Supporting Information

From Benzopyrroles to Phenylpyrroles: Remodeling of Indoles Enabled by Photoredox Catalysis

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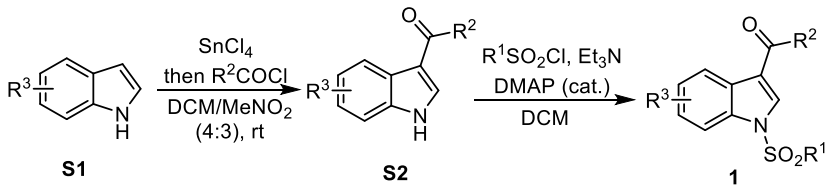
General Information

Reagents were purchased from commercial sources and were used as received unless otherwise noted. Anhydrous CH_2Cl_2 was refluxed with CaH_2 and freshly distilled prior to use. Ultradry *N*,*N*-dimethylformamide was used as obtained from commercial sources without further purification. Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded on a *JEOL-400YH* (^{1}H NMR at 400 MHz, ^{13}C NMR at 100 MHz and ^{19}F NMR at 376 MHz) spectrometer with tetramethylsilane (TMS) or deuterated solvent resonance as the internal standard (^{1}H NMR: TMS at 0.00 ppm; ^{13}C NMR: $CDCl_3$ at 77.0 ppm). All spectra are reported as parts per million. ^{1}H, ^{13}C and ^{19}F NMR data are reported as follows: chemical shift (ppm), multiplicity (app = apparent, s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, dd = doublet of doublets, td = triplet of doublets, ddd = double of doublet of doublets, m = multiplet), coupling constants (Hz), and integration. High Resolution Mass Spectra (HRMS) were performed by Analytical Instrument Center at the State Key Laboratory of Chemical Oncogenomics of Peking University Shenzhen Graduate School on an Electron Spray Injection (ESI) mass spectrometer. Melting point was recorded on an SGW® X-4A melting point apparatus.

General Synthesis of *N*-Sulfonyl-3-Acyl Indoles



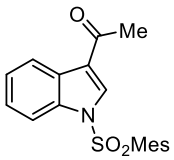
Commercially unavailable 3-acyl indoles **S2** were prepared via acylation of indoles following the practical protocol developed by Ottoni's group in 2001 (Ref: *Org. Lett.* **2001**, *3*, 1005-1007), and used directly for *N*-sulfonylation without any purification.

To a solution of indole **S1** (1.0 eq.) in anhydrous DCM at 0 °C under N_2 was added $SnCl_4$ (1.5 eq.) in a single portion via syringe. After the ice bath was removed, the mixture was stirred vigorously at room temperature for 30 min, and then acyl chloride (R^2COCl, 1.2 eq.) was added in small portions to the dark suspension, followed by the addition of $MeNO_2$. The reaction was quenched with cold water after it was stirred for 2 h at room temperature. Then the mixture was filtered under reduced pressure and the filtrate was extracted with ethyl acetate for three times. The combined organic phases were dried over anhydrous Na_2SO_4 and concentrated *in vacuo*, and the residue was used directly for next step.

The crude 3-acyl indole **S2** was suspended in DCM, then DMAP (0.1 eq.) and sulfonyl chloride (R^1SO_2Cl, 2.0 eq.) were added, followed by the addition of triethylamine (3.0 eq.) via

syringe at room temperature. The resulting mixture was stirred for 0.5–12 h for full consumption of 3-acyl indole **S2**, according to the result monitored by TLC. The volatile was carefully removed *in vacuo* before ethyl acetate was added, and the mixture was stirred vigorously for 10 min, then filtered. The filtrate was concentrated *in vacuo* to give a residue, which was purified through column chromatography with petroleum/ether ethyl acetate as the eluent to give the titled product **1**.

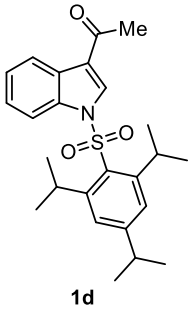
Characterization data of unknown substrates



1c

1-(1-(mesitylsulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1c**)

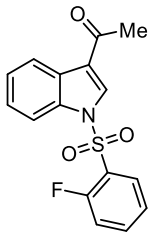
white powder, **M. p.** = 112–113 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.36 (dt, J = 8.1, 1.1 Hz, 1H), 8.32 (s, 1H), 7.33–7.27 (m, 1H), 7.25–7.18 (m, 2H), 6.98 (s, 2H), 2.58 (s, 3H), 2.54 (s, 6H), 2.29 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.5, 144.9, 140.3, 134.7, 132.7, 132.6, 131.6, 127.1, 125.3, 124.4, 123.1, 119.5, 111.8, 27.7, 22.5, 21.0; **HRMS** (ESI) *m/z*: calcd for $C_{19}H_{20}NO_3S^+$ $[M+H]^+$, 342.1158; found, 342.1156;



1d

1-(1-((2,4,6-triisopropylphenyl)sulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1d**)

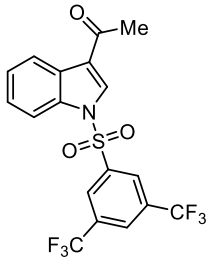
white powder, **M. p.** = 137–139 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.35 (dt, J = 8.0, 1.1 Hz, 1H), 8.26 (s, 1H), 7.32–7.27 (m, 1H), 7.25–7.17 (m, 4H), 4.16 (sept, J = 6.8 Hz, 2H), 2.91 (sept, J = 6.9 Hz, 1H), 2.58 (s, 3H), 1.24 (d, J = 6.9 Hz, 6H), 1.12 (d, J = 6.8 Hz, 12H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.4, 155.4, 151.5, 135.0, 131.6, 130.3, 126.9, 125.2, 124.5, 124.3, 123.0, 120.1, 111.9, 34.2, 29.6, 27.7, 24.3, 23.3; **HRMS** (ESI) *m/z*: calcd for $C_{25}H_{32}NO_3S^+$ $[M+H]^+$, 426.2097; found, 426.2108;



1f

1-(1-((2-fluorophenyl)sulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1f**)

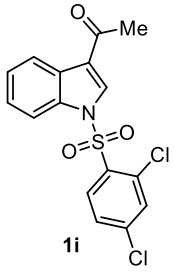
white powder, **M. p.** = 115–117 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.38–8.32 (m, 2H), 8.14 (ddd, *J* = 7.9, 7.1, 1.8 Hz, 1H), 7.79–7.71 (m, 1H), 7.62–7.52 (m, 1H), 7.36–7.27 (m, 3H), 7.09 (ddd, *J* = 10.2, 8.4, 1.1 Hz, 1H), 2.59 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.4, 158.9 (d, *J* = 259.1 Hz), 137.1 (d, *J* = 8.8 Hz), 134.4, 133.0 (d, *J* = 2.9 Hz), 130.3, 127.3, 125.5, 125.2 (d, *J* = 13.3 Hz), 124.8, 124.7, 123.0, 121.0, 117.6 (*J* = 20.7 Hz), 112.6, 27.6; **^{19}F NMR** (376 MHz, $CDCl_3$): δ -107.4 (m, 1F); **HRMS** (ESI) *m/z*: calcd for $C_{16}H_{13}FNO_3S^+$ $[M+H]^+$, 318.0595; found, 318.0591;



1h

1-(1-((3,5-bis(trifluoromethyl)phenyl)sulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1h**)

white powder, **M. p.** = 161–163 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.40 (s, 2H), 8.34 (d, *J* = 7.1 Hz, 1H), 8.18 (s, 1H), 8.10 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.49–7.34 (m, 2H), 2.59 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.2, 140.0, 134.7, 133.6 (q, *J* = 34.9 Hz), 131.3, 128.2 (q, *J* = 3.6 Hz), 127.7, 127.2 (q, *J* = 3.8 Hz), 126.5, 125.6, 123.6, 123.0, 122.0 (q, *J* = 273.6 Hz), 112.6, 27.9; **^{19}F NMR** (376 MHz, $CDCl_3$): δ –63.0 (s, 6F); **HRMS** (ESI) *m/z*: calcd for $C_{18}H_{12}F_6NO_3S^+$ $[M+H]^+$, 436.0437; found, 436.0433;

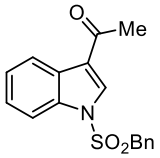


1i

1-(1-((2,4-dichlorophenyl)sulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1i**)

white powder, **M. p.** = 102–104 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.40–8.34 (m, 2H), 8.28 (d, *J* = 8.5 Hz, 1H), 7.58–7.54 (m, 1H), 7.52–7.45 (m, 2H), 7.35 (td, *J* = 7.6, 1.2 Hz, 1H), 7.30 (ddd, *J* =

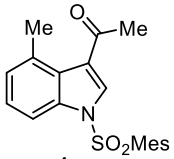
8.6, 7.3, 1.4 Hz, 1H), 2.60 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.4, 141.9, 134.4, 133.91, 133.87, 133.5, 132.8, 132.5, 127.9, 127.5, 125.7, 125.1, 123.5, 120.7, 112.4, 27.8; **HRMS** (ESI) *m/z*: calcd for $C_{16}H_{12}Cl_2NO_3S^+$ $[M+H]^+$, 367.9909; found, 367.9908;



1l

1-(1-(benzylsulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1l**)

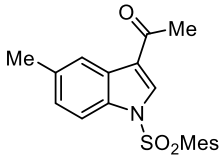
white powder, **M. p.** = 104–106 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.41–8.34 (m, 1H), 7.88–7.80 (m, 1H), 7.44–7.36 (m, 3H), 7.33–7.27 (m, 1H), 7.17 (t, J = 7.8 Hz, 2H), 6.86–6.78 (m, 2H), 4.56 (s, 2H), 2.29 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.4, 135.2, 133.5, 130.3, 129.6, 128.8, 127.1, 126.2, 125.8, 124.9, 123.2, 120.2, 112.6, 59.8, 27.4; **HRMS** (ESI) *m/z*: calcd for $C_{17}H_{16}NO_3S^+$ $[M+H]^+$, 314.0845; found, 314.0843;



1p

1-(1-(mesitylsulfonyl)-4-methyl-1*H*-indol-3-yl)ethan-1-one (**1p**)

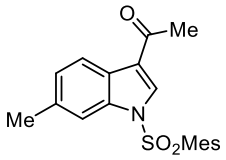
light yellow crystal, **M. p.** = 143–144 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.32 (s, 1H), 7.12–7.06 (m, 1H), 7.06–6.99 (m, 2H), 6.96 (s, 2H), 2.71 (s, 3H), 2.61 (s, 3H), 2.52 (s, 6H), 2.27 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.1, 144.8, 140.2, 135.3, 134.0, 133.1, 132.6, 131.7, 126.4, 125.8, 125.3, 121.8, 109.3, 29.0, 22.7, 22.5, 21.0; **HRMS** (ESI) *m/z*: calcd for $C_{20}H_{22}NO_3S^+$ $[M+H]^+$, 356.1315; found, 356.1323;



1q

1-(1-(mesitylsulfonyl)-5-methyl-1*H*-indol-3-yl)ethan-1-one (**1q**)

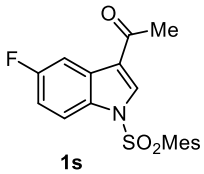
brown powder, **M. p.** = 142–144 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.28 (s, 1H), 8.16 (dt, J = 1.8, 0.8 Hz, 1H), 7.10–7.01 (m, 2H), 6.97 (s, 2H), 2.57 (s, 3H), 2.53 (s, 6H), 2.41 (s, 3H), 2.29 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.7, 144.8, 140.3, 134.3, 132.9, 132.8, 132.6, 131.7, 127.3, 126.7, 122.9, 119.3, 111.4, 27.7, 22.5, 21.3, 21.0; **HRMS** (ESI) *m/z*: calcd for $C_{20}H_{22}NO_3S^+$ $[M+H]^+$, 356.1315; found, 356.1309;



1r

1-(1-(mesitylsulfonyl)-6-methyl-1*H*-indol-3-yl)ethan-1-one (**1r**)

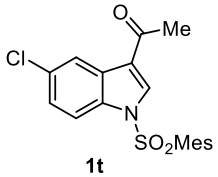
clear crystal, **M. p.** = 166–168 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.24–8.18 (m, 2H), 7.13 (ddd, *J* = 8.1, 1.5, 0.7 Hz, 1H), 7.04 (dt, *J* = 1.6, 0.8 Hz, 1H), 6.99 (s, 2H), 2.56 (s, 3H), 2.55 (s, 6H), 2.35 (s, 3H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.6, 144.9, 140.3, 135.5, 135.2, 132.6, 132.2, 131.8, 126.0, 124.8, 122.7, 119.7, 112.0, 27.7, 22.6, 21.9, 21.1; **HRMS** (ESI) *m/z*: calcd for $C_{20}H_{22}NO_3S^+$ $[M+H]^+$, 356.1315; found, 356.1318;



1s

1-(5-fluoro-1-(mesitylsulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1s**)

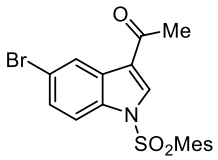
white powder, **M. p.** = 154–155 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.32 (s, 1H), 8.05 (dd, *J* = 9.2, 2.6 Hz, 1H), 7.14 (dd, *J* = 9.0, 4.3 Hz, 1H), 7.00 (s, 2H), 6.96 (td, *J* = 9.0, 2.6 Hz, 1H), 2.57 (s, 3H), 2.54 (s, 6H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.2, 160.3 (d, *J* = 241.4 Hz), 145.2, 140.3, 133.9, 132.7, 131.4, 131.0, 128.3 (d, *J* = 11.0 Hz), 119.4 (d, *J* = 4.2 Hz), 113.6 (d, *J* = 26.1 Hz), 112.8 (d, *J* = 9.4 Hz), 108.9 (d, *J* = 25.2 Hz), 27.6, 22.6, 21.1; **^{19}F NMR** (376 MHz, $CDCl_3$): δ -117.6 (m, 1F); **HRMS** (ESI) *m/z*: calcd for $C_{19}H_{19}FNO_3S^+$ $[M+H]^+$, 360.1064; found, 360.1076;



1t

1-(5-chloro-1-(mesitylsulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1t**)

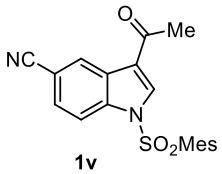
brown powder, **M. p.** = 160–162 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.37 (d, *J* = 2.0 Hz, 1H), 8.30 (s, 1H), 7.18 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.12 (dd, *J* = 8.8, 0.7 Hz, 1H), 6.99 (s, 2H), 2.57 (s, 3H), 2.52 (s, 6H), 2.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.1, 145.2, 140.3, 133.5, 133.0, 132.7, 131.3, 130.5, 128.2, 125.7, 122.8, 118.9, 112.8, 27.6, 22.5, 21.0; **HRMS** (ESI) *m/z*: calcd for $C_{19}H_{19}ClNO_3S^+$ $[M+H]^+$, 376.0769; found, 376.0776;



1u

1-(5-bromo-1-(mesitylsulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1u**)

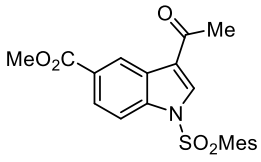
brown powder, **M. p.** = 178–179 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.53 (d, J = 2.0 Hz, 1H), 8.28 (s, 1H), 7.31 (dd, J = 8.8, 2.0 Hz, 1H), 7.07 (d, J = 8.8 Hz, 1H), 6.99 (s, 2H), 2.57 (s, 3H), 2.52 (s, 6H), 2.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.1, 145.2, 140.3, 133.4, 133.3, 132.7, 131.3, 128.7, 128.3, 125.8, 118.8, 118.2, 113.2, 27.6, 22.5, 21.0; **HRMS** (ESI) *m/z*: calcd for $C_{19}H_{19}BrNO_3S^+$ $[M+H]^+$, 420.0264; found, 420.0258;



1v

3-acetyl-1-(mesitylsulfonyl)-1*H*-indole-5-carbonitrile (**1v**)

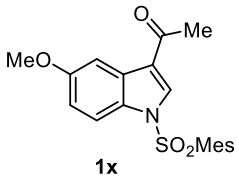
brown powder, **M. p.** = 190–192 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.75 (dd, J = 1.7, 0.8 Hz, 1H), 8.38 (s, 1H), 7.48 (dd, J = 8.6, 1.6 Hz, 1H), 7.32 (dd, J = 8.7, 0.8 Hz, 1H), 7.03 (s, 2H), 2.60 (s, 3H), 2.54 (s, 6H), 2.33 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 192.9, 145.7, 140.4, 136.3, 134.1, 132.9, 131.0, 128.4, 128.3, 127.2, 119.0, 118.9, 112.9, 108.2, 27.7, 22.6, 21.1; **HRMS** (ESI) *m/z*: calcd for $C_{20}H_{19}N_2O_3S^+$ $[M+H]^+$, 367.1111; found, 367.1122;



1w

methyl 3-acetyl-1-(mesitylsulfonyl)-1*H*-indole-5-carboxylate (**1w**)

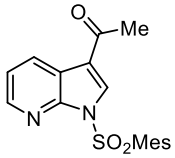
offwhite powder, **M. p.** = 155–157 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.04 (d, J = 1.8 Hz, 1H), 8.38 (s, 1H), 7.94 (dd, J = 8.8, 1.7 Hz, 1H), 7.26 (d, J = 8.8 Hz, 1H), 6.99 (s, 2H), 3.91 (s, 3H), 2.62 (s, 3H), 2.53 (s, 6H), 2.29 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.0, 166.8, 145.2, 140.2, 137.0, 133.6, 132.6, 131.2, 126.8, 126.6, 126.4, 125.2, 119.7, 111.6, 52.0, 27.7, 22.4, 21.0; **HRMS** (ESI) *m/z*: calcd for $C_{21}H_{22}NO_5S^+$ $[M+H]^+$, 400.1213; found, 400.1212;



1x

1-(1-(mesitylsulfonyl)-5-methoxy-1*H*-indol-3-yl)ethan-1-one (**1x**)

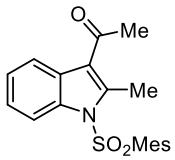
gray powder, **M. p.** = 144–146 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.27 (s, 1H), 7.85 (d, J = 2.5 Hz, 1H), 7.07 (dd, J = 8.9, 0.6 Hz, 1H), 6.98 (s, 2H), 6.83 (dd, J = 9.0, 2.6 Hz, 1H), 3.84 (s, 3H), 2.57 (s, 3H), 2.53 (s, 6H), 2.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.7, 157.3, 144.9, 140.3, 133.1, 132.7, 131.7, 129.3, 128.2, 119.4, 115.3, 112.6, 104.5, 55.7, 27.6, 22.5, 21.1; **HRMS** (ESI) *m/z*: calcd for $C_{20}H_{22}NO_4S^+$ $[M+H]^+$, 372.1264; found, 372.1260;



1y

1-(1-(mesitylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)ethan-1-one (**1y**)

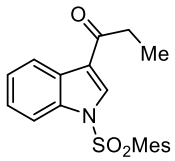
white powder, **M. p.** = 133–134 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.56 (dd, J = 8.0, 1.7 Hz, 1H), 8.49 (s, 1H), 8.26 (dd, J = 4.8, 1.7 Hz, 1H), 7.21 (dd, J = 7.9, 4.7 Hz, 1H), 6.96 (s, 2H), 2.71 (s, 6H), 2.60 (s, 3H), 2.27 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.3, 147.3, 145.8, 144.7, 141.3, 132.2, 132.0, 131.4, 131.3, 120.1, 119.7, 117.6, 27.2, 22.8, 21.0; **HRMS** (ESI) *m/z*: calcd for $C_{18}H_{19}N_2O_3S^+$ $[M+H]^+$, 343.1111; found, 343.1123;



1z

1-(1-(mesitylsulfonyl)-2-methyl-1*H*-indol-3-yl)ethan-1-one (**1z**)

brown powder, **M. p.** = 124–126 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.17–8.09 (m, 1H), 7.97–7.88 (m, 1H), 7.34–7.27 (m, 2H), 6.95 (s, 2H), 2.64 (s, 3H), 2.57 (s, 3H), 2.38 (s, 6H), 2.29 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 195.9, 144.4, 142.9, 139.6, 136.6, 134.4, 132.3, 125.7, 124.4, 123.7, 120.7, 119.3, 114.7, 32.1, 22.2, 21.0, 13.0; **HRMS** (ESI) *m/z*: calcd for $C_{20}H_{22}NO_3S^+$ $[M+H]^+$, 356.1315; found, 356.1311;

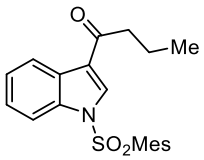


1A

1-(1-(mesitylsulfonyl)-1*H*-indol-3-yl)propan-1-one (**1A**)

brown powder, **M. p.** = 131–133 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.38 (dt, J = 8.0, 1.1 Hz, 1H), 8.34 (s, 1H), 7.33–7.27 (m, 1H), 7.23–7.17 (m, 2H), 6.97 (s, 2H), 2.95 (q, J = 7.4 Hz, 2H), 2.54 (s, 6H), 2.28 (s, 3H), 1.26 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 196.8, 144.9, 140.2, 134.6, 132.6, 132.0, 131.7, 127.3, 125.2, 124.3, 123.1, 118.8, 111.8, 33.1, 22.5, 21.0, 8.4; **HRMS**

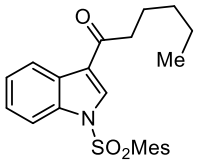
(ESI) *m/z*: calcd for $C_{20}H_{22}NO_3S^+$ [M+H]$^+$, 356.1315; found, 356.1325;



1B

1-(1-(mesitylsulfonyl)-1*H*-indol-3-yl)butan-1-one (**1B**)

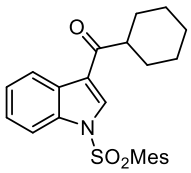
colorless crystal, **M. p.** = 131–133 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.38 (dt, J = 8.0, 1.1 Hz, 1H), 8.34 (s, 1H), 7.33–7.27 (m, 1H), 7.24–7.17 (m, 2H), 6.97 (s, 2H), 2.89 (t, J = 7.4 Hz, 2H), 2.54 (s, 6H), 2.28 (s, 3H), 1.87–1.76 (m, 2H), 1.03 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 196.4, 144.9, 140.2, 134.6, 132.6, 132.2, 131.7, 127.3, 125.2, 124.4, 123.2, 119.2, 111.8, 41.9, 22.5, 21.0, 18.1, 13.9; **HRMS** (ESI) *m/z*: calcd for $C_{21}H_{24}NO_3S^+$ [M+H]$^+$, 370.1471; found, 370.1471;



1C

1-(1-(mesitylsulfonyl)-1*H*-indol-3-yl)hexan-1-one (**1C**)

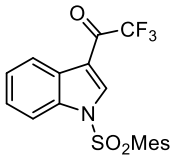
colorless crystal, **M. p.** = 115–117 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.38 (dt, J = 8.0, 1.1 Hz, 1H), 8.32 (s, 1H), 7.31 (ddd, J = 8.1, 6.5, 1.8 Hz, 1H), 7.24–7.17 (m, 2H), 6.99 (s, 2H), 2.90 (t, J = 7.2 Hz, 2H), 2.54 (s, 6H), 2.30 (s, 3H), 1.84–1.73 (m, 2H), 1.44–1.32 (m, 4H), 0.97–0.87 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 196.7, 144.9, 140.3, 134.7, 132.7, 132.2, 131.8, 127.4, 125.3, 124.4, 123.3, 119.2, 111.8, 40.1, 31.6, 24.5, 22.6, 22.5, 21.1, 13.9; **HRMS** (ESI) *m/z*: calcd for $C_{23}H_{28}NO_3S^+$ [M+H]$^+$, 398.1784; found, 398.1786;



1D

cyclohexyl(1-(mesitylsulfonyl)-1*H*-indol-3-yl)methanone (**1D**)

white powder, **M. p.** = 156–158 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.38 (dt, J = 8.0, 1.1 Hz, 1H), 8.35 (s, 1H), 7.30 (ddd, J = 8.1, 7.0, 1.3 Hz, 1H), 7.23–7.12 (m, 2H), 6.98 (s, 2H), 3.07 (tt, J = 11.7, 3.3 Hz, 1H), 2.54 (s, 6H), 2.30 (s, 3H), 1.99–1.83 (m, 4H), 1.81–1.71 (m, 1H), 1.67–1.55 (m, 2H), 1.49–1.37 (m, 2H), 1.31 (tt, J = 12.3, 3.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 200.1, 144.9, 140.3, 134.7, 132.7, 131.9, 131.8, 127.8, 125.3, 124.4, 123.4, 118.0, 111.7, 48.0, 29.7, 25.9, 25.8, 22.6, 21.1; **HRMS** (ESI) *m/z*: calcd for $C_{24}H_{28}NO_3S^+$ [M+H]$^+$, 410.1784; found, 410.1785



1E

2,2,2-trifluoro-1-(1-(mesitylsulfonyl)-1*H*-indol-3-yl)ethan-1-one (**1E**)

colorless crystal, **M. p.** = 116–118 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.54 (q, J = 1.7 Hz, 1H), 8.36 (dt, J = 8.0, 1.0 Hz, 1H), 7.38 (ddd, J = 8.1, 7.0, 1.4 Hz, 1H), 7.30 (td, J = 8.4, 1.4 Hz, 1H), 7.28–7.23 (m, 1H), 7.01 (s, 2H), 2.56 (s, 6H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.0 (q, J = 36.3 Hz), 145.5, 140.5, 135.7 (q, J = 5.1 Hz), 134.3, 132.9, 131.1, 127.2, 126.3, 125.3, 122.8, 116.4 (q, J = 290.9 Hz), 112.2, 111.8, 22.6, 21.1; **^{19}F NMR** (376 MHz, $CDCl_3$): δ -72.8 (s, 3F); **HRMS** (ESI) *m/z*: calcd for $C_{19}H_{17}F_3NO_3S^+$ $[M+H]^+$, 396.0876; found, 396.0869;

Photochemical set-up

All the photoreactions were carried out using ROGER OHSP-350UV parallel photoreactor (provided by Beijing Nuozhi Technology Co., Ltd) equipped with 10 W blue LED for each reaction site, with a circling ethanol-cooled jacket. Light type of light reactor is 3A3A4100–455 nm from Nuozhi Technology.

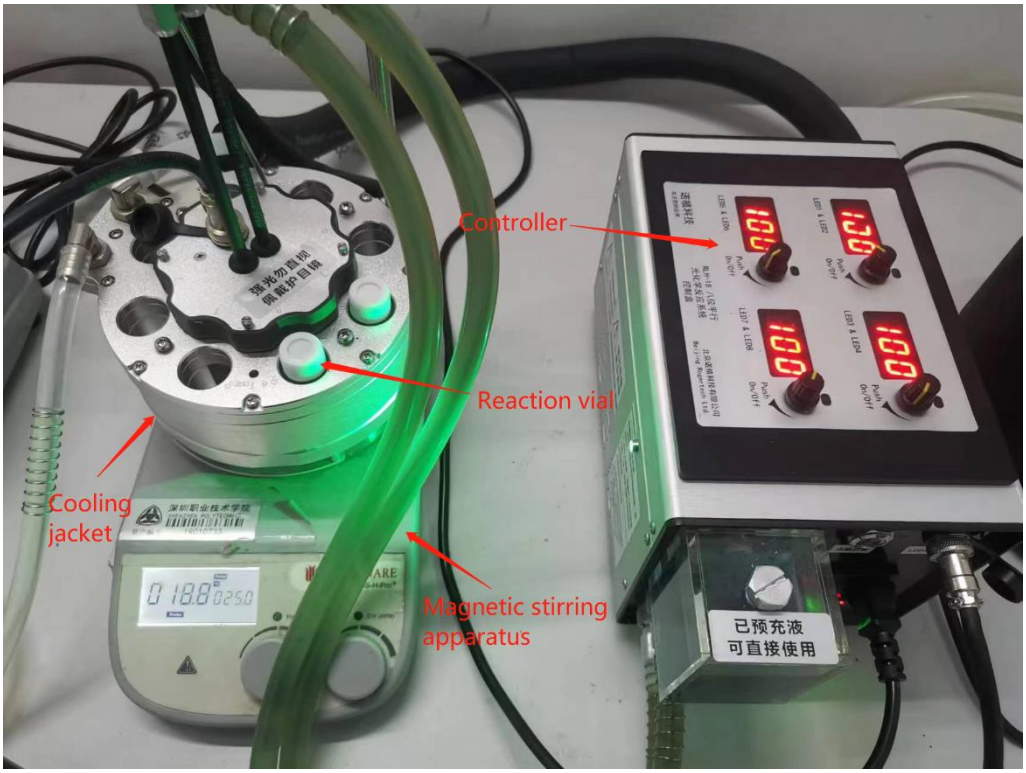


Figure S1 The photochemical set-up

The emission spectrum (see below) of the blue LED reactor shows a maximum intensity at a wavelength of $\lambda(\text{emission})_{max}$ = 453.0 nm. The photophysical data of LEDs (Figure S2) was provided by Beijing Nuozhi Technology Co., Ltd.

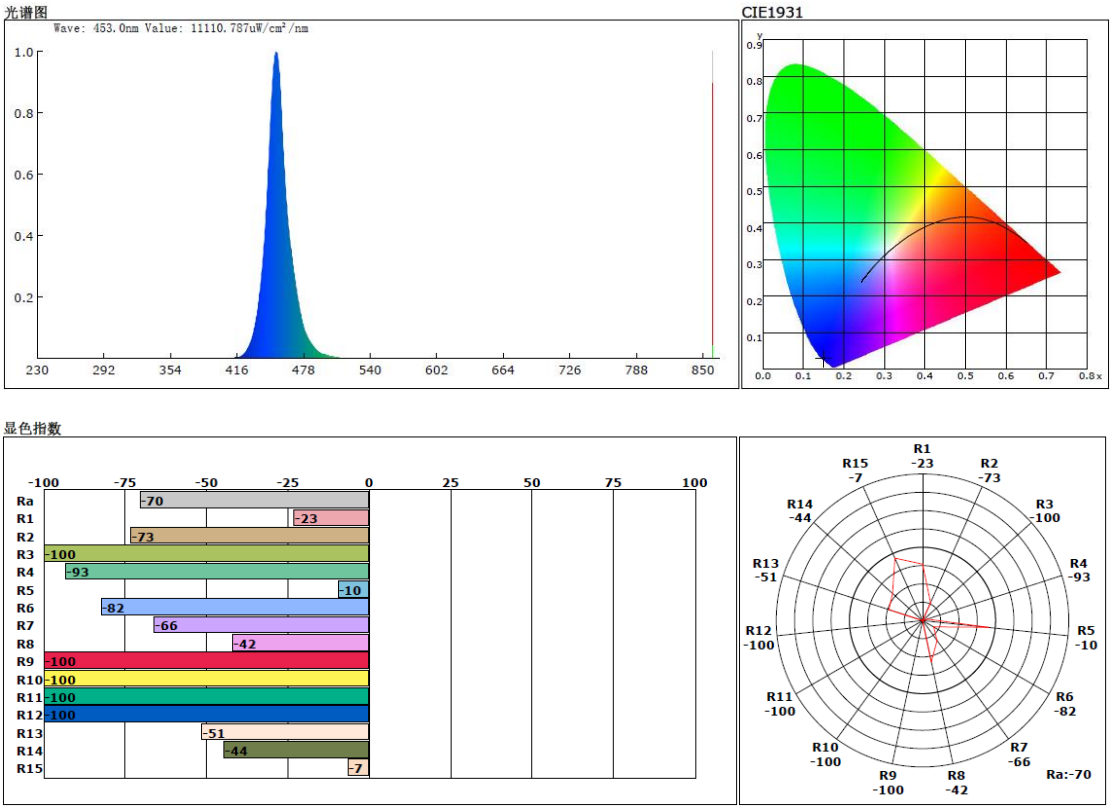
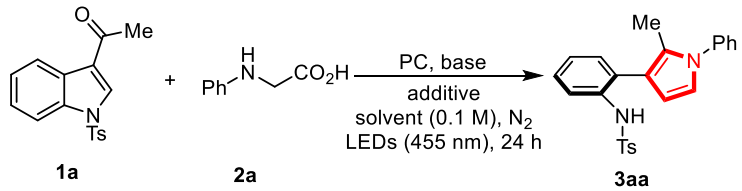


Figure S2 Photophysical property of LEDs used during our exploration

Optimization of reaction conditions[a]



1a **2a** **3aa**

entry	PC	solvent	base	additive	yield of **3aa** (%)[b]
1	4CzIPN (**PC1**)	MeCN	K_2CO_3	none	29
2	*fac*-Ir(ppy)$_3$ (**PC2**)	MeCN	K_2CO_3	none	N.D.
3	[Ir(dF(CF$_3$)ppy)$_2$(5,5'-di-CF$_3$bpy)]PF$_6$ (**PC3**)	MeCN	K_2CO_3	none	29
4	[Ir(dFppy)$_2$(dtbbpy)]PF$_6$ (**PC4**)	MeCN	K_2CO_3	none	22
5	[Ir(Me(Me)ppy)$_2$(dtbbpy)]PF$_6$ (**PC5**)	MeCN	K_2CO_3	none	22
6	[Ir(ppy)$_2$(dtbbpy)]PF$_6$ (**PC6**)	MeCN	K_2CO_3	none	18
7	[Ir(dF(CF$_3$)ppy)$_2$(dtbbpy)]PF$_6$ (**PC7**)	MeCN	K_2CO_3	none	32
8	[Ir(dF(CF$_3$)ppy)$_2$(bpy)]PF$_6$ (**PC8**)	MeCN	K_2CO_3	none	37 (37)[c]
9	*fac*-(*p*-CF$_3$-ppy)$_3$ (**PC9**)	MeCN	K_2CO_3	none	N.D.
10	4DPAIPN (**PC10**)	MeCN	K_2CO_3	none	9.7
11	3DPA2FBN (**PC11**)	MeCN	K_2CO_3	none	N.D.
12	DPZ (**PC12**)	MeCN	K_2CO_3	none	9.8
13	CsPbBr$_3$ (**PC13**)	MeCN	K_2CO_3	none	N.D.
14	**PC8**	DCE	K_2CO_3	none	18
15	**PC8**	THF	K_2CO_3	none	12

16	**PC8**	Dioxane	K_2CO_3	none	trace
17	**PC8**	DMF	K_2CO_3	none	62
18	**PC8**	DMSO	K_2CO_3	none	47
19	**PC8**	MeOH	K_2CO_3	none	27
20	**PC8**	DCM	K_2CO_3	none	15
21	**PC8**	EtOAc	K_2CO_3	none	17
22	**PC8**	PhMe	K_2CO_3	none	13
23	**PC8**	DMC	K_2CO_3	none	N.D.
24	**PC8**	DME	K_2CO_3	none	19
25	**PC8**	Benzene	K_2CO_3	none	18
26	**PC8**	DMF	K_2CO_3	Na_2SO_4	62
27	**PC8**	**DMF**	**K_2CO_3**	**4 Å MS**	**76 (67)[d]**
28	**PC8**	DMF	none	4 Å MS	N.D.
29	**PC8**	DMF	Li_2CO_3	4 Å MS	61
30	**PC8**	DMF	Na_2CO_3	4 Å MS	74
31	**PC8**	DMF	Cs_2CO_3	4 Å MS	58
32	**PC8**	DMF	NaOAc	4 Å MS	67
33	**PC8**	DMF	$NaHCO_3$	4 Å MS	38
34	**PC8**	DMF	K_3PO_4	4 Å MS	66
35	**PC8**	DMF	K_2HPO_4	4 Å MS	69
36	**PC8**	DMF	KH_2PO_4	4 Å MS	12
37	**PC8**	DMF	Na_2HPO_4	4 Å MS	15
38	**PC8**	DMF	NaOH	4 Å MS	13
39	**PC8**	DMF	Et_3N	4 Å MS	27
40	**PC8**	DMF	DIPEA	4 Å MS	22
41	**PC8**	DMF	DBU	4 Å MS	22
42	none	DMF	K_2CO_3	4 Å MS	24
43[e]	**PC8**	DMF	K_2CO_3	4 Å MS	N.D.
44[f]	**PC8**	DMF	K_2CO_3	4 Å MS	N.D.

[a]Unless otherwise specified, the reaction was conducted as follows: **1a** (0.1 mmol, 1equiv), **2a** (1.1 equiv), **PC** (1 mol %), base (1.5 equiv), additive (5 equiv of Na_2SO_4 or 50 mg of 4 Å MS, if used), solvent (1 mL), N_2, blue LEDs irradiation (10 W), rt, 24 h. [b]NMR yield was determined using 1,3,5-trimethoxybenzene as the internal standard. [c]Isolated yield. [d]Isolated yield on a 0.2 mmol scale of indole **1a**. [e]The reaction was carried out in the dark. [f]The reaction was conducted in the open air.

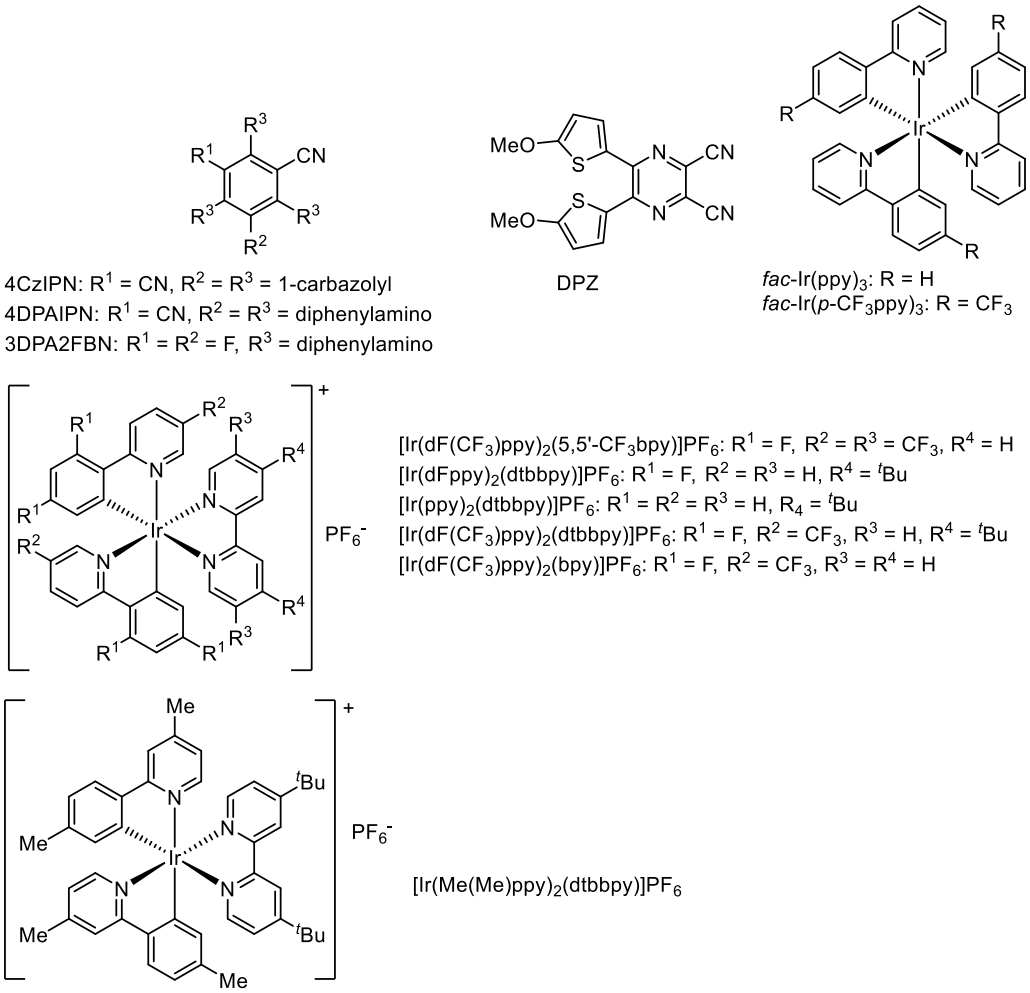
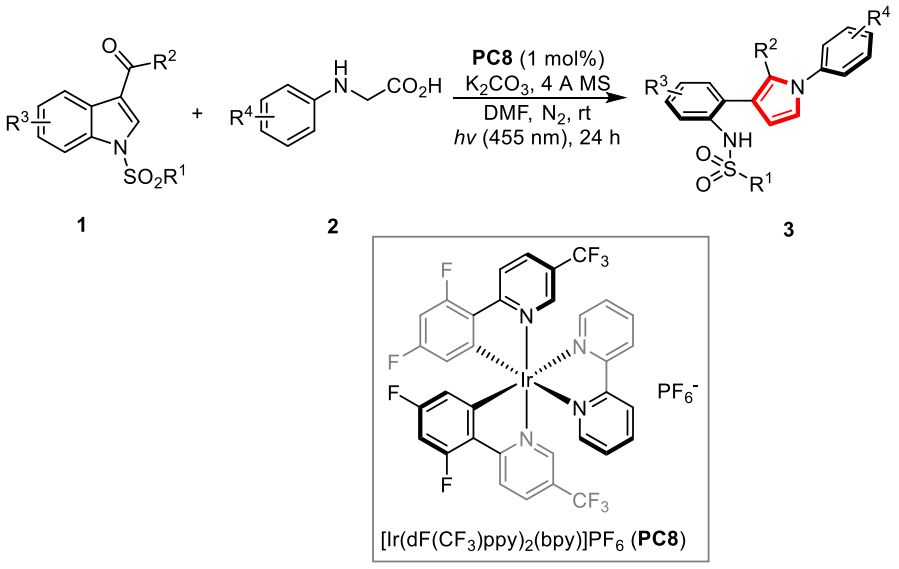


Figure S3 The structures of photocatalysts used for optimization of reaction conditions

General procedure for the synthesis of 3-(*o*-aminophenyl)pyrroles

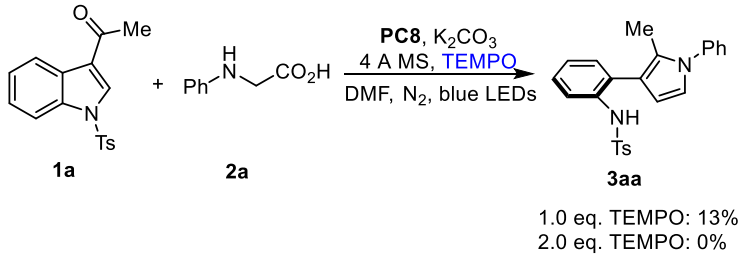


To a 15-mL transparent glass vial with magnetic stir bar were successively added *N*-sulfonyl-3-acyl indole **1** (0.20 mmol), *N*-phenylglycine **2** (0.22 mmol), K_2CO_3 (41.4 mg, 0.30

mmol), 4 Å molecular sieve (100 mg), [Ir(dF(CF_3)ppy)(bpy)]PF_6 (**PC8**, 2.0 mg, 2 μmol) and anhydrous DMF (2 mL). The vial was then sealed up with the open-topped cap equipped with silicone septa and placed under N_2 atmosphere in the photoreactor under the irradiation of blue LED (455 nm, 10 W). The reaction was stirred for 24 h cooled with a circling chiller (ethanol as the refrigerant at 25 °C). Then the mixture was filtered *in vacuo* and washed with dichloromethane (2 mL×3). Then the filtrate was concentrated *in vacuo* to give a residue, which was purified through column chromatography with petroleum/ether ethyl acetate as the eluent to give 3-(2-aminophenyl)pyrrole **3**.

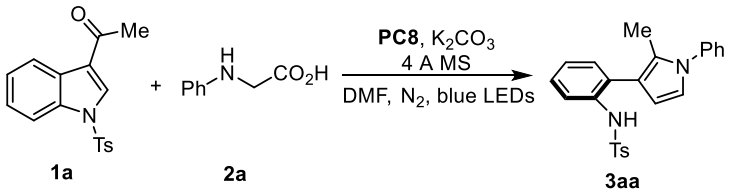
Mechanistic investigation

Radical trapping experiment with TEMPO



Two parallel reactions were performed. To a 15-mL transparent glass vial with magnetic stir bar were successively added *N*-sulfonyl-3-acyl indole **1a** (62.6 mg, 0.20 mmol), *N*-phenylglycine **2a** (33.3 mg, 0.22 mmol), K_2CO_3 (41.4 mg, 0.30 mmol), 4 Å molecular sieve (100 mg), [Ir(dF(CF_3)ppy)(bpy)]PF_6 (**PC8**, 2.0 mg, 2 μmol), TEMPO (2,2,6,6-tetramethyl-1-piperidinyloxy, 31.3 mg for 1.0 eq. and 62.5 mg for 2.0 eq.) and anhydrous DMF (2 mL) under N_2 atmosphere. The vial was then sealed up with the open-topped cap equipped with silicone septa and placed under N_2 in the photoreactor under the irradiation of blue LED (455 nm, 10 W). The reaction was stirred for 24 h cooled with a circling chiller (ethanol as the refrigerant at 25 °C). After that, internal standard 1,3,5-trimethoxybenzene (10.0 mg) was added to the reaction system and the resulting mixture was vigorously stirred for 20 min before being kept still for 20 min. A fraction of the reaction liquid (*ca*. 50 μL) was extracted and diluted with $CDCl_3$ (0.5 mL) for NMR analysis. The NMR yields of biaryl **3aa** were identified as 13% and 0% by the erosion of 1.0 and 2.0 equiv. of TEMPO, respectively.

Light on/off experiment



Six standard reactions were set up parallel on a 0.10 mmol scale with 1,3,5-trimethoxybenzene

(5.0 mg) as an internal standard. One of the reaction vials was unsealed for NMR analysis before the irradiation of the remained ones with blue LEDs for 2 h. Then the second parallel reaction was NMR analyzed and the remained four vials were kept in the dark for another 2 h. All the six parallel reactions were analyzed after alternant treatment with irradiation and darkness in a period of 2 h. The NMR yield of each reaction is listed as follows.

Time (h)	0	2	4	6	8	10
On/Off	Off	On	Off	On	Off	On
Yield (%)	0	19	23	39	42	53

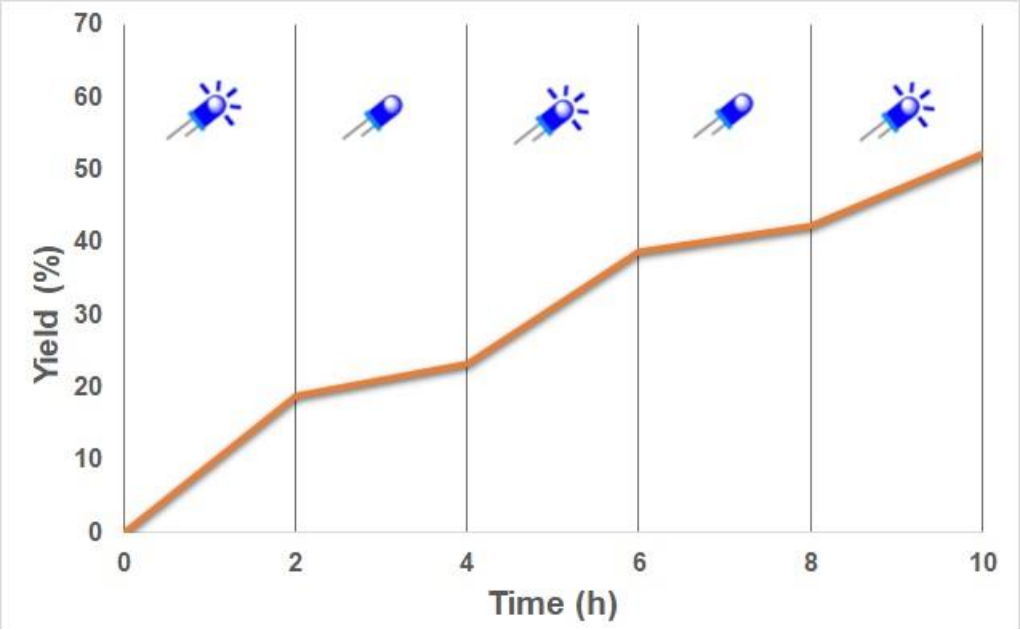
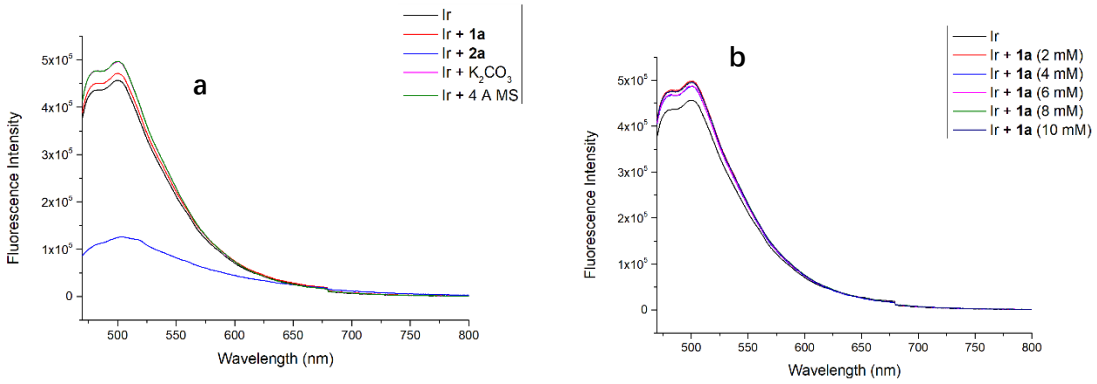


Figure S4 The results of the light on/off experiment

Emission Quenching Experiments (Stern–Volmer Studies)

Emission intensities were recorded using an FLS1000 Transient/Steady-state Fluorescence Spectrometer. The emission intensity was collected with the excitation wavelength at 480 nm. The fluorescence was measured from 470 nm to 800 nm. The fluorescence intensity for exploration of the relationship between I_0/I and the concentration of **1a**/**2a** was collected at maximum emission wavelength of 499 nm.



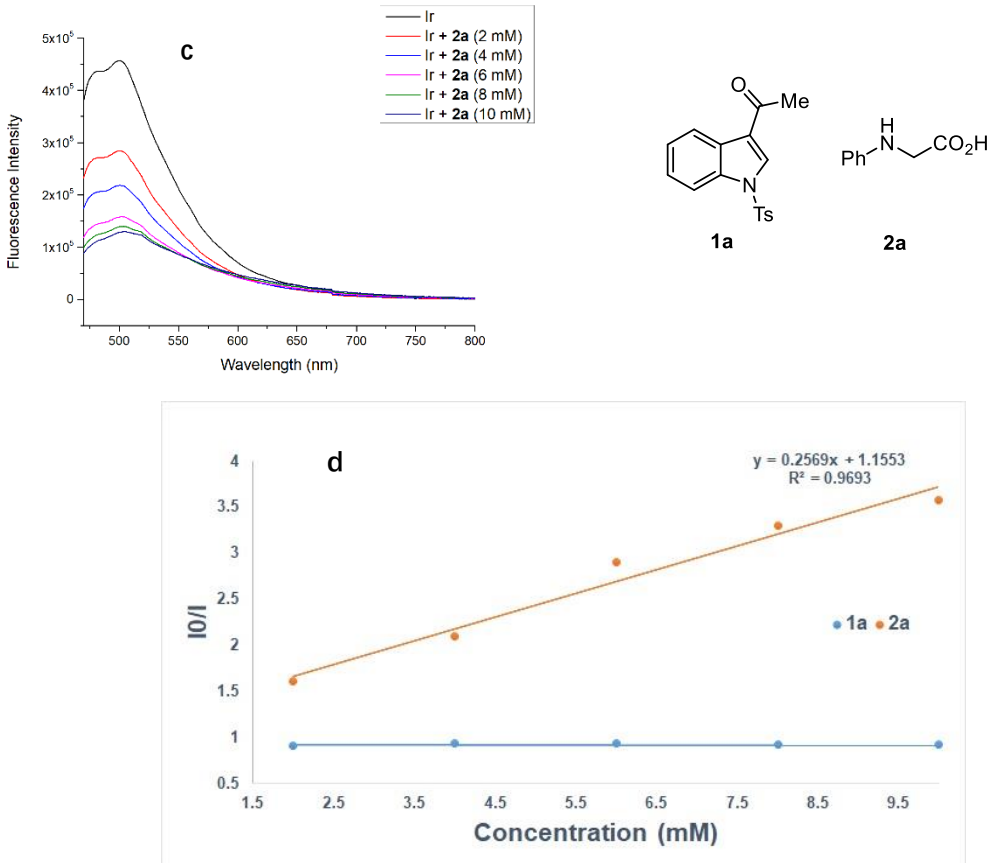


Figure S5 Stern–Volmer studies

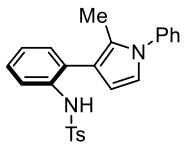
a: The emission spectra of 5 × 10^{-5} M solutions of [Ir(dF(CF_3)ppy)$_2$(bpy)]PF_6 in DMF with (or without) different reaction components (blank, **1a**, **2a**, K_2CO_3, 4 Å molecular sieve);

b: The emission spectra of 5 × 10^{-5} M solutions of [Ir(dF(CF_3)ppy)$_2$(bpy)]PF_6 in DMF with various concentration of **1a**;

c: The emission spectra of 5 × 10^{-5} M solutions of [Ir(dF(CF_3)ppy)$_2$(bpy)]PF_6 in DMF with various concentration of **2a**;

d: The relationship between fluorescence quenching ratio (I_0/I) and the increasing concentration of **1a**/**2a**.

Characterization data of products

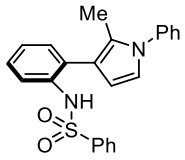


3aa

4-methyl-*N*-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3aa**)

54 mg (67%), yellowish powder, **M. p.** = 51–53 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.67 (dd, J = 8.2, 1.2 Hz, 1H), 7.61 (d, J = 8.3 Hz, 2H), 7.53–7.46 (m, 2H), 7.43–7.37 (m, 1H), 7.36–7.31 (m, 2H), 7.27–7.22 (m, 1H), 7.20–7.16 (m, 2H), 7.15–7.10 (m, 2H), 7.07 (td, J = 7.4, 1.2 Hz, 1H),

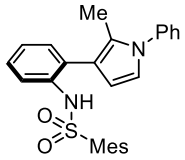
6.82 (d, *J* = 2.9 Hz, 1H), 5.87 (d, *J* = 2.9 Hz, 1H), 2.33 (s, 3H), 1.86 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 143.6, 139.9, 136.5, 135.2, 131.2, 129.5, 129.2, 127.8, 127.6, 127.4, 127.2, 127.1, 125.7, 124.0, 121.9, 119.2, 117.2, 108.8, 21.5, 11.0; **HRMS** (ESI) *m/z*: calcd for $C_{24}H_{23}N_2O_2S^+$ $[M+H]^+$, 403.1475; found, 403.1492;



3ab

N-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**1ab**)

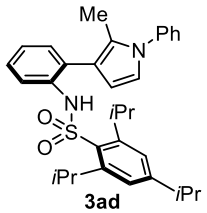
53 mg (68%), yellowish oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.75–7.67 (m, 3H), 7.53–7.45 (m, 3H), 7.42–7.35 (m, 3H), 7.35–7.30 (m, 2H), 7.25 (td, *J* = 8.5, 1.9 Hz, 1H), 7.16 (br s, 1H), 7.13 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.08 (td, *J* = 7.4, 1.2 Hz, 1H), 6.81 (d, *J* = 2.9 Hz, 1H), 5.84 (d, *J* = 2.9, Hz, 1H), 1.83 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 139.8, 139.4, 135.0, 132.8, 131.2, 129.2, 128.8, 127.8, 127.7, 127.3, 127.1, 125.7, 124.2, 121.9, 119.4, 117.1, 108.7, 11.0 (1C is merged with other peaks); **HRMS** (ESI) *m/z*: calcd for $C_{23}H_{21}N_2O_2S^+$ $[M+H]^+$, 389.1318; found, 389.1332;



3ac

2,4,6-trimethyl-*N*-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3ac**)

61 mg (71%), offwhite powder, **M. p.** = 113–114 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54–7.46 (m, 3H), 7.43–7.38 (m, 1H), 7.36–7.32 (m, 2H), 7.31 (br s, 1H), 7.23–7.13 (m, 2H), 7.06 (td, *J* = 7.5, 1.3 Hz, 1H), 6.86 (d, *J* = 2.9 Hz, 1H), 6.80 (s, 2H), 6.13 (d, *J* = 2.9 Hz, 1H), 2.42 (s, 6H), 2.19 (s, 3H), 1.84 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.2, 139.9, 139.3, 135.2, 133.9, 131.8, 131.2, 129.3, 127.8, 127.6, 127.3, 127.0, 125.6, 124.0, 121.8, 119.6, 117.6, 109.0, 22.8, 20.8, 11.0; **HRMS** (ESI) *m/z*: calcd for $C_{26}H_{27}N_2O_2S^+$ $[M+H]^+$, 431.1778; found, 431.1793

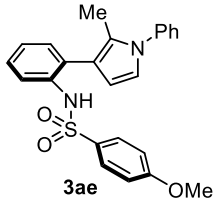


3ad

2,4,6-triisopropyl-*N*-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3ad**)

63 mg (61%), white powder, **M. p.** = 122–123 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.50–7.44 (m, 2H), 7.40–7.35 (m, 1H), 7.35–7.30 (m, 2H), 7.24 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.19 (dd, *J* = 7.5, 1.6

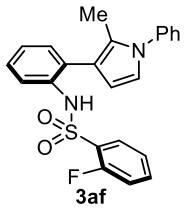
Hz, 1H), 7.18–7.13 (m, 3H), 7.07 (br s, 1H), 7.05 (td, *J* = 7.4, 1.3 Hz, 1H), 6.84 (d, *J* = 2.9 Hz, 1H), 6.17 (d, *J* = 2.9 Hz, 1H), 4.12 (sept, *J* = 6.8 Hz, 2H), 2.89 (sept, *J* = 6.8 Hz, 1H), 2.01 (s, 3H), 1.24 (d, *J* = 6.8 Hz, 6H), 1.17 (d, *J* = 6.8 Hz, 12H); **^{13}C NMR** (100 MHz, $CDCl_3$): *δ* 152.9, 150.3, 139.9, 135.8, 133.5, 131.4, 129.2, 127.42, 127.40, 127.2, 127.0, 125.7, 123.9, 123.5, 121.7, 118.9, 117.6, 109.2, 34.1, 29.8, 24.7, 23.5, 11.3; **HRMS** (ESI) *m/z*: calcd for $C_{32}H_{39}N_2O_2S^+$ $[M+H]^+$, 515.2727; found, 515.2744;



3ae

4-methoxy-*N*-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3ae**)

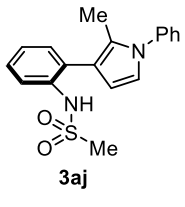
52 mg (62%), brown oil, **^{1}H NMR** (400 MHz, $CDCl_3$): *δ* 7.71–7.61 (m, 3H), 7.52–7.45 (m, 2H), 7.42–7.36 (m, 1H), 7.36–7.32 (m, 2H), 7.24 (td, *J* = 7.2, 1.8 Hz, 1H), 7.17–7.11 (m, 2H), 7.07 (td, *J* = 7.4, 1.2 Hz, 1H), 6.86–6.80 (m, 3H), 5.89 (d, *J* = 2.9 Hz, 1H), 3.75 (s, 3H), 1.86 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): *δ* 162.9, 139.8, 135.2, 131.2, 131.0, 129.24, 129.21, 127.7, 127.6, 127.3, 127.1, 125.7, 124.0, 121.8, 119.3, 117.2, 114.0, 108.7, 55.4, 11.0; **HRMS** (ESI) *m/z*: calcd for $C_{24}H_{23}N_2O_3S^+$ $[M+H]^+$, 419.1424; found, 419.1458;



3af

2-fluoro-*N*-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3af**)

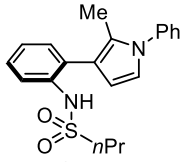
44 mg (54%), yellowish powder, **M. p.** = 130–131 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): *δ* 7.88 (td, *J* = 7.5, 1.8 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 1H), 7.53–7.44 (m, 4H), 7.43–7.35 (m, 3H), 7.23–7.14 (m, 3H), 7.09–6.98 (m, 2H), 6.87 (d, *J* = 2.9 Hz, 1H), 6.11 (d, *J* = 2.9 Hz, 1H), 1.91 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): *δ* 158.9 (d, *J* = 256.4 Hz), 140.0, 135.2 (d, *J* = 8.4 Hz), 134.7, 131.3, 130.9, 129.2, 127.7, 127.5, 127.4, 127.2 (d, *J* = 13.4 Hz), 127.0, 125.8, 124.2 (d, *J* = 3.8 Hz), 124.0, 122.0, 118.5, 117.0 (d, *J* = 2.2 Hz), 116.8, 108.8, 11.0; **^{19}F NMR** (376 MHz, $CDCl_3$): *δ* -109.4 (m, 1F); **HRMS** (ESI) *m/z*: calcd for $C_{23}H_{20}FN_2O_2S^+$ $[M+H]^+$, 407.1224; found, 407.1224;



3aj

N-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)methanesulfonamide (**3aj**)

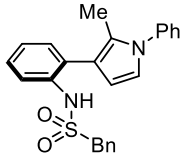
39 mg (59%), yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65 (dd, J = 8.2, 1.2 Hz, 1H), 7.53–7.46 (m, 2H), 7.43–7.39 (m, 1H), 7.39–7.32 (m, 3H), 7.31–7.28 (m, 1H), 7.16 (td, J = 7.5, 1.2 Hz, 1H), 6.93 (br s, 1H), 6.89 (d, J = 2.9 Hz, 1H), 6.20 (d, J = 2.9 Hz, 1H), 2.96 (s, 3H), 2.08 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 139.8, 135.5, 131.7, 129.2, 128.2, 127.4, 127.2, 127.0, 125.8, 124.0, 122.2, 118.0, 117.3, 108.9, 39.3, 11.3; **HRMS** (ESI) *m/z*: calcd for $C_{18}H_{19}N_2O_2S^+$ $[M+H]^+$, 327.1162; found, 327.1159;



3ak

N-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)propane-1-sulfonamide (**3ak**)

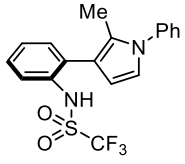
34 mg (48%), brown oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65 (dd, J = 8.2, 1.2 Hz, 1H), 7.53–7.45 (m, 2H), 7.43–7.34 (m, 3H), 7.34–7.24 (m, 2H), 7.15 (td, J = 7.5, 1.2 Hz, 1H), 6.90 (br s, 1H), 6.89 (d, J = 2.9 Hz, 1H), 6.21 (d, J = 2.9 Hz, 1H), 3.08–2.99 (m, 2H), 2.08 (s, 3H), 1.79–1.68 (m, 2H), 0.97 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 139.8, 135.6, 131.6, 129.2, 128.1, 127.4, 127.0, 126.8, 125.8, 123.7, 122.2, 117.8, 117.3, 108.8, 53.2, 17.0, 12.8, 11.2; **HRMS** (ESI) *m/z*: calcd for $C_{20}H_{23}N_2O_2S^+$ $[M+H]^+$, 355.1475; found, 355.1484;



3al

N-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-1-phenylmethanesulfonamide (**3al**)

43 mg (54%), yellowish powder, **M. p.** = 50–52 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65 (dd, J = 8.2, 1.2 Hz, 1H), 7.49–7.43 (m, 2H), 7.40–7.35 (m, 1H), 7.34–7.25 (m, 7H), 7.22–7.18 (m, 2H), 7.14 (td, J = 7.4, 1.2 Hz, 1H), 6.84 (br s, 1H), 6.77 (d, J = 2.9 Hz, 1H), 5.93 (d, J = 2.9 Hz, 1H), 4.39 (s, 2H), 2.04 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 139.8, 135.6, 131.7, 130.6, 129.2, 128.8, 128.5, 128.0, 127.3, 127.0, 126.0, 125.8, 123.3, 122.0, 117.0, 116.3, 108.6, 57.2, 11.3 (1C is merged with other peaks); **HRMS** (ESI) *m/z*: calcd for $C_{24}H_{23}N_2O_2S^+$ $[M+H]^+$, 403.1475; found, 403.1494;

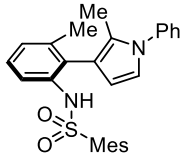


3am

1,1,1-trifluoro-*N*-(2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)methanesulfonamide (**3am**)

36 mg (47%), yellowish oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65 (dd, J = 8.2, 1.2 Hz, 1H),

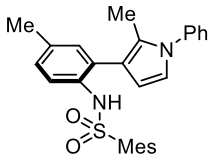
7.53–7.46 (m, 2H), 7.44–7.38 (m, 1H), 7.38–7.29 (m, 4H), 7.28–7.21 (m, 2H), 6.90 (d, *J* = 2.9 Hz, 1H), 6.22 (d, *J* = 2.9 Hz, 1H), 2.07 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): *δ* 139.8, 133.2, 131.6, 129.3, 128.3, 128.1, 127.6, 127.5, 125.9, 125.5, 122.4, 119.7 (q, *J* = 323.0 Hz), 119.1, 116.5, 108.6, 11.1; **^{19}F NMR** (376 MHz, $CDCl_3$): *δ* -75.9 (s, 3F); **HRMS** (ESI) *m/z*: calcd for $C_{18}H_{16}F_3N_2O_2S^+$ $[M+H]^+$, 381.0879; found, 381.0880;



3ap

2,4,6-trimethyl-*N*-(3-methyl-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3ap**)

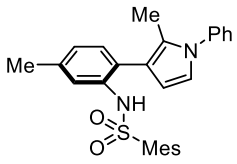
33 mg (37%), yellow powder, **M. p.** = 129–131 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): *δ* 7.53–7.47 (m, 2H), 7.43–7.37 (m, 1H), 7.36–7.31 (m, 3H), 7.14–7.06 (m, 2H), 6.96 (dt, *J* = 7.6, 1.1 Hz, 1H), 6.89 (d, *J* = 2.8 Hz, 1H), 6.82 (s, 2H), 5.97 (d, *J* = 2.9 Hz, 1H), 2.45 (s, 6H), 2.21 (s, 3H), 2.07 (s, 3H), 1.72 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): *δ* 142.1, 140.0, 139.3, 138.9, 135.9, 134.2, 131.9, 129.2, 127.4, 127.2, 127.1, 126.7, 125.5, 125.3, 122.0, 116.1, 115.7, 109.2, 22.9, 20.8, 20.5, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1952;



3aq

2,4,6-trimethyl-*N*-(4-methyl-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3aq**)

53 mg (59%), brown foam, **^{1}H NMR** (400 MHz, $CDCl_3$): *δ* 7.54–7.46 (m, 2H), 7.43–7.37 (m, 2H), 7.35–7.30 (m, 2H), 7.19 (br s, 1H), 7.01 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.96 (d, *J* = 2.1 Hz, 1H), 6.84 (d, *J* = 2.9 Hz, 1H), 6.79 (s, 2H), 6.08 (d, *J* = 2.9 Hz, 1H), 2.39 (s, 6H), 2.27 (s, 3H), 2.18 (s, 3H), 1.81 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): *δ* 142.0, 139.9, 139.3, 134.0, 133.7, 132.5, 131.8, 131.7, 129.2, 128.2, 128.1, 127.3, 126.9, 125.6, 121.7, 120.2, 117.8, 109.0, 22.8, 20.8, 20.7, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1962;

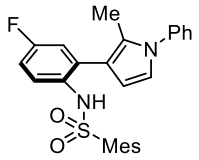


3ar

2,4,6-trimethyl-*N*-(5-methyl-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide

(**3ar**)

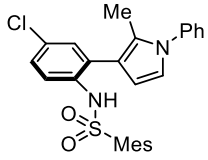
66 mg (74%), brown powder, **M. p.** = 148–149 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54–7.45 (m, 2H), 7.44–7.37 (m, 1H), 7.36–7.30 (m, 3H), 7.27 (br s, 1H), 7.03 (d, *J* = 7.7 Hz, 1H), 6.88 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.85 (d, *J* = 2.9 Hz, 1H), 6.80 (s, 2H), 6.11 (d, *J* = 2.9 Hz, 1H), 2.42 (s, 6H), 2.30 (s, 3H), 2.19 (s, 3H), 1.83 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.1, 139.9, 139.3, 137.4, 134.9, 133.9, 131.8, 130.9, 129.2, 127.3, 127.0, 125.6, 124.78, 124.75, 121.7, 120.1, 117.5, 109.1, 22.7, 21.3, 20.8, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1964;



3as

N-(4-fluoro-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3as**)

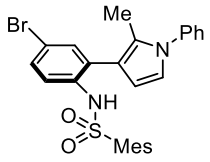
64 mg (71%), yellowish foam, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55–7.47 (m, 3H), 7.45–7.39 (m, 1H), 7.35–7.29 (m, 2H), 7.21 (br s, 1H), 6.92 (ddd, *J* = 9.0, 8.0, 3.0 Hz, 1H), 6.88–6.83 (m, 2H), 6.78 (s, 2H), 6.08 (d, *J* = 2.9 Hz, 1H), 2.36 (s, 6H), 2.18 (s, 3H), 1.78 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 159.4 (d, *J* = 244.2 Hz), 142.2, 139.7, 139.3, 133.7, 131.8, 131.0 (d, *J* = 2.8 Hz), 130.7 (d, *J* = 8.5 Hz), 129.3, 127.5, 127.1, 125.6, 122.6 (d, *J* = 8.6 Hz), 122.0, 117.6 (d, *J* = 22.1 Hz), 116.9, 114.1 (d, *J* = 22.3 Hz), 108.6, 22.8, 20.8, 10.8; **^{19}F NMR** (376 MHz, $CDCl_3$): δ -118.2 (m, 1F); **HRMS** (ESI) *m/z*: calcd for $C_{26}H_{26}FN_2O_2S^+$ $[M+H]^+$, 449.1694; found, 449.1714;



3at

N-(4-chloro-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3at**)

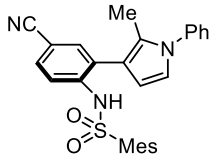
57 mg (61%), yellow powder, **M. p.** = 136–137 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54–7.48 (m, 2H), 7.47–7.39 (m, 2H), 7.35–7.30 (m, 2H), 7.27 (br s, 1H), 7.19–7.12 (m, 2H), 6.86 (d, *J* = 2.9 Hz, 1H), 6.81 (s, 2H), 6.10 (d, *J* = 2.9 Hz, 1H), 2.40 (s, 6H), 2.20 (s, 3H), 1.83 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.4, 139.7, 139.2, 133.8, 133.6, 131.9, 130.9, 129.7, 129.3, 129.2, 127.5, 127.4, 127.2, 125.7, 122.1, 120.9, 116.5, 108.8, 22.8, 20.8, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{26}H_{26}ClN_2O_2S^+$ $[M+H]^+$, 465.1398; found, 465.1400;



3au

N-(4-bromo-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3au**)

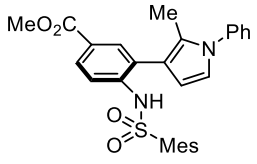
54 mg (53%), brown powder, **M. p.** = 157–158 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54–7.47 (m, 2H), 7.45–7.39 (m, 1H), 7.39–7.35 (m, 1H), 7.34–7.29 (m, 3H), 7.29 (s, 1H), 7.26 (br s, 1H), 6.86 (d, J = 2.9 Hz, 1H), 6.82 (s, 2H), 6.10 (d, J = 2.9 Hz, 1H), 2.41 (s, 6H), 2.20 (s, 3H), 1.85 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.5, 139.7, 139.2, 134.4, 133.8, 133.6, 132.0, 130.4, 129.9, 129.3, 127.5, 127.3, 125.7, 122.1, 121.0, 116.8, 116.4, 108.8, 22.8, 20.8, 11.0; **HRMS** (ESI) *m/z*: calcd for $C_{26}H_{26}BrN_2O_2S^+$ $[M+H]^+$, 509.0893; found, 509.0921;



3av

N-(4-cyano-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3av**)

69 mg (76%), brown powder, **M. p.** = 177–178 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (br s, 1H), 7.54–7.49 (m, 2H), 7.48–7.40 (m, 4H), 7.37–7.31 (m, 2H), 6.91 (d, J = 2.9 Hz, 1H), 6.89 (s, 2H), 6.17 (d, J = 2.9 Hz, 1H), 2.50 (s, 6H), 2.24 (s, 3H), 1.94 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 143.1, 139.7, 139.5, 139.2, 134.9, 133.2, 132.2, 131.6, 129.4, 127.7, 127.60, 127.55, 125.8, 122.6, 118.8, 117.6, 115.1, 108.6, 106.6, 22.7, 20.9, 11.0; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{26}N_3O_2S^+$ $[M+H]^+$, 456.1740; found, 456.1747;

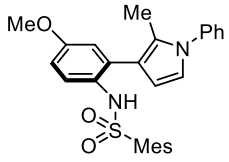


3aw

methyl 3-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)-4-((2,4,6-trimethylphenyl)sulfonamido)benzoate (**3aw**)

67 mg (68%), brown powder, **M. p.** = 144–145 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.89–7.82 (m, 2H), 7.55–7.48 (m, 3H), 7.46–7.39 (m, 2H), 7.37–7.33 (m, 2H), 6.90 (d, J = 2.9 Hz, 1H), 6.85 (s, 2H), 6.17 (d, J = 2.9 Hz, 1H), 3.85 (s, 3H), 2.49 (s, 6H), 2.22 (3H), 1.93 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.6, 142.7, 139.7, 139.6, 139.2, 133.4, 132.7, 132.1, 129.3, 129.2, 127.5, 127.4,

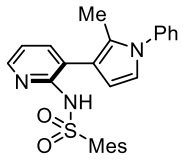
126.6, 125.7, 125.0, 122.2, 117.1, 116.4, 108.9, 51.9, 22.7, 20.9, 11.0; **HRMS** (ESI) *m/z*: calcd for $C_{28}H_{29}N_2O_4S^+$ $[M+H]^+$, 489.1843; found, 489.1861;



3ax

N-(4-methoxy-2-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3ax**)

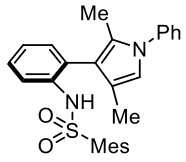
70 mg (76%), yellowish crystal, **M. p.** = 127–128 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55–7.47 (m, 3H), 7.43–7.37 (m, 1H), 7.34–7.29 (m, 2H), 7.11 (br s, 1H), 6.83 (d, J = 2.9 Hz, 1H), 6.78 (dd, J = 8.9, 3.0 Hz, 1H), 6.74 (s, 2H), 6.68 (d, J = 3.0 Hz, 1H), 6.05 (d, J = 2.9 Hz, 1H), 3.75 (s, 3H), 2.32 (s, 6H), 2.15 (s, 3H), 1.74 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 156.5, 141.9, 139.8, 139.3, 133.9, 131.7, 130.6, 129.3, 127.9, 127.3, 126.9, 125.5, 123.3, 121.7, 118.0, 116.2, 112.7, 108.8, 55.4, 22.9, 20.8, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_3S^+$ $[M+H]^+$, 461.1893; found, 461.1905;



3ay

2,4,6-trimethyl-*N*-(3-(2-methyl-1-phenyl-1*H*-pyrrol-3-yl)pyridin-2-yl)benzenesulfonamide (**3ay**)

75 mg (87%), brown oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.02 (br s, 1H), 7.64 (br s, 1H), 7.53–7.46 (m, 2H), 7.45–7.39 (m, 2H), 7.39–7.35 (m, 2H), 6.93 (s, 2H), 6.88 (d, J = 3.0 Hz, 1H), 6.87–6.83 (m, 1H), 6.26 (d, J = 2.9 Hz, 1H), 2.75 (s, 6H), 2.72 (s, 3H), 2.09 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.1, 146.1, 142.2, 140.0, 139.7, 139.0, 134.3, 131.6, 129.2, 127.5, 127.4, 125.8, 122.2, 119.2, 117.7, 115.9, 108.6, 22.8, 20.9, 11.3; **HRMS** (ESI) *m/z*: calcd for $C_{25}H_{26}N_3O_2S^+$ $[M+H]^+$, 432.1740; found, 432.1747;

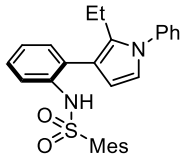


3az

N-(2-(2,4-dimethyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3az**)

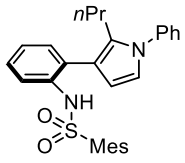
16 mg (18%), light red powder, **M. p.** = 61–63 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (dd, J = 8.2, 1.2 Hz, 1H), 7.51–7.45 (m, 2H), 7.40–7.35 (m, 1H), 7.34–7.29 (m, 2H), 7.22 (ddd, J = 8.2, 7.1, 1.9 Hz, 1H), 7.14–7.03 (m, 3H), 6.80 (s, 2H), 6.68 (d, J = 1.1 Hz, 1H), 2.41 (s, 6H), 2.19 (s, 3H), 1.82 (s, 3H), 1.76 (d, J = 1.1 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.2, 140.0, 139.2,

135.6, 134.0, 131.9, 131.8, 129.2, 127.8, 127.0, 126.7, 126.6, 125.5, 123.9, 119.8, 119.0, 118.2, 118.0, 22.7, 20.8, 11.2, 10.2; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1969;



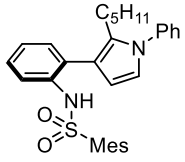
3aA

N-(2-(2-ethyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3aA**)
44 mg (49%), brown powder, **M. p.** = 141–143 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.53–7.47 (m, 2H), 7.45–7.35 (m, 4H), 7.28 (br s, 1H), 7.22–7.15 (m, 2H), 7.04 (td, *J* = 7.4, 1.3 Hz, 1H), 6.87 (s, 2H), 6.81 (d, *J* = 2.9 Hz, 1H), 6.06 (d, *J* = 2.9 Hz, 1H), 2.50 (s, 6H), 2.37 (q, *J* = 7.5 Hz, 2H), 2.25 (s, 3H), 0.70 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.3, 140.2, 139.3, 135.5, 134.1, 133.3, 132.0, 131.4, 129.3, 127.68, 127.65, 127.3, 126.2, 123.5, 122.4, 118.4, 116.8, 109.1, 22.9, 20.9, 17.9, 14.5; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1949;



3aB

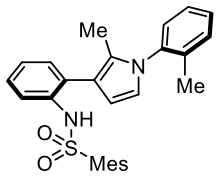
2,4,6-trimethyl-*N*-(2-(1-phenyl-2-propyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3aB**)
20 mg (22%), brown foam, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.53–7.47 (m, 2H), 7.45–7.33 (m, 4H), 7.26 (br s, 1H), 7.21–7.15 (m, 2H), 7.04 (td, *J* = 8.0, 1.2 Hz, 1H), 6.87 (s, 2H), 6.81 (d, *J* = 2.9 Hz, 1H), 6.05 (d, *J* = 2.9 Hz, 1H), 2.50 (s, 6H), 2.32 (t, *J* = 8.0 Hz, 2H), 2.25 (s, 3H), 1.12–1.00 (m, 2H), 0.55 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.3, 140.2, 139.3, 135.4, 134.1, 132.0, 131.8, 131.4, 129.3, 127.63, 127.59, 127.3, 126.1, 123.5, 122.5, 118.3, 117.3, 109.1, 26.6, 22.9, 20.9, 13.7 (1C is merged with other peaks); **HRMS** (ESI) *m/z*: calcd for $C_{28}H_{31}N_2O_2S^+$ $[M+H]^+$, 459.2101; found, 459.2100;



3aC

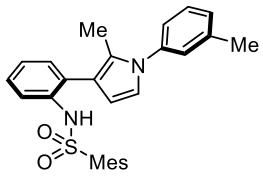
2,4,6-trimethyl-*N*-(2-(2-pentyl-1-phenyl-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3aC**)

28 mg (29%), yellowish oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.53–7.46 (m, 2H), 7.45–7.39 (m, 2H), 7.38–7.33 (m, 2H), 7.27 (br s, 1H), 7.21–7.15 (m, 2H), 7.03 (td, J = 7.4, 1.2 Hz, 1H), 6.87 (s, 2H), 6.80 (d, J = 2.9 Hz, 1H), 6.05 (d, J = 2.9 Hz, 1H), 2.49 (s, 6H), 2.31 (t, J = 8.0 Hz, 2H), 2.24 (s, 3H), 1.09–1.00 (m, 2H), 1.00–0.86 (m, 4H), 0.64 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.2, 140.2, 139.3, 135.4, 134.2, 132.0, 131.3, 129.2, 127.6, 127.4, 126.1, 123.5, 122.4, 118.4, 117.2, 109.1, 31.2, 29.1, 24.4, 22.9, 21.8, 20.9, 13.7 (2C are merged with other peaks); **HRMS** (ESI) *m/z*: calcd for $C_{30}H_{35}N_2O_2S^+$ $[M+H]^+$, 487.2414; found, 487.2404;



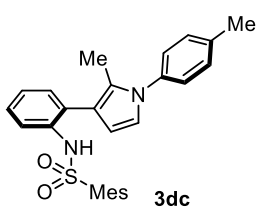
3bc

2,4,6-trimethyl-*N*-(2-(2-methyl-1-(*o*-tolyl)-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3bc**)
59 mg (66%), yellowish foam, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.42–7.29 (m, 5H), 7.27–7.23 (m, 1H), 7.19–7.12 (m, 2H), 7.02 (td, J = 7.4, 1.2 Hz, 1H), 6.85 (s, 2H), 6.71 (d, J = 2.8 Hz, 1H), 6.16 (d, J = 2.8 Hz, 1H), 2.50 (s, 6H), 2.22 (s, 3H), 2.08 (s, 3H), 1.76 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.3, 139.3, 138.9, 135.9, 135.3, 133.8, 131.9, 131.3, 130.9, 128.6, 127.9, 127.6, 127.5, 127.1, 126.6, 123.4, 121.7, 117.9, 116.3, 108.6, 22.8, 20.9, 17.2, 10.3; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1969



3cc

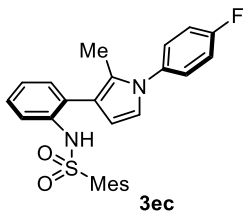
2,4,6-trimethyl-*N*-(2-(2-methyl-1-(*m*-tolyl)-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3cc**)
55 mg (62%), yellowish powder, **M. p.** = 144–145 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.48 (dd, J = 8.2, 1.2 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 7.31 (br s, 1H), 7.24–7.11 (m, 5H), 7.06 (td, J = 7.4, 1.3 Hz, 1H), 6.85 (d, J = 2.9 Hz, 1H), 6.81 (s, 2H), 6.11 (d, J = 2.9 Hz, 1H), 2.45 (s, 3H), 2.42 (s, 6H), 2.20 (s, 3H), 1.83 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.1, 139.9, 139.3, 135.2, 134.0, 131.8, 131.2, 129.0, 128.1, 127.9, 127.5, 127.0, 126.3, 124.0, 122.7, 121.8, 119.6, 117.4, 108.8, 22.8, 21.4, 20.8, 10.9 (1C is merged with other peaks); **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1966



3dc

2,4,6-trimethyl-*N*-(2-(2-methyl-1-(*p*-tolyl)-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3dc**)

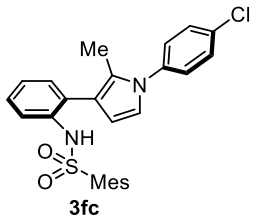
50 mg (56%), yellowish oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.48 (dd, J = 8.1, 1.2 Hz, 1H), 7.34–7.27 (m, 3H), 7.23–7.13 (m, 4H), 7.05 (td, J = 7.5, 1.3 Hz, 1H), 6.83 (d, J = 2.9 Hz, 1H), 6.80 (s, 2H) 6.11 (d, J = 2.9 Hz, 1H), 2.44 (s, 3H), 2.42 (s, 6H), 2.19 (s, 3H), 1.82 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.1, 139.3, 137.4, 137.3, 135.2, 133.9, 131.8, 131.2, 129.8, 127.9, 127.5, 127.1, 125.5, 124.0, 121.9, 119.6, 117.3, 108.7, 22.8, 21.0, 20.8, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_2S^+$ $[M+H]^+$, 445.1944; found, 445.1964;



3ec

N-(2-(1-(4-fluorophenyl)-2-methyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3ec**)

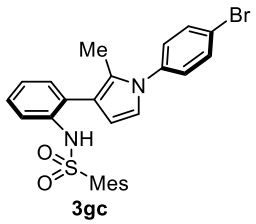
45 mg (50%), yellowish crystal, **M. p.** = 137–139 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.44 (dd, J = 8.1, 1.2 Hz, 1H), 7.34–7.28 (m, 2H), 7.25 (br s, 1H), 7.22–7.16 (m, 3H), 7.14 (dd, J = 7.6, 1.7 Hz, 1H), 7.06 (td, J = 7.4, 1.2 Hz, 1H), 6.84–6.79 (m, 3H), 6.13 (d, J = 2.9 Hz, 1H), 2.44 (s, 6H), 2.21 (s, 3H), 1.83 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 161.7 (d, J = 247.5 Hz), 142.2, 139.3, 136.0 (d, J = 3.2 Hz), 135.2, 134.0, 131.9, 131.2, 127.64, 127.60, 127.4 (d, J = 8.6 Hz), 127.2, 123.9, 121.9, 119.4, 117.6, 116.2 (d, J = 22.7 Hz), 109.1, 22.8, 20.8, 10.8; **^{19}F NMR** (376 MHz, $CDCl_3$): δ -114.0 (s, 1F); **HRMS** (ESI) *m/z*: calcd for $C_{26}H_{26}FN_2O_2S^+$ $[M+H]^+$, 449.1694; found, 449.1719;



3fc

N-(2-(1-(4-chlorophenyl)-2-methyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3fc**)

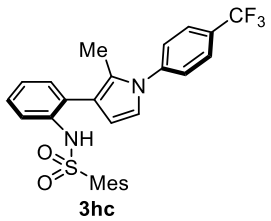
68 mg (73%), white powder, **M. p.** = 129–130 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.50–7.45 (m, 2H), 7.44 (dd, J = 8.1, 1.2 Hz, 1H), 7.31–7.26 (m, 2H), 7.23 (br s, 1H), 7.19 (td, J = 7.8, 1.8 Hz, 1H), 7.13 (dd, J = 7.6, 1.7 Hz, 1H), 7.06 (td, J = 7.4, 1.2 Hz, 1H), 6.83 (d, J = 2.9 Hz, 1H), 6.81 (s, 2H), 6.14 (d, J = 2.9 Hz, 1H), 2.43 (s, 6H), 2.20 (s, 3H), 1.84 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.2, 139.2, 138.4, 135.2, 133.9, 133.1, 131.9, 131.2, 129.4, 127.7, 127.5, 127.0, 126.8, 124.0, 121.7, 119.5, 118.0, 109.4, 22.8, 20.8, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{26}H_{26}ClN_2O_2S^+$ $[M+H]^+$, 465.1398; found, 465.1405;



3gc

N-(2-(1-(4-bromophenyl)-2-methyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3gc**)

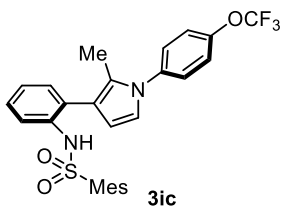
58 mg (57%), offwhite powder, **M. p.** = 147–148 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65–7.60 (m, 2H), 7.44 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.25–7.16 (m, 4H), 7.13 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.06 (td, *J* = 7.4, 1.3 Hz, 1H), 6.83 (d, *J* = 2.9 Hz, 1H), 6.81 (s, 2H), 6.14 (d, *J* = 2.9 Hz, 1H), 2.43 (s, 6H), 2.20 (s, 3H), 1.84 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.2, 139.2, 138.9, 135.2, 133.9, 132.4, 131.9, 131.2, 127.7, 127.5, 127.1, 126.9, 124.0, 121.6, 121.0, 119.5, 118.0, 109.5, 22.7, 20.8, 10.9; **HRMS** (ESI) *m/z*: calcd for $C_{26}H_{26}BrN_2O_2S^+$ $[M+H]^+$, 509.0893; found, 509.0897;



3hc

2,4,6-trimethyl-*N*-(2-(2-methyl-1-(4-(trifluoromethyl)phenyl)-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3hc**)

21 mg (21%), yellowish powder, **M. p.** = 175–176 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.82–7.73 (m, 2H), 7.51–7.45 (m, 2H), 7.42 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.23–7.17 (m, 2H), 7.15 (dd, 7.5, 1.7 Hz, 1H), 7.07 (td, *J* = 7.4, 1.2 Hz, 1H), 6.89 (d, *J* = 3.0 Hz, 1H), 6.82 (s, 2H), 6.19 (d, *J* = 2.9 Hz, 1H), 2.44 (s, 6H), 2.21 (s, 3H), 1.90 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 142.8, 142.3, 139.3, 135.2, 134.0, 131.9, 131.2, 129.3 (q, *J* = 32.7 Hz), 127.8, 127.3, 127.0, 126.6 (q, *J* = 3.6 Hz), 125.6, 124.0, 123.8 (q, *J* = 272.2 Hz), 121.6, 119.5, 118.7, 110.1, 22.8, 20.8, 11.1; **^{19}F NMR** (376 MHz, $CDCl_3$): δ -62.2 (s, 3F); **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{26}F_3N_2O_2S^+$ $[M+H]^+$, 499.1662; found, 499.1667

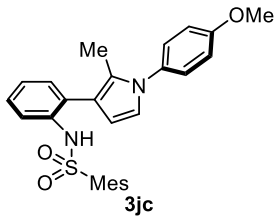


3ic

2,4,6-trimethyl-*N*-(2-(2-methyl-1-(4-(trifluoromethoxy)phenyl)-1*H*-pyrrol-3-yl)phenyl)benzenesulfonamide (**3ic**)

58 mg (56%), yellow foam, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.43 (dd, *J* = 8.1, 1.2 Hz, 1H),

7.41–7.33 (m, 4H), 7.23–7.17 (m, 2H), 7.14 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.06 (td, *J* = 7.4, 1.2 Hz, 1H), 6.85 (d, *J* = 2.9 Hz, 1H), 6.82 (s, 2H), 6.15 (d, *J* = 2.9 Hz, 1H), 2.44 (s, 6H), 2.21 (s, 3H), 1.86 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 148.0, 142.3, 139.3, 138.4, 135.2, 134.0, 131.9, 131.2, 127.7, 127.4, 127.1, 127.0, 124.0, 121.83, 121.8, 120.4 (q, *J* = 257.8 Hz), 119.5, 118.1, 109.6, 22.8, 20.8, 11.0; **^{19}F NMR** (376 MHz, $CDCl_3$): δ -57.8 (s, 3F); **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{26}F_3N_2O_3S^+$ $[M+H]^+$, 515.1611; found, 515.1630;

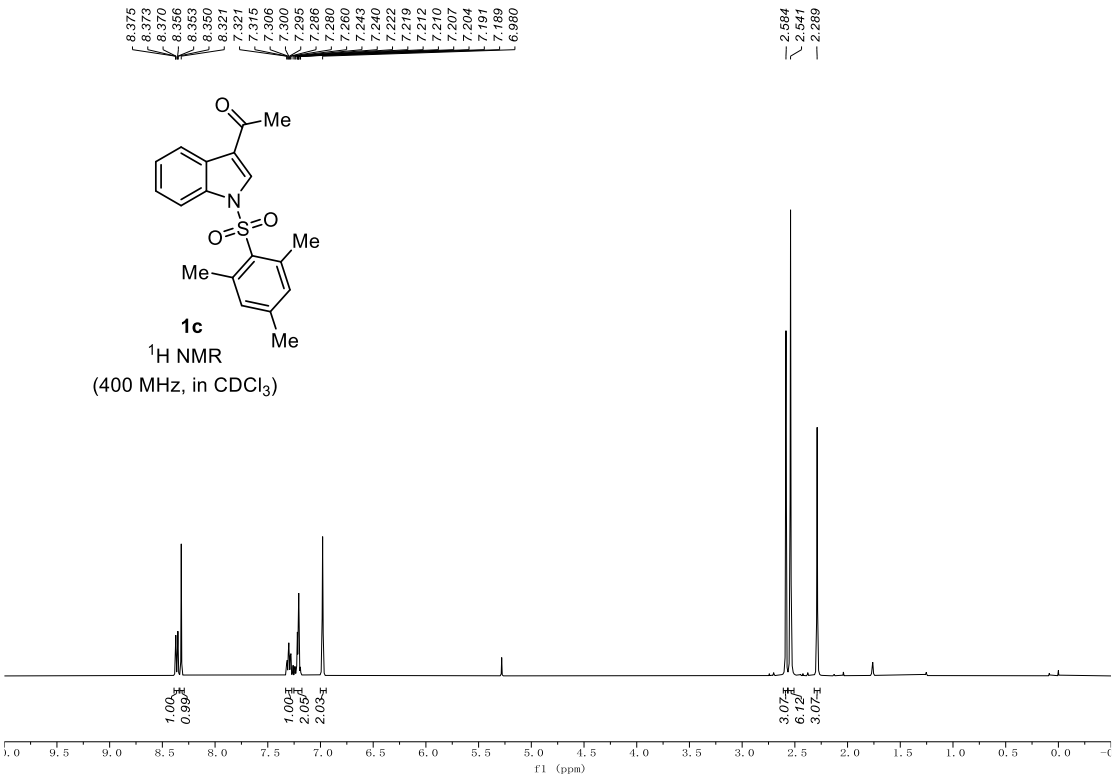


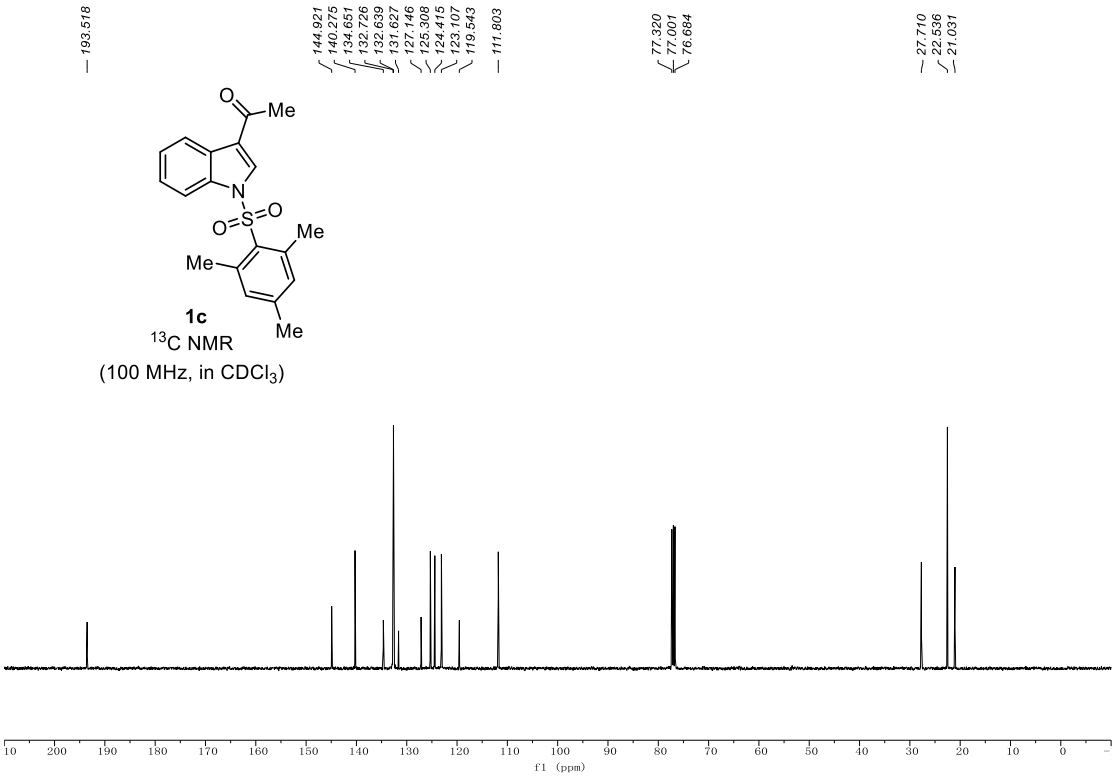
3jc

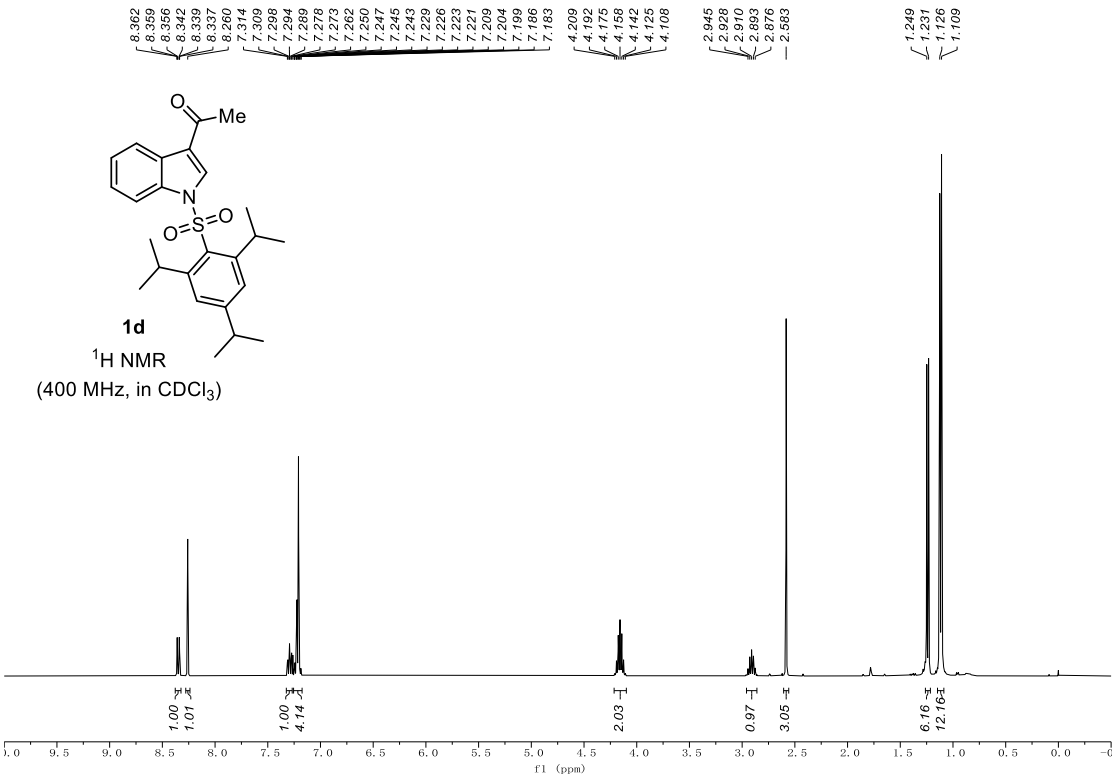
N-(2-(1-(4-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)phenyl)-2,4,6-trimethylbenzenesulfonamide (**3jc**)

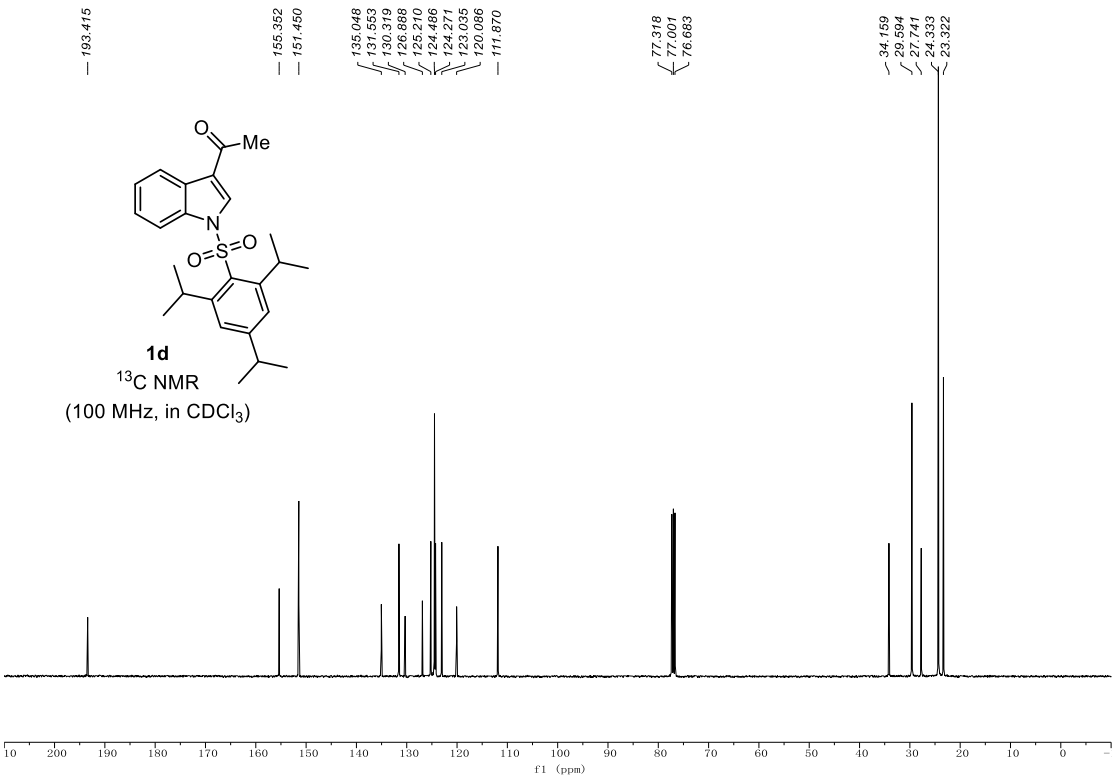
60 mg (65%), yellowish foam, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.47 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.33 (br s, 1H), 7.27–7.23 (m, 2H), 7.21–7.16 (m, 1H), 7.14 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.05 (td, *J* = 7.4, 1.3 Hz, 1H), 7.03–6.98 (m, 2H), 6.81 (d, *J* = 2.9 Hz, 1H), 6.80 (s, 2H), 6.10 (d, *J* = 2.9 Hz, 1H), 3.88 (s, 3H), 2.42 (s, 6H), 2.20 (s, 3H), 1.80 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 158.8, 142.1, 139.3, 135.1, 133.9, 132.9, 131.8, 131.2, 127.9, 127.5, 127.3, 127.0, 123.9, 122.0, 119.5, 117.0, 114.3, 108.5, 55.5, 22.8, 20.8, 10.8; **HRMS** (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O_3S^+$ $[M+H]^+$, 461.1893; found, 461.1906;

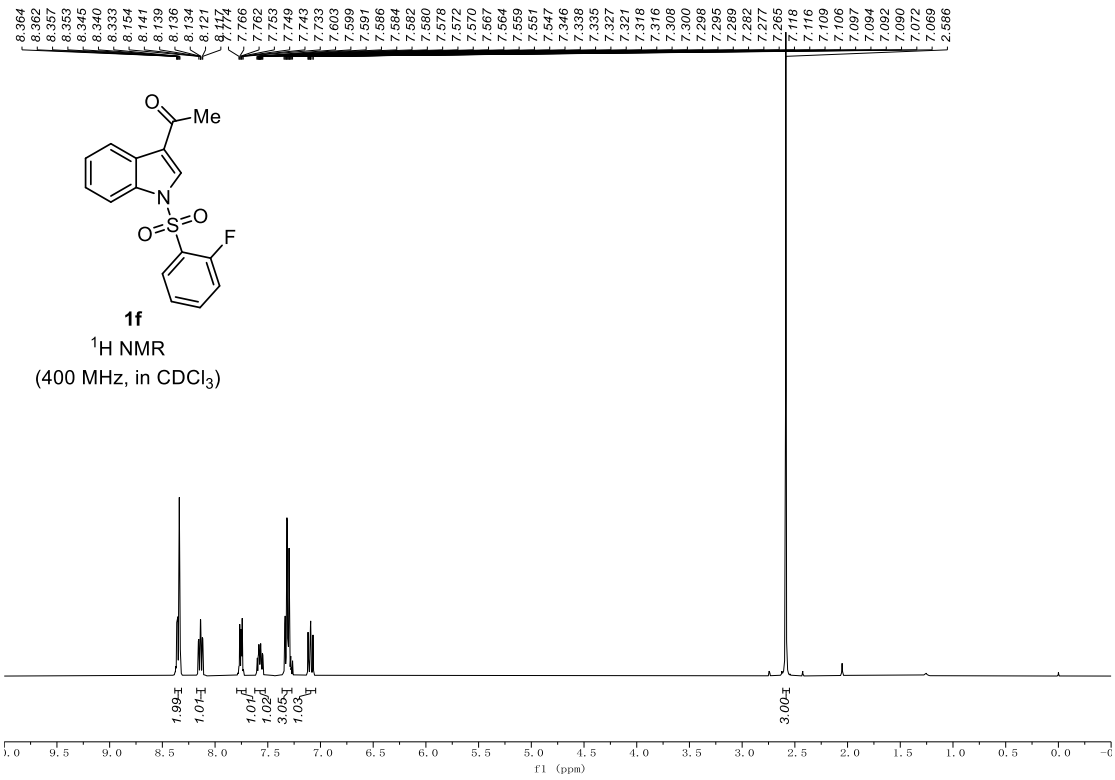
Copies of NMR spectra of unknown substrates and products






8.362
8.359
8.356
8.342
8.339
8.337
8.260
7.314
7.309
7.298
7.294
7.289
7.278
7.273
7.262
7.250
7.247
7.245
7.243
7.229
7.226
7.223
7.221
7.209
7.204
7.199
7.186
7.183
4.209
4.192
4.175
4.158
4.142
4.125
4.108
2.945
2.928
2.910
2.893
2.876
2.583
1.249
1.231
1.126
1.109
O
Me
N
O=S=O
1d
1H NMR
(400 MHz, in CDCl3)
1.00
1.01
1.00
4.14
2.03
0.97
3.05
6.16
12.16
f1 (ppm)

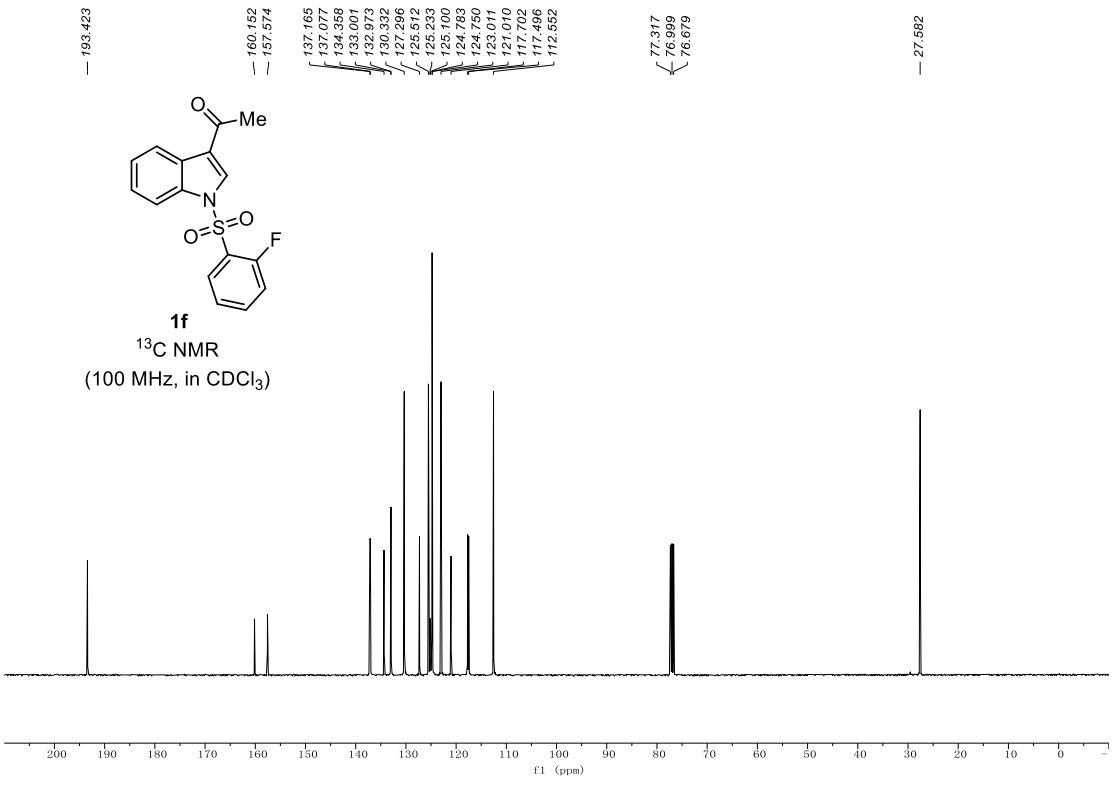

193.415
155.352
151.450
135.048
131.553
130.319
126.888
125.210
124.486
124.271
123.035
120.086
111.870
77.318
77.001
76.683
34.159
29.594
27.741
24.333
23.322
O
Me
N
O=S=O
1d
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)



1f

^{1}H NMR

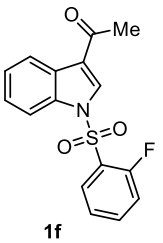
(400 MHz, in $CDCl_3$)



1f

^{13}C NMR

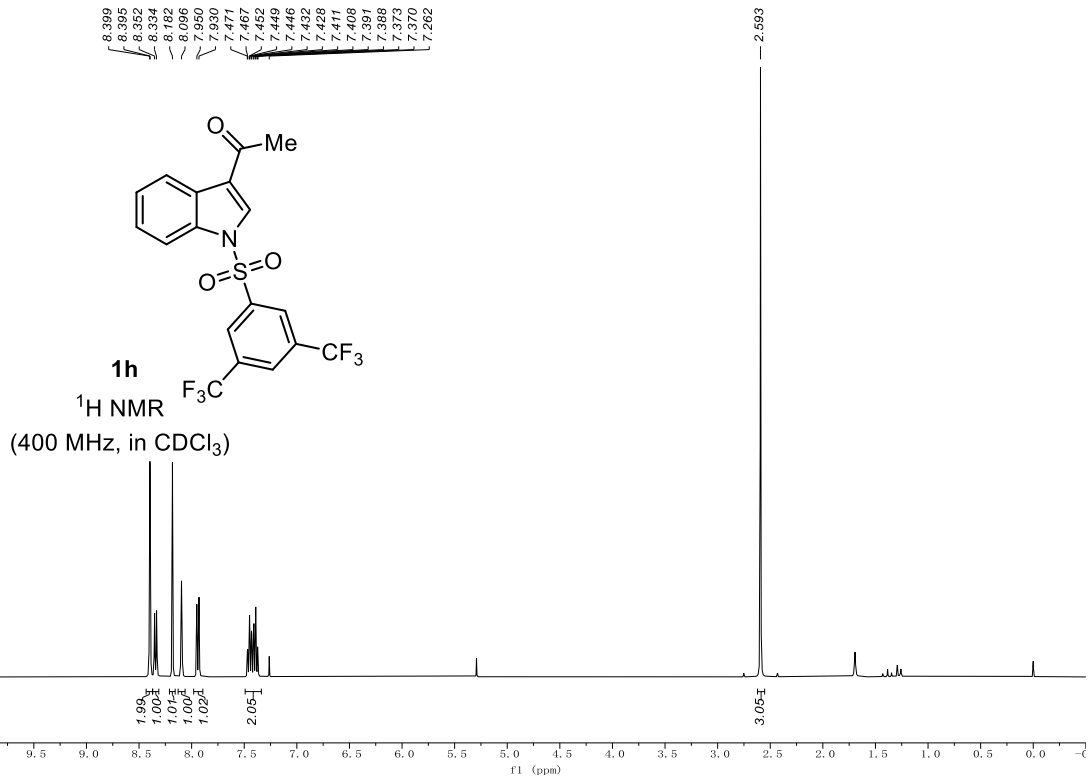
(100 MHz, in $CDCl_3$)



1f

^{19}F NMR

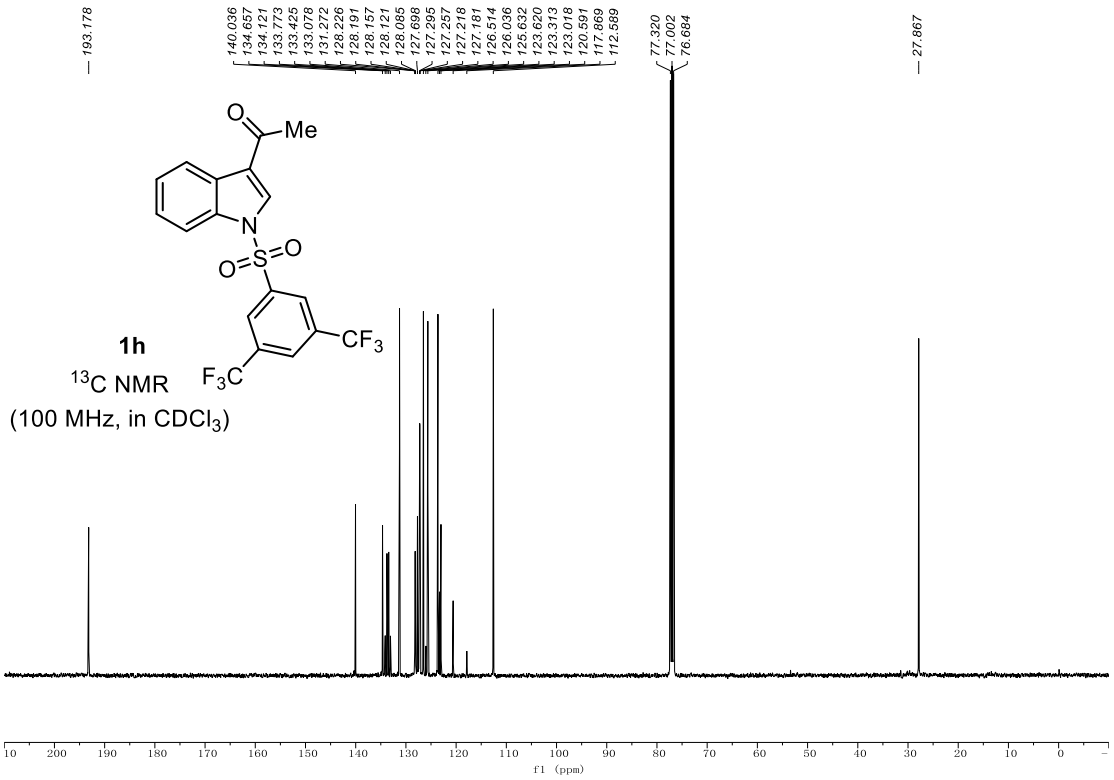
(376 MHz, in $CDCl_3$)

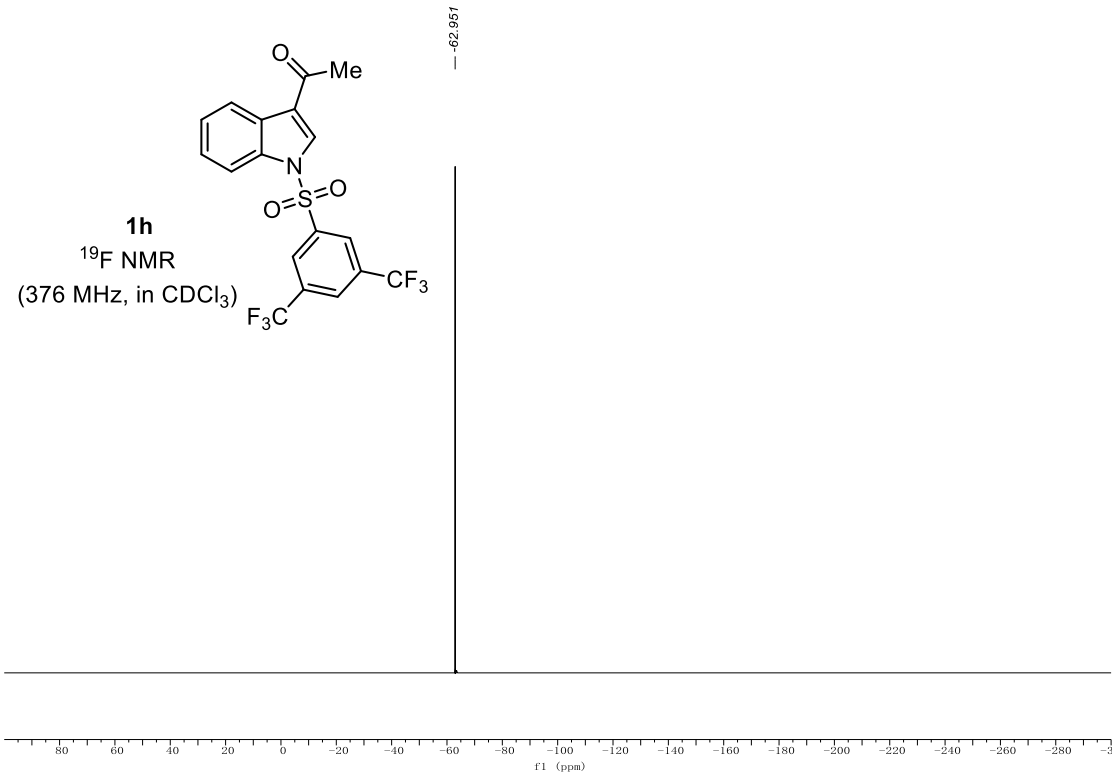


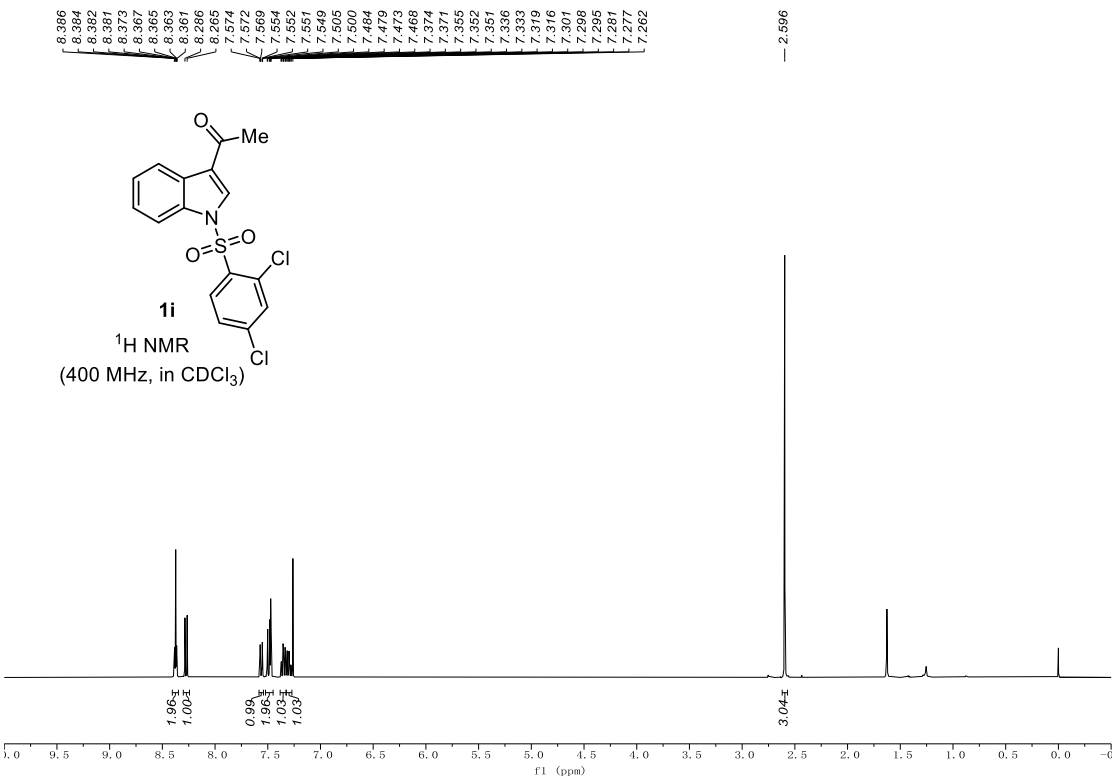
1h

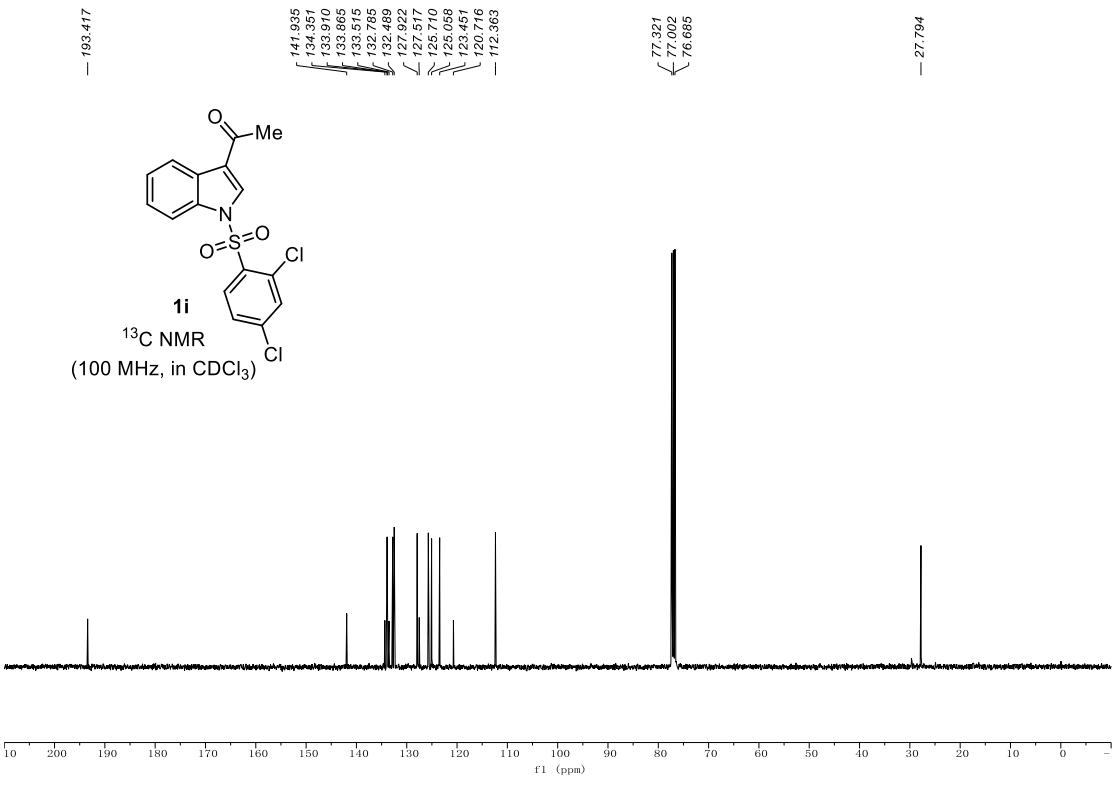
^{1}H NMR

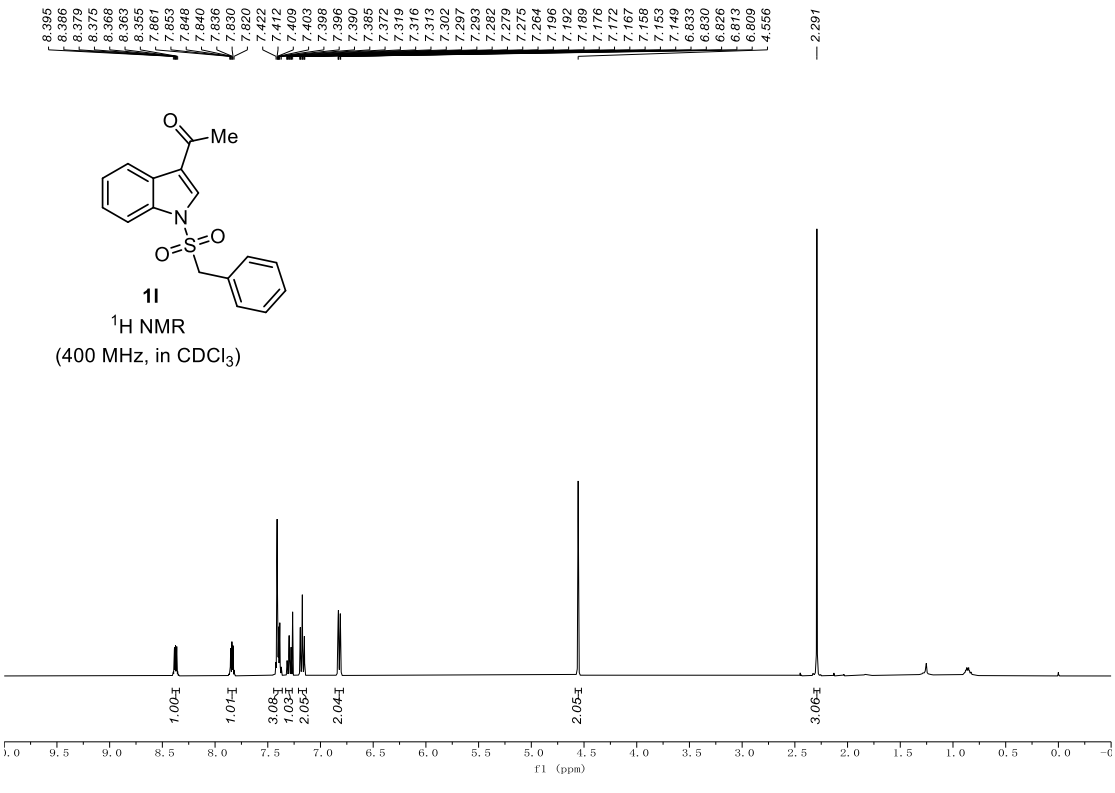
(400 MHz, in $CDCl_3$)

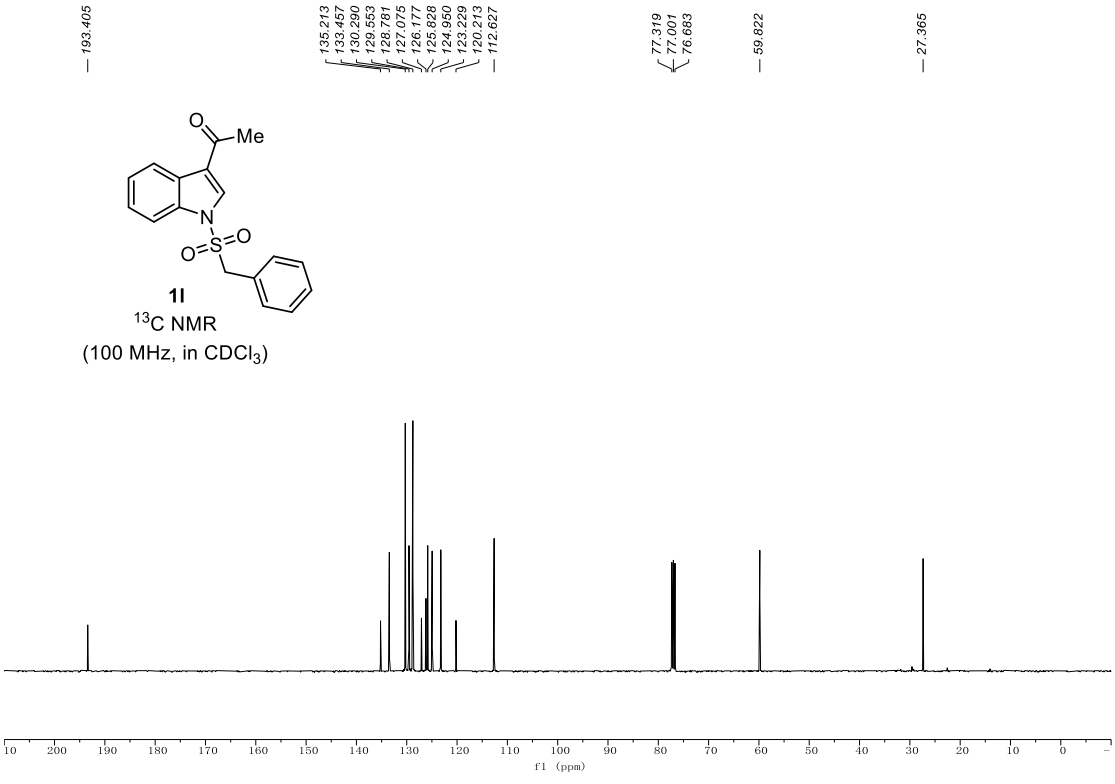

193.178
140.036
134.657
134.121
133.773
133.425
133.078
131.272
128.226
128.191
128.157
128.121
128.085
127.698
127.295
127.257
127.218
127.181
126.514
126.036
125.632
123.620
123.313
123.018
120.591
117.869
112.589
77.320
77.002
76.684
27.867
O
Me
N
O=S=O
CF3
F3C
1h
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

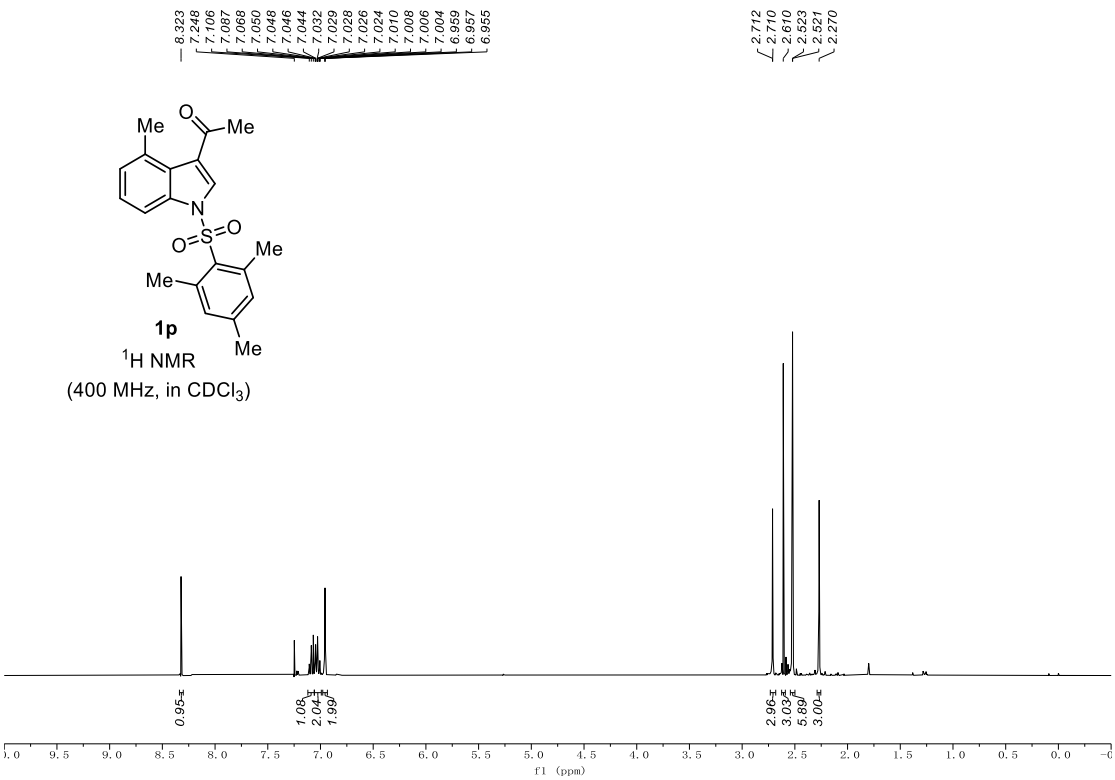

-62.951
O
Me
N
O=S=O
CF3
F3C
1h
19F NMR
(376 MHz, in CDCl3)
f1 (ppm)


8.386
8.384
8.382
8.381
8.373
8.367
8.365
8.363
8.361
8.286
8.265
7.574
7.572
7.569
7.554
7.552
7.551
7.549
7.505
7.500
7.464
7.479
7.473
7.468
7.374
7.371
7.355
7.352
7.351
7.336
7.333
7.319
7.316
7.301
7.298
7.295
7.281
7.277
7.262
2.596
O
Me
N
O=S=O
Cl
Cl
1i
1H NMR
(400 MHz, in CDCl3)
1.96
1.00
0.99
1.96
1.03
1.03
3.04
f1 (ppm)

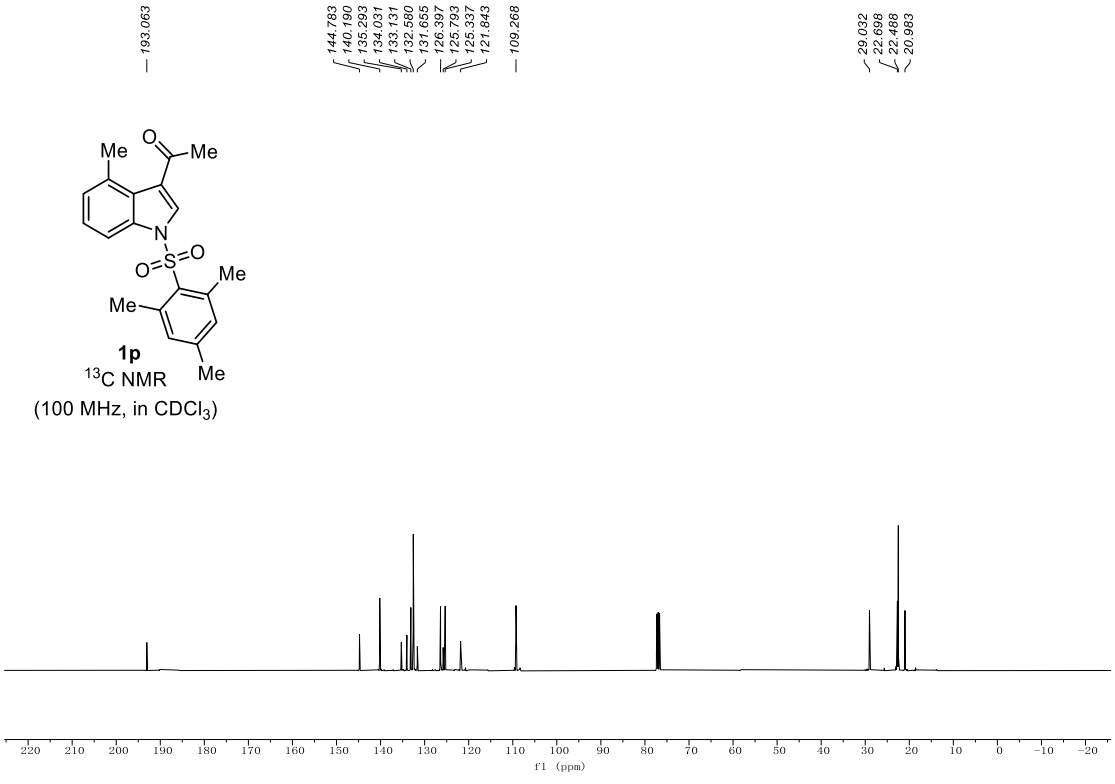

193.417
141.935
134.351
133.910
133.865
133.515
132.785
132.489
127.922
127.517
125.710
125.058
123.451
120.716
112.363
77.321
77.002
76.685
27.794
O
Me
N
O=S=O
Cl
Cl
1i
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)


8.395
8.386
8.379
8.375
8.368
8.363
8.355
7.861
7.853
7.848
7.840
7.836
7.830
7.820
7.422
7.412
7.409
7.403
7.398
7.396
7.390
7.385
7.372
7.319
7.316
7.313
7.302
7.297
7.293
7.282
7.279
7.275
7.264
7.196
7.192
7.189
7.176
7.172
7.167
7.158
7.153
7.149
6.833
6.830
6.826
6.813
6.809
4.556
2.291
O
Me
N
S
O
O
1l
1H NMR
(400 MHz, in CDCl3)
1.00
1.01
3.08
1.03
2.05
2.04
2.05
3.06
f1 (ppm)

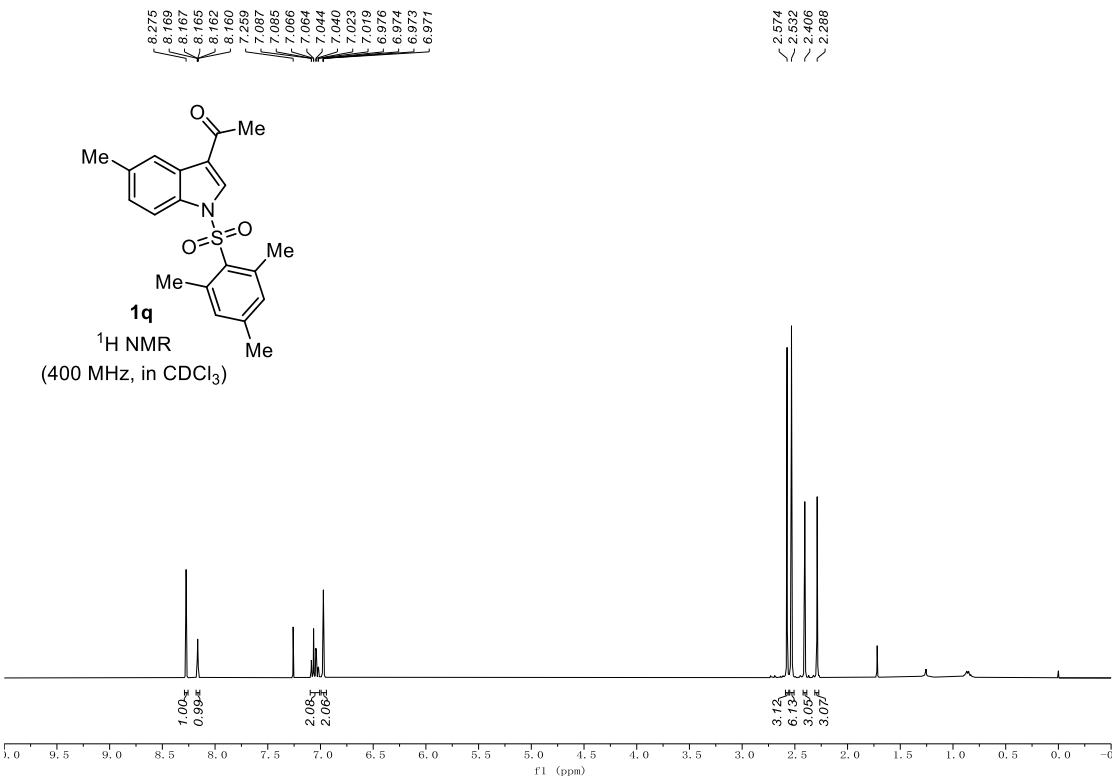

193.405
135.213
133.457
130.290
129.553
128.781
127.075
126.177
125.828
124.950
123.229
120.213
112.627
77.319
77.001
76.683
59.822
27.365
O
Me
N
S
O
O
1l
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

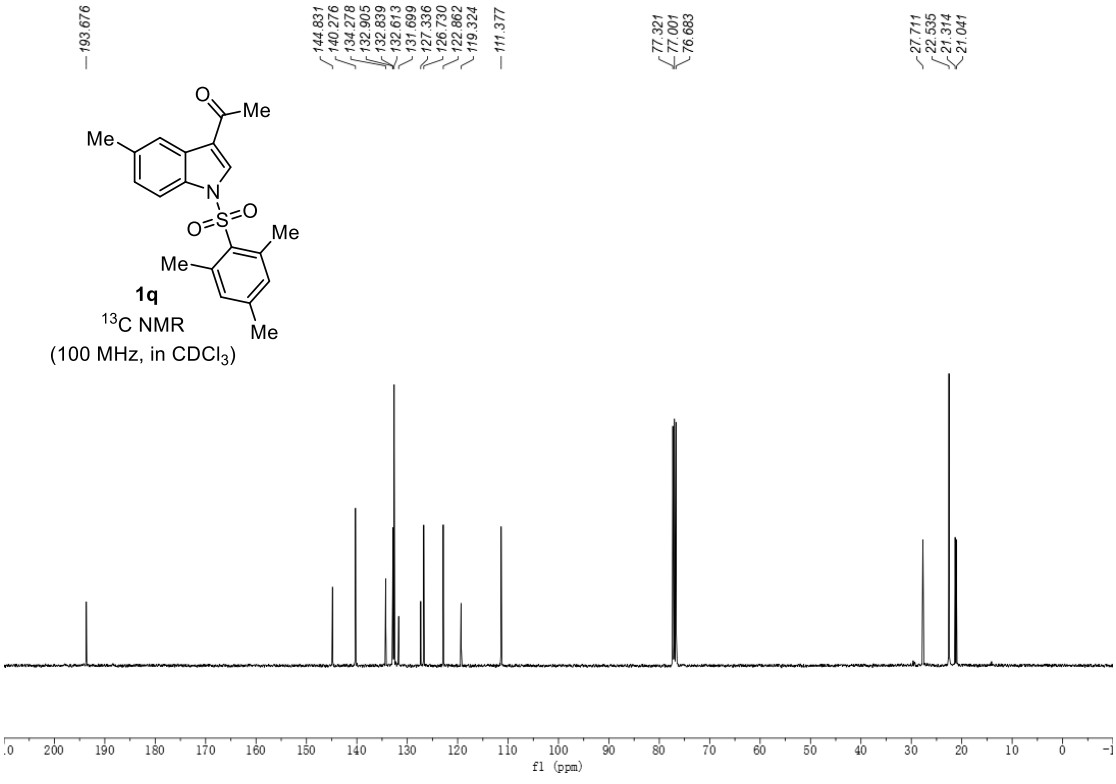


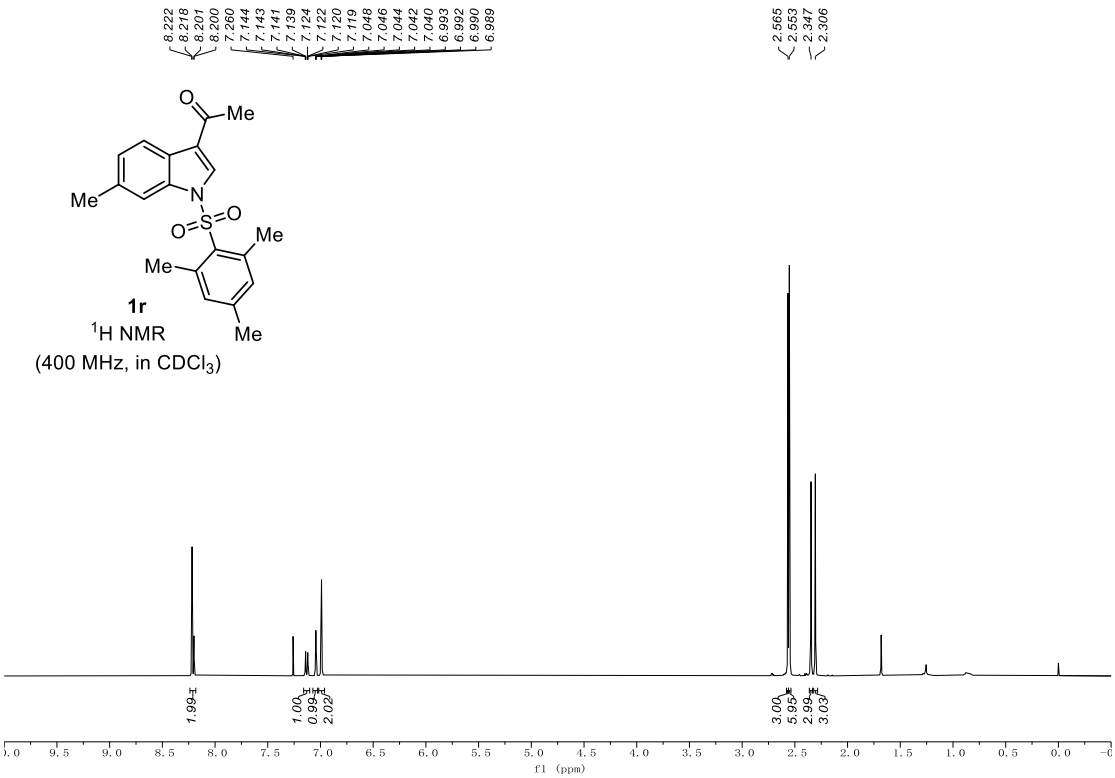
^{1}H NMR
(400 MHz, in $CDCl_3$)



^{13}C NMR
(100 MHz, in $CDCl_3$)


8.275
8.169
8.167
8.165
8.162
8.160
7.259
7.087
7.085
7.066
7.064
7.044
7.040
7.023
7.019
6.976
6.974
6.973
6.971
2.574
2.532
2.406
2.288
Me
Me
O
Me
N
O=S=O
Me
Me
Me
1q
1H NMR
(400 MHz, in CDCl3)
1.00
0.99
2.08
2.06
3.12
6.13
3.05
3.07
f1 (ppm)

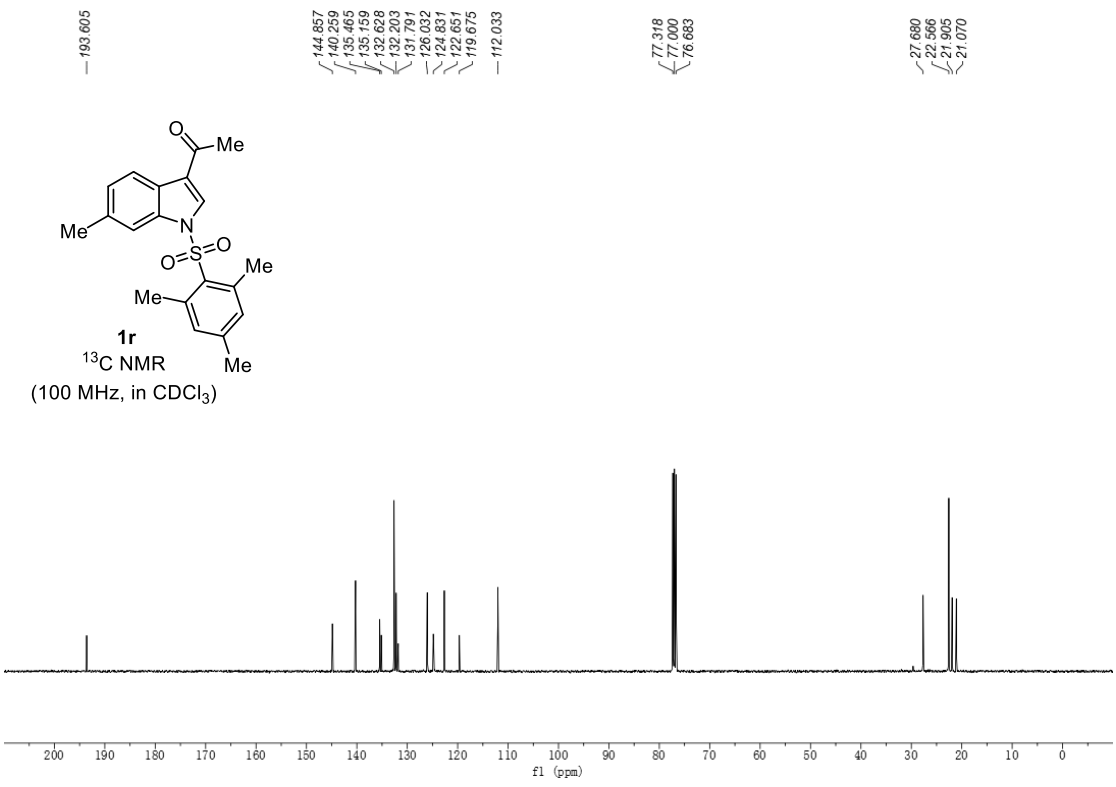

193.676
144.831
140.276
134.278
132.905
132.839
132.613
131.699
127.336
126.730
122.862
119.324
111.377
77.321
77.001
76.683
27.711
22.535
21.314
21.041
Me
Me
O
Me
N
O=S=O
Me
Me
Me
1q
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)



1r

^{1}H NMR

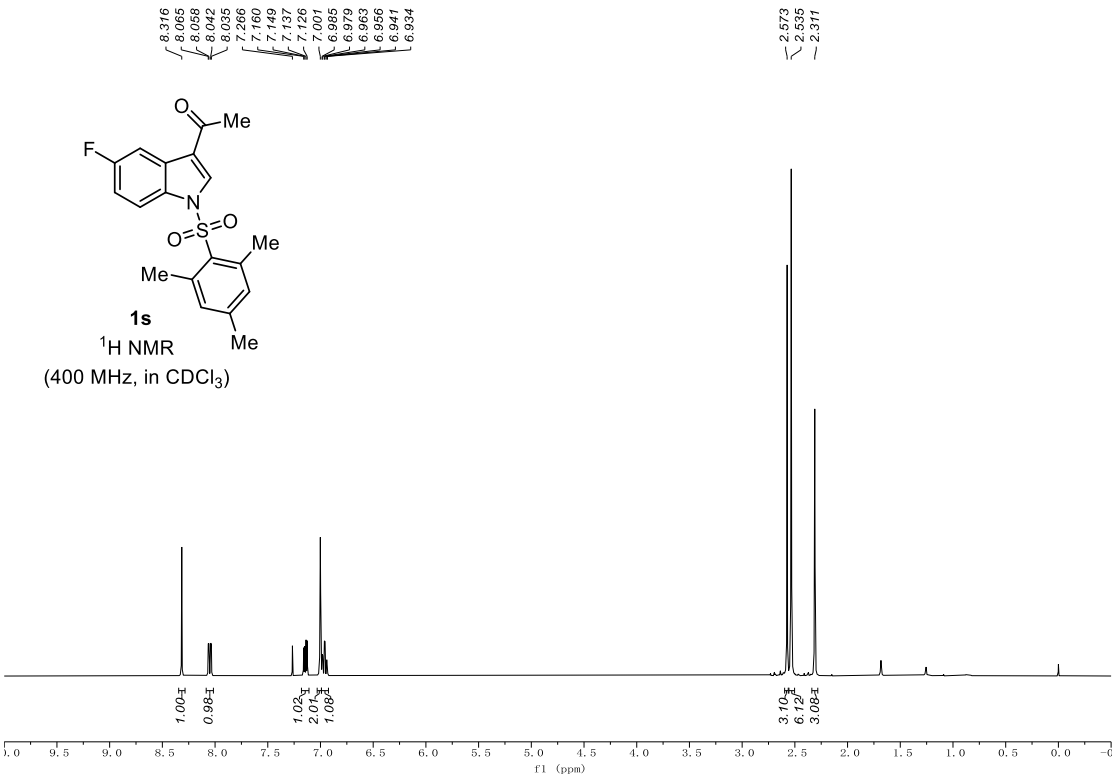
(400 MHz, in $CDCl_3$)



1r

^{13}C NMR

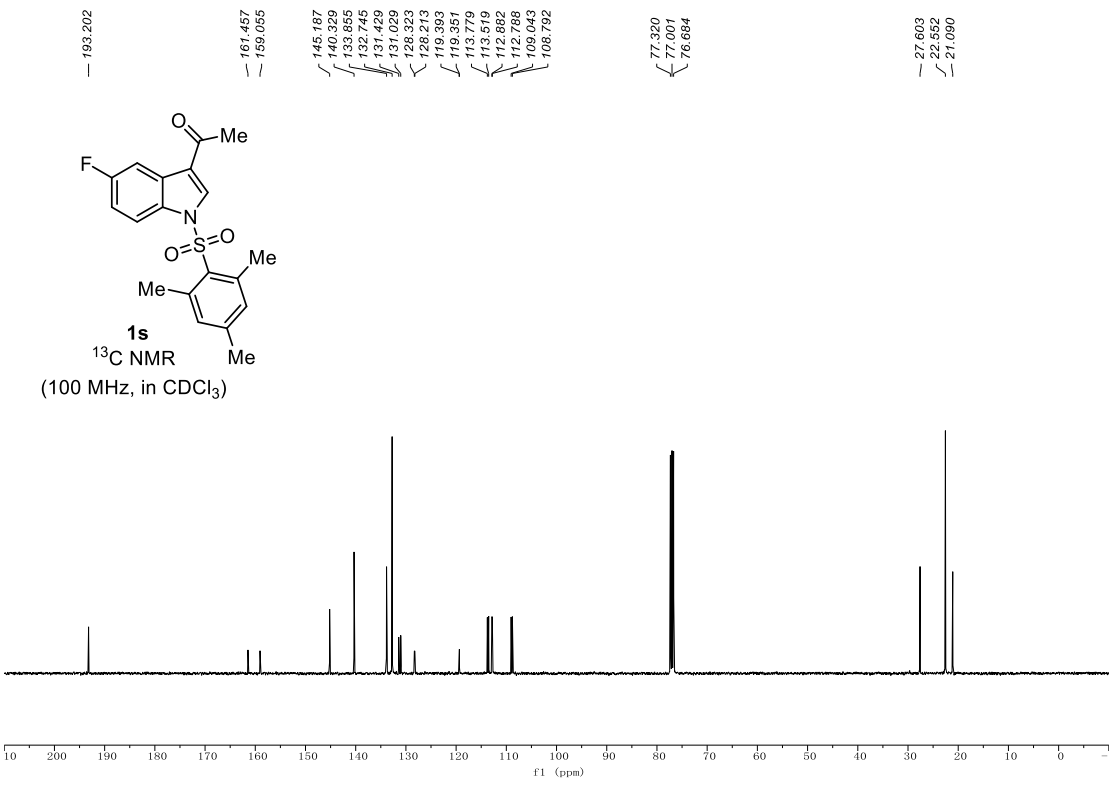
(100 MHz, in $CDCl_3$)



1s

^{1}H NMR

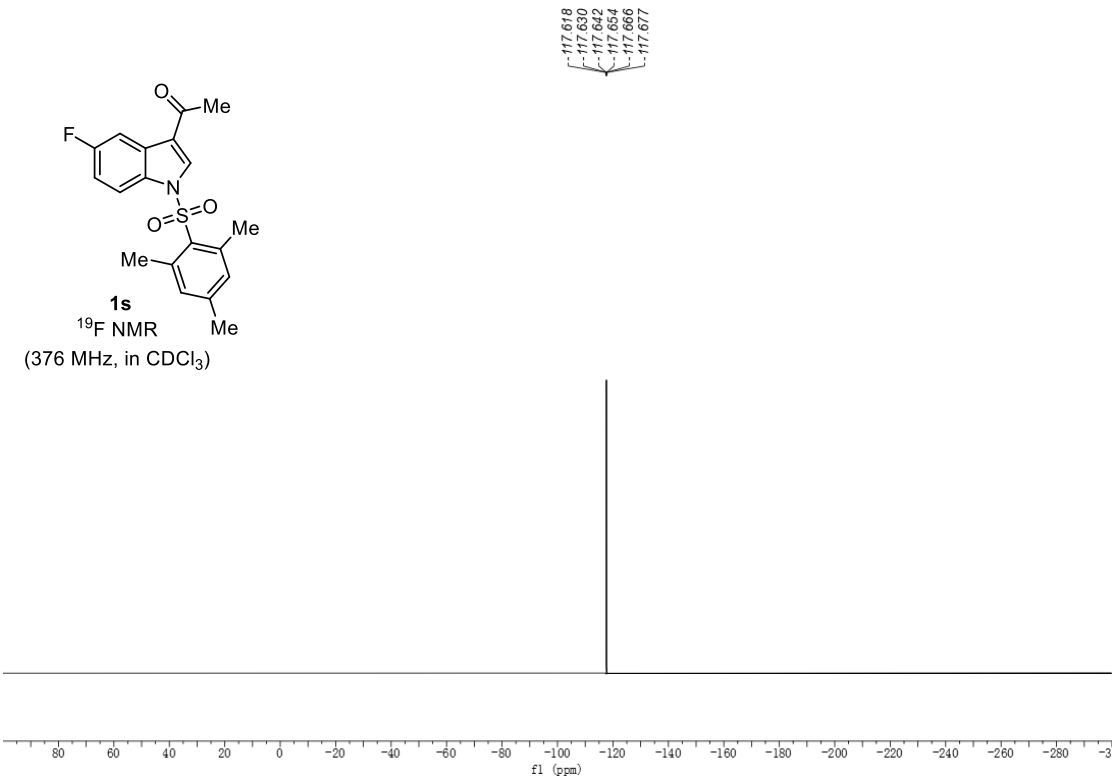
(400 MHz, in $CDCl_3$)

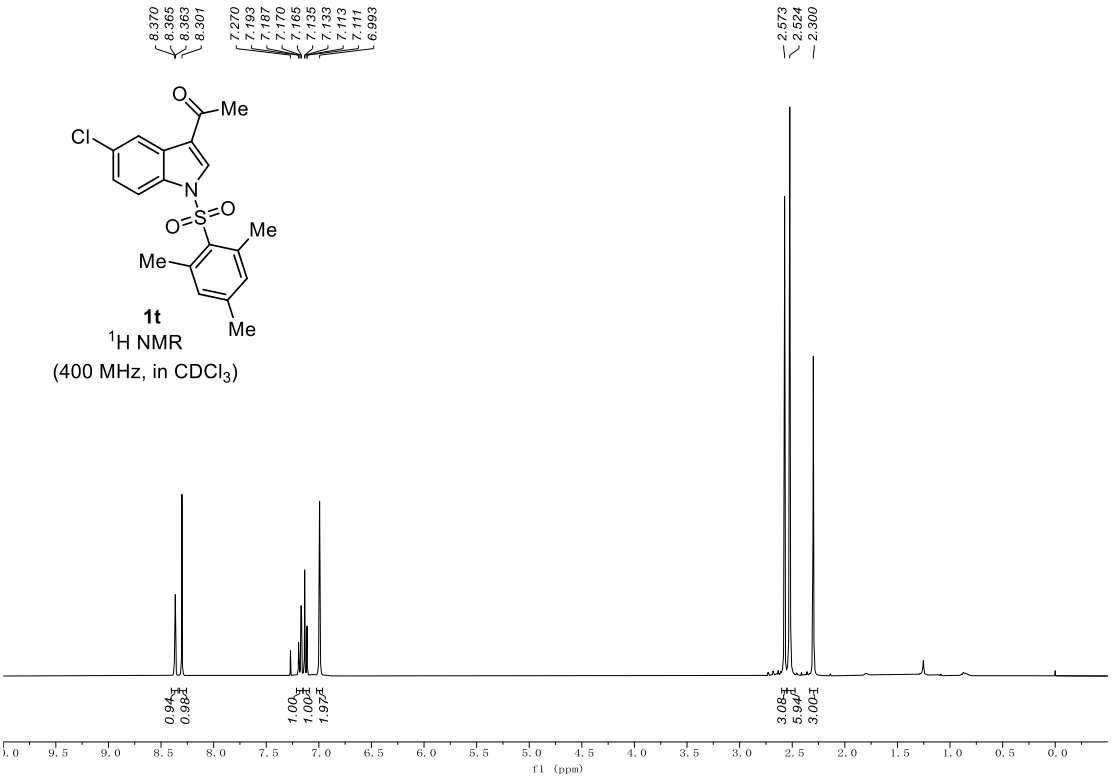


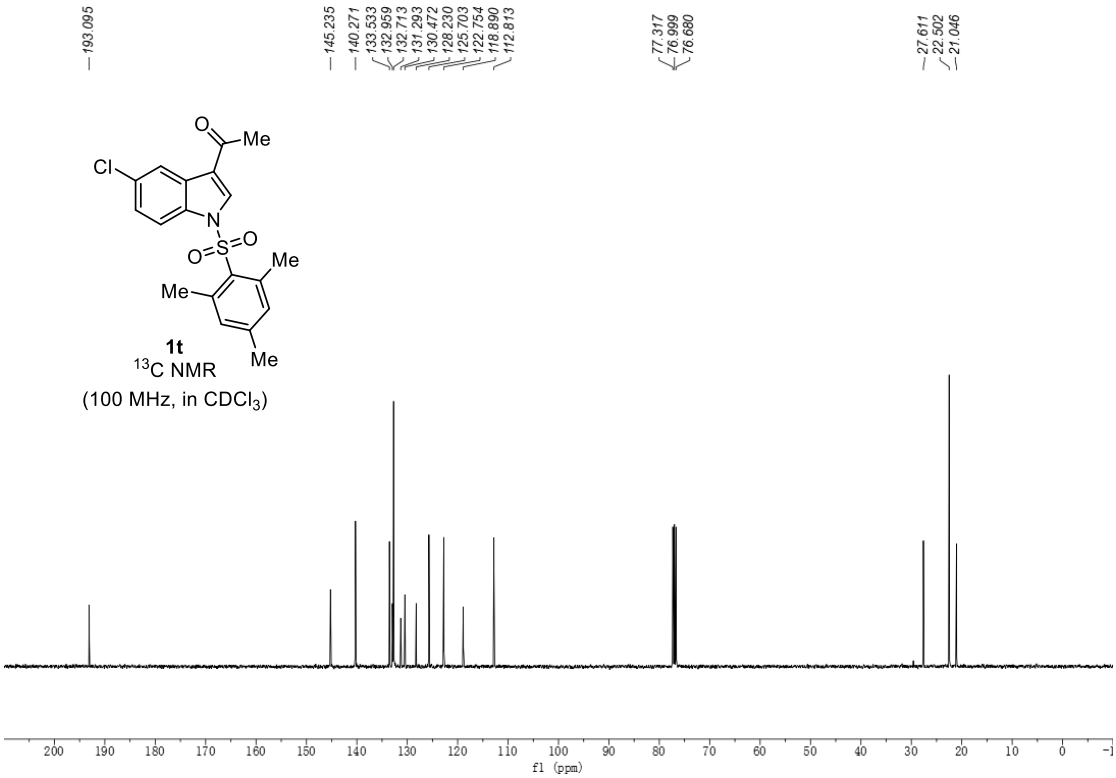
1s

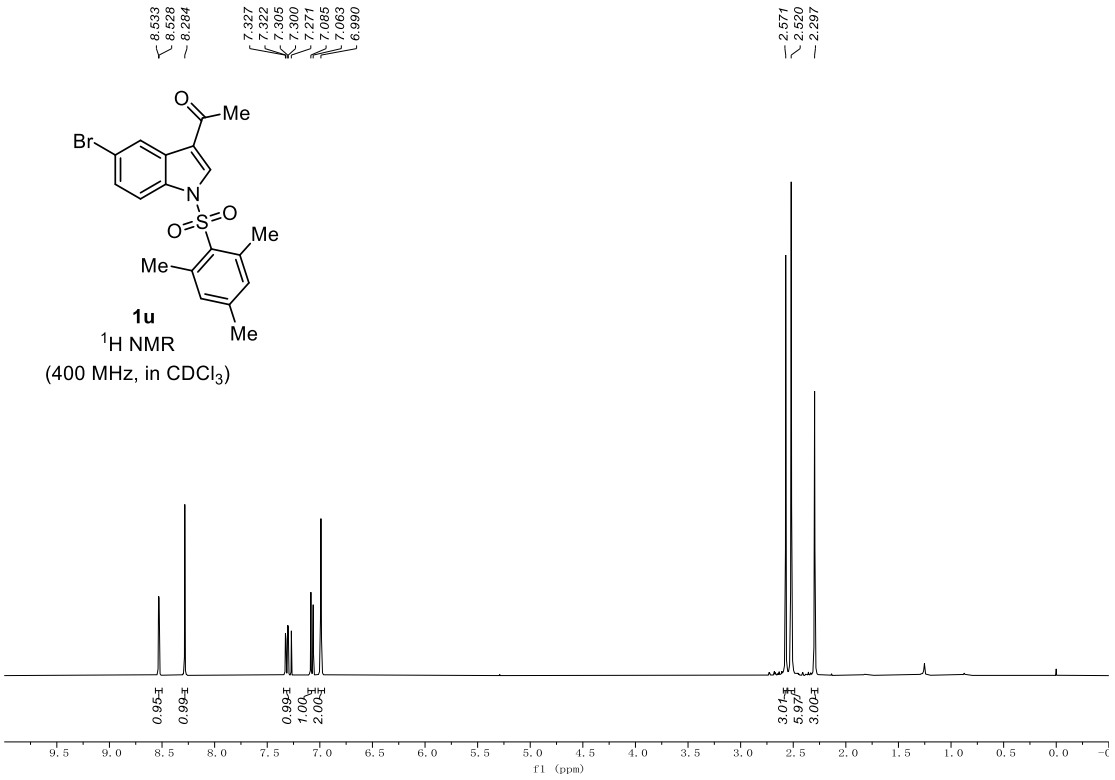
^{13}C NMR

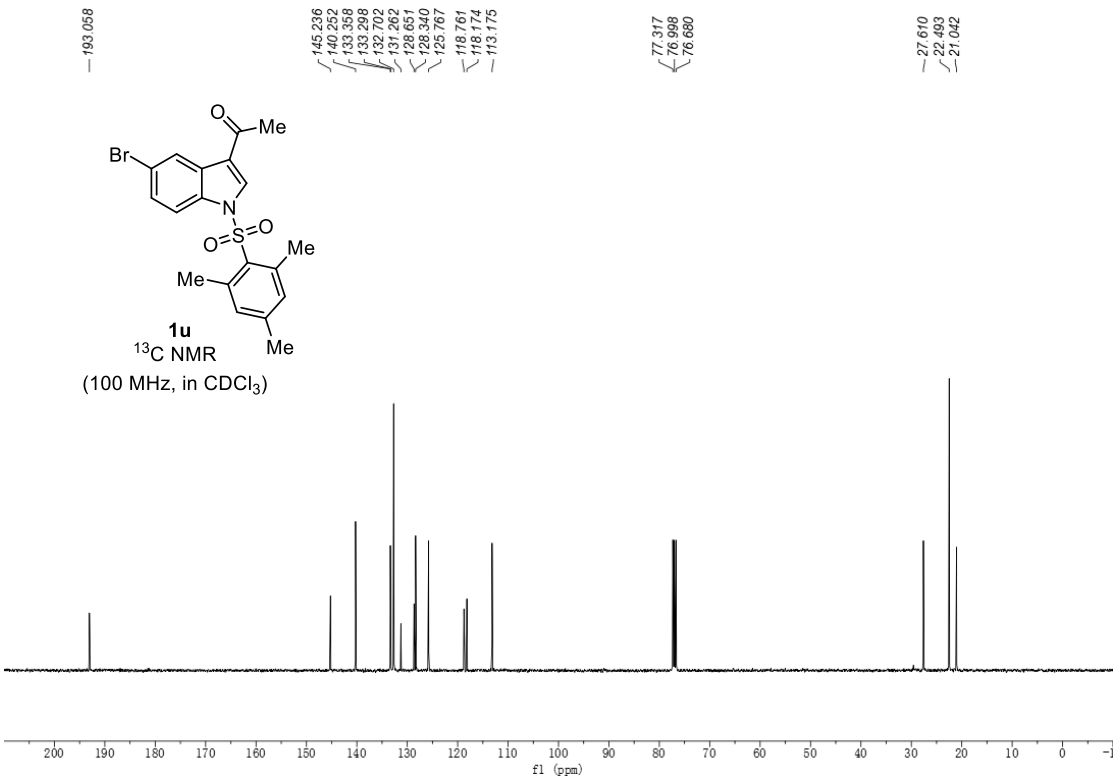
(100 MHz, in $CDCl_3$)

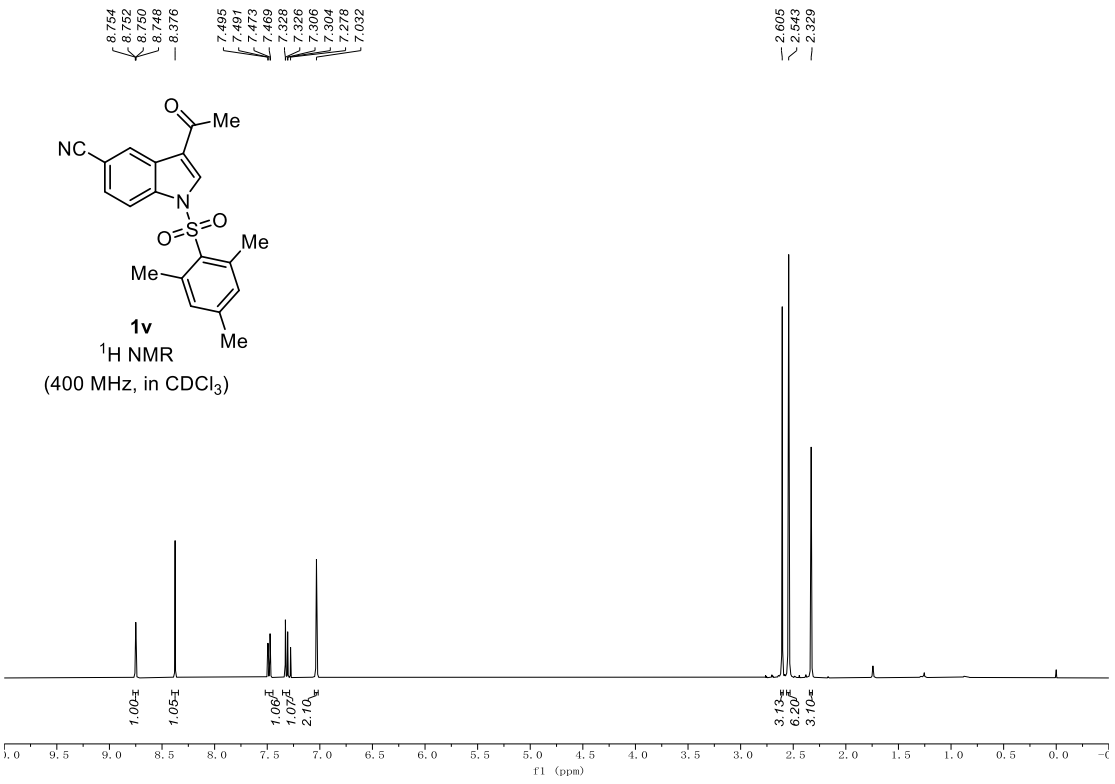

117.618
117.630
117.642
117.654
117.666
117.677
O
Me
F
N
O
S
O
Me
Me
Me
1s
19F NMR
(376 MHz, in CDCl3)
80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -3
f1 (ppm)

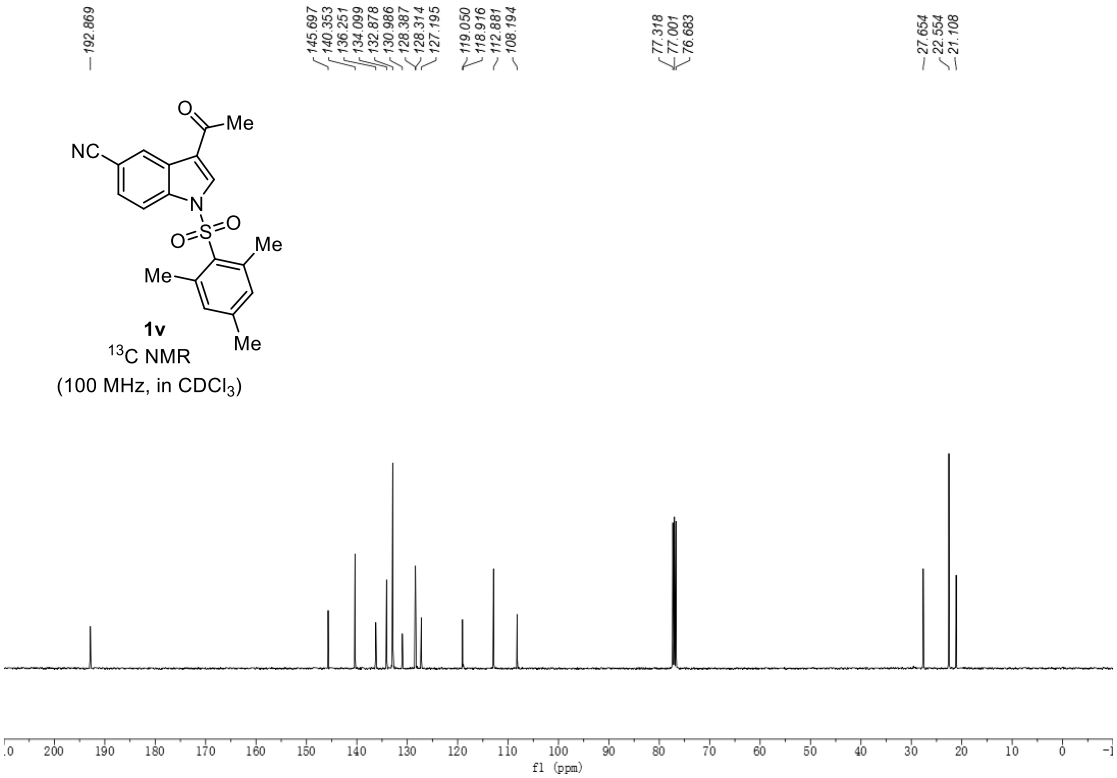

8.370
8.365
8.363
8.301
7.270
7.193
7.187
7.170
7.165
7.135
7.133
7.113
7.111
6.993
2.573
2.524
2.300
O
Me
Cl
N
O
S
O
Me
Me
Me
1t
1H NMR
(400 MHz, in CDCl3)
0.94
0.98
1.00
1.00
1.97
3.08
5.94
3.00
f1 (ppm)

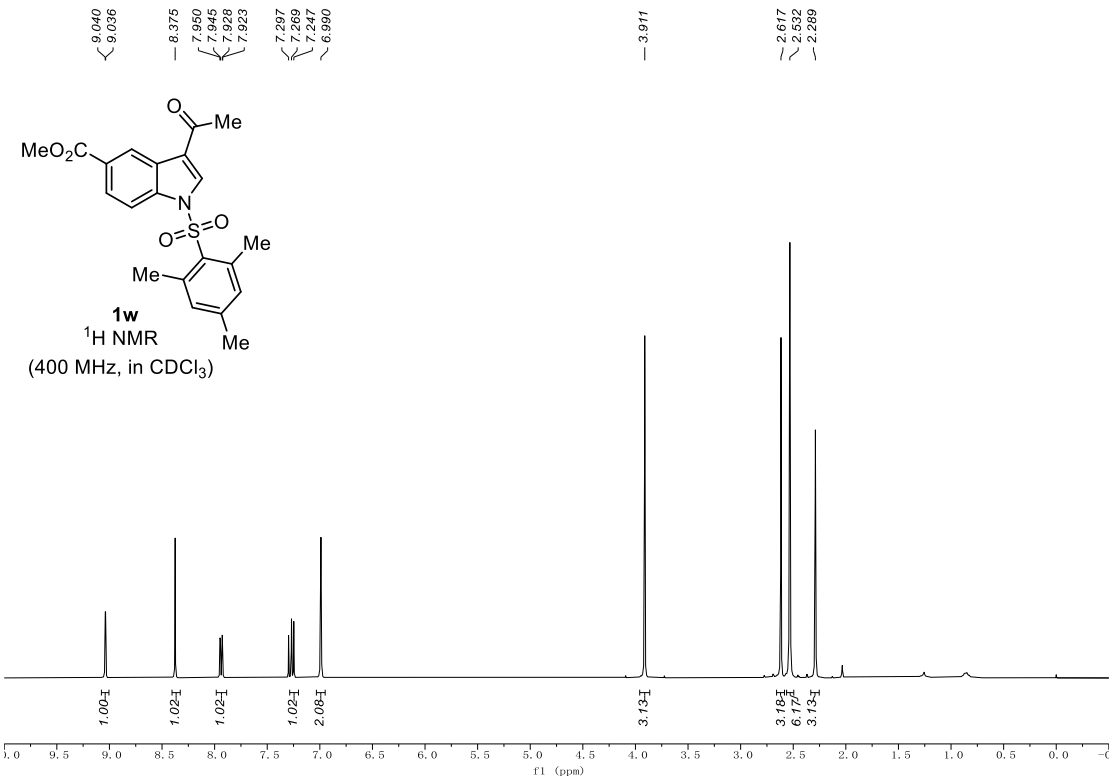

193.095
145.235
140.271
133.533
132.959
132.713
131.293
130.472
128.230
125.703
122.754
118.890
112.813
77.317
76.999
76.680
27.611
22.502
21.046
Cl
O
Me
N
O=S=O
Me
Me
Me
1t
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

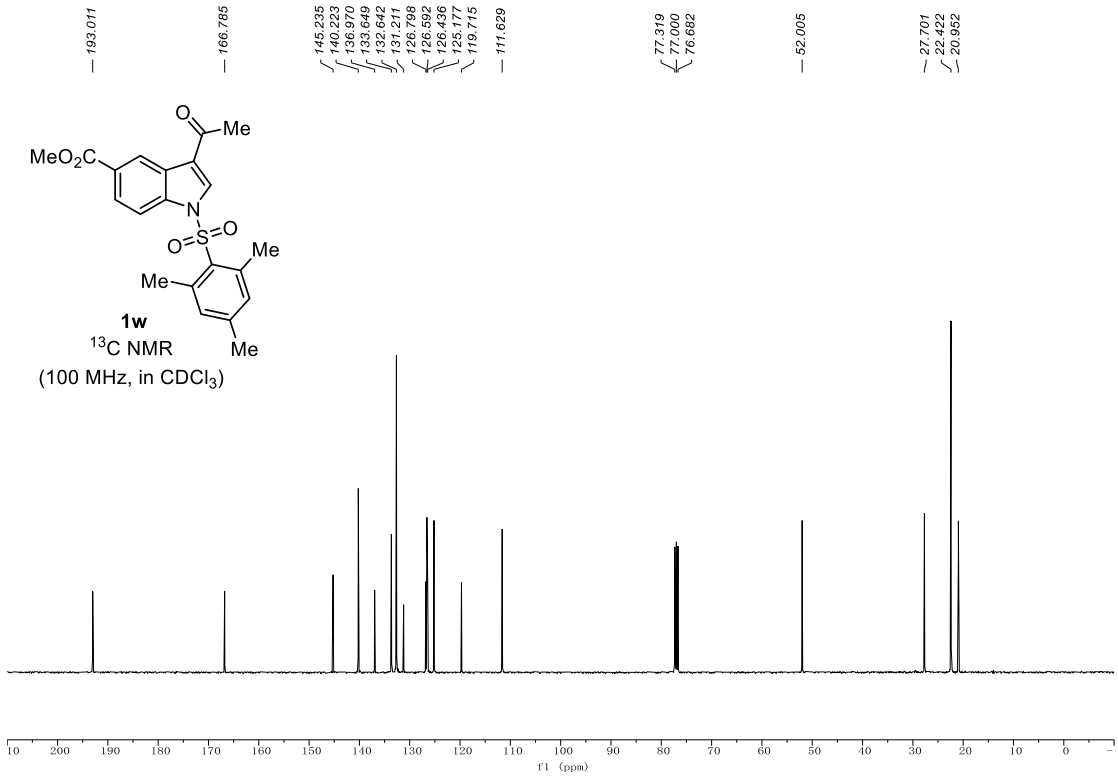

8.533
8.528
8.284
7.327
7.322
7.305
7.300
7.271
7.085
7.063
6.990
2.571
2.520
2.297
Br
O
Me
N
O=S=O
Me
Me
Me
1u
1H NMR
(400 MHz, in CDCl3)
0.95
0.99
0.99
1.00
2.00
3.01
5.97
3.00
f1 (ppm)

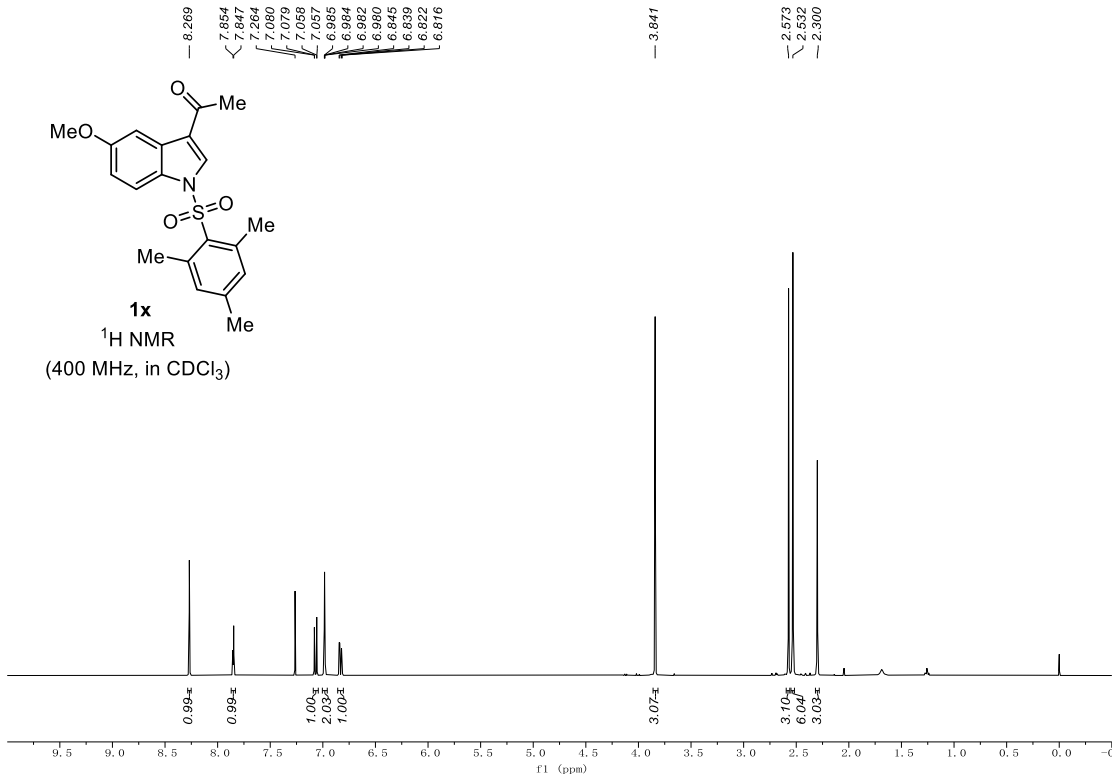

193.058
145.236
140.252
133.358
133.298
132.702
131.262
128.651
128.340
125.767
118.761
118.174
113.175
77.317
76.998
76.680
27.610
22.493
21.042
Br
O
Me
N
O=S=O
Me
Me
Me
1u
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

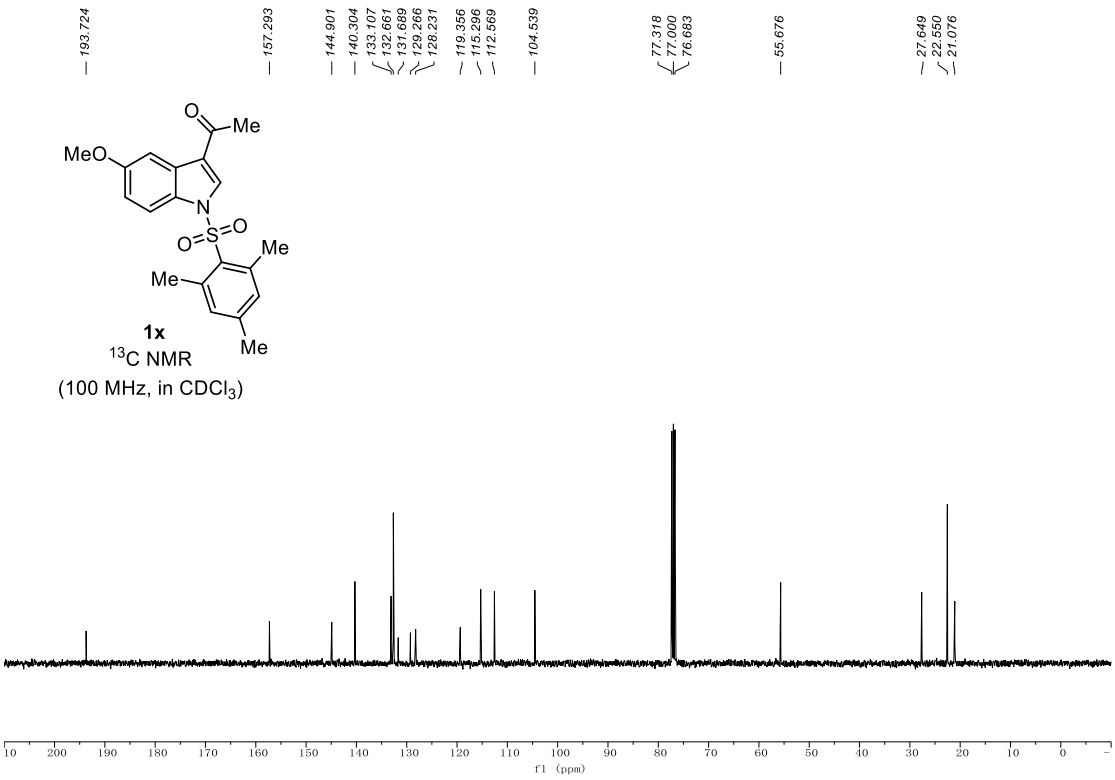

8.754
8.752
8.750
8.748
8.376
7.495
7.491
7.473
7.469
7.328
7.326
7.306
7.304
7.278
7.032
2.605
2.543
2.329
NC
O
Me
N
O=S=O
Me
Me
Me
1v
1H NMR
(400 MHz, in CDCl3)
1.00
1.05
1.06
1.07
2.10
3.13
6.20
3.10
f1 (ppm)

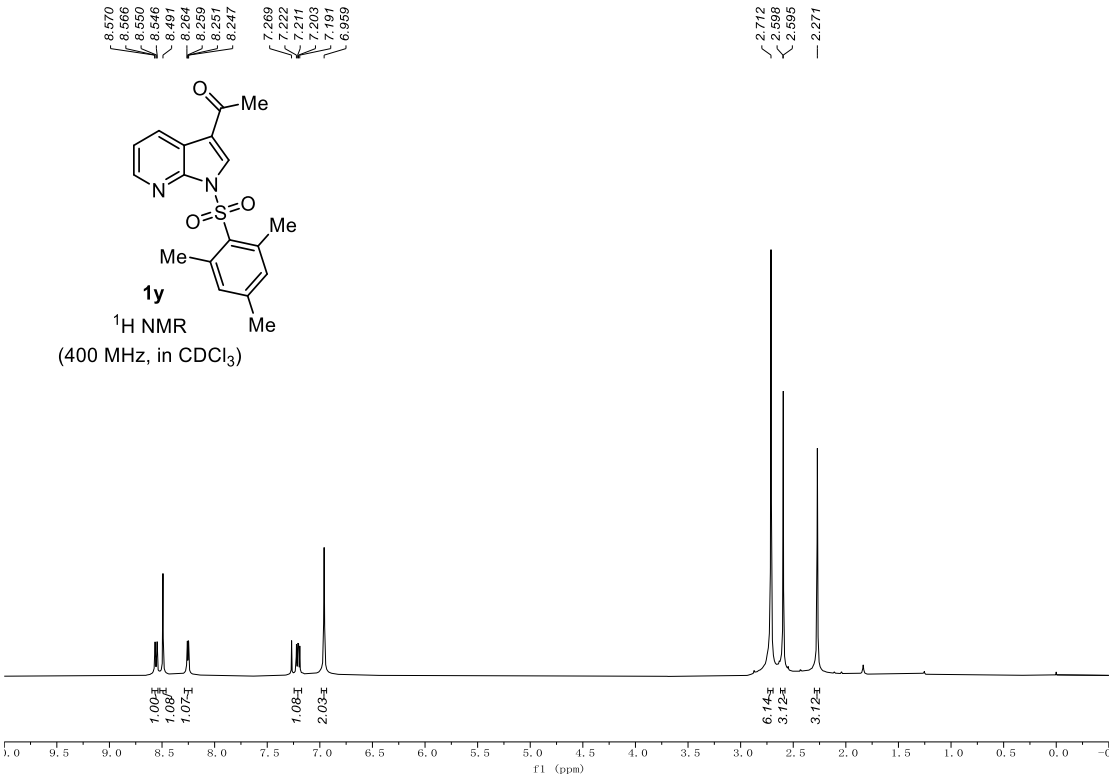

192.869
145.697
140.353
136.251
134.099
132.878
130.986
128.387
128.314
127.195
119.050
118.916
112.881
108.194
77.318
77.001
76.683
27.654
22.554
21.108
O
Me
NC
N
O=S=O
Me
Me
Me
1v
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

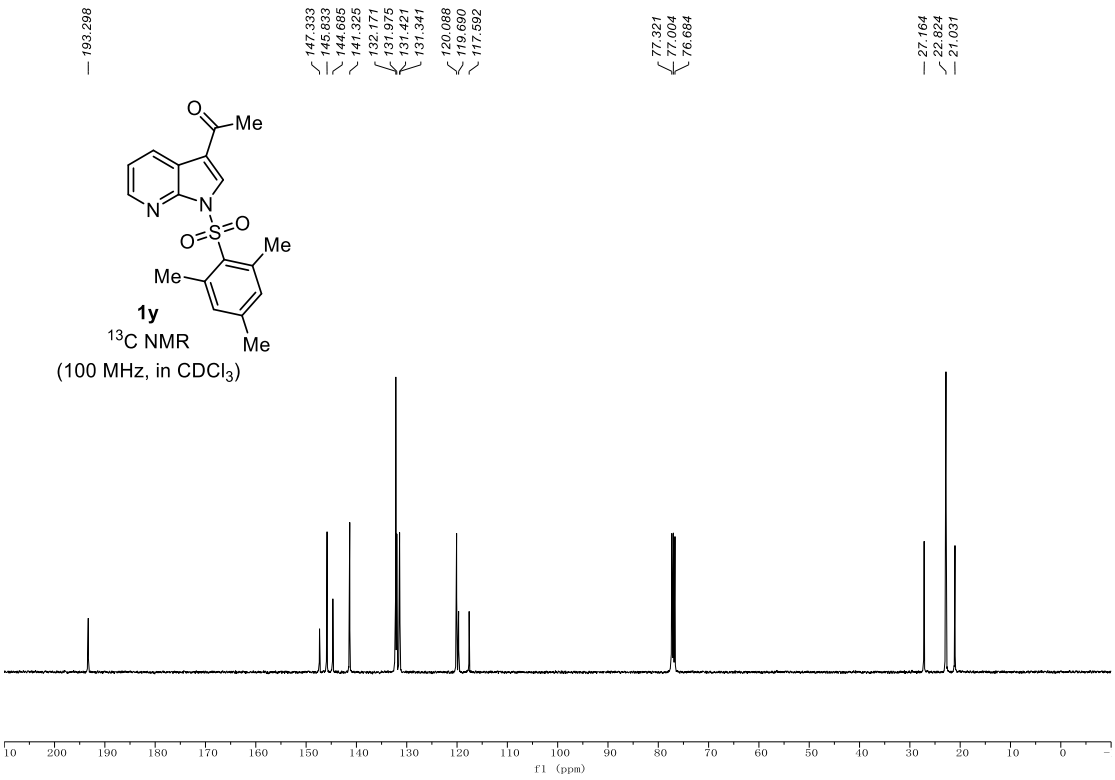

9.040
9.036
8.375
7.950
7.945
7.928
7.923
7.297
7.269
7.247
6.990
3.911
2.617
2.532
2.289
O
Me
MeO2C
N
O=S=O
Me
Me
Me
1w
1H NMR
(400 MHz, in CDCl3)
1.00
1.02
1.02
1.02
2.08
3.13
3.18
6.17
3.13
f1 (ppm)


193.011
166.785
145.235
140.223
136.970
133.649
132.642
131.211
126.798
126.592
126.436
125.177
119.715
111.629
77.319
77.000
76.682
52.005
27.701
22.422
20.952
MeO2C
Me
N
O=S=O
Me
Me
Me
1w
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)


8.269
7.854
7.847
7.264
7.080
7.079
7.058
7.057
6.985
6.984
6.982
6.980
6.845
6.839
6.822
6.816
3.841
2.573
2.532
2.300
MeO
Me
N
O=S=O
Me
Me
Me
1x
1H NMR
(400 MHz, in CDCl3)
0.99
0.99
1.00
2.03
1.00
3.07
3.10
6.04
3.03
f1 (ppm)


193.724
157.293
144.901
140.304
133.107
132.661
131.689
129.266
128.231
119.356
115.296
112.569
104.539
77.318
77.000
76.683
55.676
27.649
22.550
21.076
MeO
Me
N
O
S
O
Me
Me
Me
1x
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)


8.570
8.566
8.550
8.546
8.491
8.264
8.259
8.251
8.247
7.269
7.222
7.211
7.203
7.191
6.959
2.712
2.598
2.595
2.271
Me
N
N
O
S
O
Me
Me
Me
1y
1H NMR
(400 MHz, in CDCl3)
1.00
1.08
1.07
1.08
2.03
6.14
3.12
3.12
f1 (ppm)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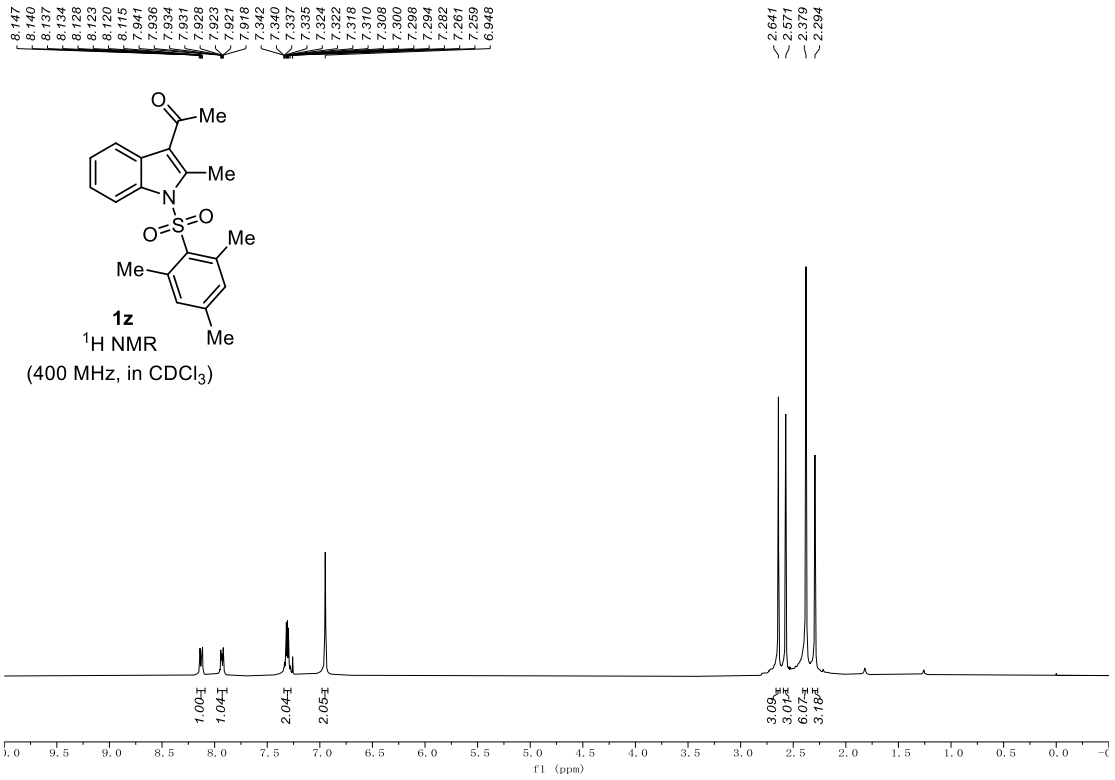
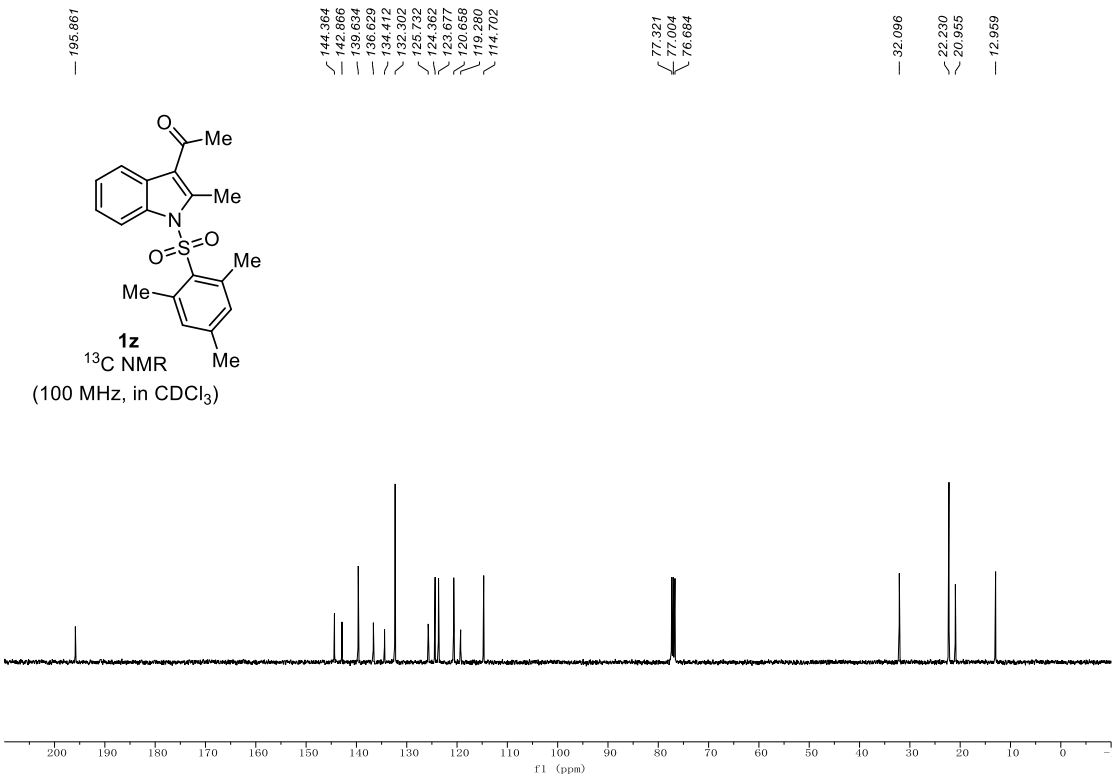
147.333
145.833
144.685
141.325
132.171
131.975
131.421
131.341
120.088
119.690
117.592
77.321
77.004
76.684
27.164
22.824
21.031
Me
N
N
O
S
O
Me
Me
Me
1y
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)


8.147
8.140
8.137
8.134
8.128
8.123
8.120
8.115
7.941
7.936
7.934
7.931
7.928
7.923
7.921
7.918
7.342
7.340
7.337
7.335
7.324
7.322
7.318
7.310
7.308
7.300
7.298
7.294
7.282
7.261
7.259
6.948
2.641
2.571
2.379
2.294
Me
Me
N
O
S
O
Me
Me
Me
1z
1H NMR
(400 MHz, in CDCl3)
1.00
1.04
2.04
2.05
3.09
3.01
6.07
3.18
f1 (ppm)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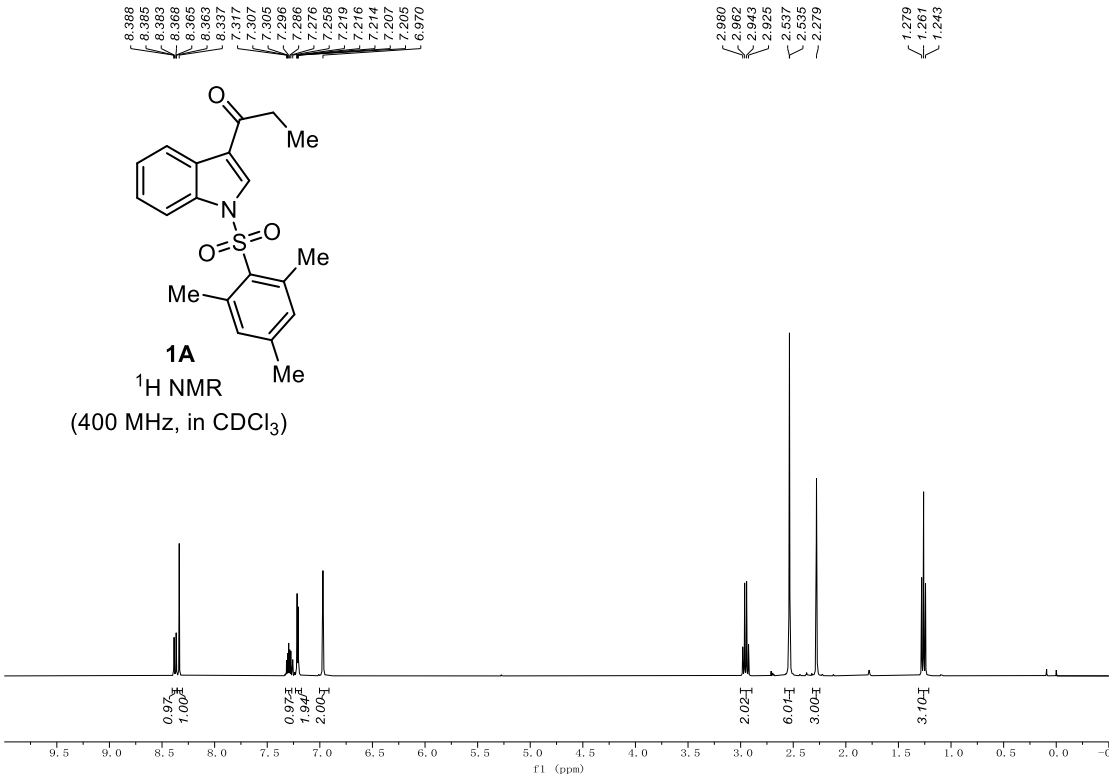
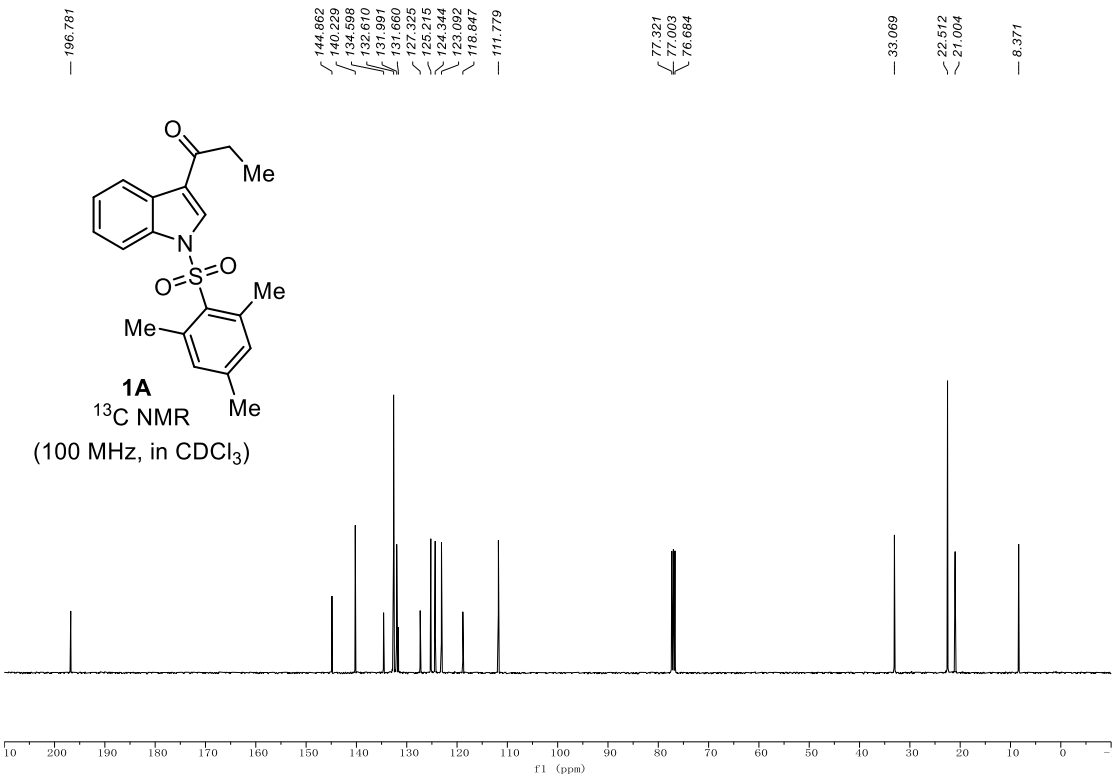
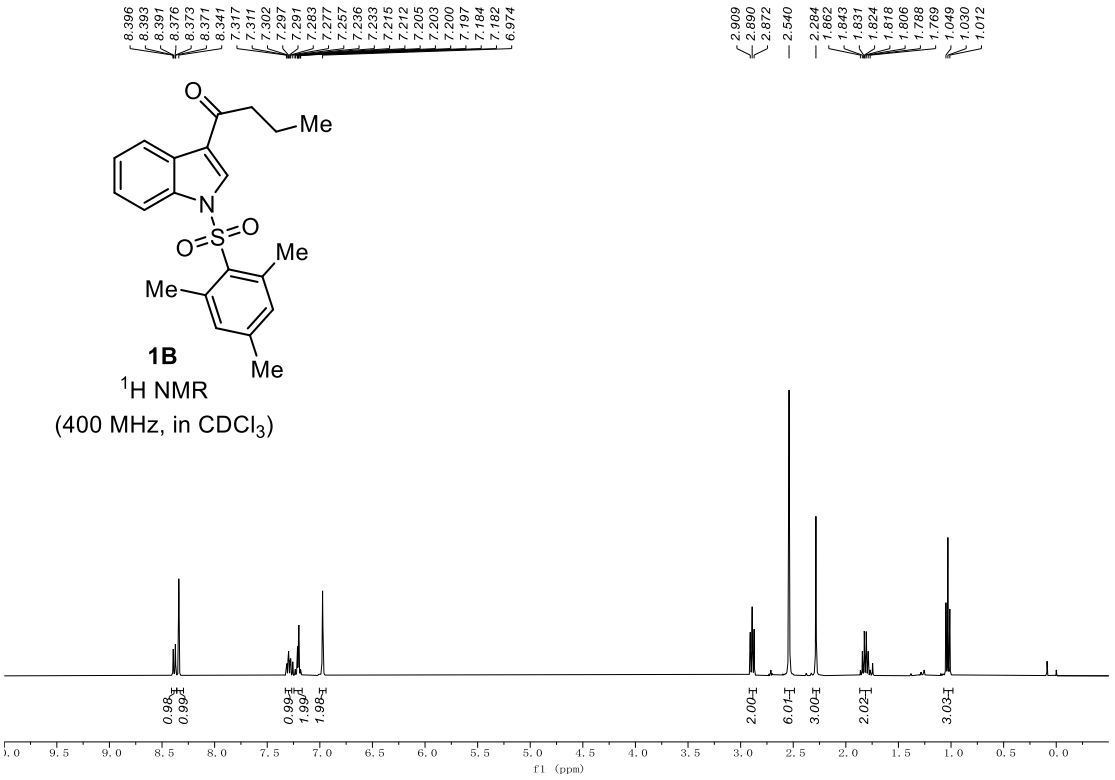
144.364
142.866
139.634
136.629
134.412
132.302
125.732
124.362
123.677
120.658
119.280
114.702
77.321
77.004
76.684
32.096
22.230
20.955
12.959
Me
Me
N
O=S=O
Me
Me
Me
1z
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)


8.388
8.385
8.383
8.368
8.365
8.363
8.337
7.317
7.307
7.305
7.296
7.286
7.276
7.258
7.219
7.216
7.214
7.207
7.205
6.970
2.980
2.962
2.943
2.925
2.537
2.535
2.279
1.279
1.261
1.243
Me
N
O=S=O
Me
Me
Me
1A
1H NMR
(400 MHz, in CDCl3)
0.97
1.00
0.97
1.94
2.00
2.02
6.01
3.00
3.10
f1 (ppm)


196.781
144.862
140.229
134.598
132.610
131.991
131.660
127.325
125.215
124.344
123.092
118.847
111.779
77.321
77.003
76.684
33.069
22.512
21.004
8.371
Me
Me
Me
Me
1A
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)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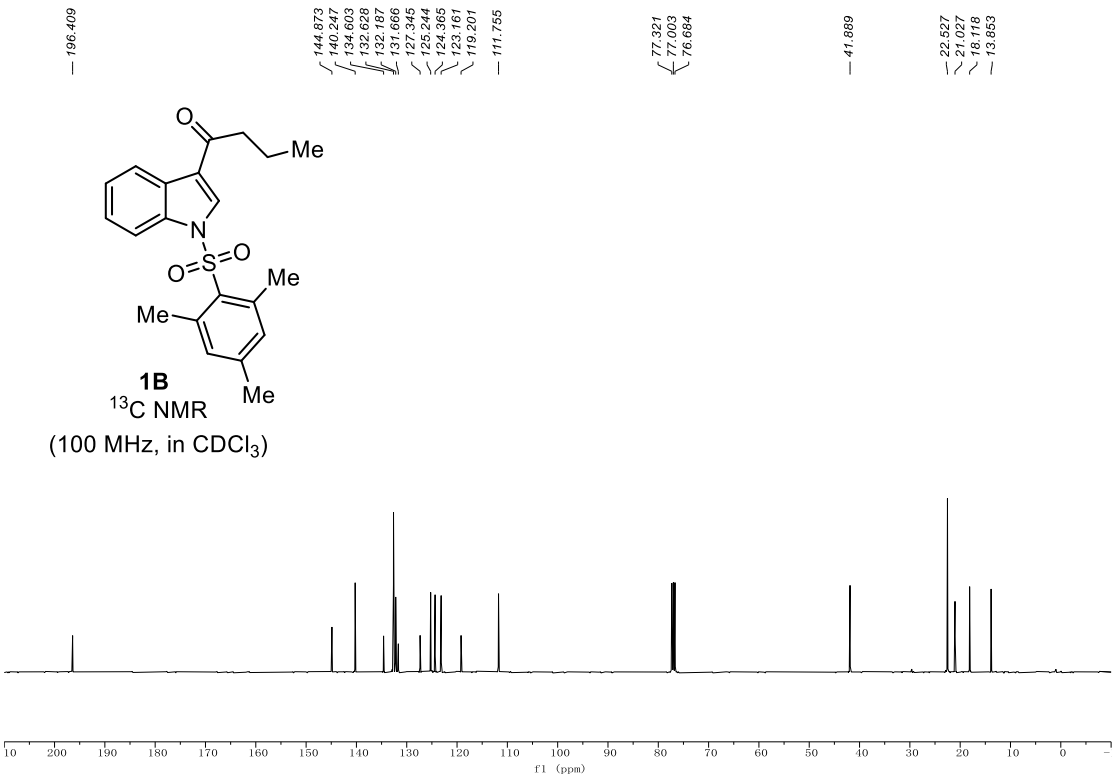
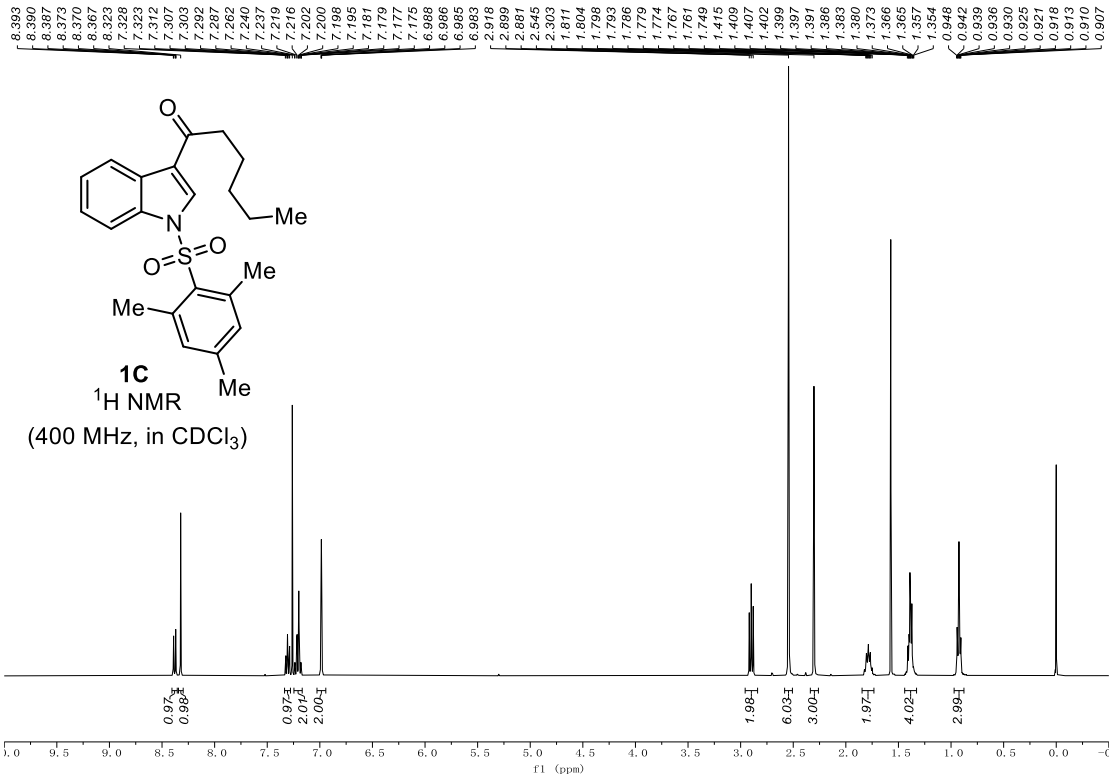
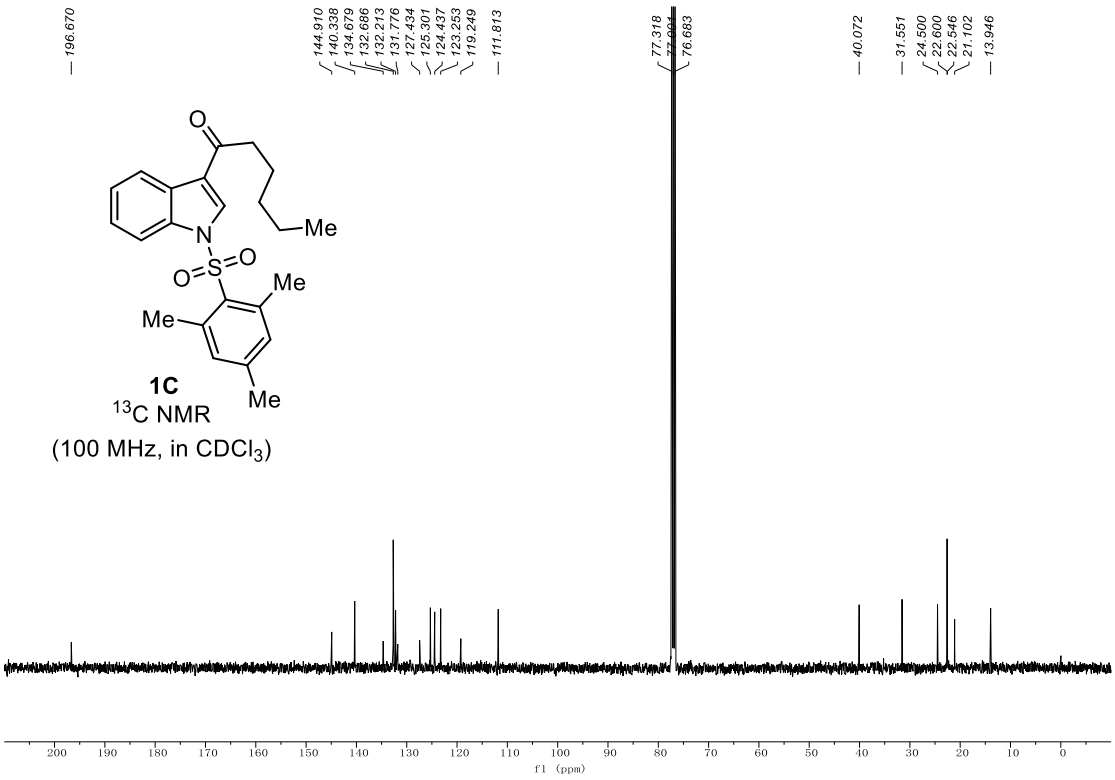
8.393
8.391
8.376
8.373
8.371
8.341
7.317
7.311
7.302
7.297
7.291
7.283
7.277
7.257
7.236
7.233
7.215
7.212
7.205
7.203
7.200
7.197
7.184
7.182
6.974
2.909
2.890
2.872
2.540
2.284
1.862
1.843
1.831
1.824
1.818
1.806
1.788
1.769
1.049
1.030
1.012
Me
Me
Me
Me
1B
1H NMR
(400 MHz, in CDCl3)
0.98
0.99
0.99
1.99
1.98
2.00
6.01
3.00
2.02
3.03
f1 (ppm)


196.409
144.873
140.247
134.603
132.628
132.187
131.666
127.345
125.244
124.365
123.161
119.201
111.755
77.321
77.003
76.684
41.889
22.527
21.027
18.118
13.853
O
Me
N
O=S=O
Me
Me
Me
1B
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)


8.393
8.390
8.387
8.373
8.370
8.367
8.323
7.328
7.323
7.312
7.307
7.303
7.292
7.287
7.262
7.240
7.237
7.219
7.216
7.202
7.200
7.198
7.195
7.181
7.179
7.177
7.175
6.988
6.986
6.985
6.983
2.918
2.899
2.881
2.545
2.303
1.811
1.804
1.798
1.793
1.786
1.779
1.774
1.767
1.761
1.749
1.415
1.409
1.407
1.402
1.399
1.397
1.391
1.386
1.383
1.380
1.373
1.366
1.365
1.357
1.354
0.948
0.942
0.939
0.936
0.930
0.925
0.921
0.918
0.913
0.910
0.907
O
Me
N
O=S=O
Me
Me
Me
1C
1H NMR
(400 MHz, in CDCl3)
0.97
0.98
0.97
2.01
2.00
1.98
6.03
3.00
1.97
4.02
2.99
f1 (ppm)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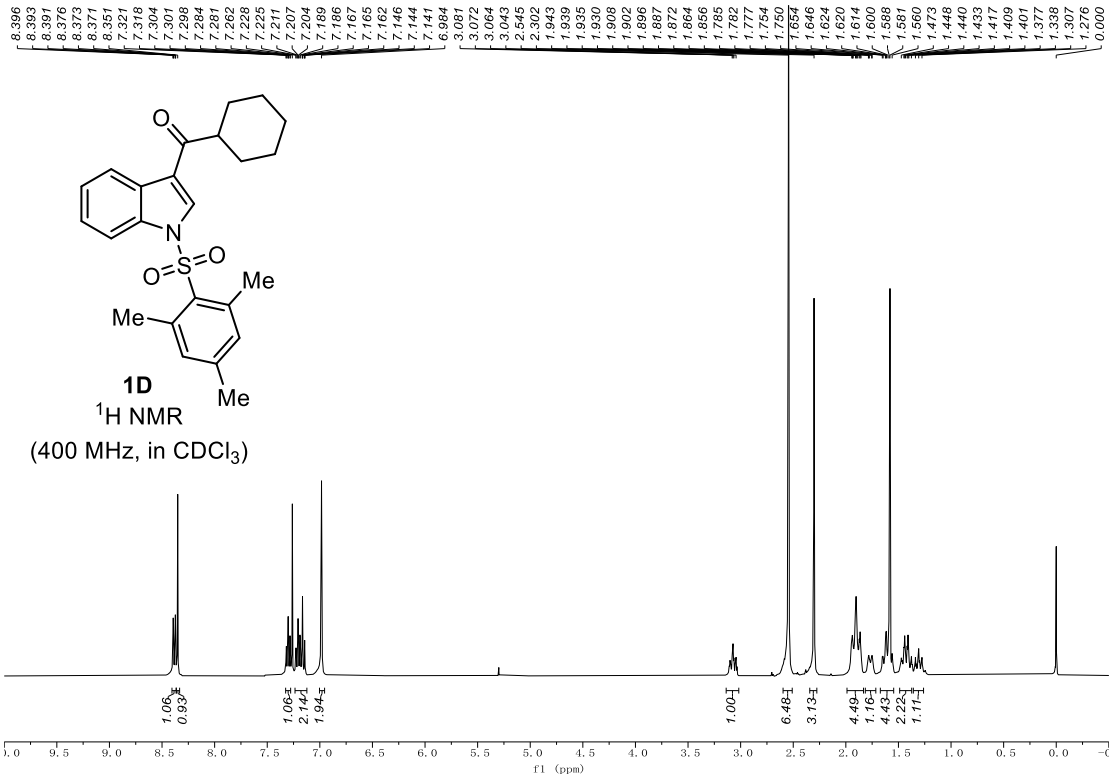
140.338
134.679
132.686
132.213
131.776
127.434
125.301
124.437
123.253
119.249
111.813
77.318
77.001
76.683
40.072
31.551
24.500
22.600
22.546
21.102
13.946
Me
Me
Me
Me
1C
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)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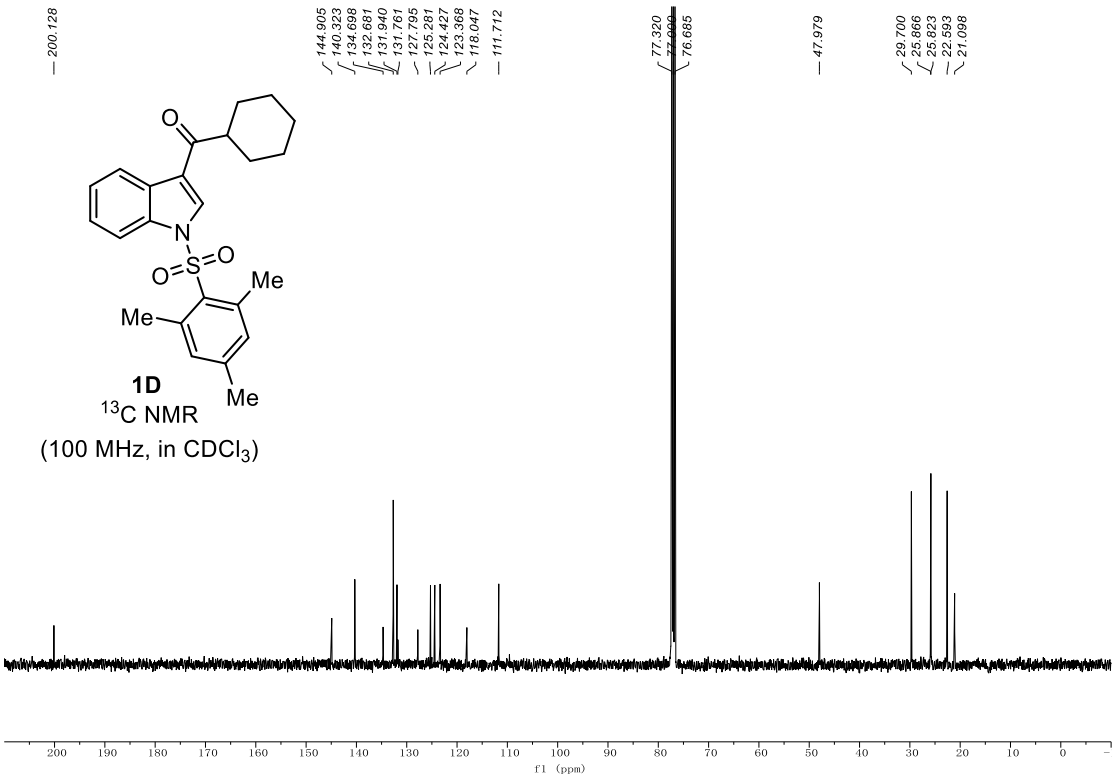
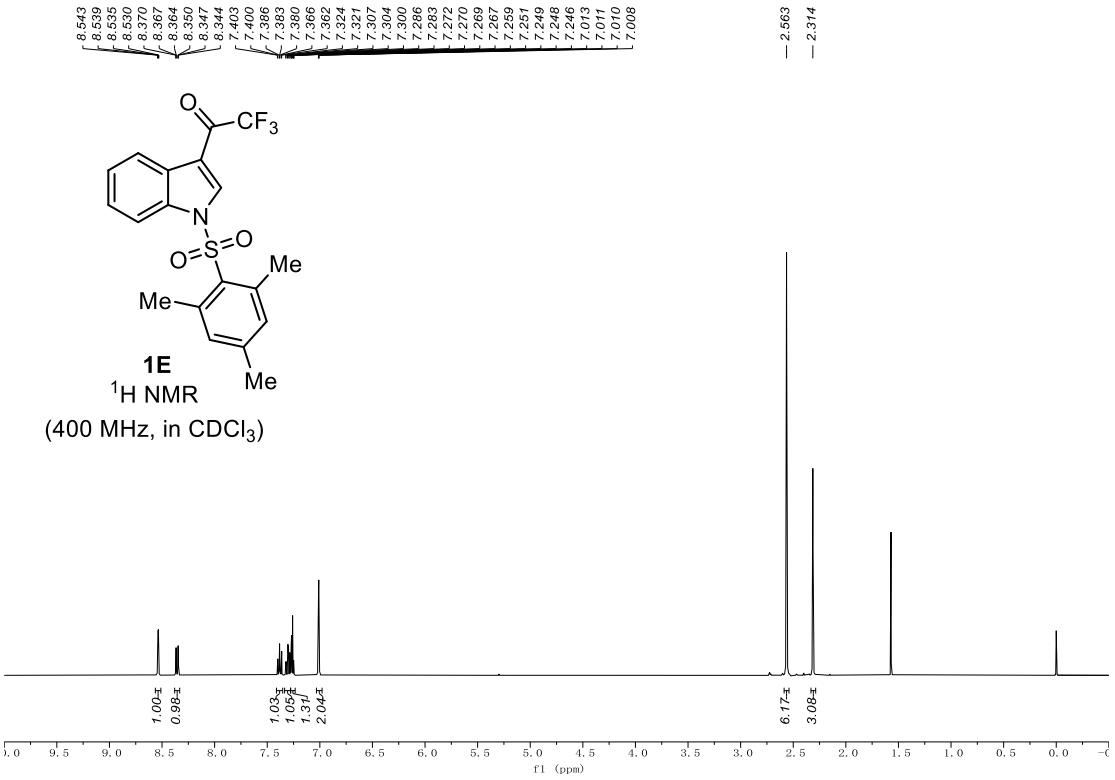
8.393
8.391
8.376
8.373
8.371
8.351
7.321
7.318
7.304
7.301
7.298
7.284
7.281
7.262
7.228
7.225
7.211
7.207
7.204
7.189
7.186
7.167
7.165
7.162
7.146
7.144
7.141
6.984
3.081
3.072
3.064
3.043
2.545
2.302
1.943
1.939
1.935
1.930
1.908
1.902
1.896
1.887
1.872
1.864
1.856
1.785
1.782
1.777
1.754
1.750
1.654
1.646
1.624
1.620
1.614
1.600
1.588
1.581
1.560
1.473
1.448
1.440
1.433
1.417
1.409
1.401
1.377
1.338
1.307
1.276
0.000
Me
Me
Me
1D
1H NMR
(400 MHz, in CDCl3)
1.06
0.93
1.06
2.14
1.94
1.00
6.48
3.13
4.49
1.16
4.43
2.22
1.11
f1 (ppm)


200.128
144.905
140.323
134.698
132.681
131.940
131.761
127.795
125.281
124.427
123.368
118.047
111.712
77.320
77.000
76.685
47.979
29.700
25.866
25.823
22.593
21.098
O
N
O=S=O
Me
Me
Me
1D
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)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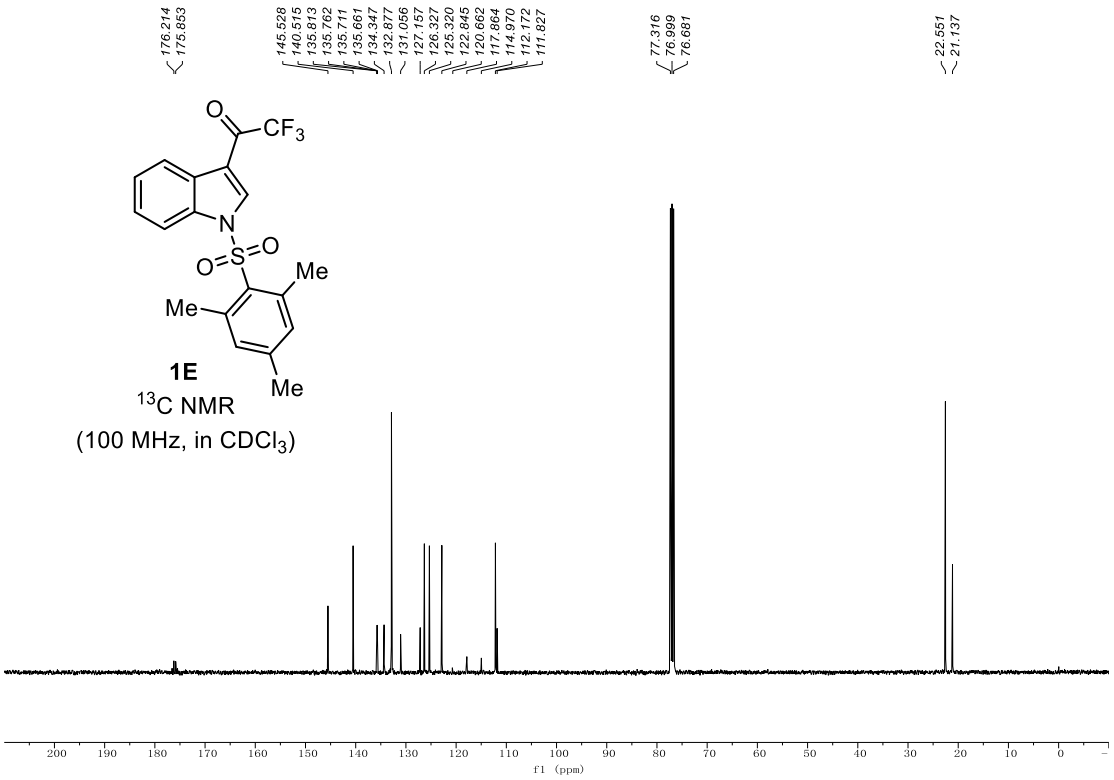
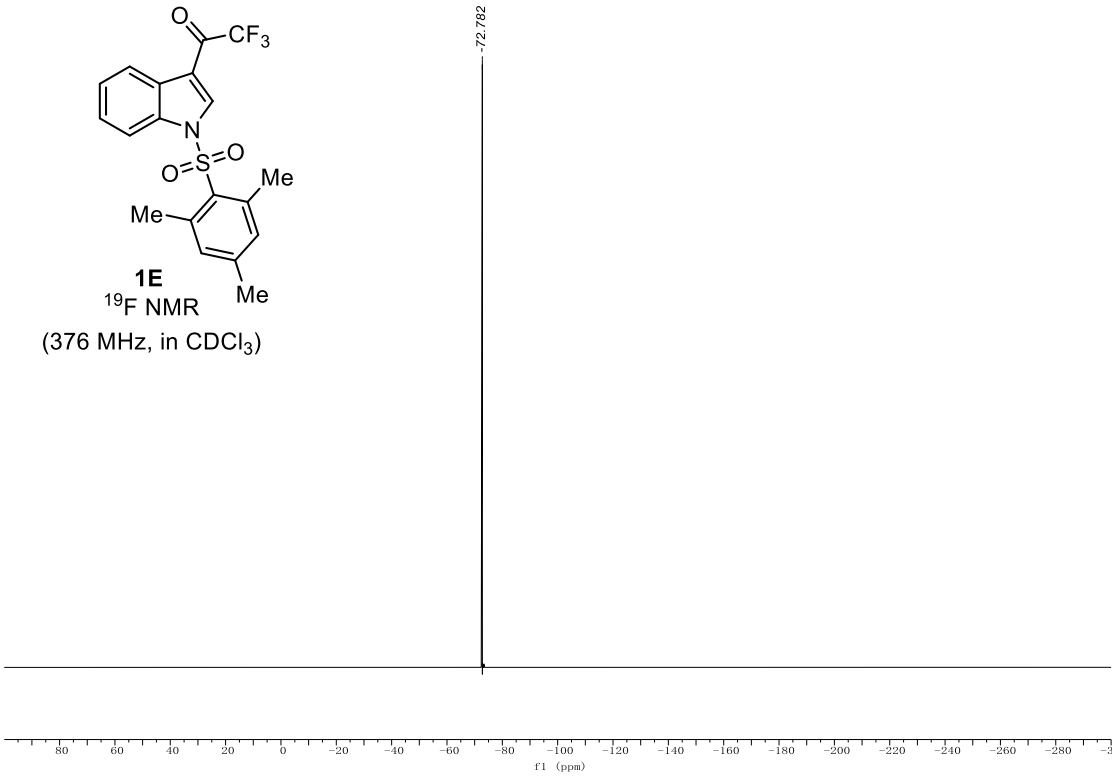
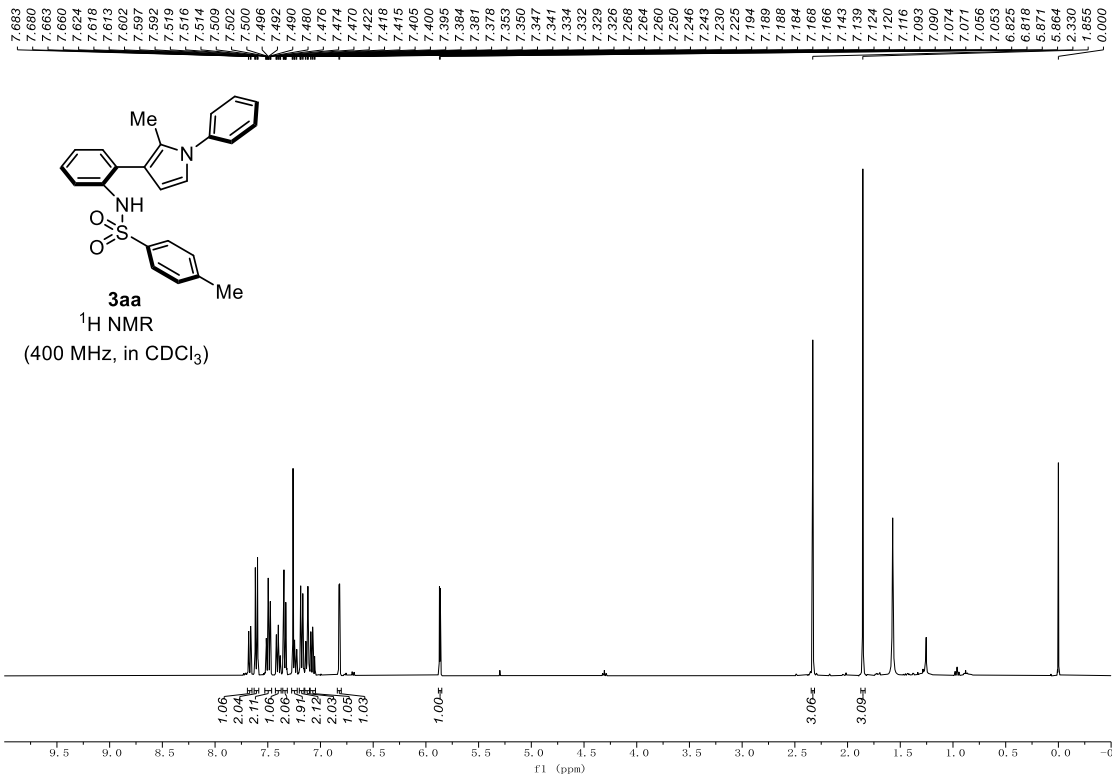
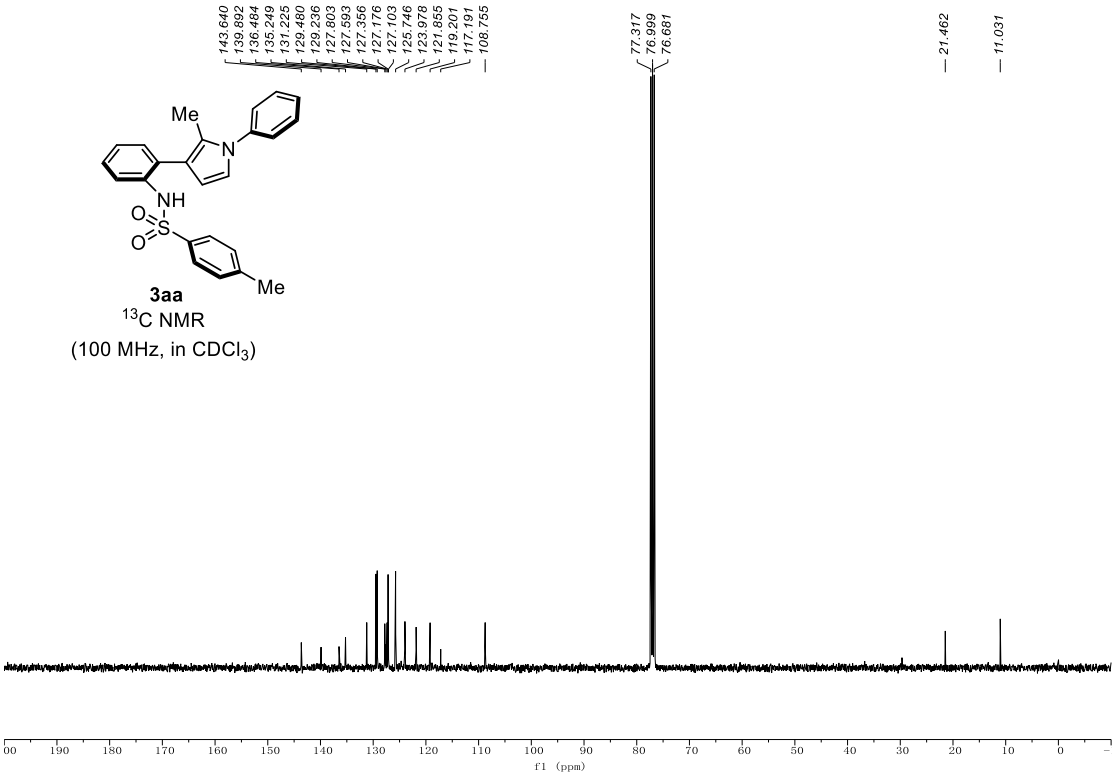
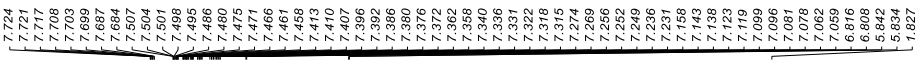
8.539
8.535
8.530
8.370
8.367
8.364
8.350
8.347
8.344
7.403
7.400
7.386
7.383
7.380
7.366
7.362
7.324
7.321
7.307
7.304
7.300
7.286
7.283
7.272
7.270
7.269
7.267
7.259
7.251
7.249
7.248
7.246
7.013
7.011
7.010
7.008
2.563
2.314
O
CF3
N
O=S=O
Me
Me
Me
1E
1H NMR
(400 MHz, in CDCl3)
1.00
0.98
1.03
1.05
1.31
2.04
6.17
3.08
f1 (ppm)

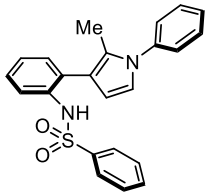

176.214
175.853
145.528
140.515
135.813
135.762
135.711
135.661
134.347
132.877
131.056
127.157
126.327
125.320
122.845
120.662
117.864
114.970
112.172
111.827
77.316
76.999
76.681
22.551
21.137
O
CF3
N
O=S=O
Me
Me
Me
1E
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)


-72.782
O
CF3
N
O=S=O
Me
Me
Me
1E
19F NMR
(376 MHz, in CDCl3)
f1 (ppm)


7.683 7.680 7.663 7.660 7.624 7.618 7.613 7.602 7.597 7.592 7.519 7.516 7.514 7.509 7.502 7.500 7.496 7.492 7.490 7.480 7.476 7.474 7.470 7.422 7.418 7.415 7.405 7.400 7.395 7.384 7.381 7.378 7.353 7.350 7.347 7.341 7.334 7.332 7.329 7.326 7.268 7.264 7.260 7.250 7.246 7.243 7.230 7.225 7.194 7.189 7.188 7.184 7.168 7.166 7.143 7.139 7.124 7.120 7.116 7.093 7.090 7.074 7.071 7.056 7.053 6.825 6.818 5.871 5.864 2.330 1.855 0.000
Me
N
NH
O
S
O
Me
3aa
1H NMR
(400 MHz, in CDCl3)
1.06 2.04 2.11 1.06 2.06 1.91 2.12 2.03 1.05 1.03 1.00 3.06 3.09
f1 (ppm)


143.640 139.892 136.484 135.249 131.225 129.480 129.236 127.803 127.593 127.356 127.176 127.103 125.746 123.978 121.855 119.201 117.191 108.755
77.317 76.999 76.681
21.462
11.031
Me
N
NH
O
S
O
Me
3aa
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

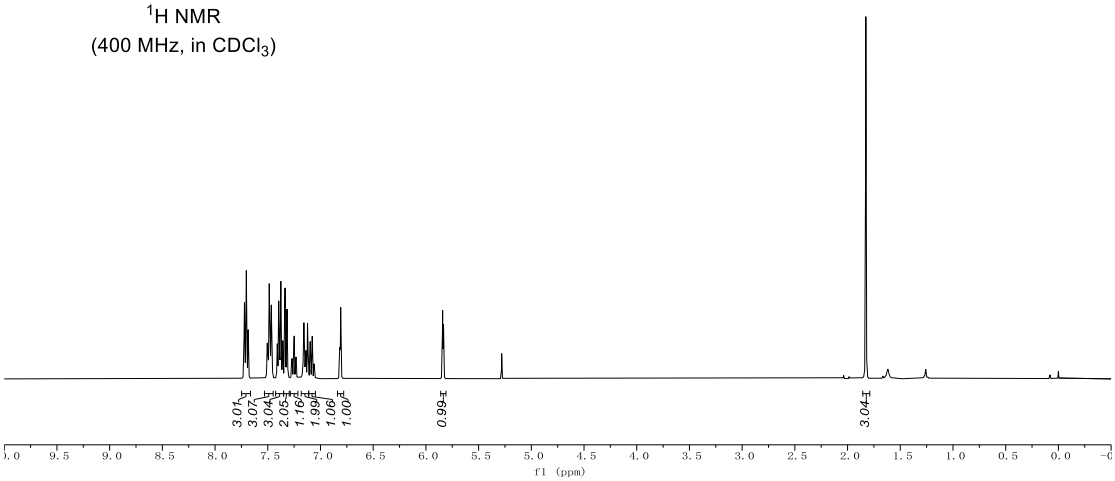


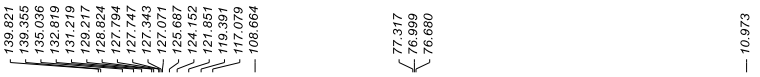


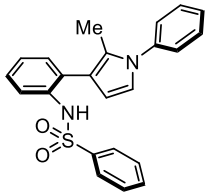
3ab

^{1}H NMR

(400 MHz, in $CDCl_3$)



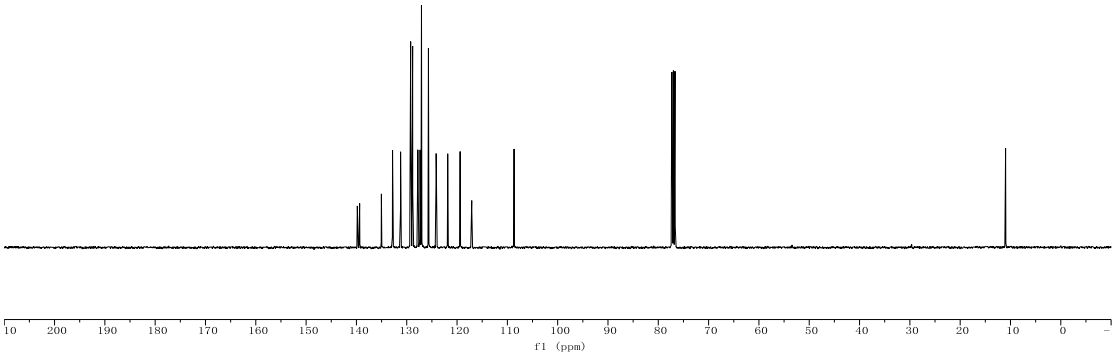


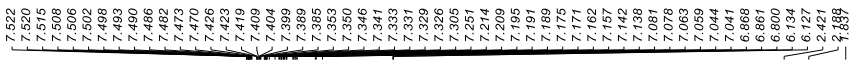


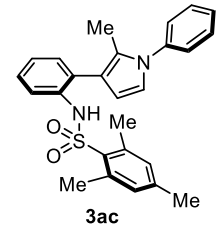
3ab

^{13}C NMR

(100 MHz, in $CDCl_3$)



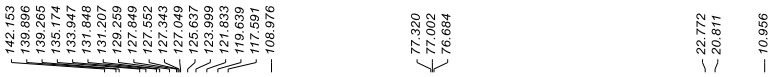


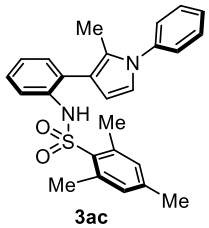


3ac

^{1}H NMR

(400 MHz, in $CDCl_3$)

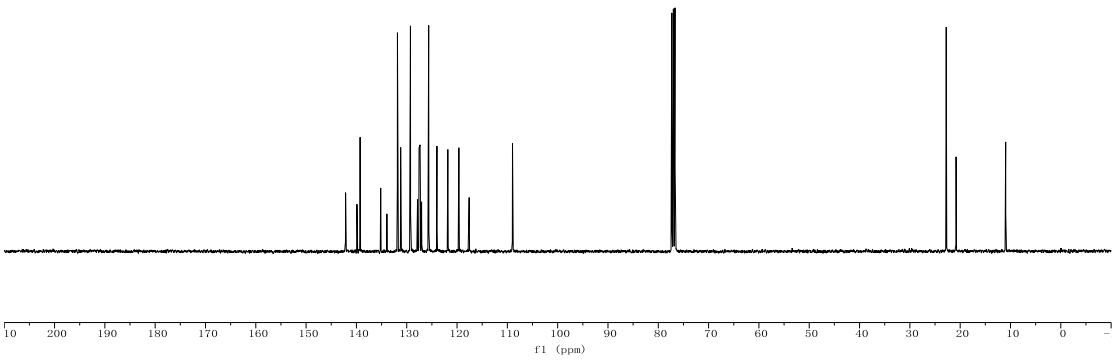


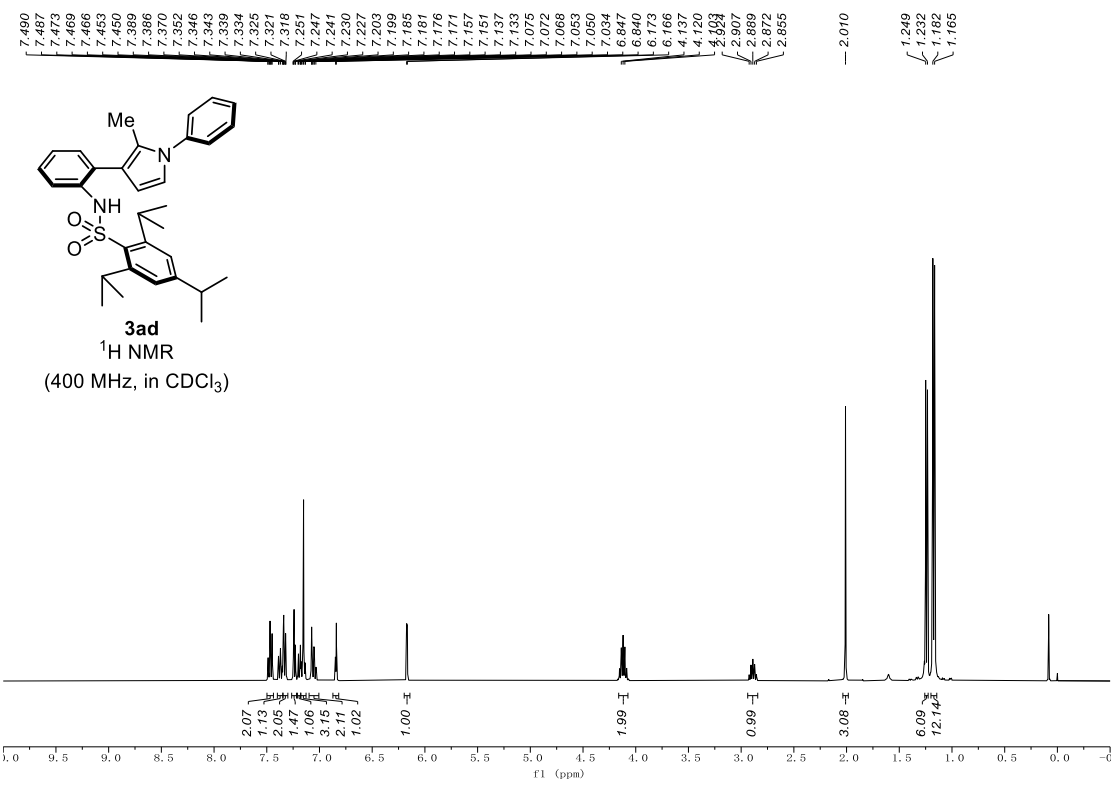


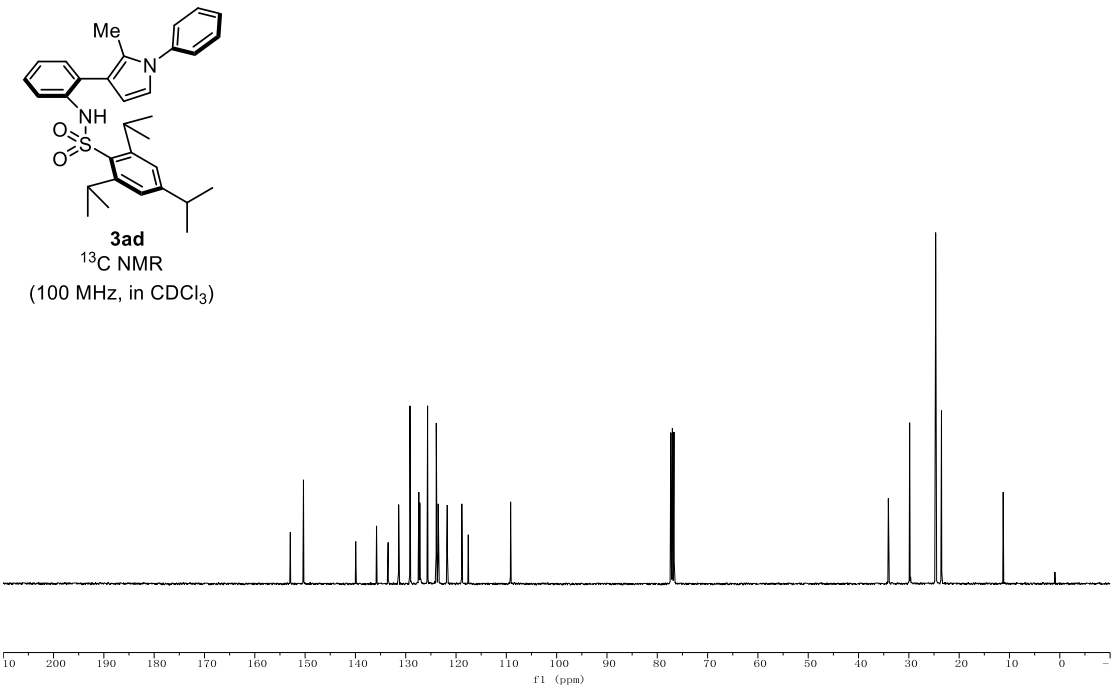
3ac

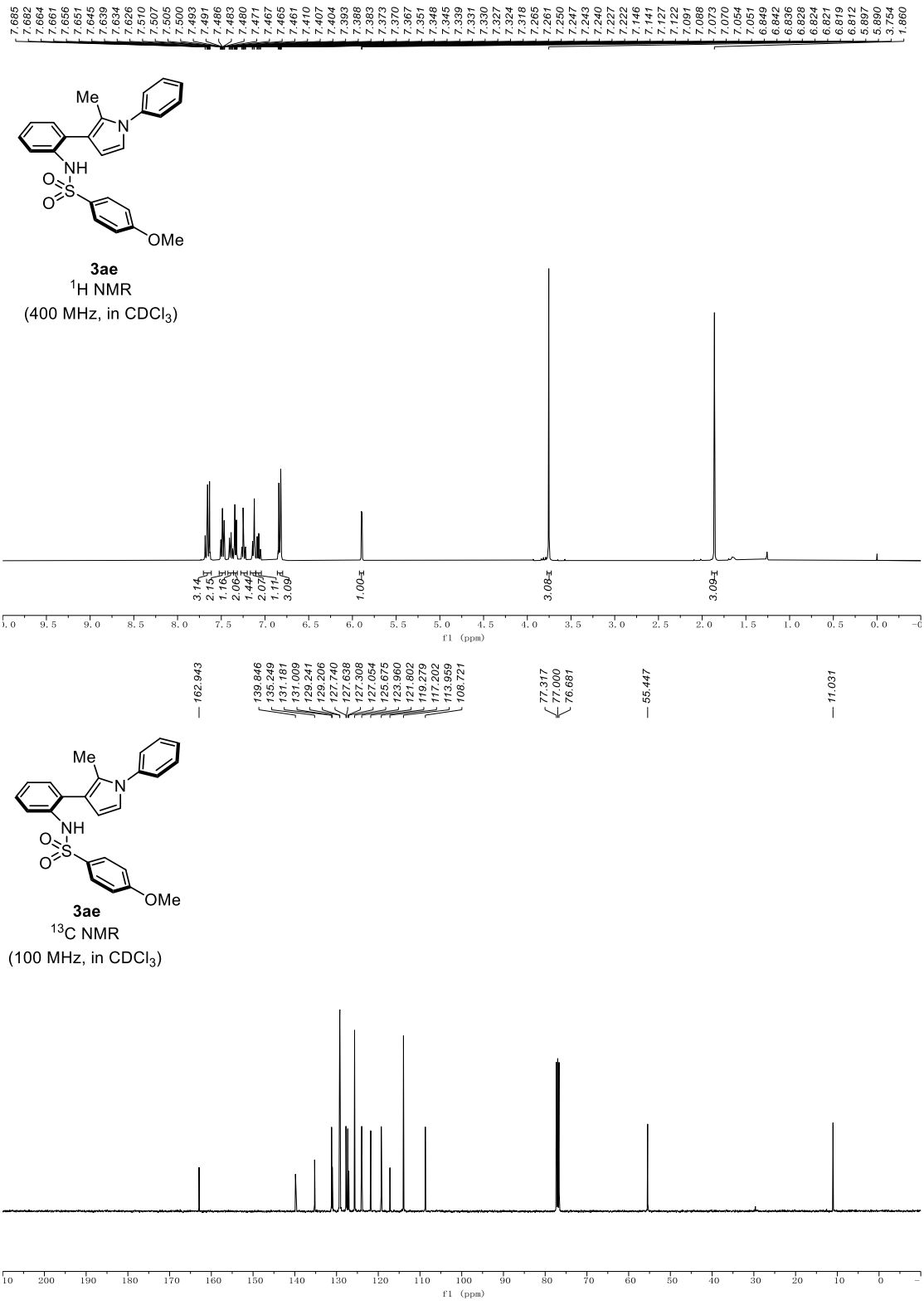
^{13}C NMR

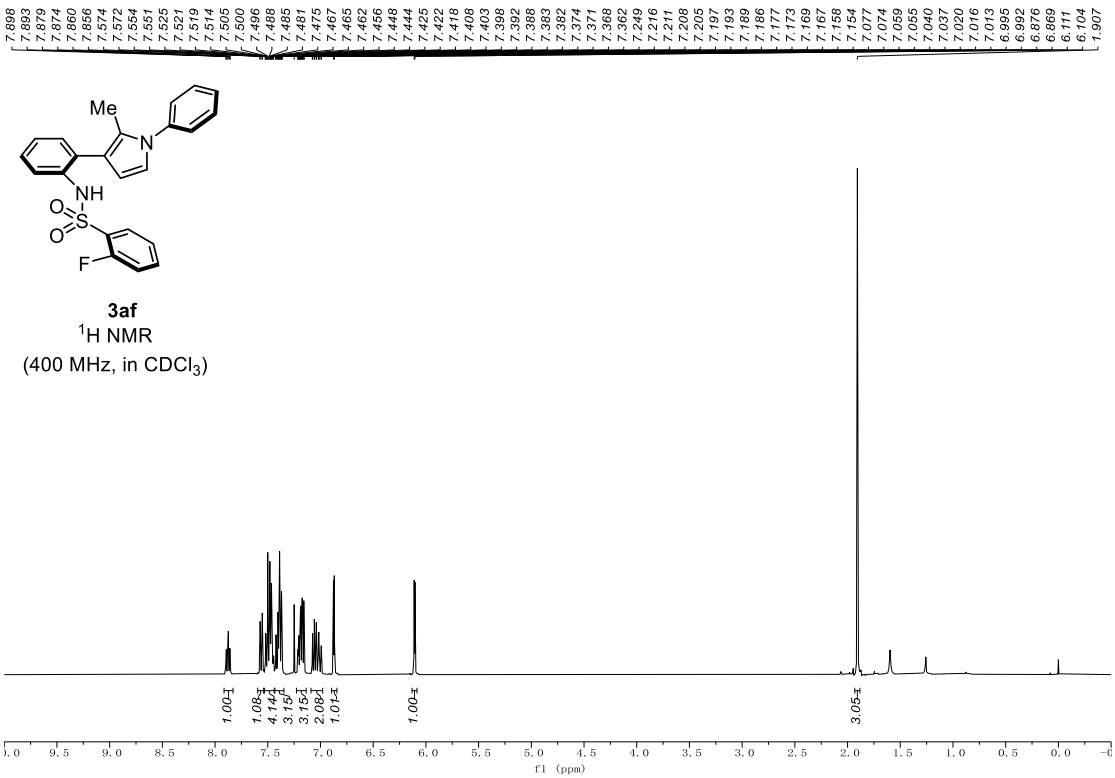
(100 MHz, in $CDCl_3$)



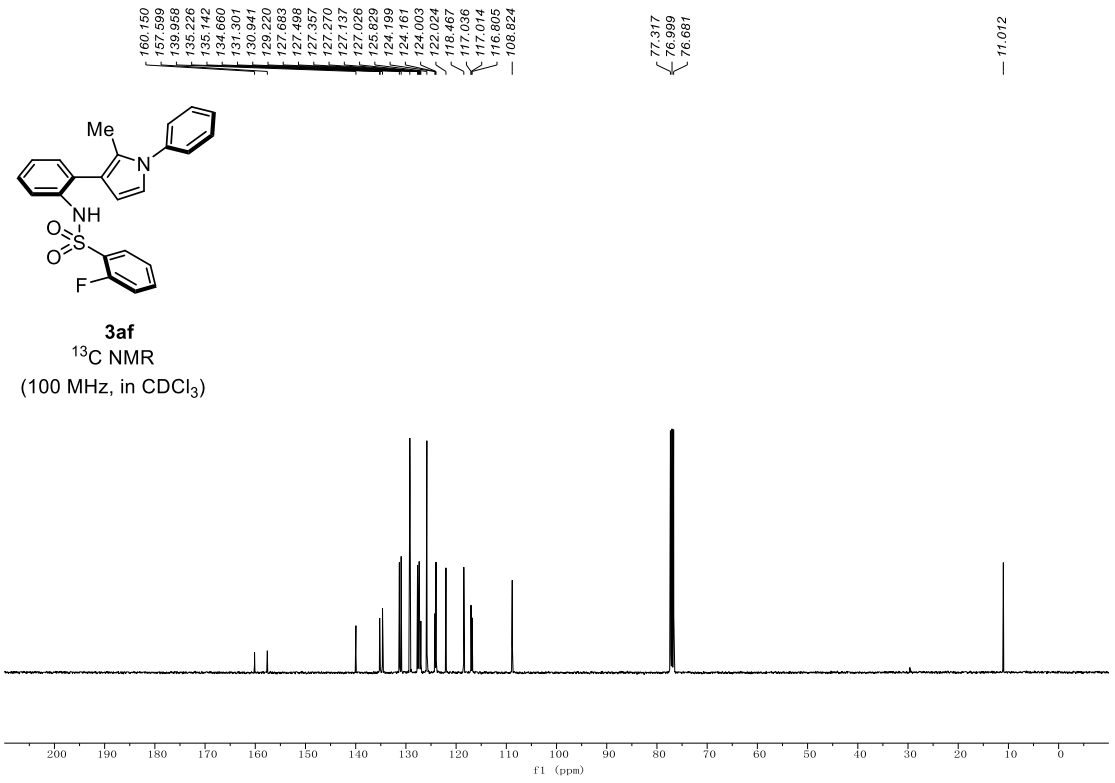

Me
N
NH
O
S
O
3ad
1H NMR
(400 MHz, in CDCl3)
f1 (ppm)


Me
N
NH
O
S
O
3ad
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

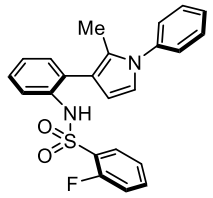

7.685
7.682
7.664
7.661
7.656
7.651
7.645
7.639
7.634
7.626
7.510
7.507
7.505
7.500
7.493
7.491
7.486
7.483
7.480
7.471
7.467
7.465
7.461
7.410
7.407
7.404
7.393
7.388
7.383
7.373
7.370
7.367
7.351
7.348
7.345
7.339
7.331
7.330
7.327
7.324
7.318
7.265
7.261
7.250
7.247
7.243
7.240
7.227
7.222
7.146
7.141
7.127
7.122
7.091
7.088
7.073
7.070
7.054
7.051
6.849
6.842
6.836
6.828
6.824
6.821
6.819
6.812
5.897
5.890
3.754
1.860
Me
N
NH
O
S
O
OMe
3ae
1H NMR
(400 MHz, in CDCl3)
3.14
2.15
1.16
2.06
1.44
2.07
1.11
3.09
1.00
3.06
3.09
f1 (ppm)
162.943
139.846
135.249
131.181
131.009
129.241
129.206
127.740
127.638
127.308
127.054
125.675
123.960
121.802
119.279
117.202
113.959
108.721
77.317
77.000
76.681
55.447
11.031
Me
N
NH
O
S
O
OMe
3ae
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)



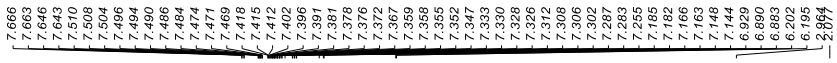
3af
^{1}H NMR
(400 MHz, in $CDCl_3$)

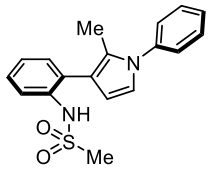


3af
^{13}C NMR
(100 MHz, in $CDCl_3$)

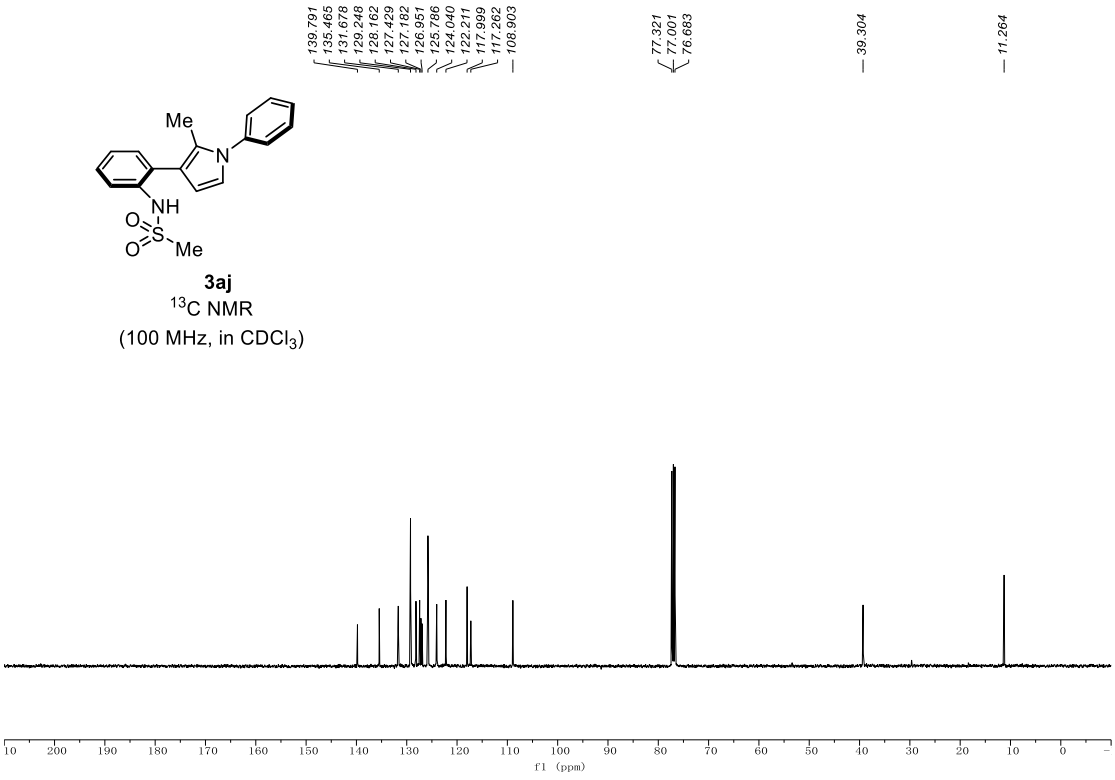


3af
^{19}F NMR
(376 MHz, in $CDCl_3$)





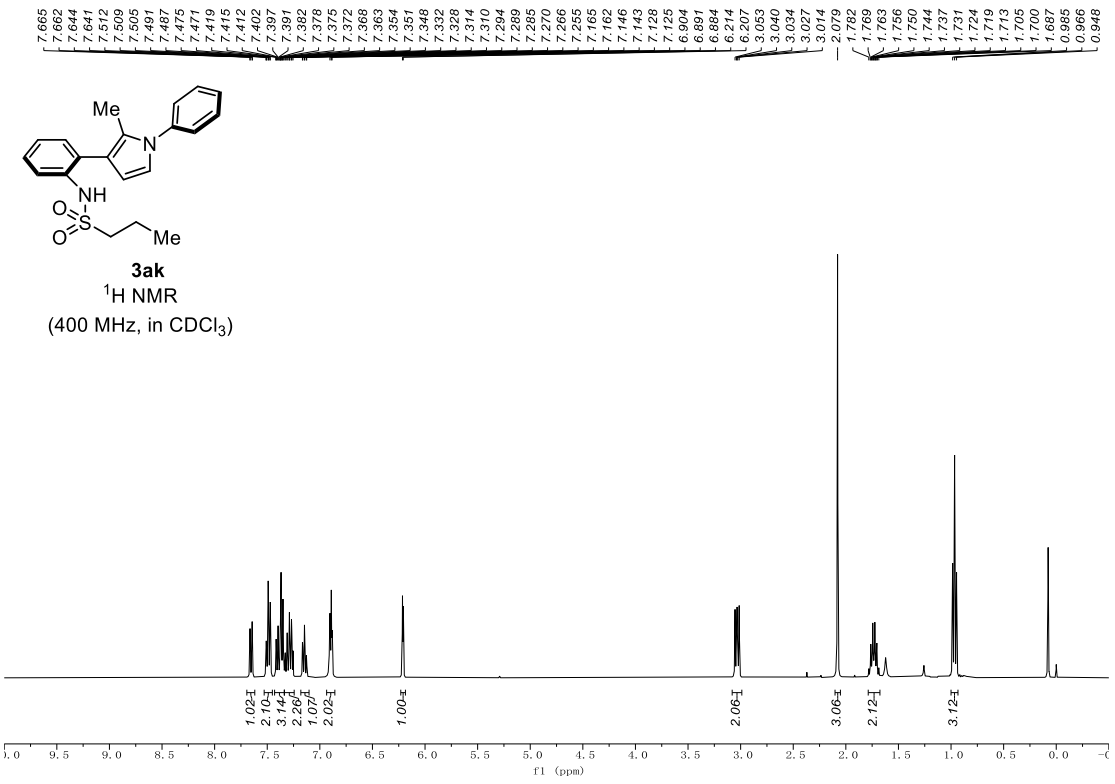
3aj
^{1}H NMR
(400 MHz, in $CDCl_3$)



3aj

^{13}C NMR

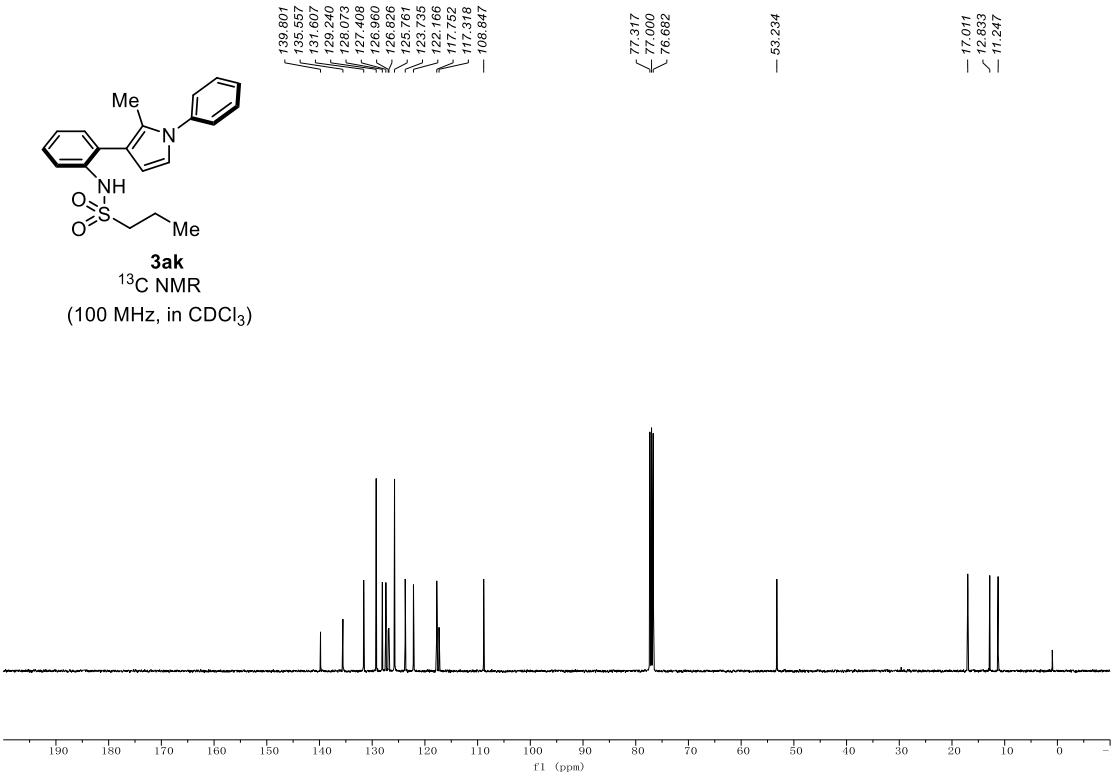
(100 MHz, in $CDCl_3$)



3ak

^{1}H NMR

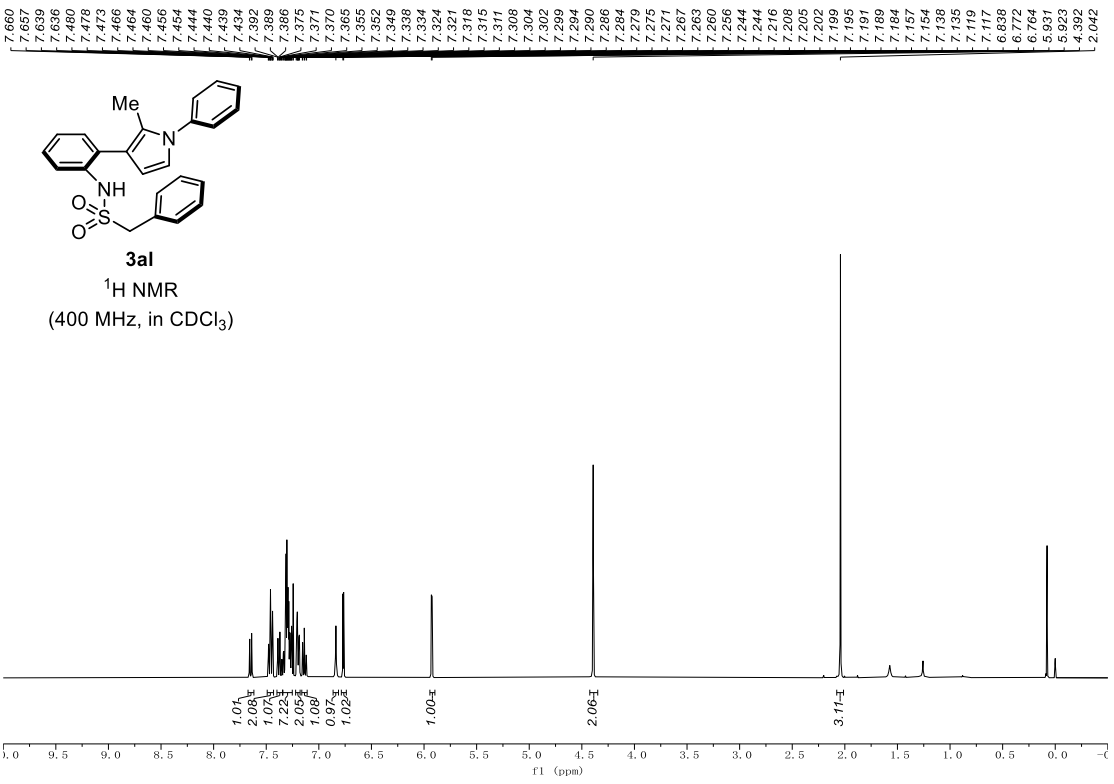
(400 MHz, in $CDCl_3$)



3ak

^{13}C NMR

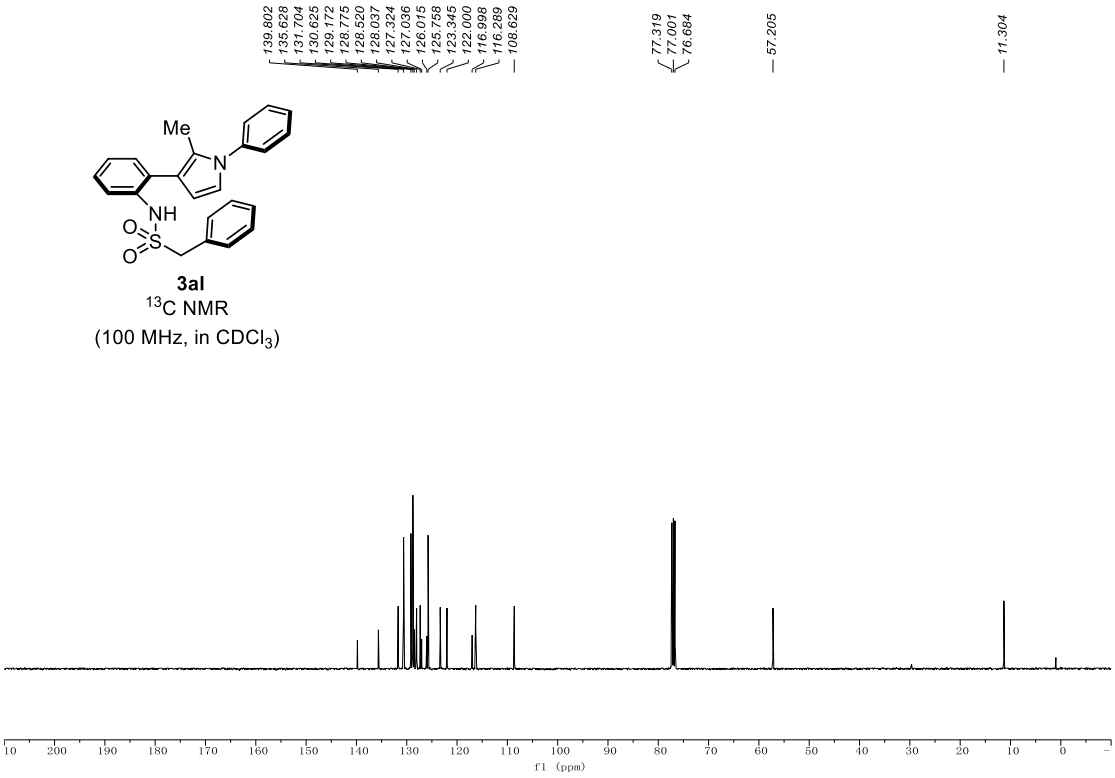
(100 MHz, in $CDCl_3$)



3al

^{1}H NMR

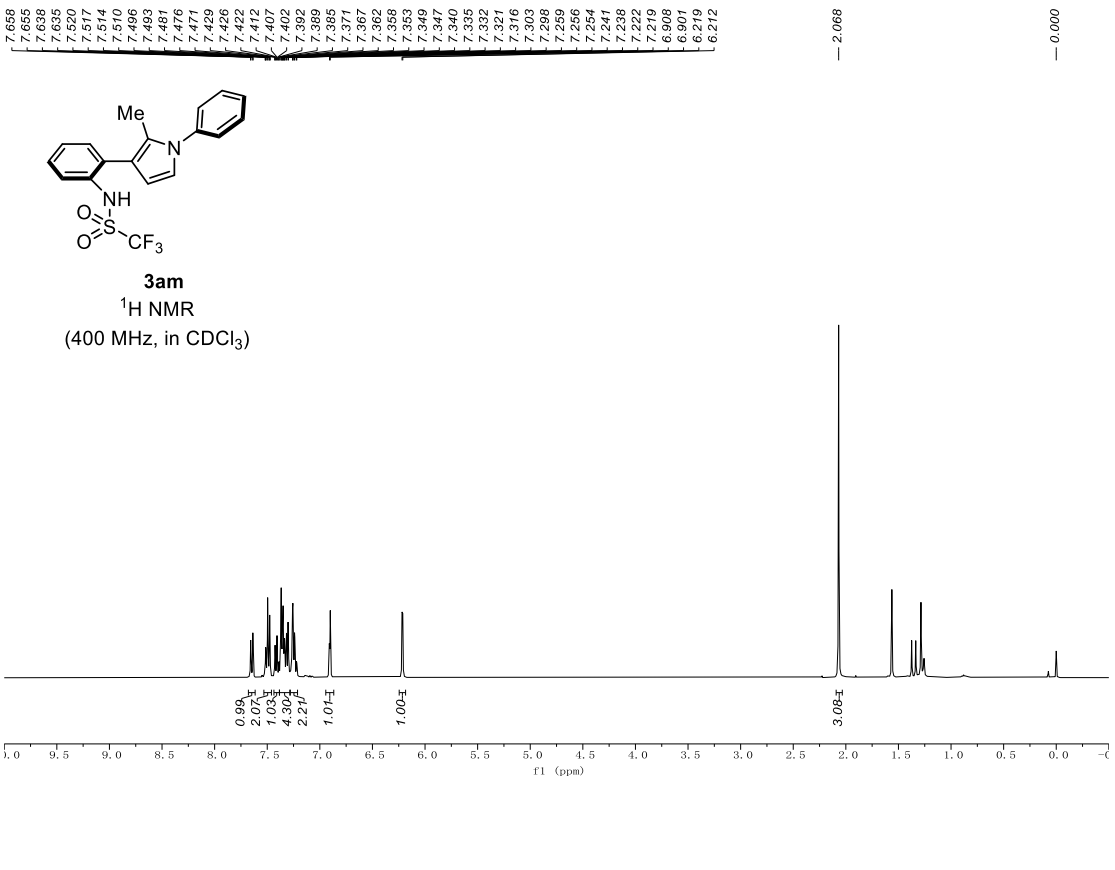
(400 MHz, in $CDCl_3$)



3al

^{13}C NMR

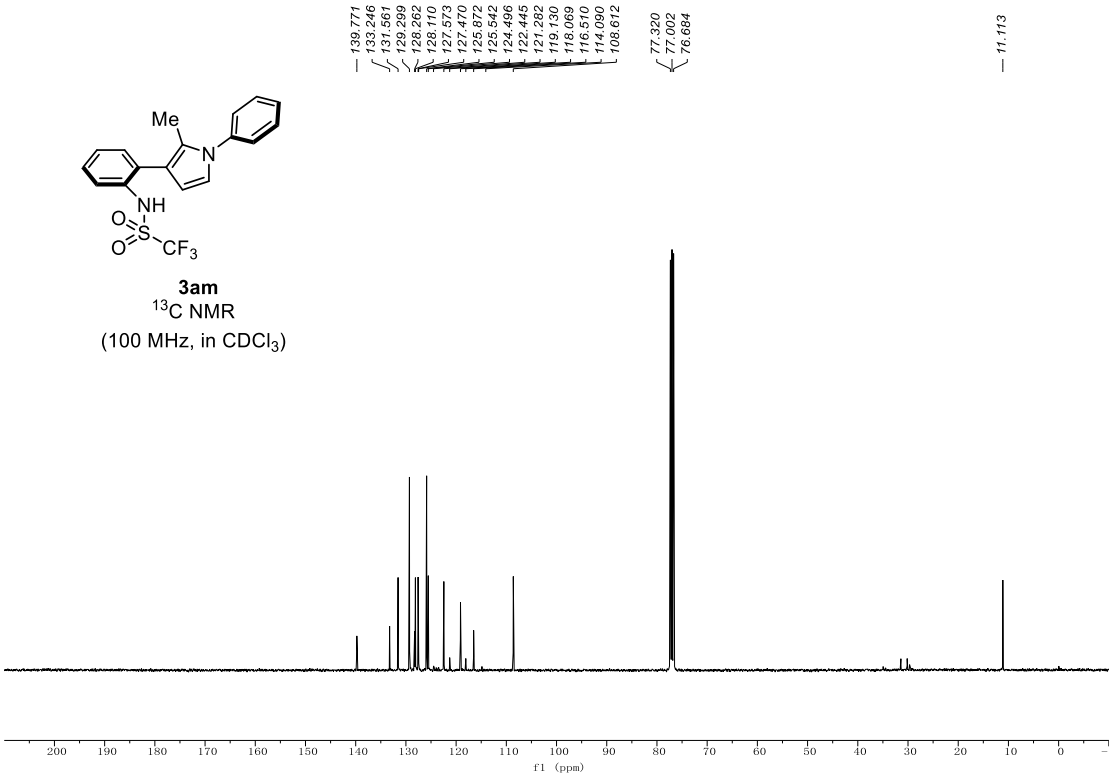
(100 MHz, in $CDCl_3$)



3am

^{1}H NMR

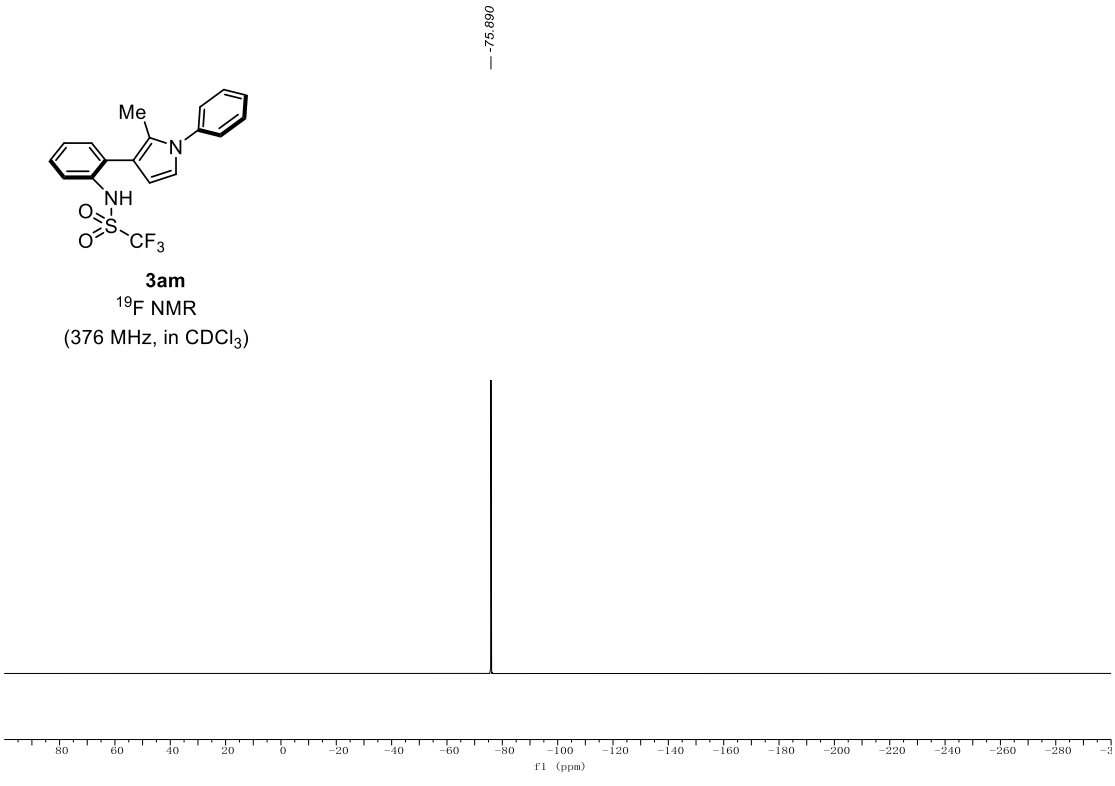
(400 MHz, in $CDCl_3$)



3am

^{13}C NMR

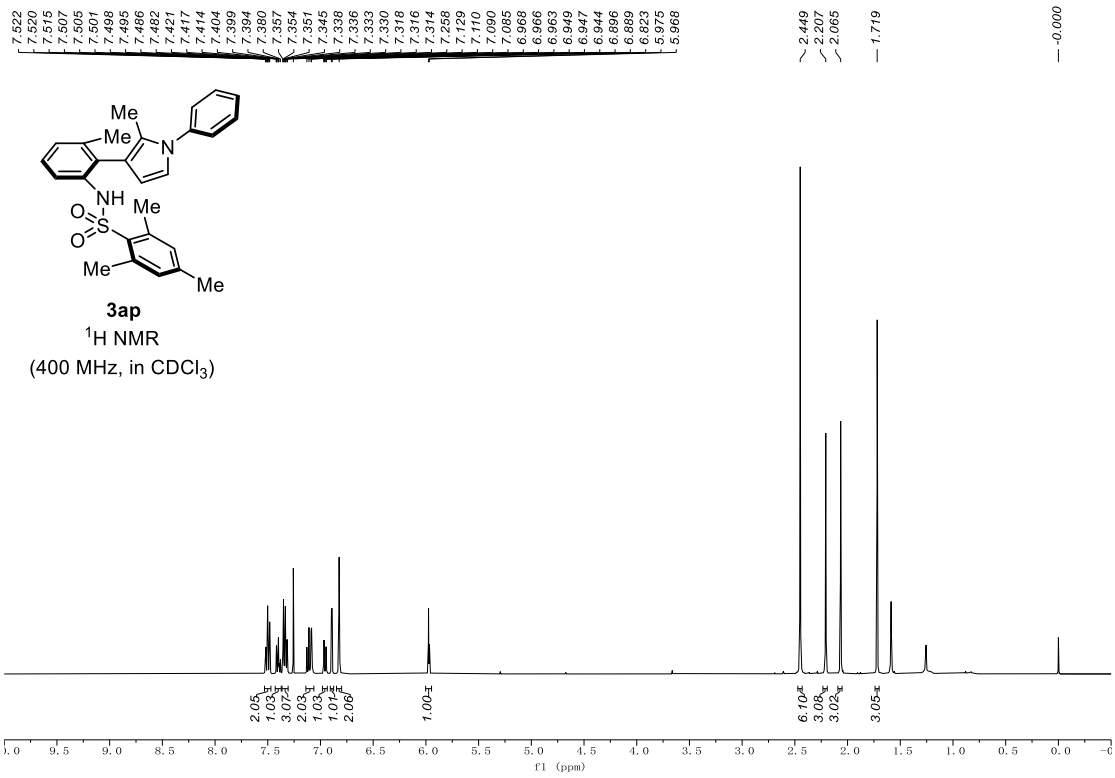
(100 MHz, in $CDCl_3$)



3am

^{19}F NMR

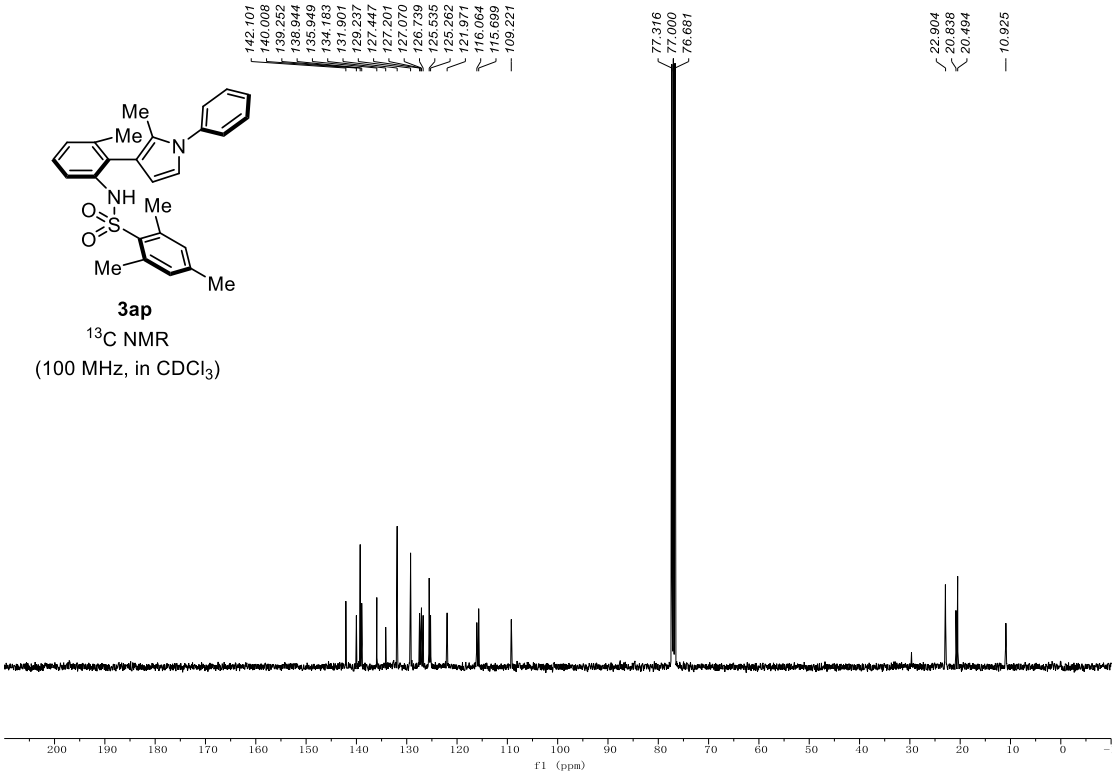
(376 MHz, in $CDCl_3$)



3ap

^{1}H NMR

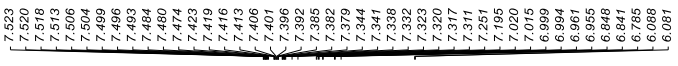
(400 MHz, in $CDCl_3$)

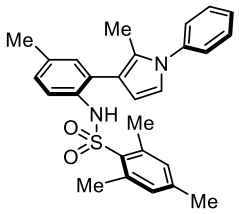


3ap

^{13}C NMR

(100 MHz, in $CDCl_3$)

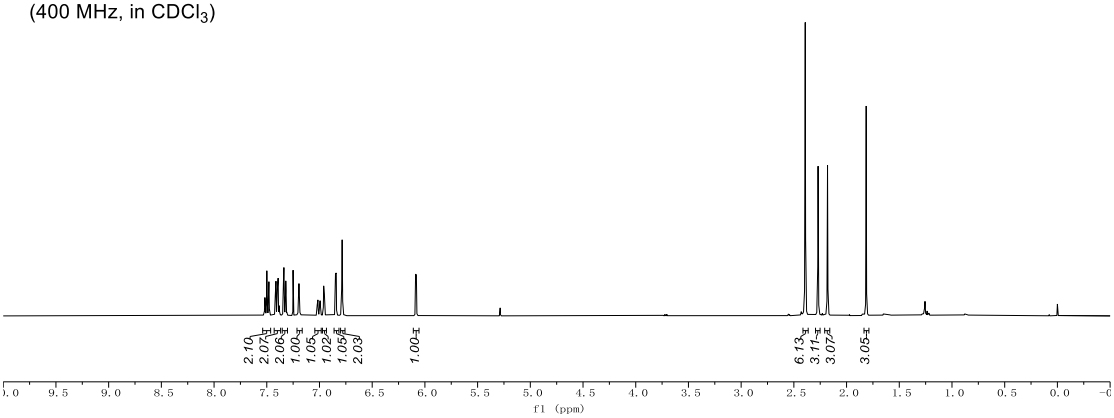


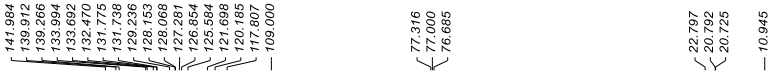


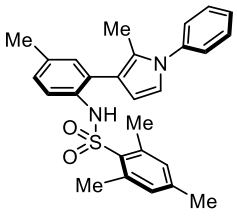
3aq

^{1}H NMR

(400 MHz, in $CDCl_3$)



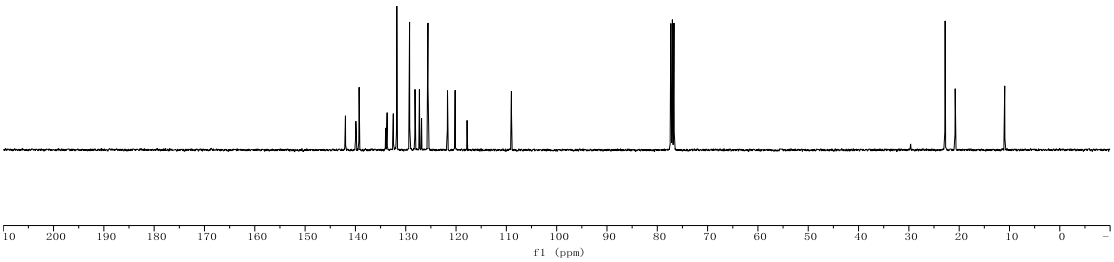


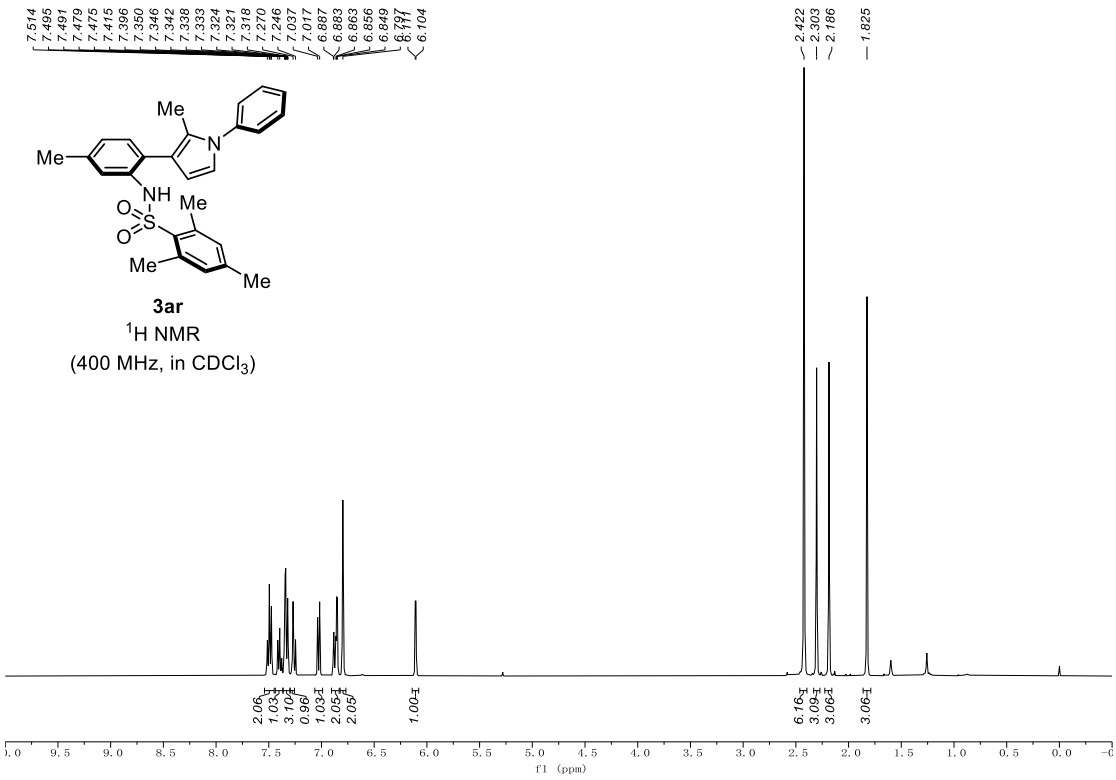


3aq

^{13}C NMR

(100 MHz, in $CDCl_3$)

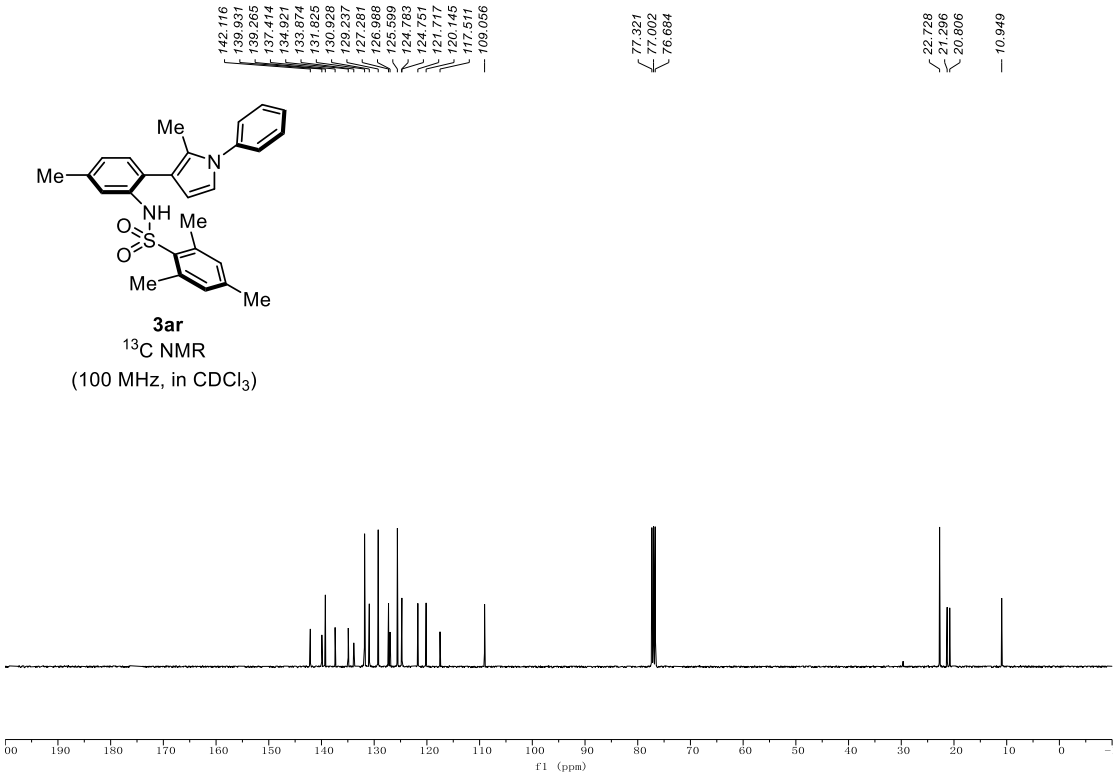




3ar

^{1}H NMR

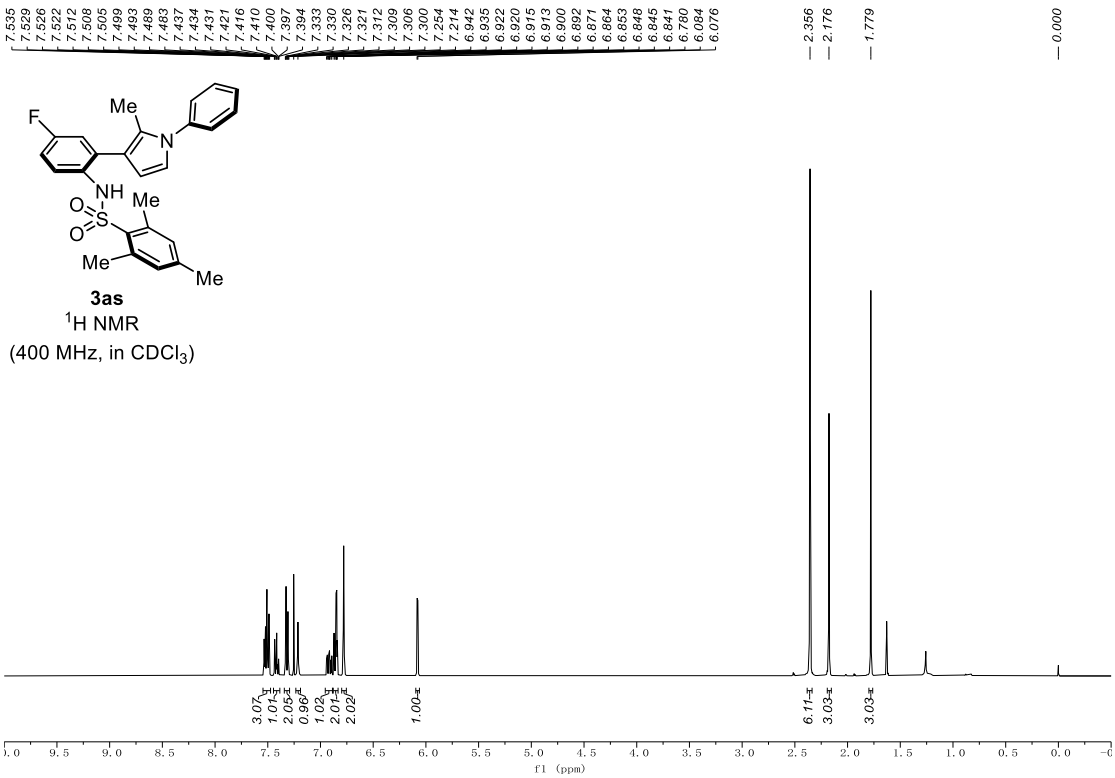
(400 MHz, in $CDCl_3$)



3ar

^{13}C NMR

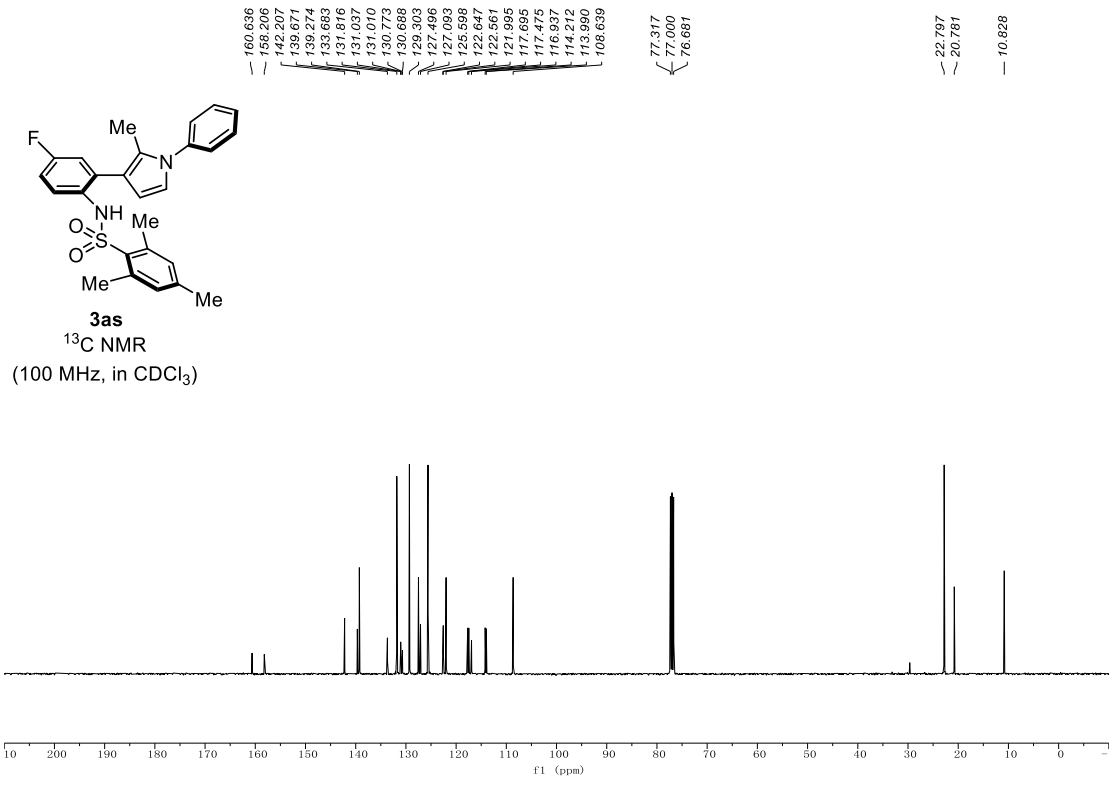
(100 MHz, in $CDCl_3$)



3as

^{1}H NMR

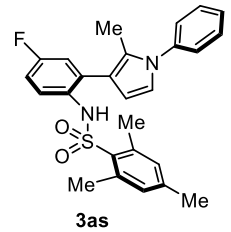
(400 MHz, in $CDCl_3$)



3as

^{13}C NMR

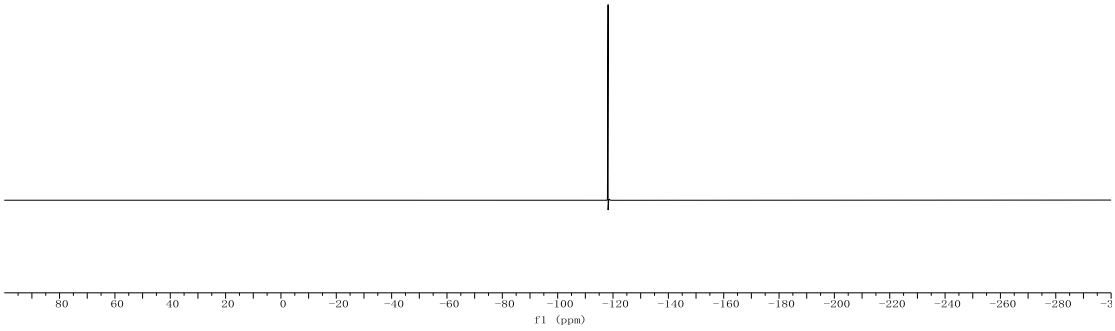
(100 MHz, in $CDCl_3$)

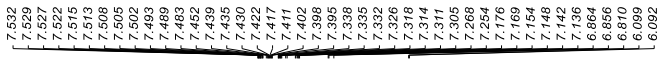


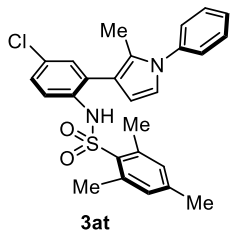
3as

^{19}F NMR

(376 MHz, in $CDCl_3$)



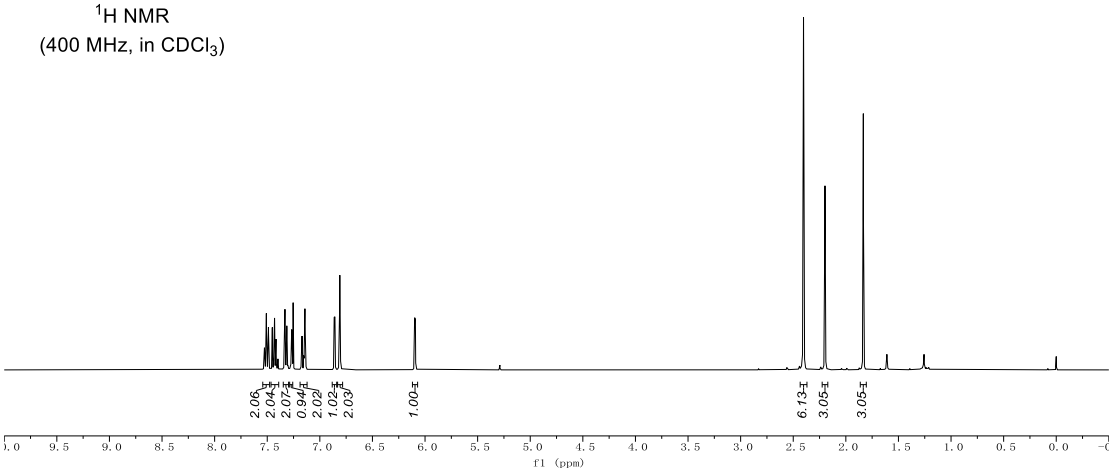


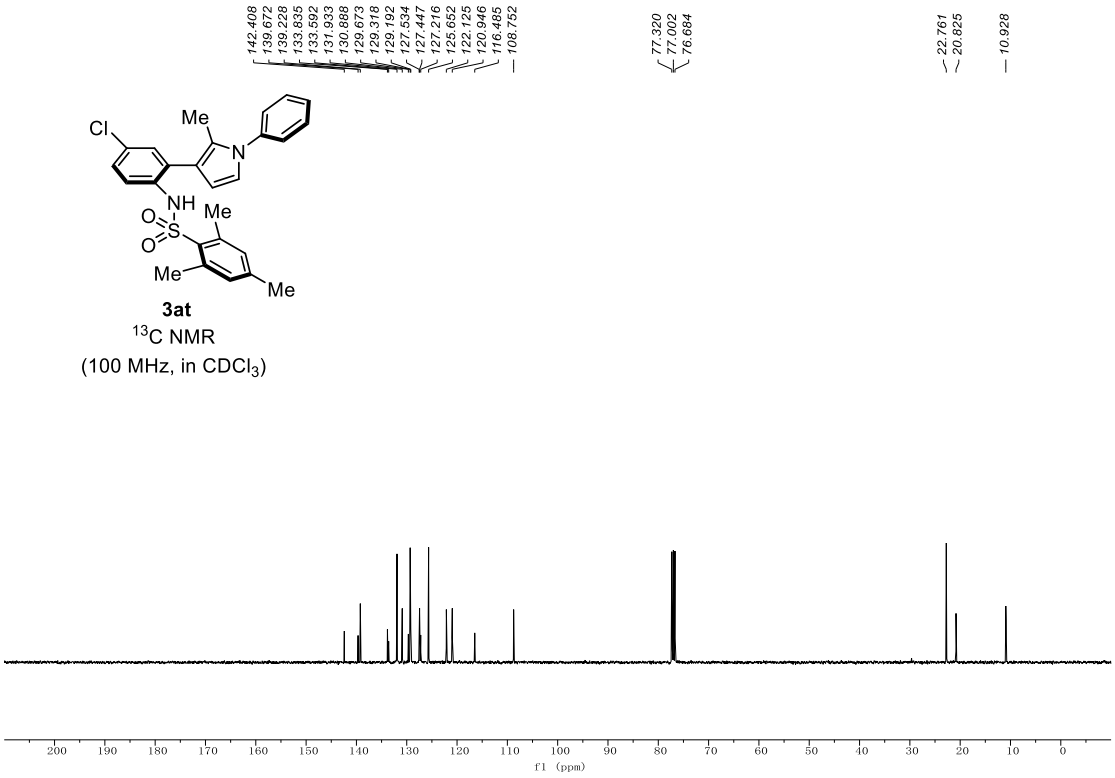


3at

^{1}H NMR

(400 MHz, in $CDCl_3$)

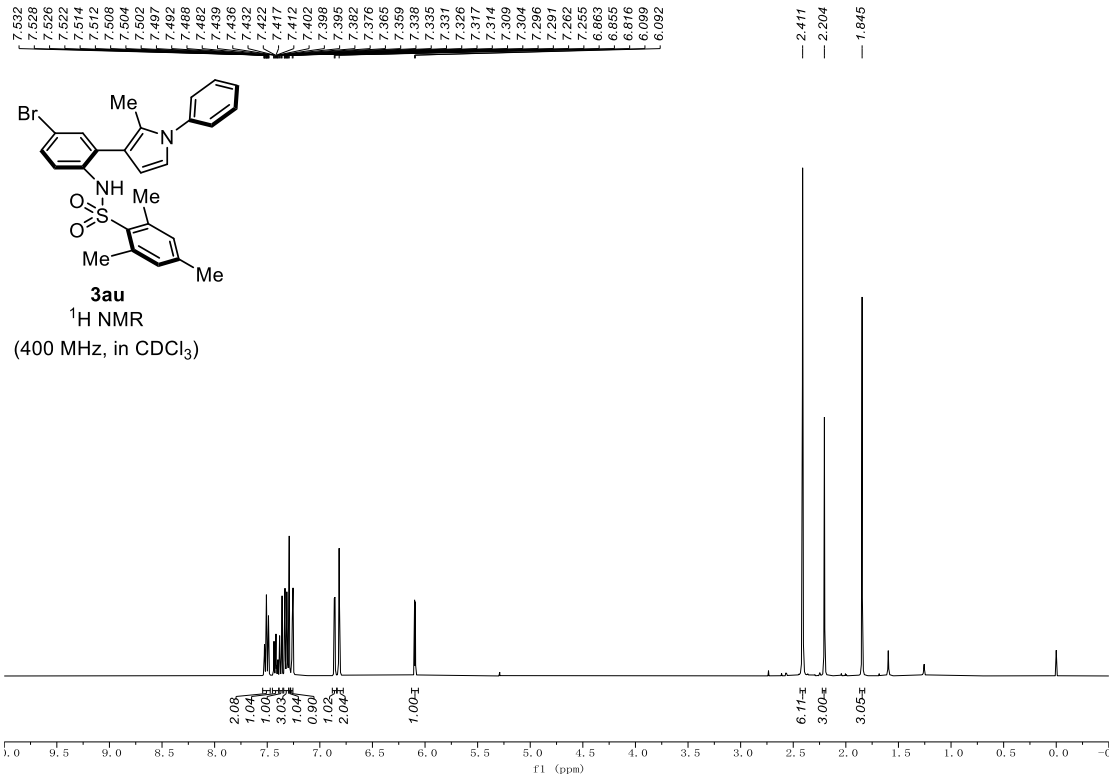




3at

^{13}C NMR

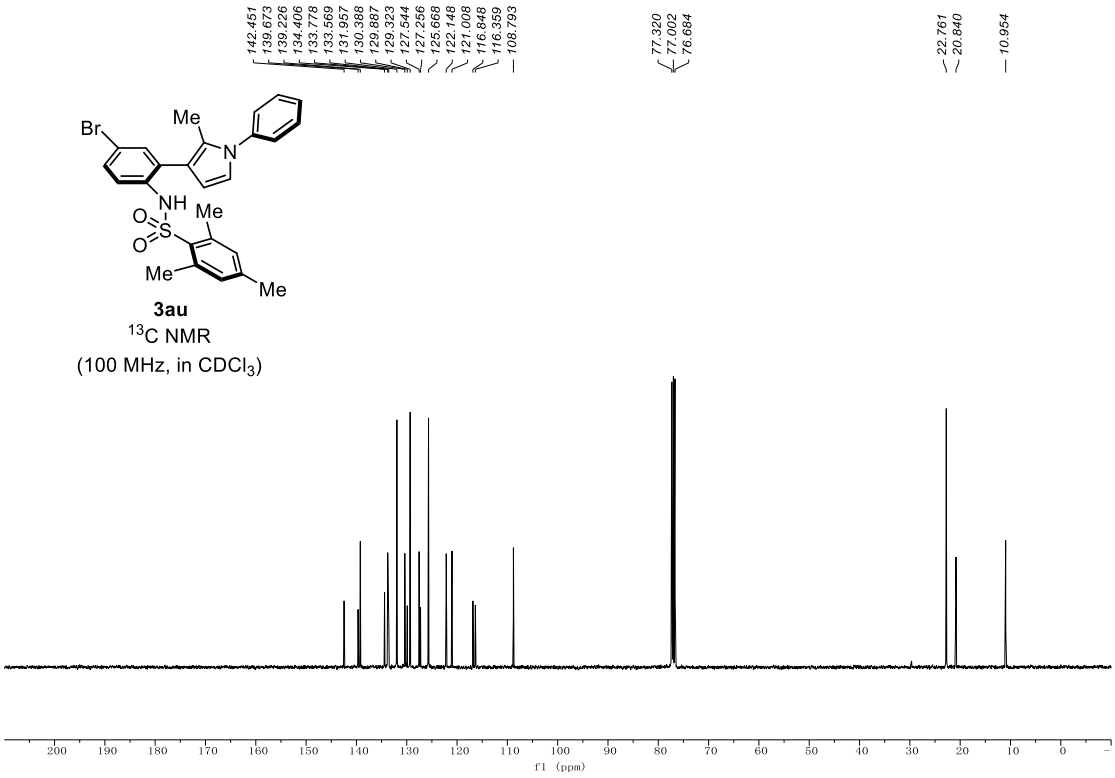
(100 MHz, in $CDCl_3$)



3au

^{1}H NMR

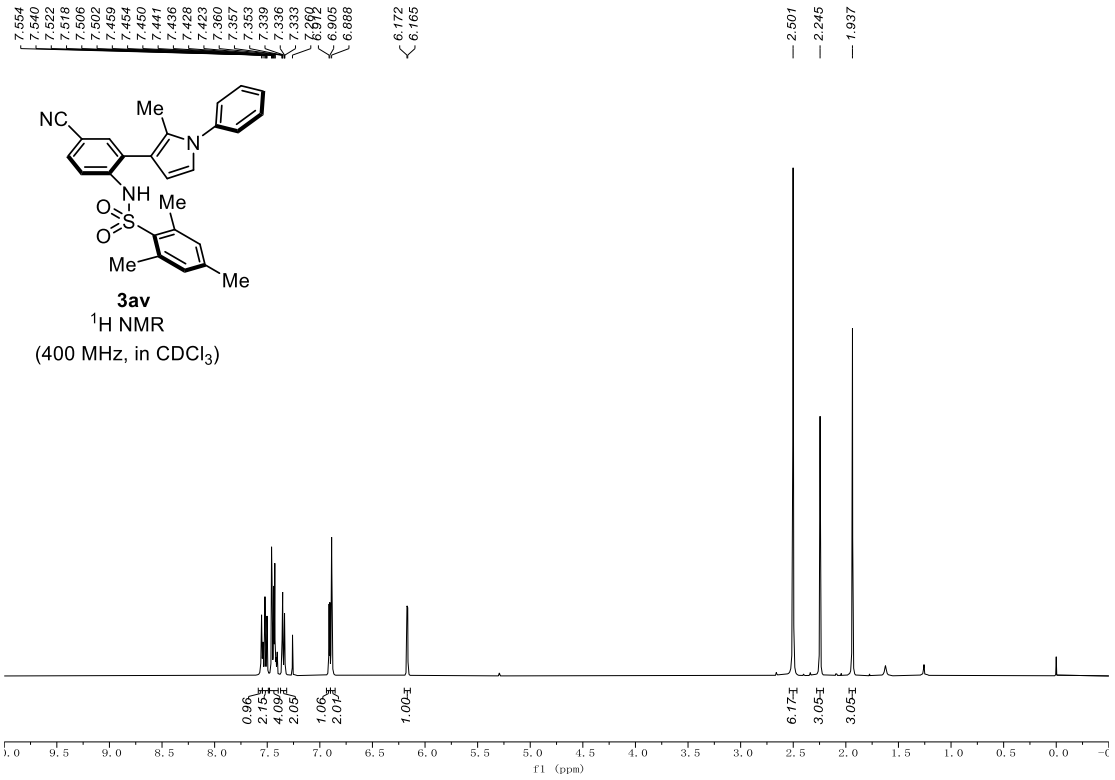
(400 MHz, in $CDCl_3$)



3au

^{13}C NMR

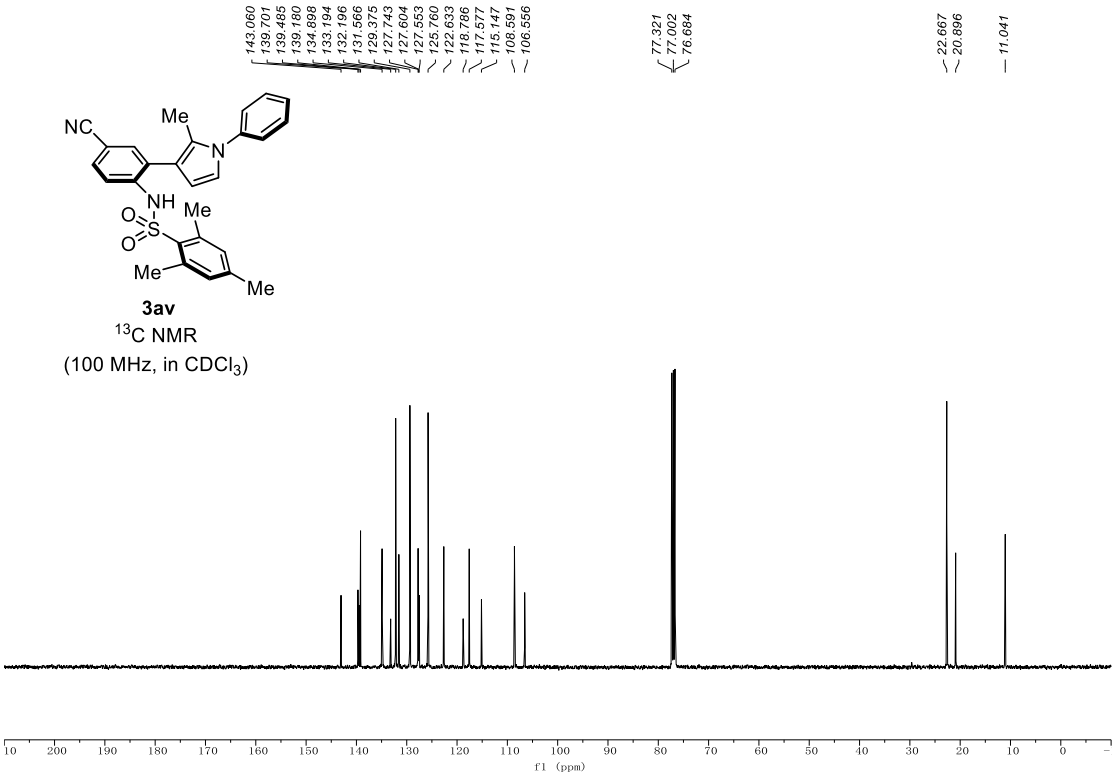
(100 MHz, in $CDCl_3$)

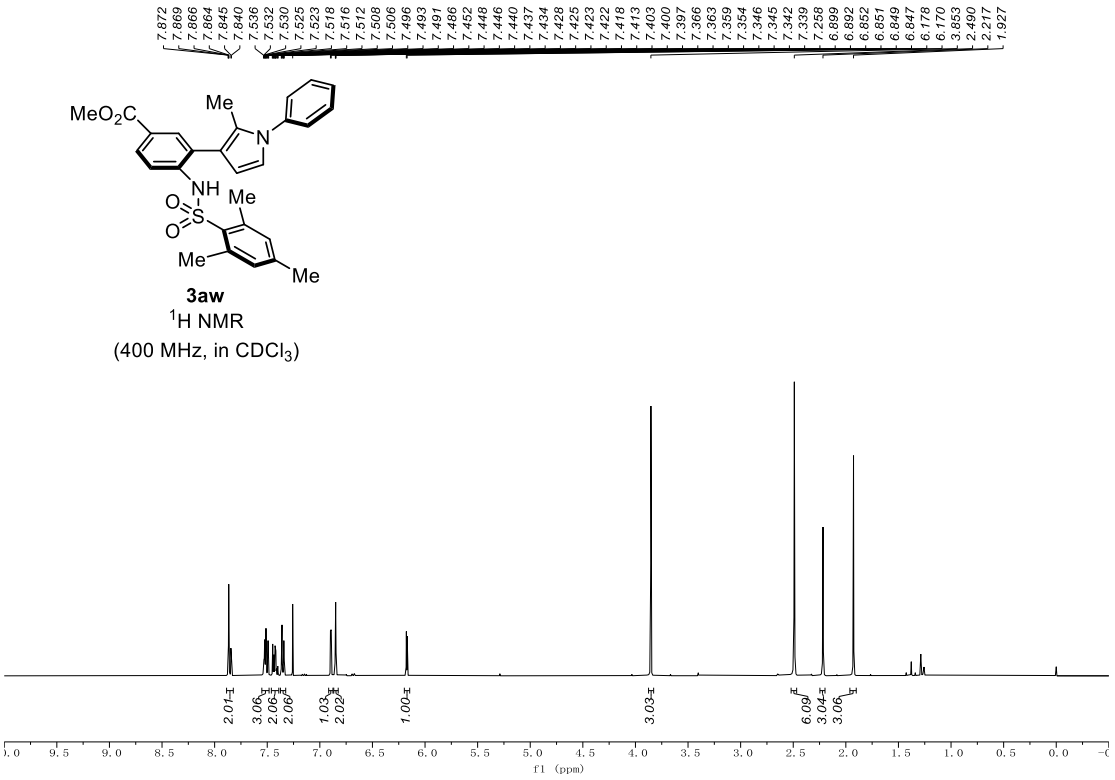


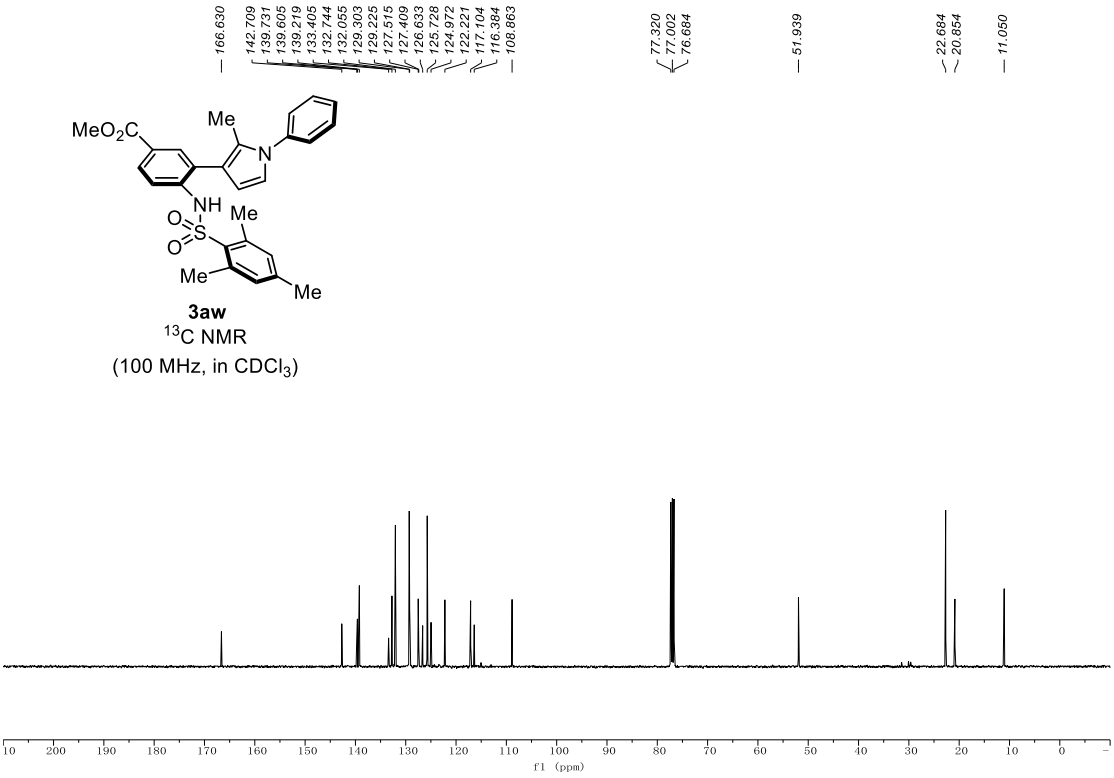
3av

^{1}H NMR

(400 MHz, in $CDCl_3$)


143.060
139.701
139.485
139.180
134.898
133.194
132.196
131.566
129.375
127.743
127.604
127.553
125.760
122.633
118.786
117.577
115.147
108.591
106.556
77.321
77.002
76.684
22.667
20.896
11.041
NC
Me
N
NH
Me
O
S
O
Me
Me
3av
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

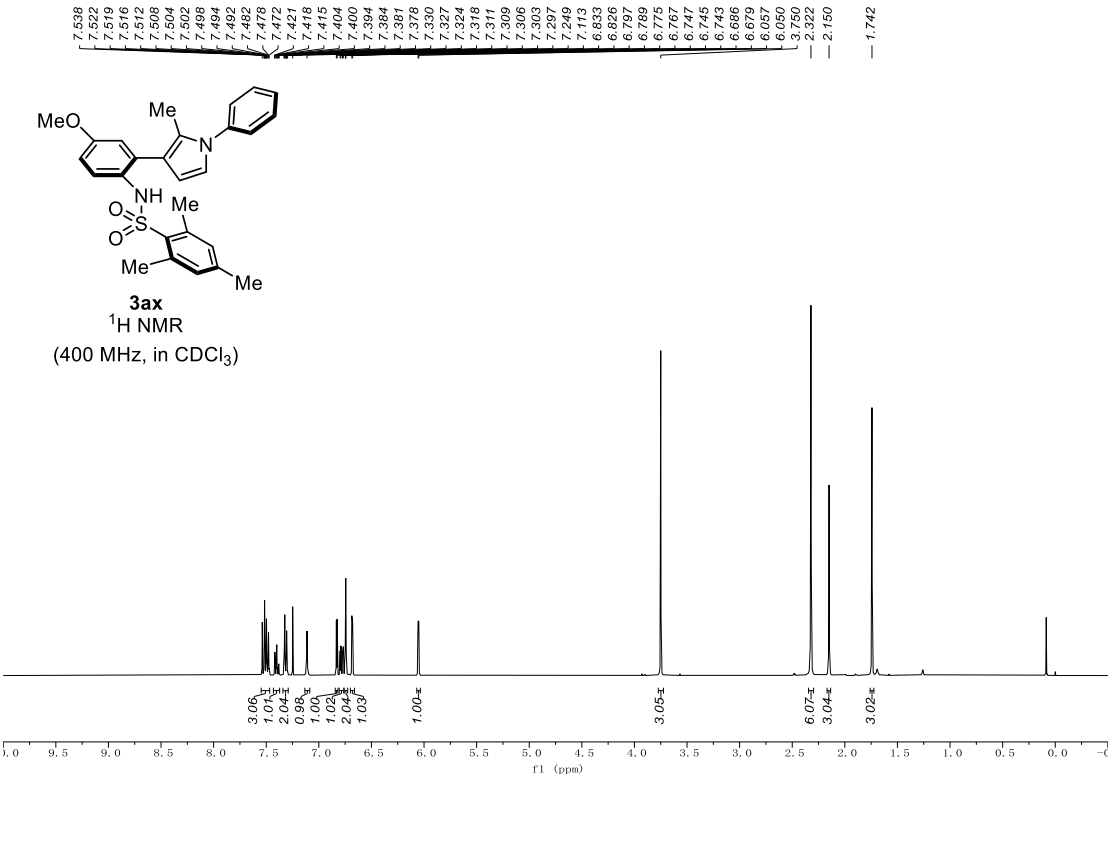

7.872
7.869
7.866
7.864
7.845
7.840
7.536
7.532
7.530
7.525
7.523
7.518
7.516
7.512
7.508
7.506
7.496
7.493
7.491
7.486
7.452
7.448
7.446
7.440
7.437
7.434
7.428
7.425
7.423
7.422
7.418
7.413
7.403
7.400
7.397
7.366
7.363
7.359
7.354
7.346
7.345
7.342
7.339
7.258
6.899
6.892
6.852
6.851
6.849
6.847
6.178
6.170
3.853
2.490
2.217
1.927
MeO2C
Me
N
NH
Me
O
S
O
Me
Me
3aw
1H NMR
(400 MHz, in CDCl3)
2.01
3.06
2.06
2.06
1.03
2.02
1.00
3.03
6.09
3.04
3.06
f1 (ppm)



3aw

^{13}C NMR

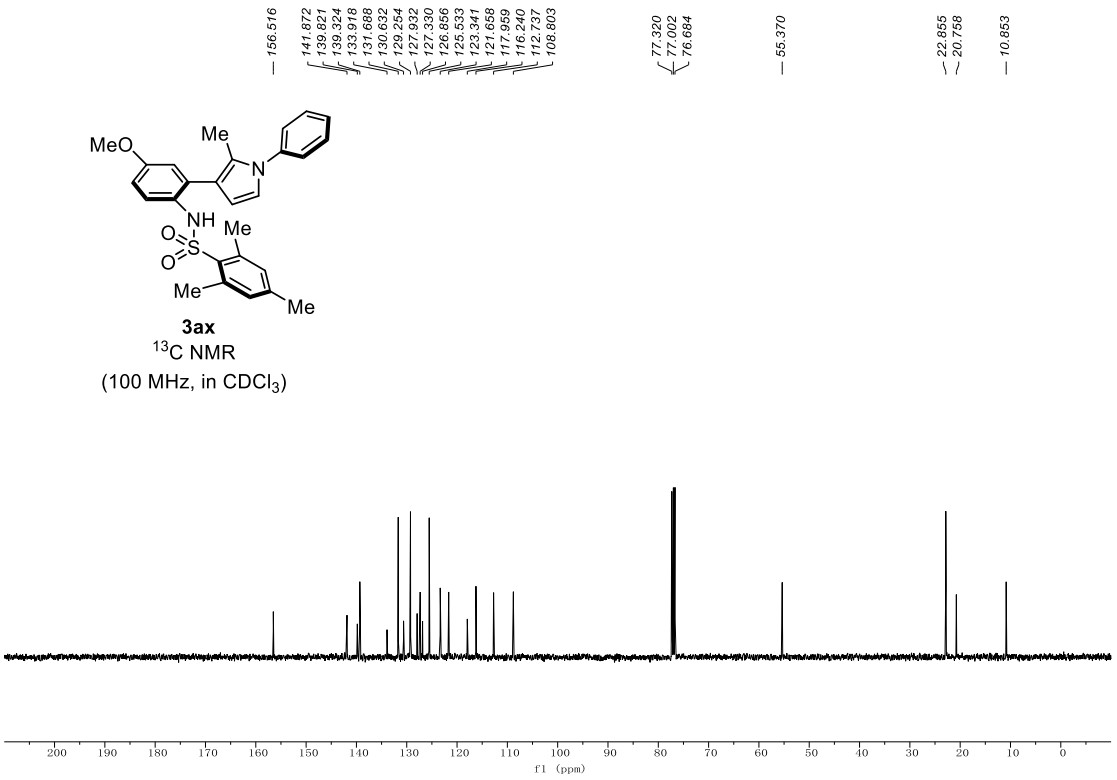
(100 MHz, in $CDCl_3$)



3ax

^{1}H NMR

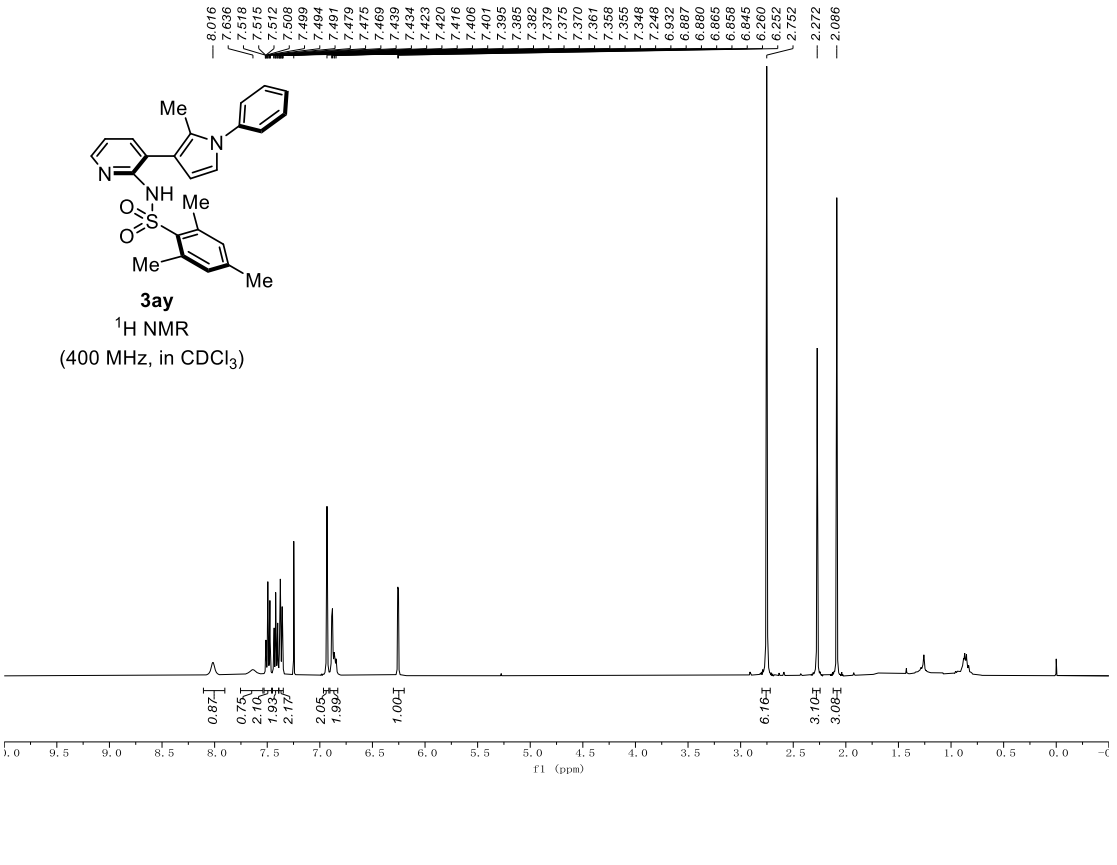
(400 MHz, in $CDCl_3$)



3ax

^{13}C NMR

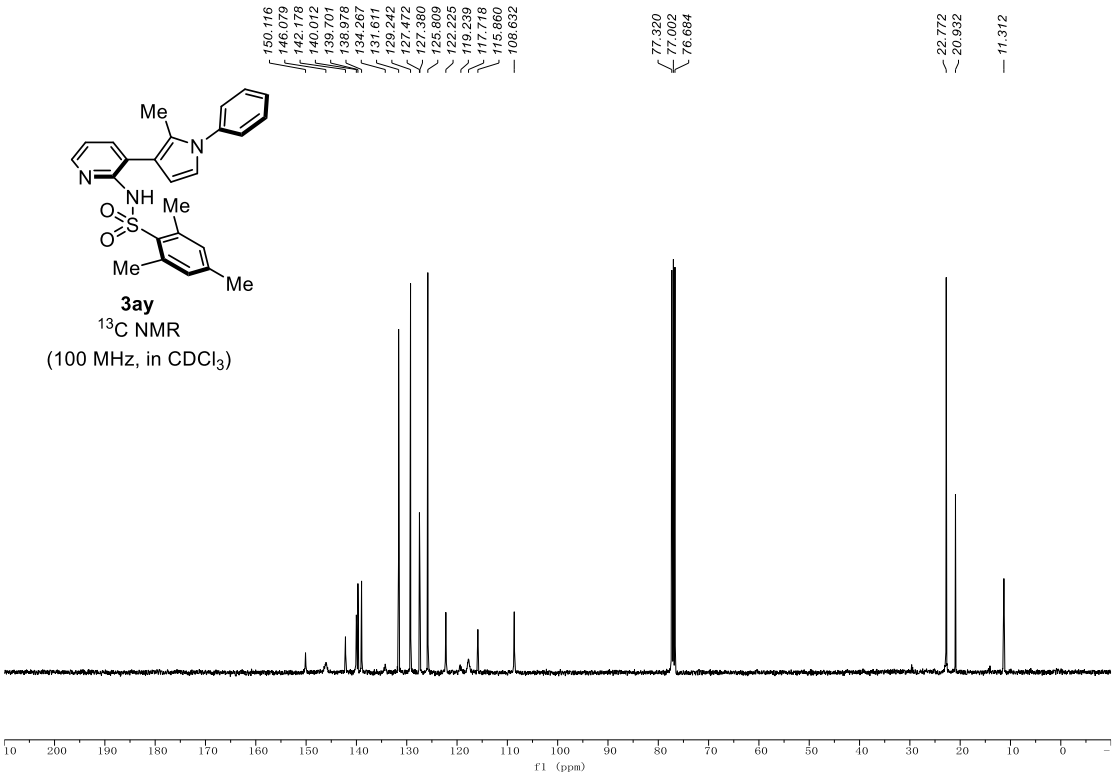
(100 MHz, in $CDCl_3$)



3ay

^{1}H NMR

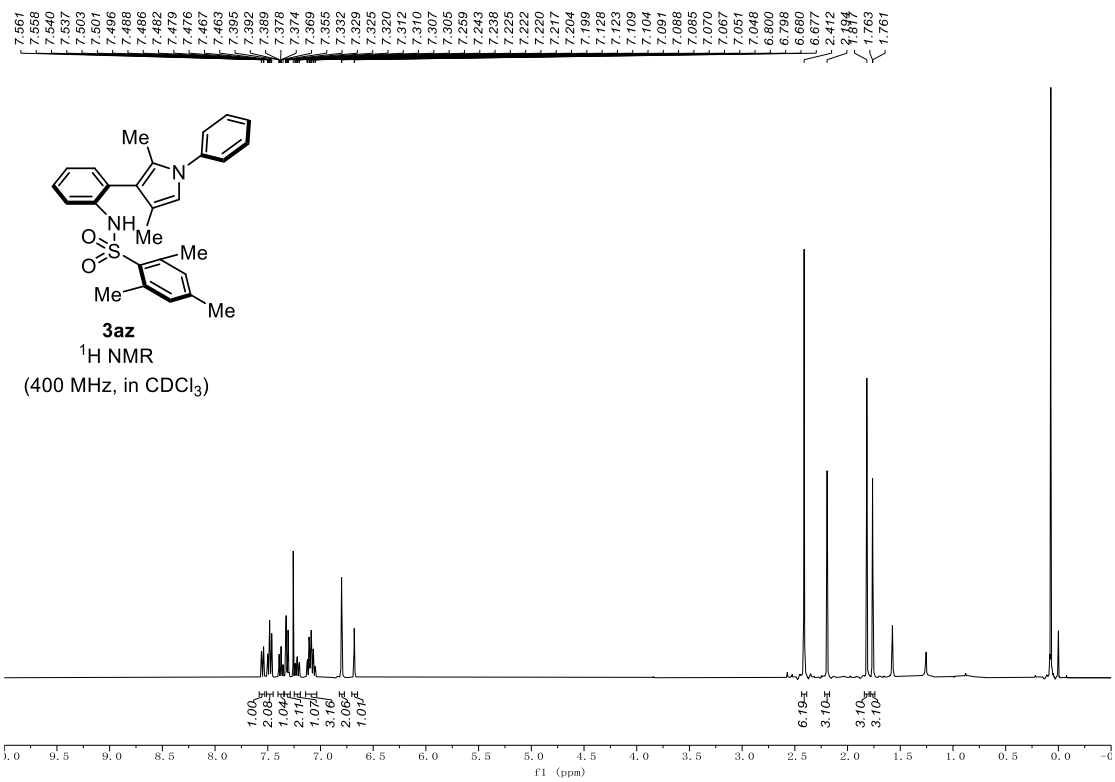
(400 MHz, in $CDCl_3$)



3ay

^{13}C NMR

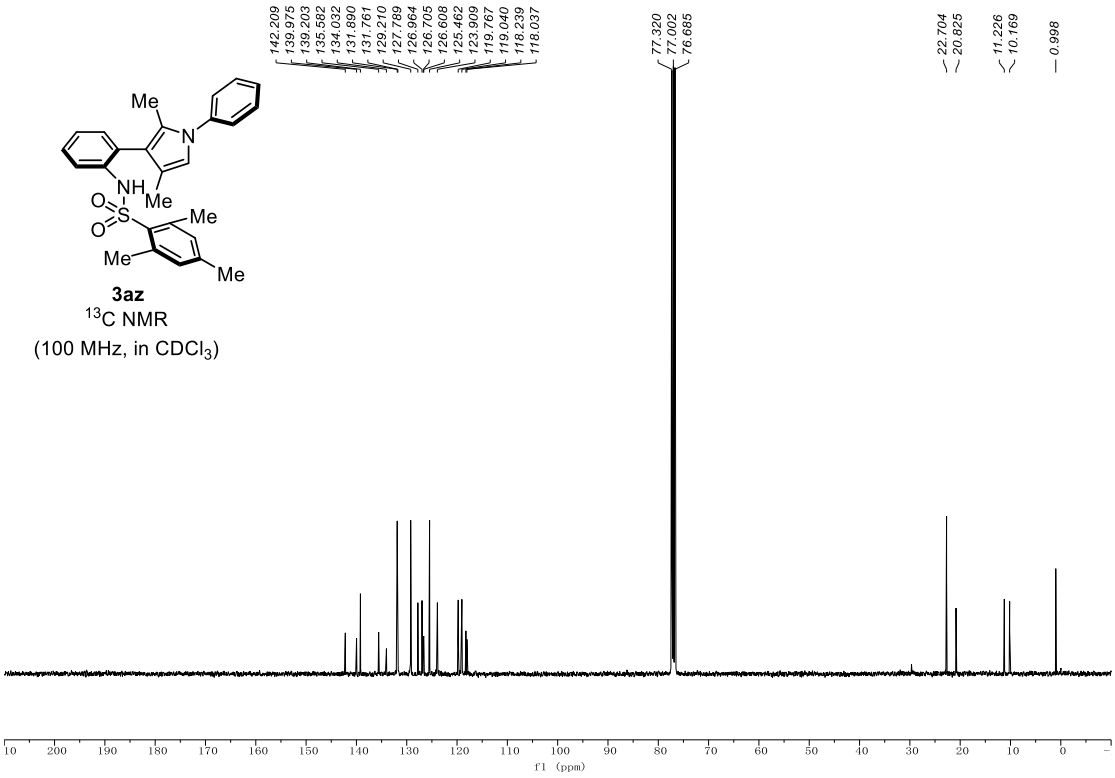
(100 MHz, in $CDCl_3$)



3az

^{1}H NMR

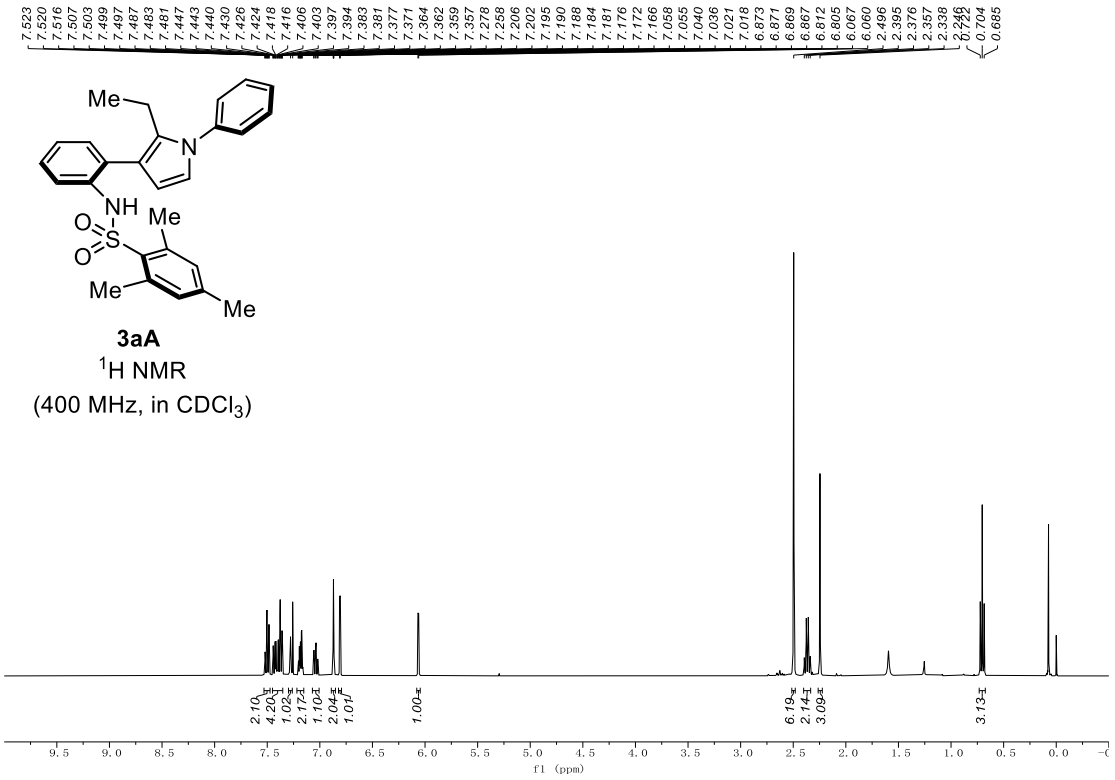
(400 MHz, in $CDCl_3$)



3az

^{13}C NMR

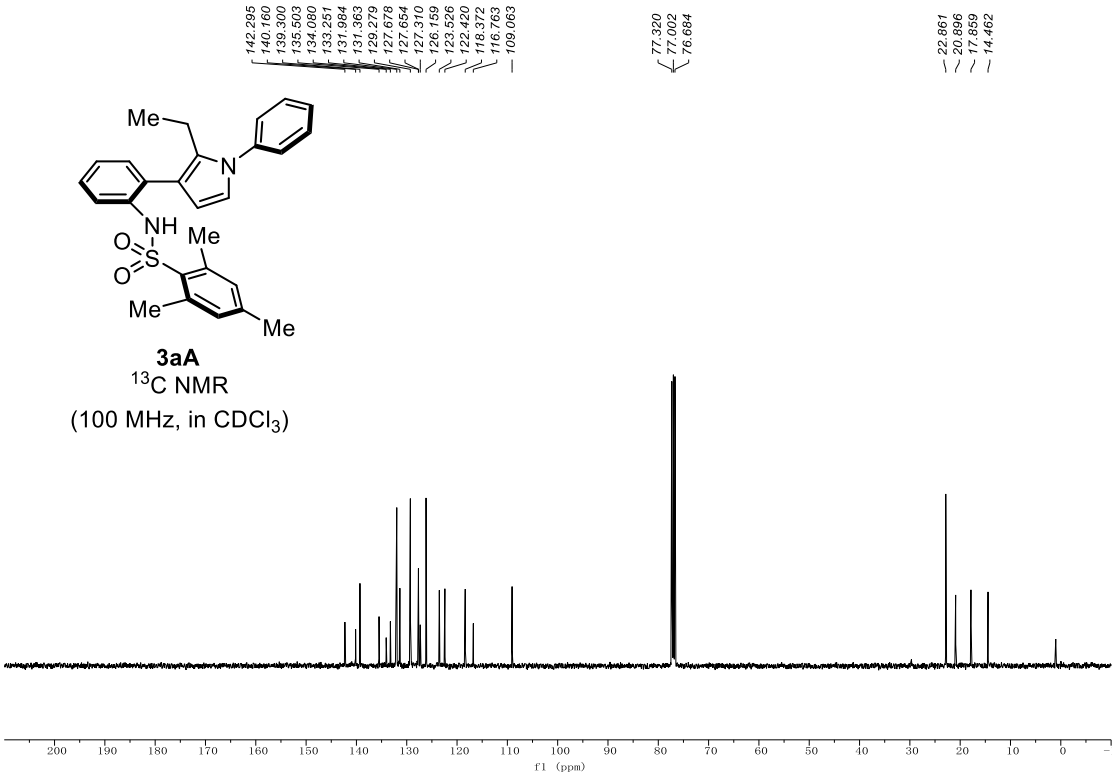
(100 MHz, in $CDCl_3$)



3aA

^{1}H NMR

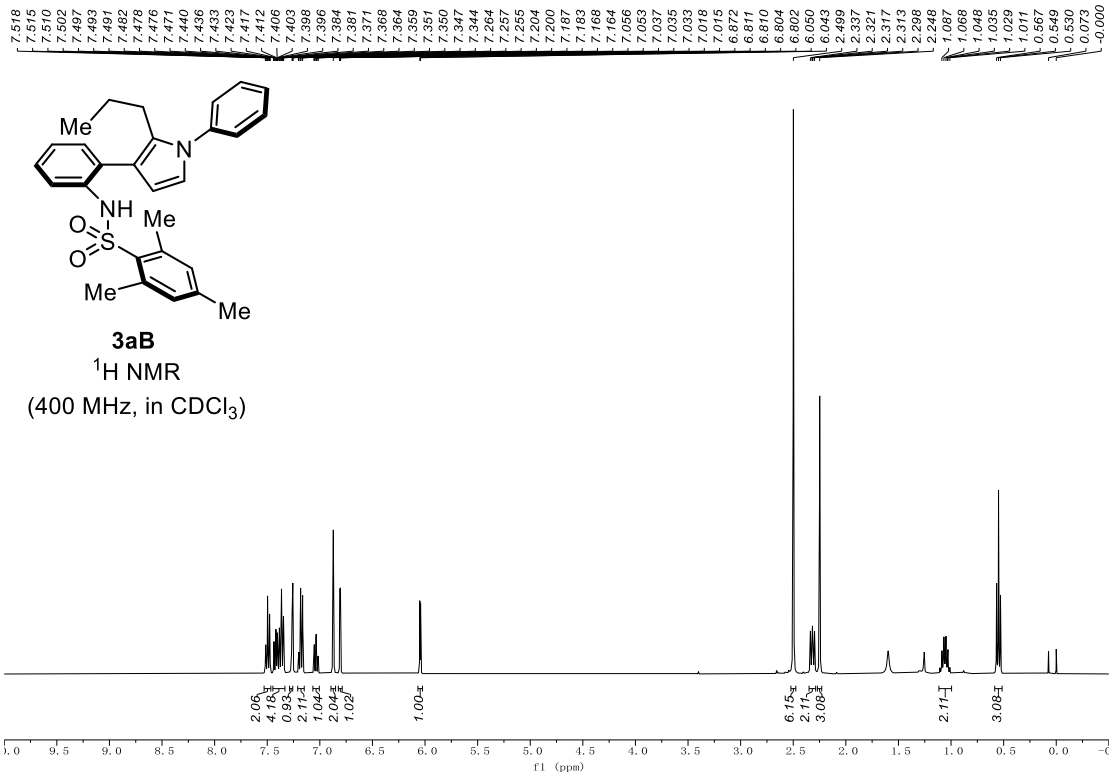
(400 MHz, in $CDCl_3$)



3aA

^{13}C NMR

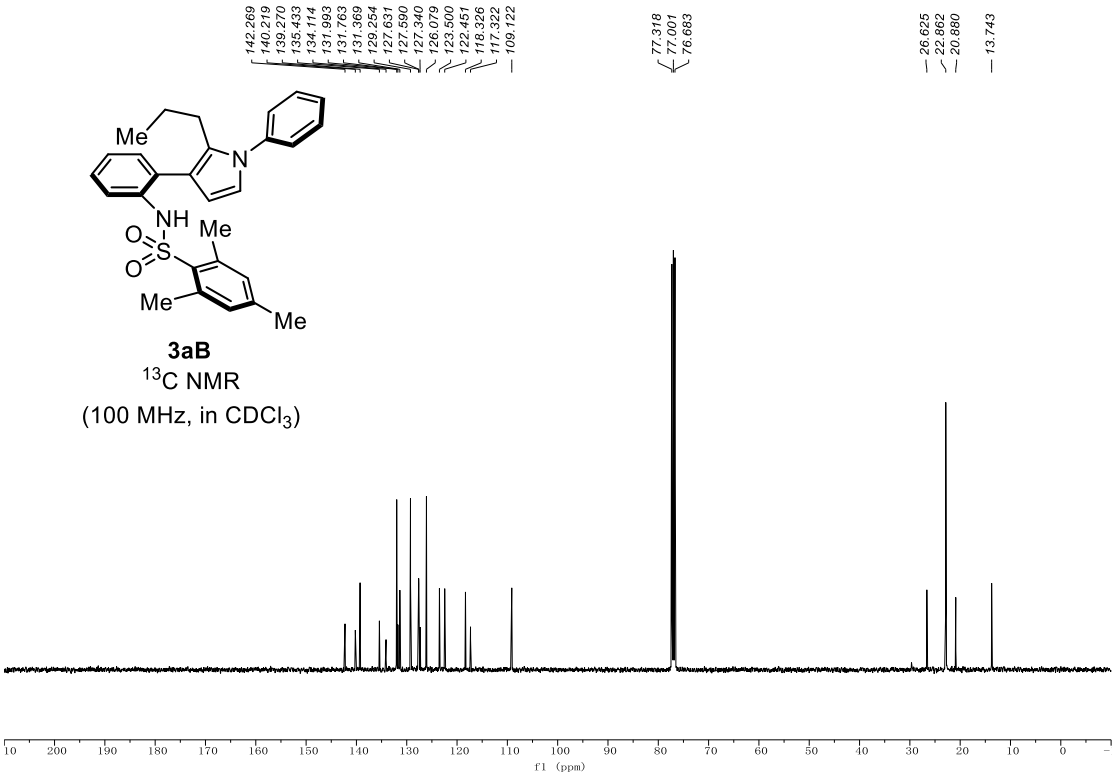
(100 MHz, in $CDCl_3$)



3aB

^{1}H NMR

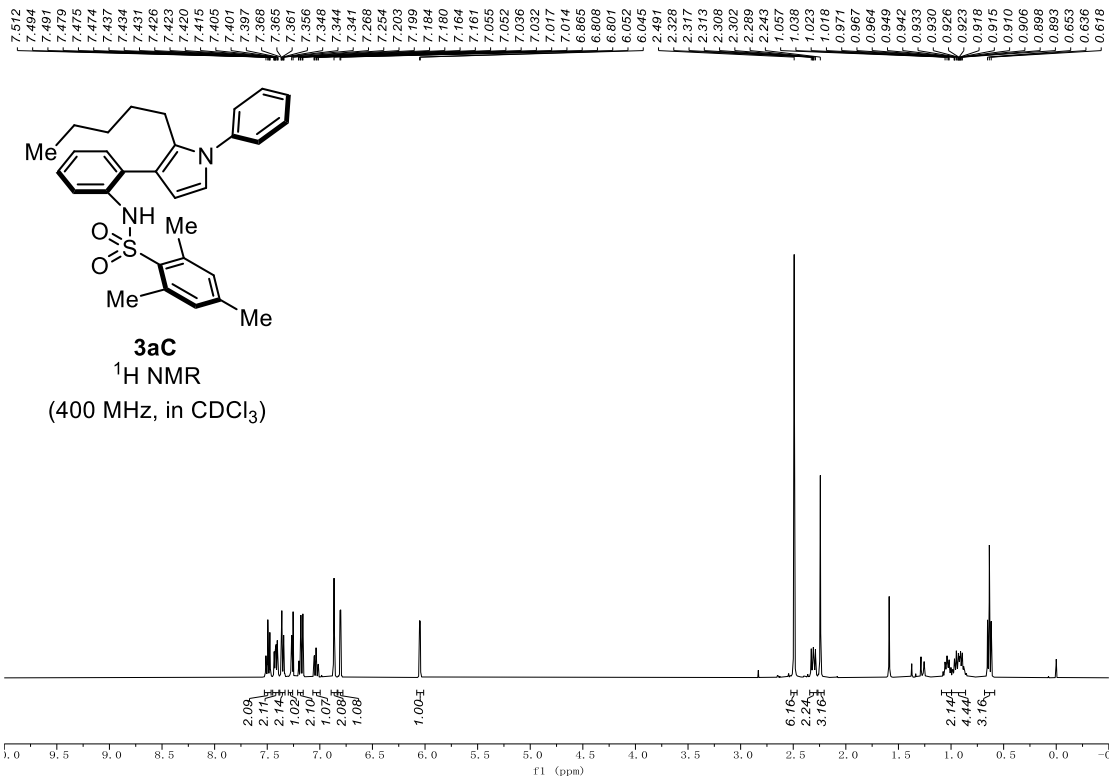
(400 MHz, in $CDCl_3$)



3aB

^{13}C NMR

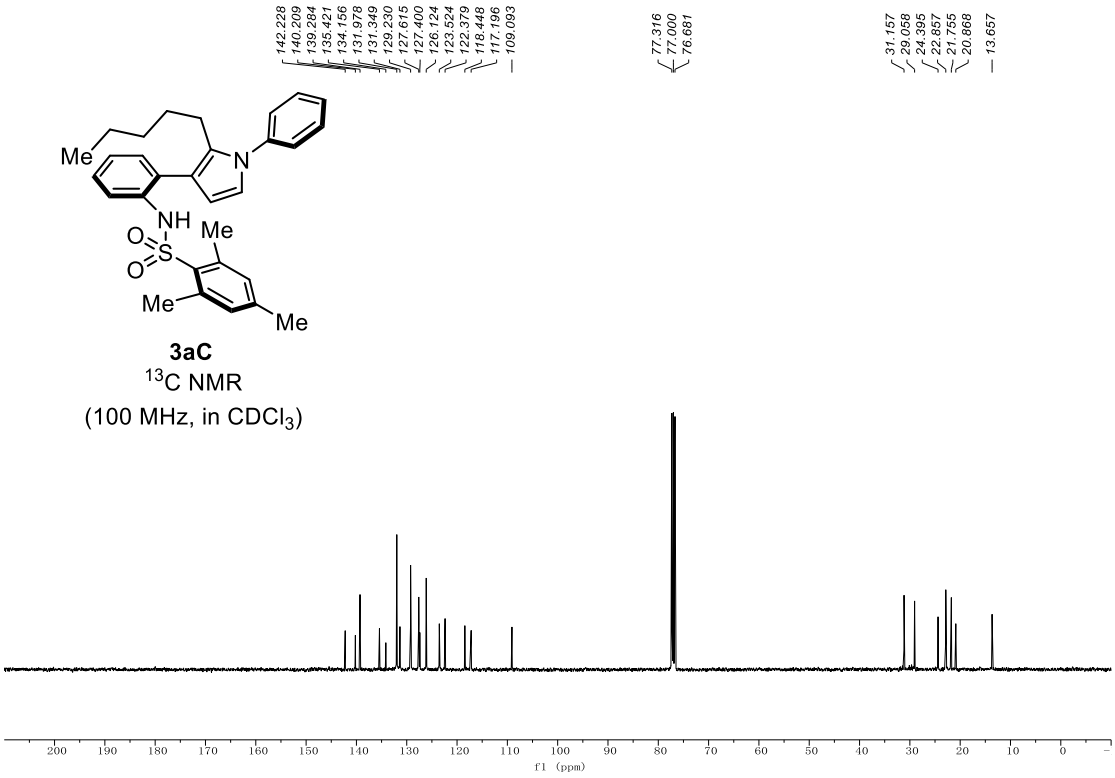
(100 MHz, in $CDCl_3$)



3aC

^{1}H NMR

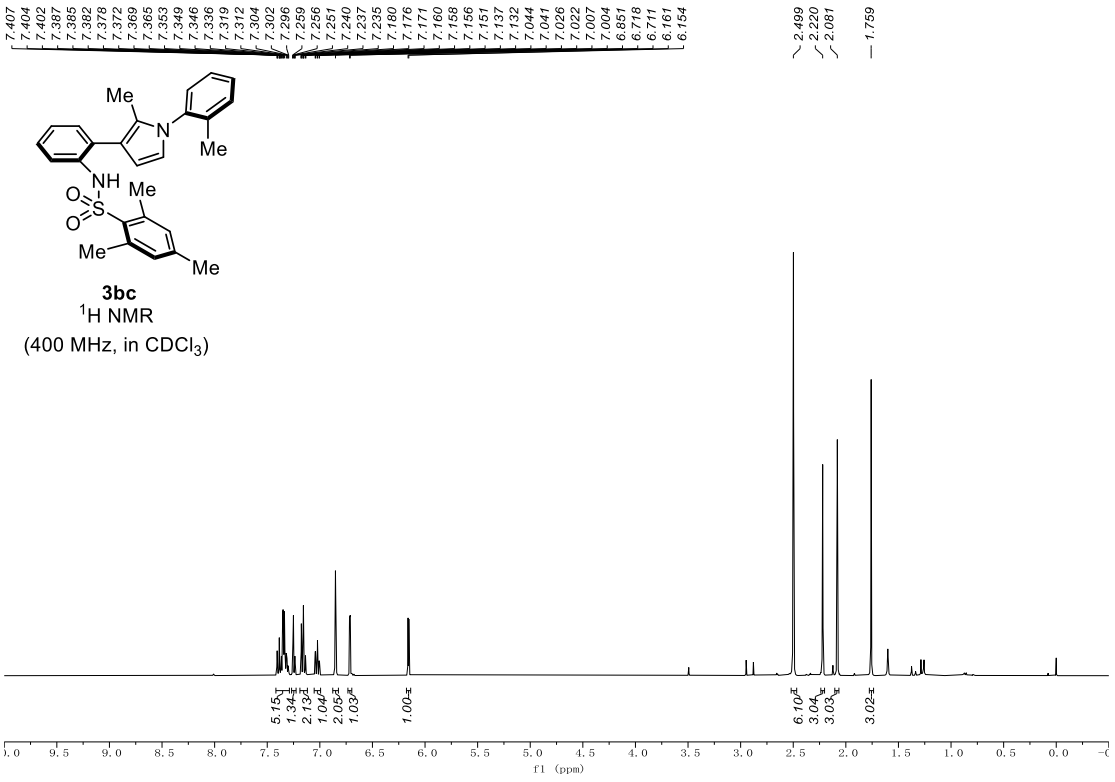
(400 MHz, in $CDCl_3$)



3aC

^{13}C NMR

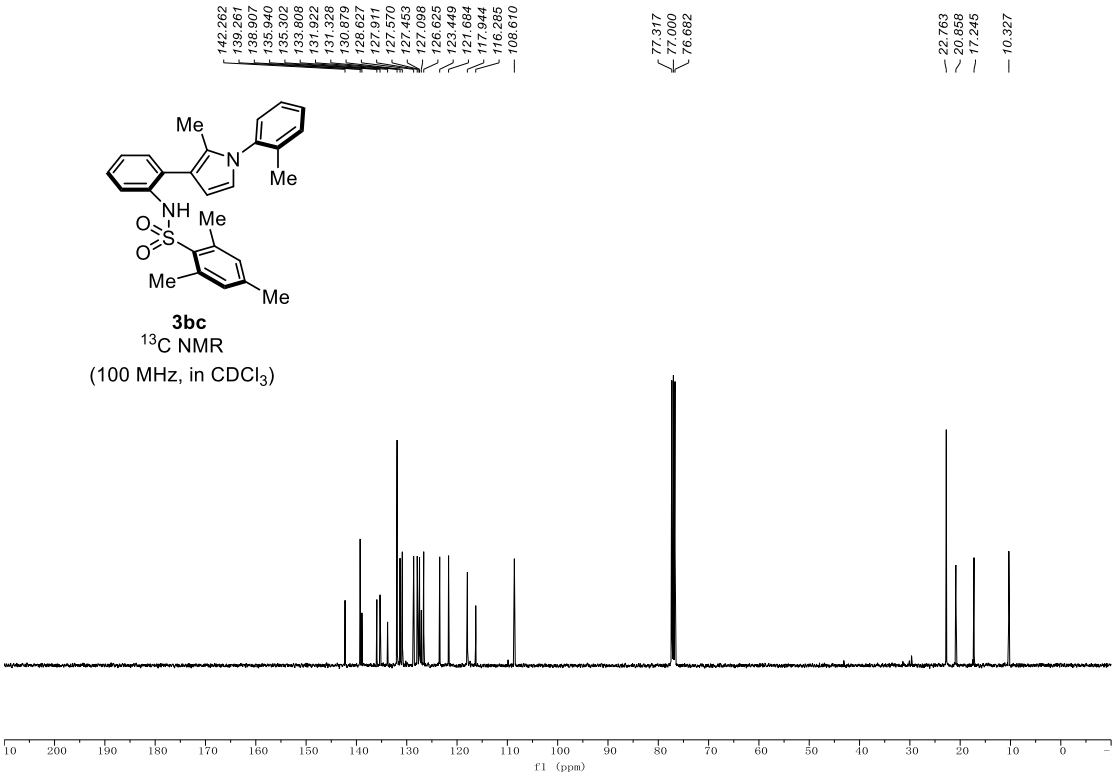
(100 MHz, in $CDCl_3$)



3bc

^{1}H NMR

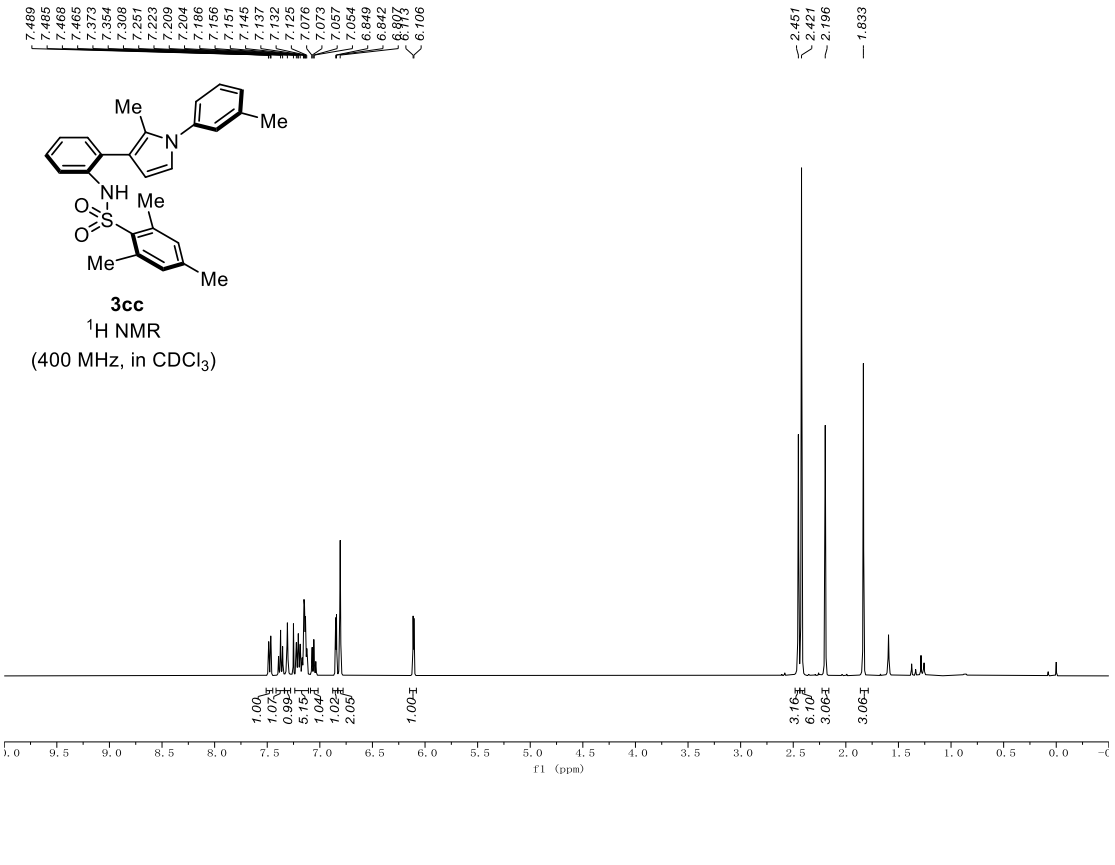
(400 MHz, in $CDCl_3$)



3bc

^{13}C NMR

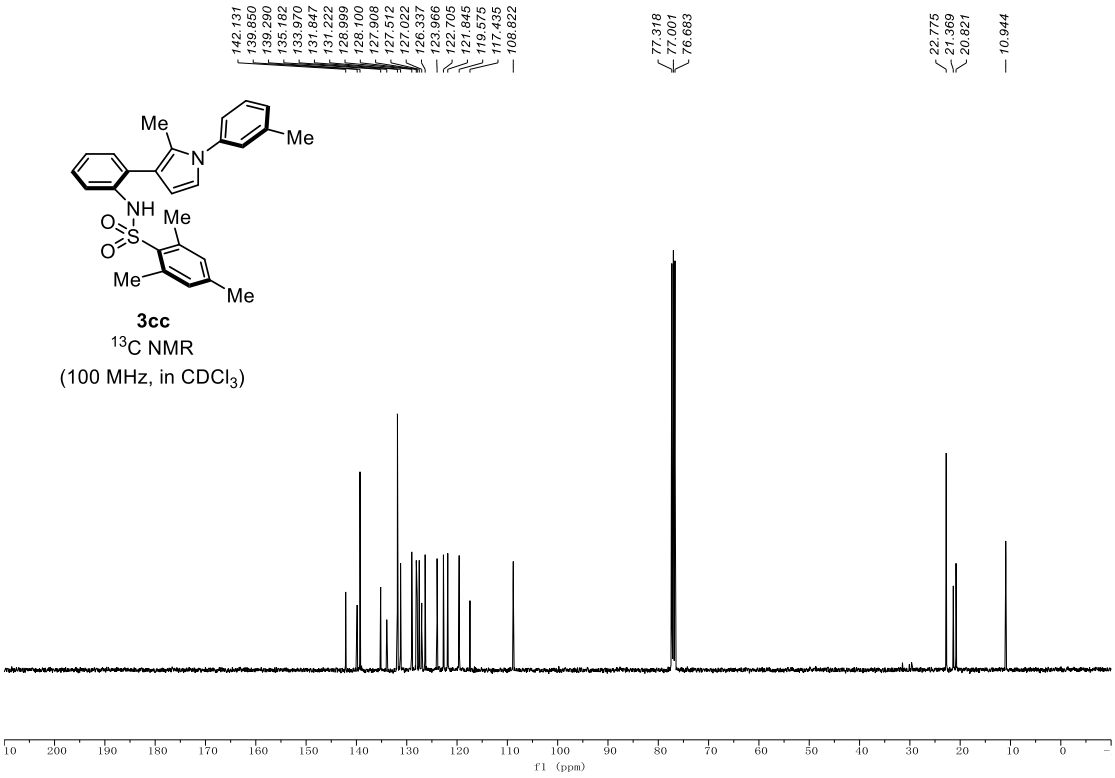
(100 MHz, in $CDCl_3$)

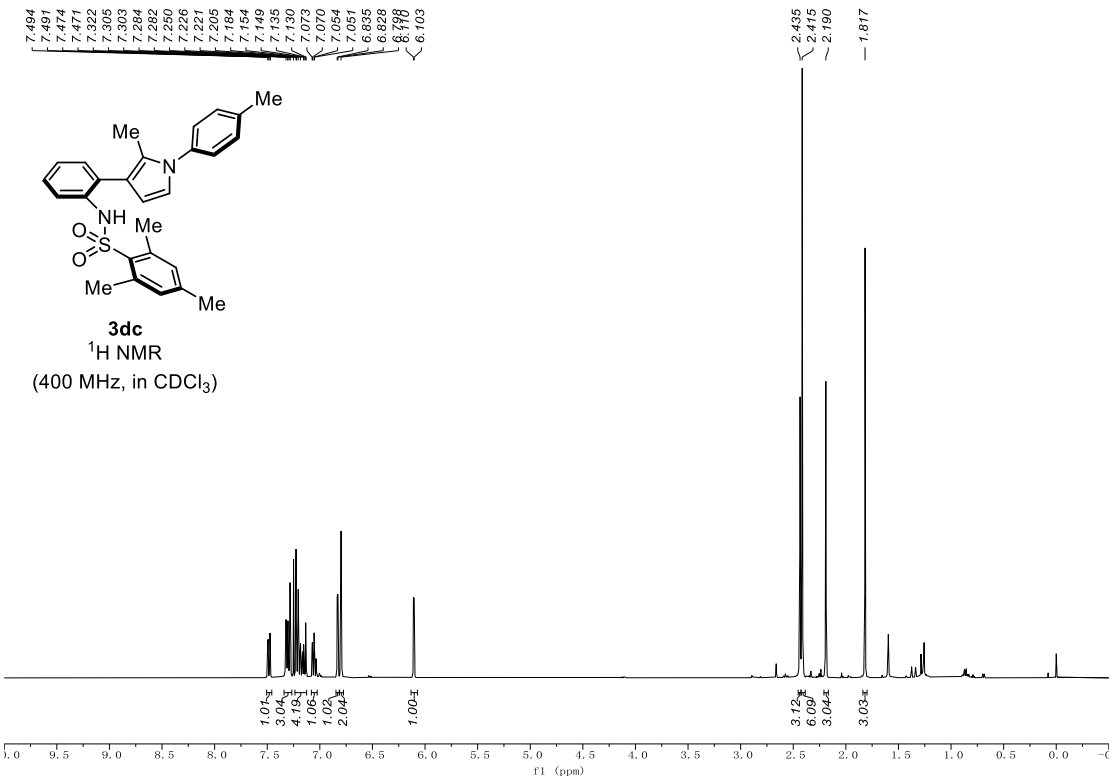


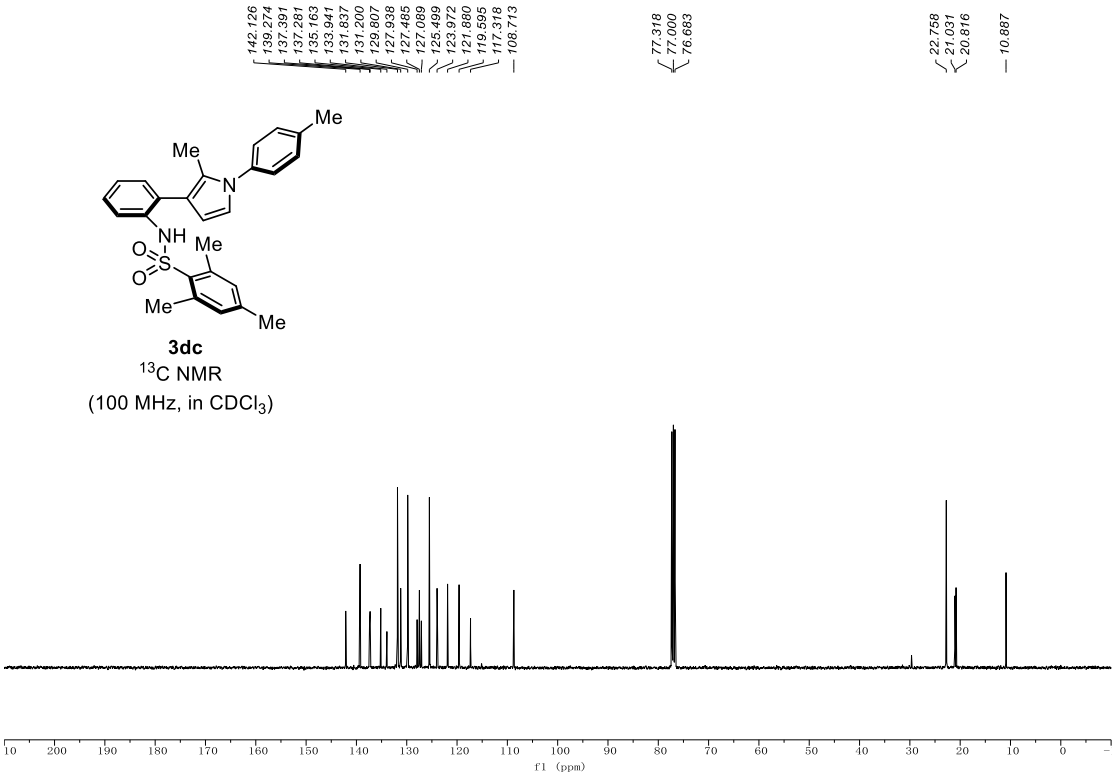
3cc

^{1}H NMR

(400 MHz, in $CDCl_3$)


142.131
139.850
139.290
135.182
133.970
131.847
131.222
128.999
128.100
127.908
127.512
127.022
126.337
123.966
122.705
121.845
119.575
117.435
108.822
77.318
77.001
76.683
22.775
21.369
20.821
10.944
Me
N
Me
NH
O
S
O
Me
Me
Me
3cc
13C NMR
(100 MHz, in CDCl3)
f1 (ppm)

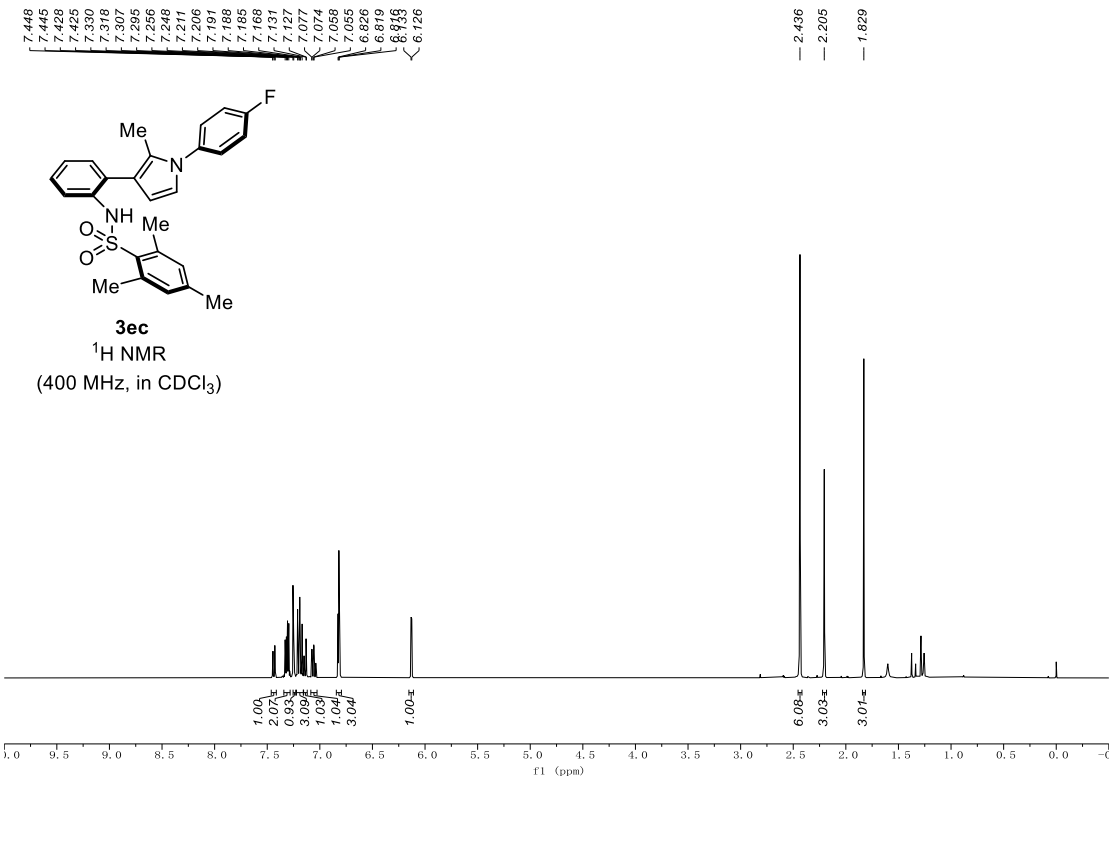

7.494
7.491
7.474
7.471
7.322
7.305
7.303
7.284
7.282
7.250
7.226
7.221
7.205
7.184
7.154
7.149
7.135
7.130
7.073
7.070
7.054
7.051
6.835
6.828
6.178
6.175
6.103
2.435
2.415
2.190
1.817
Me
N
Me
NH
O
S
O
Me
Me
Me
3dc
1H NMR
(400 MHz, in CDCl3)
1.01
3.04
4.19
1.06
1.02
2.04
1.00
3.12
6.09
3.04
3.03
f1 (ppm)



3dc

^{13}C NMR

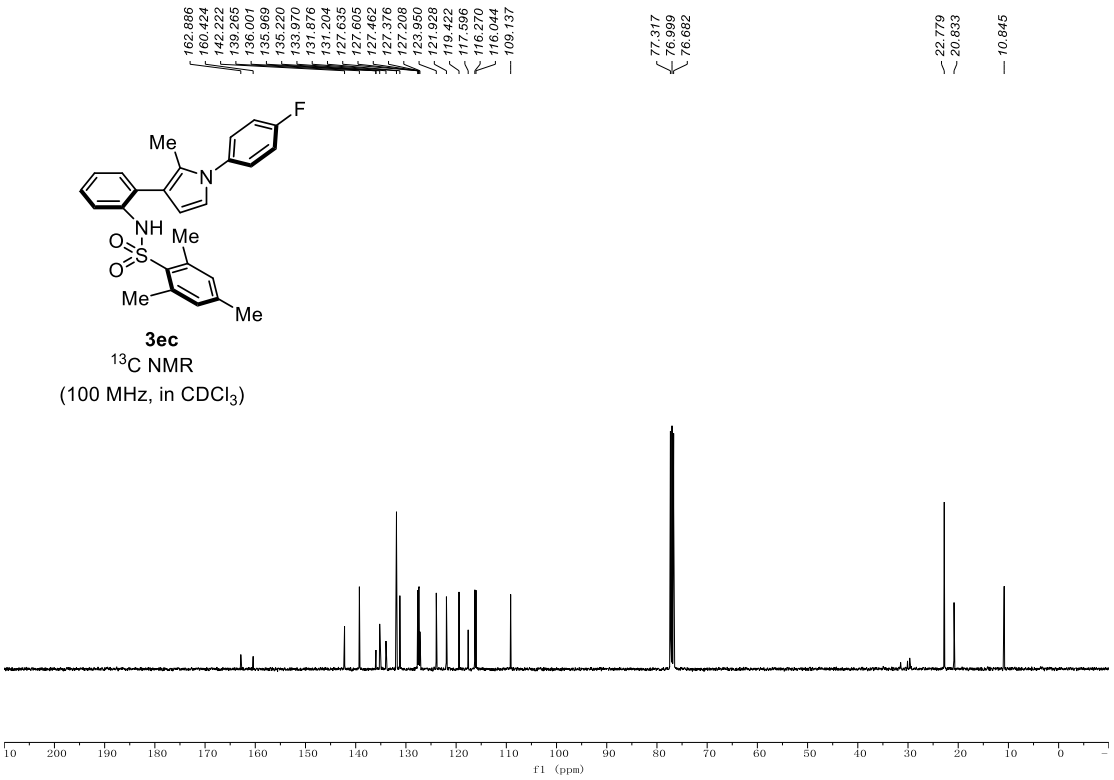
(100 MHz, in $CDCl_3$)



3ec

^{1}H NMR

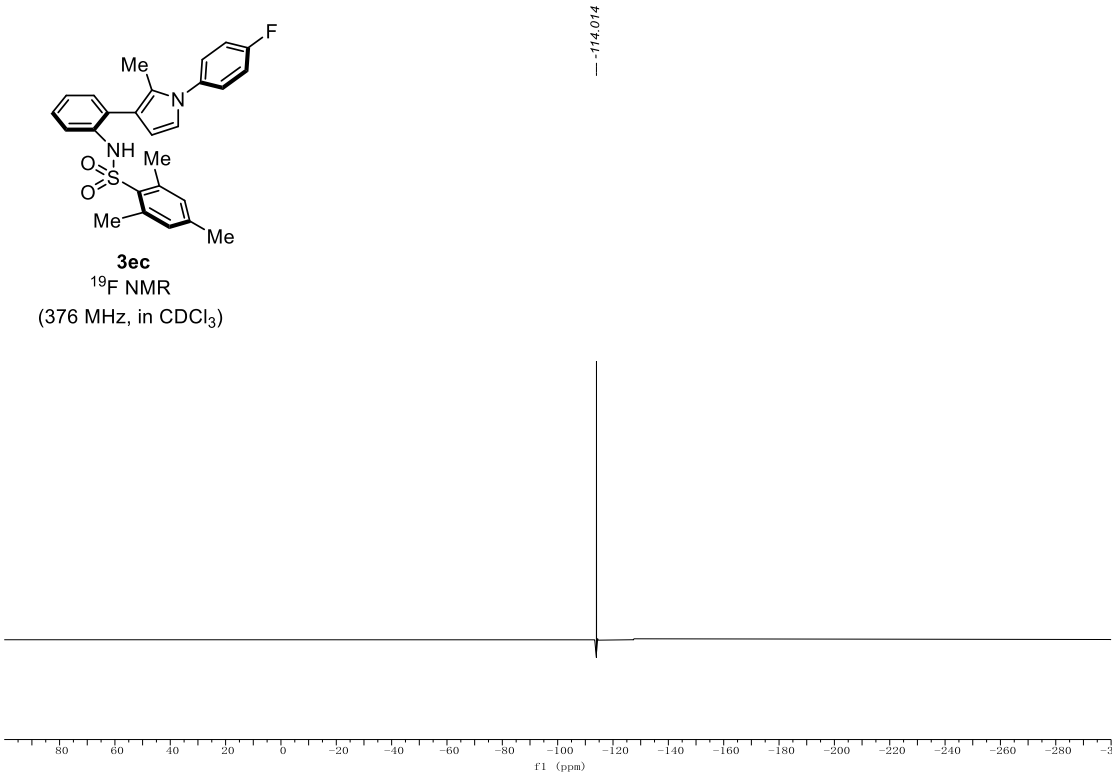
(400 MHz, in $CDCl_3$)



3ec

^{13}C NMR

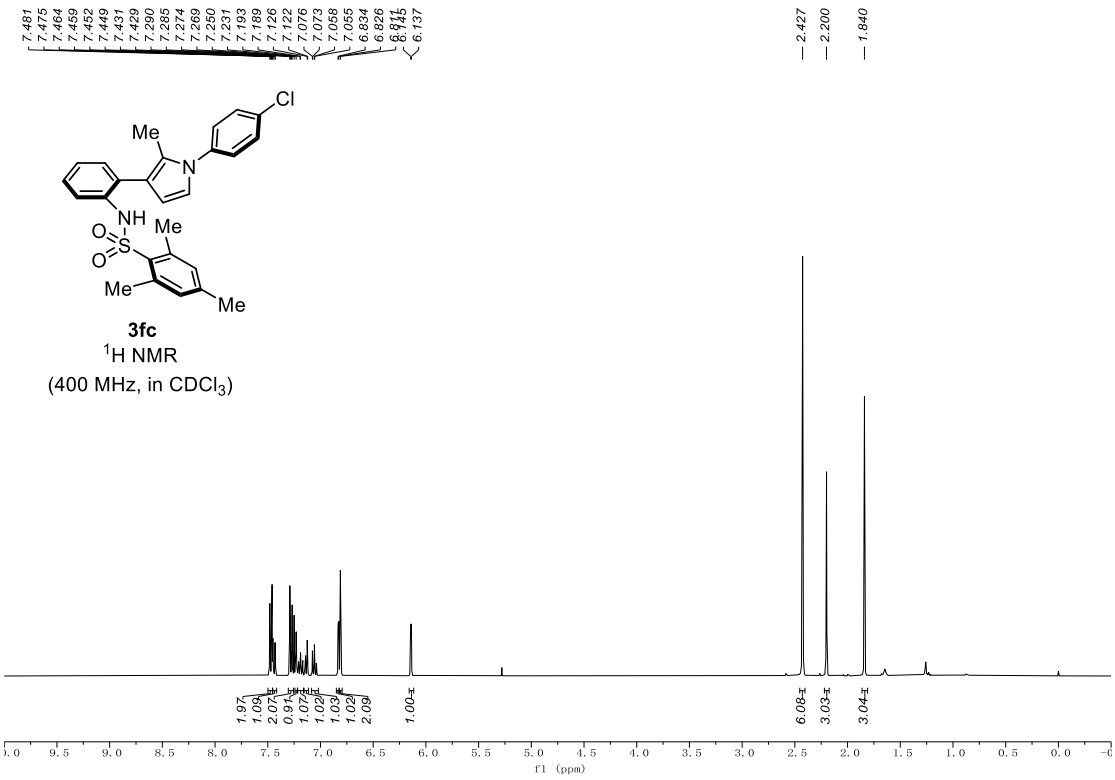
(100 MHz, in $CDCl_3$)



3ec

^{19}F NMR

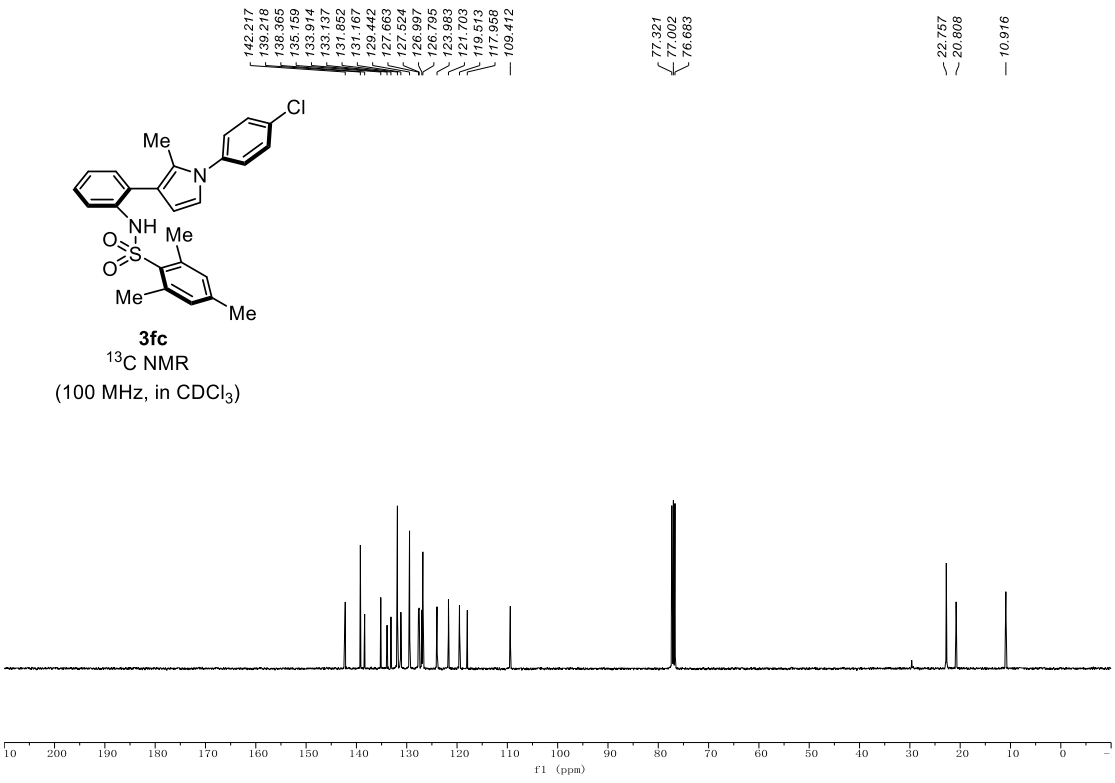
(376 MHz, in $CDCl_3$)



3fc

^{1}H NMR

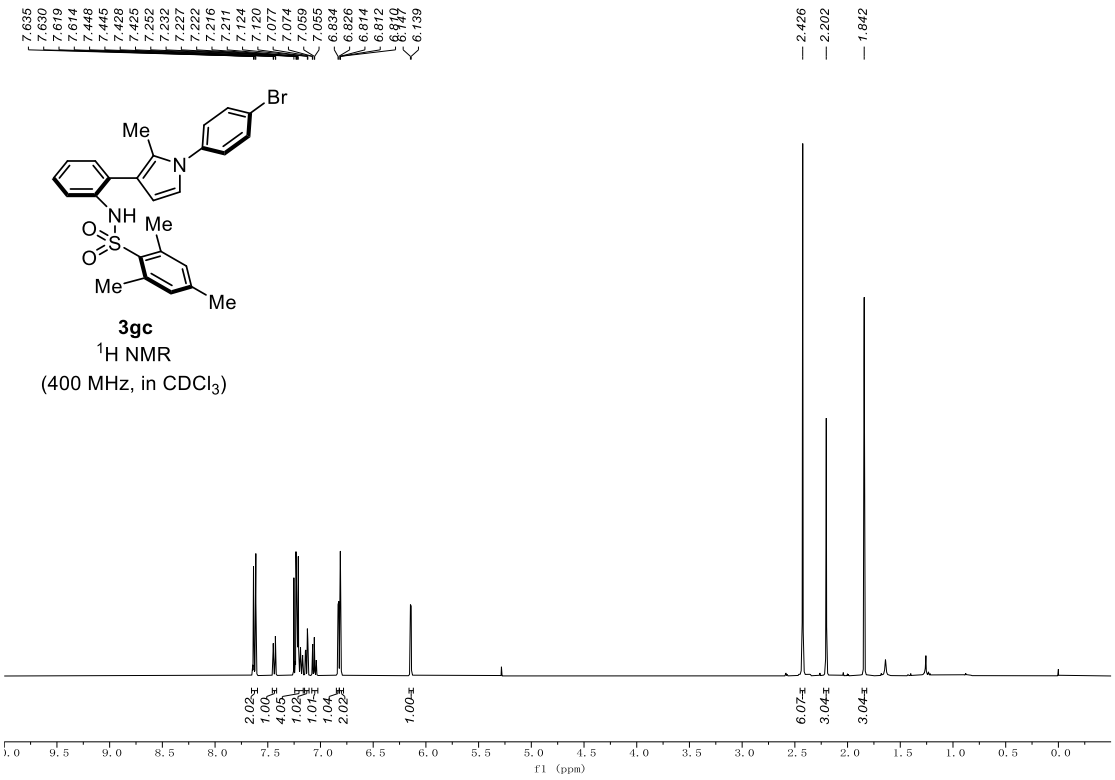
(400 MHz, in $CDCl_3$)



3fc

^{13}C NMR

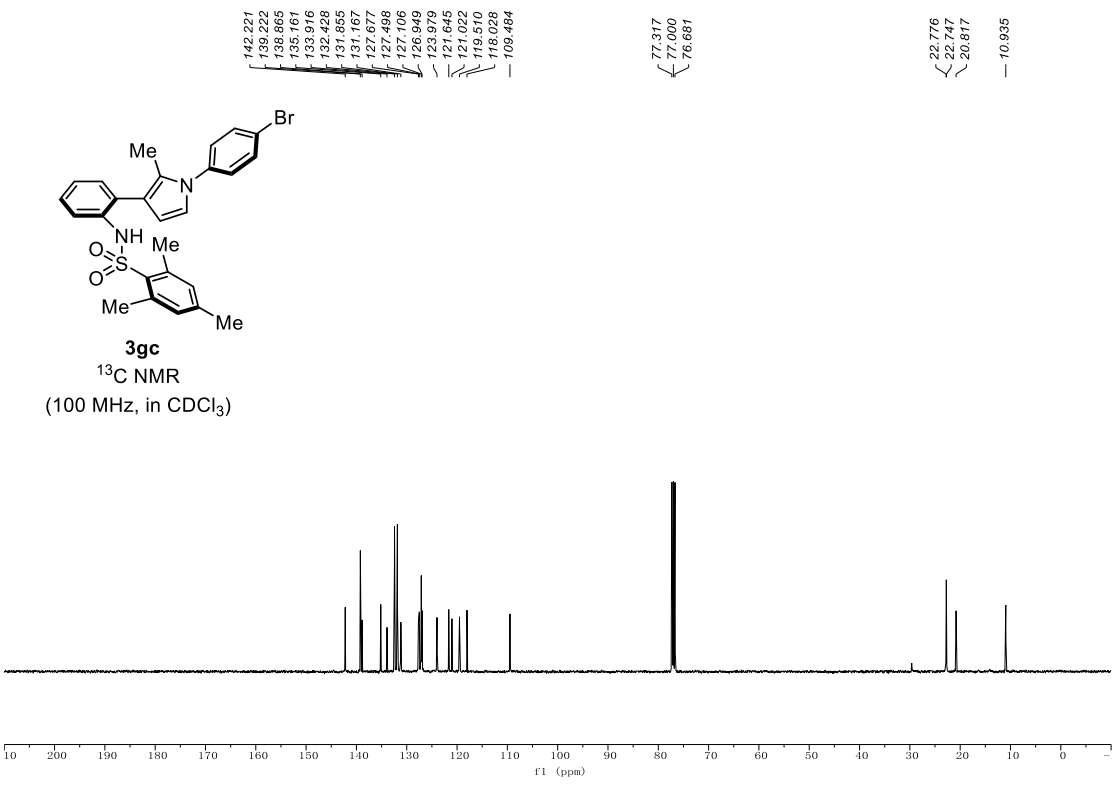
(100 MHz, in $CDCl_3$)



3gc

^{1}H NMR

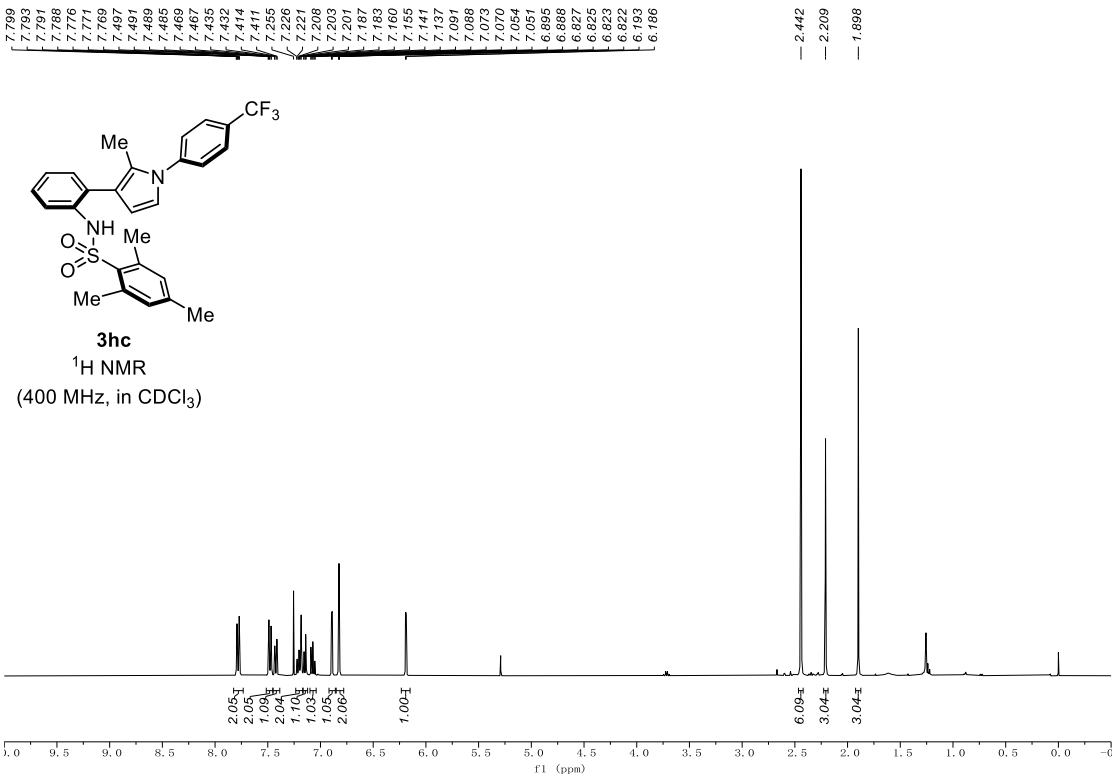
(400 MHz, in $CDCl_3$)



3gc

^{13}C NMR

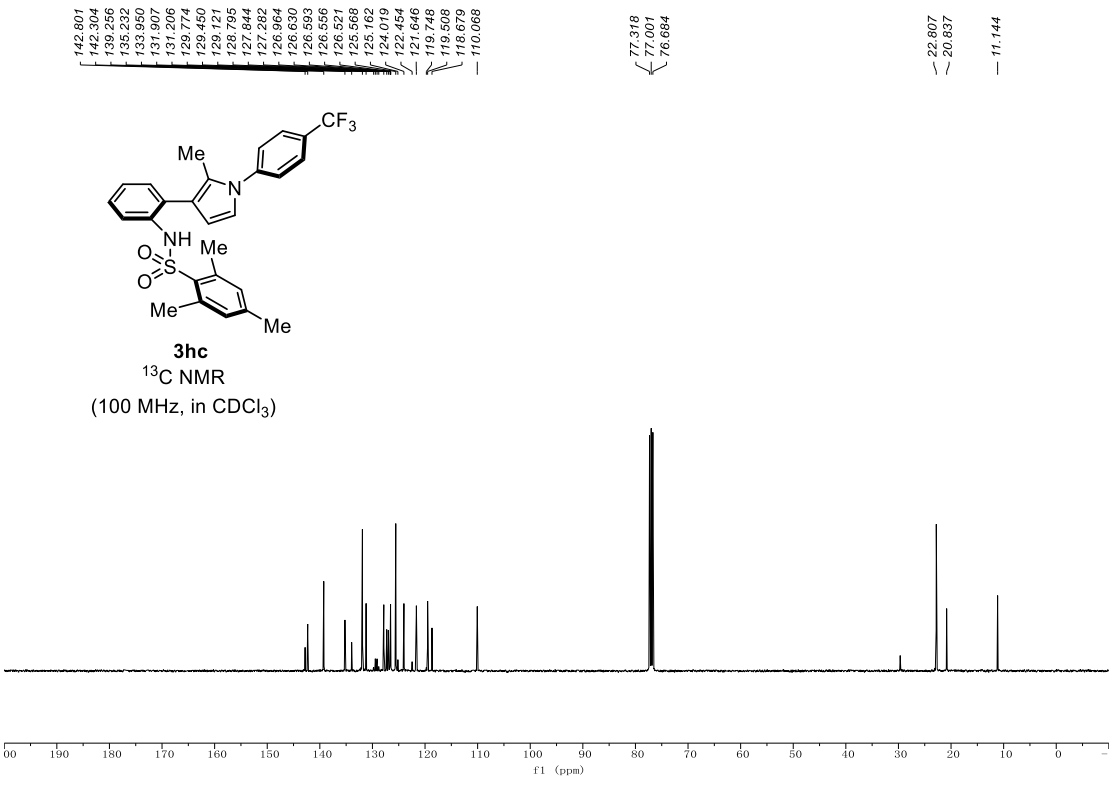
(100 MHz, in $CDCl_3$)



3hc

^{1}H NMR

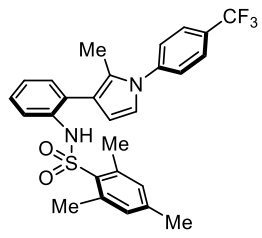
(400 MHz, in $CDCl_3$)



3hc

^{13}C NMR

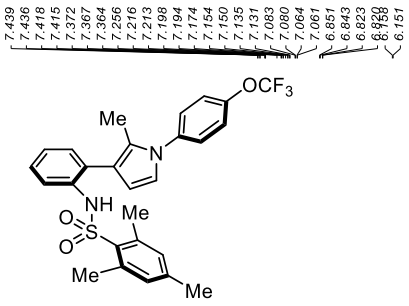
(100 MHz, in $CDCl_3$)



3hc

^{19}F NMR

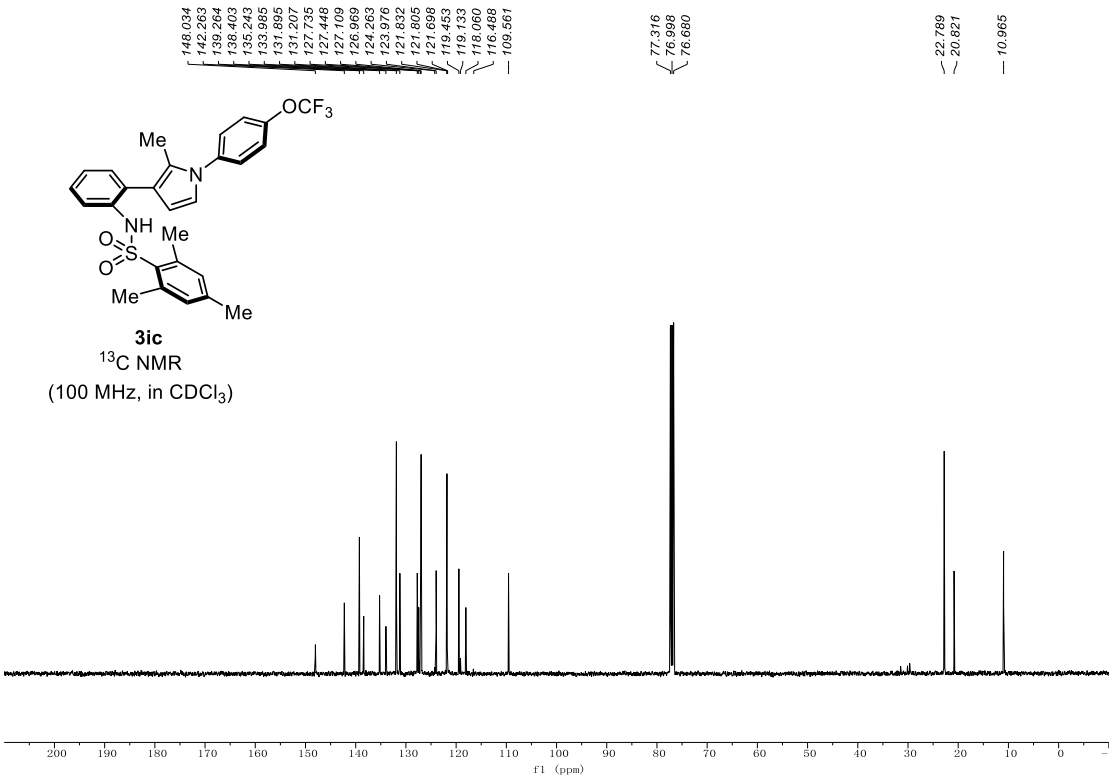
(376 MHz, in $CDCl_3$)



3ic

^{1}H NMR

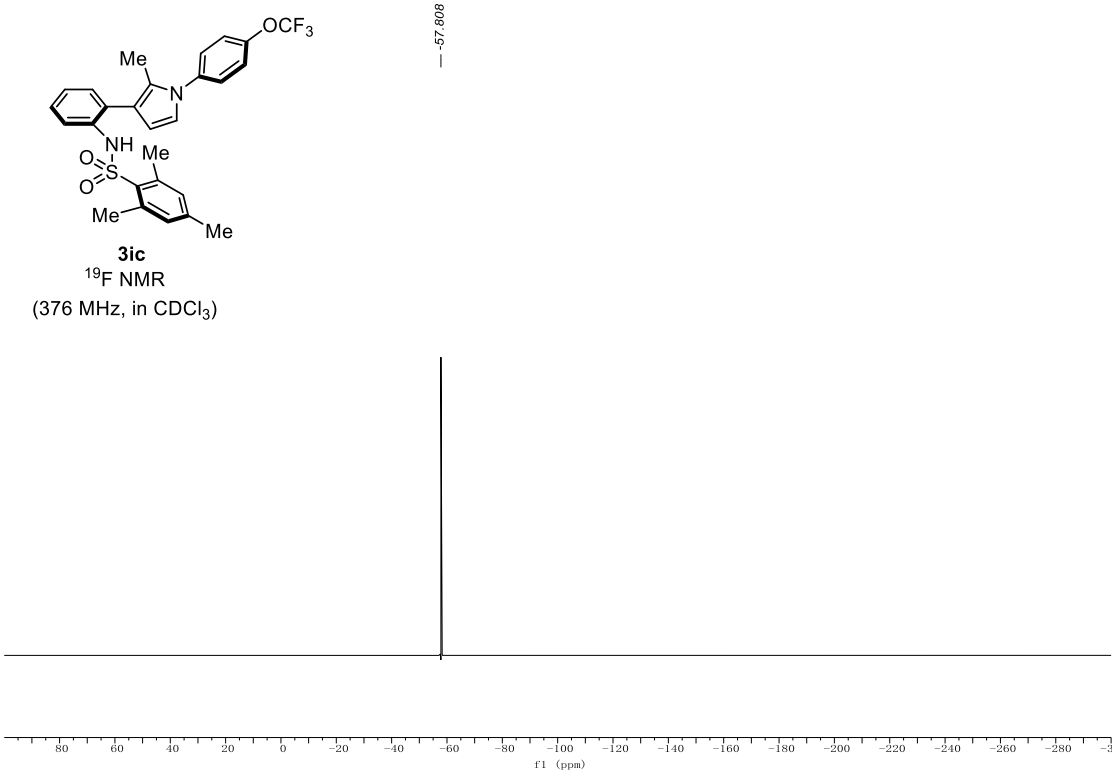
(400 MHz, in $CDCl_3$)



3ic

^{13}C NMR

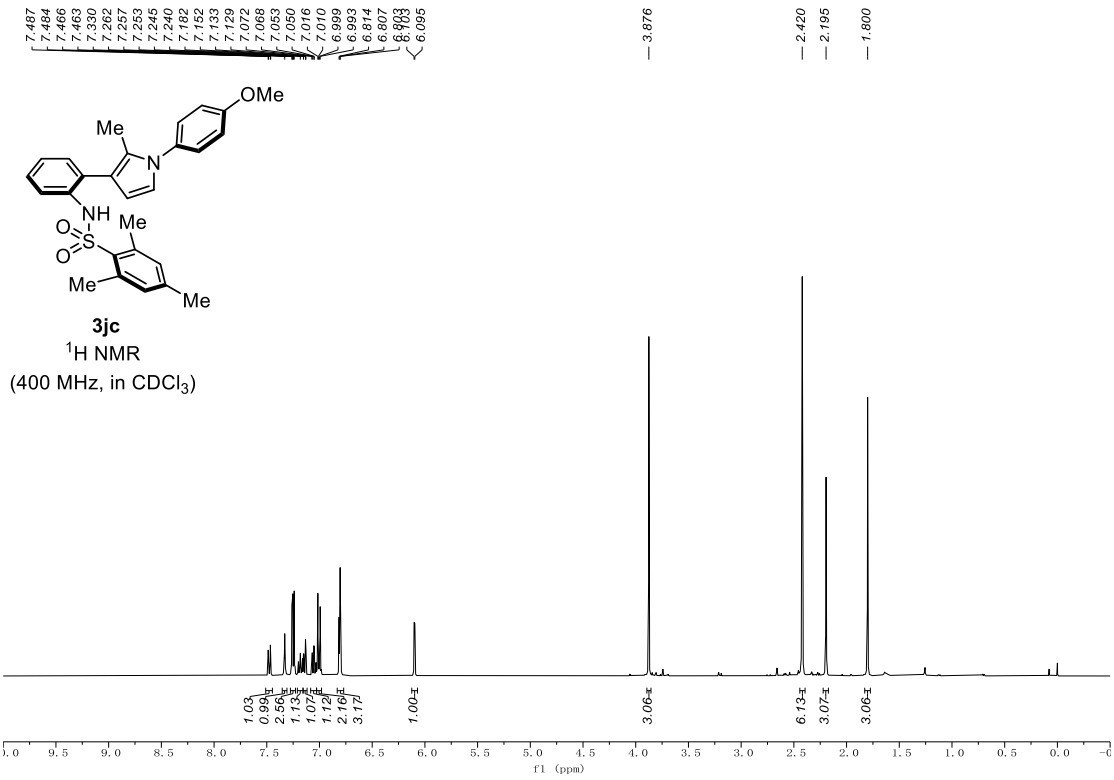
(100 MHz, in $CDCl_3$)



3ic

^{19}F NMR

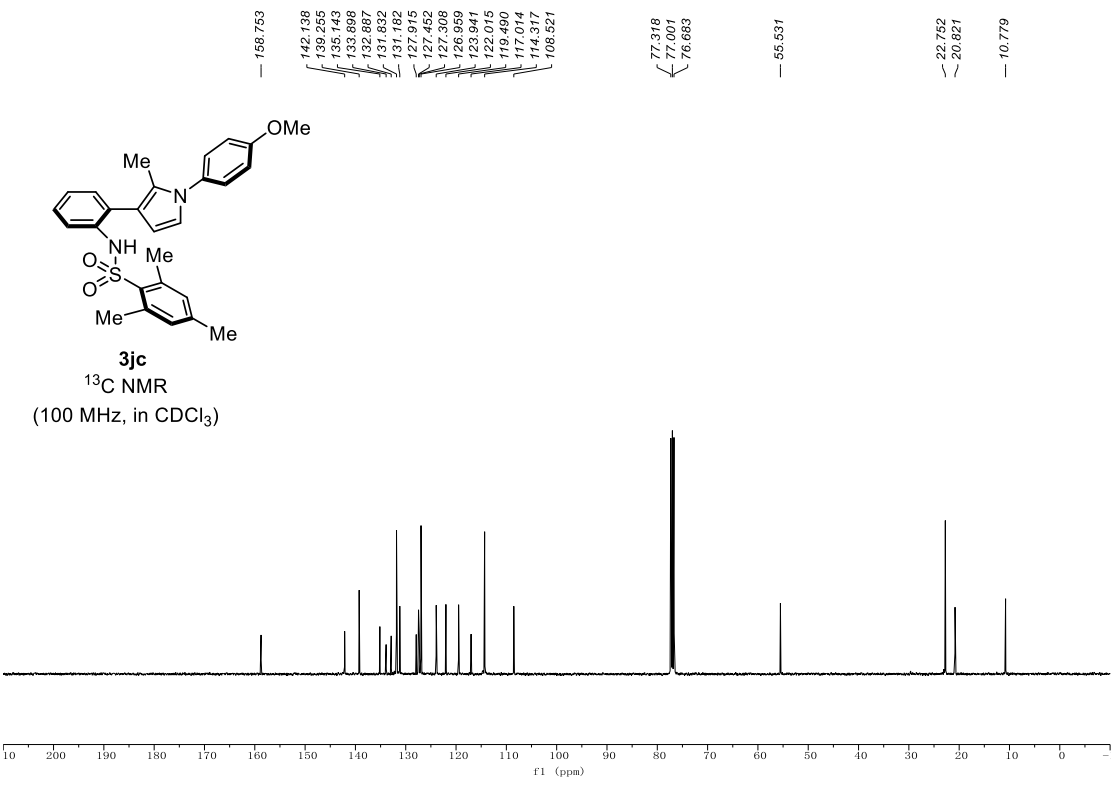
(376 MHz, in $CDCl_3$)



3jc

^{1}H NMR

(400 MHz, in $CDCl_3$)



3jc

^{13}C NMR

(100 MHz, in $CDCl_3$)