Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Iron-catalyzed Cross-Dehydrogenative C–H Amidation of Benzofurans and Benzothiophenes with Anilines

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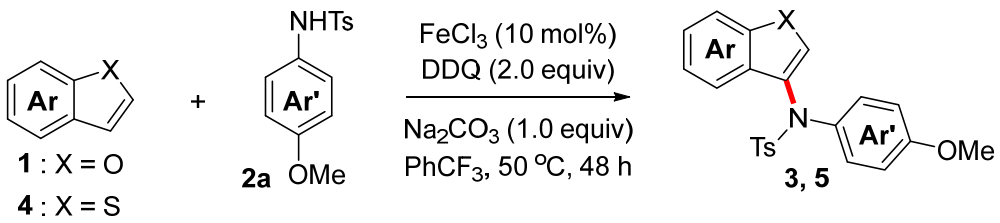
1. General Information

Compounds and solvents were purchased from commercial sources and were used as received without further purification unless stated otherwise. All products were purified by flash chromatography on silica gel (200-300 mesh). The chemical yields referred are isolated products. ^{1}H NMR and ^{13}C NMR spectra were recorded on 400 MHz or 600 MHz Bruker spectrometers. Chemical shifts are reported in part per million relative to residual solvent of $CDCl_3$ (7.26 ppm for ^{1}H NMR, 77.16 ppm for ^{13}C NMR). Infrared spectra (IR) were recorded on Bruker EQUINAX55 spectrometer. Circular dichrorism (CD) spectra were recorded on a JASCO J-810 spectrometer. Circular polarized luminescence (CPL) spectra were measured on a JASCO CPL-200 spectrometer. The used abbreviations are as follows: s (singlet), d (doublet), t (triplet), quart. (quartet), quint. (quintet), m (multiplet), br (broad). Multiplets which arise from accidental equality of coupling constants of magnetically non-equivalent protons are marked as virtual (virt.). High resolution mass spectra (HRMS) data were measured on a ESI-microTOF Ⅱ. Melting points were measured on a SGW® X-4B and are not corrected. Reactions were monitored by TLC analysis using silica gel 60 Å F-254 thin layer plates and compounds were visualized with a UV light at 254 nm or 365 nm. Further visualization was achieved by staining with iodine, or $KMnO_4$ followed by heating on a hot plate. Flash column chromatography was performed on silica gel 60 Å, 10–40 μm.

2. Synthetic Procedures

General procedures for direct amidation of aromatic C–H bond.



To a stirred solution of aniline **2** (0.4 mmol), DDQ (0.4 mmol, 90.8 mg), $FeCl_3$ (0.02

mmol, 3.24 mg) and Na_2CO_3 (0.2 mmol, 21.2 mg) in 2.0 mL dry $PhCF_3$, were added benzofuran or benzothiophene **1** (0.2 mmol) under air and the resulting mixture heated to 50 °C for 48 h. The reaction was then cooled, the mixture was concentrated under vacuum, and the crude product was purified by flash chromatography on silica gel with petroleum ether/ethyl acetate (60/1 to 30/1 to 15/1) as an eluent to afford the product.

3. Mechanistic Experiments

3.1 EPR experiment

Procedure for EPR studies of the reaction between DDQ and aniline 2a.

To a stirred solution of aniline **2a** (0.1 mmol, 27.7 mg) and DDQ (0.12 mmol, 27.2 mg) in 2.5 mL dry $PhCF_3$ under air and the resulting mixture heated to 50 °C. After 1 hour, 20.0 μL of the reaction mixture was taken out into a small tube and analyzed by EPR at room temperature (Figure S1).

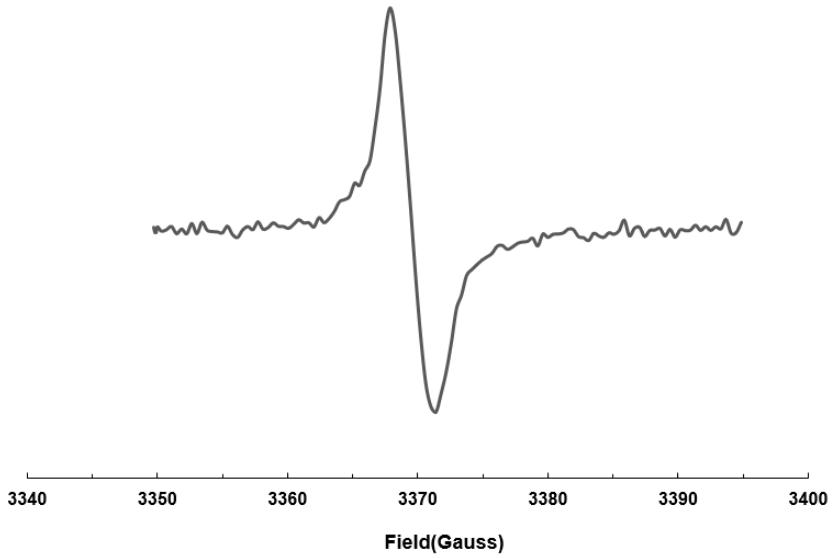
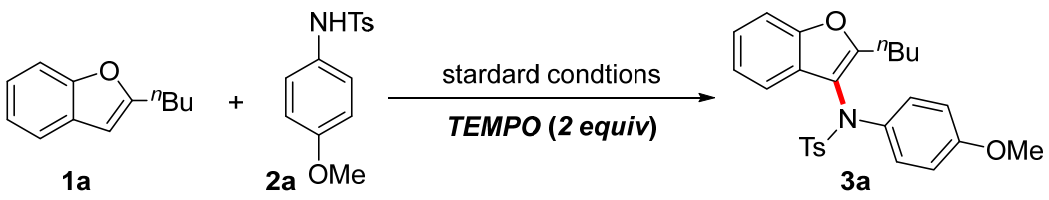


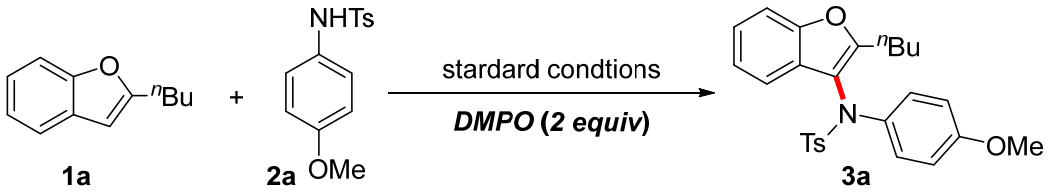
Figure S1. EPR spectra of DDQ and aniline **2a** mixture in $PhCF_3$.

3.2 The radical trapping experiments



To a stirred solution of aniline **2a** (0.4 mmol, 110.8 mg), DDQ (0.4 mmol, 90.8 mg), $FeCl_3$ (0.02 mmol, 3.24 mg), Na_2CO_3 (0.2 mmol, 21.2 mg) and TEMPO (0.4 mol, 62.5 mg) in 2.0 mL dry $PhCF_3$, were added 2-butylbenzofuran **1a** (0.2 mmol, 34.9 mg) under air and the resulting was mixture heated to 50 °C for 48 h.

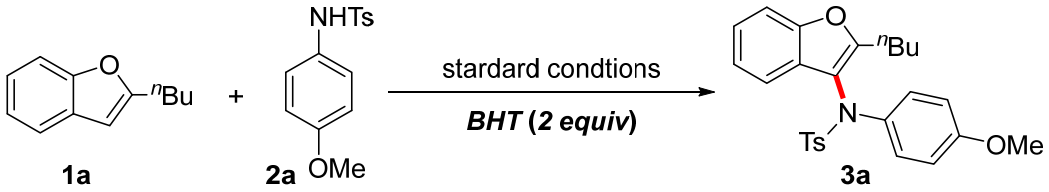
It was found that no reaction took place and only starting materials were detected (**1a** and **2a** was recovered in 99% and 75% respectively).



1a 2a 3a

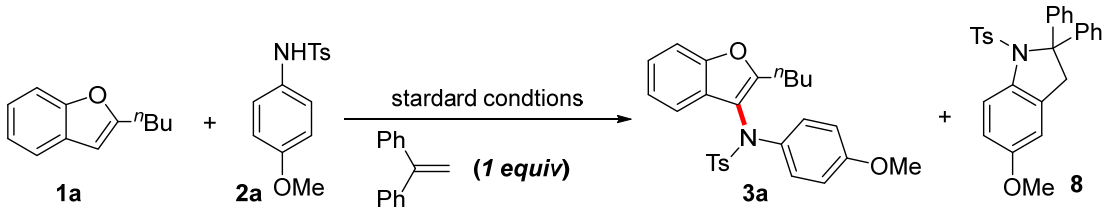
To a stirred solution of aniline **2a** (0.4 mmol, 110.8 mg), DDQ (0.4 mmol, 90.8 mg), $FeCl_3$ (0.02 mmol, 3.24 mg), Na_2CO_3 (0.2 mmol, 21.2 mg) and DMPO (0.4 mol, 45.2 mg) in 2.0 mL dry $PhCF_3$, were added 2-butylbenzofuran **1a** (0.2 mmol, 34.9 mg) under air and the resulting mixture was heated to 50 °C for 48 h.

It was found that no reaction took place and only starting materials were detected.



1a 2a 3a

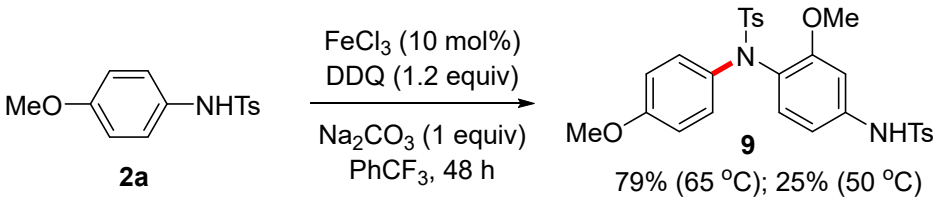
To a stirred solution of aniline **2a** (0.2 mmol, 55.4 mg), DDQ (0. 4 mmol, 90.8 mg), $FeCl_3$ (0.02 mmol, 3.24 mg), Na_2CO_3 (0.2 mmol, 21.6 mg) and BHT (0.4 mol, 88.2 mg) in 2.0 mL dry $PhCF_3$, were added 2-butylbenzofuran **1a** (0.2 mmol, 34.9 mg) under air and the resulting mixture was heated to 50 °C for 48 h. The reaction was then cooled, the mixture was concentrated under vacuum, and the crude product was purified by flash chromatography on silica gel with petroleum ether/ethyl acetate (60/1 to 30/1 to 15/1) as an eluent to afford the product **3a** (3.5 mg, <5%). The majority of starting materials **1a** and **2a** was recovered.



To a stirred solution of aniline **2a** (0.2 mmol, 55.4 mg), DDQ (0. 4 mmol, 90.8 mg), $FeCl_3$ (0.02 mmol, 3.24 mg), Na_2CO_3 (0.2 mmol, 21.6 mg) in 2.0 mL dry $PhCF_3$, were added 2-butylbenzofuran **1a** (0.2 mmol, 34.9 mg), 1,1-diphenylethylene (0.2 mol, 36.5 mg) under air and the resulting mixture was heated to 50 °C for 48 h. The reaction was then cooled, the mixture was concentrated under vacuum, and the crude product was purified by flash chromatography on silica gel with petroleum ether/ethyl acetate (60/1 to 30/1 to 15/1) as an eluent to afford the product **3a** (27.8 mg, 31%) and **8** (8.2 mg, 9%).

The above radical trapping experiments suggested that a radical mechanism is likely involved in the present amination reaction.

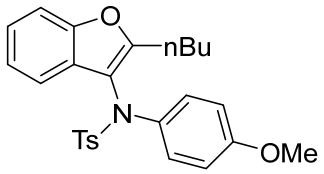
3.4 self-amidation of aniline 2a



To a stirred solution of aniline **2a** (0.2 mmol, 55.4 mg), DDQ (0.24 mmol, 54.5 mg), $FeCl_3$ (0.02 mmol, 3.24 mg) and Na_2CO_3 (0.2 mmol, 21.2 mg) in 2.0 mL dry $PhCF_3$, under air and the resulting mixture heated to 50°C or 65 °C for 48h. The reaction was then cooled, the mixture was concentrated under vacuum, and the crude product was purified by flash chromatography on silica gel with petroleum ether/ethyl acetate (20/1 to 10/1) as an eluent to afford the product.

4. Analytical Data of Products.

N-(2-Butylbenzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methylbenzenesulfonamide (3a)



3a

Compound **3a** was synthesized following the general procedure.

A white solid, 74.6 mg, 83% yield.

m.p.: 65 ºC – 67 ºC

TLC: R_f = 0.47 (Hexane/EtOAc = 6:1)

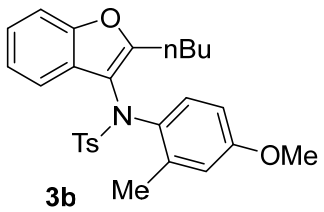
IR (KBr): 2960, 1604, 1508, 1453, 1349, 1252, 1165, 747, 668, 592, 550 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.67 – 7.63 (m, 2H), 7.42 – 7.37 (m, 1H), 7.39 – 7.33 (m, 2H), 7.31 – 7.26 (m, 2H), 7.25 – 7.19 (m, 1H), 7.15 – 7.09 (m, 1H), 7.08 – 7.03 (m, 1H), 6.87 – 6.81 (m, 2H), 3.79 (s, 3H), 2.80 – 2.74 (m, 2H), 2.48 (s, 3H), 1.69 – 1.62 (m, 2H), 1.41 – 1.33 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 159.0, 158.6, 153.1, 143.7, 137.7, 134.2, 129.54, 128.7, 127.9, 126.3, 123.7, 122.8, 119.1, 118.3, 114.3, 111.4, 55.4, 29.3, 25.9, 22.6, 21.6, 13.8.

HRMS (ESI): $C_{26}H_{28}NO_4S$ $[M+H]^+$: calcd.: 450.1734; found: 450.1734.

N-(2-Butylbenzofuran-3-yl)-*N*-(4-Methoxy-2-methylphenyl)-4-Methylbenzenesulfonamide (3b)



3b

Compound **3b** was synthesized following the general procedure.

A colorless oil, 79.7 mg, 86% yield.

TLC: R_f = 0.46 (Hexane/EtOAc = 6:1)

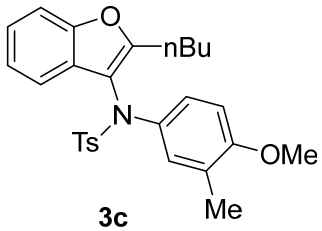
IR (KBr): 2959, 1603, 1498, 1453, 1353, 1223, 1164, 1046, 748, 670, 601, 544 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.65 – 7.61 (m, 2H), 7.41 – 7.36 (m, 1H), 7.30 – 7.23 (m, 4H), 7.23 – 7.19 (m, 1H), 7.15 – 7.08 (m, 1H), 6.79 – 6.74 (m, 1H), 6.67 (dd, *J* = 8.8, 3.0 Hz, 1H), 3.78 (s, 3H), 2.81 – 2.70 (m, 2H), 2.47 (s, 3H), 2.46 (s, 3H), 1.60 – 1.54 (m, 2H), 1.41 – 1.34 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.9, 158.2, 153.0, 143.7, 139.8, 137.6, 132.5, 129.7, 129.5, 128.1, 126.2, 123.5, 122.6, 120.2, 117.5, 116.6, 111.4, 111.2, 55.3, 29.4, 26.8, 22.7, 21.6, 19.6, 13.8.

HRMS (ESI): $C_{27}H_{30}NO_4S$ $[M+H]^+$: calcd.: 464.1890; found: 464.1889.

***N*-(2-Butylbenzofuran-3-yl)-*N*-(4-Methoxy-3-methylphenyl)-4-Methylbenzenesulfonamide (3c)**



3c

Compound **3c** was synthesized following the general procedure.

A white solid, 69.5 mg, 75% yield.

m.p.: 84 ºC – 86 ºC

TLC: R_f = 0.42 (Hexane/EtOAc = 6:1)

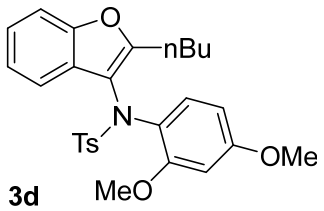
IR (KBr): 2955, 1600, 1502, 1454, 1350, 1228, 1165, 1032, 745, 667, 607, 566 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.70 – 7.63 (m, 2H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.25 – 7.18 (m, 3H), 7.15 – 7.07 (m, 2H), 6.74 (d, *J* = 8.3 Hz, 1H), 3.81 (s, 3H), 2.78 (m, 2H), 2.48 (s, 3H), 2.18 (s, 3H), 1.70 – 1.60 (m, 2H), 1.41 – 1.35 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.9, 157.0, 153.1, 143.6, 137.8, 133.6, 130.0, 129.5, 127.9, 127.6, 126.3, 125.9, 123.7, 122.8, 119.1, 118.4, 111.3, 110.0, 55.4, 29.4, 25.9, 22.7, 21.6, 16.3, 13.8.

HRMS (ESI): $C_{27}H_{30}NO_4S$ $[M+H]^+$: calcd.: 464.1890; found: 464.1887.

***N*-(2-Butylbenzofuran-3-yl)-*N*-(2,4-Dimethoxyphenyl)-4-Methylbenzenesulfonamide (3d)**



3d

Compound **3d** was synthesized following the general procedure.

A colorless oil, 74.8 mg, 78% yield.

TLC: R_f = 0.46 (Hexane/EtOAc = 6:1)

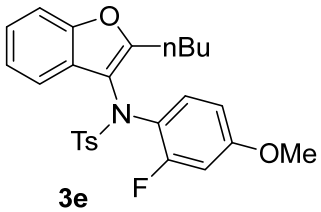
IR (KBr): 2927, 1606, 1507, 1455, 1350, 1210, 1164, 1036, 750, 672, 557 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.71 – 7.62 (m, 2H), 7.41 – 7.32 (m, 3H), 7.27 – 7.22 (m, 2H), 7.23 – 7.08 (m, 2H), 6.50 – 6.37 (m, 2H), 3.79 (s, 3H), 3.74 (s, 3H), 2.80 – 2.69 (m, 2H), 2.46 (s, 3H), 1.62 – 1.50 (m, 2H), 1.43 – 1.32 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 160.6, 159.1, 157.4, 153.0, 143.2, 138.1, 131.2, 129.1, 128.1, 126.7, 123.4, 122.7, 122.5, 119.9, 117.8, 111.0, 104.2, 99.5, 55.4, 55.0, 29.4, 26.0, 22.8, 21.5, 13.8.

HRMS (ESI): $C_{27}H_{30}NO_5S$ $[M+H]^+$: calcd.: 480.1839; found: 480.1837.

***N*-(2-Butylbenzofuran-3-yl)-*N*-(2-Fluoro-4-methoxyphenyl)-4-Methylbenzenesulfonamide (3e)**



3e

Compound **3e** was synthesized following the general procedure.

A white solid, 71.1 mg, 76% yield.

m.p.: 58 ºC – 60 ºC

TLC: R_f = 0.42 (Hexane/EtOAc = 6:1)

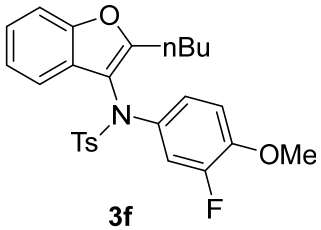
IR (KBr): 2925, 1618, 1510, 1455, 1355, 1223, 1163, 1090, 748, 670, 539 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.71 – 7.65 (m, 2H), 7.45 – 7.34 (m, 2H), 7.31 – 7.26 (m, 3H), 7.25 – 7.18 (m, 1H), 7.18 – 7.12 (m, 1H), 6.71 – 6.63 (m, 2H), 3.79 (s, 3H), 2.71 (m, 2H), 2.47 (s, 3H), 1.60 – 1.53 (m, 2H), 1.37 – 1.31 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, CDCl3): δ (ppm) 160.54 (d, J = 10.6 Hz), 159.88 (d, J = 251.1 Hz), 159.47 , 153.09 , 143.85 , 137.27 , 131.30 , 129.45 , 128.13 , 126.18 , 123.31 (d, J = 87.0 Hz), 121.39 (d, J = 13.3 Hz), 119.38 (d, J = 3.0 Hz), 117.50 , 111.23 , 110.14 (d, J = 3.0 Hz), 102.84 , 102.60 , 55.75 , 29.34 , 25.74 (d, J = 2.8 Hz), 22.67 , 21.60 , 13.81 .

HRMS (ESI): $C_{26}H_{27}FNO_4S$ $[M+H]^+$: calcd.: 468.1639; found: 468.1638.

***N*-(2-Butylbenzofuran-3-yl)-*N*-(3-Fluoro-4-methoxyphenyl)-4-Methylbenzenesulfonamide (3f)**



3f

Compound **3f** was synthesized following the general procedure.

A white solid, 67.3 mg, 72% yield.

m.p.: 81 ºC – 83 ºC

TLC: R_f = 0.44 (Hexane/EtOAc = 6:1)

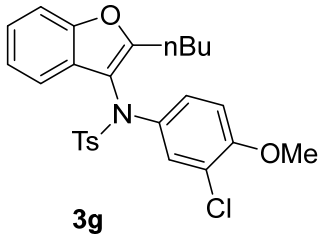
IR (KBr): 2922, 1514, 1454, 1348, 1270, 1224, 1166, 1026, 749, 668, 622, 558 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.68 – 7.61 (m, 2H), 7.44 – 7.38 (m, 1H), 7.30 – 7.28 (m, 2H), 7.26 – 7.14 (m, 3H), 7.14 – 7.08 (m, 1H), 6.98 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.88 (t, *J* = 8.9 Hz, 1H), 3.88 (s, 3H), 2.74 (m, 2H), 2.48 (s, 3H), 1.68 –1.59 (m, 2H), 1.39 – 1.29 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) δ (ppm) 159.3, 153.2, 151.2 (d, *J* = 248.0 Hz), 146.8 (d, *J* = 10.6 Hz), 144.0, 137.3, 134.2, 129.6, 127.9, 126.0, 123.9, 123.0 (d, *J* = 3.9 Hz), 123.0, 118.9, 117.9, 115.2 (d, *J* = 20.0 Hz), 113.1(d, *J* = 2.6 Hz), 111.5, 56.3, 29.3, 25.8, 22.6, 21.6, 13.8.

HRMS (ESI): $C_{26}H_{27}FNO_4S$ $[M+H]^+$: calcd.: 468.1639; found: 468.1640.

***N*-(2-Butylbenzofuran-3-yl)-*N*-(3-Chloro-4-methoxyphenyl)-4-Methylbenzenesulfonamide (3g)**



3g

Compound **3g** was synthesized following the general procedure.

A colorless oil, 70.7 mg, 73% yield.

TLC: R_f = 0.49 (Hexane/EtOAc = 6:1)

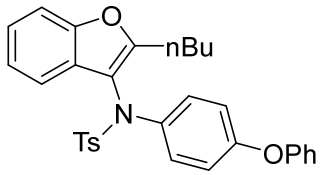
IR (KBr): 2925, 1496, 1454, 1356, 1263, 1165, 1062, 749, 670, 608, 562 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.69 – 7.60 (m, 2H), 7.44 – 7.38 (m, 2H), 7.33 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.30 – 7.29 (m, 1H), 7.26 – 7.19 (m, 1H), 7.17 – 7.08 (m, 1H), 7.04 – 6.95 (m, 1H), 6.86 (d, *J* = 8.9 Hz, 1H), 3.89 (s, 3H), 2.73 (m, 2H), 2.48 (s, 3H), 1.67 – 1.61 (m, 2H), 1.38 – 1.30 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 159.2, 154.1, 153.1, 144.0, 137.3, 134.5, 129.6, 128.9, 127.9, 126.6, 126.0, 123.9, 123.0, 122.5, 118.9, 117.9, 111.9, 111.5, 56.3, 29.3, 25.8, 22.6, 21.6, 13.8.

HRMS (ESI): $C_{26}H_{27}{}^{35}ClNO_4S$ $[M+H]^+$: calcd.: 484.1344; found: 484.1342.

N-(2-Butylbenzofuran-3-yl)-4-Methyl-*N*-(4-Phenoxyphenyl)-Benzenesulfonamide (3h)



3h

Compound **3h** was synthesized following the general procedure.

A white solid, 61.4 mg, 60% yield.

m.p.: 84 ºC – 86 ºC

TLC: R_f = 0.51 (Hexane/EtOAc = 6:1)

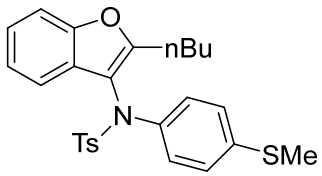
IR (KBr): 2925, 1590, 1489, 1353, 1224, 1165, 1096, 751, 665 594, 564 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.70 – 7.63 (m, 2H), 7.43 – 7.32 (m, 5H), 7.30 – 7.29 (m, 1H), 7.28 – 7.27 (m, 1H), 7.25 – 7.19 (m, 1H), 7.17 – 7.08 (m, 2H), 7.05 – 6.98 (m, 3H), 6.95 – 6.89 (m, 2H), 2.84 – 2.67 (m, 2H), 2.47 (s, 3H), 1.70 – 1.64 (m, 2H), 1.38 – 1.31 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 159.1, 156.5, 156.4, 153.1, 143.8, 137.5, 136.4, 129.8, 129.5, 128.4, 127.9, 126.2, 123.8, 123.7, 122.9, 119.3, 119.0, 118.9, 118.1, 111.4, 29.3, 25.9, 22.6, 21.6, 13.8.

HRMS (ESI): $C_{31}H_{30}NO_4S$ $[M+H]^+$: calcd.: 512.1890; found: 512.1890.

N-(2-Butylbenzofuran-3-yl)-4-Methyl-*N*-(4-(Methylthio)-Phenyl-Benzenesulfonamide (3i)



3i

Compound **3i** was synthesized following the general procedure.

A white solid, 52.1 mg, 56% yield.

m.p.: 71 ºC – 73 ºC

TLC: R_f = 0.46 (Hexane/EtOAc = 6:1)

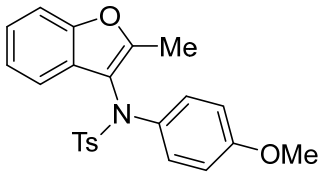
IR (KBr): 2923, 1594, 1490, 1453, 1350, 1234, 1163, 961, 815, 748, 666, 572 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.69 – 7.62 (m, 2H), 7.43 – 7.37 (m, 1H), 7.36 – 7.32 (m, 2H), 7.31 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.16 (m, 2H), 7.14 – 7.07 (m, 1H), 7.01 – 6.95 (m, 1H), 2.77 – 2.70 (m, 2H), 2.47 (s, 3H), 2.46 (s, 3H), 1.68 – 1.60 (m, 2H), 1.39 – 1.31 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 159.3, 153.1, 143.9, 138.6, 137.5, 137.4, 129.6, 127.9, 127.0, 126.8, 126.2, 123.8, 122.9, 119.0, 117.9, 111.4, 29.2, 25.8, 22.6, 21.6, 15.8, 13.8.

HRMS (ESI): $C_{26}H_{28}NO_3S_2$ $[M+H]^+$: calcd.: 466.1505; found: 466.1506.

***N*-(4-Methoxyphenyl)-4-Methyl-*N*-(2-Methylbenzofuran-3-yl)-Benzenesulfonamide (3j)**



3j

Compound **3j** was synthesized following the general procedure.

A white solid, 72.5 mg, 89% yield.

m.p.: 81 ºC – 83 ºC

TLC: R_f = 0.47 (Hexane/EtOAc = 6:1)

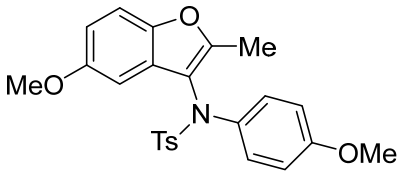
IR (KBr): 2926, 1600, 1505, 1348, 1250, 1165, 1089, 1032, 754, 671, 560 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.67 – 7.63 (m, 2H), 7.41 – 7.36 (m, 1H), 7.37 – 7.34 (m, 2H), 7.32 – 7.26 (m, 2H), 7.24 – 7.18 (m, 1H), 7.15 – 7.09 (m, 1H), 7.08 – 7.04 (m, 1H), 6.87 – 6.82 (m, 2H), 3.79 (s, 3H), 2.47 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.7, 155.2, 153.1, 143.8, 137.7, 134.0, 129.6, 128.8, 127.8, 126.3, 123.8, 122.9, 118.9, 118.9, 114.4, 111.3, 55.4, 21.6, 12.0.

HRMS (ESI): $C_{23}H_{22}NO_4S$ $[M+H]^+$: calcd.: 408.1264; found: 408.1267.

***N*-(5-Methoxy-2-Methylbenzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3k)**



3k

Compound **3k** was synthesized following the general procedure.

A white solid, 76.1 mg, 87% yield.

m.p.: 81 ºC – 83 ºC

TLC: R_f = 0.46 (Hexane/EtOAc = 6:1)

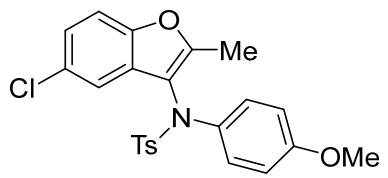
IR (KBr): 2921, 1604, 1506, 1471, 1353, 1247, 1165, 1030, 803, 662, 565 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.71 – 7.63 (m, 2H), 7.38 – 7.32 (m, 2H), 7.32 – 7.27 (m, 2H), 7.26 (d, *J* = 8.9 Hz, 1H), 6.88 – 6.82 (m, 2H), 6.80 (dd, *J* = 8.9, 2.6 Hz, 1H), 6.44 (d, *J* = 2.6 Hz, 1H), 3.80 (s, 3H), 3.71 (s, 3H), 2.46 (s, 3H), 2.38 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.6, 156.2, 156.0, 148.0, 143.7, 137.9, 134.1, 129.6, 128.6, 127.9, 126.8, 119.0, 114.4, 112.3, 111.8, 101.5, 55.7, 55.4, 21.5, 12.1.

HRMS (ESI): $C_{24}H_{24}NO_5S$ $[M+H]^+$: calcd.: 438.1370; found: 438.1373.

***N*-(5-Chloro-2-Methylbenzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3l)**



3l

Compound **3l** was synthesized following the general procedure.

A white solid, 72.5 mg, 82% yield.

m.p.: 138 ºC – 140 ºC

TLC: R_f = 0.47 (Hexane/EtOAc = 6:1)

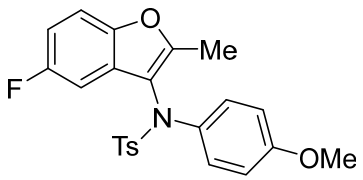
IR (KBr): 2918, 1601, 1506, 1451, 1348, 1253, 1163, 1092, 823, 663, 568 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.63 – 7.59 (m, 2H), 7.35 – 7.26 (m, 5H), 7.15 (dd, *J* = 8.7, 2.2 Hz, 1H), 6.90 – 6.84 (m, 2H), 6.68 (d, *J* = 2.2 Hz, 1H), 3.81 (s, 3H), 2.50 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.8, 157.2, 151.4, 144.3, 137.4, 133.8, 129.7, 128.7, 127.9, 127.5, 123.9, 118.5, 118.5, 114.8, 114.5, 112.3, 55.4, 21.6, 12.1.

HRMS (ESI): $C_{23}H_{21}{}^{35}ClNO_4S$ $[M+H]^+$: calcd.: 442.0874; found: 442.0880.

***N*-(5-Fluoro-2-Methylbenzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3m)**



3m

Compound **3m** was synthesized following the general procedure.

A colorless oil, 72.3 mg, 85% yield.

m.p.: 131 ºC – 133 ºC

TLC: R_f = 0.45 (Hexane/EtOAc = 6:1)

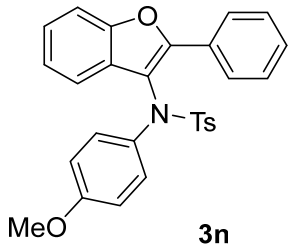
IR (KBr): 2928, 1602, 1506, 1469, 1345, 1245, 1165, 1100, 1031, 825, 665, 568 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.67 – 7.61 (m, 2H), 7.34 – 7.27 (m, 5H), 6.92 (td, *J* = 9.0, 2.6 Hz, 1H), 6.88 – 6.83 (m, 2H), 6.62 (dd, *J* = 8.5, 2.6 Hz, 1H), 3.80 (s, 3H), 2.48 (s, 3H), 2.42 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 159.2 (d, *J* = 238.9 Hz), 158.8, 157.3, 149.2, 144.1, 137.5, 133.8, 129.7, 128.8, 127.8, 127.1 (d, *J* = 10.2 Hz), 119.2 (d, *J* = 3.7 Hz), 114.5, 112.1 (d, *J* = 9.6 Hz), 111.4 (d, *J* = 26.4 Hz), 104.6 (d, *J* = 26.3 Hz), 55.4, 21.6, 12.2.

HRMS (ESI): $C_{23}H_{21}FNO_4S$ $[M+H]^+$: calcd.: 426.1170; found: 426.1174.

N-(4-Methoxyphenyl)-4-Methyl-*N*-(2-Phenylbenzofuran-3-yl)-Benzenesulfonamide (3n)



3n

Compound **3n** was synthesized following the general procedure.

A white solid, 62.0 mg, 66% yield.

m.p.: 120 ºC – 122 ºC

TLC: R_f = 0.47 (Hexane/EtOAc = 6:1)

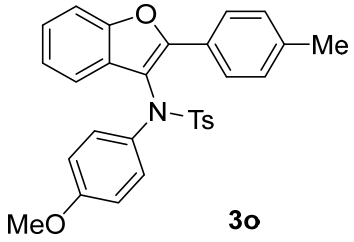
IR (KBr): 2922, 1598, 1507, 1358, 1251, 1164, 1019, 817, 749, 665, 556 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.16 – 8.06 (m, 2H), 7.67 – 7.60 (m, 2H), 7.55 – 7.47 (m, 1H), 7.49 – 7.37 (m, 5H), 7.33 – 7.29 (m, 1H), 7.26 – 7.21 (m, 2H), 7.19 – 7.10 (m, 1H), 7.04 – 6.97 (m, 1H), 6.82 – 6.74 (m, 2H), 3.76 (s, 3H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.4, 153.1, 152.9, 144.0, 137.3, 134.0, 129.4, 129.3, 128.9, 128.5, 128.2, 127.6, 127.4, 126.8, 124.8, 123.1, 120.2, 118.5, 114.3, 111.7, 55.3, 21.6.

HRMS (ESI): $C_{28}H_{24}NO_4S$ $[M+H]^+$: calcd.: 470.1421; found: 470.1425.

N-(4-Methoxyphenyl)-4-Methyl-*N*-(2-(*p*-Tolyl)-Benzofuran-3-yl)-Benzenesulfonamide (3o)



3o

Compound **3o** was synthesized following the general procedure.

A white solid, 67.7 mg, 70% yield.

m.p.: 109 ºC – 111 ºC

TLC: R_f = 0.45 (Hexane/EtOAc = 6:1)

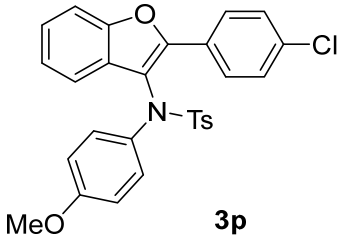
IR (KBr): 2920, 1600, 1505, 1449, 1351, 1251, 1166, 1028, 816, 745, 670, 555 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.06 – 7.97 (m, 2H), 7.68 – 7.59 (m, 2H), 7.52 – 7.46 (m, 1H), 7.42 – 7.36 (m, 2H), 7.32 – 7.24 (m, 5H), 7.15 – 7.08 (m, 1H), 7.00 – 6.93 (m, 1H), 6.84 – 6.73 (m, 2H), 3.76 (s, 3H), 2.47 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.4, 153.4, 152.8, 143.9, 139.5, 137.4, 134.1, 129.4, 129.2, 128.2, 127.6, 127.4, 126.7, 126.1, 124.6, 123.0, 120.0, 117.9, 114.3, 111.7, 55.3, 21.6, 21.4.

HRMS (ESI): $C_{29}H_{26}NO_4S$ $[M+H]^+$: calcd.: 484.1577; found: 484.1582.

***N*-(2-(4-Chlorophenyl)-Benzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3p)**



3p

Compound **3p** was synthesized following the general procedure.

A white solid, 73.6 mg, 73% yield.

m.p.: 96 ºC – 98 ºC

TLC: R_f = 0.44 (Hexane/EtOAc = 6:1)

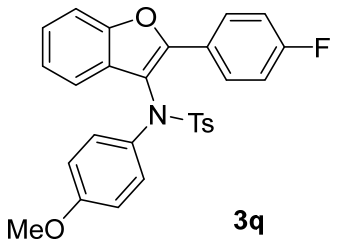
IR (KBr): 2924, 1601, 1507, 1448, 1354, 1255, 1165, 1092, 1030, 831, 744, 670 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.13 – 8.03 (m, 2H), 7.67 – 7.60 (m, 2H), 7.53 – 7.47 (m, 1H), 7.46 – 7.41 (m, 2H), 7.40 – 7.35 (m, 2H), 7.34 – 7.29 (m, 1H), 7.27 – 7.24 (m, 2H), 7.17 – 7.10 (m, 1H), 7.01 – 6.95 (m, 1H), 6.82 – 6.75 (m, 2H), 3.76 (s, 3H), 2.48 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.5, 152.9, 152.0, 144.2, 137.2, 135.3, 133.8, 129.5, 128.8, 128.2, 128.0, 127.5, 127.4, 127.2, 125.1, 123.3, 120.2, 118.9, 114.4, 111.8, 55.4, 21.6.

HRMS (ESI): $C_{28}H_{23}{}^{35}ClNO_4S$ $[M+H]^+$: calcd.: 504.1031; found: 504.1035.

N-(2-(4-Fluorophenyl)-Benzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3q)



3q

Compound **3q** was synthesized following the general procedure.

A white solid, 62.4 mg, 64% yield.

m.p.: 142 ºC – 144 ºC

TLC: R_f = 0.45 (Hexane/EtOAc = 6:1)

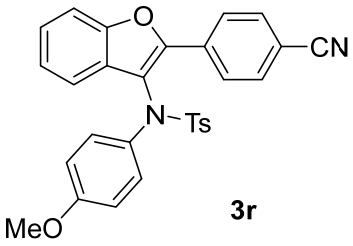
IR (KBr): 2922, 1601, 1504, 1450, 1353, 1229, 1163, 1094, 747, 671, 588, 545 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.15 – 8.04 (m, 2H), 7.60 (d, *J* = 7.9 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 1H), 7.34 (d, *J* = 8.6 Hz, 2H), 7.28 – 7.20 (m, 2H), 7.17 – 7.06 (m, 3H), 6.91 (d, *J* = 7.8 Hz, 1H), 6.76 (d, *J* = 8.9 Hz, 2H), 3.73 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 163.2 (d, *J* = 250.2 Hz), 158.5, 152.9, 152.3, 144.2, 137.2, 133.9, 129.5, 128.9 (d, *J* = 8.4 Hz), 128.2, 127.5, 127.2, 125.2 (d, *J* = 3.4 Hz), 124.9, 123.2, 120.1, 118.3, 115.7 (d, *J* = 21.9 Hz), 114.4, 111.7, 55.4, 21.6.

HRMS (ESI): $C_{28}H_{23}FNO_4S$ $[M+H]^+$: calcd.: 488.1326; found: 488.1331.

N-(2-(4-Cyanophenyl)-Benzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3r)



3r

Compound **3r** was synthesized following the general procedure.

A colorless oil, 65.3 mg, 66% yield.

m.p.: 188 ºC – 190 ºC

TLC: R_f = 0.67 (Hexane/EtOAc = 6:1)

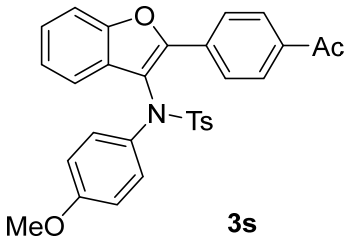
IR (KBr): 2922, 2222, 1604, 1507, 1353, 1255, 1163, 1091, 743, 671, 546 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.31 – 8.24 (m, 2H), 7.80 – 7.71 (m, 2H), 7.67 – 7.60 (m, 2H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.45 – 7.33 (m, 3H), 7.31 – 7.24 (m, 2H), 7.22 – 7.13 (m, 1H), 7.01 – 6.95 (m, 1H), 6.86 – 6.70 (m, 2H), 3.77 (s, 3H), 2.49 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.6, 153.3, 150.6, 144.5, 137.0, 133.5, 133.0, 132.3, 129.6, 128.2, 127.4, 126.9, 126.0, 123.6, 121.1, 120.6, 118.6, 114.5, 112.3, 112.0, 55.4, 21.6.

HRMS (ESI): $C_{29}H_{23}N_2O_4S$ $[M+H]^+$: calcd.: 495.1373; found: 495.1374.

***N*-(2-(4-Acetylphenyl)-Benzofuran-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3s)**



3s

Compound **3s** was synthesized following the general procedure.

A colorless oil, 67.5 mg, 66% yield.

TLC: R_f = 0.40 (Hexane/EtOAc = 6:1)

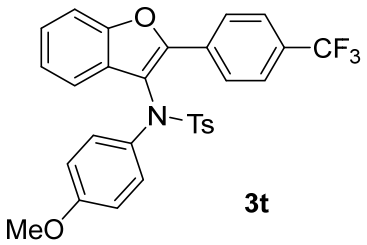
IR (KBr): 2921, 1679, 1603, 1507, 1351, 1254, 1161, 1089, 1031, 753, 668, 589 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.30 – 8.22 (m, 2H), 8.10 – 8.03 (m, 2H), 7.69 – 7.61 (m, 2H), 7.56 – 7.51 (m, 1H), 7.46 – 7.24 (m, 5H), 7.20 – 7.13 (m, 1H), 7.06 – 7.00 (m, 1H), 6.86 – 6.72 (m, 2H), 3.76 (s, 3H), 2.67 (s, 3H), 2.47 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 197.5, 158.6, 153.2, 151.6, 144.3, 137.1, 137.0, 133.7, 133.1, 129.6, 128.5, 128.2, 127.5, 127.2, 126.6, 125.6, 123.5, 120.5, 120.4, 114.4, 112.0, 55.4, 26.7, 21.6.

HRMS (ESI): $C_{30}H_{26}NO_5S$ $[M+H]^+$: calcd.: 512.1526; found: 512.1529.

N-(4-Methoxyphenyl)-4-Methyl-*N*-(2-(4-(Trifluoromethyl)-Phenyl-Benzofuran-3-yl)-Benzenesulfonamide (3t)



3t

Compound **3t** was synthesized following the general procedure.

A white solid, 66.6 mg, 62% yield.

m.p.: 175 ºC – 177 ºC

TLC: R_f = 0.42 (Hexane/EtOAc = 6:1)

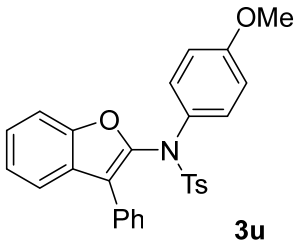
IR (KBr): 2923, 1612, 1508, 1356, 1323, 1162, 1111, 1032, 745, 668, 543 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.27 – 8.17 (m, 2H), 7.73 – 7.66 (m, 2H), 7.62 – 7.56 (m, 2H), 7.54 – 7.47 (m, 1H), 7.42 – 7.27 (m, 3H), 7.24 – 7.18 (m, 2H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.04 – 6.95 (m, 1H), 6.78 (d, *J* = 8.6 Hz, 2H), 3.73 (s, 3H), 2.42 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.5, 153.2, 151.2, 144.3, 137.0, 133.7, 132.2, 130.7(q, J = 32.7 Hz), 129.5, 128.1, 127.3, 127.1, 126.8, 125.6, 125.5(q, J = 3.8 Hz), 123.5, 120.5, 114.5, 112.0, 55.4, 21.5.

HRMS (ESI): $C_{29}H_{23}F_3NO_4S$ $[M+H]^+$: calcd.: 538.1294; found: 538.1297.

N-(4-Methoxyphenyl)-4-Methyl-*N*-(3-Phenylbenzofuran-2-yl)-Benzenesulfonamide (3u)



3u

Compound **3u** was synthesized following the general procedure.

A white solid, 72.3 mg, 77% yield.

m.p.: 112 ºC – 114 ºC

TLC: R_f = 0.47 (Hexane/EtOAc = 6:1)

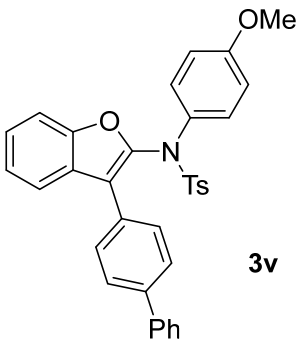
IR (KBr): 2922, 1621, 1507, 1453, 1356, 1253, 1165, 1032, 749, 667, 551 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.79 – 7.74 (m, 2H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.67–7.65 (m, 2H), 7.56 – 7.52 (m, 2H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.42 – 7.38 (m, 1H), 7.32 – 7.27 (m, 3H), 7.17 – 7.12 (m, 2H), 6.76 – 6.72 (m, 2H), 3.76 (s, 3H), 2.49 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 159.3, 152.0, 144.5, 144.1, 135.6, 131.9, 130.6, 129.7, 129.3, 129.0, 128.7, 128.6, 127.9, 127.7, 125.5, 123.1, 120.9, 117.9, 114.2, 111.4, 55.3, 21.7.

HRMS (ESI): $C_{28}H_{24}NO_4S$ $[M+H]^+$: calcd.: 470.1421; found: 470.1426.

***N*-(3-([1,1'-Biphenyl]-4-yl)-Benzofuran-2-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (3v)**



3v

Compound **3v** was synthesized following the general procedure.

A white solid, 69.8 mg, 64% yield

m.p.: 162 ºC – 164 ºC

TLC: R_f = 0.44 (Hexane/EtOAc = 6:1)

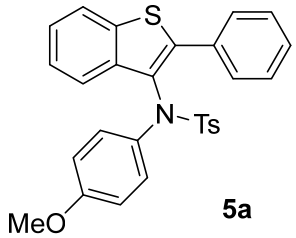
IR (KBr): 2921, 1600, 1505, 1446, 1360, 1251, 1161, 841, 725, 668, 555 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.84 – 7.78 (m, 2H), 7.77 – 7.66 (m, 5H), 7.65 – 7.58 (m, 2H), 7.54 – 7.43 (m, 3H), 7.43 – 7.34 (m, 3H), 7.33 – 7.25 (m, 2H), 7.19 – 7.12 (m, 2H), 6.75 – 6.66 (m, 2H), 3.72 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 159.3, 152.1, 144.5, 144.1, 140.7, 140.5, 135.7, 132.0, 129.7, 129.3, 128.8, 128.6, 127.3, 127.0, 125.5, 123.2, 121.0, 117.6, 114.2, 111.4, 55.3, 21.6.

HRMS (ESI): $C_{34}H_{28}NO_4S$ $[M+H]^+$: calcd.: 546.1734; found: 546.1737.

***N*-(4-Methoxyphenyl)-4-Methyl-*N*-(2-Phenylbenzo[b]thiophen-3-yl)-Benzenesulfonamide (5a)**



5a

Compound **5a** was synthesized following the general procedure.

A white solid, 71.9 mg, 74% yield.

m.p.: 155 ºC – 157 ºC

TLC: R_f = 0.50 (Hexane/EtOAc = 6:1)

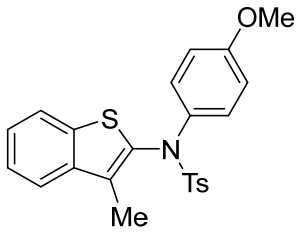
IR (KBr): 2928, 1509, 1354, 1252, 1162, 1091, 1027, 923, 815, 766, 656, 560 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.85 – 7.78 (m, 1H), 7.70 – 7.59 (m, 3H), 7.58 – 7.51 (m, 2H), 7.49 – 7.33 (m, 5H), 7.23 – 7.15 (m, 2H), 7.12 – 7.01 (m, 2H), 6.75 – 6.66 (m, 2H), 3.74 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.0, 143.7, 143.4, 137.8, 137.5, 136.6, 134.1, 132.4, 129.7, 129.2, 128.9, 128.9, 128.4, 128.0, 127.3, 124.8, 124.8, 123.0, 122.5, 114.1, 55.3, 21.6.

HRMS (ESI): $C_{28}H_{24}NO_3S_2$ $[M+H]^+$: calcd.: 486.1192; found: 486.1197.

***N*-(4-Methoxyphenyl)-4-Methyl-*N*-(3-Methylbenzo[b]thiophen-2-yl)-Benzenesulfonamide (5b)**



5b

Compound **5b** was synthesized following the general procedure.

A white solid, 77.1 mg, 91% yield.

m.p.: 91 ºC – 93 ºC

TLC: R_f = 0.68 (Hexane/EtOAc = 6:1)

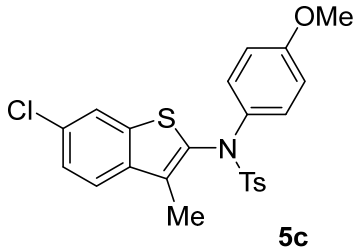
IR (KBr): 2925, 1506, 1349, 1245, 1162, 1086, 951, 753, 665, 615, 568 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.72 – 7.66 (m, 4H), 7.41 – 7.35 (m, 2H), 7.34 – 7.31 (m, 4H), 6.90 – 6.85 (m, 2H), 3.80 (s, 3H), 2.49 (s, 3H), 2.49 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 159.1, 144.1, 137.9, 137.6, 136.7, 135.8, 133.4, 132.4, 129.9, 129.5, 128.6, 125.4, 124.3, 122.8, 122.3, 114.4, 55.4, 21.7, 11.8.

HRMS (ESI): $C_{23}H_{22}NO_3S_2$ $[M+H]^+$: calcd.: 424.1036; found: 424.1040.

***N*-(6-Chloro-3-Methylbenzo[b]thiophen-2-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (5c)**



5c

Compound **5c** was synthesized following the general procedure.

A white solid, 80.6 mg, 88% yield.

m.p.: 146 ºC – 148 ºC

TLC: R_f = 0.51 (Hexane/EtOAc = 6:1)

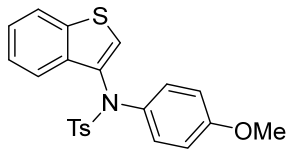
IR (KBr): 2921, 1599, 1507, 1355, 1250, 1165, 1083, 1035, 667, 576 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.69 – 7.63 (m, 3H), 7.62 – 7.57 (m, 1H), 7.37 – 7.26 (m, 5H), 6.91 – 6.83 (m, 2H), 3.80 (s, 3H), 2.49 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 159.2, 144.2, 139.1, 138.5, 135.7, 135.5, 133.2, 131.8, 130.6, 129.9, 129.5, 128.6, 125.8, 123.5, 122.5, 114.5, 55.4, 21.7, 11.8.

HRMS (ESI): $C_{23}H_{21}{}^{35}ClNO_3S_2$ $[M+H]^+$: calcd.: 458.0646; found: 458.0647.

***N*-(Benzo[b]thiophen-3-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (5d)**



5d

Compound **5d** was synthesized following the general procedure.

A colorless oil, 31.9 mg, 39% yield.

TLC: R_f = 0.52 (Hexane/EtOAc = 6:1)

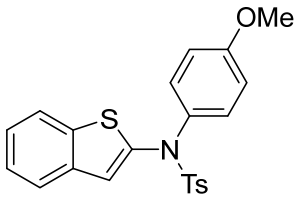
IR (KBr): 2923, 1600, 1505, 1352, 1253, 1163, 1088, 1030, 807, 759, 663, 560 cm^{-1}

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.92–7.90 (m, 1H), 7.86–7.83 (m, 1H), 7.67–7.65 (m, 1H), 7.48 – 7.43 (m, 3H), 7.33 – 7.30 (m, 1H), 7.05 – 7.01 (m, 2H), 6.94–6.92 (m, 2H), 6.59–6.57 (m, 2H), 3.69 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 158.0, 143.5, 139.5, 138.8, 137.4, 137.3, 134.2, 129.2, 127.8, 127.7, 125.1, 124.9, 124.6, 123.1, 122.4, 114.0, 55.3, 21.5.

HRMS (ESI): $C_{22}H_{20}NO_3S_2$ $[M+H]^+$: calcd.: 410.0879; found: 410.0883.

***N*-(Benzo[b]thiophen-2-yl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (5d')**



5d'

Compound **5d'** was synthesized following the general procedure.

A white solid, 39.3 mg, 48% yield.

m.p.: 103 ºC – 105 ºC

TLC: R_f = 0.51 (Hexane/EtOAc = 6:1)

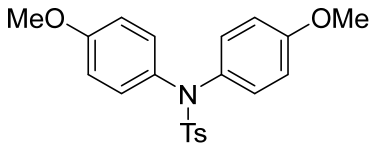
IR (KBr): 2920, 1600, 1507, 1350, 1255, 1231, 1165, 1028, 760, 662, 552 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.88 – 7.84 (m, 1H), 7.81 – 7.76 (m, 1H), 7.68 – 7.61 (m, 2H), 7.41 – 7.33 (m, 4H), 7.32 – 7.27 (m, 3H), 6.89 – 6.82 (m, 2H), 3.79 (s, 3H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.8, 143.8, 137.9, 136.7, 136.3, 133.6, 133.1, 129.5, 129.5, 128.0, 125.1, 124.7, 123.8, 122.8, 122.0, 114.3, 55.4, 21.6.

HRMS (ESI): $C_{22}H_{20}NO_3S_2$ $[M+H]^+$: calcd.: 410.0879; found: 410.0882.

***N*, *N*-Bis(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (7a)**



7a

Compound **7a** was synthesized following the general procedure.

A white solid, 67.5 mg, 88% yield.

m.p.: 117 ºC – 119 ºC

TLC: R_f = 0.49 (Hexane/EtOAc = 6:1)

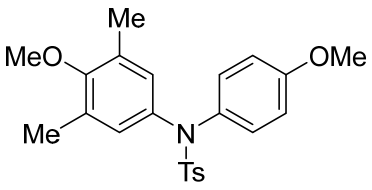
IR (KBr): 2933, 1601, 1504, 1350, 1299, 1244, 1158, 1031, 674, 575, 546 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.65 – 7.54 (m, 2H), 7.33 – 7.27 (m, 2H), 7.25 – 7.17 (m, 4H), 6.88 – 6.80 (m, 4H), 3.80 (s, 6H), 2.47 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.7, 143.3, 137.5, 134.5, 129.7, 129.4, 127.8, 114.4, 55.4, 21.6.

HRMS (ESI): $C_{21}H_{22}NO_4S$ $[M+H]^+$: calcd.: 384.1264; found: 384.1267.

***N*-(4-Methoxy-3,5-Dimethylphenyl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (7b)**



7b

Compound **7b** was synthesized following the general procedure.

A white solid, 69.1 mg, 84% yield.

m.p.: 153 ºC – 155 ºC

TLC: R_f = 0.51 (Hexane/EtOAc = 6:1)

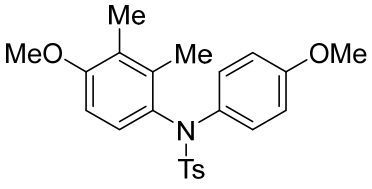
IR (KBr): 2948, 1599, 1508, 1347, 1239, 1166, 1093, 1033, 1010, 819, 660, 541 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.63 – 7.57 (m, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.23 – 7.17 (m, 2H), 6.93 (s, 2H), 6.87 – 6.80 (m, 2H), 3.79 (s, 3H), 3.70 (s, 3H), 2.46 (s, 3H), 2.23 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.8, 156.1, 143.3, 137.6, 137.0, 134.2, 131.7, 130.0, 129.3, 128.4, 127.8, 114.3, 59.6, 55.4, 21.6, 16.2.

HRMS (ESI): $C_{23}H_{26}NO_4S$ $[M+H]^+$: calcd.: 412.1577; found: 412.1579.

***N*-(4-Methoxy-2,3-Dimethylphenyl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (7c)**



7c

Compound **7c** was synthesized following the general procedure.

A white solid, 70.8 mg, 86% yield.

m.p.: 139 ºC – 141 ºC

TLC: R_f = 0.50 (Hexane/EtOAc = 6:1)

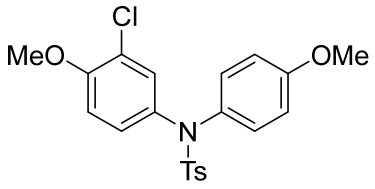
IR (KBr): 2924, 1587, 1506, 1481, 1348, 1255, 1164, 1106, 1033, 669, 562 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.62 – 7.54 (m, 2H), 7.33 – 7.26 (m, 4H), 6.92 – 6.79 (m, 3H), 6.64 (d, *J* = 8.7 Hz, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 2.47 (s, 3H), 2.36 (s, 3H), 2.15 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.1, 157.2, 143.2, 138.7, 137.6, 134.2, 132.9, 129.3, 128.9, 127.9, 126.8, 126.7, 114.1, 107.5, 55.5, 55.4, 21.6, 15.4, 12.4.

HRMS (ESI): $C_{23}H_{26}NO_4S$ $[M+H]^+$: calcd.: 412.1577; found: 412.1581.

N-(3-Chloro-4-Methoxyphenyl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (7d)



7d

Compound **7d** was synthesized following the general procedure.

A white solid, 64.3 mg, 77% yield.

m.p.: 135 ºC – 137 ºC

TLC: R_f = 0.51 (Hexane/EtOAc = 6:1)

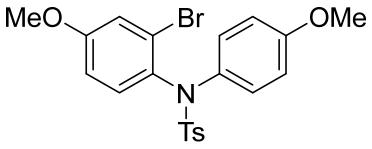
IR (KBr): 2919, 1598, 1504, 1348, 1298, 1260, 1165, 1091, 1021, 665, 588, 543 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.61 – 7.54 (m, 2H), 7.33 – 7.25 (m, 3H), 7.24 – 7.15 (m, 3H), 6.90 – 6.78 (m, 3H), 3.89 (s, 3H), 3.80 (s, 3H), 2.47 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.9, 154.2, 143.6, 137.1, 134.8, 133.9, 130.0, 129.9, 129.5, 127.8, 127.8, 122.4, 114.5, 111.9, 56.3, 55.4, 21.6.

HRMS (ESI): $C_{21}H_{21}{}^{35}ClNO_4S$ $[M+H]^+$: calcd.: 418.0874; found: 418.0877.

N-(2-Bromo-4-Methoxyphenyl)-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (7e)



7e

Compound **7e** was synthesized following the general procedure.

A white solid, 83.2 mg, 90% yield.

m.p.: 82 ºC – 84 ºC

TLC: R_f = 0.49 (Hexane/EtOAc = 6:1)

IR (KBr): 2921, 1596, 1507, 1485, 1353, 1160, 1034, 974, 670, 557 cm^{-1}

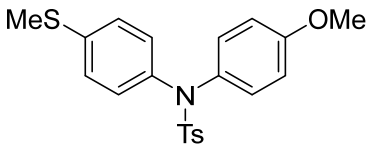
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.62 – 7.54 (m, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.28 – 7.18 (m, 3H), 7.16 – 7.09 (m, 1H), 6.85 – 6.71 (m, 3H), 3.75 (s, 3H), 3.75 (s, 3H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 159.6, 158.7, 143.6, 137.0, 133.1, 132.8, 131.3, 130.0, 129.4, 128.1, 126.5, 118.9, 114.1, 113.9, 55.7, 55.4, 21.6.

HRMS (ESI): $C_{21}H_{21}{}^{79}BrNO_4S$ $[M+H]^+$: calcd.: 462.0369; found: 462.0371;

$C_{21}H_{21}{}^{81}BrNO_4S$ $[M+H]^+$: calcd.: 464.0349; found: 464.0350.

***N*-(4-Methoxyphenyl)-4-Methyl-*N*-(4-Methylthio)-Phenyl-Benzenesulfonamide (7f)**



7f

Compound **7f** was synthesized following the general procedure.

A white solid, 72.7 mg, 91% yield.

m.p.: 111 ºC – 113 ºC

TLC: R_f = 0.48 (Hexane/EtOAc = 6:1)

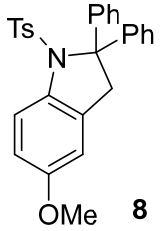
IR (KBr): 2924, 1599, 1505, 1349, 1249, 1164, 1093, 1026, 982, 720, 664, 575 cm^{-1}

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.63 – 7.55 (m, 2H), 7.32 – 7.25 (m, 2H), 7.24 – 7.14 (m, 6H), 6.89 – 6.80 (m, 2H), 3.80 (s, 3H), 2.46 (s, 3H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.9, 143.5, 138.9, 137.7, 137.4, 134.0, 130.0, 129.5, 128.2, 127.8, 127.0, 114.4, 55.4, 21.6, 15.7.

HRMS (ESI): $C_{21}H_{22}NO_3S_2$ $[M+H]^+$: calcd.: 400.1036; found: 400.1040.

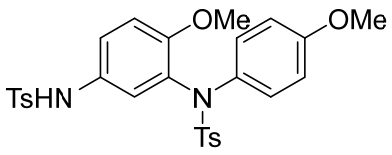
5-Methoxy-2,2-diphenyl-1-tosylindoline (8)



8

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.77 (d, *J* = 9.0 Hz, 1H), 7.45 – 7.38 (m, 4H), 7.28 – 7.22 (m, 6H), 6.94 – 6.84 (m, 4H), 6.80 (dd, *J* = 9.0, 2.7 Hz, 1H), 6.62 (d, *J* = 2.6 Hz, 1H), 3.81 (s, 2H), 3.75 (s, 3H), 2.29 (s, 3H).

N-(2-Methoxy-5-(4-Methylphenyl)-Sulfonamido-Phenyl-*N*-(4-Methoxyphenyl)-4-Methyl-Benzenesulfonamide (9)



9

A white solid, 41.0 mg, 74% yield.

m.p.: 158 ºC – 160 ºC

TLC: R_f = 0.34 (Hexane/EtOAc = 2:1)

IR (KBr): 2927, 1601, 1506, 1357, 1305, 1257, 1163, 1088, 1034, 816, 654, 548 cm^{-1}

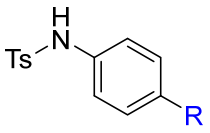
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.64 – 7.55 (m, 3H), 7.53 (s, 1H), 7.50 – 7.45 (m, 2H), 7.31 – 7.23 (m, 1H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.00 – 6.91 (m, 2H), 6.82 (dd, *J* = 9.1, 2.9 Hz, 1H), 6.74 – 6.65 (m, 2H), 6.40 (d, *J* = 2.9 Hz, 1H), 3.79 (s, 3H), 3.63 (s, 3H), 2.45 (s, 3H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.7, 156.3, 144.4, 143.5, 136.7, 135.5, 132.8, 132.7, 129.6, 129.5, 128.8, 128.6, 128.2, 127.1, 123.1, 115.3, 114.3, 114.3, 55.4, 55.4, 21.6, 21.5.

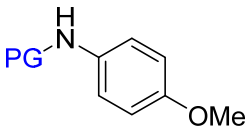
HRMS (ESI): $C_{28}H_{29}N_2O_6S_2$ $[M+H]^+$: calcd.: 553.1462; found: 553.1464.

Unsuccessful substrates:

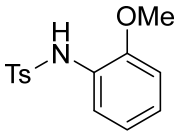
Amides:



R = OAc, OCF_3, NHTs, Me:
No reaction
R = NMe_2: con% <15%

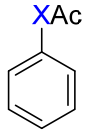


PG = Ac, CO_2Me:
No reaction
PG = Ms: con% <20%

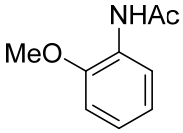


No reaction

Arenes:



X = O, NH
No reaction



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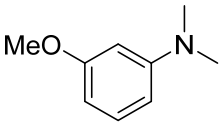

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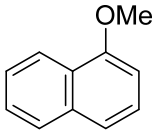

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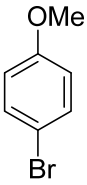
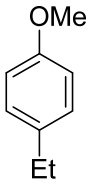
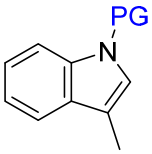


con% <15%



con% <20%

X = O, S
con% <20%



PG = H, Me, Ac, Ts
No reaction

5. X-Ray Crystallographic Analysis

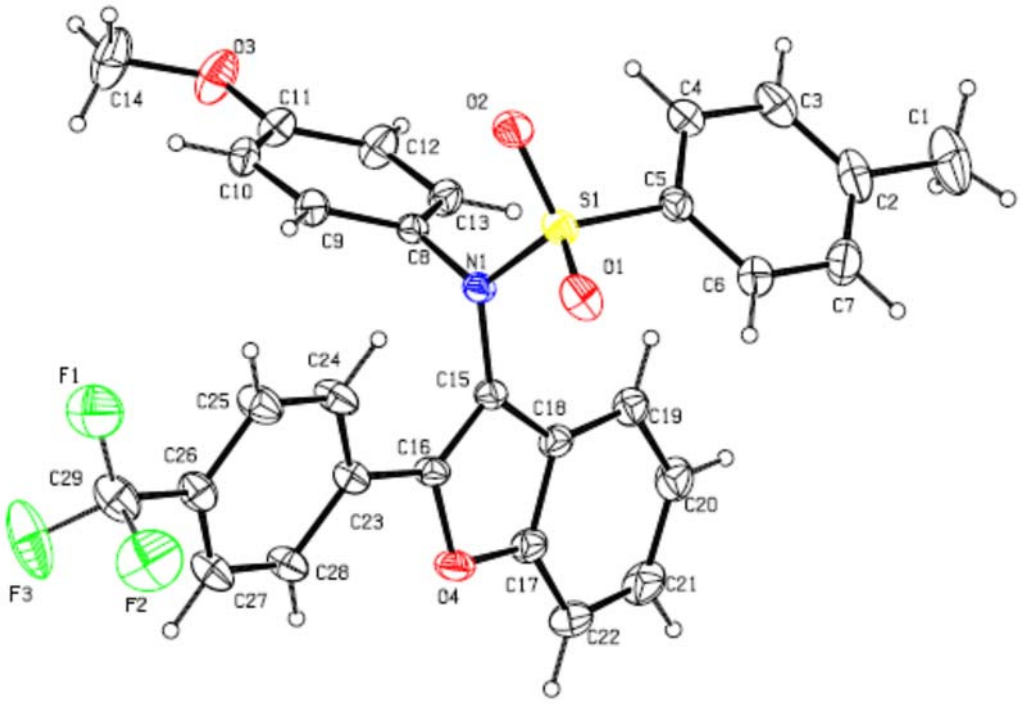


Table S2 Crystallographic data and structural refinement for compound **3t**

Complex	**Compound 1**
Formula	$C_{29}H_{22}F_3NO_4S$
Formula weight	537.53.
Temp (K)	297(15)
λ (Mo, Kα), Å	0.71073
Crystal system	Triclinic
Space group	P-1
a (Å)	10.359(2)
b (Å)	11.887(3)
c (Å)	12.512(3)
α (deg)	73.639(4)
β (deg)	86.075(4)
γ (deg)	89.672(4)
V ($Å^3$)	1474.7(6)

Z	2
ρ_{calc}g/cm^3	1.211
Absorption coefficient	0.160 mm^{-1}
F(000)	556
Crystal size/mm^3	0.3 × 0.2 × 2
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14
Reflections collected	10483
Independent reflections	5153 [R_{int} = 0.0387]
Data/restraints/parameters	5153/57/374
Largest diff. peak/hole / e Å^{-3}	0.274/-0.323
Flack parameter	0.01(3)
Theta range for data collection (deg)	1.700–24.996
Final R1a, wR2b	0.0594, 0.1719
Goodness-of-fit on F2	1.063

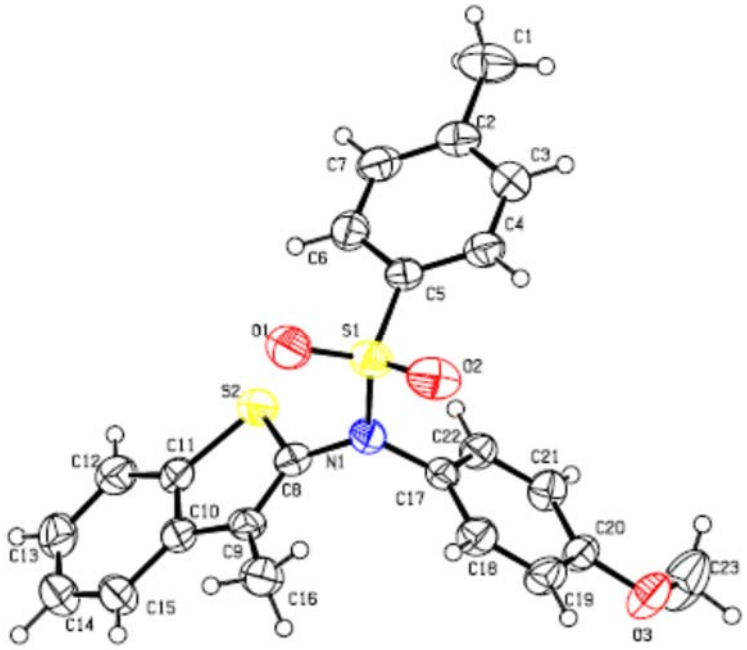


Table S3 Crystallographic data and structural refinement for compound **5b**

Complex	**Compound 1**

Formula	$C_{23}H_{21}NO_3S_2$
Formula weight	423.53
Temp (K)	297(2)
λ (Mo, Kα), Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	8.2878(17)
b (Å)	21.266(4)
c (Å)	11.819(2)
α (deg)	90
β (deg)	100.442(5)
γ (deg)	90
V ($Å^3$)	2048.5(7)
Z	4
$\rho_{calc}g/cm^3$	1.373
Absorption coefficient	0.285
F(000)	888
Crystal size/mm^3	0.12 × 0.10 × 0.10
Index ranges	$-9 \leq h \leq 9$, $-25 \leq k \leq 25$, $-11 \leq l \leq 13$
Reflections collected	10005
Independent reflections	3510 [$R_{int} = 0.0439$]
Data/restraints/parameters	3510/0/266
Largest diff. peak/hole / e $Å^{-3}$	0.226/-0.235
Flack parameter	0.0000(3)
Theta range for data collection (deg)	1.915–24.995
Final R1a, wR2b	0.0555, 0.0971
Goodness-of-fit on F2	1.010

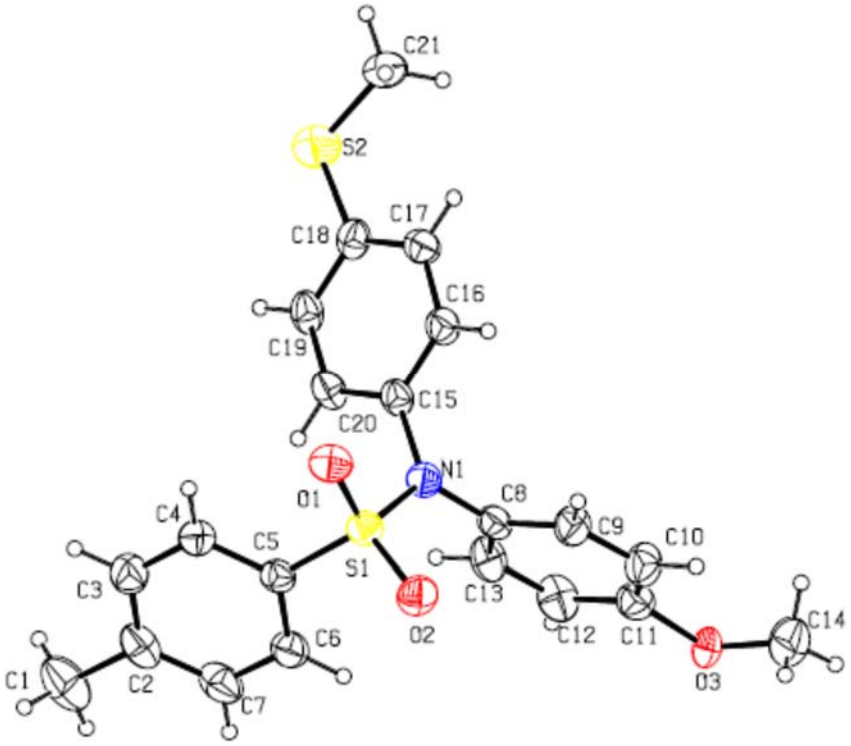
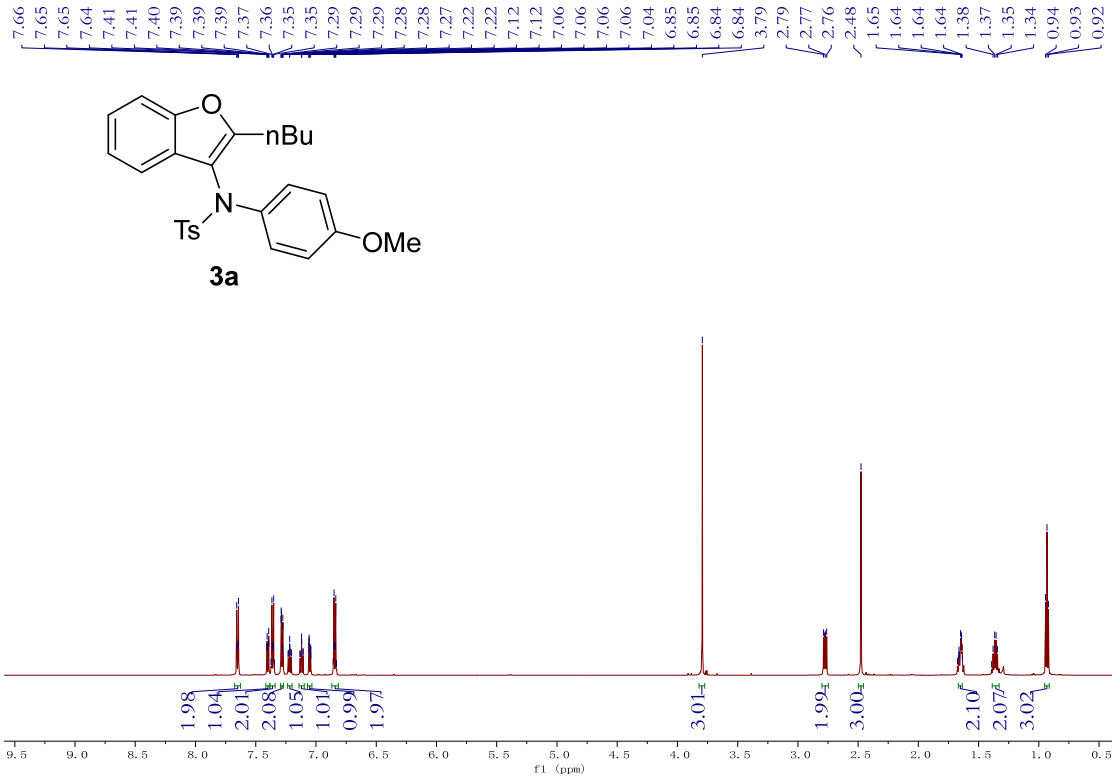


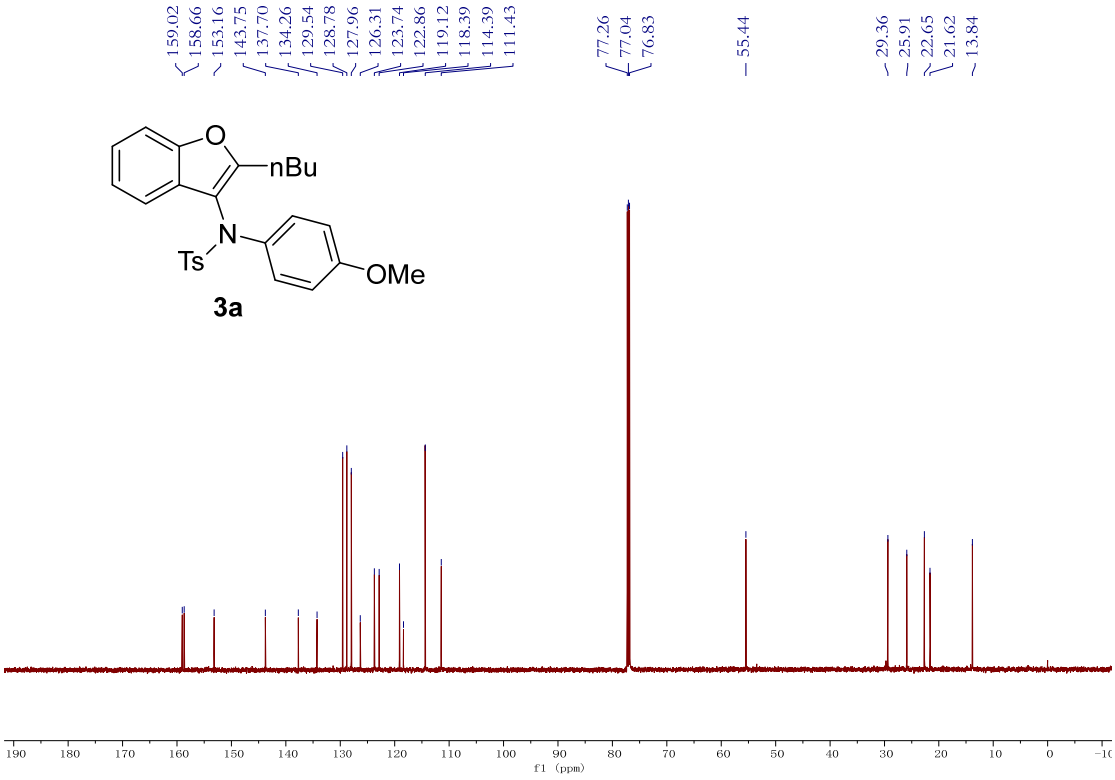
Table S4 Crystallographic data and structural refinement for compound **7f**

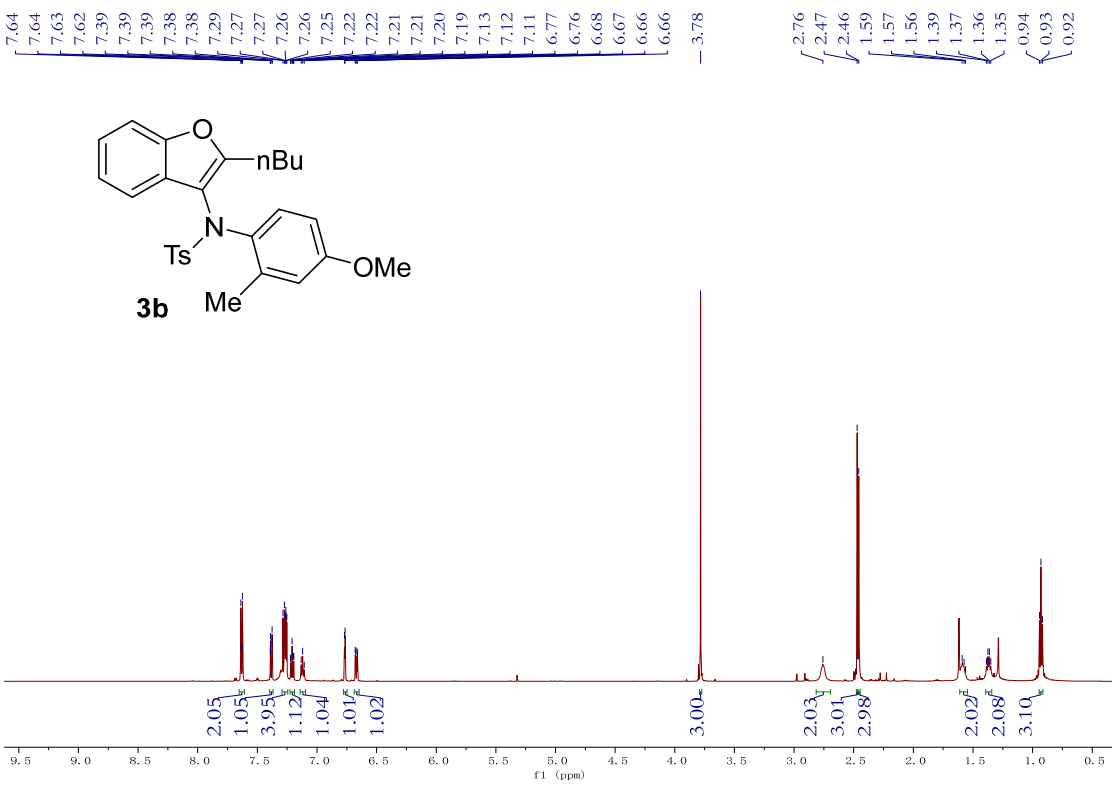
Complex	**Compound 1**
Formula	$C_{21}H_{21}NO_3S_2$
Formula weight	399.51
Temp (K)	297(15)
λ (Mo, Kα), Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	12.583(3)
b (Å)	13.374(3)
c (Å)	11.959(3)
α (deg)	90
β (deg)	98.369(4)
γ (deg)	90
V ($Å^3$)	1991.0(7)
Z	4
$\rho_{calc}g/cm^3$	1.333

Absorption coefficient	0.288
F(000)	840
Crystal size/mm^3	0.20 × 0.20 × 0.10
Index ranges	$-14 \leq h \leq 14$, $-15 \leq k \leq 15$, $-14 \leq l \leq 13$
Reflections collected	13308
Independent reflections	3427 [$R_{int} = 0.0375$]
Data/restraints/parameters	3427/20/241
Largest diff. peak/hole / e $Å^{-3}$	0.968/-0.883
Flack parameter	n/a
Theta range for data collection (deg)	2.235–24.996
Final R1a, wR2b	0.0677, 0.1885
Goodness-of-fit on F^2	1.030

6. NMR Spectra of Products



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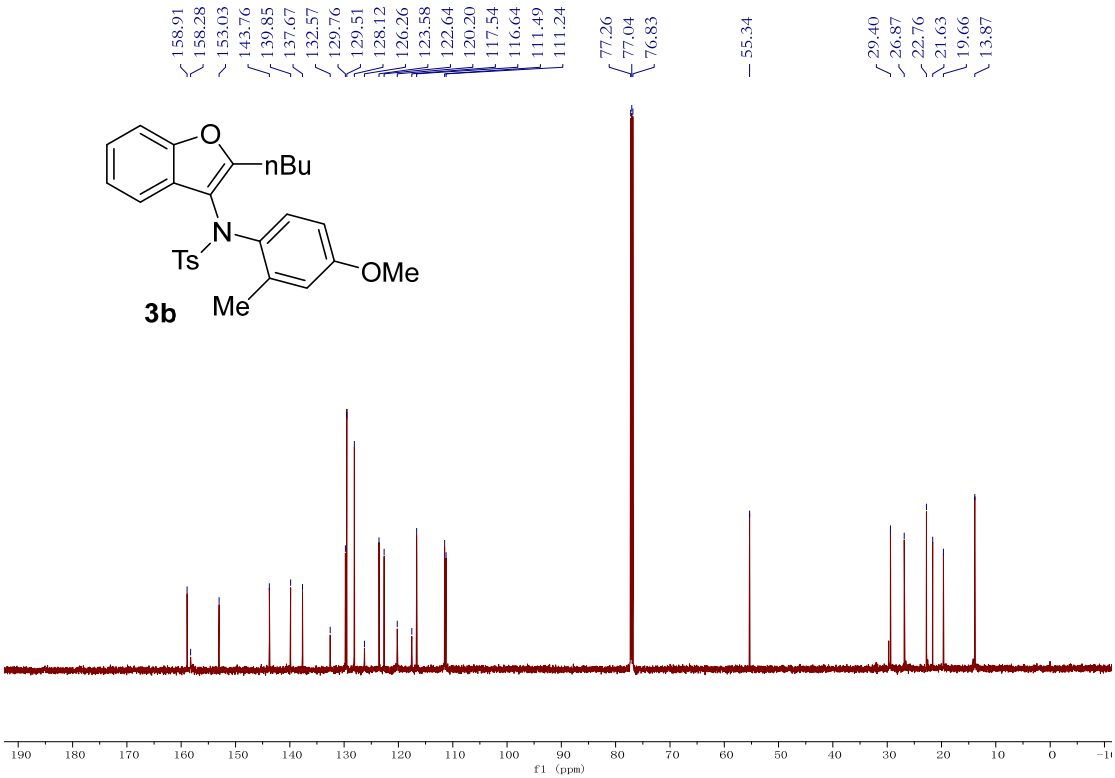
2.76 2.47 2.46 1.59 1.57 1.56 1.39 1.37 1.36 1.35 0.94 0.93 0.92
O
nBu
N
Ts
OMe
Me
3b
2.05 1.05 3.95 1.12 1.04 1.01 1.02 3.00 2.03 3.01 2.98 2.02 2.08 3.10
f1 (ppm)


158.91 158.28 153.03 143.76 139.85 137.67 132.57 129.76 129.51 128.12 126.26 123.58 122.64 120.20 117.54 116.64 111.49 111.24 77.26 77.04 76.83 55.34 29.40 26.87 22.76 21.63 19.66 13.87
O
nBu
N
Ts
OMe
Me
3b
f1 (ppm)


7.68
7.67
7.67
7.66
7.41
7.39
7.29
7.29
7.28
7.24
7.23
7.23
7.22
7.22
7.21
7.21
7.21
7.15
7.13
7.13
7.12
7.12
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7.10
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1.67
1.66
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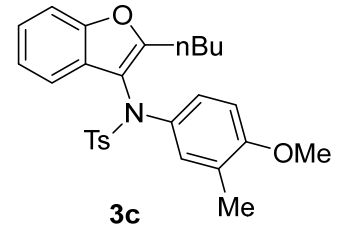
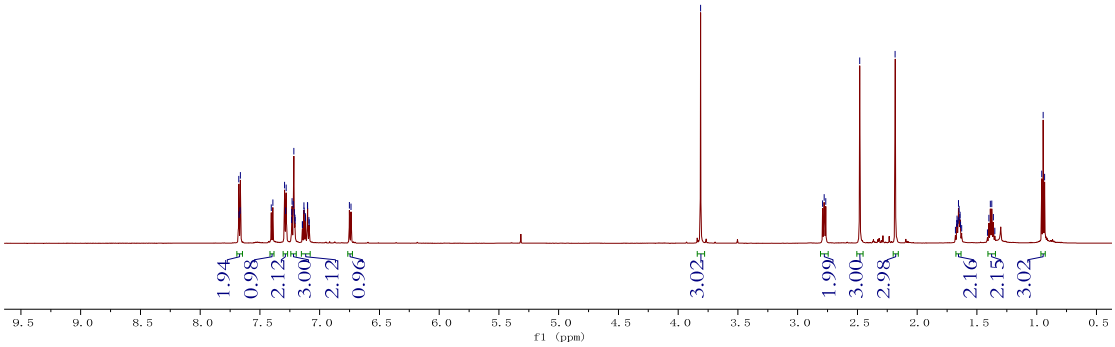
0.95
0.93


O
nBu
N
Ts
OMe
Me

3c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3.00
2.12
0.96
3.02
1.99
3.00
2.98
2.16
2.15
3.02
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)


158.92
157.00
153.16
143.69
137.85
133.67
130.06
129.51
127.98
127.61
126.37
125.96
123.71
122.86
119.18
118.49
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77.08
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25.94
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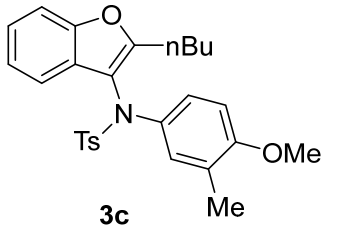
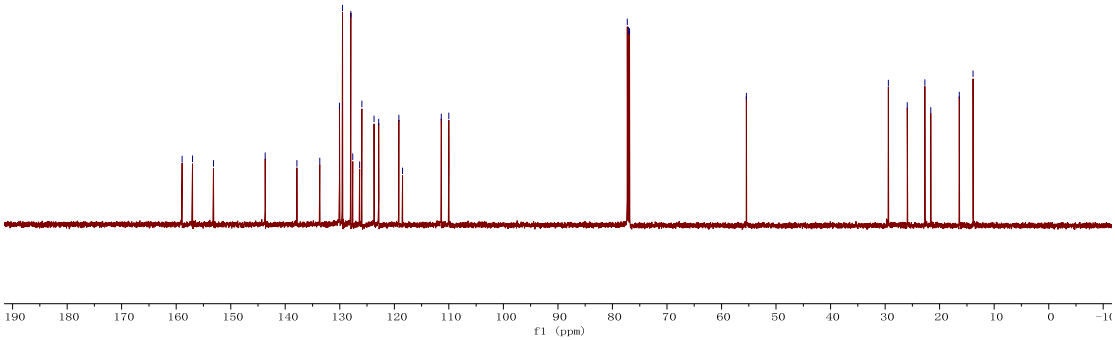
21.63
16.39
13.87


O
nBu
N
Ts
OMe
Me

3c


190
180
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90
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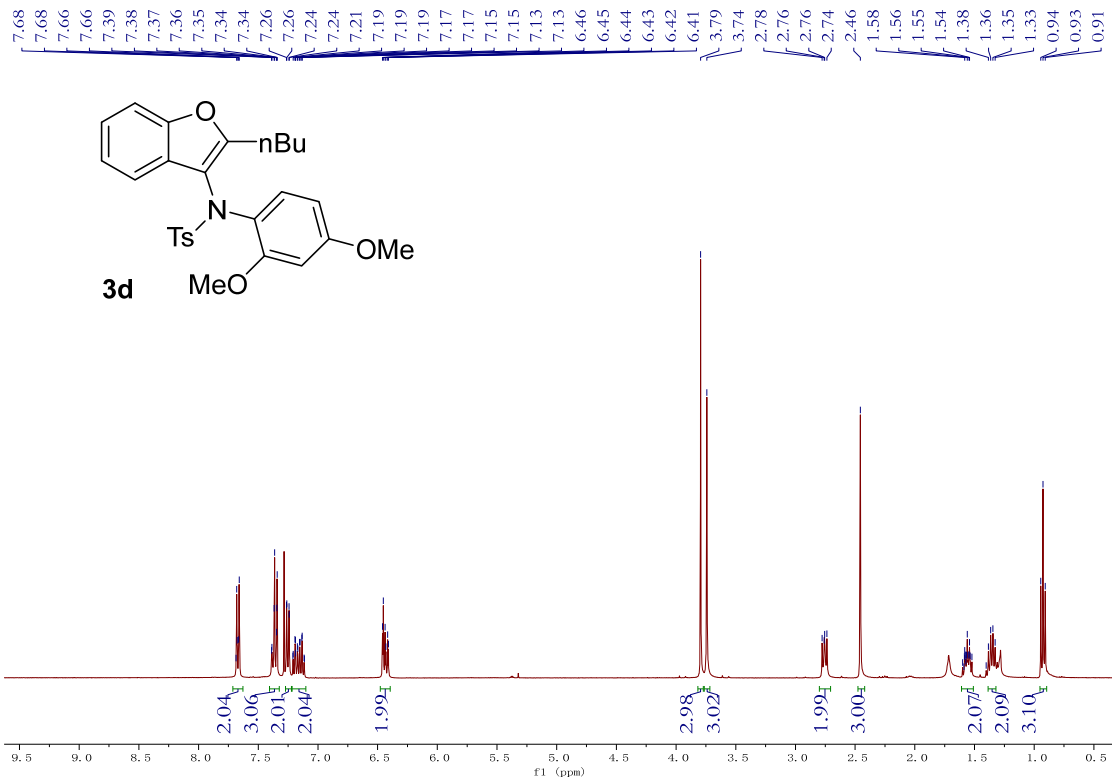
70
60
50
40
30
20
10
0
f1 (ppm)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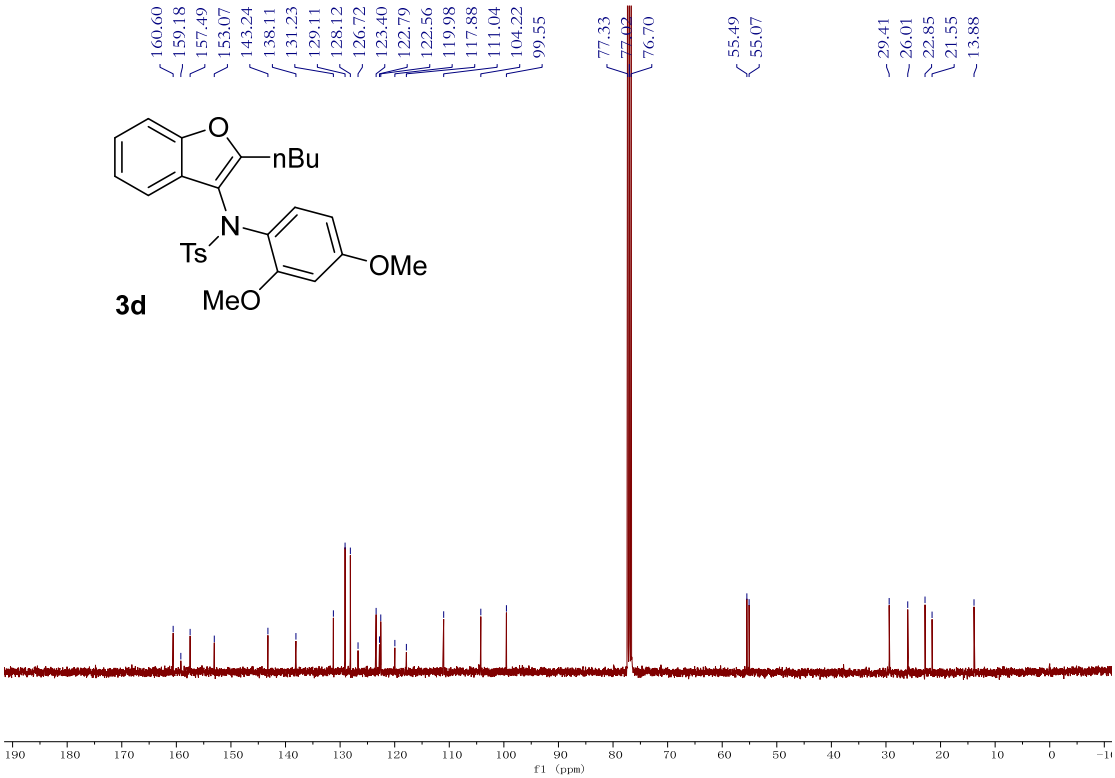
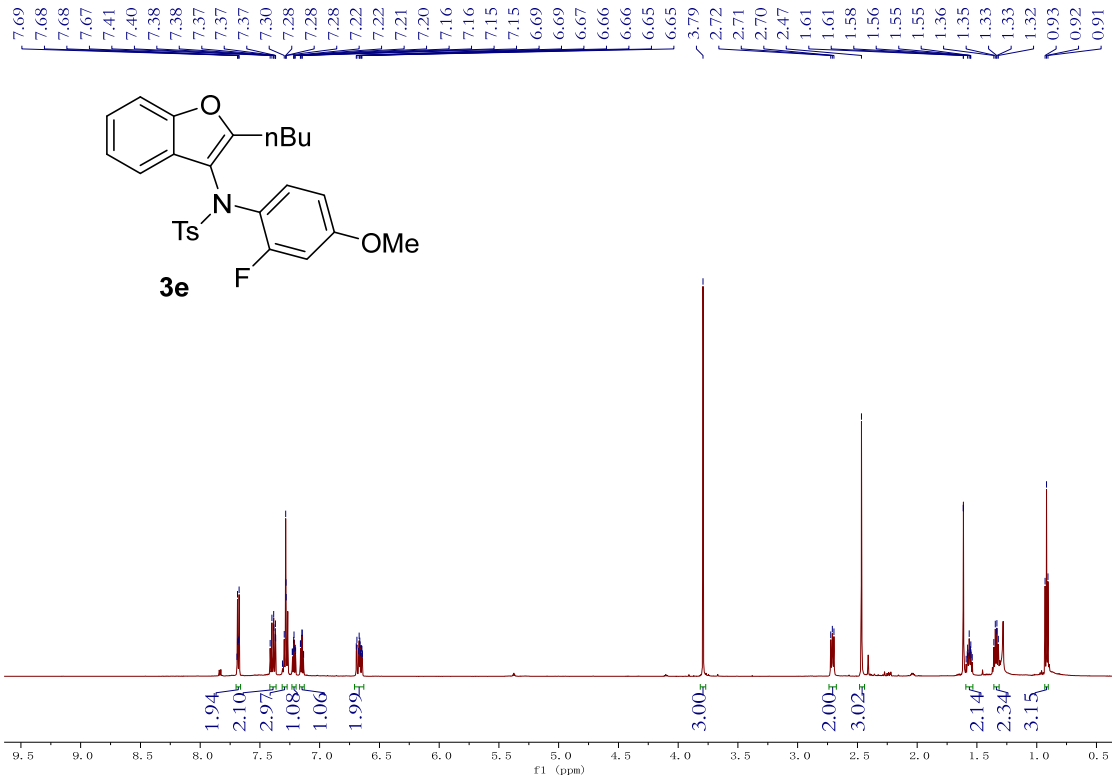
O
nBu
N
Ts
OMe
MeO
3d
2.04 3.06 2.01 2.04 1.99 2.98 3.02 1.99 3.00 2.07 2.09 3.10
f1 (ppm)


160.60 159.18 157.49 153.07 143.24 138.11 131.23 129.11 128.12 126.72 123.40 122.79 122.56 119.98 117.88 111.04 104.22 99.55 77.33 77.02 76.70 55.49 55.07 29.41 26.01 22.85 21.55 13.88
O
nBu
N
Ts
OMe
MeO
3d
f1 (ppm)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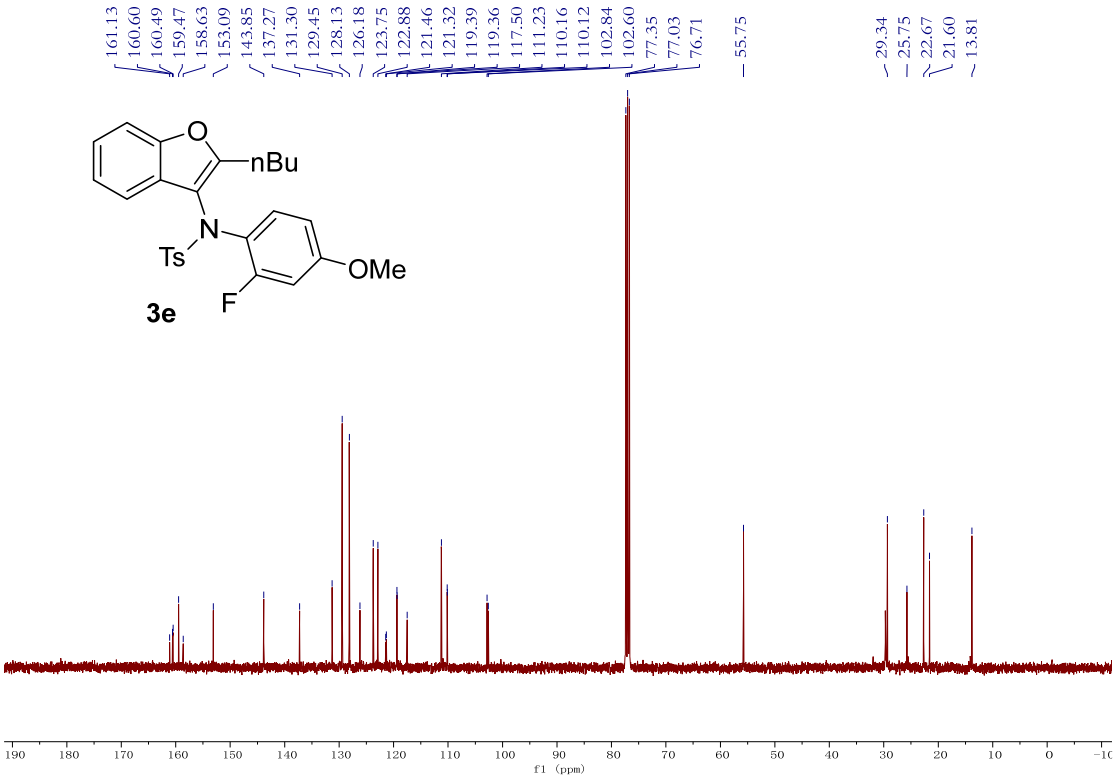
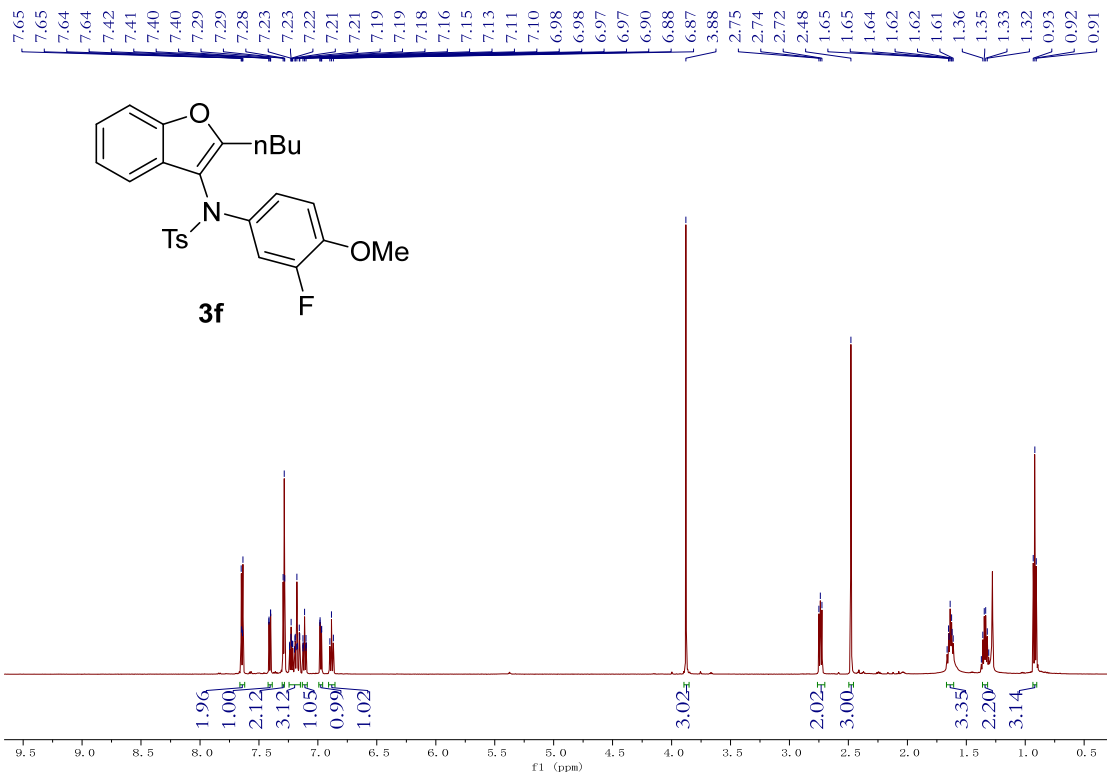
O
nBu
N
Ts
OMe
F
3e
1.94 2.10 2.97 1.08 1.06 1.99 3.00 2.00 3.02 2.14 2.34 3.15
f1 (ppm)


161.13 160.60 160.49 159.47 158.63 153.09 143.85 137.27 131.30 129.45 128.13 126.18 123.75 122.88 121.46 121.32 119.39 119.36 117.50 111.23 110.16 110.12 102.84 102.60 77.35 77.03 76.71 55.75 29.34 25.75 22.67 21.60 13.81
O
nBu
N
Ts
OMe
F
3e
f1 (ppm)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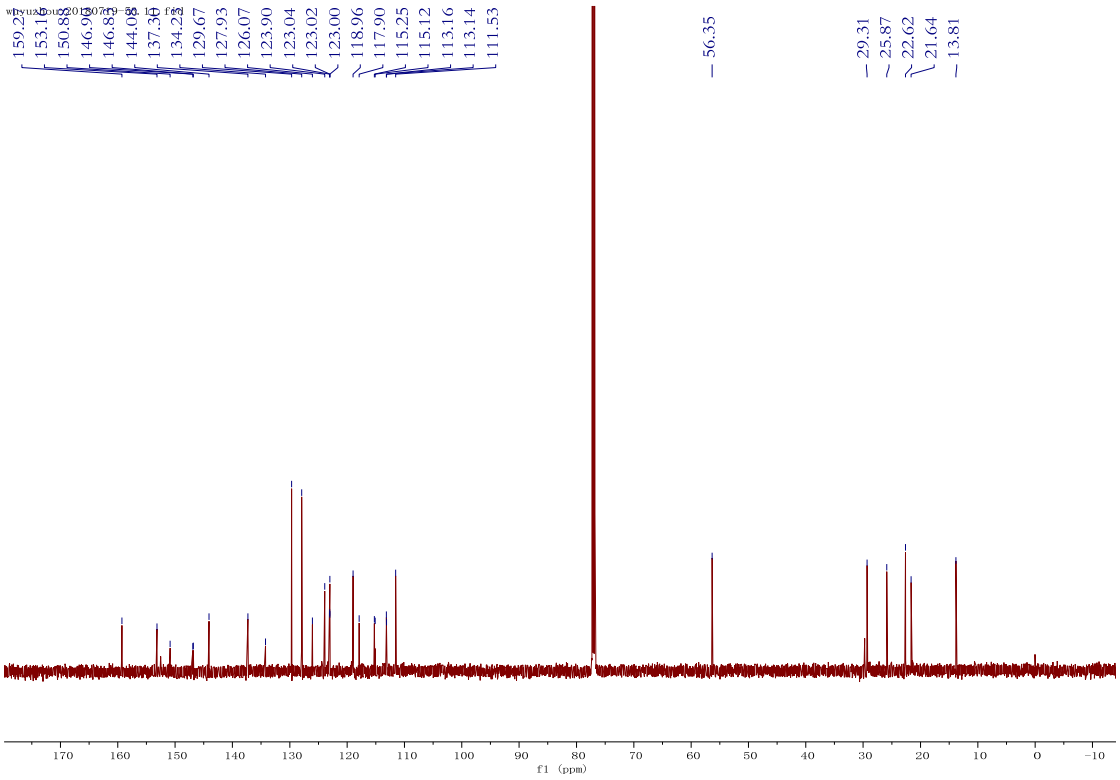
O
nBu
N
Ts
OMe
F
3f
1.96 1.00 2.12 3.12 1.05 0.99 1.02 3.02 2.02 3.00 3.35 2.20 3.14
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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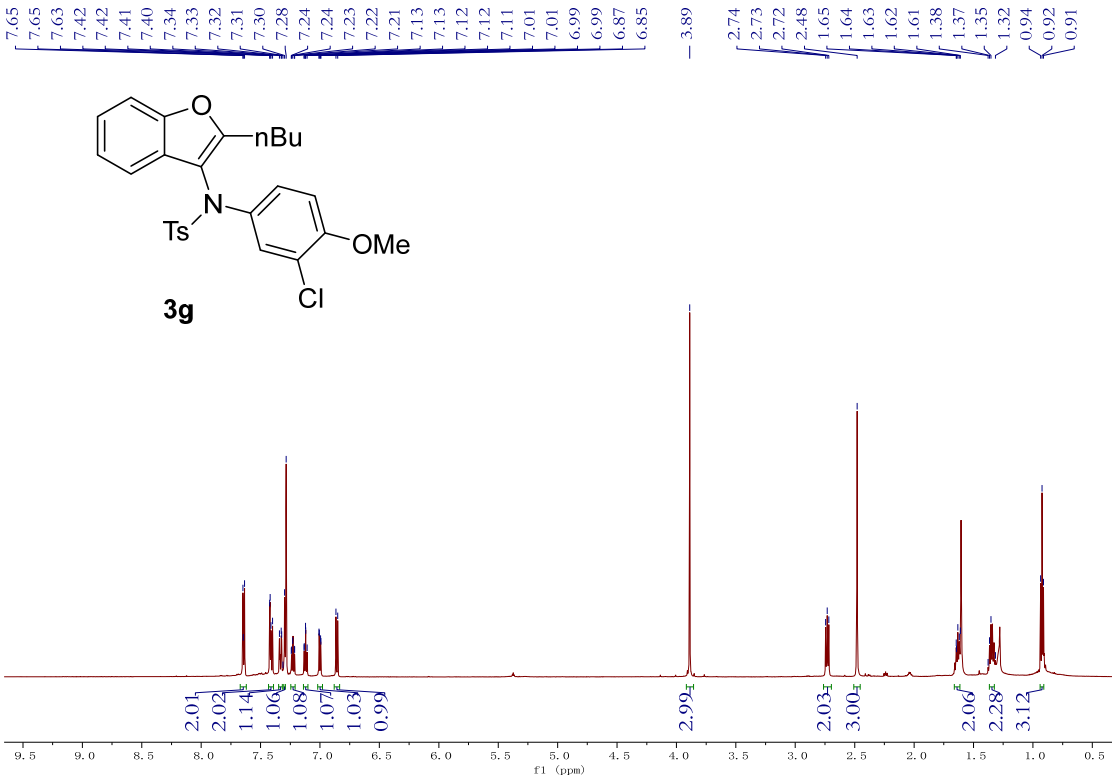
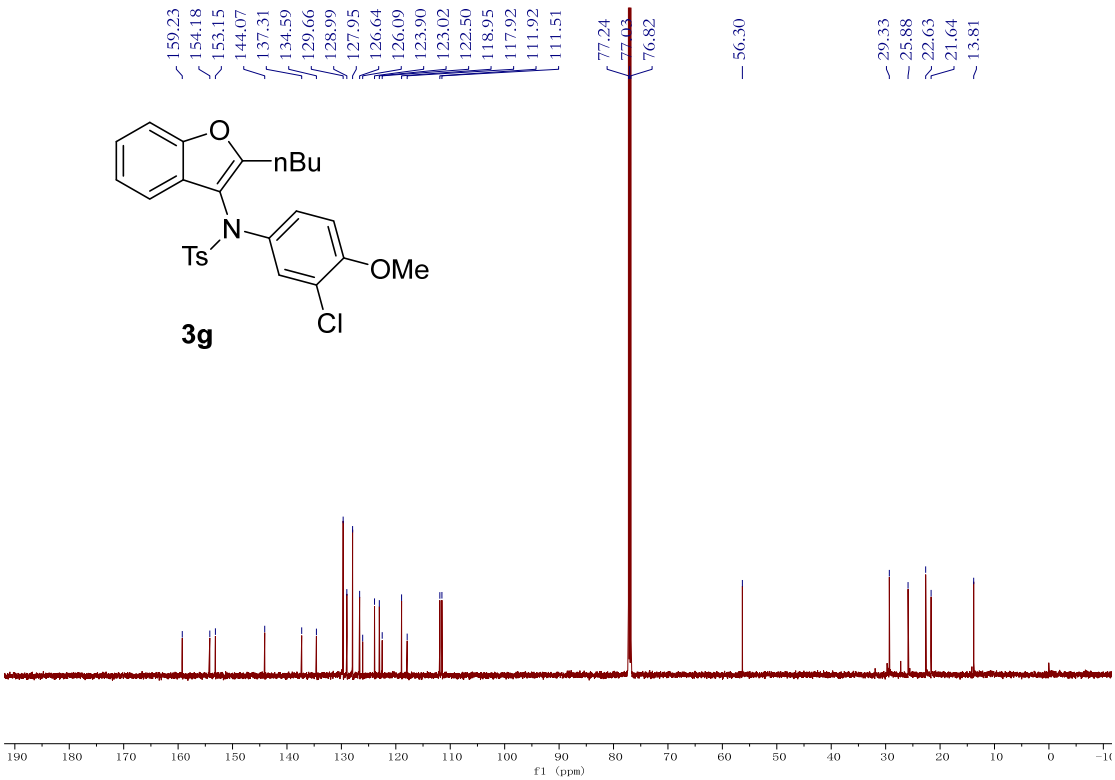
f1 (ppm)


7.65 7.65 7.63 7.42 7.42 7.41 7.40 7.34 7.33 7.32 7.31 7.30 7.28 7.24 7.24 7.23 7.22 7.21 7.13 7.13 7.12 7.12 7.11 7.01 7.01 6.99 6.99 6.87 6.85 3.89 2.74 2.73 2.72 2.48 1.65 1.64 1.63 1.62 1.61 1.38 1.37 1.35 1.32 0.94 0.92 0.91
O
nBu
N
Ts
OMe
Cl
3g
2.01 2.02 1.14 1.06 1.08 1.07 1.03 0.99 2.99 2.03 3.00 2.06 2.28 3.12
f1 (ppm)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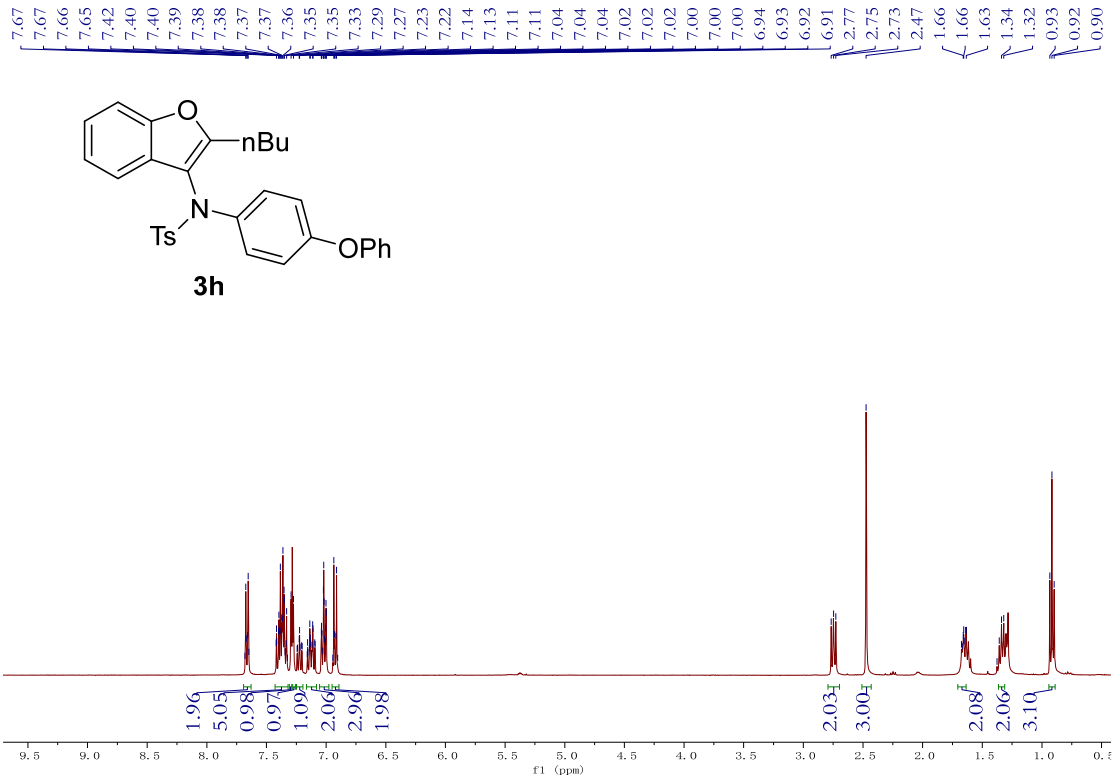
nBu
N
Ts
OMe
Cl
3g
f1 (ppm)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O
nBu
N
Ts
OPh
3h
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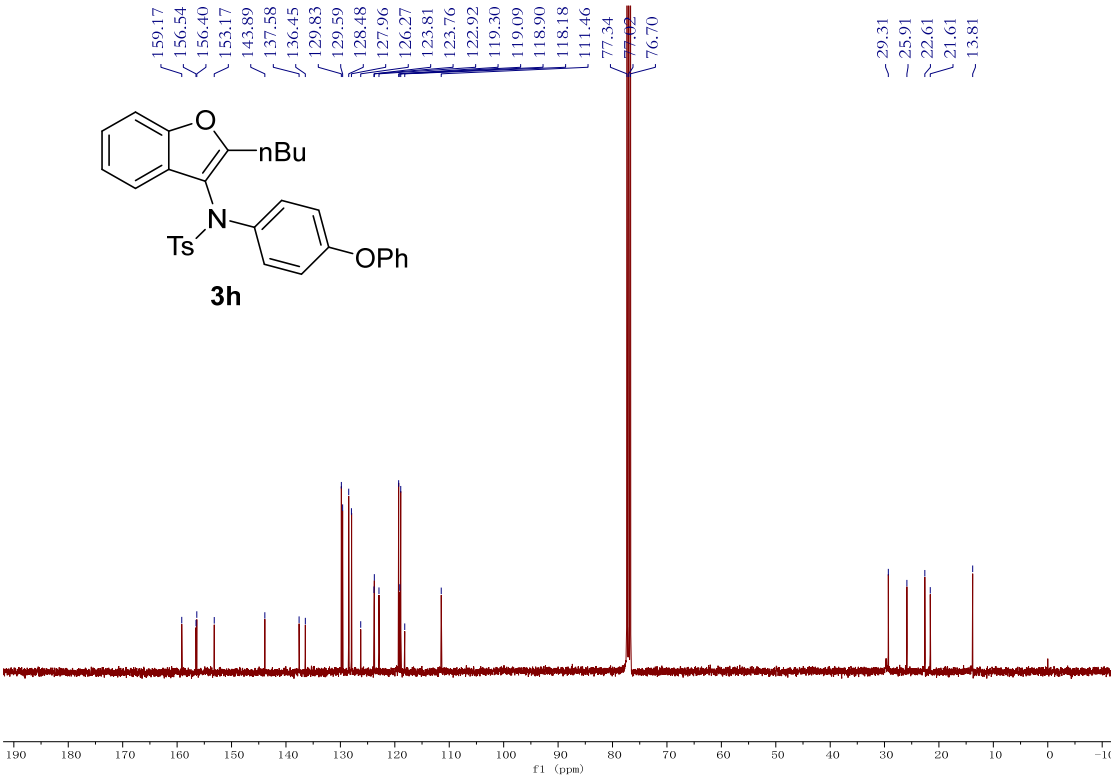
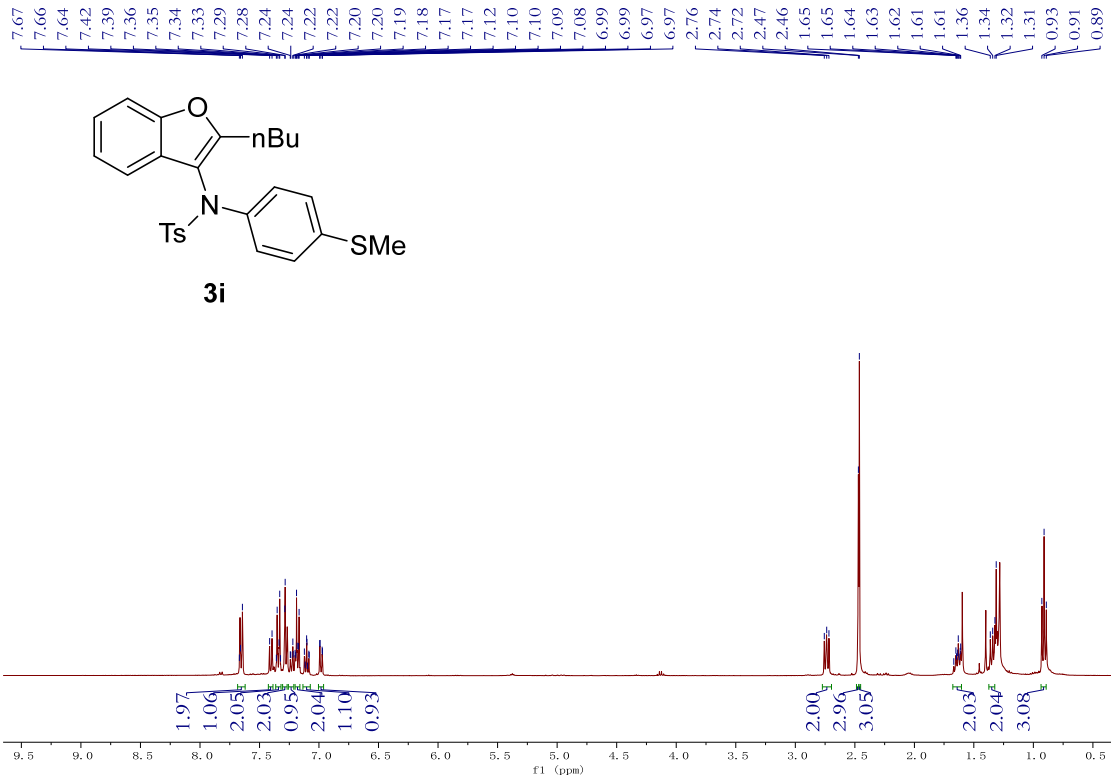
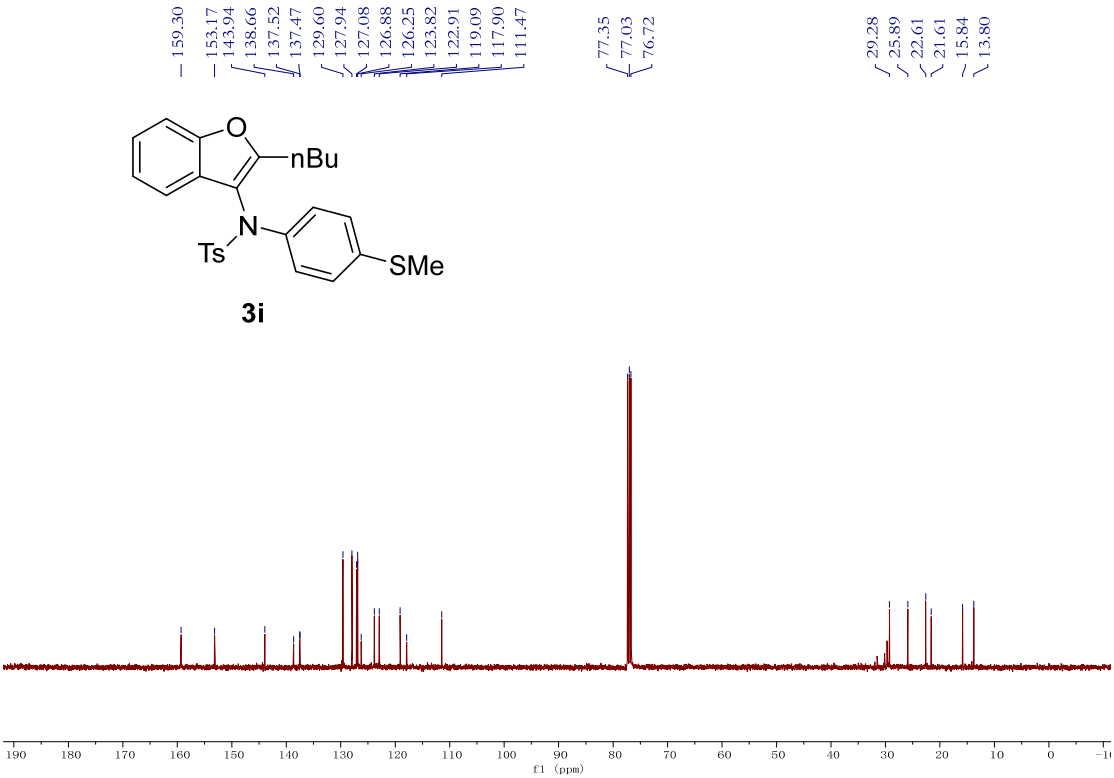
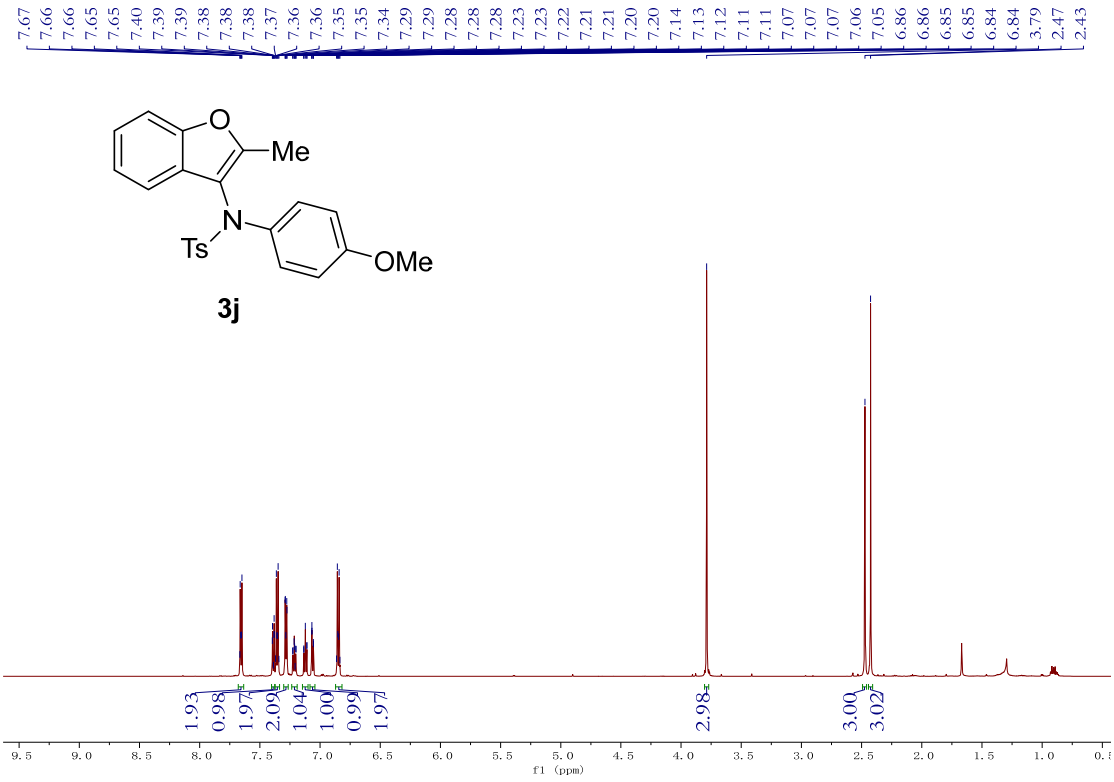
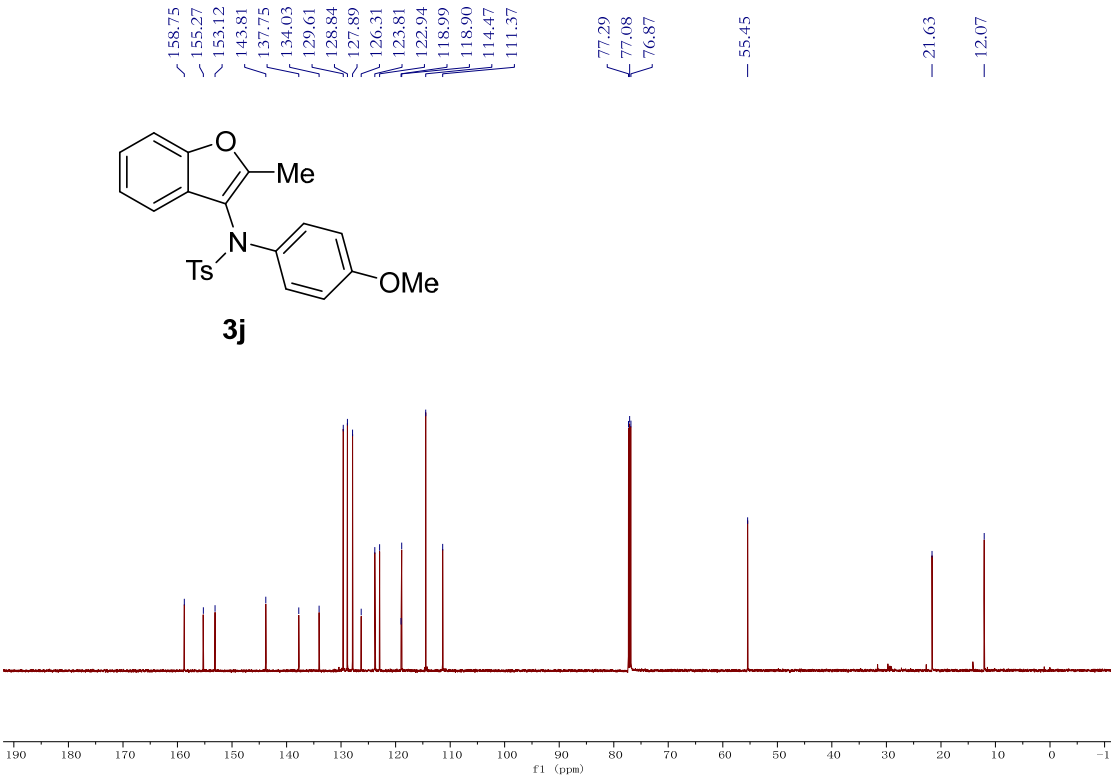
f1 (ppm)

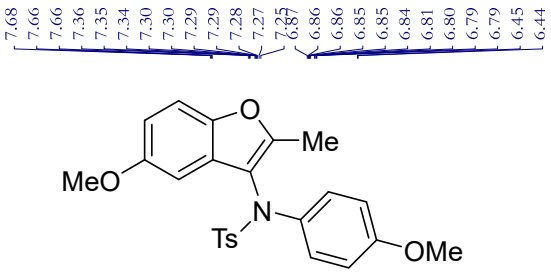

159.17 156.54 156.40 153.17 143.89 137.58 136.45 129.83 129.59 128.48 127.96 126.27 123.81 123.76 122.92 119.30 119.09 118.90 118.18 111.46 77.34 77.02 76.70 29.31 25.91 22.61 21.61 13.81
O
nBu
N
Ts
OPh
3h
f1 (ppm)


7.67 7.66 7.64 7.42 7.39 7.36 7.35 7.34 7.33 7.29 7.28 7.24 7.24 7.22 7.22 7.20 7.20 7.19 7.18 7.17 7.17 7.12 7.10 7.10 7.09 7.08 6.99 6.99 6.97 6.97
2.76 2.74 2.72 2.47 2.46 1.65 1.65 1.64 1.63 1.62 1.61 1.61 1.36 1.34 1.32 1.31 0.93 0.91 0.89
O
nBu
N
Ts
SMe
3i
1.97 1.06 2.05 2.03 0.95 2.04 1.10 0.93
2.00 2.96 3.05 2.03 2.04 3.08
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)

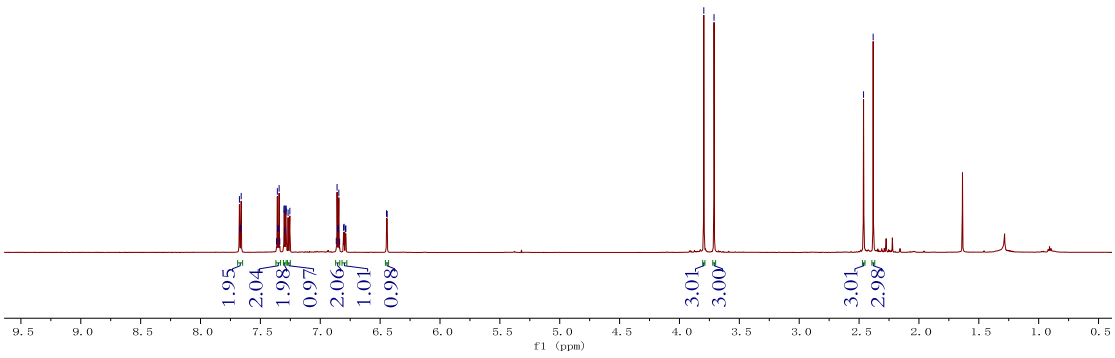

159.30 153.17 143.94 138.66 137.52 137.47 129.60 127.94 127.08 126.88 126.25 123.82 122.91 119.09 117.90 111.47
77.35 77.03 76.72
29.28 25.89 22.61 21.61 15.84 13.80
O
nBu
N
Ts
SMe
3i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

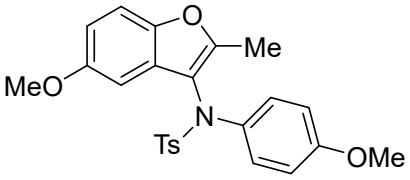

7.67 7.66 7.66 7.65 7.65 7.40 7.39 7.39 7.38 7.38 7.38 7.37 7.36 7.36 7.35 7.35 7.34 7.29 7.29 7.28 7.28 7.28 7.23 7.23 7.22 7.21 7.21 7.20 7.20 7.14 7.13 7.12 7.11 7.11 7.07 7.07 7.07 7.06 7.05 6.86 6.86 6.85 6.85 6.84 6.84 3.79 2.47 2.43
O
Me
N
Ts
OMe
3j
1.93 0.98 1.97 2.09 1.04 1.00 0.99 1.97 2.98 3.00 3.02
f1 (ppm)


158.75 155.27 153.12 143.81 137.75 134.03 129.61 128.84 127.89 126.31 123.81 122.94 118.99 118.90 114.47 111.37 77.29 77.08 76.87 55.45 21.63 12.07
O
Me
N
Ts
OMe
3j
f1 (ppm)



3k





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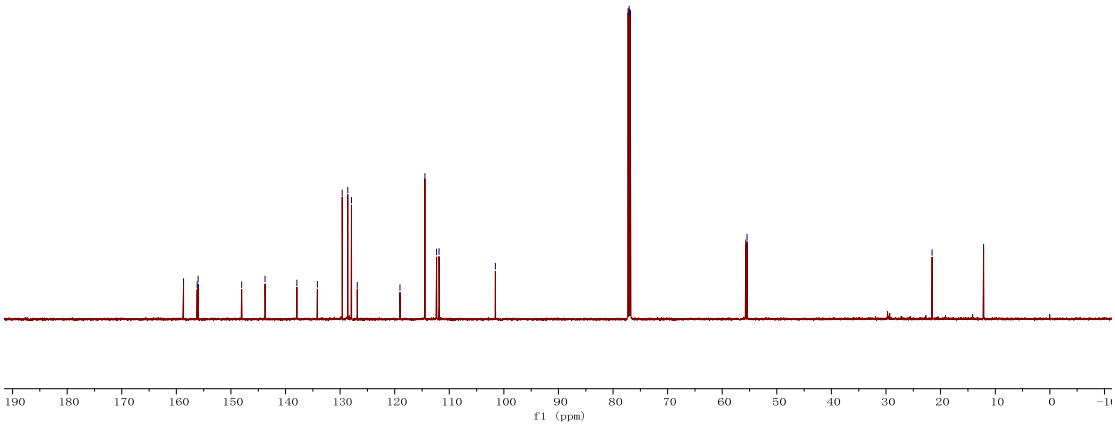

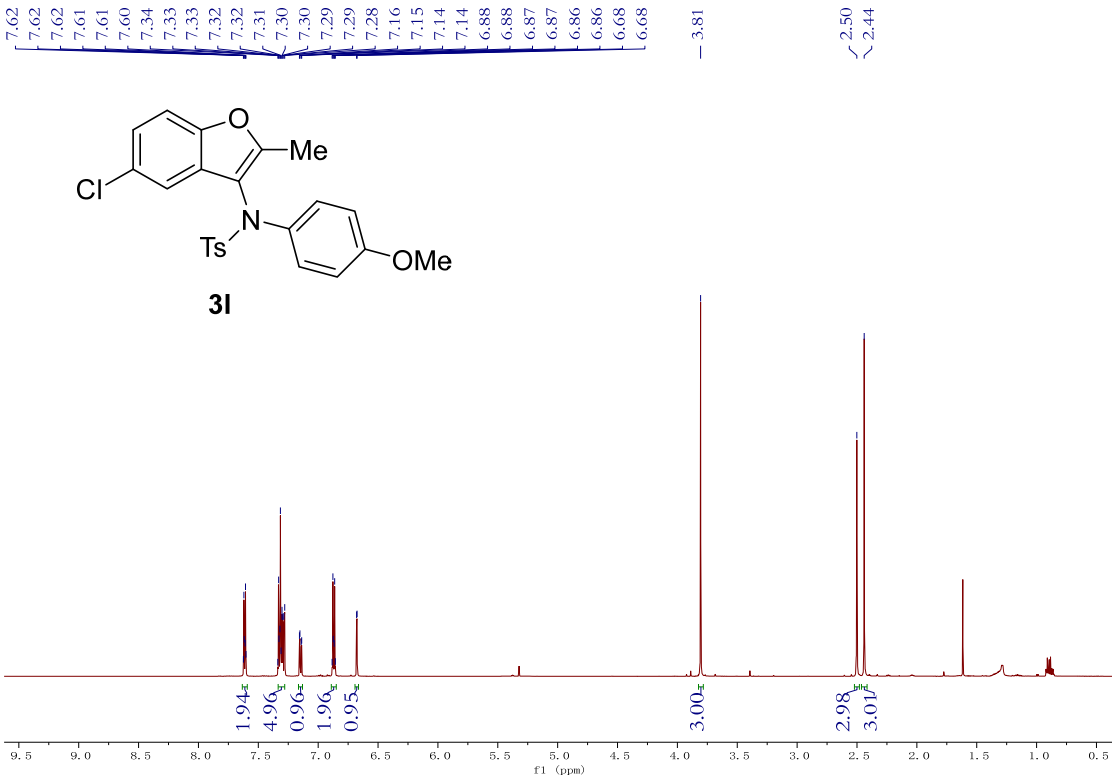
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7.62
7.61
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7.60
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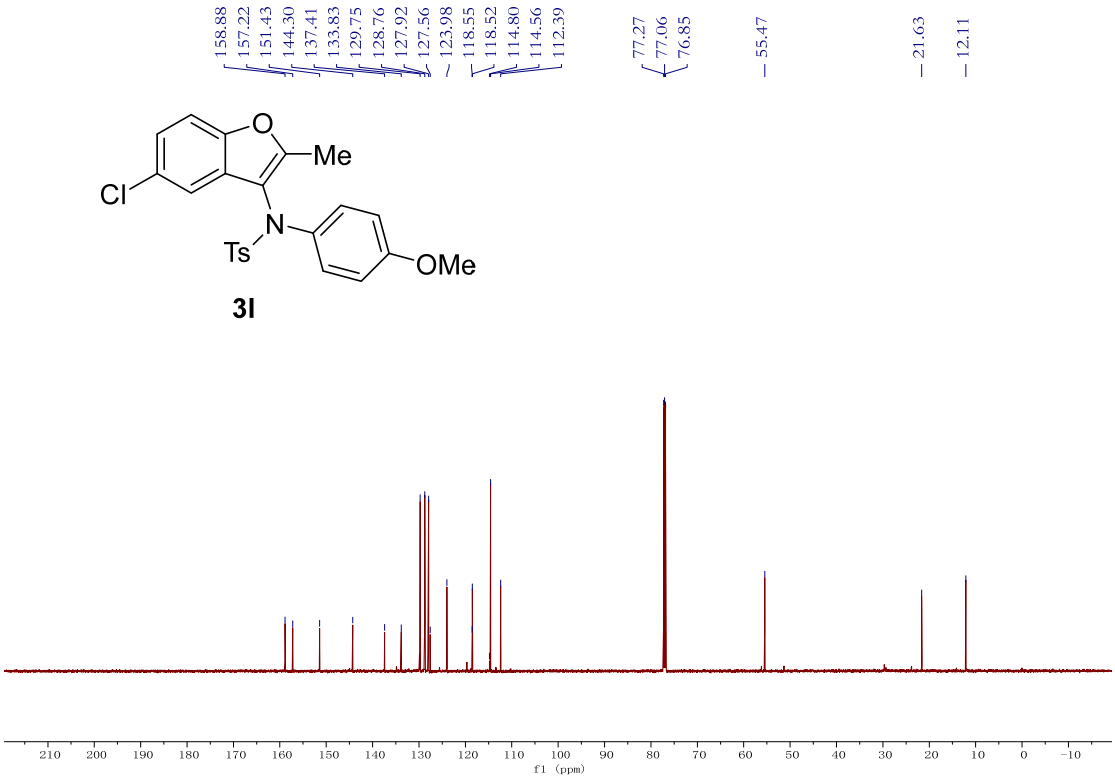
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.16
7.15
7.14
7.14
6.88
6.88
6.87
6.87
6.86
6.86
6.68
6.68
3.81
2.50
2.44
O
Me
Cl
N
Ts
OMe
1.94
4.96
0.96
1.96
0.95
3.00
2.98
3.01
f1 (ppm)

3l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128.76
127.92
127.56
123.98
118.55
118.52
114.80
114.56
112.39
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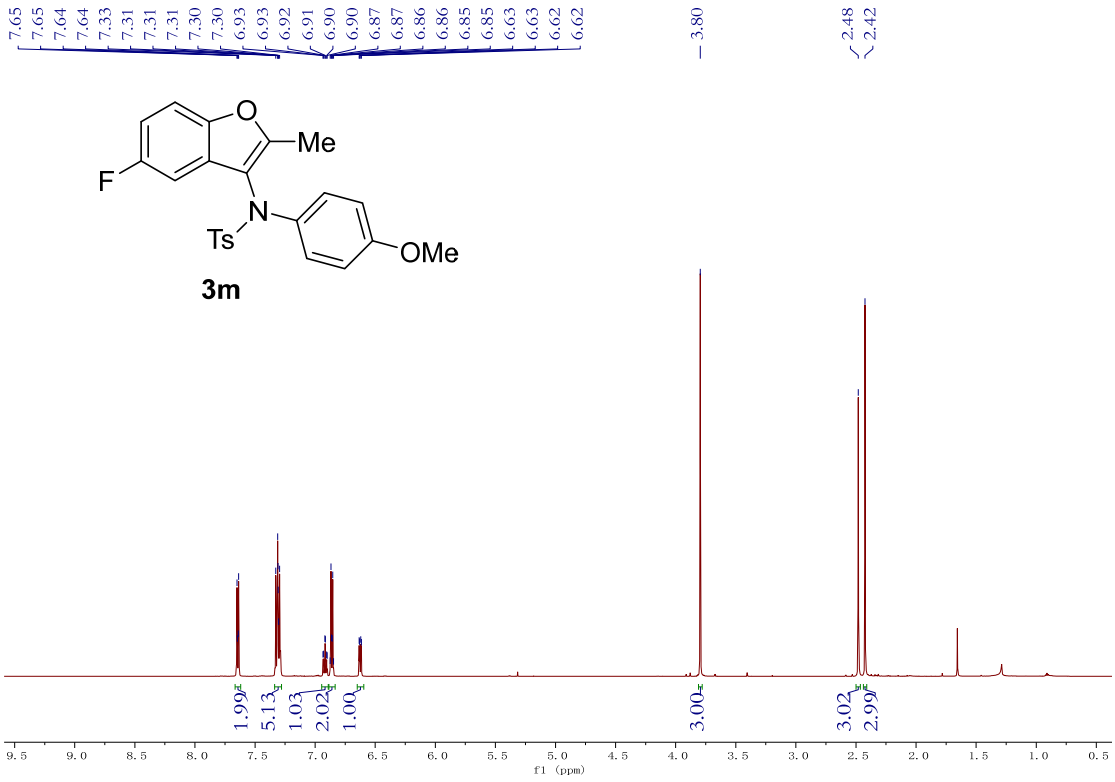
76.85
55.47
21.63
12.11
O
Me
Cl
N
Ts
OMe
f1 (ppm)

3l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7.65
7.64
7.64
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7.31
7.31
7.31
7.30
7.30
6.93
6.93
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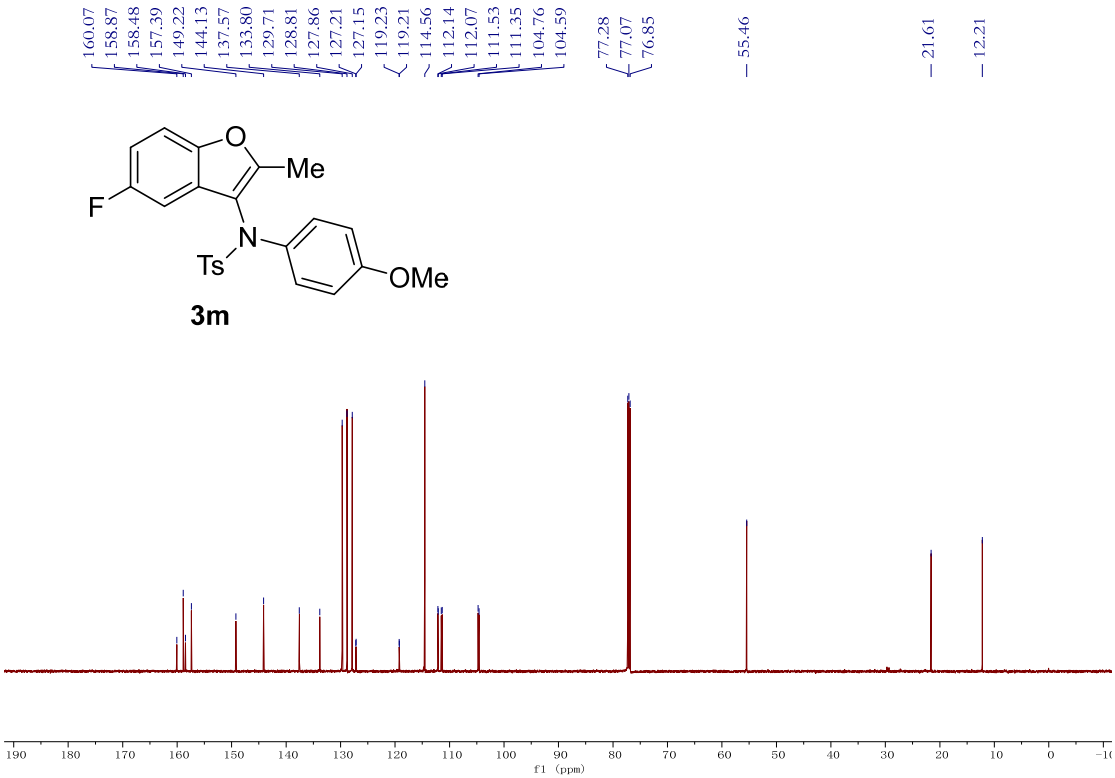
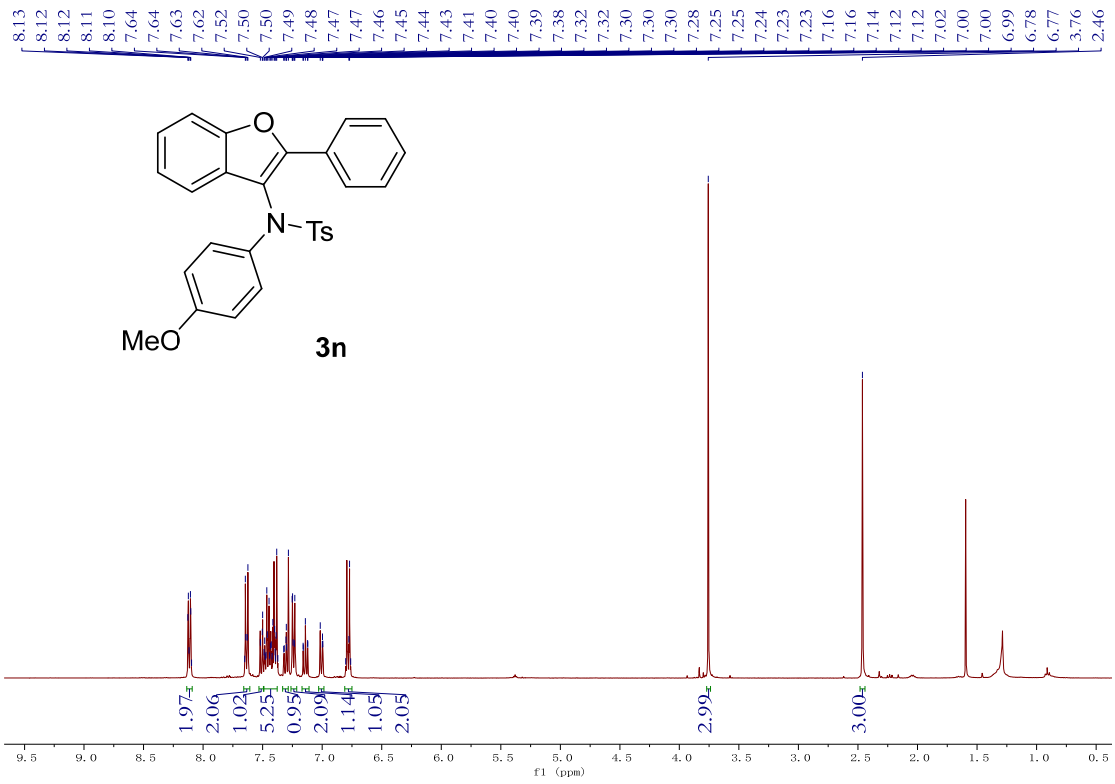
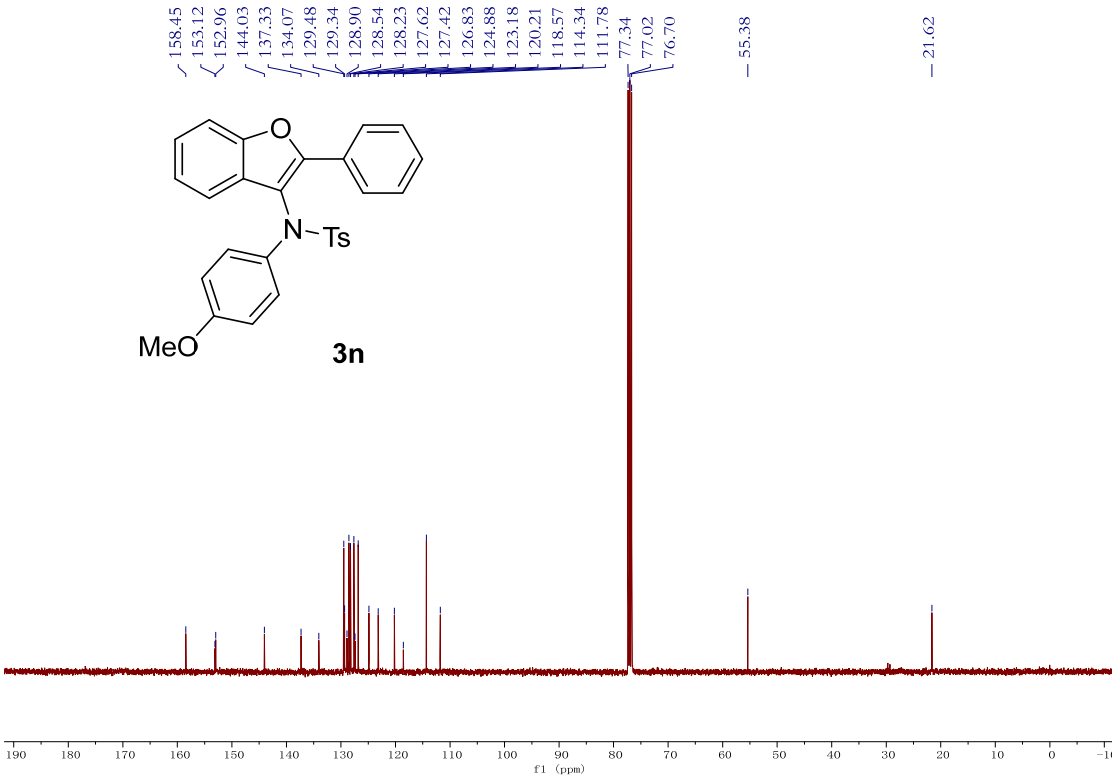
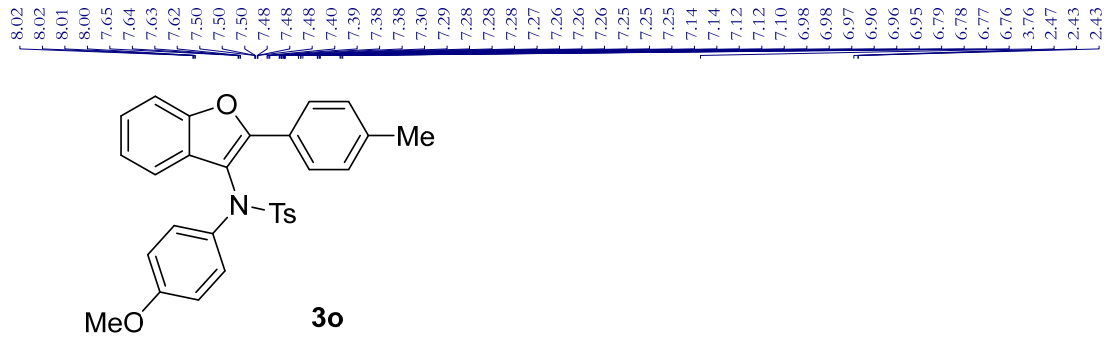
6.91
6.90
6.90
6.87
6.87
6.86
6.86
6.85
6.85
6.63
6.63
6.62
6.62
3.80
2.48
2.42
O
Me
F
N
Ts
OMe
3m
1.99
5.13
1.03
2.02
1.00
3.00
3.02
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


160.07
158.87
158.48
157.39
149.22
144.13
137.57
133.80
129.71
128.81
127.86
127.21
127.15
119.23
119.21
114.56
112.14
112.07
111.53
111.35
104.76
104.59
77.28
77.07
76.85
55.46
21.61
12.21
O
Me
F
N
Ts
OMe
3m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

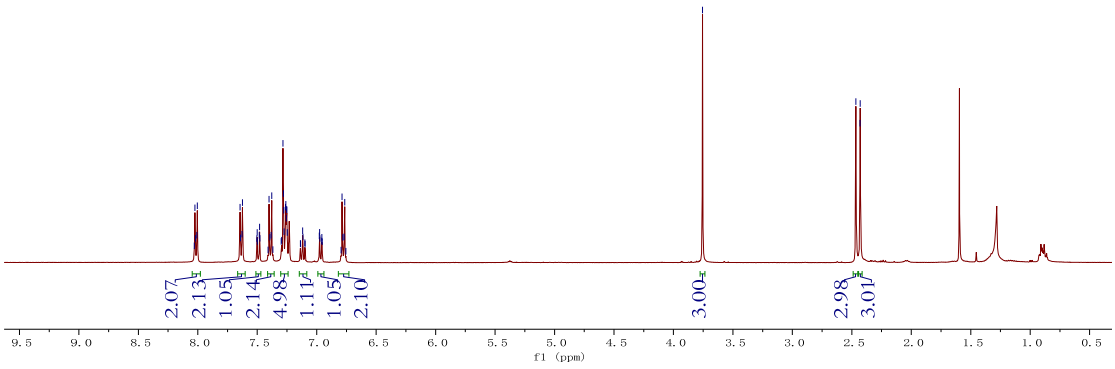

8.13 8.12 8.12 8.11 8.10 7.64 7.64 7.63 7.62 7.52 7.50 7.50 7.49 7.48 7.47 7.47 7.46 7.45 7.44 7.43 7.41 7.40 7.40 7.39 7.38 7.32 7.32 7.30 7.30 7.30 7.28 7.25 7.25 7.24 7.23 7.23 7.16 7.16 7.14 7.12 7.12 7.02 7.00 7.00 6.99 6.78 6.77 3.76 2.46
O
N
Ts
MeO
3n
1.97 2.06 1.02 5.25 0.95 2.09 1.14 1.05 2.05 2.99 3.00
f1 (ppm)

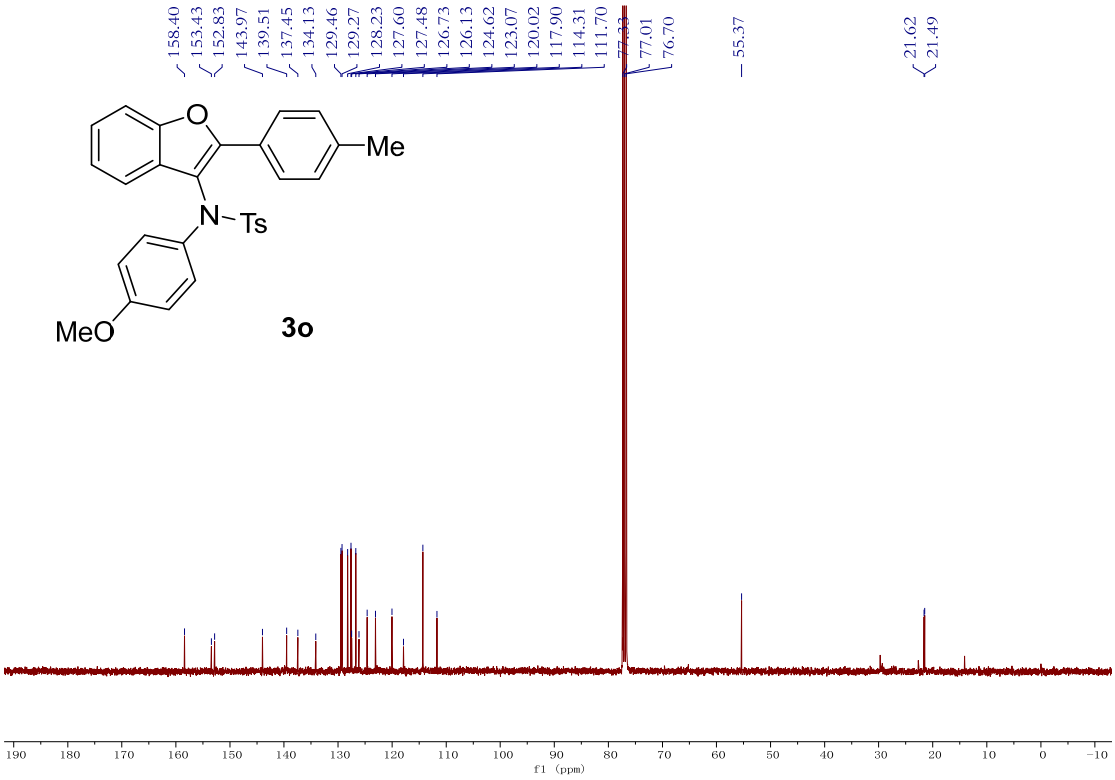

158.45 153.12 152.96 144.03 137.33 134.07 129.48 129.34 128.90 128.54 128.23 127.62 127.42 126.83 124.88 123.18 120.21 118.57 114.34 111.78 77.34 77.02 76.70 55.38 21.62
O
N
Ts
MeO
3n
f1 (ppm)


8.02 8.02 8.01 8.00 7.65 7.64 7.63 7.62 7.50 7.50 7.50 7.48 7.48 7.48 7.40 7.39 7.38 7.38 7.30 7.29 7.28 7.28 7.28 7.27 7.26 7.26 7.26 7.25 7.25 7.25 7.14 7.14 7.12 7.12 7.10 6.98 6.98 6.97 6.96 6.96 6.95 6.79 6.78 6.77 6.76 3.76 2.47 2.43 2.43

O
Me
N
Ts
MeO

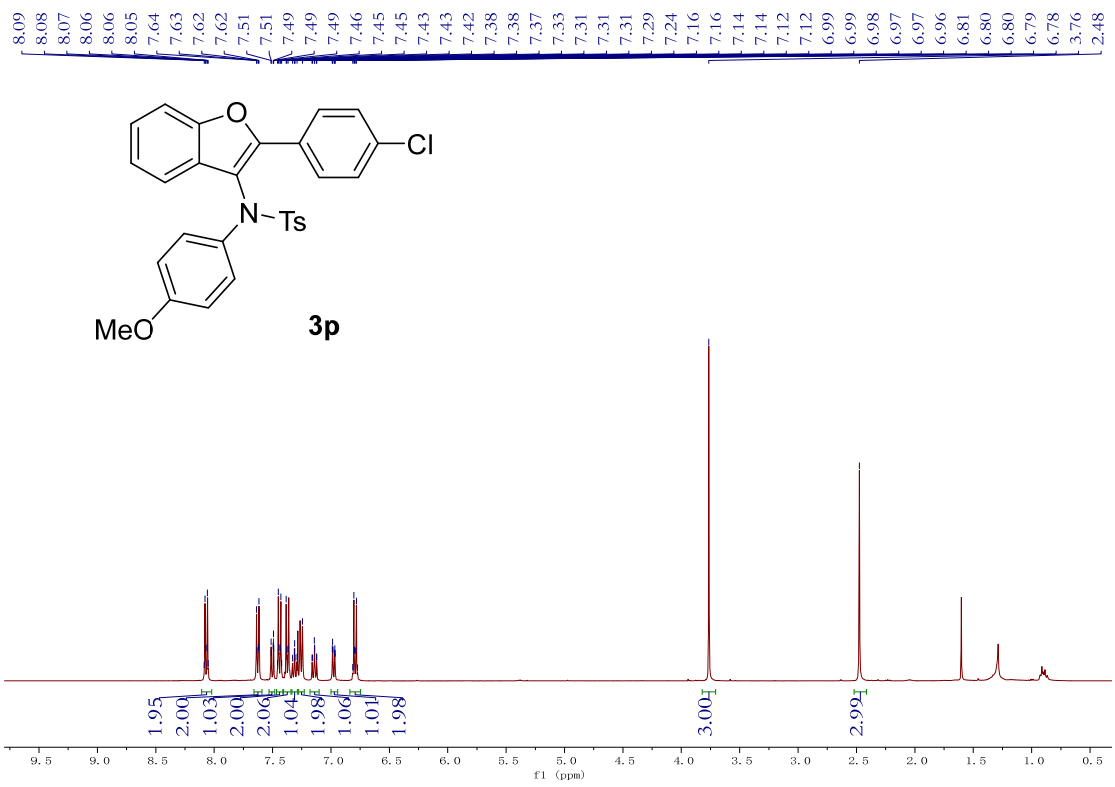
3o

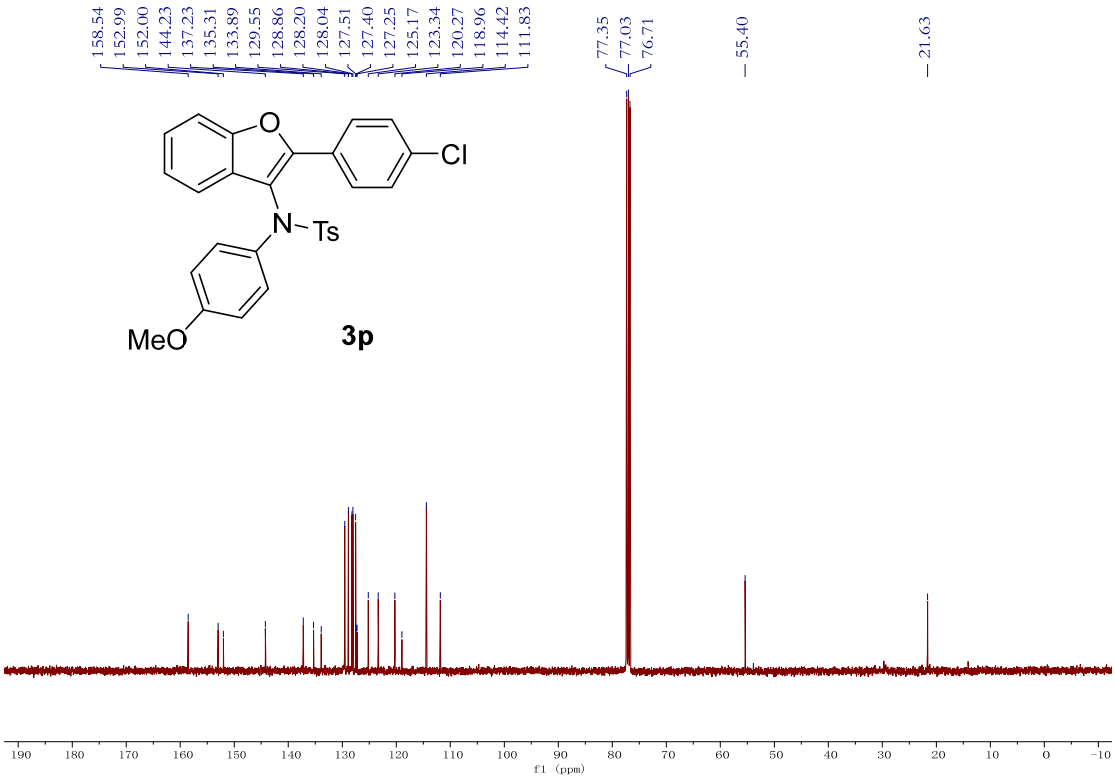

2.07 2.13 1.05 2.14 4.98 1.11 1.05 2.10 3.00 2.98 3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


158.40 153.43 152.83 143.97 139.51 137.45 134.13 129.46 129.27 128.23 127.60 127.48 126.73 126.13 124.62 123.07 120.02 117.90 114.31 111.70 77.33 77.01 76.70 55.37 21.62 21.49
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

O
Me
N
Ts
MeO

3o


8.09 8.08 8.07 8.06 8.06 8.05 7.64 7.63 7.62 7.62 7.51 7.51 7.49 7.49 7.49 7.46 7.45 7.45 7.43 7.43 7.42 7.38 7.38 7.37 7.33 7.31 7.31 7.31 7.29 7.24 7.16 7.16 7.14 7.14 7.12 7.12 6.99 6.99 6.98 6.97 6.97 6.96 6.81 6.80 6.80 6.79 6.78 3.76 2.48
O
Cl
N
Ts
MeO
3p
1.95 2.00 1.03 2.00 2.06 1.04 1.99 1.06 1.01 1.98 3.00 2.99
f1 (ppm)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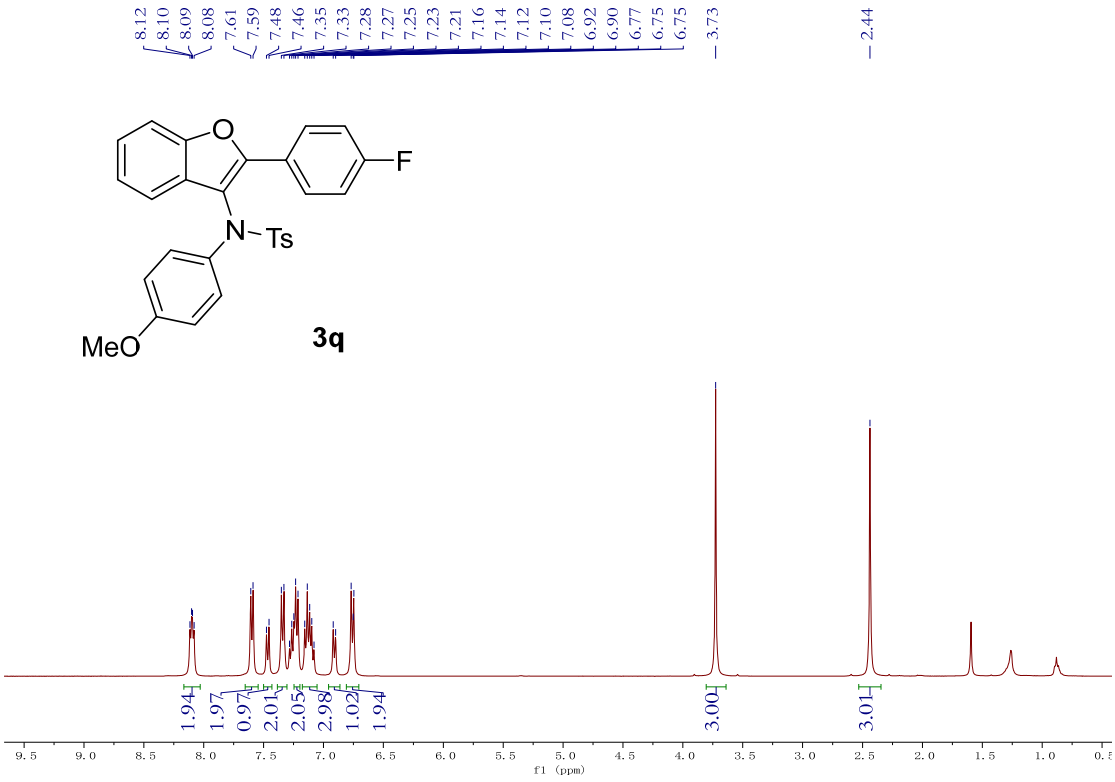
77.35 77.03 76.71
55.40
21.63
O
Cl
N
Ts
MeO
3p
f1 (ppm)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8.09
8.08
7.61
7.59
7.48
7.46
7.35
7.33
7.28
7.27
7.25
7.23
7.21
7.16
7.14
7.12
7.10
7.08
6.92
6.90
6.77
6.75
6.75
3.73
2.44
O
F
N
Ts
MeO
3q
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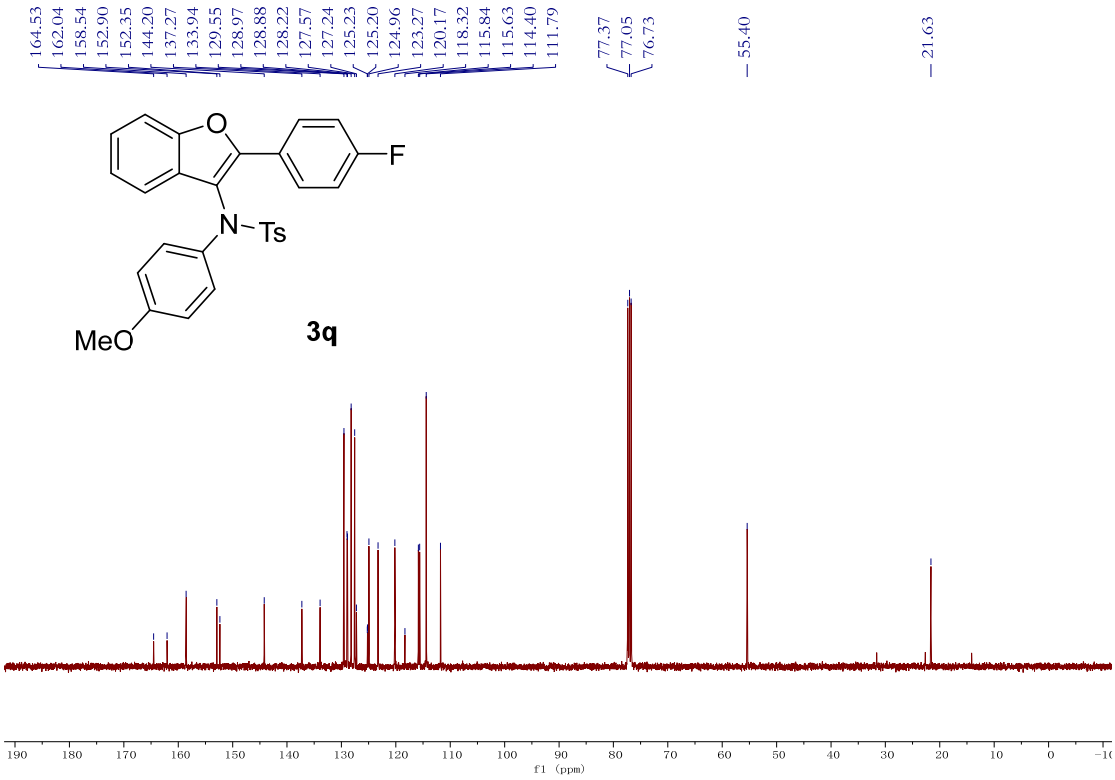
0.97
2.01
2.05
2.98
1.02
1.94
3.00
3.01
f1 (ppm)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128.88
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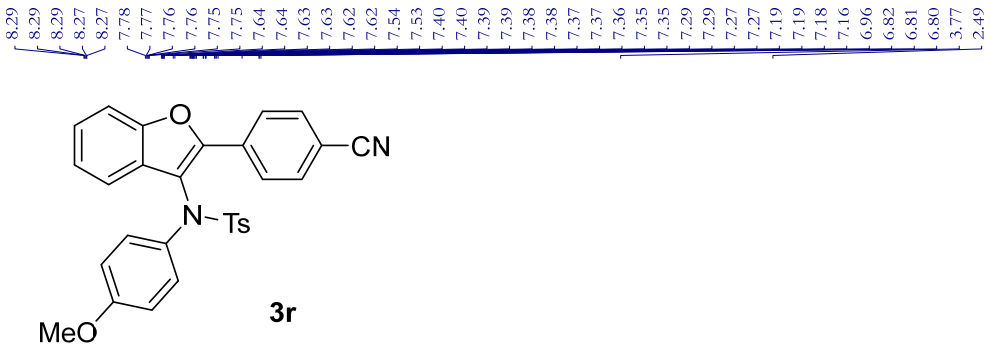
127.57
127.24
125.23
125.20
124.96
123.27
120.17
118.32
115.84
115.63
114.40
111.79
77.37
77.05
76.73
55.40
21.63
O
F
N
Ts
MeO
3q
f1 (ppm)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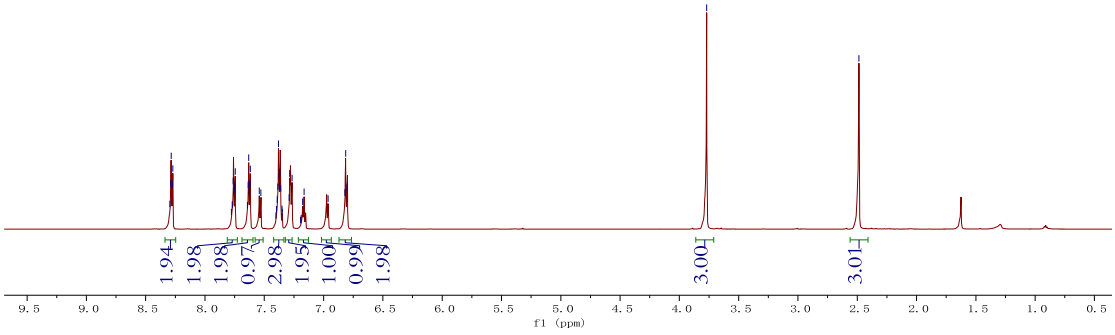
O
CN
N
Ts
MeO

3r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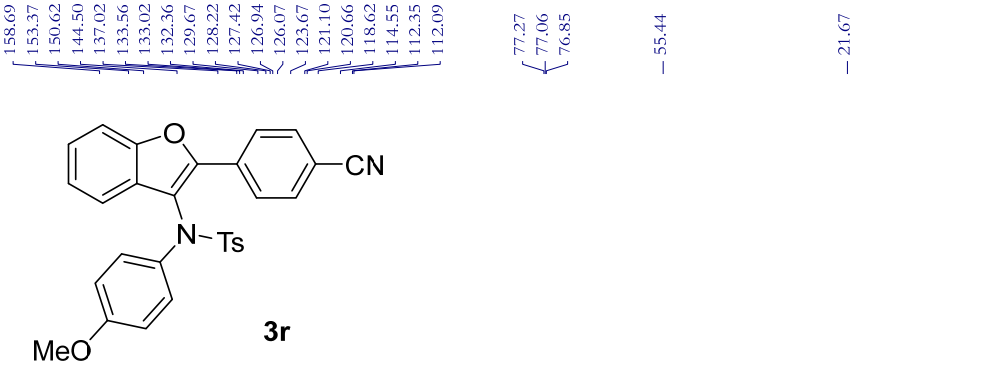
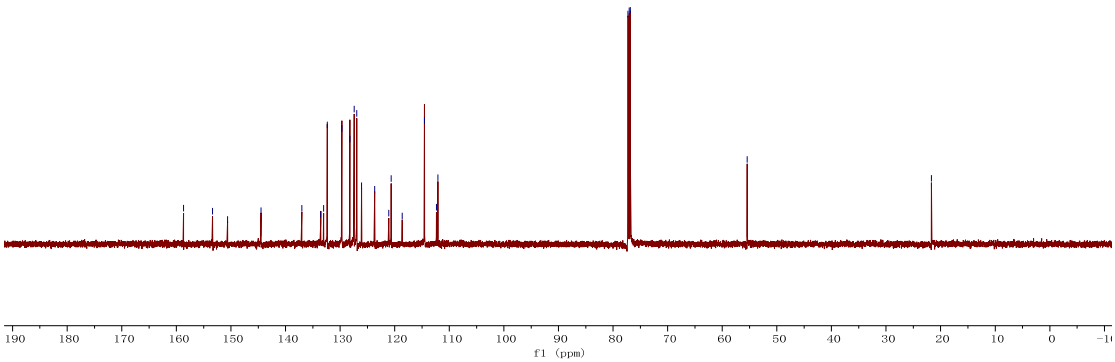
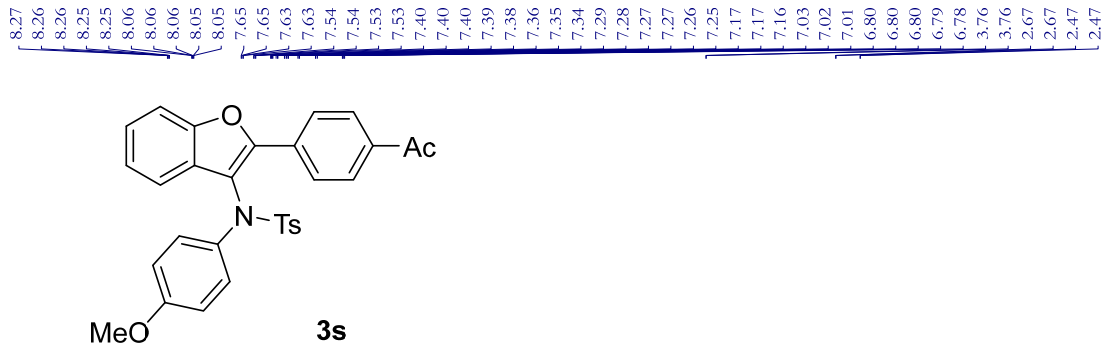
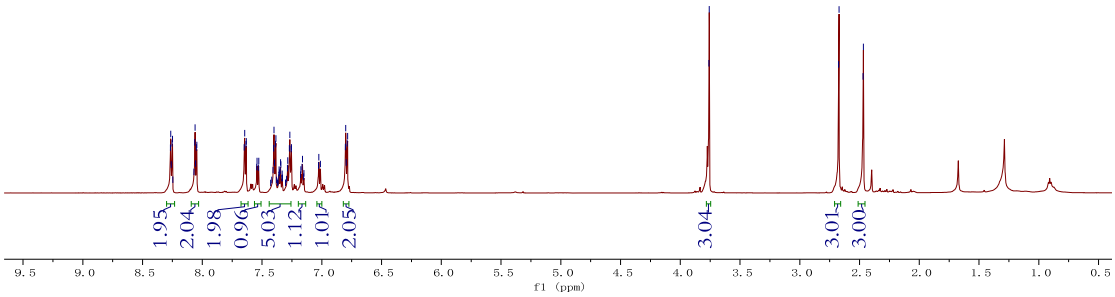
f1 (ppm)


158.69 153.37 150.62 144.50 137.02 133.56 133.02 132.36 129.67 128.22 127.42 126.94 126.07 123.67 121.10 120.66 118.62 114.55 112.35 112.09 77.27 77.06 76.85 55.44 21.67
O
CN
N
Ts
MeO

3r


f1 (ppm)


8.27 8.26 8.26 8.25 8.25 8.06 8.06 8.06 8.05 8.05 7.65 7.65 7.63 7.63 7.54 7.54 7.53 7.53 7.40 7.40 7.40 7.39 7.38 7.36 7.35 7.34 7.29 7.28 7.27 7.27 7.26 7.25 7.17 7.17 7.16 7.03 7.02 7.01 6.80 6.80 6.79 6.78 3.76 3.76 2.67 2.47 2.47
O
Ac
N
Ts
MeO
3s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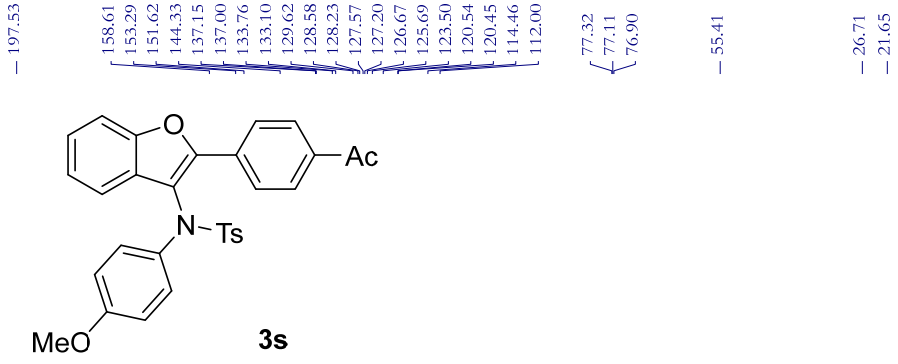
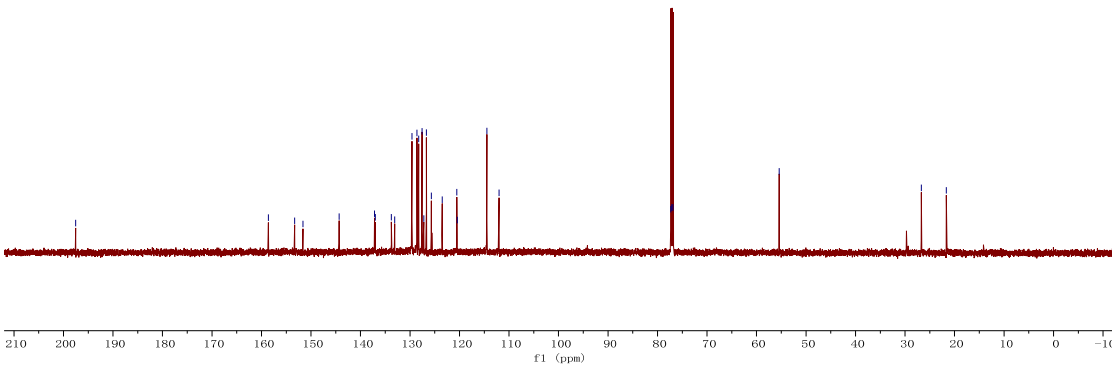
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


197.53
158.61 153.29 151.62 144.33 137.15 137.00 133.76 133.10 129.62 128.58 128.23 127.57 127.20 126.67 125.69 123.50 120.54 120.45 114.46 112.00
77.32 77.11 76.90
55.41
26.71 21.65
O
Ac
N
Ts
MeO
3s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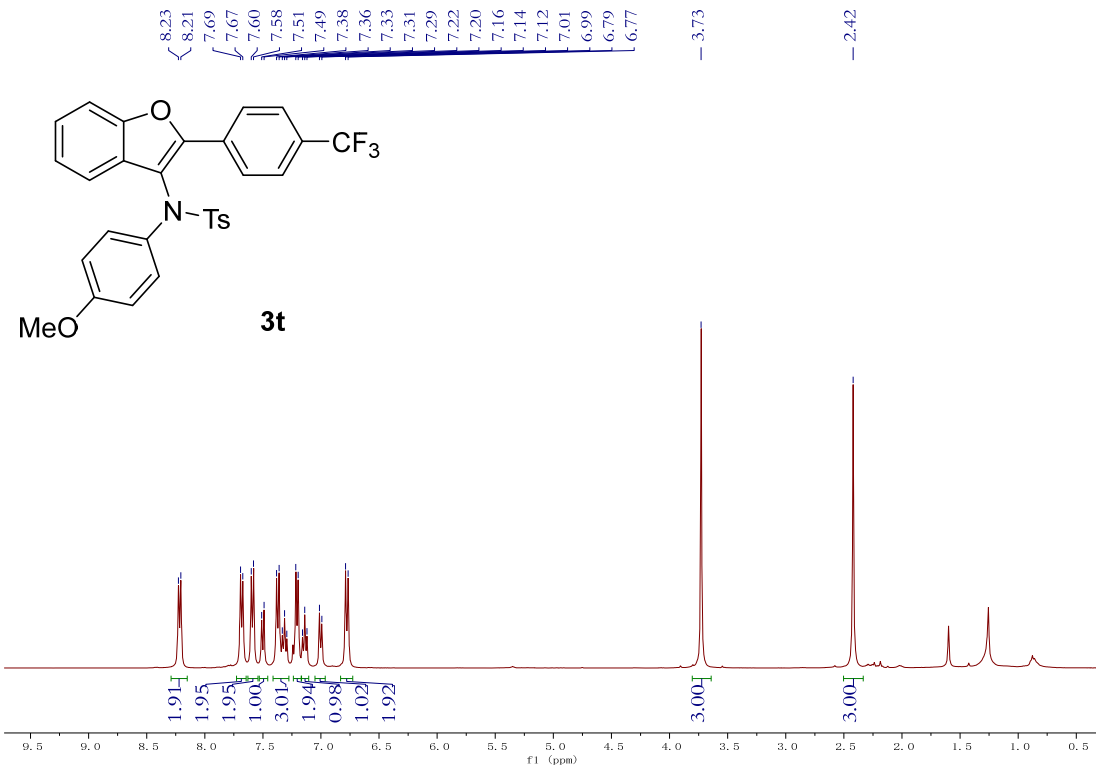
f1 (ppm)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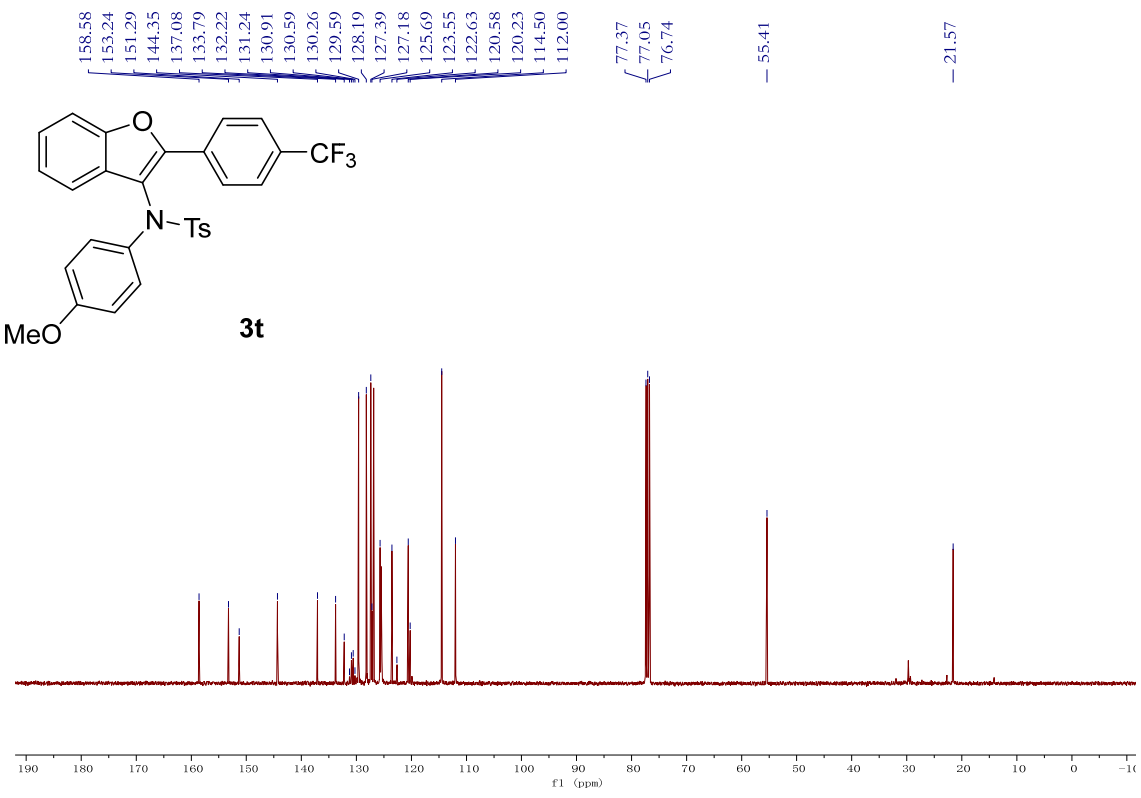
7.51
7.49
7.38
7.36
7.33
7.31
7.29
7.22
7.20
7.16
7.14
7.12
7.01
6.99
6.79
6.77
3.73
2.42
O
CF3
N
Ts
MeO
3t
1.91
1.95
1.95
1.00
3.01
1.94
0.98
1.02
1.92
3.00
3.00
f1 (ppm)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132.22
131.24
130.91
130.59
130.26
129.59
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127.39
127.18
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122.63
120.58
120.23
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77.05
76.74
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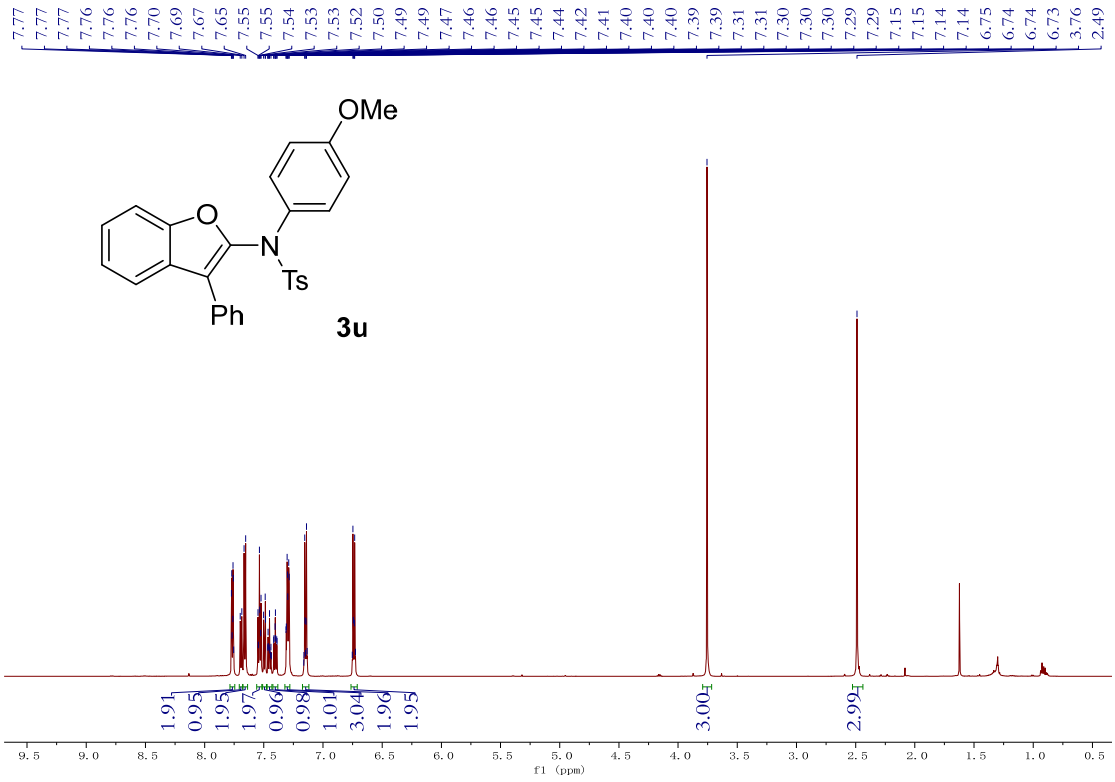
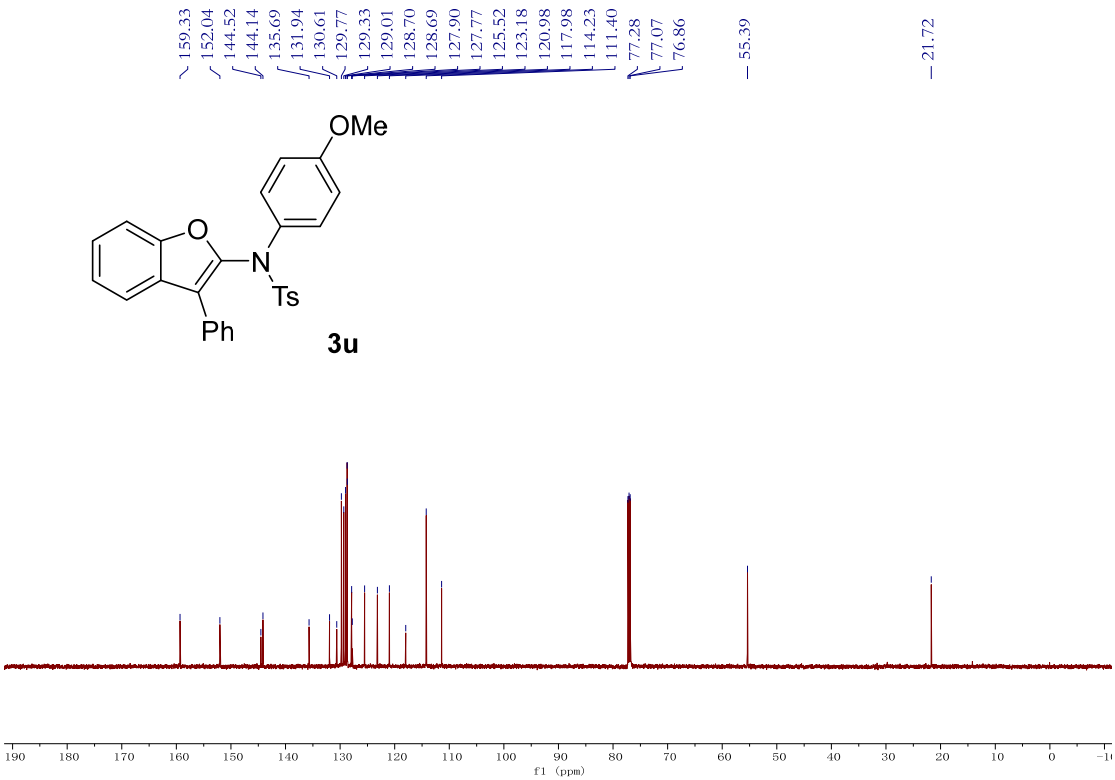
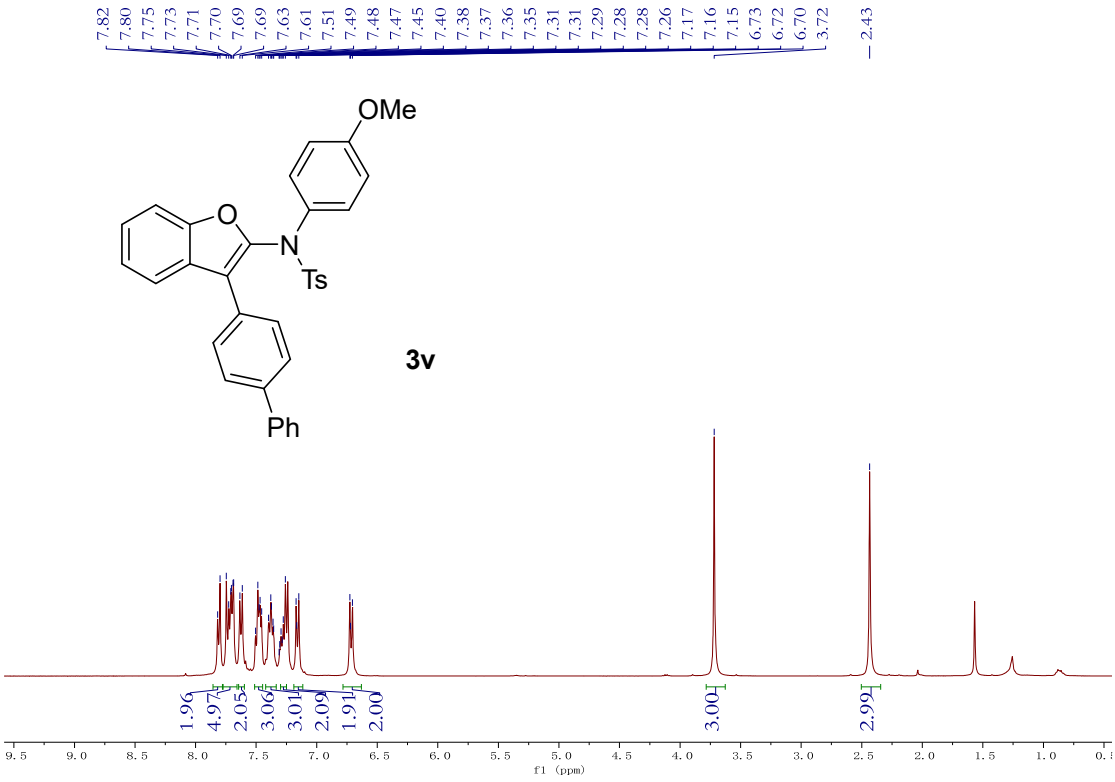
21.57
O
CF3
N
Ts
MeO
3t
f1 (ppm)


7.77 7.77 7.77 7.76 7.76 7.76 7.70 7.69 7.67 7.65 7.55 7.55 7.54 7.53 7.53 7.52 7.50 7.49 7.49 7.47 7.46 7.46 7.45 7.45 7.44 7.42 7.41 7.40 7.40 7.40 7.39 7.39 7.31 7.31 7.30 7.30 7.30 7.29 7.29 7.15 7.15 7.14 7.14 6.75 6.74 6.74 6.73 3.76 2.49
OMe
O
N
Ts
Ph
3u
1.91 0.95 1.95 1.97 0.99 0.98 1.01 3.04 1.96 1.95 3.00 2.99
f1 (ppm)


159.33 152.04 144.52 144.14 135.69 131.94 130.61 129.77 129.33 129.01 128.70 128.69 127.90 127.77 125.52 123.18 120.98 117.98 114.23 111.40 77.28 77.07 76.86 55.39 21.72
OMe
O
N
Ts
Ph
3u
f1 (ppm)


7.82
7.80
7.75
7.73
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7.70
7.69
7.69
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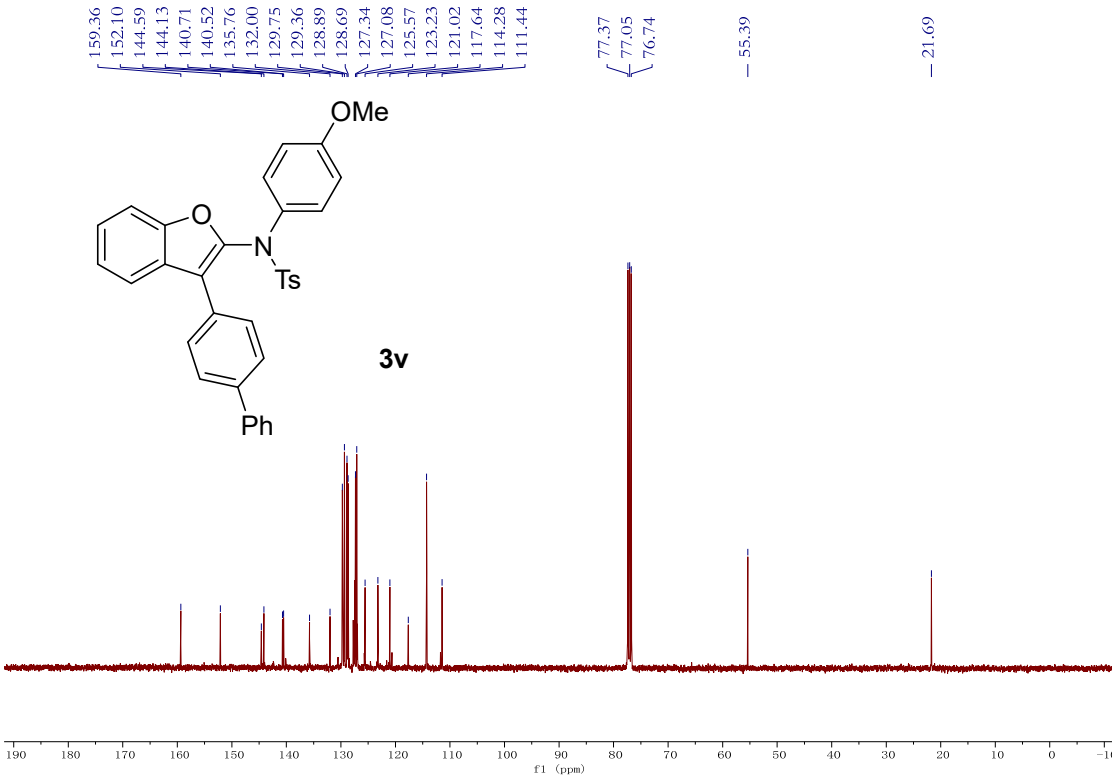
7.61
7.51
7.49
7.48
7.47
7.45
7.40
7.38
7.37
7.36
7.35
7.31
7.31
7.29
7.28
7.28
7.26
7.17
7.16
7.15
6.73
6.72
6.70
3.72
2.43
OMe
O
N
Ts
Ph
3v
1.96
4.97
2.05
3.06
3.01
2.09
1.91
2.00
3.00
2.99
f1 (ppm)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144.59
144.13
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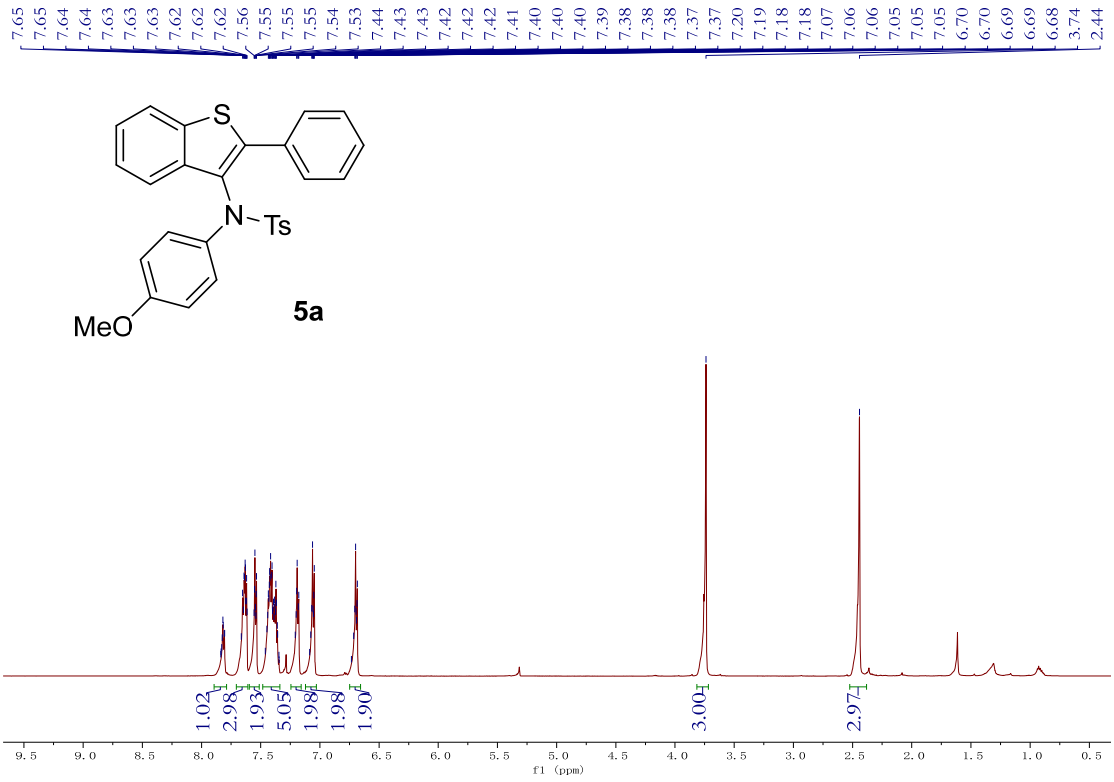
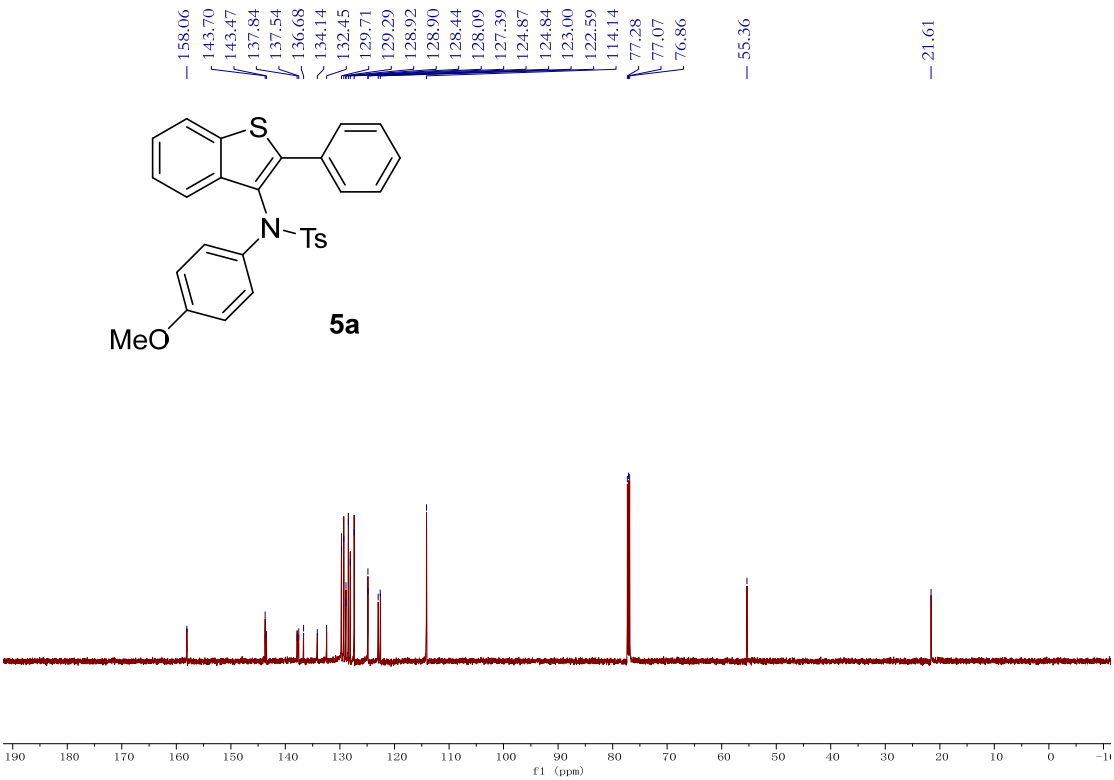
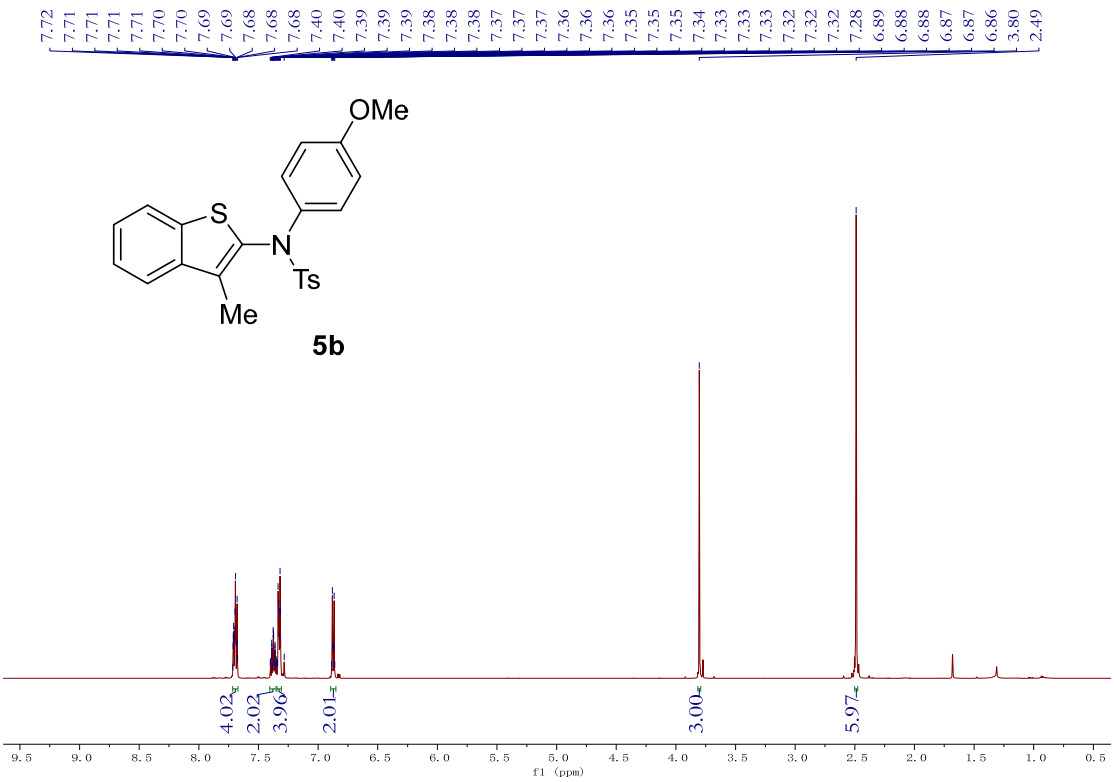
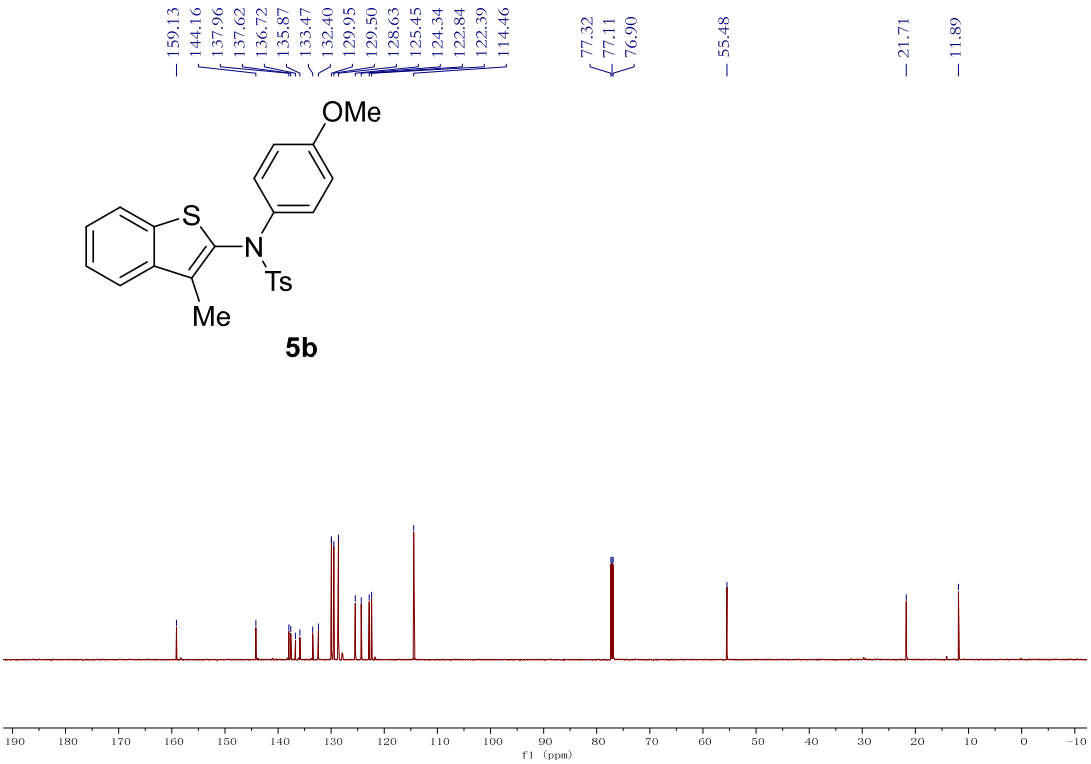
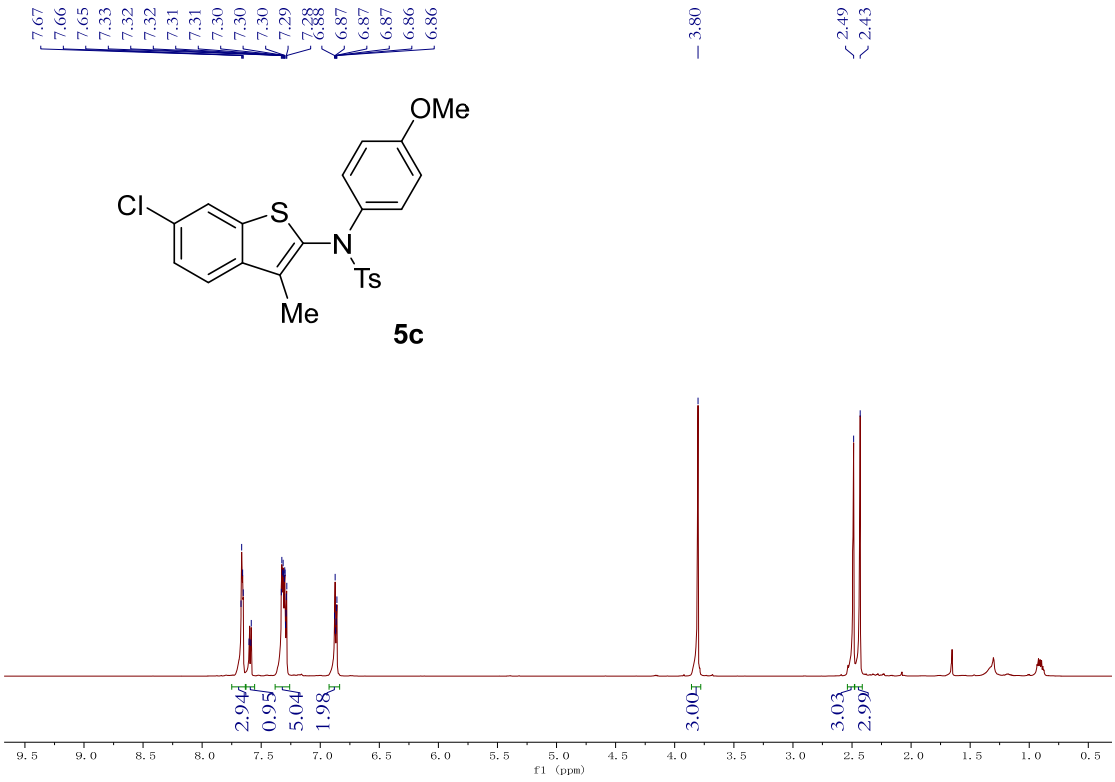
140.52
135.76
132.00
129.75
129.36
128.89
128.69
127.34
127.08
125.57
123.23
121.02
117.64
114.28
111.44
77.37
77.05
76.74
55.39
21.69
OMe
O
N
Ts
Ph
3v
f1 (ppm)


7.65 7.65 7.64 7.64 7.63 7.63 7.63 7.62 7.62 7.62 7.56 7.55 7.55 7.55 7.54 7.53 7.44 7.43 7.43 7.42 7.42 7.42 7.41 7.40 7.40 7.40 7.39 7.38 7.38 7.38 7.37 7.37 7.20 7.19 7.18 7.18 7.07 7.06 7.06 7.05 7.05 7.05 6.70 6.70 6.69 6.69 6.68 3.74 2.44
S
N
Ts
MeO
5a
1.02 2.98 1.93 5.05 1.98 1.98 1.90 3.00 2.97
f1 (ppm)


158.06 143.70 143.47 137.84 137.54 136.68 134.14 132.45 129.71 129.29 128.92 128.90 128.44 128.09 127.39 124.87 124.84 123.00 122.59 114.14 77.28 77.07 76.86 55.36 21.61
S
N
Ts
MeO
5a
f1 (ppm)


7.72 7.71 7.71 7.71 7.71 7.70 7.70 7.69 7.69 7.68 7.68 7.68 7.40 7.40 7.39 7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.37 7.36 7.36 7.36 7.35 7.35 7.35 7.34 7.33 7.33 7.33 7.32 7.32 7.32 7.28 6.89 6.88 6.88 6.87 6.87 6.86 3.80 2.49
OMe
S
N
Ts
Me
5b
4.02 2.02 3.98 2.01 3.00 5.97
f1 (ppm)


159.13 144.16 137.96 137.62 136.72 135.87 133.47 132.40 129.95 129.50 128.63 125.45 124.34 122.84 122.39 114.46
77.32 77.11 76.90
55.48
21.71
11.89
OMe
S
N
Ts
Me
5b
f1 (ppm)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7.66
7.65
7.33
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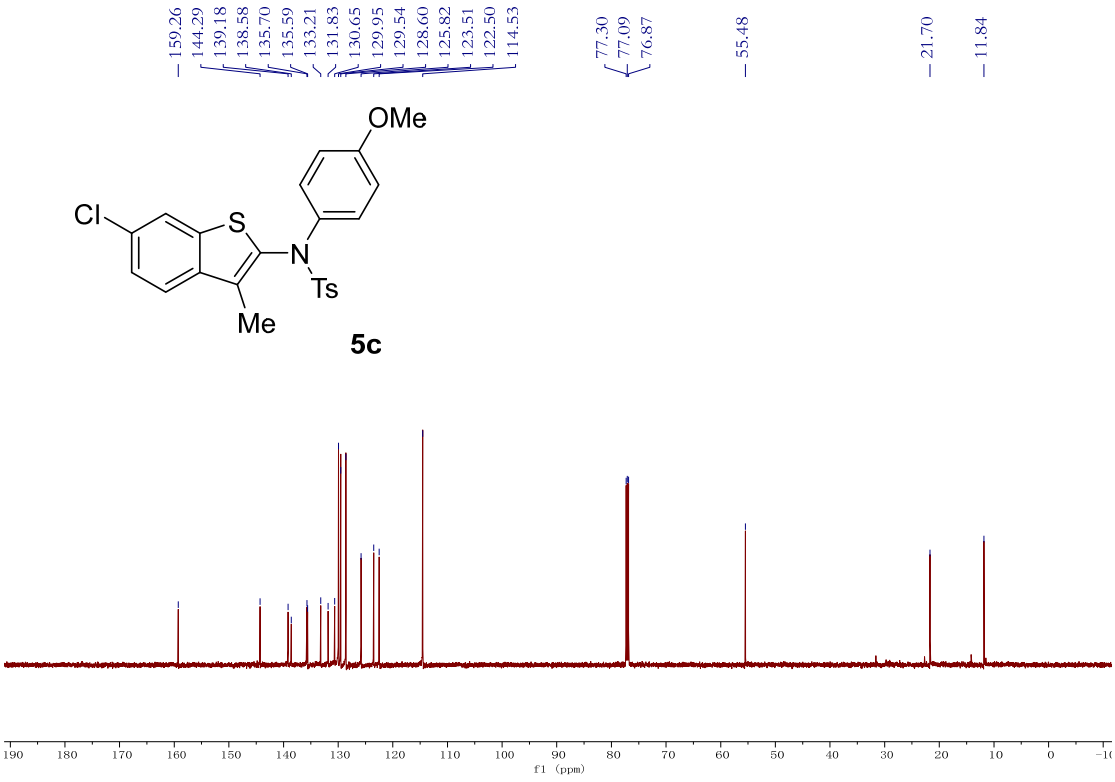
7.32
7.31
7.31
7.30
7.30
7.30
7.29
7.28
6.88
6.87
6.87
6.86
6.86
3.80
2.49
2.43
OMe
Cl
S
N
Ts
Me
5c
2.94
0.95
5.04
1.98
3.00
3.03
2.99
f1 (ppm)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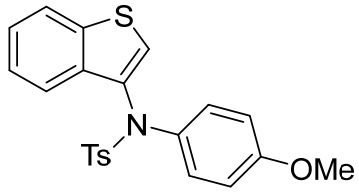
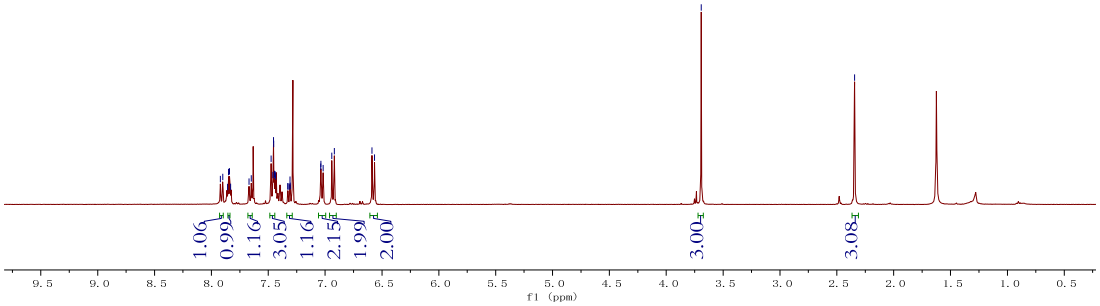
144.29
139.18
138.58
135.70
135.59
133.21
131.83
130.65
129.95
129.54
128.60
125.82
123.51
122.50
114.53
77.30
77.09
76.87
55.48
21.70
11.84
OMe
Cl
S
N
Ts
Me
5c
f1 (ppm)


7.92
7.90
7.86
7.85
7.84
7.83
7.67
7.65
7.48
7.46
7.45
7.45
7.45
7.44
7.44
7.44
7.33
7.33
7.31
7.31
7.31
7.04
7.04
7.02
6.94
6.92
6.59
6.57
3.69
2.34


S
N
Ts
OMe

5d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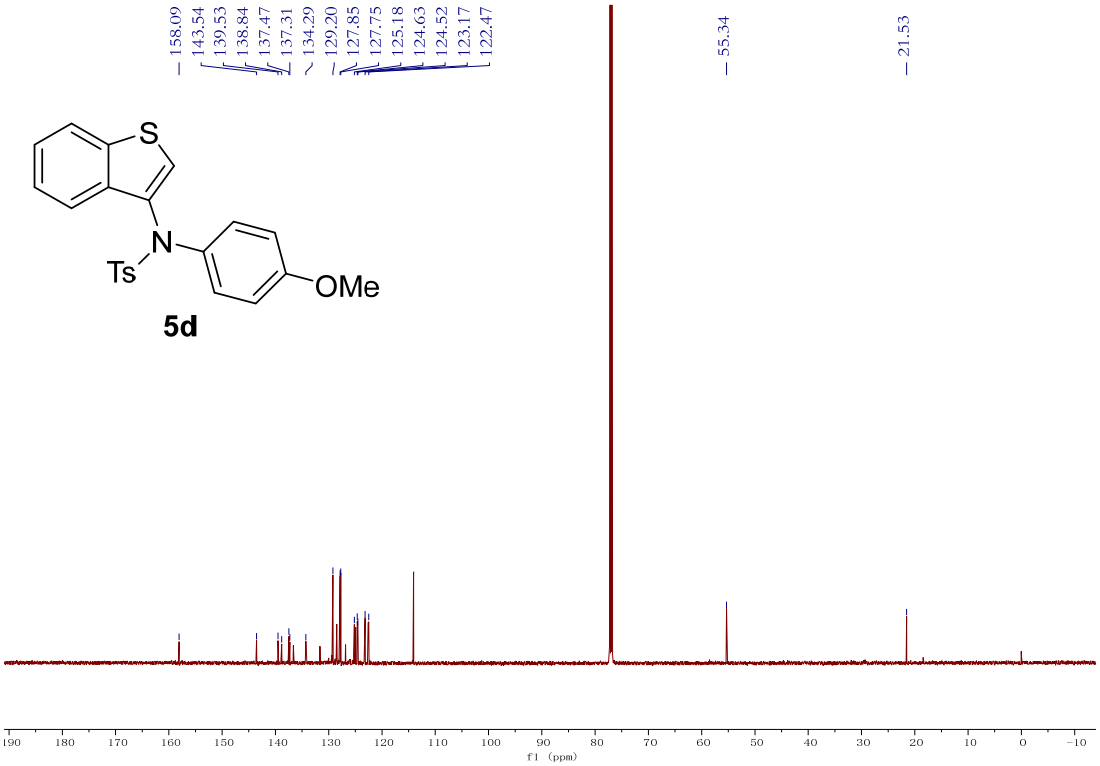
0.99
1.16
3.05
1.16
2.15
1.99
2.00
3.00
3.08
f1 (ppm)


158.09
143.54
139.53
138.84
137.47
137.31
134.29
129.20
127.85
127.75
125.18
124.63
124.52
123.17
122.47
55.34
21.53
f1 (ppm)

S
N
Ts
OMe

5d


7.88
7.87
7.87
7.86
7.85
7.85
7.85
7.80
7.80
7.80
7.79
7.78
7.78
7.78
7.66
7.65
7.64
7.64
7.63
7.41
7.39
7.39
7.38
7.38
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.31
7.29
7.28
7.27
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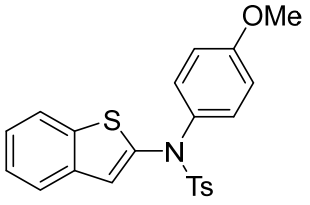
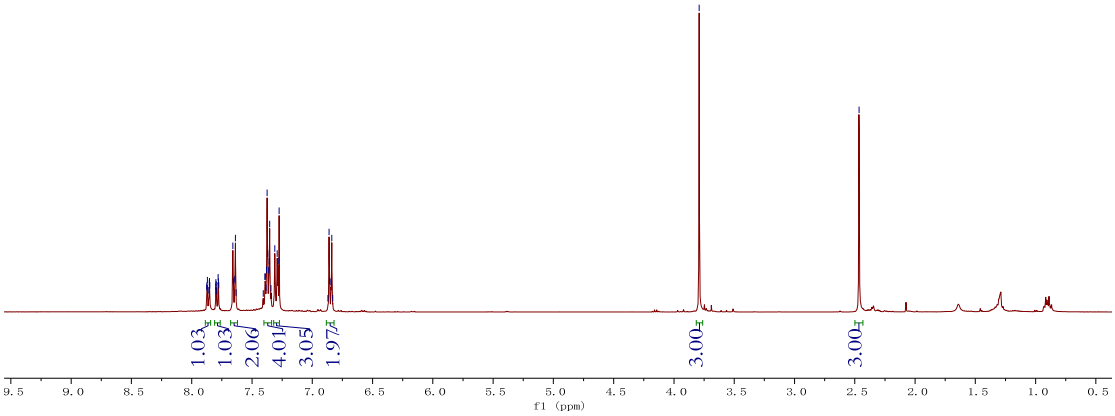
6.86
6.86
6.84
6.84
6.83
3.79
2.46


OMe
S
N
Ts

5d'


1.03
1.03
2.06
4.01
3.05
1.97
3.00
3.00
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)


158.87
143.83
137.93
136.70
136.35
133.69
133.14
129.55
129.51
128.09
125.13
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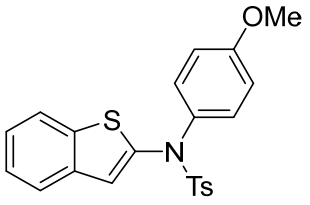
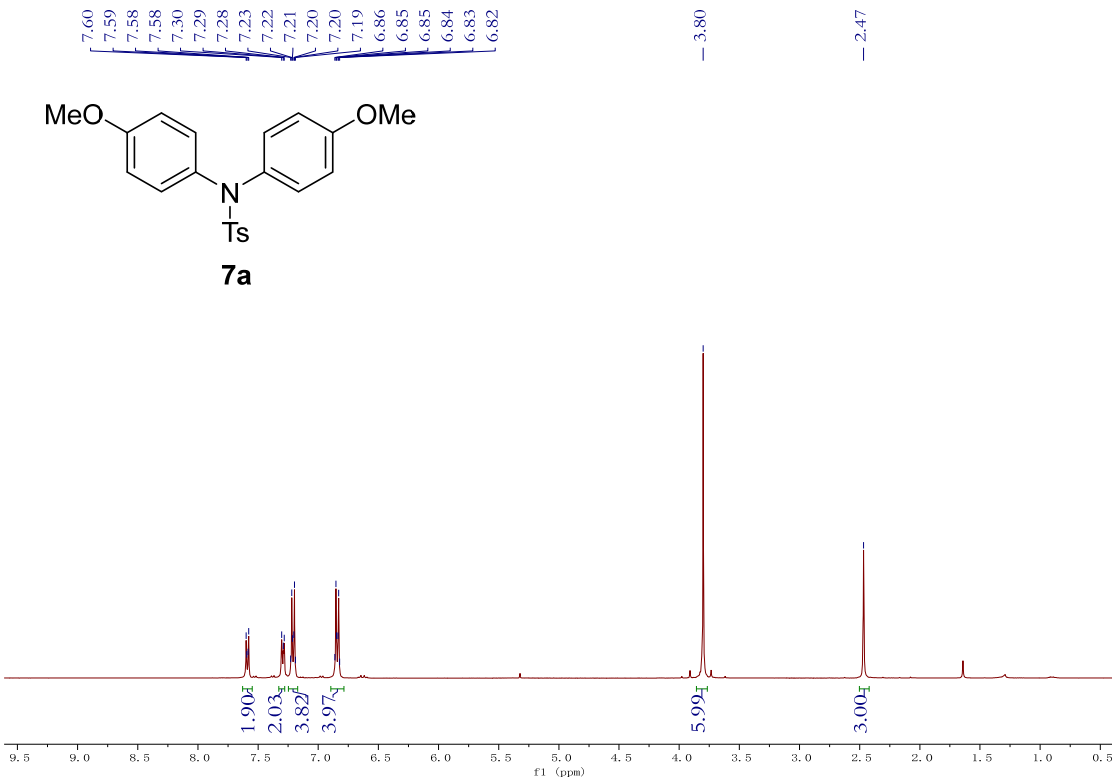
123.86
122.82
122.08
114.33
77.36
77.04
76.72
55.45
21.62


OMe
S
N
Ts

5d'

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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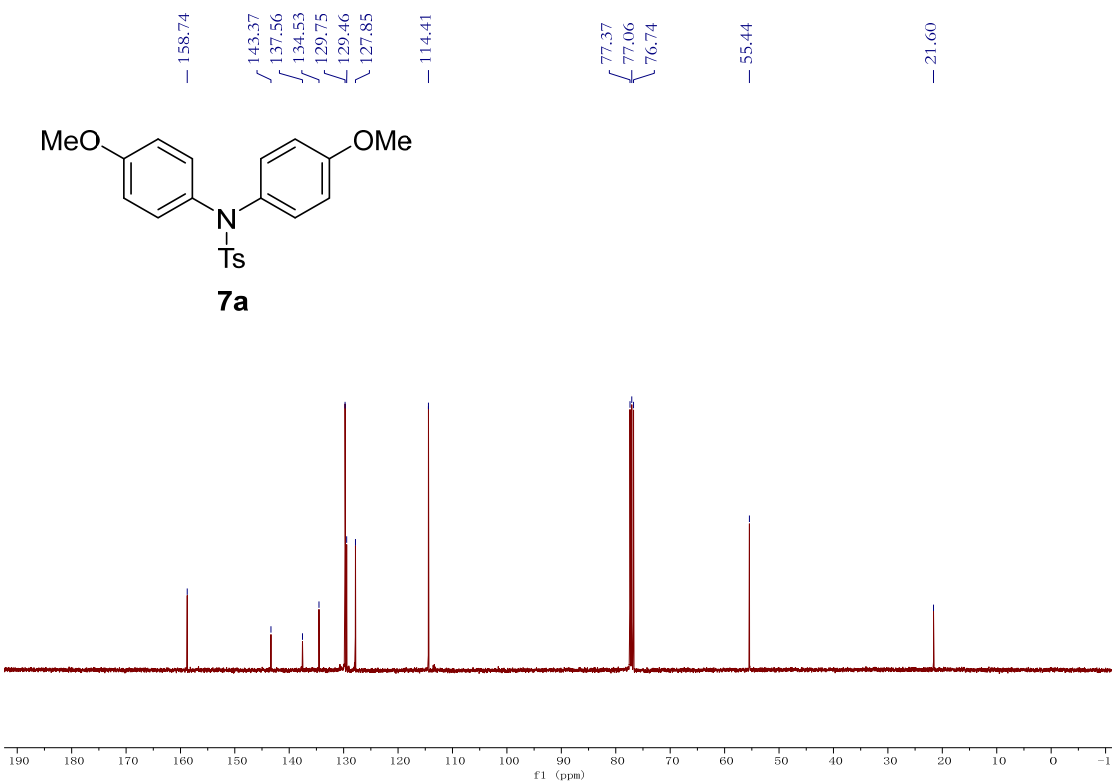
7.59
7.58
7.58
7.30
7.29
7.28
7.23
7.22
7.21
7.20
7.20
7.19
6.86
6.85
6.85
6.84
6.83
6.82
3.80
2.47
MeO
OMe
N
Ts
1.90
2.03
3.82
3.97
5.99
3.00
f1 (ppm)

7a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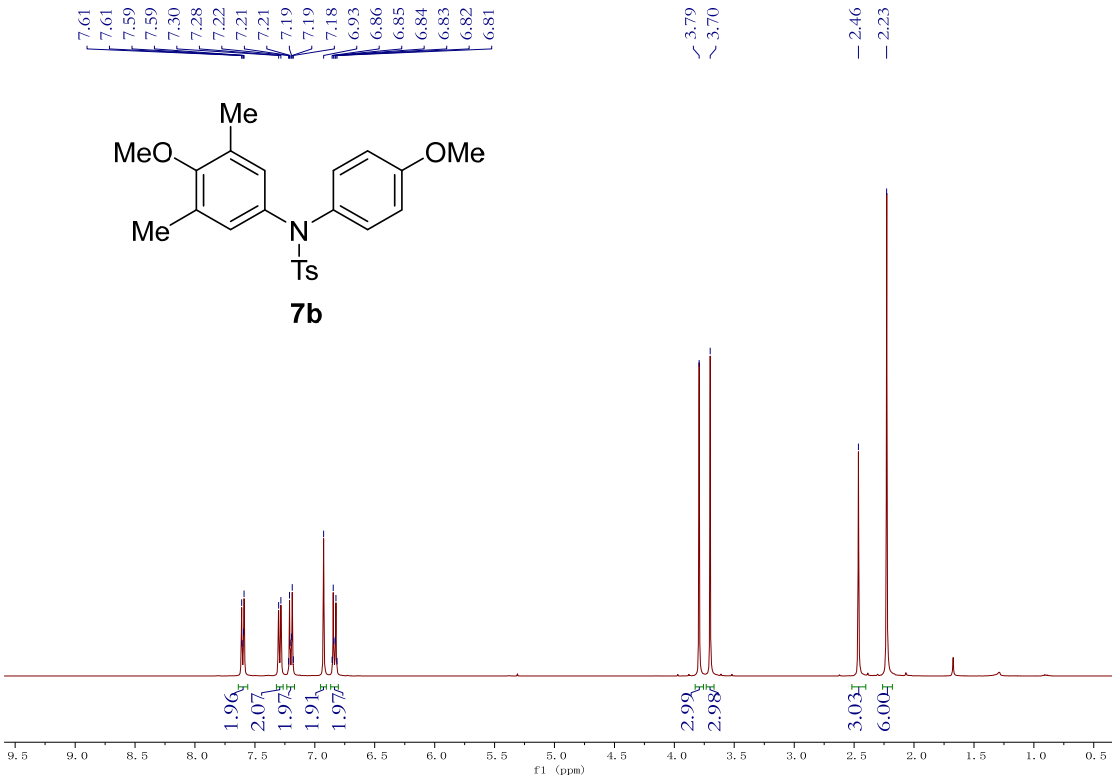
143.37
137.56
134.53
129.75
129.46
127.85
114.41
77.37
77.06
76.74
55.44
21.60
MeO
OMe
N
Ts
f1 (ppm)

7a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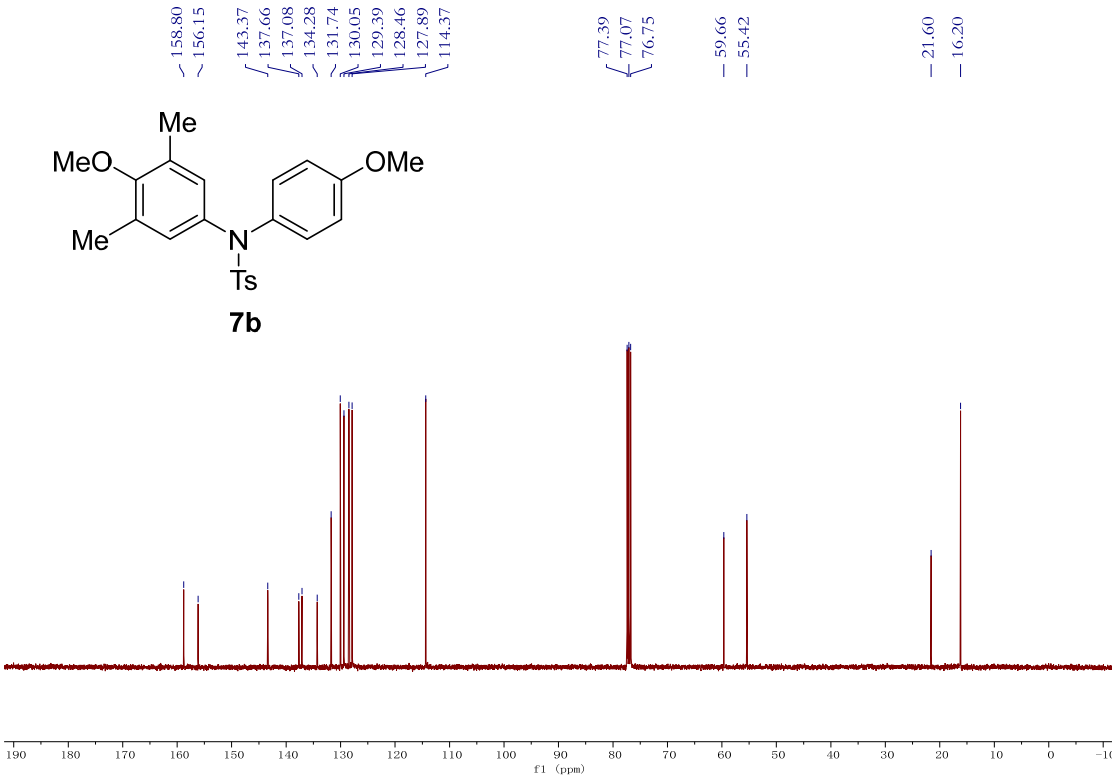
7.61
7.59
7.59
7.30
7.28
7.22
7.21
7.21
7.19
7.19
7.18
6.93
6.86
6.85
6.84
6.83
6.82
6.81
3.79
3.70
2.46
2.23
Me
MeO
OMe
Me
N
Ts
1.96
2.07
1.97
1.91
1.97
2.99
2.98
3.03
6.00
f1 (ppm)

7b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156.15
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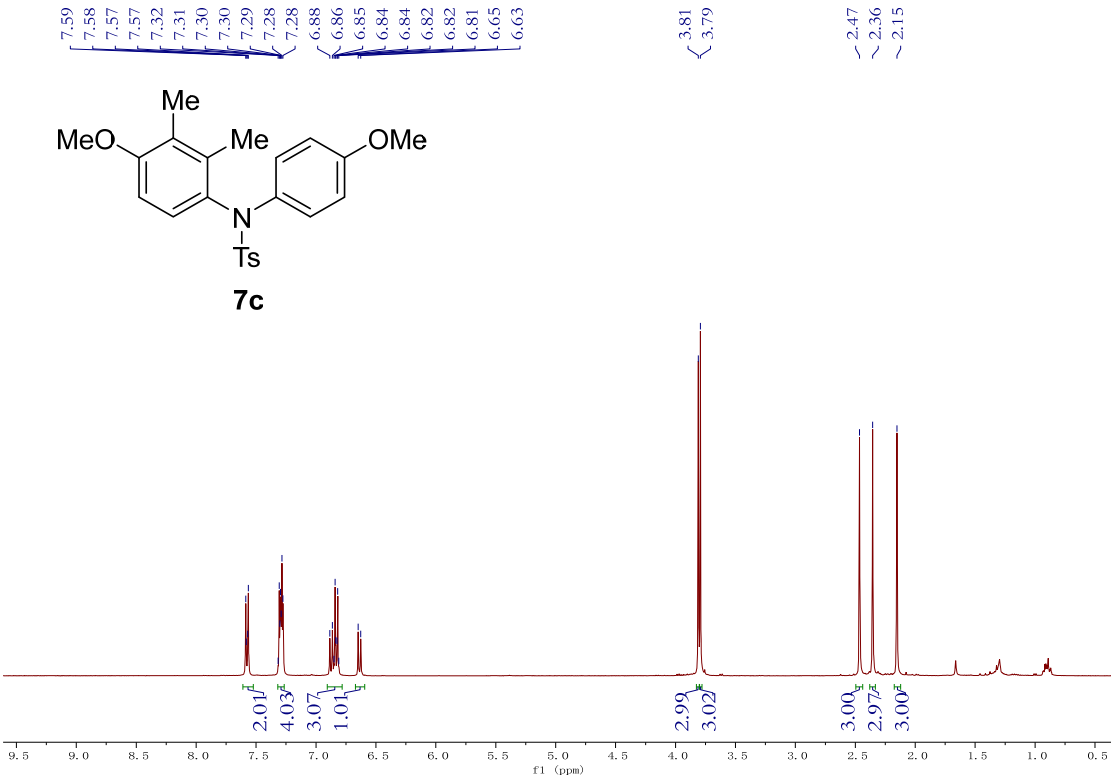
137.08
134.28
131.74
130.05
129.39
128.46
127.89
114.37
77.39
77.07
76.75
59.66
55.42
21.60
16.20
Me
MeO
OMe
Me
N
Ts
f1 (ppm)

7b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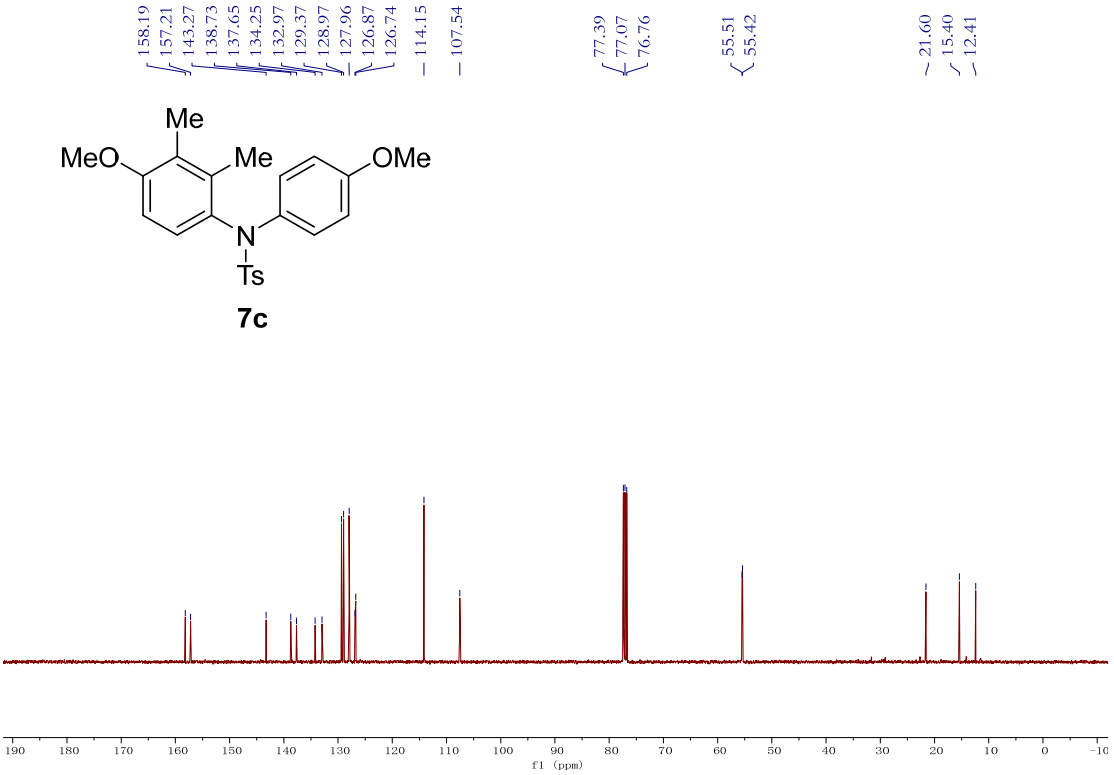
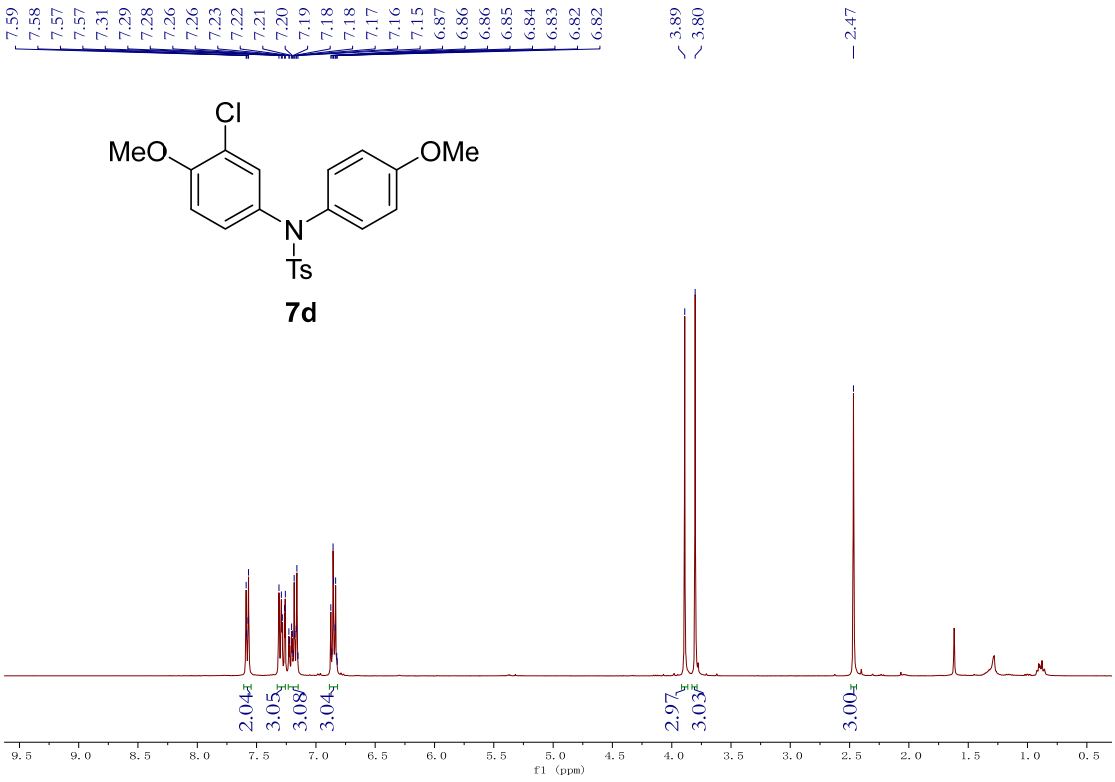
7.58
7.57
7.57
7.32
7.31
7.30
7.30
7.29
7.28
7.28
6.88
6.86
6.85
6.84
6.84
6.82
6.82
6.81
6.65
6.63
3.81
3.79
2.47
2.36
2.15
Me
MeO
Me
OMe
N
Ts
2.01
4.03
3.07
1.01
2.99
3.02
3.00
2.97
3.00
f1 (ppm)

7c


158.19
157.21
143.27
138.73
137.65
134.25
132.97
129.37
128.97
127.96
126.87
126.74
114.15
107.54
77.39
77.07
76.76
55.51
55.42
21.60
15.40
12.41
Me
MeO
Me
OMe
N
Ts
f1 (ppm)

7c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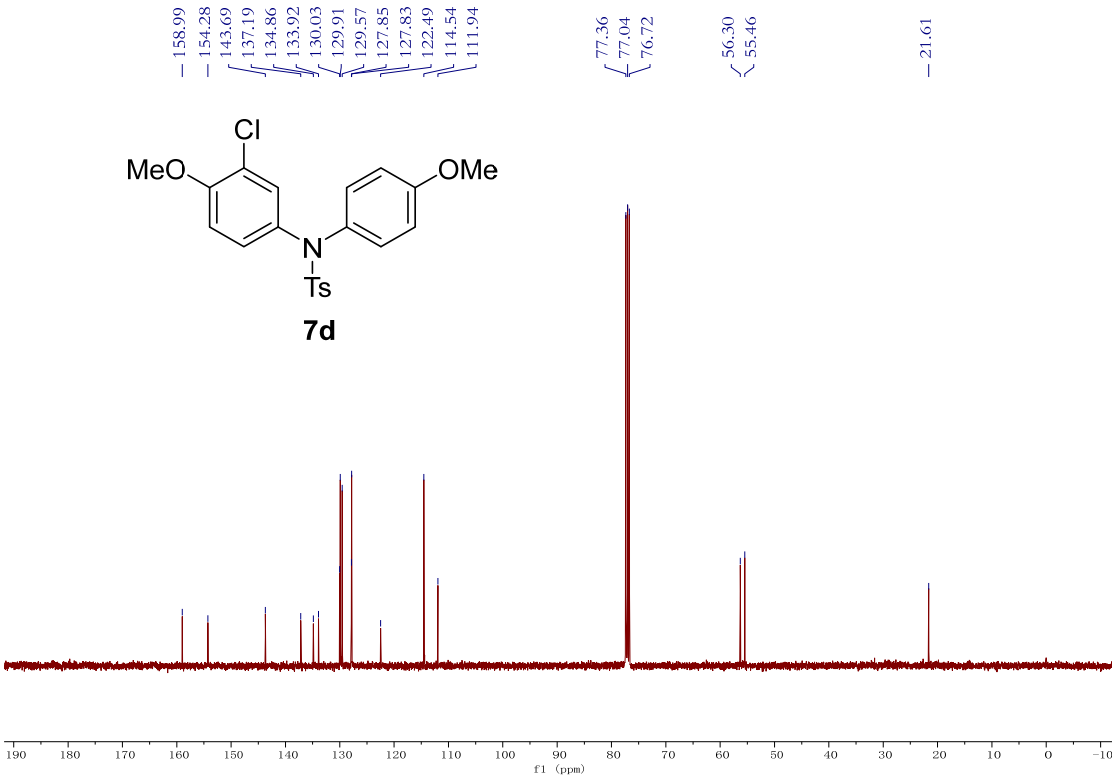
7.58
7.57
7.57
7.31
7.29
7.28
7.26
7.26
7.23
7.22
7.21
7.20
7.19
7.18
7.18
7.17
7.16
7.15
6.87
6.86
6.86
6.85
6.84
6.83
6.82
6.82
3.89
3.80
2.47
Cl
MeO
OMe
N
Ts
7d
2.04
3.05
3.08
3.04
2.97
3.03
3.00
f1 (ppm)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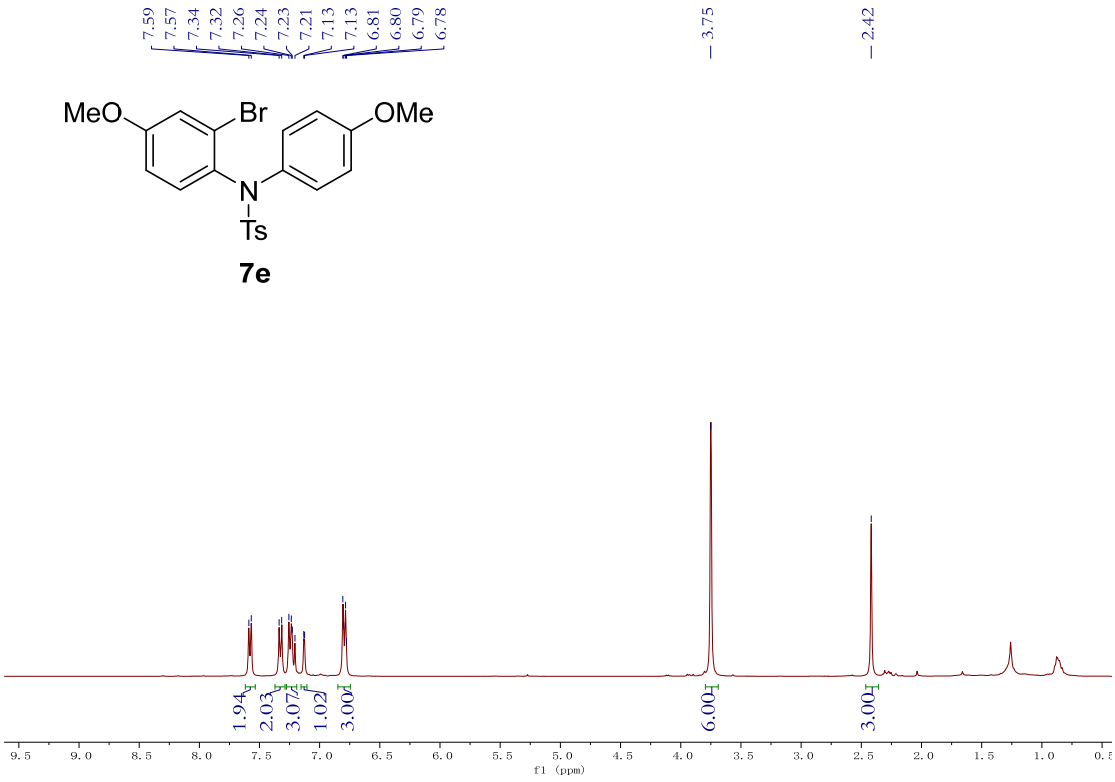
137.19
134.86
133.92
130.03
129.91
129.57
127.85
127.83
122.49
114.54
111.94
77.36
77.04
76.72
56.30
55.46
21.61
Cl
MeO
OMe
N
Ts
7d
f1 (ppm)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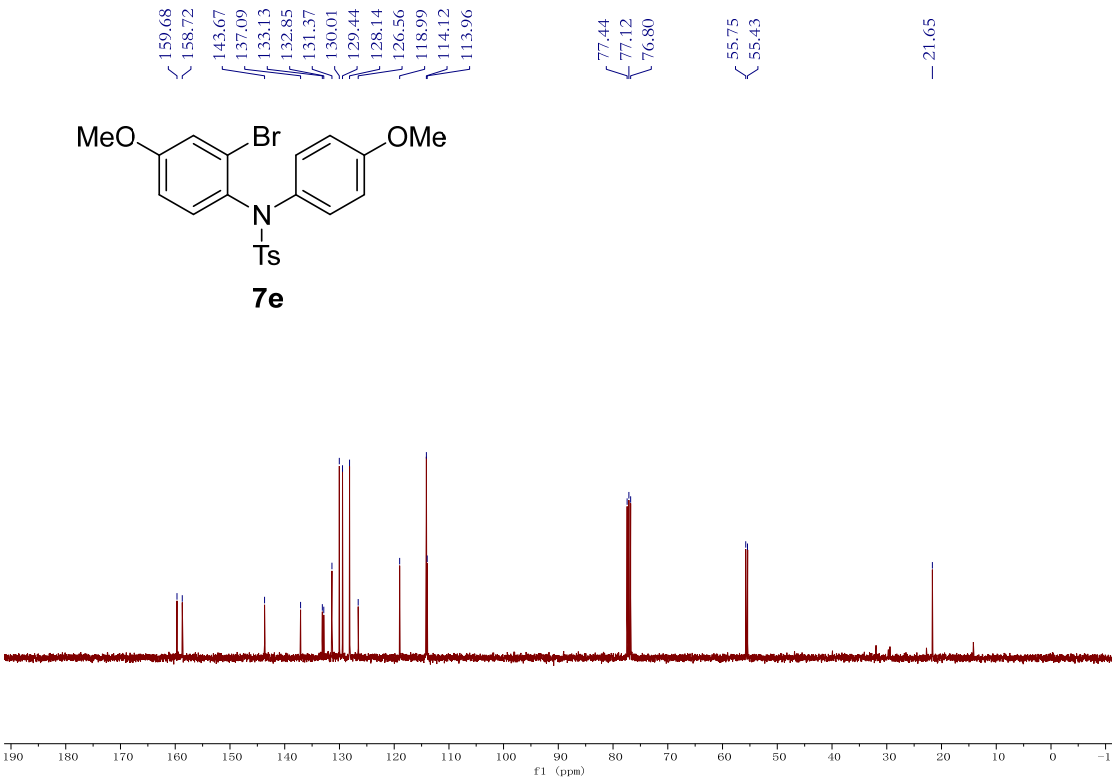
7.57
7.34
7.32
7.26
7.24
7.23
7.21
7.13
7.13
6.81
6.80
6.79
6.78
3.75
2.42
MeO
Br
OMe
N
Ts
1.94
2.03
3.07
1.02
3.00
6.00
3.00
f1 (ppm)

7e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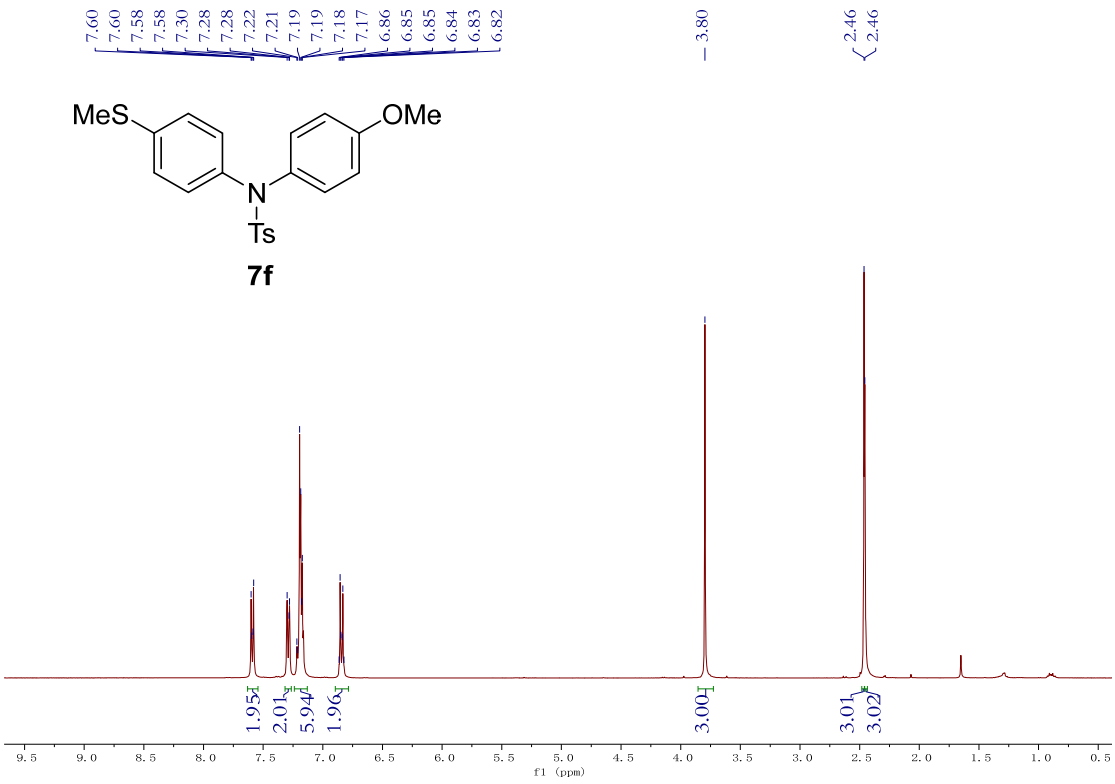
132.85
131.37
130.01
129.44
128.14
126.56
118.99
114.12
113.96
77.44
77.12
76.80
55.75
55.43
21.65
MeO
Br
OMe
N
Ts
f1 (ppm)

7e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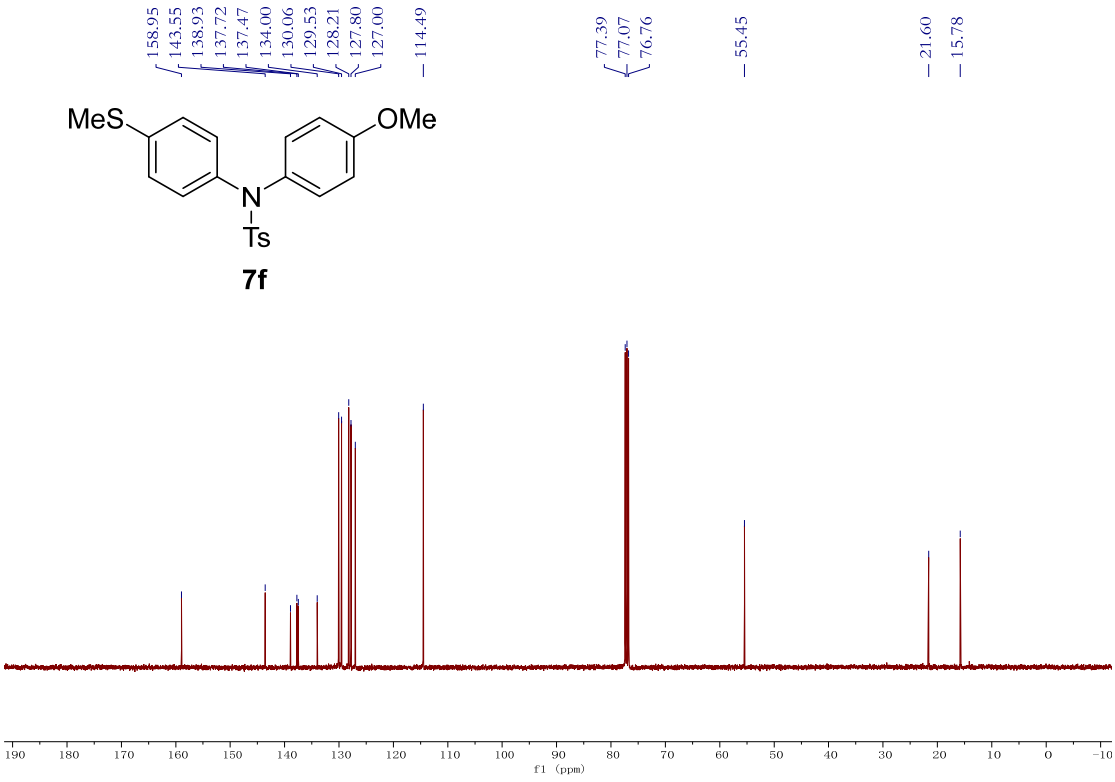
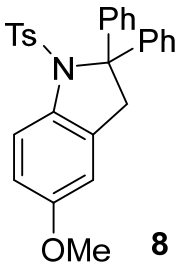
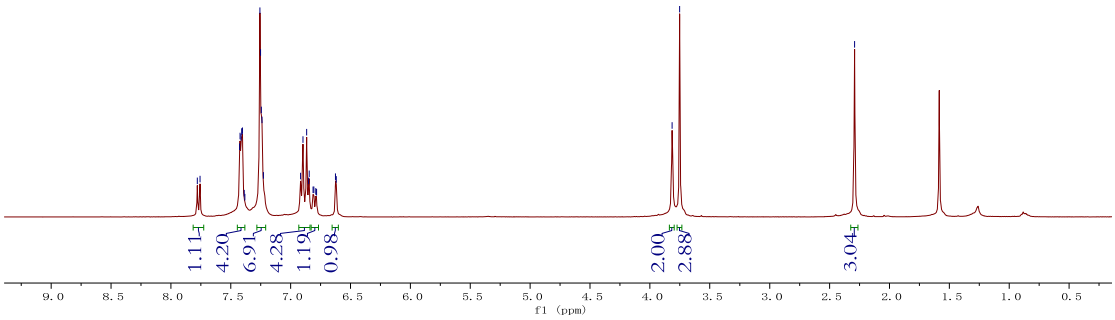
7.60
7.58
7.58
7.30
7.28
7.28
7.22
7.21
7.19
7.19
7.18
7.17
6.86
6.85
6.85
6.84
6.83
6.82
3.80
2.46
2.46
MeS
OMe
N
Ts
7f
1.95
2.01
5.94
1.96
3.00
3.01
3.02
f1 (ppm)


158.95
143.55
138.93
137.72
137.47
134.00
130.06
129.53
128.21
127.80
127.00
114.49
77.39
77.07
76.76
55.45
21.60
15.78
MeS
OMe
N
Ts
7f
f1 (ppm)

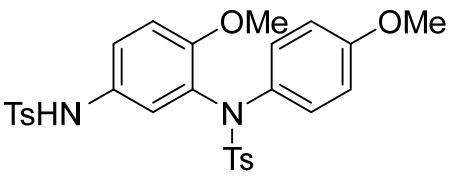

7.78
7.76
7.43
7.42
7.41
7.41
7.40
7.39
7.38
7.26
7.25
7.24
7.24
7.23
6.92
6.90
6.87
6.85
6.85
6.81
6.81
6.79
6.78
6.63
6.62
3.81
3.75
2.29


Ts
N
Ph
Ph
OMe

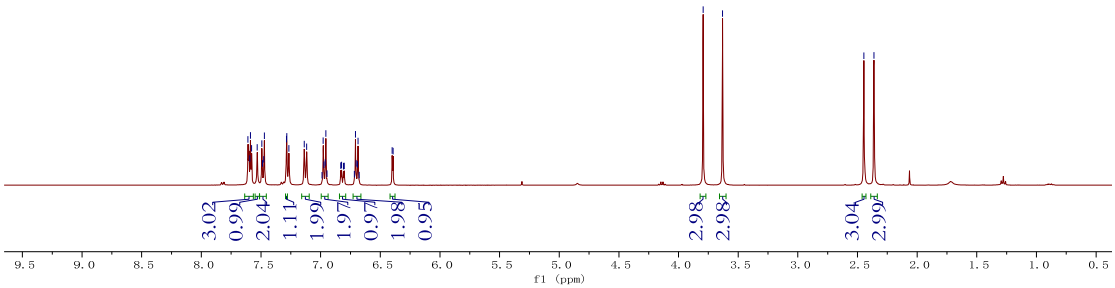
8

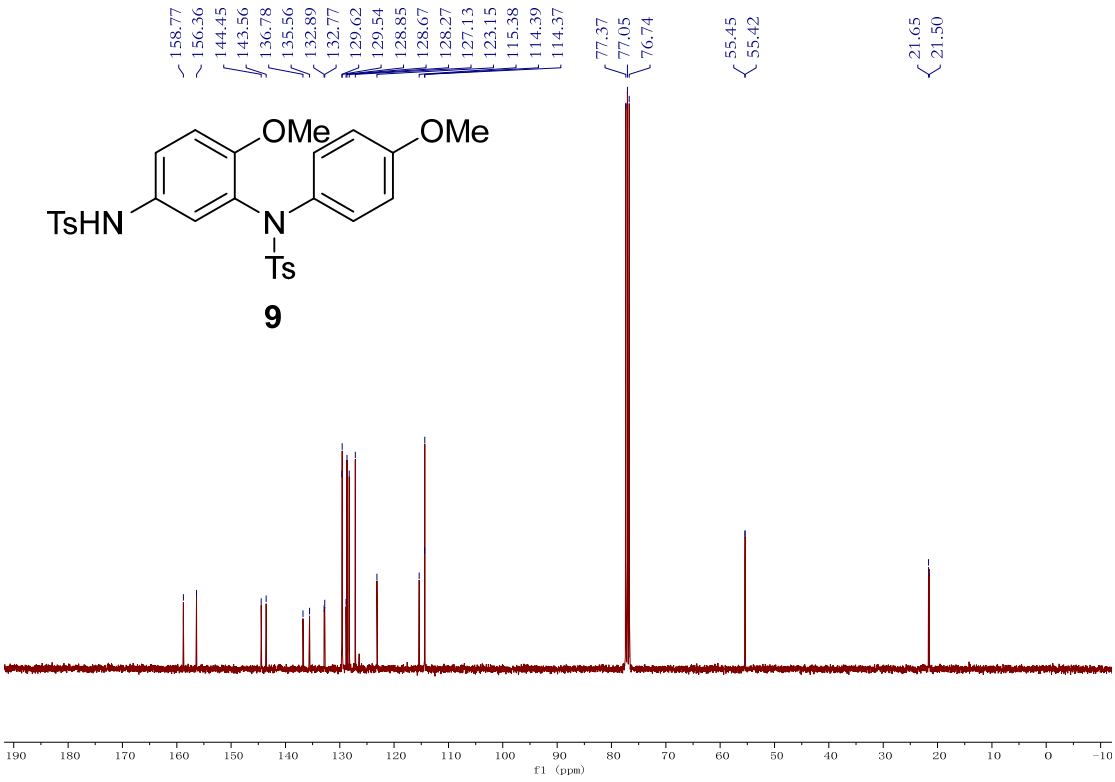

1.11
4.20
6.91
4.28
1.19
0.98
2.00
2.88
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


7.61
7.59
7.59
7.58
7.53
7.49
7.49
7.48
7.47
7.29
7.28
7.27
7.14
7.12
6.99
6.98
6.97
6.96
6.96
6.95
6.83
6.82
6.81
6.80
6.72
6.71
6.70
6.69
6.69
6.68
6.40
6.39
3.79
3.63
2.45
2.36


OMe
OMe
TsHN
N
Ts

9


3.02
0.99
2.04
1.11
1.99
1.97
0.97
1.98
0.95
2.98
2.98
3.04
2.99
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)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156.36
144.45
143.56
136.78
135.56
132.89
132.77
129.62
129.54
128.85
128.67
128.27
127.13
123.15
115.38
114.39
114.37
77.37
77.05
76.74
55.45
55.42
21.65
21.50
OMe
OMe
TsHN
N
Ts
9
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)