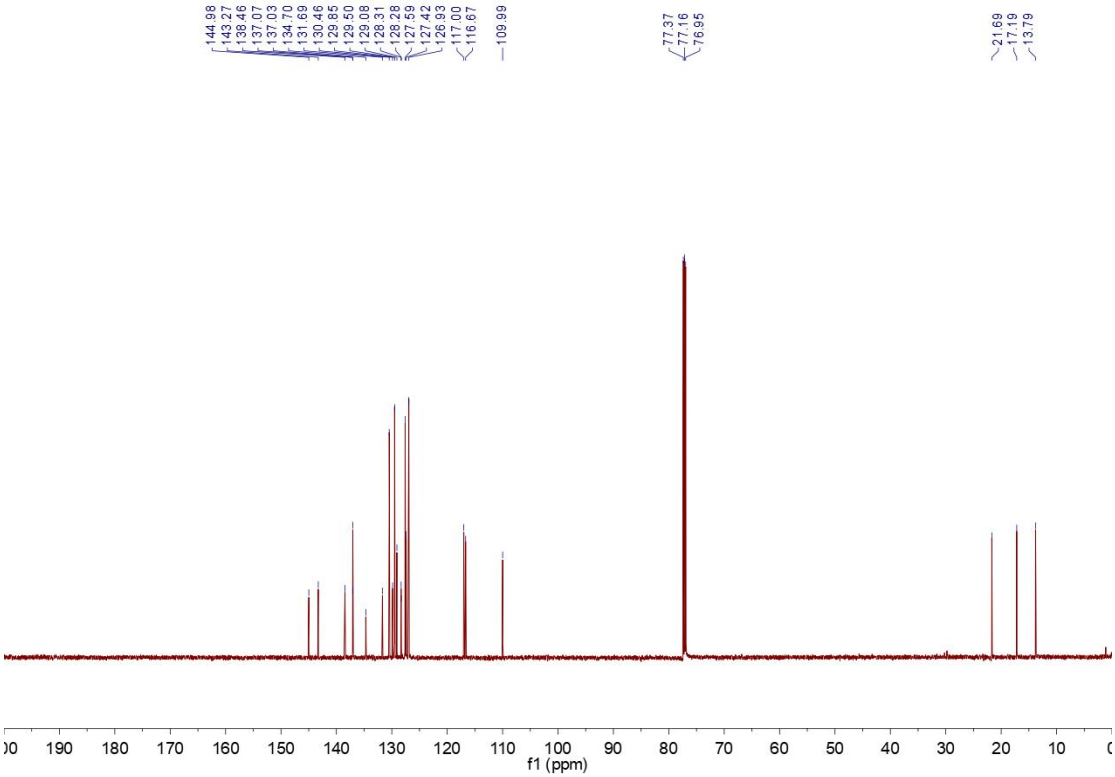
3v:


8.280
8.259
7.408
7.388
7.365
7.346
7.292
7.271
7.260
7.239
7.219
7.056
7.044
7.024
6.795
6.049
2.269
2.246
2.245
2.227
2.215
2.196
2.178
2.158
2.140
2.085
1.401
1.394
1.382
1.072
1.054
1.035
0.672
0.654
0.636
N
N
N
Ts
1.00
5.03
1.01
2.01
3.01
1.02
1.01
3.05
2.04
3.02
2.02
2.03
3.00
f1 (ppm)

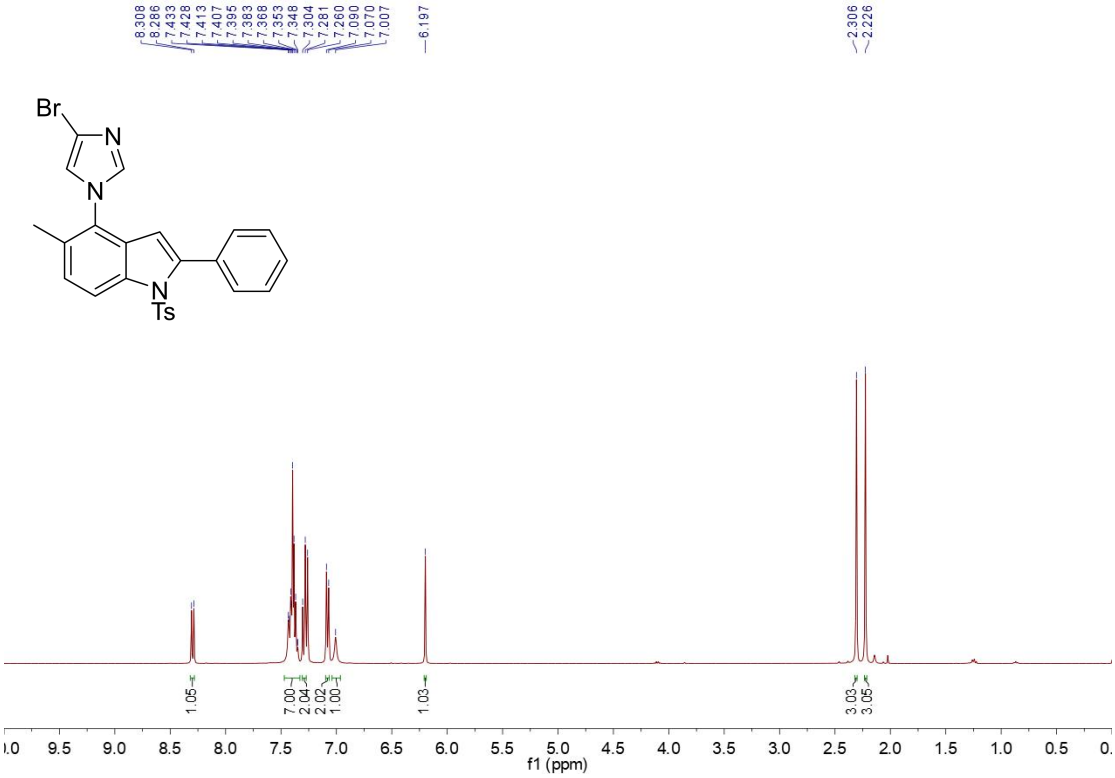

149.14
144.86
143.82
137.22
134.27
131.57
131.21
130.25
129.24
129.19
129.04
128.14
128.08
127.56
127.27
126.79
120.06
117.29
110.06
77.48
77.16
76.84
29.77
26.40
22.12
21.53
16.74
13.61
f1 (ppm)

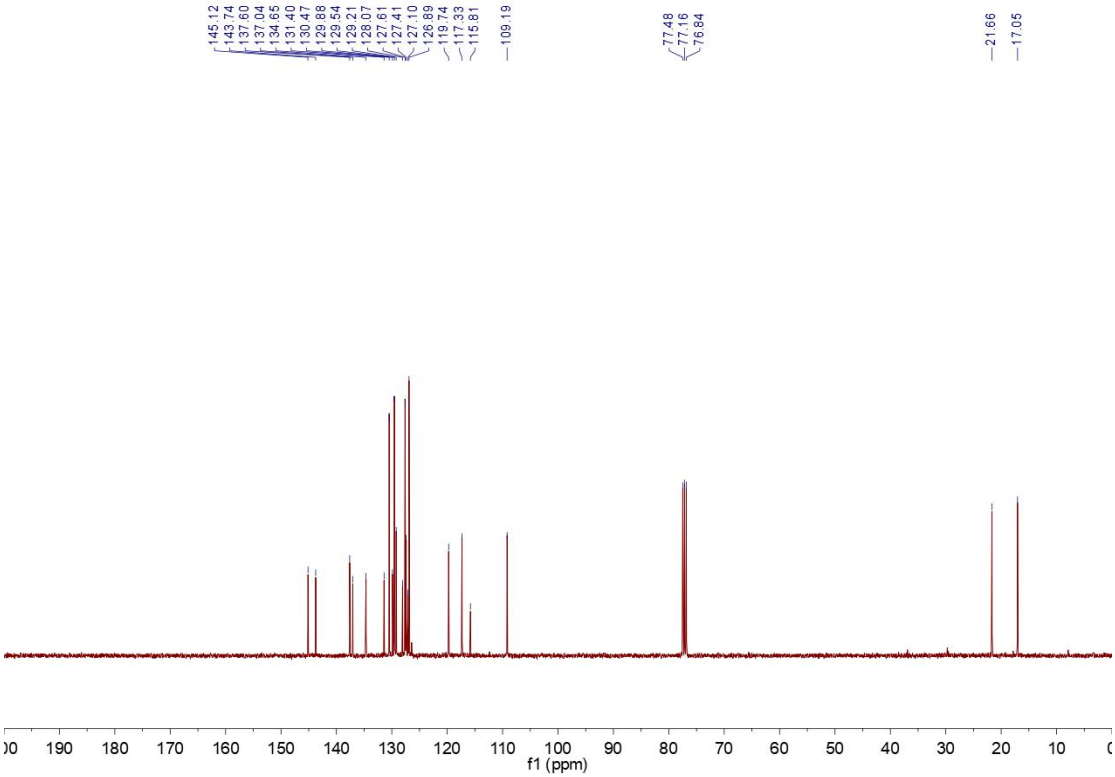
3w:


8.263
8.248
7.426
7.424
7.410
7.387
7.283
7.269
7.083
6.719
6.230
2.311
2.274
2.222
N
N
N
Ts
1.00
4.03
2.02
3.03
2.04
1.00
1.00
3.03
3.02
3.04
f1 (ppm)

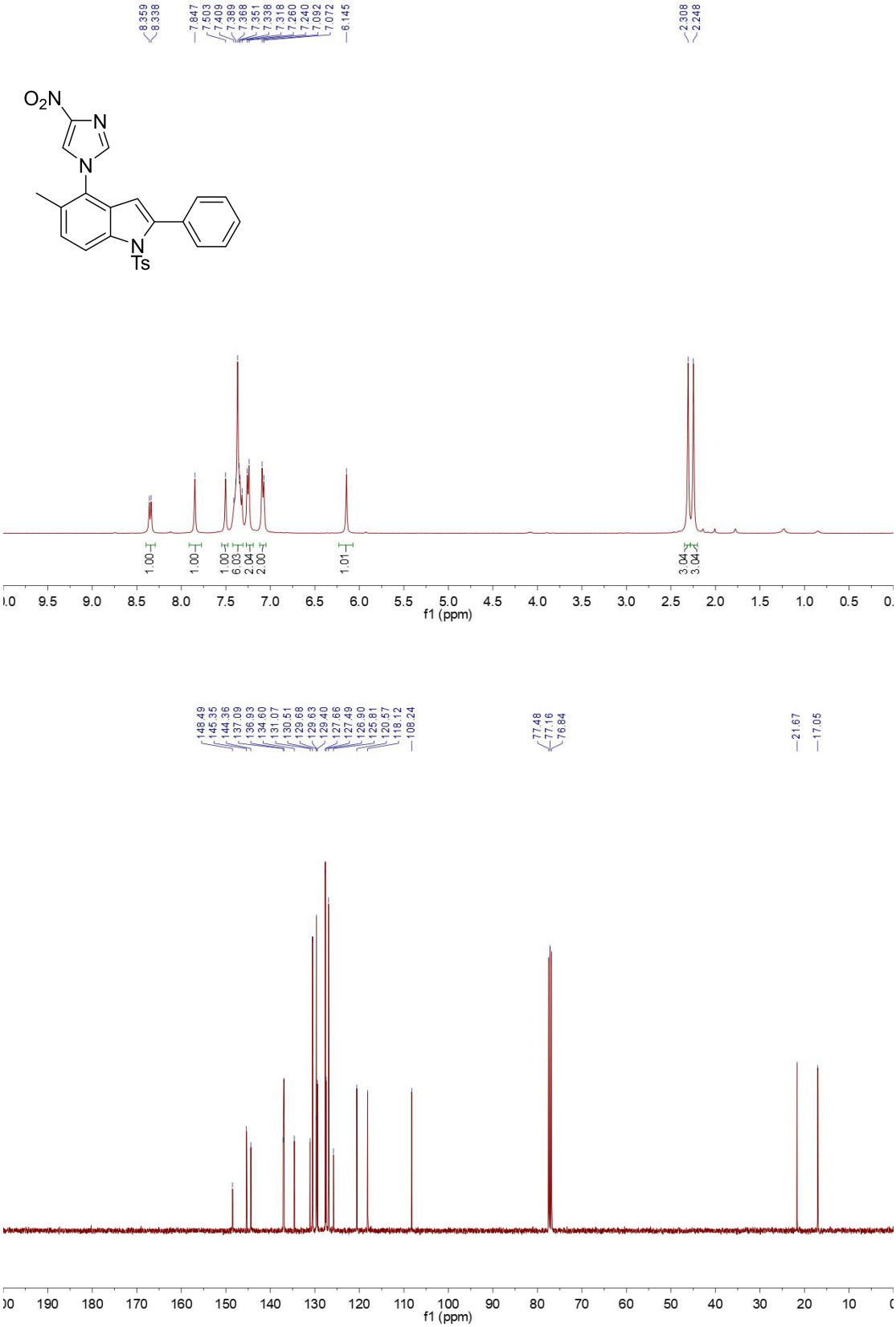

144.98
143.27
138.46
137.07
137.03
134.70
131.69
130.46
129.85
129.50
129.08
128.31
128.28
127.59
127.42
126.93
117.00
116.67
109.99
77.37
77.16
76.95
21.69
17.19
13.79
f1 (ppm)

3x:

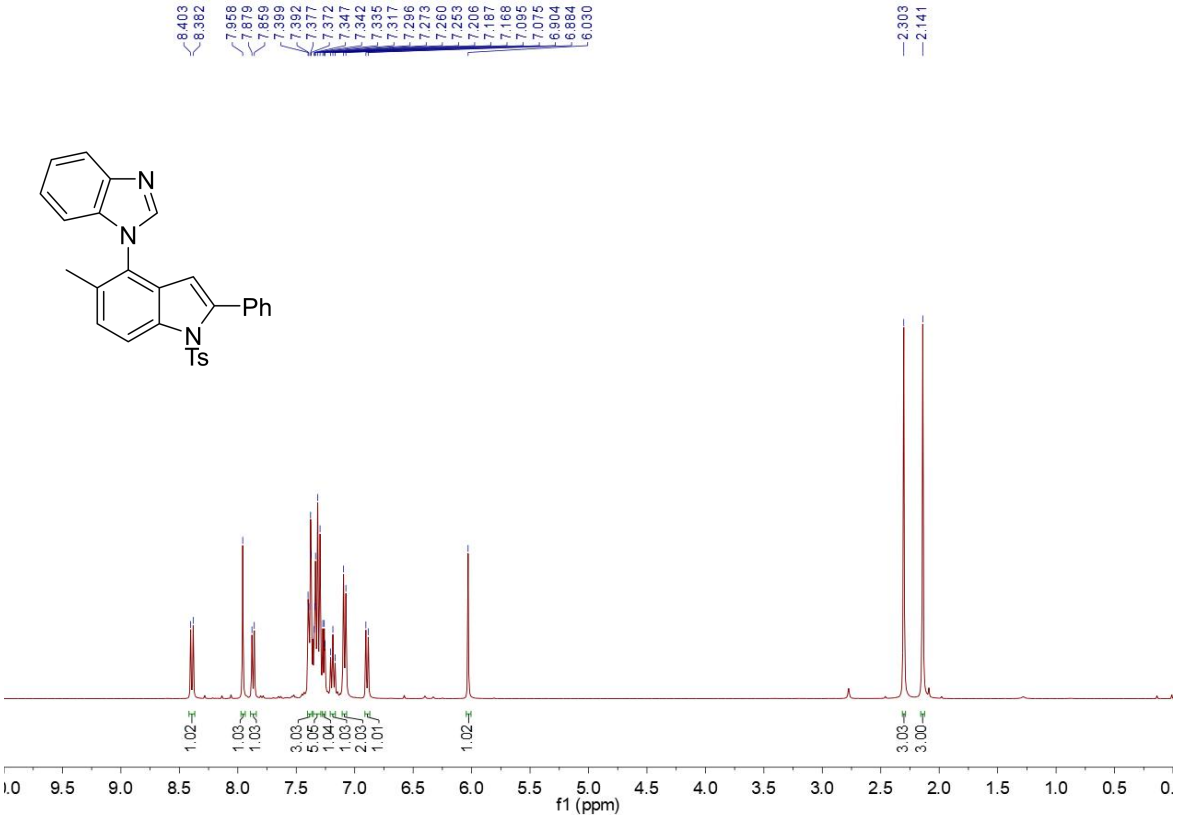

8.308
8.286
7.433
7.428
7.413
7.407
7.395
7.383
7.368
7.353
7.348
7.304
7.281
7.260
7.090
7.070
7.007
6.197
2.306
2.226
Br
N
N
N
Ts
1.05
7.00
2.04
2.02
1.00
1.03
3.03
3.05
f1 (ppm)

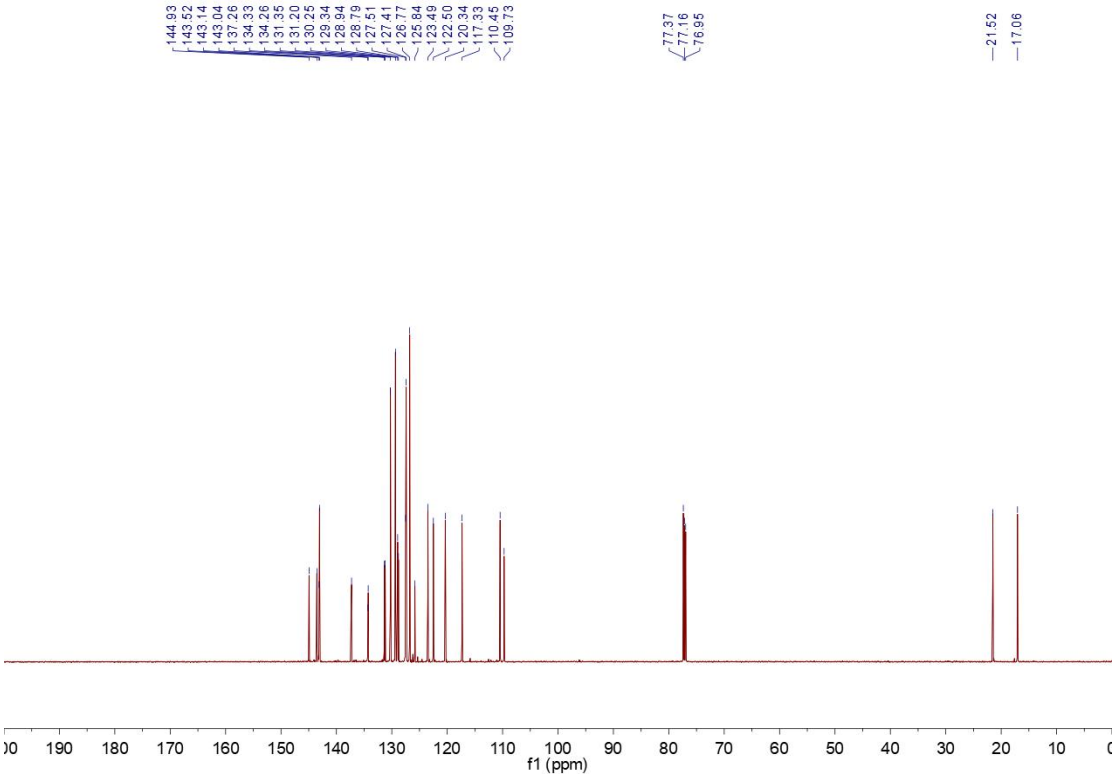

145.12
143.74
137.60
137.04
134.65
131.40
130.47
129.88
129.54
129.21
128.07
127.61
127.41
127.10
126.89
119.74
117.33
115.81
109.19
77.48
77.16
76.84
21.66
17.05
f1 (ppm)

3y:

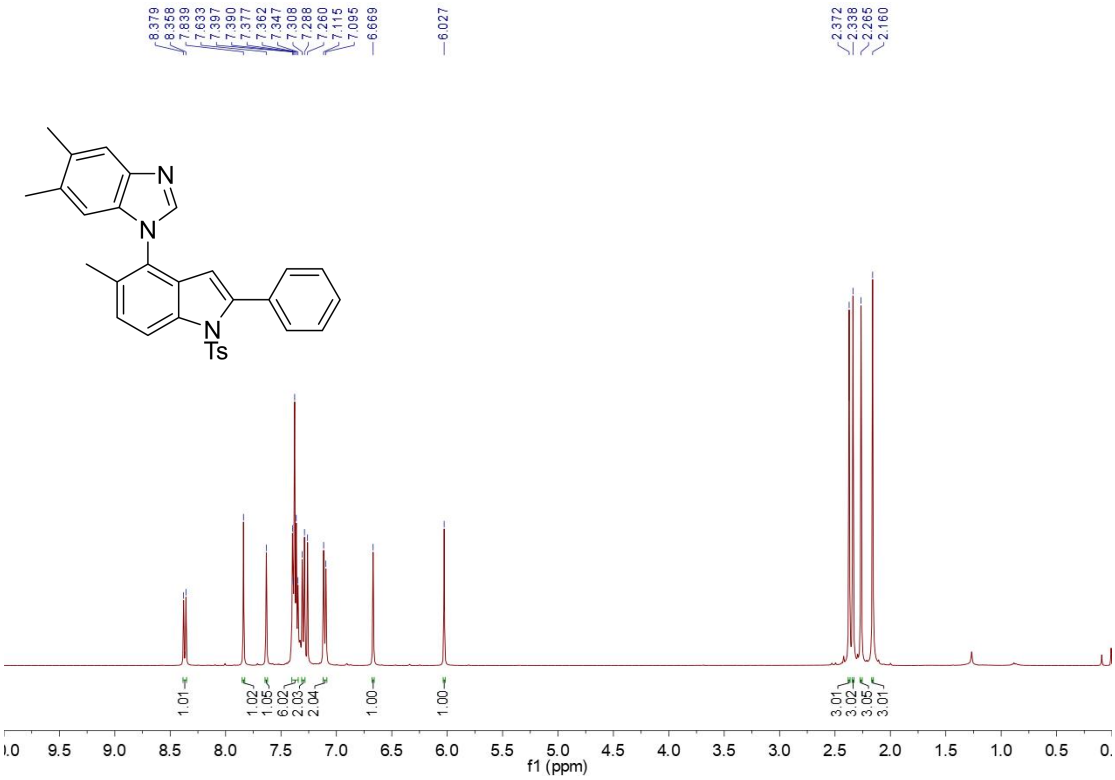

8.359
8.338
7.847
7.503
7.409
7.389
7.368
7.351
7.338
7.318
7.260
7.240
7.092
7.072
6.145
2.308
2.248
O2N
N
N
N
Ts
1.00
1.00
1.00
6.03
2.04
2.00
1.01
3.04
3.04
f1 (ppm)
148.49
145.35
144.36
137.09
136.93
134.60
131.07
130.51
129.68
129.63
129.40
127.66
127.49
126.90
125.81
120.57
118.12
108.24
77.48
77.16
76.84
21.67
17.05
f1 (ppm)

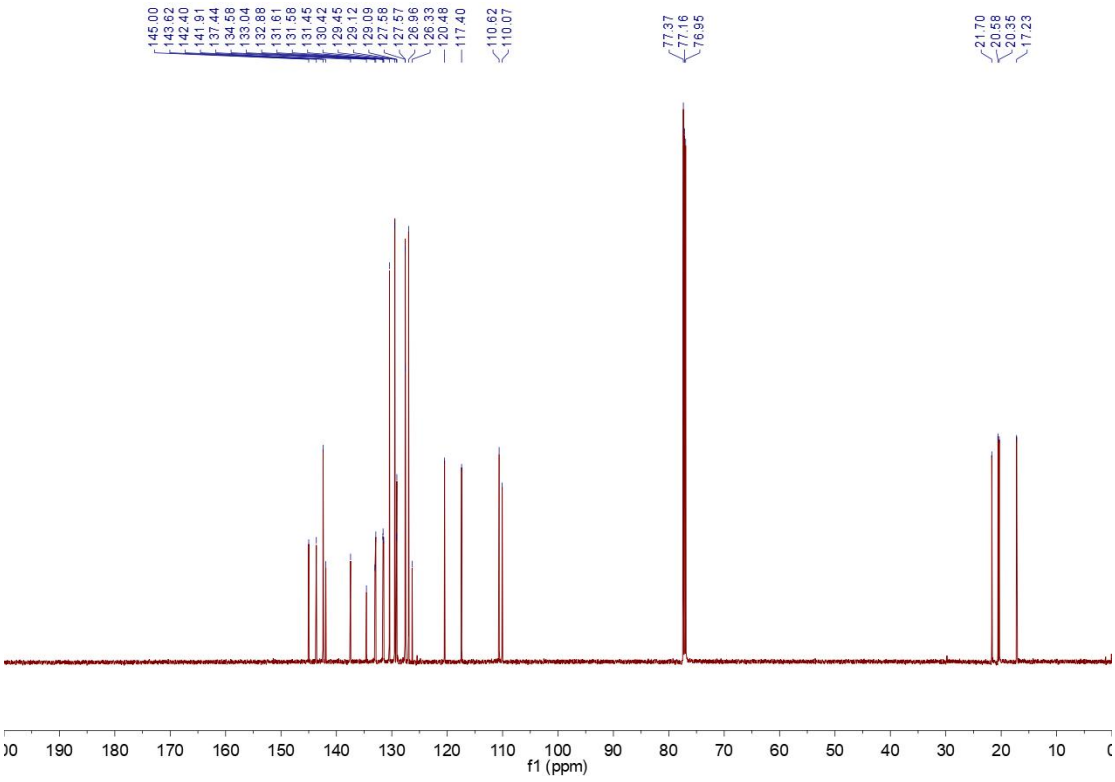
3z:


8.403
8.382
7.958
7.879
7.859
7.399
7.392
7.377
7.372
7.347
7.342
7.335
7.317
7.296
7.273
7.260
7.253
7.206
7.187
7.168
7.095
7.075
6.904
6.884
6.030
2.303
2.141
N
N
Ph
N
Ts
1.02
1.03
1.03
3.03
5.05
1.04
1.03
2.03
1.01
1.02
3.03
3.00
f1 (ppm)

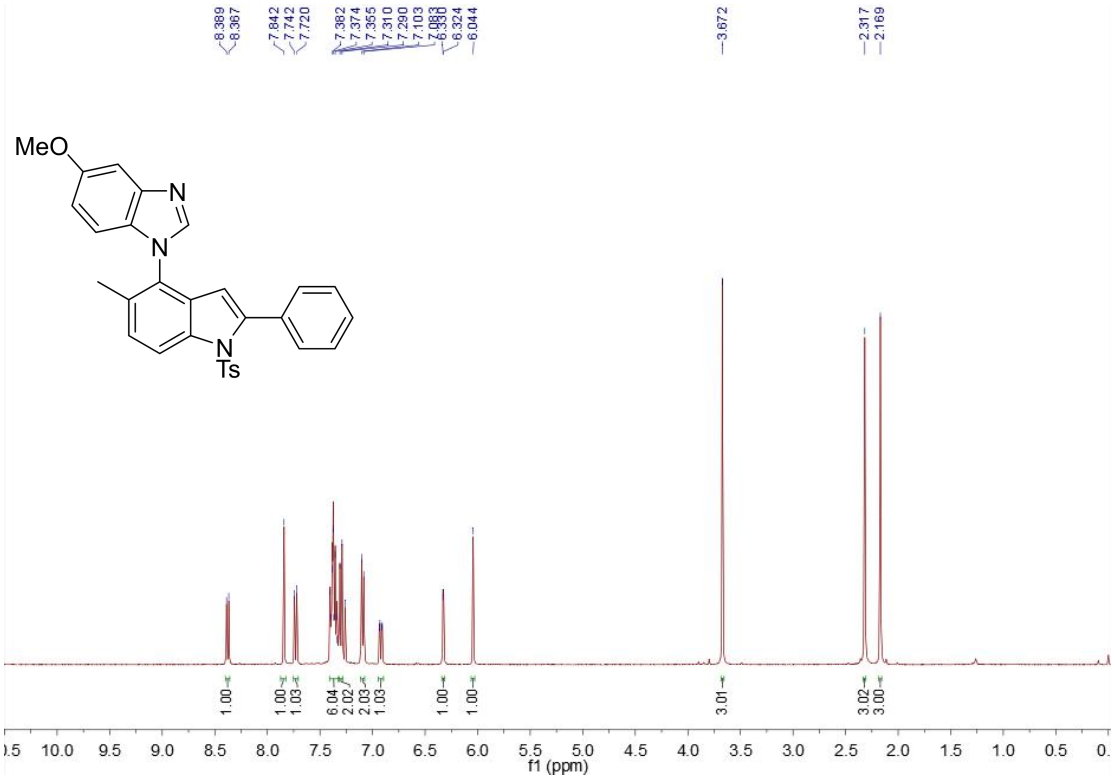

144.93
143.52
143.14
143.04
137.26
134.33
134.26
131.35
131.20
130.25
129.34
128.94
128.79
127.51
127.41
126.77
125.84
123.49
122.50
120.34
117.33
110.45
109.73
77.37
77.16
76.95
21.52
17.06
f1 (ppm)

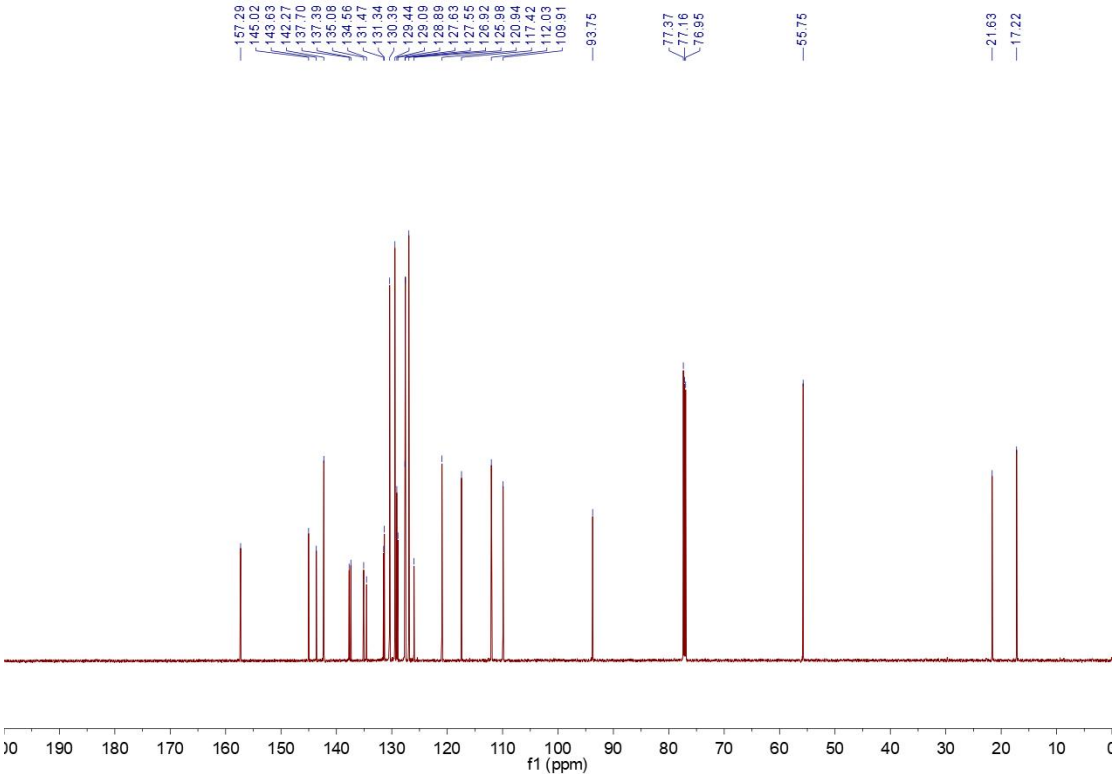
3aa:


8.379
8.358
7.839
7.633
7.397
7.390
7.377
7.362
7.347
7.308
7.288
7.260
7.115
7.095
6.669
6.027
2.372
2.338
2.265
2.160
N
N
N
Ts
1.01
1.02
1.05
6.02
2.03
2.04
1.00
1.00
3.01
3.02
3.05
3.01
f1 (ppm)

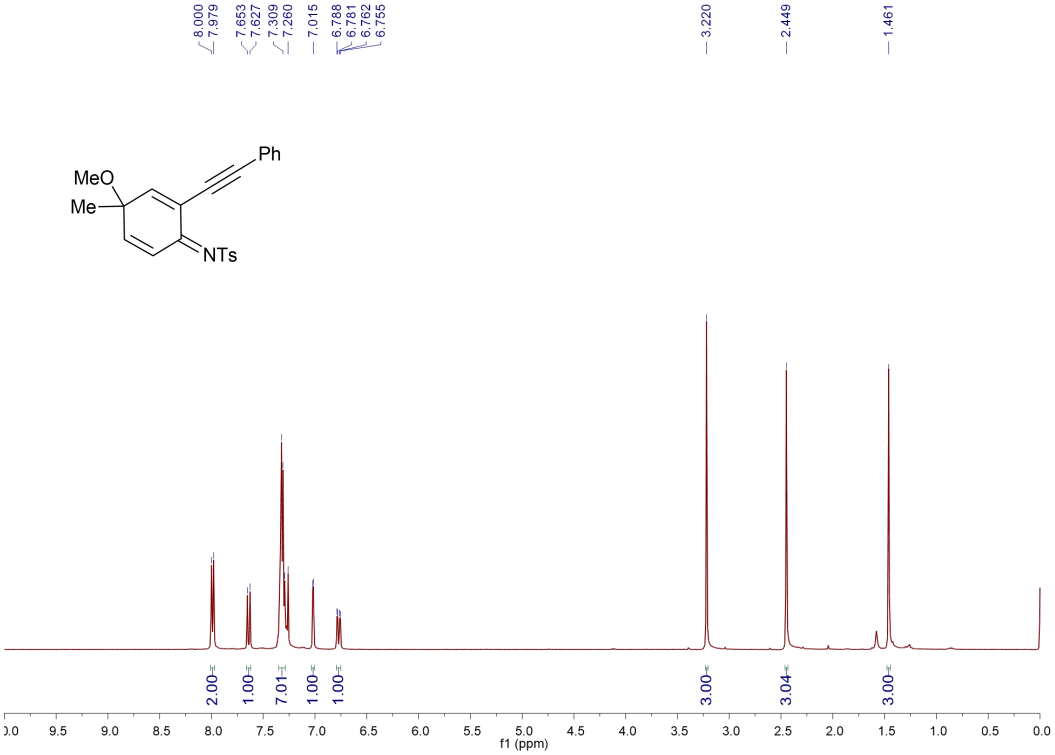

145.00
143.62
142.40
141.91
137.44
134.58
133.04
132.88
131.61
131.58
131.45
130.42
129.45
129.12
129.09
127.58
127.57
126.96
126.33
120.48
117.40
110.62
110.07
77.37
77.16
76.95
21.70
20.58
20.35
17.23
f1 (ppm)

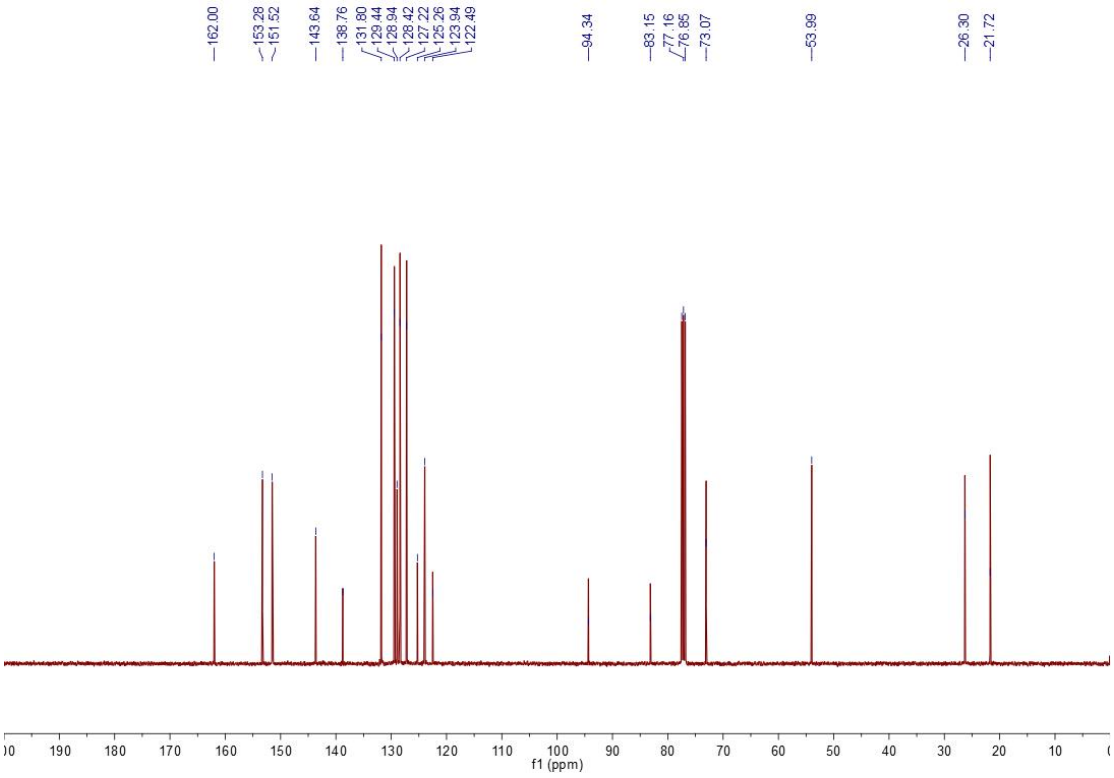
3ab:


8.389
8.367
7.842
7.742
7.720
7.382
7.374
7.355
7.310
7.290
7.103
7.083
6.330
6.324
6.044
3.672
2.317
2.169
MeO
N
N
N
Ts
1.00
1.00
1.03
6.04
2.02
2.03
1.03
1.00
1.00
3.01
3.02
3.00
f1 (ppm)

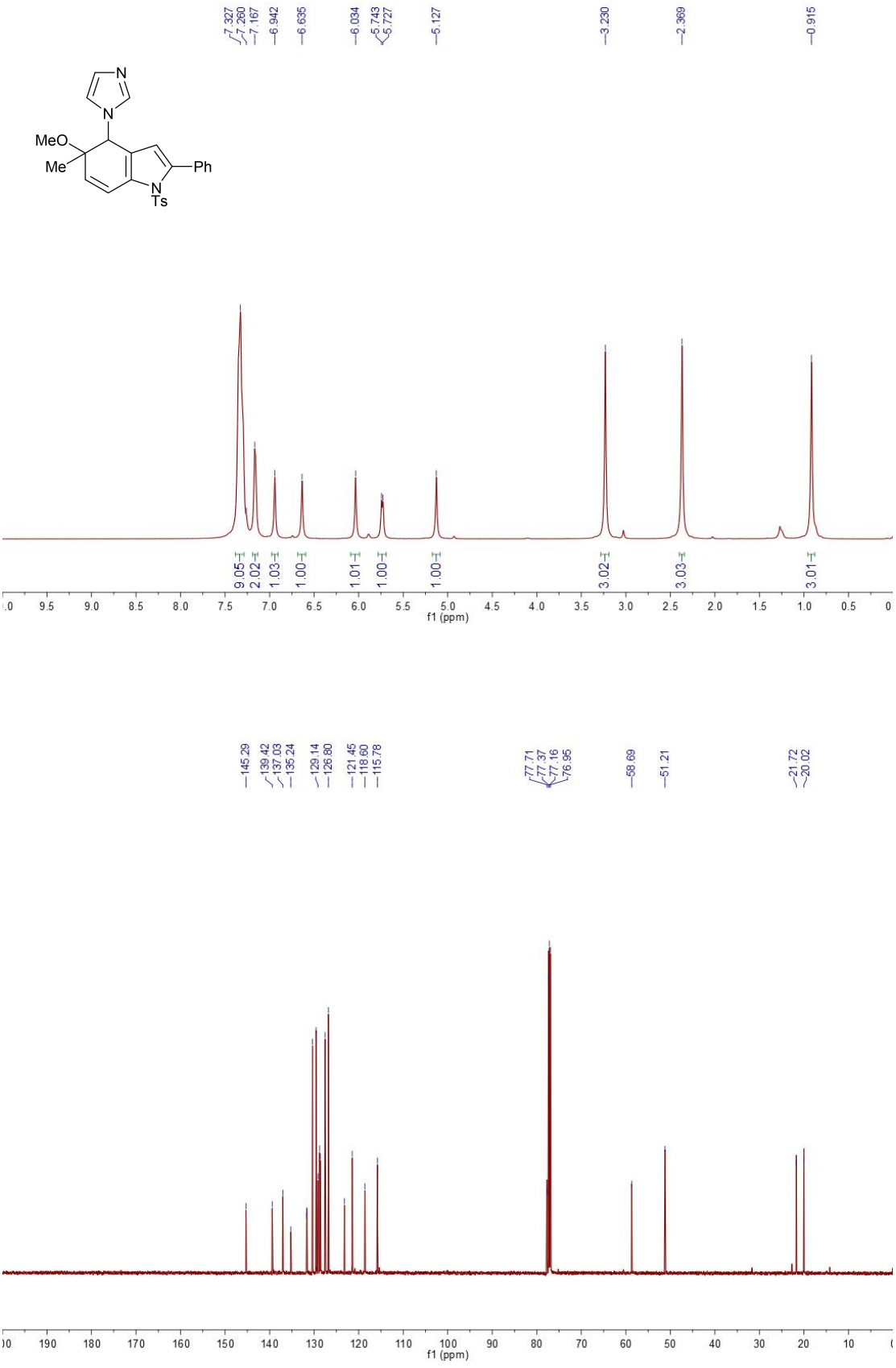

157.29
145.02
143.63
142.27
137.70
137.39
135.08
134.56
131.47
131.34
130.39
129.44
129.09
128.89
127.63
127.55
126.92
125.98
120.94
117.42
112.03
109.91
93.75
77.37
77.16
76.95
55.75
21.63
17.22
f1 (ppm)

Intermediate 4a:

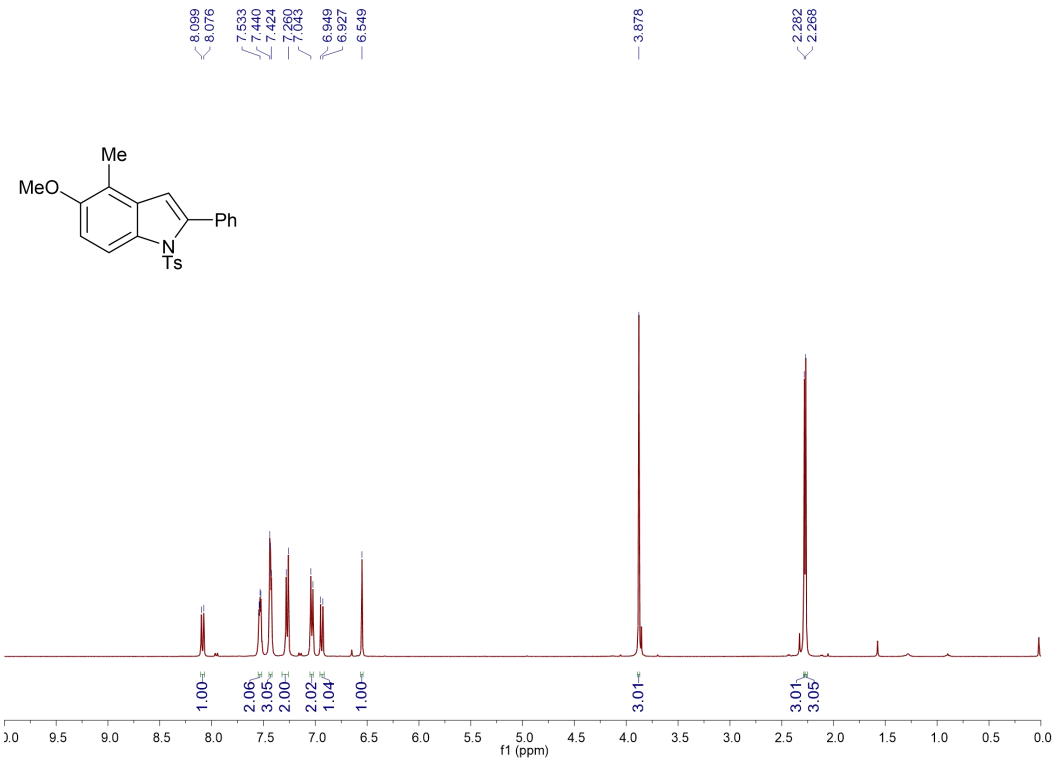


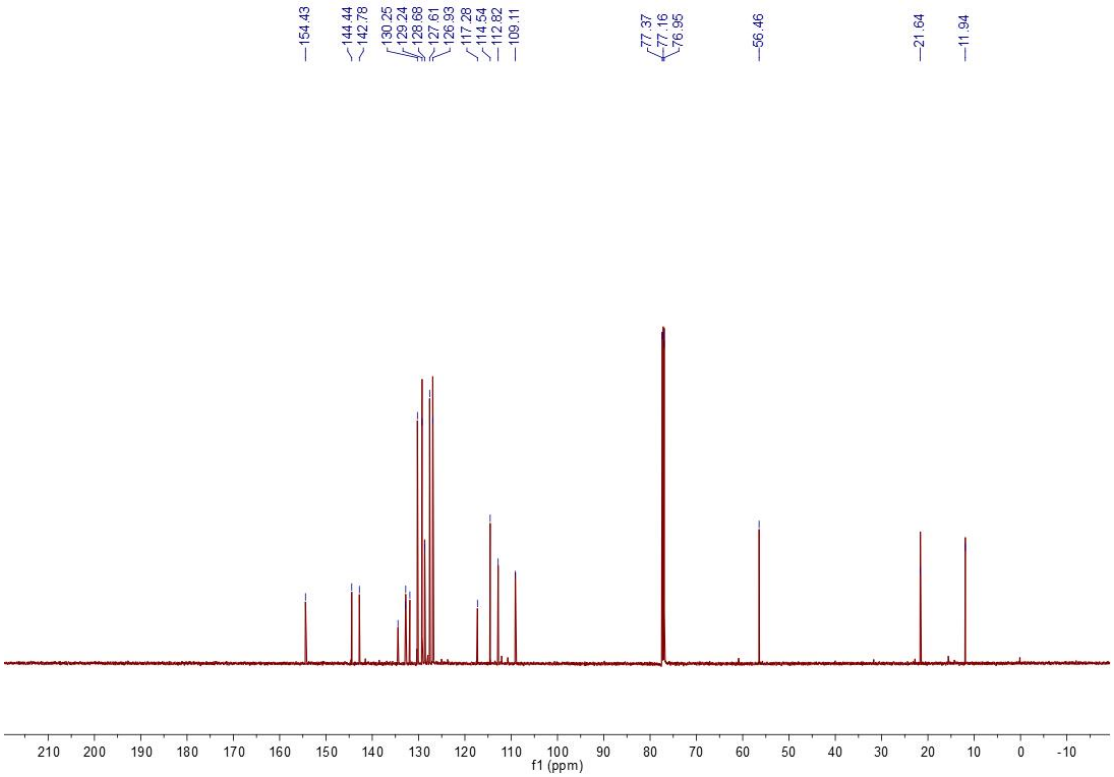


by-Product 5a:

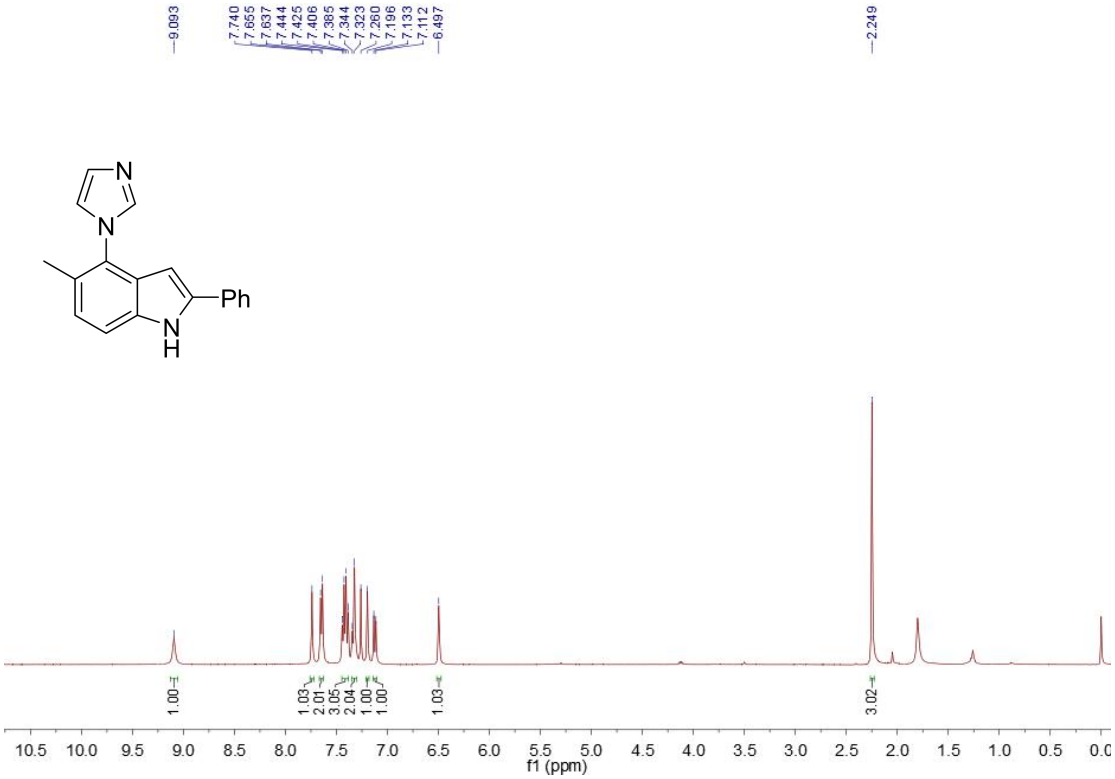


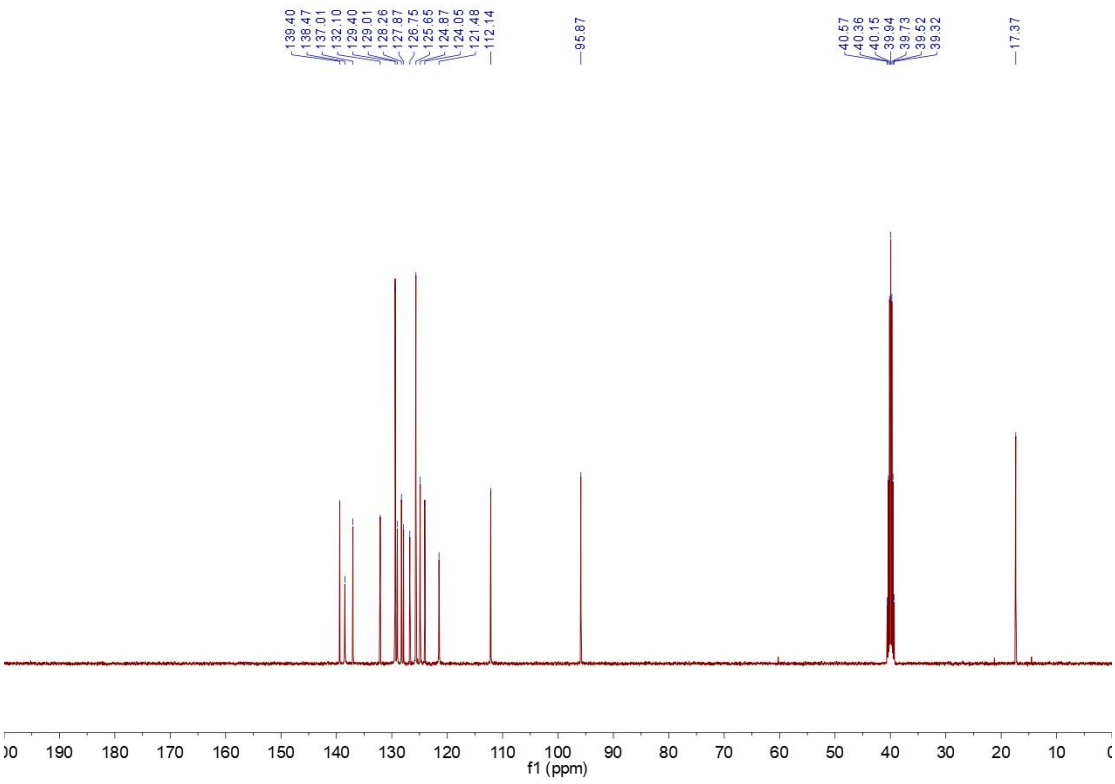
by-Product 6a:



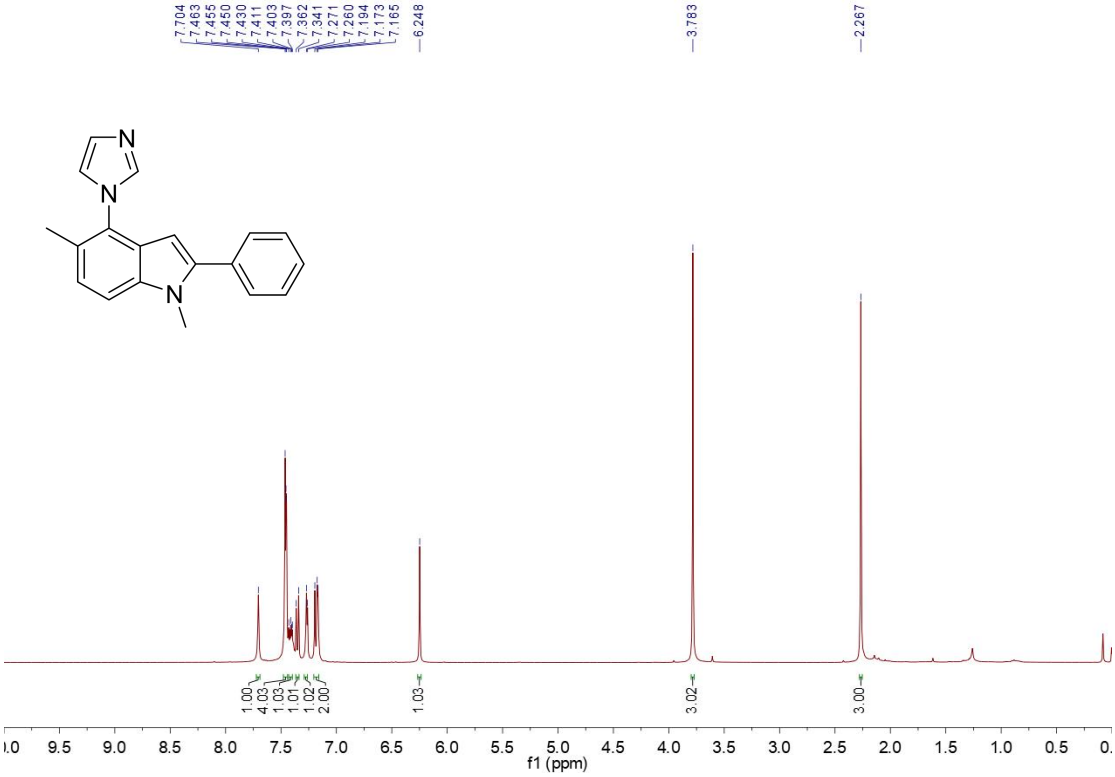


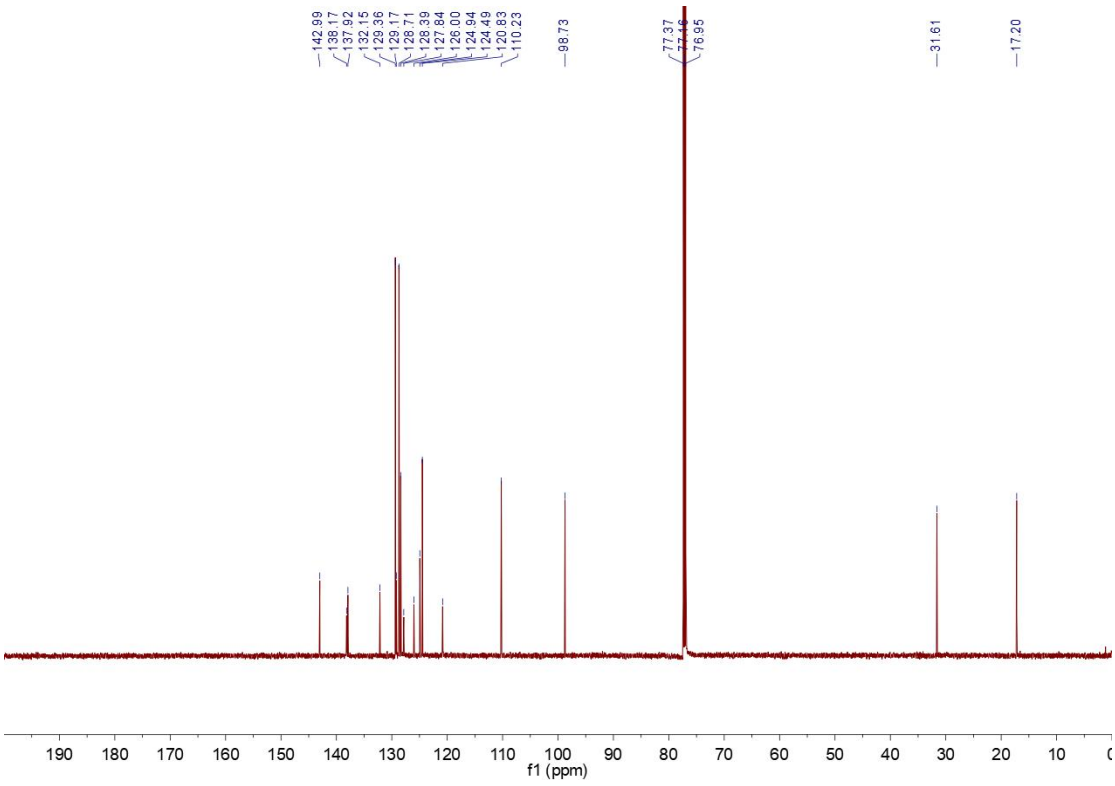
Derivative 7a:



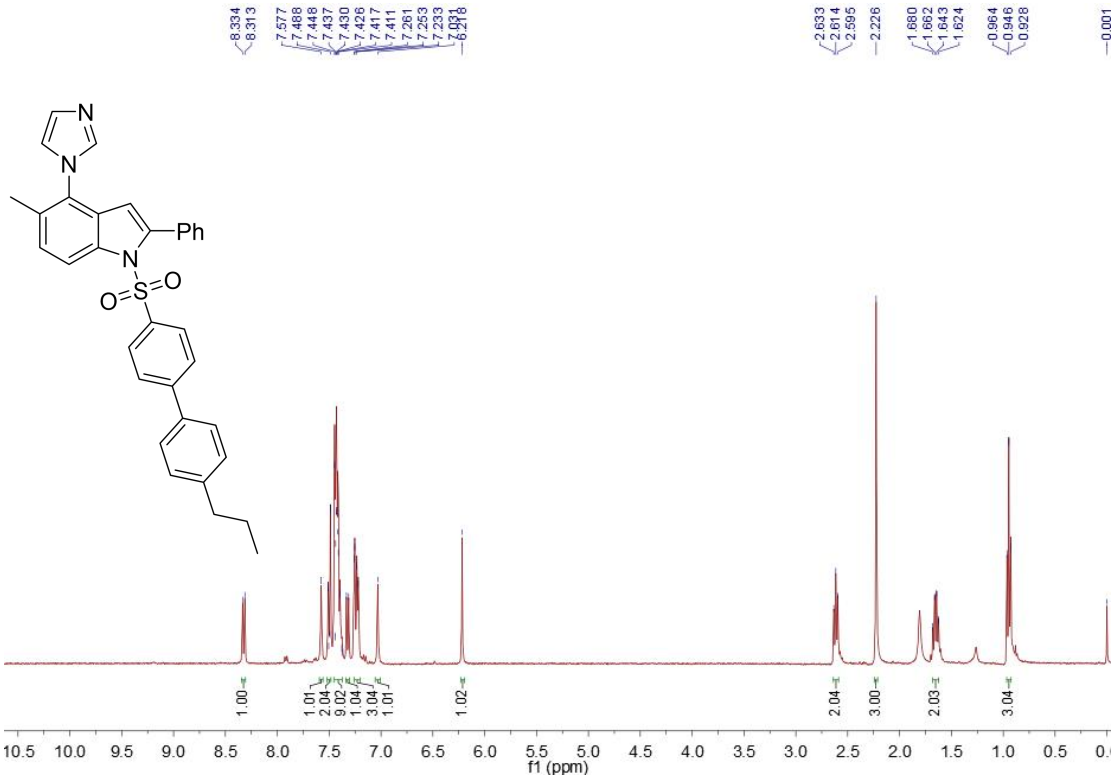


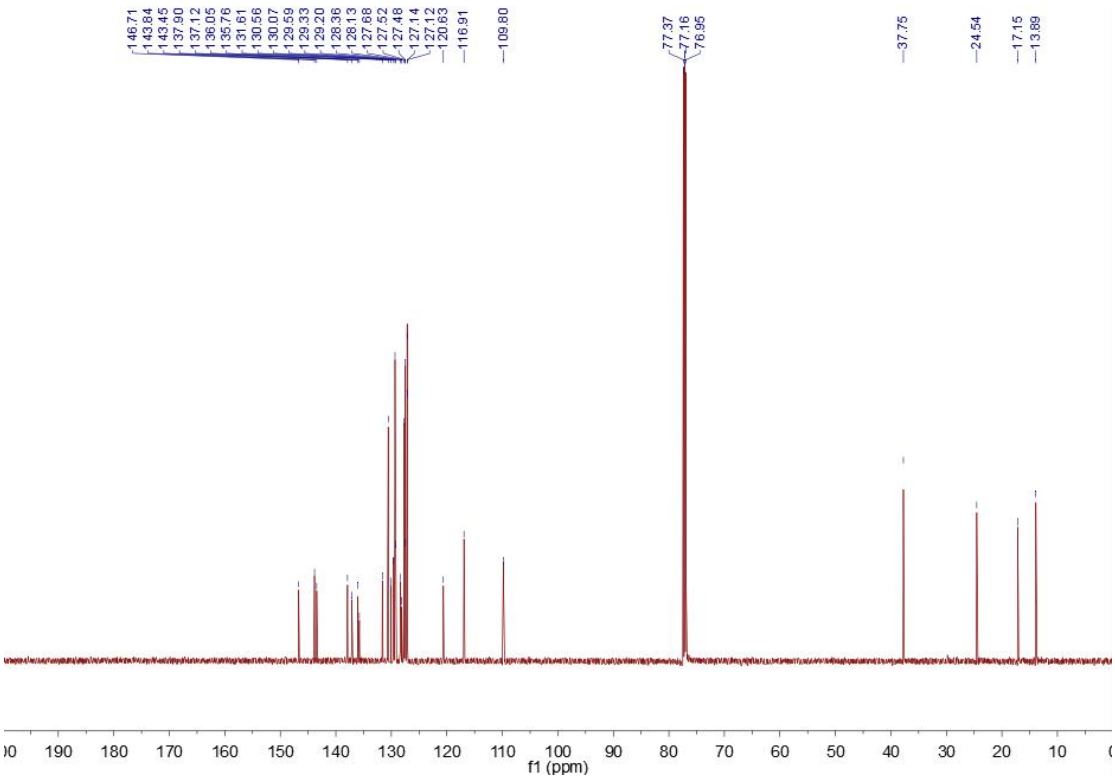
Derivative 8a:



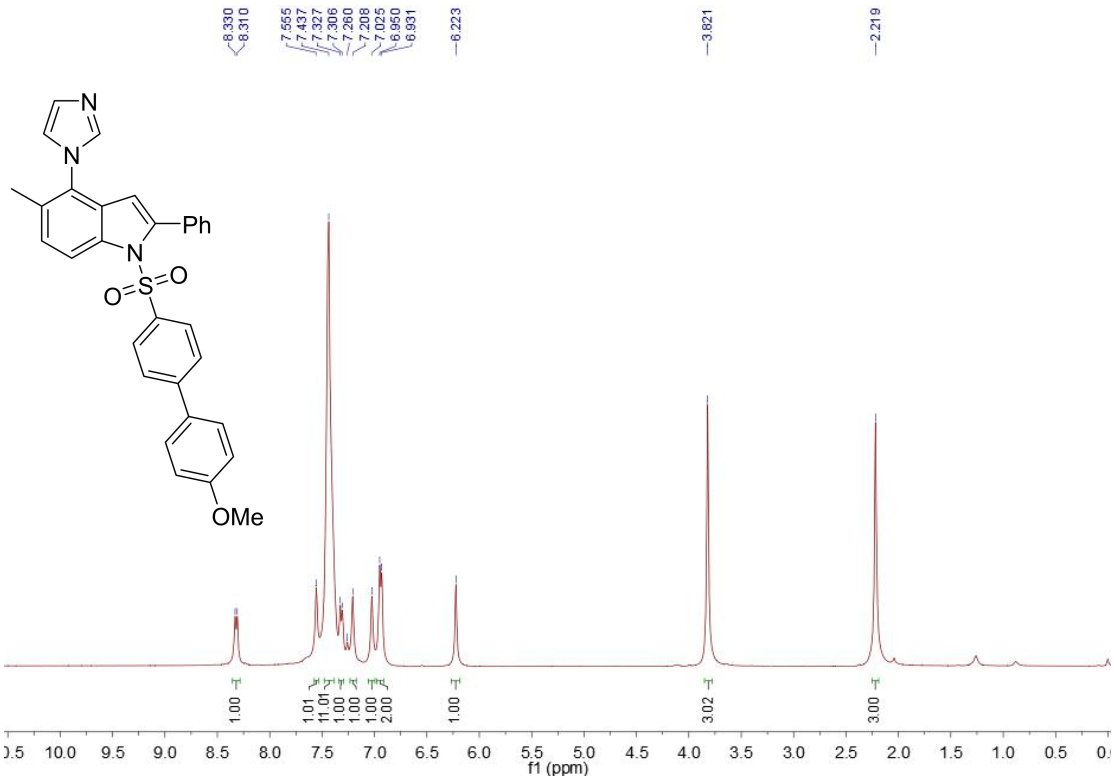


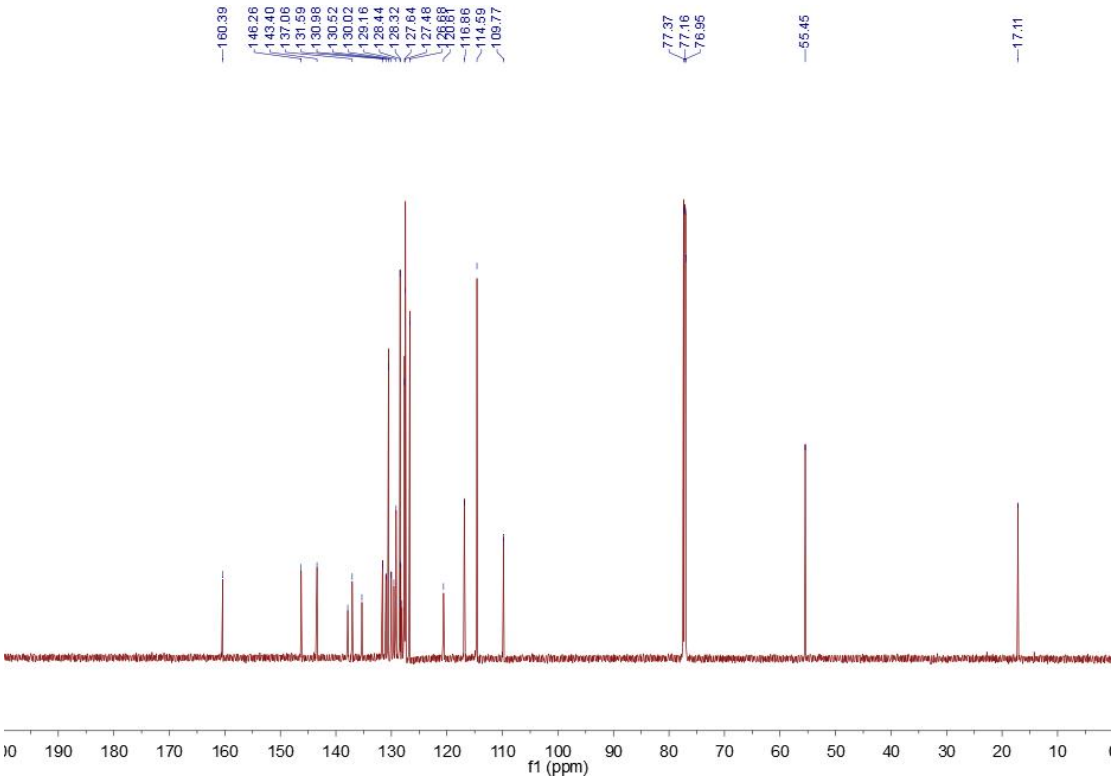
Derivative 9a:





9b:


8.330
8.310
7.555
7.437
7.327
7.306
7.260
7.208
7.025
6.950
6.931
6.223
3.821
2.219
N
N
Ph
N
O=S=O
OMe
1.00
1.01
11.01
1.00
1.00
1.00
2.00
1.00
3.02
3.00
f1 (ppm)


160.39
146.26
143.40
137.06
131.59
130.98
130.52
130.02
129.16
128.44
128.32
127.64
127.48
116.86
114.59
109.77
77.37
77.16
76.95
55.45
17.11
f1 (ppm)