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# Synthesis of novel pyridinium 1,5-zwitterions and their reactivity with isatin-based α-(trifluoromethyl)imines: a sulfur-controlled domino reaction

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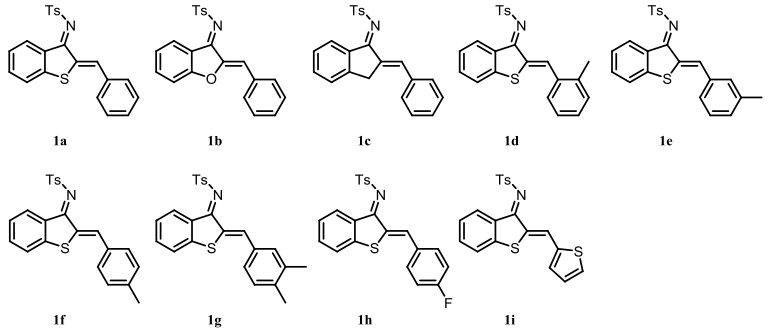
## 1. General information and materials

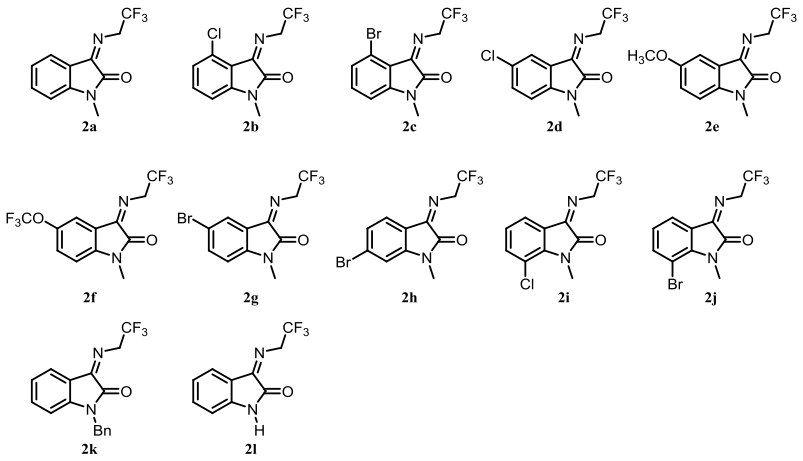
All reactions were performed under Ar atmospheres in oven-dried glassware with magnetic stirring. Unless otherwise stated, all reagents were purchased from commercial suppliers (Aldrich, TCI or Alfa Aesar) and used without further purification. All solvents were purified and dried according to standard methods prior to use. TLC monitored all reactions with silica gel-coated plates. Flash column chromatography was performed using 200-300 mesh silica gel. $^{1}$H- and $^{13}$C NMR spectra were recorded at ambient temperature on Bruker 400 or 600 instruments. All spectra were referenced to $CDCl_3$ ($^{1}$H δ 7.26 ppm and $^{13}$C NMR δ 77.00 ppm). $^{19}$F NMR spectrum was recorded on Bruker 400 (376 MHz) spectrometers with $CFCl_3$ as external standard. HRMS were obtained on Waters Xevo Q-TOF MS with ESI resource. Melting points were measured on a RY-I apparatus and are reported uncorrected. IR was measured on a Perkin-Elmer 983G apparatus. Compound **1a**, **1c**, **1d**, **1f**, **1g** was synthesized according to the reported method[1], [2], and the synthesis method of **1b**, **1e** are similar to **1a**. Compound **2** was synthesized according to the reported method[3].

## 2. The structure of 1-azadiene 1 and Isatin-derived α-(trifluoromethyl)imine 2

1-azadiene **1**




Isatin-derived α-(trifluoromethyl)imine **2**




## 3. General procedure for the synthesis of 3a, 4 and 5

**3a**

Under Ar atmosphere, **1a** (79.3 mg, 0.20 mmol) and DMAP (24.6 mg, 0.2 mmol) were dissolved in $CH_3CN$ 2 mL. The mixture was stirred at 20 ºC for 1min and white solid was obtained. After filtration, **3a** was obtained in 83% yield (86 mg).

**4a** as an example

Under Ar atmosphere, **1a** (39.15 mg, 0.10 mmol) and DMAP (2.45 mg, 0.02 mmol) were dissolved in $CH_3CN$ 1 mL. To the above reaction mixture, **2a** (29.06 mg, 0.12 mmol) was added. Then, the mixture

was stirred at 20 °C until the reaction was completed monitored by TLC analysis about 1 min. After the reaction completed, the reaction mixture was extracted with ethyl acetate (2 × 10 mL). The combined organic layers were dried over anhydrous $Mg_2SO_4$ and evaporated under vacuum. The reside was purified by column chromatography (ethyl acetate: petroleum ether = 1:5) to give **4a** (53 mg, 82%) as white solid. **5a** as an example

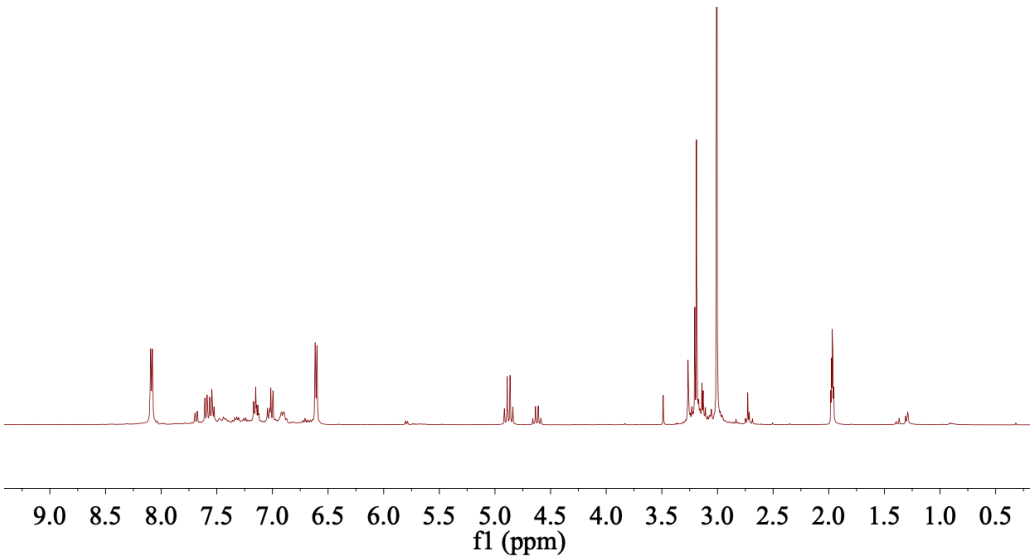
Under Ar atmosphere, **1a** (39.15 mg, 0.10 mmol) and DMAP (2.45 mg, 0.02 mmol) were dissolved in $CH_3CN$ 1 mL. To the above reaction mixture, **2a** (29.06 mg, 0.12 mmol) was added. The resulting reaction mixture was allowed to warm to reflux and stirred for 30 min. After the reaction completed (monitored by TLC), the reaction mixture was extracted with ethylacetate (2 × 10 mL). The combined organic layers were dried over anhydrous $Mg_2SO_4$ and evaporated under vacuum. The reside was purified by column chromatography (ethyl acetate: petroleum ether = 1:5) to give **5a** (40 mg, 63%) as yellow solid.

## 4. Procedure for the 1 mmol Scale Reaction of 4a and 5a

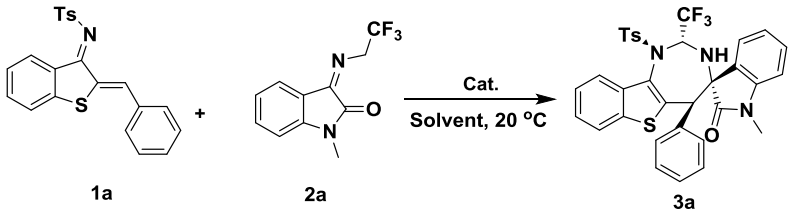
Under Ar atmosphere, **1a** (391.5 mg, 1.00 mmol) and DMAP (24.5 mg, 0.20 mmol) were dissolved in $CH_3CN$ 10 mL. To the above reaction mixture, **2a** (290.6 mg, 1.20 mmol) was added. Then, the mixture was stirred at 20 °C until the reaction was completed monitored by TLC analysis about 10 min. After the reaction completed, the reaction mixture was extracted with ethylacetate (20 × 10 mL). The combined organic layers were dried over anhydrous $Mg_2SO_4$ and evaporated under vacuum. The reside was purified by column chromatography (ethyl acetate: petroleum ether = 1:5) to give **4a** (422 mg, 66%) as white solid.

Under Ar atmosphere, **1a** (391.5 mg, 1.00 mmol) and DMAP (24.5 mg, 0.20 mmol) were dissolved in $CH_3CN$ 10 mL. To the above reaction mixture, **2a** (290.6 mg, 1.20 mmol) was added. The resulting reaction mixture was allowed to warm to reflux and stirred for 60 min. After the reaction completed (monitored by TLC), the reaction mixture was extracted with ethylacetate (20 × 10 mL). The combined organic layers were dried over anhydrous $Mg_2SO_4$ and evaporated under vacuum. The reside was purified by column chromatography (ethyl acetate: petroleum ether = 1:5) to give **5a** (305 mg, 48%) as yellow solid.

## 5. $^1$H NMR of reaction of 2a and DMAP



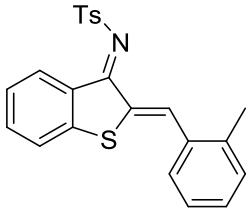
**6. Table S1 Optimization of the reaction conditions**[a]




| Entry | Cat. | Solvent | Time/min | Yield/% (**3a**)[b] |
|---|---|---|---|---|
| 1 | pyridine | $CH_3CN$ | 10 h | 50 |
| 2 | 4-Me-pyridine | $CH_3CN$ | 10 h | 57 |
| 3 | 4-MeO-pyridine | $CH_3CN$ | 8 h | 28 |
| 4 | 3-Br-pyridine | $CH_3CN$ | 10 h | 0 |
| 5 | DMAP | $CH_3CN$ | 1 | 82 |
| 6 | DABCO | $CH_3CN$ | 50 | 50 |
| 7 | DMAP | toluene | 15 | 51 |
| 8 | DMAP | $CHCl_3$ | 15 | 30 |
| 9 | DMAP | $CH_2Cl_2$ | 20 | 33 |
| 10 | DMAP | THF | 15 | 32 |
| 11 | DMAP | DMF | 15 | 45 |
| 12[c] | DMAP | $CH_3CN$ | 1 | 51 |
| 13[d] | DMAP | $CH_3CN$ | 1 | 75 |

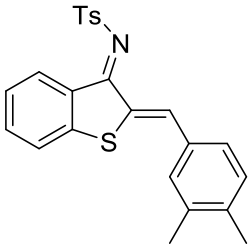
[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol) and catalyst (0.02 mmol) in solvent (1 mL) at 20 °C. [b] Isolated yields. [c] 1a:2a = 1:1. [d] 1a:2a = 1:1.5.

## 7. Characterization of all new compounds



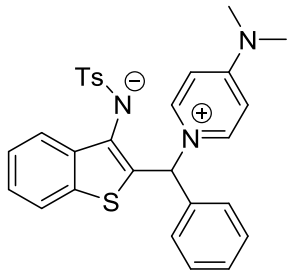

**4-methyl-*N*-((*E*)-2-((*Z*)-2-methylbenzylidene)benzo[*b*]thiophen-3(2*H*)-ylidene)benzenesulfonamide (1d)**

Red solid: 376 mg (yield 19%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.5; mp 139-141 ℃; IR (KBr) 2362, 1590, 1508, 1277, 1140, 1071, 848, 744, 545 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.0 Hz, 1H), 8.59 (s, 1H), 8.02 (d, *J* = 8.2 Hz, 2H), 7.77 – 7.65 (m, 1H), 7.59 – 7.53 (m, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.29 (m, 5H), 7.26 – 7.23 (m, 1H), 2.47 (s, 3H), 2.40 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 170.0, 147.8, 143.0, 140.1, 139.8, 135.7, 135.3, 133.8, 133.0, 131.4, 130.9, 130.5, 129.6, 129.4, 129.0, 126.6, 126.4, 125.7, 123.3, 21.6, 20.1 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{23}H_{20}NO_2S_2^+$ 406.0930, found 406.0948.



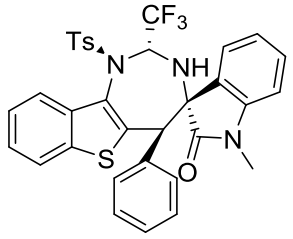

***N*-((*E*)-2-((*Z*)-3,4-dimethylbenzylidene)benzo[*b*]thiophen-3(2*H*)-ylidene)-4-methylbenzenesulfonamide (1g)**

Red solid: 387 mg (yield 20%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.5; mp 168-170 °C; IR (KBr) 2359, 1588, 1526, 1305, 1144, 1085, 813, 724, 562 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.92 (d, *J* = 8.0 Hz, 1H), 8.16 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.28 (m, 5H), 7.22 (d, *J* = 8.4 Hz, 1H), 2.48 (s, 3H), 2.31 (s, 6H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 170.4, 147.5, 142.9, 140.3, 140.23, 140.18, 137.5, 136.9, 135.1, 132.7, 132.18, 132.15, 132.0, 131.1, 130.4, 128.9, 126.7, 125.6, 123.3, 21.6, 20.0, 19.8 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{24}H_{22}NO_2S_2^+$ 420.1086, found 420.1085.




**(2-((4-(dimethylamino)pyridin-1-ium-1-yl)(phenyl)methyl)benzo[*b*]thiophen-3-yl)(tosyl)amide (3a)**

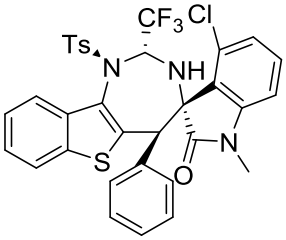
White solid: 86 mg (yield 83%, 0.2 mmol scale); mp 145-147 ℃; IR (KBr) 1647, 1149, 1118, 1079, 750, 778, 741; $^1H$ NMR (400 MHz, $CD_3CN$) δ 7.91 (d, *J* = 7.8 Hz, 2H), 7.53 (d, *J* = 8.1 Hz, 3H), 7.41 – 7.32 (m, 4H), 7.27 – 7.15 (m, 3H), 7.10 – 7.00 (m, 4H), 6.74 (d, *J* = 7.7 Hz, 2H), 3.15 (s, 6H), 2.28 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (101 MHz, $CD_3CN$) δ 156.4, 149.2, 145.3, 143.4, 140.8, 139.4, 139.0, 138.7, 137.9, 128.9, 128.7, 128.6, 127.2, 125.9, 125.1, 124.9, 123.5, 122.3, 107.3, 67.7, 39.6, 20.3 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{29}H_{28}N_3O_2S_2^+$ 514.1617, found 514.1617.




**1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4a)**

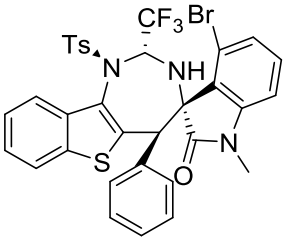
White solid: 53 mg (yield 82%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 228-230 ℃; IR (KBr) 3328, 1715, 1613, 1469, 1351, 1152, 965, 705, 592 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.83 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.39 – 7.26 (m, 2H), 7.24 – 7.07 (m, 8H), 7.01 (d, *J* = 7.2 Hz, 2H), 6.65 – 6.49 (m, 1H), 6.21 (dq, *J* = 14.0, 4.6 Hz, 1H), 4.98 (s, 1H), 3.02 (d, *J* = 14.0 Hz, 1H), 2.86 (s, 3H), 2.39 (s, 3H) ppm.$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.3, 144.8, 143.3,

143.0, 137.7, 136.5, 136.3, 133.6, 129.7, 129.6, 129.5, 128.3, 128.2, 128.1, 127.9, 125.4 (q, $^{1}J_{C\text{-}F}$ = 251.1 Hz), 124.9, 124.7, 124.5, 124.0, 123.3, 122.5, 121.8, 108.6, 65.9 (q, $^{2}J_{C\text{-}F}$ = 32.7 Hz), 63.7, 51.3, 25.9, 21.6 ppm. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -78.05 ppm. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{33}H_{27}F_3N_3O_3S_2^+$ 634.1440, found 634.1442.



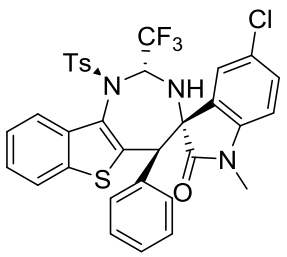

**4'-chloro-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4b)**

White solid: 56 mg (yield 82%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 226-228 °C; IR (KBr) 3448, 1713, 1610, 1457, 1351, 1192, 1162, 753, 665 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 1H), 7.39 (dd, *J* = 15.8, 8.0 Hz, 3H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.15 – 6.96 (m, 9H), 6.86 (dq, *J* = 13.6, 4.6 Hz, 1H), 6.38 (d, *J* = 7.4 Hz, 1H), 5.45 (s, 1H), 3.00 (d, *J* = 14.0 Hz, 1H), 2.97 (s, 3H), 2.30 (s, 3H) ppm. $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 173.9, 144.9, 144.4, 144.3, 142.1, 137.4, 136.5, 136.4, 135.8, 133.8, 130.7, 130.3, 129.1, 128.5, 128.3, 127.9, 125.9, 124.7, 124.6, 124.5, 122.34, 122.27, 107.0, 67.6 (q, $^{2}J_{C\text{-}F}$ = 31.9 Hz), 65.7, 47.0, 26.3, 21.4 ppm. (the C of $CF_3$ is not observed). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -78.75 ppm. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{33}H_{26}ClF_3N_3O_3S_2^+$ 668.1051, found 668.1045.



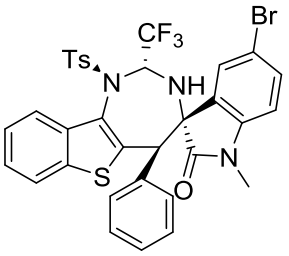

**4'-bromo-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4c)**

White solid: 58 mg (yield 80%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 212-214 °C; IR (KBr) 3322, 1713, 1605, 1454, 1350, 1194, 1161, 780, 665 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.67 (m, 1H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.31 – 7.26 (m, 2H), 7.22 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.18 – 7.06 (m, 9H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.42 (d, *J* = 7.8 Hz, 1H), 5.71 (s, 1H), 3.02 (d, *J* = 14.0 Hz, 1H), 2.99 (s, 3H), 2.31 (s, 3H) ppm. $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 174.0, 145.1, 144.4, 142.3, 137.3, 136.4, 135.8, 133.9, 130.8, 129.1, 128.44, 128.40, 128.1, 128.0, 127.8, 124.6, 124.5, 124.4, 122.3, 122.1, 118.7, 107.5, 67.7 (q, $^{2}J_{C\text{-}F}$ = 32.0 Hz), 66.2, 60.5, 46.7, 26.4, 21.5 ppm (the C of $CF_3$ is not observed). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -78.80 ppm. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0545.



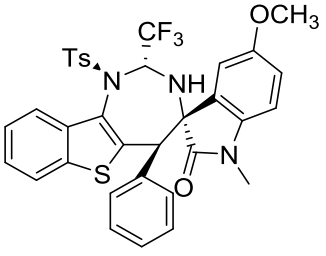
**5'-chloro-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4d)**

White solid: 55 mg (yield 80%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 218-220 ℃; IR (KBr) 3315, 1724, 1613, 1493, 1365, 1153, 789, 757, 661 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 2.0 Hz, 1H), 7.81 – 7.72 (m, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.28 (dd, *J* = 6.0, 1.6 Hz, 2H), 7.25 – 7.21 (m, 2H), 7.20 – 7.08 (m, 3H), 7.00 – 6.87 (m, 2H), 6.46 (d, *J* = 8.4 Hz, 1H), 6.11 (dq, *J* = 13.8, 4.8 Hz, 1H), 4.75 (s, 1H), 3.00 (d, *J* = 14.0 Hz, 1H), 2.83 (s, 3H), 2.41 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 173.9, 144.9, 142.1, 141.8, 137.7, 136.5, 136.2, 133.2, 130.0, 129.7, 129.62, 129.56, 128.5, 128.3, 128.11, 128.06, 125.8 (q, $^1J_{C\text{-}F}$ = 281.6 Hz), 125.1, 124.9, 124.7, 124.5, 122.5, 122.1, 109.5, 65.9 (q, $^2J_{C\text{-}F}$ = 32.9 Hz), 63.8, 51.4, 26.0, 21.6 ppm. $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -77.92 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}ClF_3N_3O_3S_2^+$ 668.1051, found 668.1047.




**5'-bromo-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4e)**

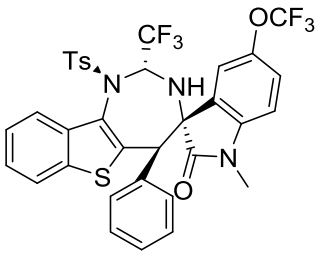
White solid: 61 mg (yield 84%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 222-224 °C; IR (KBr) 3316, 1726, 1612, 1491, 1364, 1251, 999, 812, 660 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.97 (m, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.44 – 7.39 (m, 2H), 7.38 – 7.33 (m, 1H), 7.33 – 7.26 (m, 1H), 7.26 – 7.23 (m, 2H), 7.20 – 7.14 (m, 1H), 7.10 (t, *J* = 7.4 Hz, 2H), 6.91 (d, *J* = 7.4 Hz, 2H), 6.41 (d, *J* = 8.3 Hz, 1H), 6.09 (dq, *J* = 13.8, 4.6 Hz, 1H), 4.66 (s, 1H), 3.00 (d, *J* = 14.0 Hz, 1H), 2.82 (s, 3H), 2.41 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 173.8, 145.0, 142.3, 142.0, 137.7, 136.4, 136.2, 133.2, 132.5, 130.3, 129.7, 129.5, 128.3, 128.07, 127.2, 125.7 (q, $^1J_{C\text{-}F}$ = 262.5 Hz), 125.0, 124.9, 124.8, 122.5, 122.2, 115.7, 110.0, 66.0 (q, $^2J_{C\text{-}F}$ = 33.1 Hz), 63.7, 51.4, 26.0, 21.6 ppm. $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -77.89 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0541.




**5'-methoxy-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4f)**

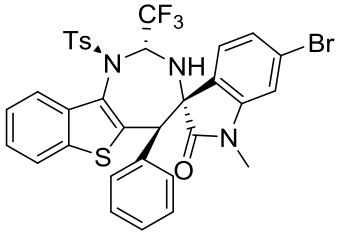
White solid: 45 mg (yield 67%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 232-234 °C; IR (KBr) 3315, 1715, 1600, 1498, 1342, 1153, 967, 668, 575 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.0 Hz, 1H), 7.60 (m, 3H), 7.37 – 7.27 (m, 1H), 7.24 – 7.04 (m, 9H), 6.80 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.46 (d, *J* = 8.5 Hz, 1H), 6.22 (dq, *J* = 14.0, 4.8 Hz, 1H), 5.04 (s, 1H), 3.96 (s, 3H), 3.03 (d, *J* = 13.6 Hz, 1H), 2.84 (s, 3H), 2.40 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.0, 156.4, 144.8, 143.2,

137.7, 136.6, 136.1, 133.7, 129.7, 129.6, 129.4, 128.2, 128.1, 128.0, 124.9, 124.6, 124.5, 122.6, 121.8, 114.2, 111.2, 109.1, 100.0, 65.8 (q, $^{2}J_{C\text{-}F}$ = 32.4 Hz), 64.0, 56.1, 51.3, 26.0, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -77.90 ppm. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{34}H_{29}F_3N_3O_4S_2^+$ 664.1546, found 664.1545.



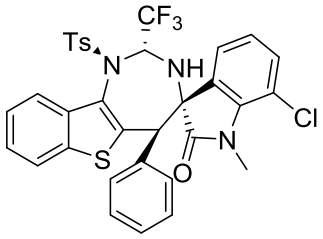

**1'-methyl-5-phenyl-1-tosyl-5'-(trifluoromethoxy)-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4g)**

White solid: 47 mg (yield 64%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 222-224 ℃; IR (KBr) 3445, 1728, 1622, 1379, 1260, 1159, 746, 666, 578 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.43 – 7.32 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.23 – 7.12 (m, 4H), 7.09 (t, *J* = 7.5 Hz, 2H), 6.93 (d, *J* = 7.4 Hz, 2H), 6.53 (d, *J* = 8.4 Hz, 1H), 6.08 (dq, *J* = 13.8, 4.6 Hz, 1H), 4.75 (s, 1H), 3.01 (d, *J* = 14.0 Hz, 1H), 2.86 (s, 3H), 2.38 (s, 3H) ppm. $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 174.1, 144.93, 144.90, 144.85, 142.0, 141.9, 137.7, 136.2, 136.1, 133.0, 129.7, 129.6, 129.4, 128.4, 128.04, 128.01, 125.1, 124.9, 124.8, 122.9, 122.6, 122.1, 118.2, 109.1, 66.4 (q, $^{2}J_{C\text{-}F}$ = 32.5 Hz), 63.8, 51.3, 26.1, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -58.22, -78.03 ppm. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{34}H_{26}F_6N_3O_4S_2^+$ 718.1263, found 718.1258.



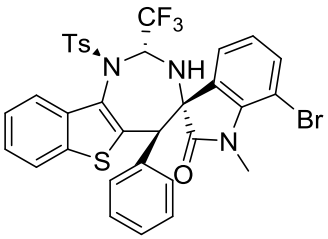

**6'-bromo-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4h)**

White solid: 60 mg (yield 82%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 220-222 °C; IR (KBr) 3302, 1723, 1606, 1491, 1371, 1153, 968, 751, 597 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.77 (t, *J* = 7.6 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.39 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.23 – 7.10 (m, 7H), 7.09 – 7.00 (m, 2H), 6.72 (d, *J* = 1.6 Hz, 1H), 6.14 (dq, *J* = 13.8, 4.6 Hz, 1H), 5.02 (s, 1H), 2.98 (d, *J* = 14.0 Hz, 1H), 2.85 (s, 3H), 2.40 (s, 3H) ppm. $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 174.2, 144.9, 144.6, 142.7, 137.7, 136.4, 136.1, 133.3, 129.60, 129.59, 128.4, 128.2, 127.3, 126.1, 125.2, 124.9, 124.7, 124.6, 123.5, 122.6, 121.7, 112.2, 65.0 (q, $^{2}J_{C\text{-}F}$ = 32.7 Hz), 63.5, 51.1, 26.0, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -78.04 ppm. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0551.



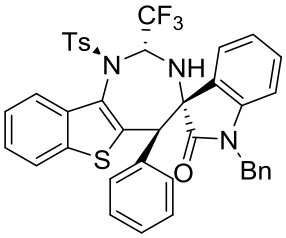
**7'-chloro-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4i)**

White solid: 57 mg (yield 83%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 222-224 °C; IR (KBr) 2923, 1719, 1637, 1560, 1458, 1364, 1163, 670, 628, 591 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.80 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.36 – 7.27 (m, 1H), 7.23 – 7.09 (m, 9H), 7.04 (d, *J* = 7.4 Hz, 2H), 6.18 (dq, *J* = 14.0, 4.8 Hz, 1H), 5.06 (s, 1H), 3.25 (s, 3H), 2.99 (d, *J* = 14.0 Hz, 1H), 2.40 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.7, 145.3, 144.9, 142.8, 139.3, 137.7, 136.4, 136.0, 133.3, 132.1, 131.05, 129.6, 128.5, 128.22, 128.17, 124.9, 124.7, 124.5, 124.1, 122.57, 122.55, 121.7, 116.1, 65.5 (q, $^2J_{C\text{-}F}$ = 32.9 Hz), 63.2, 51.3, 29.4, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.05 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}ClF_3N_3O_3S_2^+$ 668.1051, found 668.1057.



**7'-bromo-1'-methyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4j)**

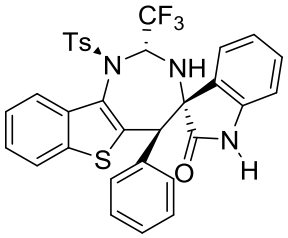
White solid: 62 mg (yield 82%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 224-226 °C; IR (KBr) 3324, 1718, 1607, 1459, 1348, 1201, 1162, 778, 672, 595 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.2 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.24 – 7.08 (m, 8H), 7.03 (d, *J* = 7.4 Hz, 2H), 6.18 (dq, *J* = 14.0, 4.8 Hz, 1H), 5.06 (s, 1H), 3.26 (s, 3H), 2.99 (d, *J* = 14.0 Hz, 1H), 2.40 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.9, 144.9, 142.8, 140.8, 137.7, 136.4, 136.0, 135.4, 133.2, 131.4, 129.6, 128.5, 128.22, 128.17, 124.9, 124.7, 124.6, 124.4, 123.1, 122.6, 121.7, 102.9, 65.5 (q, $^2J_{C\text{-}F}$ = 32.9 Hz), 63.2, 51.3, 29.7, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.05 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0541.



**1'-benzyl-5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4k)**

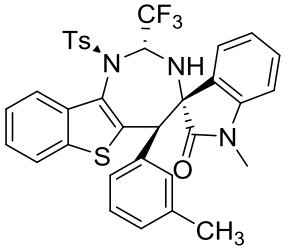
White solid: 63 mg (yield 78%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 230-232 °C; IR (KBr) 3448, 1719, 1613, 1490, 1465, 1352, 1191, 1151, 672, 546 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$)

δ 7.98 (d, *J* = 7.0 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.34 – 7.28 (m, 2H), 7.25 – 7.07 (m, 13H), 6.66 (d, *J* = 7.0 Hz, 2H), 6.41 (d, *J* = 7.6 Hz, 1H), 6.21 (dq, *J* = 14.0, 4.8 Hz, 1H), 5.17 (s, 1H), 4.83 (d, *J* = 16.0 Hz, 1H), 4.50 (d, *J* = 16.2 Hz, 1H), 3.06 (d, *J* = 13.6 Hz, 1H), 2.40 (s, 3H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 174.5, 144.8, 143.3, 142.8, 137.6, 136.5, 136.1, 134.5, 133.9, 130.1, 129.7, 129.6, 128.6, 128.4, 128.2, 128.10, 182.09, 127.4, 126.7, 124.9, 124.7, 124.5, 124.2, 123.3, 122.5, 121.8, 110.1, 65.7 (q, $^{2}J_{C\text{-}F}$ = 32.9 Hz) , 63.8, 50.5, 43.8, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -77.88 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{39}H_{31}F_3N_3O_3S_2^+$ 710.1753, found 710.1757.



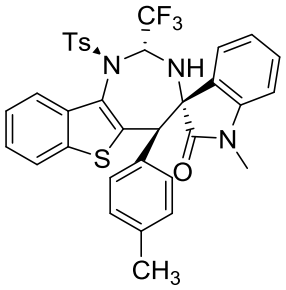

**5-phenyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4k)**

White solid: 51 mg (yield 72%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 228-230 ℃; IR (KBr) 3448, 1713, 1622, 1382, 1192, 1156, 704, 666, 570 $cm^{-1}$; $^{1}H$ NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.86 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.41 (s, 1H), 7.34 – 7.28 (m, 1H), 7.26 – 7.15 (m, 7H), 7.13 – 7.08 (m, 4H), 6.67 – 6.57 (m, 1H), 6.19 (dq, *J* = 14.2, 4.8 Hz, 1H), 5.04 (s, 1H), 2.97 (d, *J* = 14.0 Hz, 1H), 2.39 (s, 3H) ppm.$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 175.9, 144.8, 143.0, 140.2, 137.6, 136.4, 136.1, 133.6, 129.8, 129.7, 129.6, 128.5, 128.24, 128.22, 128.20, 124.9, 124.7, 124.6, 124.4, 123.4, 122.5, 121.8, 110.4, 65.6 (q, $^{2}J_{C\text{-}F}$ = 32.9 Hz) , 63.8, 50.8, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.04 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{32}H_{25}F_3N_3O_3S_2^+$ 620.1280, found 620.1289.



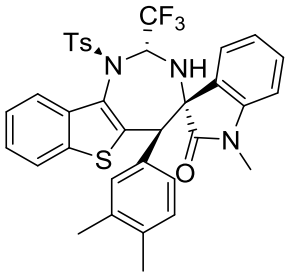

**1'-methyl-5-(m-tolyl)-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4n)**

White solid: 47 mg (yield 73%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 220-222 °C; IR (KBr) 3314, 1716, 1612, 1374, 1096, 751, 670, 572 $cm^{-1}$; $^{1}H$ NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.84 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.27 (m, 2H), 7.26 – 7.18 (m, 5H), 6.97 (dt, *J* = 14.0, 7.6 Hz, 2H), 6.88 (d, *J* = 7.4 Hz, 1H), 6.75 (s, 1H), 6.60 – 6.50 (m, 1H), 6.27 – 6.16 (m, 1H), 4.96 (s, 1H), 3.01 (d, *J* = 14.0 Hz, 1H), 2.87 (s, 3H), 2.39 (s, 3H), 2.17 (s, 3H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 174.3, 144.7, 143.3, 143.2, 137.7, 137.6, 136.5, 136.2, 133.5, 130.4, 129.6, 129.5, 128.8, 128.4, 128.2, 127.7, 126.5, 124.8, 124.6, 124.5, 124.0, 123.2, 122.5, 121.8, 108.5, 65.9 (q, $^{2}J_{C\text{-}F}$ = 32.7 Hz), 63.6, 51.2, 25.9, 21.6, 21.3 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.05 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{29}F_3N_3O_3S_2^+$ 648.1597, found 648.1599.



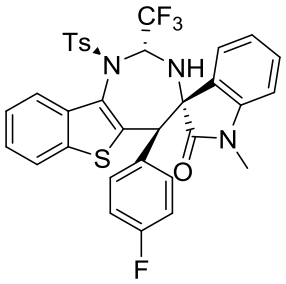
**1'-methyl-5-(p-tolyl)-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4o)**

White solid: 42 mg (yield 65%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 223-225 °C; IR (KBr) 3310, 1717, 1612, 1491, 1339, 1256, 752, 670, 594 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.85 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.35 – 7.26 (m, 3H), 7.26 – 7.18 (m, 4H), 6.95 – 6.79 (s, 4H), 6.59 – 6.52 (m, 1H), 6.19 (m, 1H), 4.91 (s, 1H), 3.00 (d, *J* = 14.0 Hz, 1H), 2.88 (s, 3H), 2.39 (s, 3H), 2.22 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.4, 144.7, 143.4, 143.3, 137.8, 137.7, 136.5, 136.2, 130.5, 129.6, 129.5, 129.4, 128.7, 128.5, 128.2, 124.7, 124.6, 124.5, 123.9, 123.2, 122.5, 121.9, 108.6, 66.0 (q, $^2J_{C\text{-}F}$ = 32.5 Hz), 63.5, 50.8, 25.9, 21.6, 21.1 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.05 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{29}F_3N_3O_3S_2^+$ 648.1597, found 648.1596.



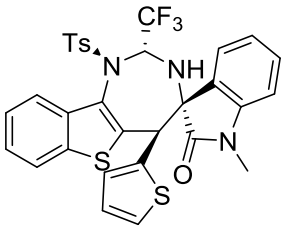
**5-(3,4-dimethylphenyl)-1'-methyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4p)**

White solid: 43 mg (yield 68%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 221-223 °C; IR (KBr) 3448, 1716, 1614, 1492, 1359, 1152, 1102, 760, 599 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.84 (m, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.35 – 7.27 (m, 2H), 7.26 – 7.17 (m, 5H), 6.85 (d, *J* = 7.8 Hz, 1H), 6.81 – 6.76 (m, 1H), 6.66 (s, 1H), 6.60 – 6.53 (m, 1H), 6.19 (dq, *J* = 14.0, 4.8 Hz, 1H), 4.87 (s, 1H), 2.99 (d, *J* = 14.0 Hz, 1H), 2.88 (s, 3H), 2.38 (s, 3H), 2.12 (s, 3H), 2.06 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.4, 144.7, 143.6, 143.3, 137.7, 136.5, 136.4, 136.2, 130.9, 130.8, 129.5, 129.2, 128.5, 128.2, 126.7, 124.6, 124.5, 123.9, 123.2, 122.5, 121.9, 108.6, 66.0 (q, $^2J_{C\text{-}F}$ = 32.3 Hz), 63.5, 50.7, 25.9, 21.6, 19.6, 19.4 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.07 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{35}H_{31}F_3N_3O_3S_2^+$ 662.1753, found 662.1754.



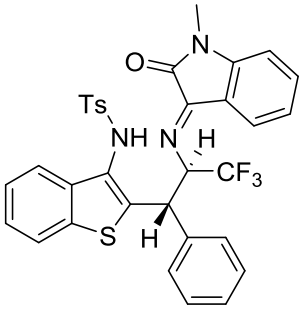
**phenyl)-1'-methyl-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4q)**

White solid: 43 mg (yield 67%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 225-227 °C; IR (KBr) 3311, 1716, 1610, 1511, 1491, 1373, 1149, 969, 753, 547 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.2 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.28 (m, 3H), 7.25 – 7.11 (m, 4H), 7.08 – 6.98 (m, 2H), 6.79 (t, *J* = 8.8 Hz, 2H), 6.65 – 6.52 (m, 1H), 6.22 (dq, *J* = 14.0, 4.6 Hz, 1H), 5.08 (s, 1H), 3.00 (d, *J* = 14.0 Hz, 1H), 2.89 (s, 3H), 2.40 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.2, 162.4 (d, *J* = 247.8 Hz), 144.8, 143.2, 142.8, 137.6, 136.4, 136.1, 131.4, 131.4, 129.8, 129.6, 128.2, 128.1, 125.0, 124.8, 124.6, 124.0, 123.5, 122.6, 121.8, 114.9 (d, *J* = 21.3 Hz), 108.7, 65.8 (q, $^2J_{C\text{-}F}$ = 32.8 Hz), 63.7, 50.4, 26.0, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.05, -113.40 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}F_4N_3O_3S_2^+$ 652.1346, found 652.1340.



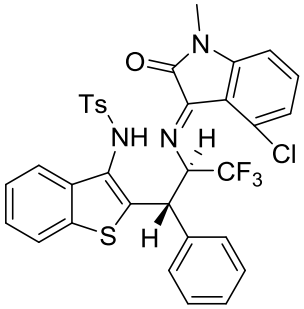
**1'-methyl-5-(thiophen-2-yl)-1-tosyl-2-(trifluoromethyl)-1,2,3,5-tetrahydrospiro[benzo[4,5]thieno[3,2-*d*][1,3]diazepine-4,3'-indolin]-2'-one (4r)**

White solid: 36 mg (yield 57%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.4; mp 226-228 °C; IR (KBr) 3448, 1718, 1615, 1491, 1352, 1196, 1162, 751, 670 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.82 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.40 – 7.26 (m, 4H), 7.26 – 7.18 (m, 3H), 7.05 – 6.99 (m, 1H), 6.98 – 6.91 (m, 1H), 6.82 (dd, *J* = 4.8, 3.6 Hz, 1H), 6.66 (d, *J* = 7.4 Hz, 1H), 6.15 (dq, *J* = 13.8, 4.8 Hz, 1H), 5.24 (s, 1H), 2.99 (d, *J* = 14.0 Hz, 1H), 2.95 (s, 3H), 2.40 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.3, 144.9, 143.6, 143.2, 137.7, 136.3, 136.2, 135.2, 129.9, 129.7, 128.3, 128.1, 127.9, 126.7, 125.1, 124.8, 124.6, 124.5, 123.9, 123.4, 122.6, 121.9, 108.7, 65.8 (q, $^2J_{C\text{-}F}$ = 36.4 Hz), 63.7, 45.7, 26.1, 21.7 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -78.06 ppm. HRMS (ESI-TOF) *m/z* $[M + Na]^+$ calcd for $C_{31}H_{24}F_3N_3O_3S_3Na^+$ 662.0824, found 662.0819.



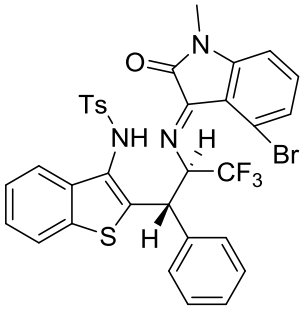
**4-methyl-*N*-(2-(3,3,3-trifluoro-2-((1-methyl-2-oxoindolin-3-ylidene)amino)-1-phenylpropyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5a)**

Yellow solid: 40 mg (yield 63%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 183-185 ℃; IR (KBr) 3448, 1718, 1615, 1491, 1352, 1196, 1162, 751, 670 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.83 – 7.70 (m, 3H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.45 – 7.35 (m, 3H), 7.32 – 7.27 (m, 3H), 7.24 – 7.12 (m, 3H), 7.01 – 6.89 (m, 1H), 6.83 – 6.74 (m, 2H), 6.64 (d, *J* = 7.8 Hz, 1H), 4.36 (d, *J* = 9.0 Hz, 1H), 3.02 (s, 3H), 2.55 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.8, 158.7, 146.1, 144.1, 138.0, 137.53, 137.47, 137.1, 136.5, 134.9, 130.0, 128.7, 128.3, 128.1, 127.7, 126.3, 124.7, 124.4, 124.0, 123.8, 123.7, 121.7, 119.7, 108.9, 67.6 (q, $^2J_{C\text{-}F}$ = 26.6 Hz), 45.1, 25.7, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.45 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{27}F_3N_3O_3S_2^+$ 634.1440, found 634.1431.




**(*E*)-*N*-(2-(2-((4-chloro-1-methyl-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5b)**

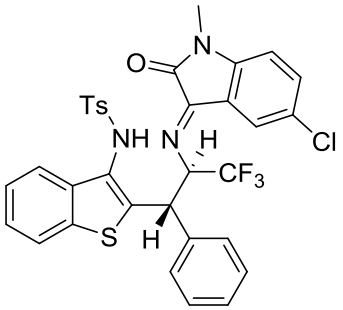
Yellow solid: 40 mg (yield 59%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 203-205 ℃; IR (KBr) 3443, 1718, 1609, 1456, 1346, 1172, 1154, 730, 670 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.81 (m, 1H), 7.78 (d, *J* = 8.2 Hz, 2H), 7.70 (s, 1H), 7.53 – 7.46 (m, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.27 (m, 4H), 7.24 – 7.16 (m, 2H), 7.14 – 7.04 (m, 2H), 6.91 – 6.74 (m, 2H), 6.52 (d, *J* = 7.8 Hz, 1H), 4.53 (d, *J* = 10.4 Hz, 1H), 2.98 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 157.7, 157.3, 147.2, 144.0, 139.3, 138.0, 137.1, 136.6, 134.7, 131.9, 130.0, 129.8, 128.7, 128.4, 128.0, 127.7, 125.8, 124.7, 124.3, 123.7, 121.7, 116.1, 110.4, 107.2, 64.2 (q, $^2J_{C\text{-}F}$ = 21.7 Hz), 45.1, 25.8, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.96 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}ClF_3N_3O_3S_2^+$ 668.1051, found 668.1049.




**(*E*)-*N*-(2-(2-((4-bromo-1-methyl-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5c)**

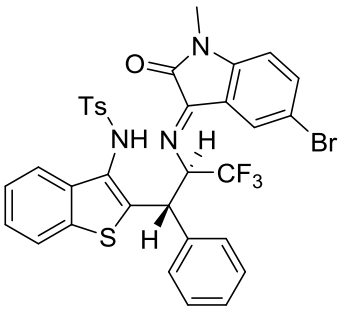
Yellow solid: 40 mg (yield 56%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 206-208 ℃; IR (KBr) 3396, 1719, 1605, 1455, 1339, 1164, 762, 669 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.85 – 7.71 (m, 3H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.46 – 7.33 (m, 3H), 7.31 – 7.28 (m, 2H), 7.24 – 7.13 (m, 3H), 6.95 (m, 1H), 6.85 – 6.74 (m, 2H), 6.64 (d, *J* = 7.8 Hz, 1H), 4.36 (d,

*J* = 9.0 Hz, 1H), 3.02 (s, 3H), 2.55 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 157.7, 157.4, 147.5, 144.0, 139.5, 138.0, 137.8, 137.0, 136.6, 134.6, 129.9, 129.0, 128.7, 128.4, 128.0, 127.7, 125.9, 124.7, 124.2, 123.6, 121.7, 119.5, 117.7, 107.7, 63.9 (q, $^2J_{C\text{-}F}$ = 28.3 Hz), 45.1, 25.7, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.45 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0563.



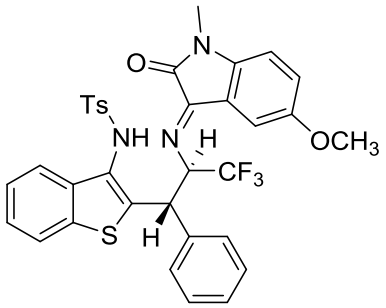

**(*E*)-*N*-(2-(2-((5-chloro-1-methyl-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5d)**

Yellow solid: 44 mg (yield 65%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 205-207 ℃; IR (KBr) 3334, 1708, 1612, 1347, 1152, 773, 662, 557 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.2 Hz, 1H), 7.81 (s, 1H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.69 (d, *J* = 2.0 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.40 – 7.35 (m, 3H), 7.32 – 7.27 (m, 4H), 7.24 – 7.15 (m, 2H), 6.93 – 6.78 (m, 3H), 6.58 (d, *J* = 8.4 Hz, 1H), 4.48 (d, *J* = 10.0 Hz, 1H), 3.01 (s, 3H), 2.53 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 158.2, 157.8, 144.4, 144.2, 138.2, 137.42, 137.37, 137.0, 136.4, 134.3, 130.0, 129.6, 128.7, 128.1, 127.7, 126.3, 124.8, 124.4, 123.6, 123.5, 122.7, 121.7, 120.9, 110.0, 63.6 (q, $^2J_{C\text{-}F}$ = 29.7 Hz), 45.1, 25.9, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.59 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}ClF_3N_3O_3S_2^+$ 668.1051, found 668.1058.



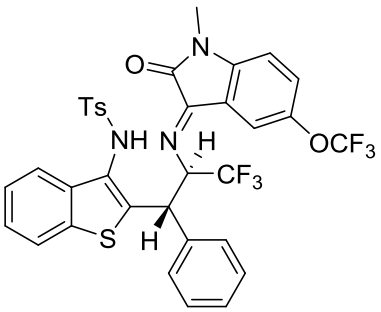

***(E)* -*N*-(2-(2-((5-bromo-1-methyl-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5e)**

Yellow solid: 46 mg (yield 57%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 209-211 ℃; IR (KBr) 3299, 1713, 1609, 1353, 1165, 816, 766, 734, 560 $cm^{-1}$;$^1H$ NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.8 Hz, 1H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.79 – 7.73 (m, 3H), 7.56 – 7.47 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.26 (m, 3H), 7.25 – 7.17 (m, 2H), 6.95 – 6.78 (m, 3H), 6.53 (d, *J* = 8.4 Hz, 1H), 4.49 (d, *J* = 9.8 Hz, 1H), 3.01 (s, 3H), 2.53 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.0, 157.6, 144.8, 144.2, 138.2, 137.42, 137.37, 137.2, 137.0, 136.4, 130.0, 128.7, 128.4, 128.1, 127.7, 126.4, 126.3, 124.8, 124.5, 123.5, 121.7, 121.2, 116.6, 110.4, 64.2 (q, $^2J_{C\text{-}F}$ = 26.7 Hz), 45.1, 25.9, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.59 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0544.



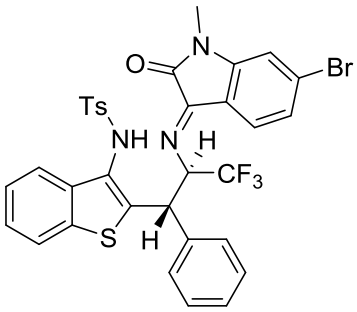

**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-2-((5-methoxy-1-methyl-2-oxoindolin-3-ylidene)amino)-1-phenylpropyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5f)**

Brown solid: 41 mg (yield 61%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 210-212 ℃; IR (KBr) 3448, 1716, 1618, 1493, 1358, 1242, 1165, 663, 563 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.43 – 7.37 (m, 3H), 7.32 – 7.27 (m, 4H), 7.24 – 7.19 (m, 1H), 7.00 – 6.94 (m, 1H), 6.95 – 6.87 (m, 1H), 6.84 – 6.74 (m, 2H), 6.55 (d, *J* = 8.4 Hz, 1H), 4.34 (d, *J* = 10.2 Hz, 1H), 3.98 (s, 3H), 2.99 (s, 3H), 2.55 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.3, 158.7, 156.8, 144.1, 140.0, 137.8, 137.6, 137.4, 137.1, 136.5, 130.0, 128.7, 128.4, 128.1, 127.6, 126.4, 124.6, 124.4, 123.7, 122.0, 121.7, 120.2, 64.3 (q, $^2J_{C\text{-}F}$ = 26.5 Hz), 56.3, 45.2, 25.7, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.18 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{29}F_3N_3O_4S_2^+$ 664.1546, found 664.1550.



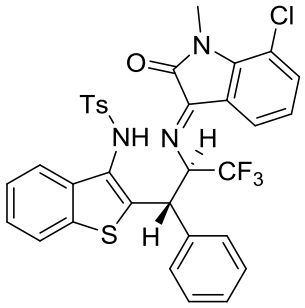

**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-2-((1-methyl-2-oxo-5-(trifluoromethoxy)indolin-3-ylidene)amino)-1-phenylpropyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5g)**

Yellow solid: 49 mg (yield 69%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 205-207 °C; IR (KBr) 3448, 1718, 1655, 1492, 1380, 1254, 1166, 759, 663 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.78 – 7.72 (m, 2H), 7.63 – 7.59 (s, 1H), 7.52 – 7.46 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.26 (m, 4H), 7.24 – 7.16 (m, 3H), 6.97 – 6.80 (m, 3H), 6.63 (d, *J* = 8.6 Hz, 1H), 4.48 (d, *J* = 9.8 Hz, 1H), 3.02 (s, 3H), 2.53 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.4, 157.6, 145.4, 144.4, 144.2, 138.1, 137.4, 137.3, 137.0, 136.4, 130.0, 128.8, 128.3, 128.2, 127.7, 126.3, 125.5, 124.8, 124.5, 123.5, 121.8, 121.6, 120.6, 119.2, 117.1, 109.7, 64.3 (q, $^2J_{C\text{-}F}$ = 27.0 Hz), 45.1, 25.9, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -58.34, -70.68 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{26}F_6N_3O_4S_2^+$ 718.1263, found 718.1268.



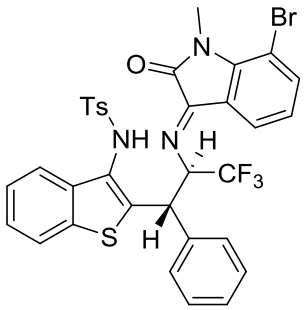
**(*E*)-*N*-(2-(2-((6-bromo-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5h)**

Yellow solid: 40 mg (yield 57%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 215-217 ℃; IR (KBr) 3283, 1716, 1607, 1367, 1261, 1163, 1134, 768, 567 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.55 – 7.45 (m, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.26 (m, 5H), 7.26 – 7.18 (m, 1H), 6.94 – 6.83 (m, 1H), 6.82 – 6.73 (m, 3H), 4.37 (d, *J* = 8.0 Hz, 1H), 3.00 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.4, 157.7, 147.0, 144.2, 137.9, 137.4, 137.3, 137.1, 136.4, 130.0, 129.5, 128.7, 128.3, 128.2, 127.7, 127.0, 126.3, 124.9, 124.8, 123.7, 121.7, 118.5, 112.6, 64.3 (q, $^2J_{C\text{-}F}$ = 26.5 Hz), 45.0, 25.9, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.51 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0545.



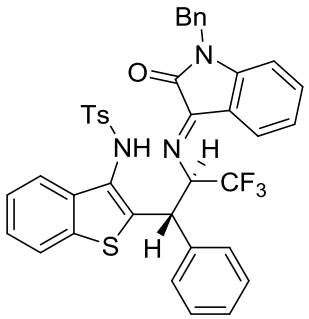
**(*E*)-*N*-(2-(2-((7-chloro-1-methyl-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5i)**

Yellow solid: 36 mg (yield 54%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 208-210 ℃; IR (KBr) 3289, 1708, 1607, 1454, 1363, 1165, 1122, 769, 661 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.96 – 7.89 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.68 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.42 – 7.27 (m, 6H), 7.25 – 7.19 (m, 2H), 7.08 (t, *J* = 7.8 Hz, 1H), 6.94 – 6.85 (m, 1H), 6.84 – 6.75 (m, 2H), 4.38 (d, *J* = 9.0 Hz, 1H), 3.38 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.7, 157.8, 144.2, 141.6, 137.9, 137.4, 137.3, 137.1, 136.9, 136.4, 130.0, 128.7, 128.3, 128.2, 127.7, 127.7, 126.2, 124.9, 124.7, 124.5, 123.6, 122.4, 122.2, 121.8, 121.7, 116.5, 64.4 (q, $^2J_{C\text{-}F}$ = 26.4 Hz), 45.0, 29.0, 21.8 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.50 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}ClF_3N_3O_3S_2^+$ 668.1051, found 668.1058.



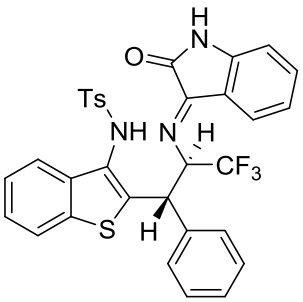

**(*E*)-*N*-(2-(2-((7-bromo-1-methyl-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5j)**

Yellow solid: 36 mg (yield 50%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 200-202 ℃; IR (KBr) 3289, 1707, 1604, 1456, 1362, 1165, 1092, 767, 659 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.96 – 7.83 (m, 1H), 7.81 – 7.59 (m, 3H), 7.55 – 7.45 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.26 (m, 3H), 7.26 – 7.19 (m, 2H), 7.06 – 6.97 (m, 1H), 6.94 – 6.84 (m, 1H), 6.83 – 6.71 (m, 2H), 4.37 (d, *J* = 12.0 Hz, 1H), 3.40 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.9, 157.7, 144.2, 143.1, 140.2, 137.9, 137.3, 137.1, 136.4, 130.0, 128.7, 128.3, 128.2, 127.7, 126.2, 125.1, 124.9, 124.5, 123.6, 122.72, 122.70, 121.8, 64.5 (q, $^2J_{C\text{-}F}$ = 26.4 Hz), 45.0, 29.1, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.53 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}BrF_3N_3O_3S_2^+$ 712.0546, found 712.0534.



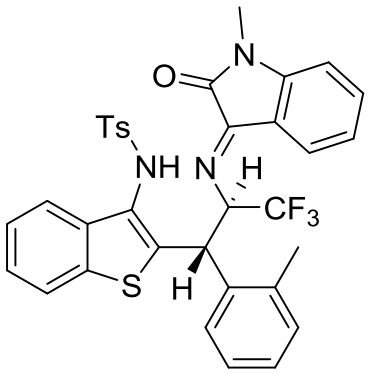

**(*E*)-*N*-(2-(2-((1-benzyl-2-oxoindolin-3-ylidene)amino)-3,3,3-trifluoro-1-phenylpropyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5k)**

Yellow solid: 43 mg (yield 61%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 226-228 ℃; IR (KBr) 3220, 1716, 1609, 1473, 1346, 1178, 1154, 645, 548 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.99 – 7.87 (m, 1H), 7.77 (t, *J* = 7.4 Hz, 3H), 7.56 – 7.45 (m, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.27 (m, 4H), 7.28 – 7.20 (m, 5H), 7.12 (m, 1H), 7.03 – 6.92 (m, 3H), 6.90 – 6.74 (m, 2H), 6.46 (d, *J* = 7.8 Hz, 1H), 4.76 (d, *J* = 15.8 Hz, 1H), 4.64 (d, *J* = 15.8 Hz, 1H), 4.38 (d, *J* = 10.0 Hz, 1H), 2.55 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.7, 158.3, 145.3, 144.1, 138.0, 137.5, 137.0, 136.4, 134.8, 134.3, 130.0, 129.0, 128.7, 128.4, 128.1, 127.9, 127.7, 126.9, 126.3, 124.8, 124.4, 123.9, 123.73, 123.68, 121.7, 119.8, 109.9, 64.3 (q, $^2J_{C\text{-}F}$ = 26.8 Hz), 45.1, 43.5, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.65 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{39}H_{31}F_3N_3O_3S_2^+$ 710.1753, found 710.1754.



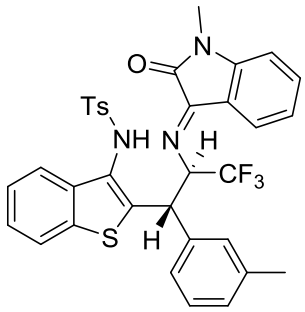
**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-2-((2-oxoindolin-3-ylidene)amino)-1-phenylpropyl)benzo[*b*]3thiophen-3-yl)benzenesulfonamide (5l)**

Yield solid: 41 mg (yield 67%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 231-233 °C; IR (KBr) 3256, 1719, 1619, 1470, 1355, 1253, 1165, 756, 663 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.95 (d, $J$ = 8.0 Hz, 1H), 7.83 – 7.68 (m, 3H), 7.50 (d, $J$ = 7.8 Hz, 1H), 7.43 – 7.32 (m, 4H), 7.30 – 7.26 (m, 3H), 7.25 – 7.12 (m, 3H), 6.92 – 6.76 (m, 3H), 6.65 (d, $J$ = 7.8 Hz, 1H), 4.41 (d, $J$ = 10.0 Hz, 1H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.5, 158.3, 144.2, 143.3, 138.7, 138.0, 137.5, 137.0, 136.5, 135.1, 130.0, 128.7, 128.3, 128.1, 127.7, 126.3, 124.8, 124.4, 124.2, 124.0, 123.7, 121.8, 120.4, 110.7, 64.0 (q, $^2J_{C\text{-}F}$ = 25.3 Hz), 45.1, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.76 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{32}H_{25}F_3N_3O_3S_2^+$ 620.1284, found 620.1284.



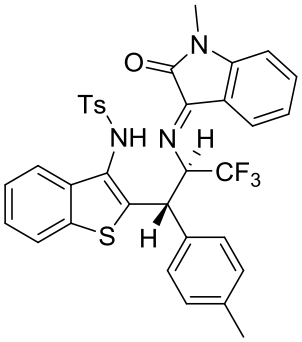
**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-2-((1-methyl-2-oxoindolin-3-ylidene)amino)-1-(o-tolyl)propyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5m)**

Yellow solid: 45 mg (yield 70%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 189-191 °C; IR (KBr) 3467, 1713, 1613, 1355, 1160, 860, 758, 563 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.83 (t, $J$ = 7.4 Hz, 3H), 7.69 – 7.58 (m, 1H), 7.56 – 7.45 (m, 2H), 7.47 – 7.38 (m, 1H), 7.31 (d, $J$ = 8.2 Hz, 2H), 7.24 – 7.09 (m, 6H), 7.08 – 7.00 (m, 1H), 6.66 (d, $J$ = 7.8 Hz, 1H), 5.37 (d, $J$ = 8.6 Hz, 1H), 3.01 (s, 3H), 2.45 (s, 3H), 1.89 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.8, 158.5, 146.2, 144.0, 138.4, 137.9, 137.3, 136.5, 136.4, 134.8, 130.9, 128.0, 127.8, 127.5, 126.7, 126.0, 124.5, 124.1, 123.84, 123.79, 123.0, 121.8, 119.9, 108.9, 63.9 (q, $^2J_{C\text{-}F}$ = 27.0 Hz), 40.5, 25.7, 21.6, 19.0 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.99 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{29}F_3N_3O_3S_2^+$ 648.1597, found 648.1597.



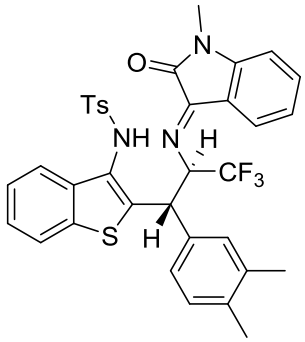
**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-2-((1-methyl-2-oxoindolin-3-ylidene)amino)-1-(m-tolyl)propyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5n)**

Yellow solid: 34 mg (yield 53%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 196-198 °C; IR (KBr) 3448, 1707, 1612, 1473, 1369, 1194, 752, 660 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.89 – 7.71 (m, 3H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.45 – 7.35 (m, 3H), 7.28 – 7.14 (m, 4H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.95 (m, 1H), 6.73 (d, *J* = 7.6 Hz, 1H), 6.65 (d, *J* = 7.8 Hz, 1H), 6.46 (s, 1H), 4.35 (d, *J* = 10.4 Hz, 1H), 3.03 (s, 3H), 2.54 (s, 3H), 2.32 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.8, 158.7, 146.1, 144.0, 138.4, 138.2, 137.7, 137.4, 137.1, 136.6, 134.9, 130.0, 129.1, 128.9, 128.5, 127.7, 126.2, 125.2, 124.7, 124.3, 124.0, 123.8, 123.7, 121.7, 119.7, 108.9, 64.0 (q, $^2J_{C\text{-}F}$ = 26.7 Hz), 45.0, 25.8, 21.7, 21.6 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.37 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{29}F_3N_3O_3S_2^+$ 648.1597, found 648.1591.



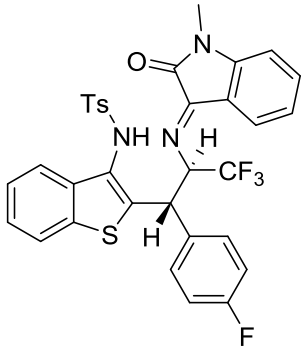
**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-2-((1-methyl-2-oxoindolin-3-ylidene)amino)-1-(p-tolyl)propyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5o)**

Yellow solid: 33 mg (yield 52%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 200-202 ℃; IR (KBr) 3390, 1712, 1614, 1495, 1470, 1168, 818, 666 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 2H), 7.77 (t, *J* = 8.5 Hz, 2H), 7.59 – 7.47 (m, 2H), 7.47 – 7.34 (m, 4H), 7.19 (dd, *J* = 11.7, 8.8 Hz, 4H), 7.08 (d, *J* = 7.8 Hz, 2H), 6.73 – 6.60 (m, 3H), 4.32 (d, 1H), 3.02 (s, 3H), 2.55 (s, 3H), 2.34 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.8, 158.7, 144.7, 143.4, 143.3, 137.8, 137.7, 136.5, 136.2, 130.5, 129.6, 129.5, 129.4, 128.7, 128.5, 128.2, 124.7, 124.6, 124.5, 123.9, 123.2, 122.5, 121.9, 108.6, 63.3 (q, $^2J_{C\text{-}F}$ = 24.6 Hz), 50.8, 25.9, 21.6, 21.1 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.37 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{29}F_3N_3O_3S_2^+$ 648.1597, found 648.1594.



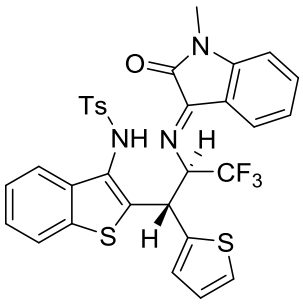
**(*E*)-*N*-(2-(1-(3,4-dimethylphenyl)-3,3,3-trifluoro-2-((1-methyl-2-oxoindolin-3-ylidene)amino)propyl)benzo[*b*]thiophen-3-yl)-4-methylbenzenesulfonamide (5p)**

Yellow solid: 40 mg (yield 60%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 209-211 °C; IR (KBr) 3441, 1711, 1613, 1370, 1165, 1050, 882, 761, 565 $cm^{-1}$; $^1$HNMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.79 (dd, *J* = 7.6, 3.4 Hz, 3H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.34 (m, 3H), 7.25 – 7.13 (m, 3H), 7.05 (d, *J* = 7.8 Hz, 1H), 6.99 – 6.86 (m, 1H), 6.64 (d, *J* = 7.8 Hz, 2H), 6.45 (s, 1H), 4.32 (d, *J* = 10.4 Hz, 1H), 3.03 (s, 3H), 2.55 (s, 3H), 2.23 (d, *J* = 5.8 Hz, 6H) ppm. $^{13}$C{$^1$H} NMR (100 MHz, $CDCl_3$) δ 158.8, 158.7, 146.1, 143.9, 138.6, 137.7, 137.1, 137.0, 136.7, 136.5, 134.8, 130.0, 129.8, 129.5, 129.0, 127.7, 127.2, 126.1, 125.4, 124.6, 124.3, 124.0, 123.7, 121.7, 119.7, 108.9, 64.1 (q, $^2J_{C\text{-}F}$ = 25.8 Hz), 44.6, 25.7, 21.8, 19.9, 19.5 ppm (the C of $CF_3$ is not observed). $^{19}$F NMR (376 MHz, $CDCl_3$) δ -70.31 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{35}H_{31}F_3N_3O_3S_2^+$ 662.1753, found 662.1750.



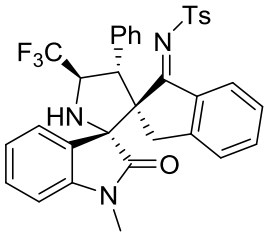
**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-1-(4-fluorophenyl)-2-((1-methyl-2-oxoindolin-3-ylidene)amino)propyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5q)**

Yellow solid: 44 mg (yield 67%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 206-208 ℃; IR (KBr) 3438, 1708, 1611, 1374, 1162, 1047, 881, 756, 563 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 8.00 – 7.88 (m, 1H), 7.76 (d, *J* = 8.4 Hz, 3H), 7.57 – 7.46 (m, 1H), 7.42 (m, 1H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.25 – 7.11 (m, 4H), 6.97 (t, *J* = 8.6 Hz, 2H), 6.93 – 6.85 (m, 1H), 6.78 (dd, *J* = 8.6, 5.2 Hz, 2H), 6.65 (d, *J* = 7.8 Hz, 1H), 4.40 (d, *J* = 10.2 Hz, 1H), 3.02 (s, 3H), 2.54 (s, 3H) ppm. $^{13}$C{$^1$H} NMR (100 MHz, $CDCl_3$) δ 162.3 (d, *J* = 246.2 Hz), 158.8, 158.6, 146.1, 144.1, 137.8, 137.5, 136.9, 136.4, 134.9, 133.3 (d, *J* = 3.2 Hz), 129.97 (d, *J* = 7.2 Hz), 129.95, 127.7, 126.3, 124.8, 124.4, 124.0, 123.71, 123.67, 121.7, 119.6, 115.6 (d, *J* = 21.4 Hz), 108.9, 64.1 (q, $^2J_{C\text{-}F}$ = 26.3 Hz), 44.3, 25.7, 21.6 ppm. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -70.43, -113.64 ppm (the C of $CF_3$ is not observed). HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{26}F_4N_3O_3S_2^+$ 652.1346, found 652.1338.



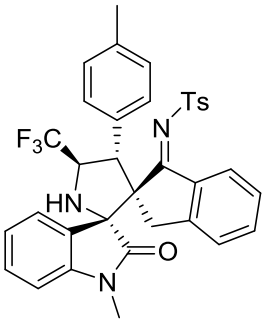
**(*E*)-4-methyl-*N*-(2-(3,3,3-trifluoro-2-((1-methyl-2-oxoindolin-3-ylidene)amino)-1-(thiophen-2-yl)propyl)benzo[*b*]thiophen-3-yl)benzenesulfonamide (5r)**

Yellow solid: 40 mg (yield 62%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.29; mp 205-207 °C; IR (KBr) 3448, 1707, 1612, 1560, 1473, 1363, 1165, 1125, 762, 564 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.83 – 7.68 (m, 3H), 7.56 – 7.49 (m, 1H), 7.45 – 7.39 (m, 1H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.25 – 7.18 (m, 3H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.02 – 6.95 (m, 1H), 6.91 – 6.84 (m, 2H), 6.65 (d, *J* = 7.8 Hz, 1H), 4.59 (d, *J* = 9.6 Hz, 1H), 3.04 (s, 3H), 2.51 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.0, 158.6, 146.2, 139.7, 138.2, 137.2, 137.0, 136.8, 135.0, 130.2, 127.3, 126.9, 126.6, 126.2, 125.3, 125.2, 124.9, 124.4, 124.0, 123.8, 123.7, 121.8, 119.7, 108.9, 65.0 (q, $^2J_{C\text{-}F}$ = 26.3 Hz), 39.6, 25.8, 21.8 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -70.54 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{31}H_{25}F_3N_3O_3S_3^+$ 640.1005, found 640.1010.



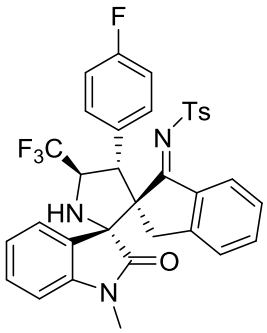
**(*E*)-4-methyl-*N*-(1''-methyl-2''-oxo-4'-phenyl-5'-(trifluoromethyl)dispiro[indene-2,3'-pyrrolidine-2',3''-indolin]-1(3*H*)-ylidene)benzenesulfonamide (6a)**

White solid: 55 mg (yield 89%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.37; mp 187-189 °C; IR (KBr) 3331, 1703, 1615, 1326, 1137, 734, 680, 560 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$ ) δ 8.10 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.33 – 7.28 (m, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 7.21 – 7.12 (m, 5H), 7.11 – 7.05 (m, 2H), 6.59 (d, *J* = 7.8 Hz, 1H), 4.82 – 4.69 (m, 1H), 4.47 (d, *J* = 11.2 Hz, 1H), 3.66 (d, *J* = 15.8 Hz, 1H), 3.04 (d, *J* = 7.8 Hz, 1H), 2.95 (d, *J* = 15.8 Hz, 1H), 2.62 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 181.0, 176.5, 150.3, 143.8, 141.5, 138.6, 134.9, 134.7, 132.4, 130.2, 129.8, 129.5, 129.33, 129.25, 128.5, 127.8, 127.2, 127.1, 125.9, 125.7, 123.1, 108.3, 100.0, 74.6, 70.8, 62.3 (q, $^2J_{C\text{-}F}$ = 29.7 Hz), 49.0, 33.4, 25.8, 21.7 ppm. (the C of $CF_3$ is not scanned). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -74.19 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{29}F_3N_3O_3S^+$ 616.1876, found 616.1880.



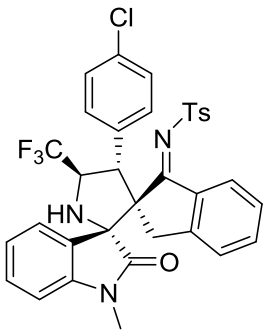

**(*E*)-4-methyl-*N*-(1''-methyl-2''-oxo-4'-(p-tolyl)-5'-(trifluoromethyl)dispiro[indene-2,3'-pyrrolidine-2',3''-indolin]-1(3*H*)-ylidene)benzenesulfonamide (6b)**

White solid: 58 mg (yield 92%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.37; mp 189-191 ℃; IR (KBr) 3330, 1706, 1616, 1324, 1157, 747, 692, 560 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.35 – 7.28 (m, 1H), 7.28 – 7.24 (m, 1H), 7.22 – 7.07 (m, 2H), 7.06 – 6.93 (m, 4H), 6.60 (d, *J* = 7.6 Hz, 1H), 4.86 – 4.61 (m, 1H), 4.44 (d, *J* = 11.0 Hz, 1H), 3.67 (d, *J* = 15.8 Hz, 1H), 3.05 (d, *J* = 8.6 Hz, 1H), 2.97 (d, *J* = 15.8 Hz, 1H), 2.60 (s, 3H), 2.54 (s, 3H), 2.27 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 180.8, 176.4, 150.5, 143.8, 141.4, 138.6, 137.5, 134.7, 132.4, 131.7, 130.0, 129.7, 129.5, 129.4, 129.3, 129.2, 127.2, 127.1, 125.9, 125.8, 123.0, 108.3, 74.5, 70.9, 62.1 (q, $^2J_{C\text{-}F}$ = 29.5 Hz), 48.6, 33.1, 25.8, 21.7, 21.0 ppm. (the C of $CF_3$ is not scanned). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -74.12 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{35}H_{31}F_3N_3O_3S^+$ 630.2033, found 630.2035.



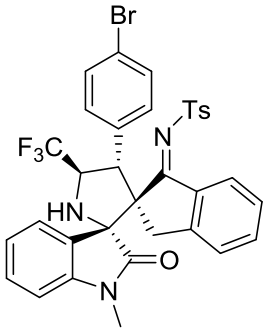

**(*E*)-*N*-(4'-(4-fluorophenyl)-1''-methyl-2''-oxo-5'-(trifluoromethyl)dispiro[indene-2,3'-pyrrolidine-2',3''-indolin]-1(3*H*)-ylidene)-4-methylbenzenesulfonamide (6c)**

White solid: 53 mg (yield 83%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.37; mp 184-186 ℃; IR (KBr) 3331, 1702, 1615, 1325, 1135, 756, 692, 541 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.8 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.33 – 7.27 (m, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.21 – 7.11 (m, 2H), 7.11 – 7.04 (m, 2H), 6.89 (t, *J* = 8.6 Hz, 2H), 6.59 (d, *J* = 7.6 Hz, 1H), 4.81 – 4.62 (m, 1H), 4.45 (d, *J* = 10.8 Hz, 1H), 3.60 (d, *J* = 15.8 Hz, 1H), 3.01 (d, *J* = 8.4 Hz, 1H), 2.88 (d, *J* = 15.8 Hz, 1H), 2.65 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 181.3, 176.5, 162.1 (d, *J* = 245.9 Hz), 150.1, 143.9, 141.5, 138.5, 134.8, 132.3, 131.8, 131.7 (d, *J* = 7.9 Hz), 130.9, 129.8, 129.6, 129.5, 129.4, 129.0, 127.3, 127.1, 125.8, 125.7, 123.1, 115.5 (d, *J* = 21.1 Hz), 108.3, 74.5, 70.5, 62.5 (q, $^2J_{C\text{-}F}$ = 29.4 Hz), 48.5, 33.6, 25.8, 21.7 ppm. $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -74.20, -114.23 ppm. (the C of $CF_3$ is not scanned). HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{28}F_4N_3O_3S^+$ 634.1782, found 634.1783.



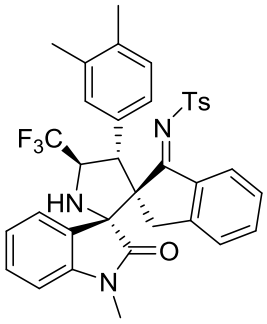

**(*E*)-*N*-(4'-(4-chlorophenyl)-1''-methyl-2''-oxo-5'-(trifluoromethyl)dispiro[indene-2,3'-pyrrolidine-2',3''-indolin]-1(3*H*)-ylidene)-4-methylbenzenesulfonamide (6d)**

White solid: 51 mg (yield 81%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.37; mp 194-196 ℃; IR (KBr) 3330, 1704, 1615, 1327, 1138, 748, 680, 560 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.51 – 7.44 (m, 3H), 7.44 – 7.37 (m, 1H), 7.33 – 7.27 (m, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.21 – 7.11 (m, 4H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.59 (d, *J* = 7.8 Hz, 1H), 4.80 – 4.52 (m, 1H), 4.43 (d, *J* = 10.8 Hz, 1H), 3.59 (d, *J* = 15.6 Hz, 1H), 3.00 (d, *J* = 8.4 Hz, 1H), 2.86 (d, *J* = 16.0 Hz, 1H), 2.65 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 181.2, 176.5, 150.1, 143.9, 141.5, 138.5, 134.8, 133.7, 133.7, 132.3, 131.5, 129.9, 129.6, 129.5, 128.9, 128.7, 127.4, 127.1, 125.8, 125.7, 123.1, 108.3, 74.5, 70.4, 62.4 (q, $^2J_{C\text{-}F}$ = 29.6 Hz), 48.6, 33.6, 25.8, 21.8 ppm. (the C of $CF_3$ is not scanned). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -74.21 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{28}ClF_4N_3O_3S^+$ 650.1487, found 650.1498.



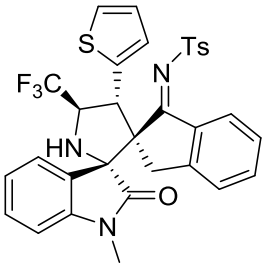

**(*E*)-*N*-(4'-(4-bromophenyl)-1''-methyl-2''-oxo-5'-(trifluoromethyl)dispiro[indene-2,3'-pyrrolidine-2',3''-indolin]-1(3*H*)-ylidene)-4-methylbenzenesulfonamide (6e)**

White solid: 52 mg (yield 82%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.37; mp 192-194 ℃; IR (KBr) 3331, 1706, 1616, 1321, 1138, 747, 692, 541 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.52 – 7.44 (m, 3H), 7.43 – 7.38 (m, 1H), 7.35 – 7.30 (m, 2H), 7.28 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.20 – 7.10 (m, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 6.59 (d, *J* = 7.6 Hz, 1H), 4.81 – 4.59 (m, 1H), 4.42 (d, *J* = 10.8 Hz, 1H), 3.59 (d, *J* = 15.8 Hz, 1H), 3.00 (d, *J* = 8.4 Hz, 1H), 2.86 (d, *J* = 15.8 Hz, 1H), 2.65 (s, 3H), 2.54 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 181.2, 176.5, 150.1, 143.9, 141.5, 138.5, 134.8, 134.2, 132.3, 131.8, 131.7, 129.9, 129.6, 129.5, 128.9, 127.4, 127.1, 125.8, 125.7, 123.1, 121.9, 108.3, 74.5, 70.4, 62.0 (q, $^2J_{C\text{-}F}$ = 30.1 Hz), 48.7, 33.6, 25.8, 21.8 ppm. (the C of $CF_3$ is not scanned). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -74.20 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{34}H_{28}BrF_4N_3O_3S^+$ 694.0981, found 694.0983.



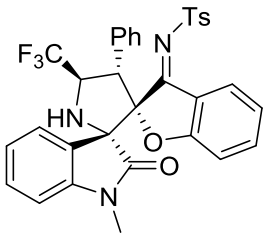

**(*E*)-*N*-(4'-(3,4-dimethylphenyl)-1''-methyl-2''-oxo-5'-(trifluoromethyl)dispiro[indene-2,3'-pyrrolidine-2',3''-indolin]-1(3*H*)-ylidene)-4-methylbenzenesulfonamide (6f)**

White solid: 57 mg (yield 90%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.37; mp 176-178 ℃; IR (KBr) 3337, 1707, 1615, 1321, 1155, 752, 679, 559 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 7.4 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.32 (m, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.21 – 7.11 (m, 2H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.86 (d, *J* = 7.8 Hz, 1H), 6.80 (s, 1H), 6.61 (d, *J* = 7.8 Hz, 1H), 4.81 – 4.63 (m, 1H), 4.43 (d, *J* = 11.2 Hz, 1H), 3.71 (d, *J* = 15.6 Hz, 1H), 3.05 (d, *J* = 8.3 Hz, 1H), 3.00 (d, *J* = 15.6 Hz, 1H), 2.58 (s, 3H), 2.54 (s, 3H), 2.16 (s, 3H), 2.08 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 176.4, 150.6, 143.7, 141.3, 138.7, 136.6, 136.1, 134.6, 132.4, 131.9, 131.6, 129.7, 129.6, 129.5, 129.3, 127.2, 127.1, 125.9, 123.0, 108.4, 74.6, 71.0, 62.1 (q, $^2J_{C\text{-}F}$ = 30.5 Hz), 48.4, 33.0, 25.8, 21.7, 19.8, 19.3 ppm. (the C of $CF_3$ is not scanned). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -74.07 ppm. HRMS (ESI-TOF) *m/z* $[M + Na]^+$ calcd for $C_{36}H_{32}F_3N_3O_3SNa^+$ 666.2009, found 666.2013.




**(*E*)-4-methyl-*N*-(1''-methyl-2''-oxo-4'-(thiophen-2-yl)-5'-(trifluoromethyl)dispiro[indene-2,3'-pyrrolidine-2',3''-indolin]-1(3*H*)-ylidene)benzenesulfonamide (6g)**

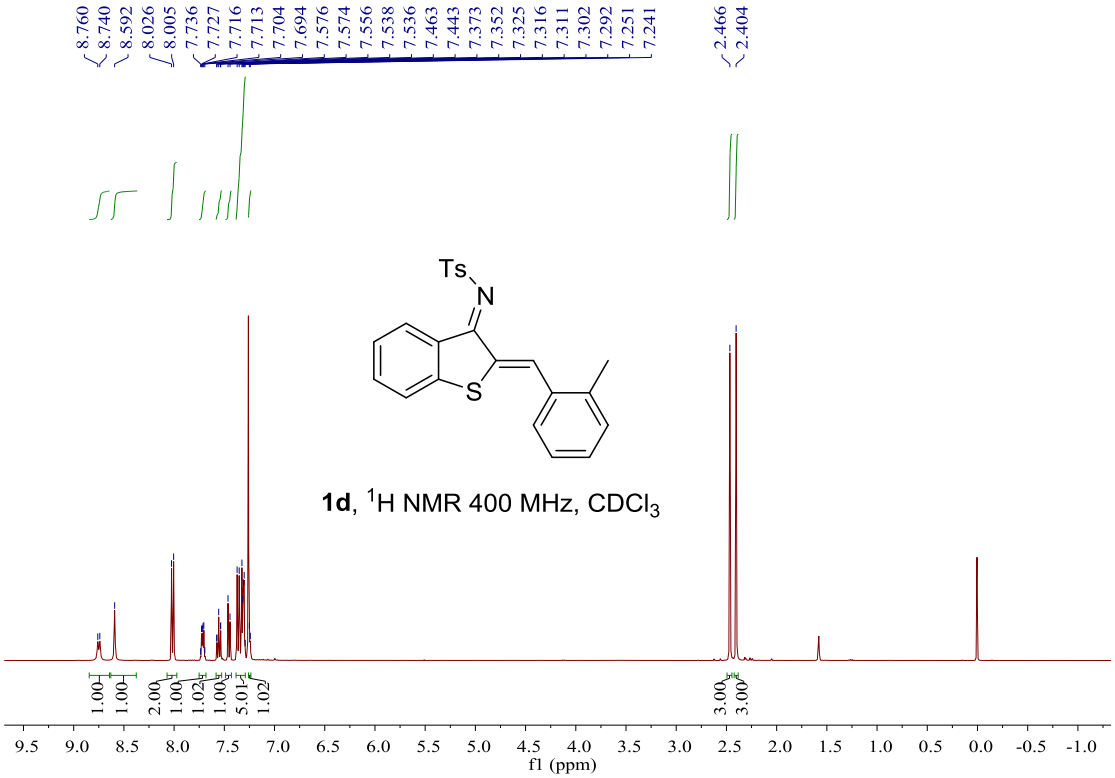
White solid: 49 mg (yield 79%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.37; mp 203-205 ℃; IR (KBr) 3325, 1704, 1615, 1326, 1156, 771, 694, 560 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 7.4 Hz, 4H), 7.36 – 7.28 (m, 2H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.19 – 7.15 (m, 1H), 7.09 – 7.02 (m, 1H), 6.93 – 6.86 (m, 1H), 6.83 (d, *J* = 3.6 Hz, 1H), 6.64 (d, *J* = 7.8 Hz, 1H), 4.73 (d, *J* = 10.8 Hz, 1H), 4.67 – 4.55 (m, 1H), 3.73 (d, *J* = 16.0 Hz, 1H), 3.14 (d, *J* = 9.0 Hz, 1H), 2.98 (d, *J* = 16.0 Hz, 1H), 2.59 (s, 3H), 2.51 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 180.2, 175.8, 150.7, 143.7, 141.3, 138.4, 137.6, 134.9, 132.4, 129.7, 129.5, 129.4, 129.3, 127.4, 127.3, 127.2, 126.7, 126.1, 125.9, 123.0, 108.5, 74.1, 70.7, 63.0 (q, $^2J_{C\text{-}F}$ = 29.7 Hz), 44.6, 32.6, 25.9, 21.7 ppm. (the C of $CF_3$ is not scanned). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -73.81 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{32}H_{27}F_3N_3O_3S_2^+$ 622.1440, found 622.1443.

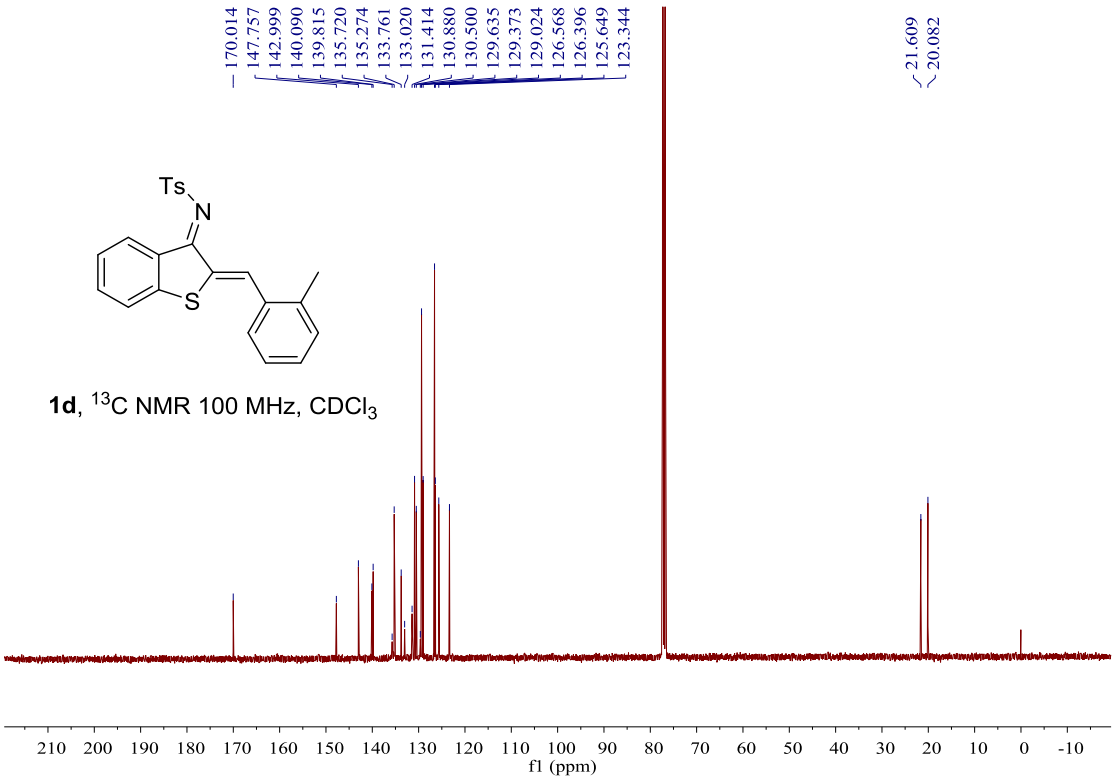


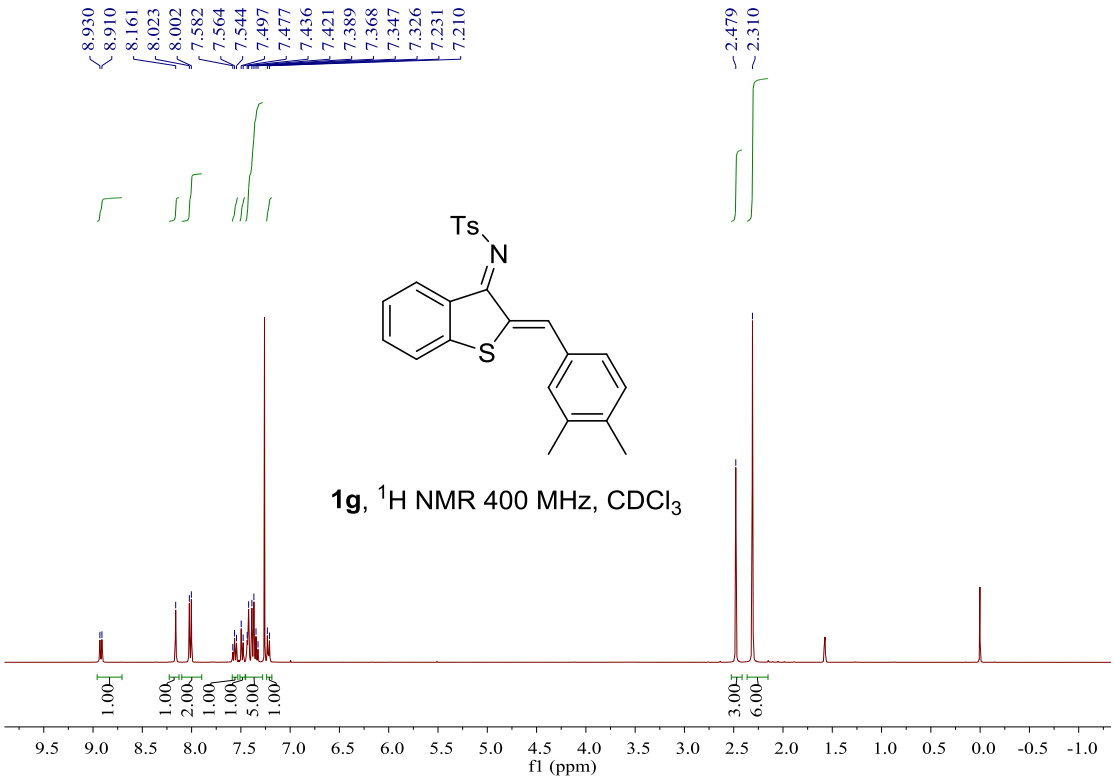

**(*E*)-4-methyl-*N*-(1''-methyl-2''-oxo-4'-phenyl-5'-(trifluoromethyl)-3*H*-dispiro[benzofuran-2,3'-pyrrolidine-2',3''-indolin]-3-ylidene)benzenesulfonamide (6h)**

White solid: 32 mg (yield 52%); $R_f$ (ethyl acetate : petroleum ether = 1:5) = 0.5; mp 198-200 °C; IR (KBr) 1709, 1616, 1462, 1370, 1089, 701, 662, 556 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.54 – 7.45 (m, 1H), 7.39 (d, *J* = 7.8 Hz, 3H), 7.25 – 7.15 (m, 6H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.95 (t, *J* = 7.6 Hz, 1H), 6.79 (t, *J* = 7.4 Hz, 1H), 6.71 (d, *J* = 7.8 Hz, 1H), 5.05 – 4.84 (m, 1H), 4.22 (d, *J* = 10.8 Hz, 1H), 3.33 (d, *J* = 9.2 Hz, 1H), 2.90 (s, 3H), 2.53 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 174.0, 173.1, 168.1, 143.7, 142.4, 138.8, 137.9, 130.9, 130.1, 129.8, 129.5, 129.3, 128.5, 128.4, 127.3, 127.1, 126.4, 122.8, 122.6, 117.8, 112.6, 108.3, 99.4, 74.7, 62.3 (q, $^2J_{C\text{-}F}$ = 30.0 Hz), 53.7, 26.7, 21.7 ppm (the C of $CF_3$ is not observed). $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -73.11 ppm. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{33}H_{27}F_3N_3O_4S^+$ 618.1669, found 618.1673.

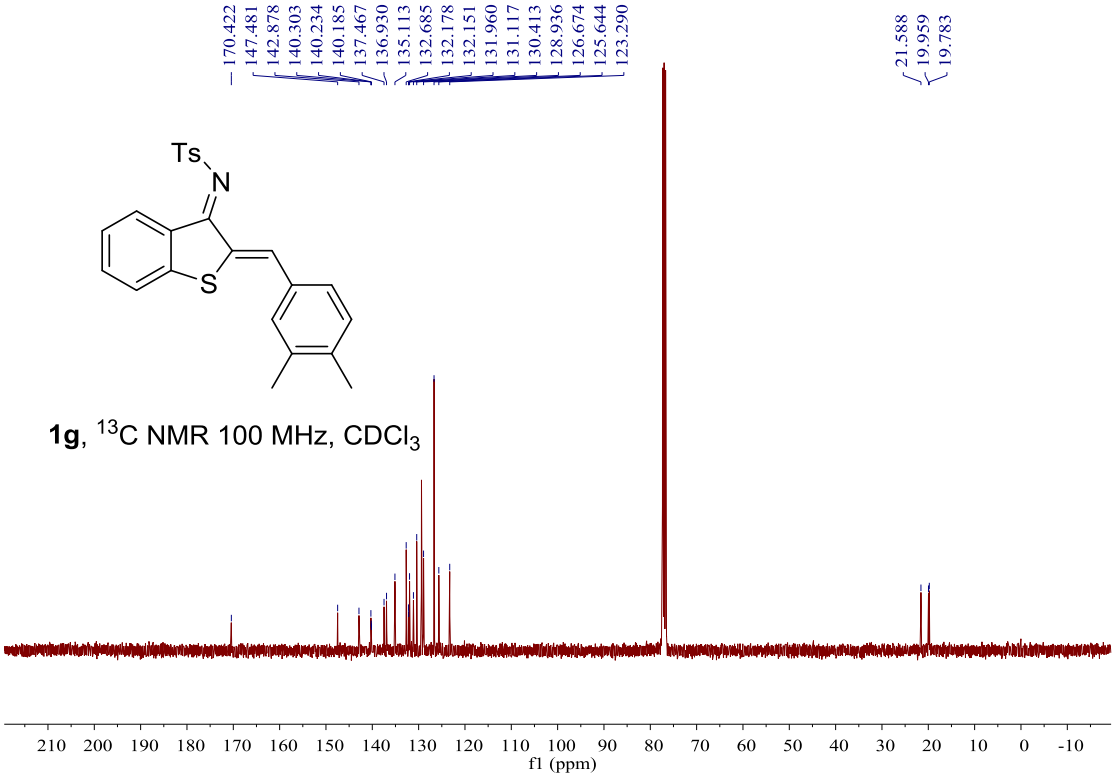
## 8. NMR spectra of all new compounds



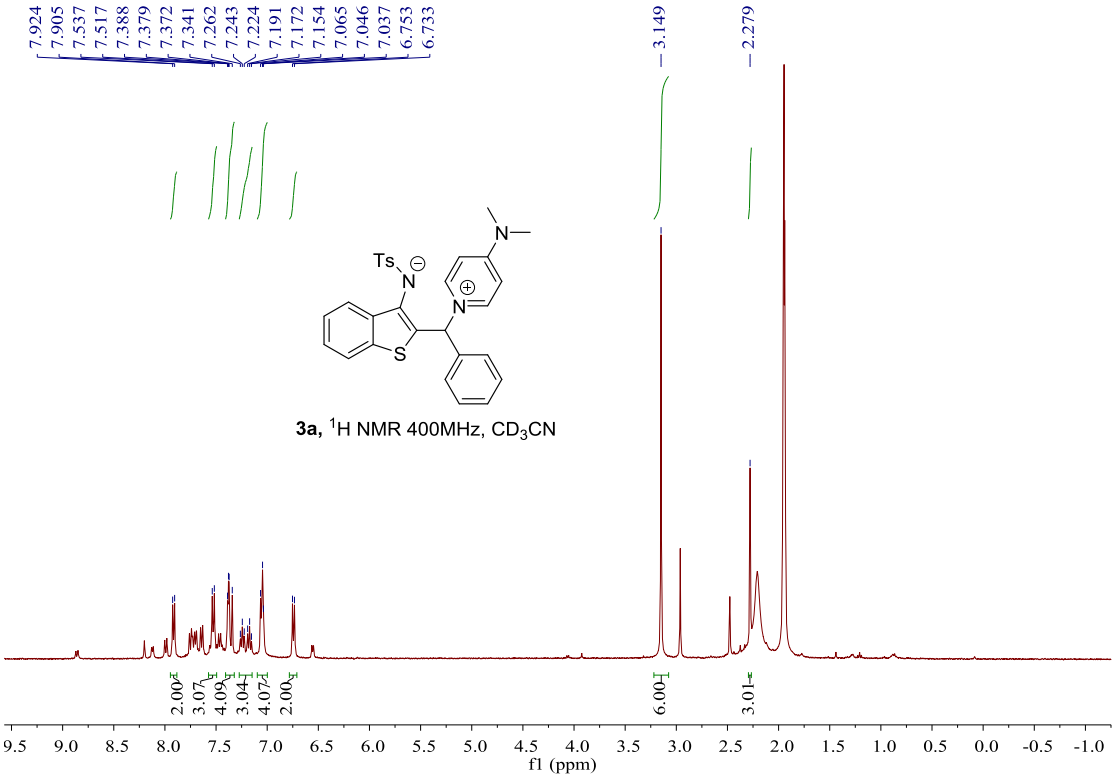





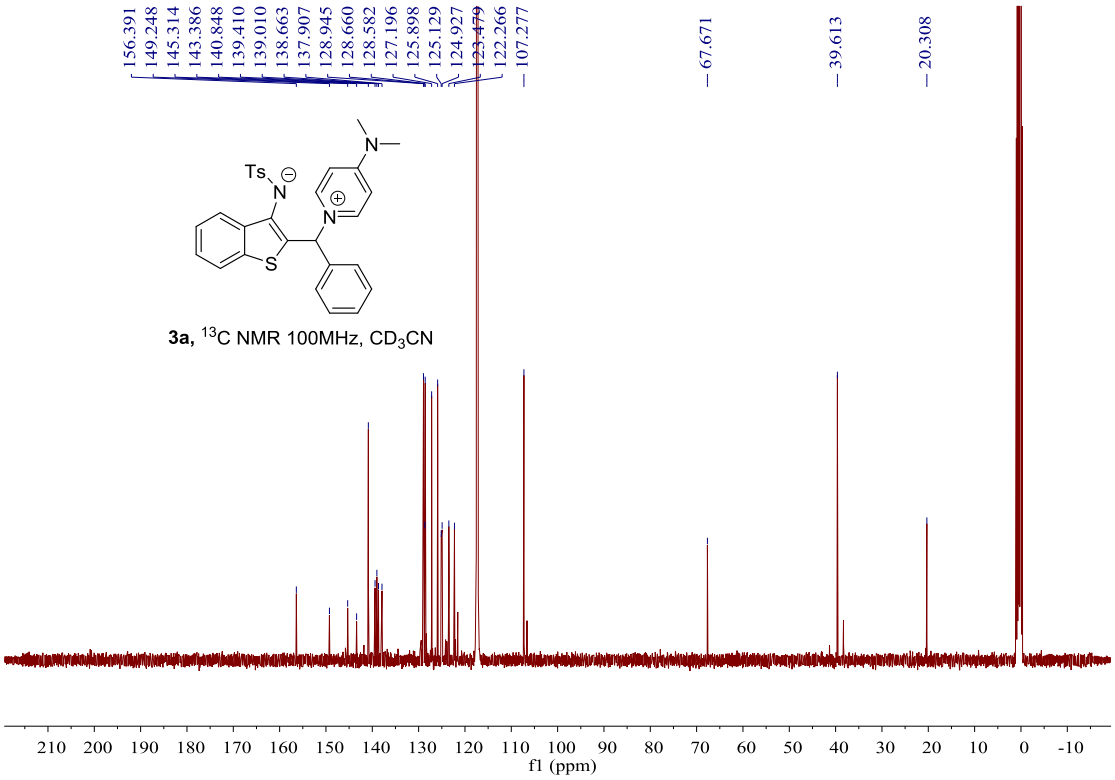

**1g**, $^{1}$H NMR 400 MHz, $CDCl_3$



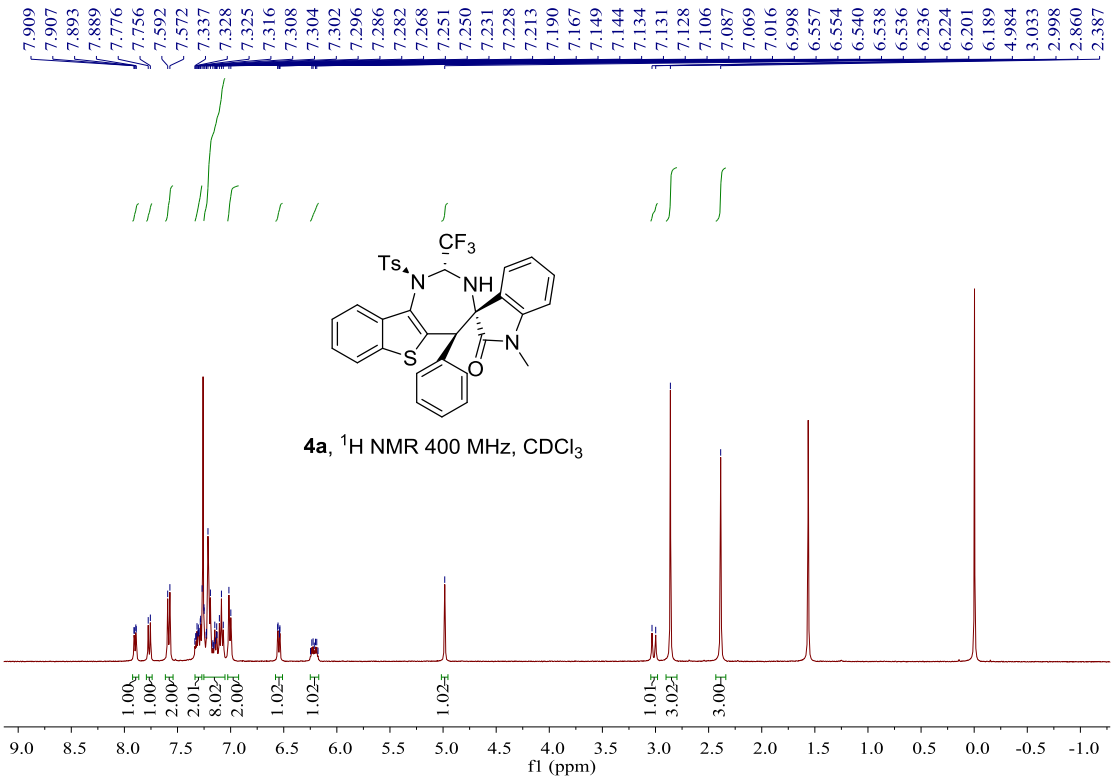

**1g**, $^{13}$C NMR 100 MHz, $CDCl_3$



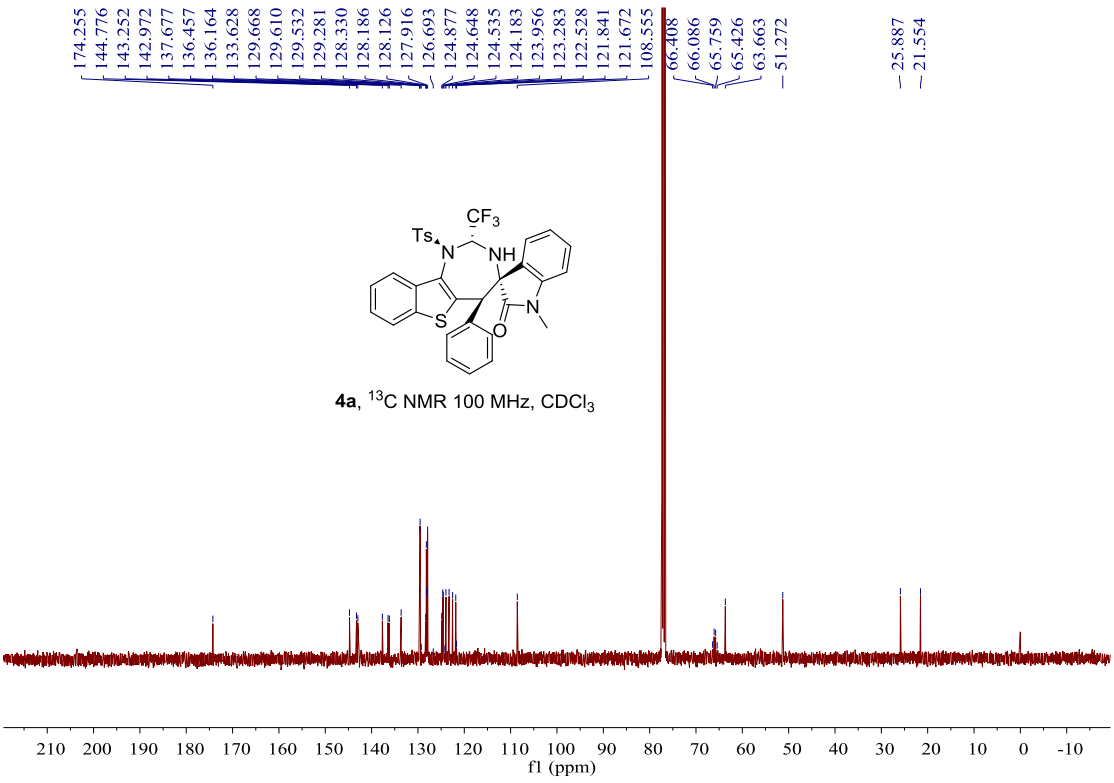

**3a,** $^{1}$H NMR 400MHz, $CD_3CN$



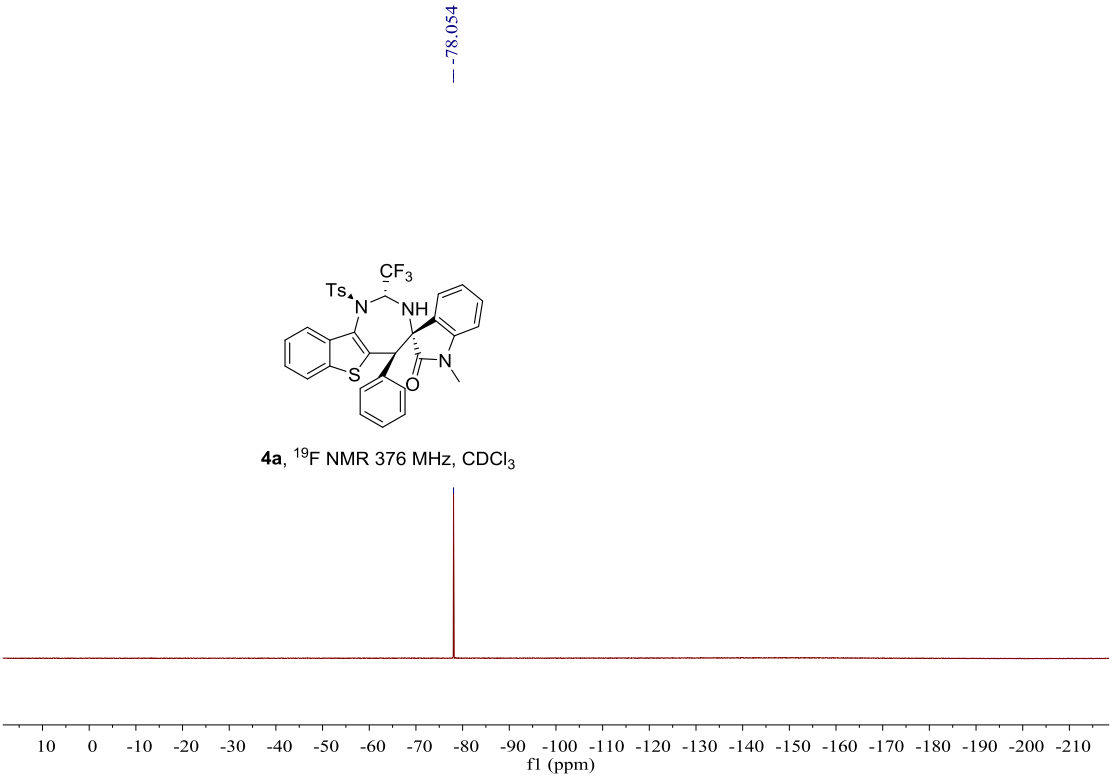

**3a,** $^{13}$C NMR 100MHz, $CD_3CN$



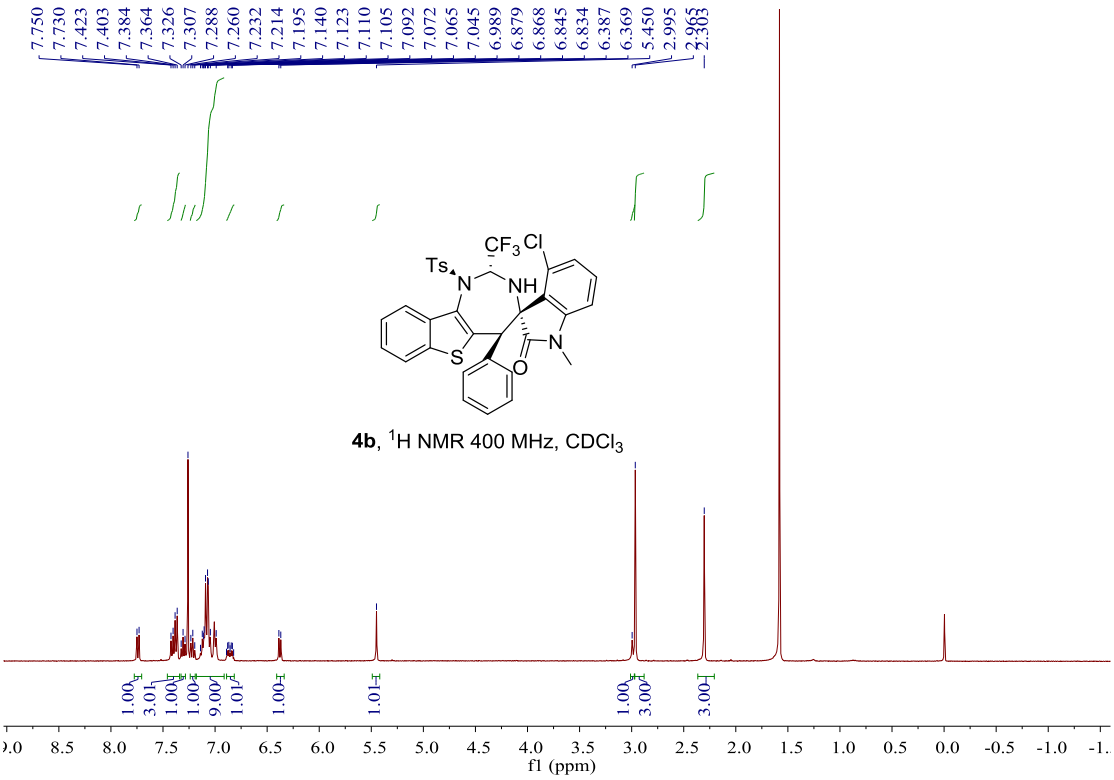

**4a**, $^{1}$H NMR 400 MHz, $CDCl_3$



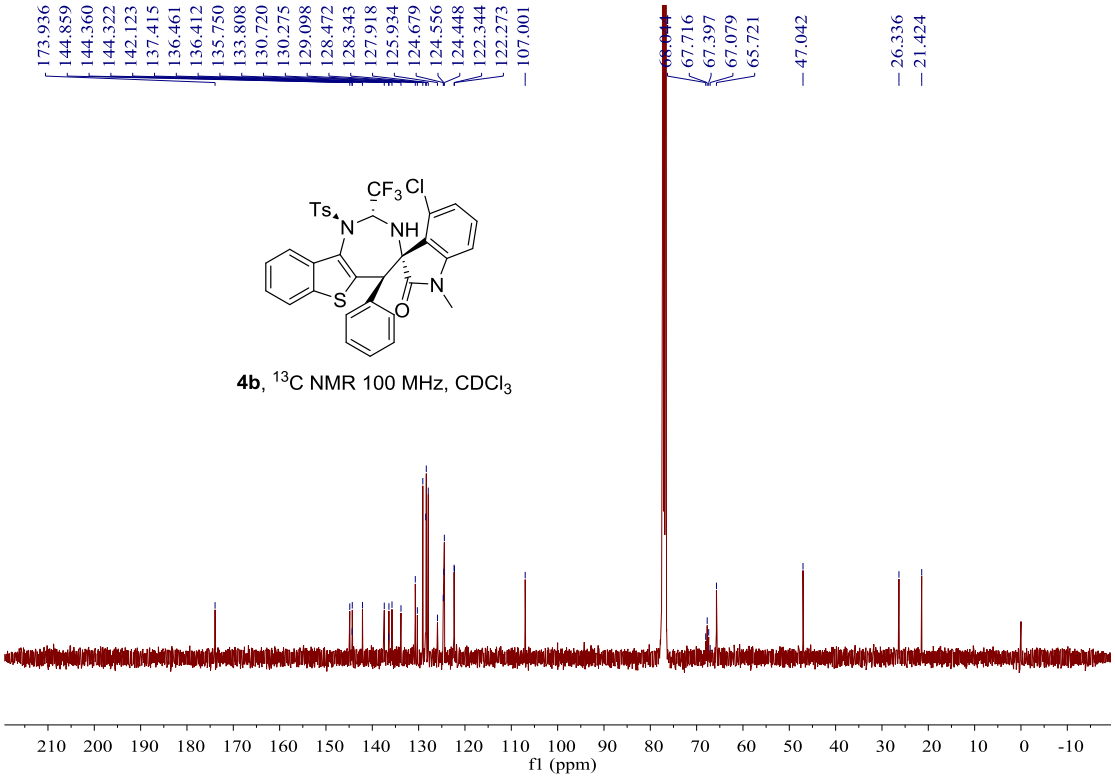

**4a**, $^{13}$C NMR 100 MHz, $CDCl_3$



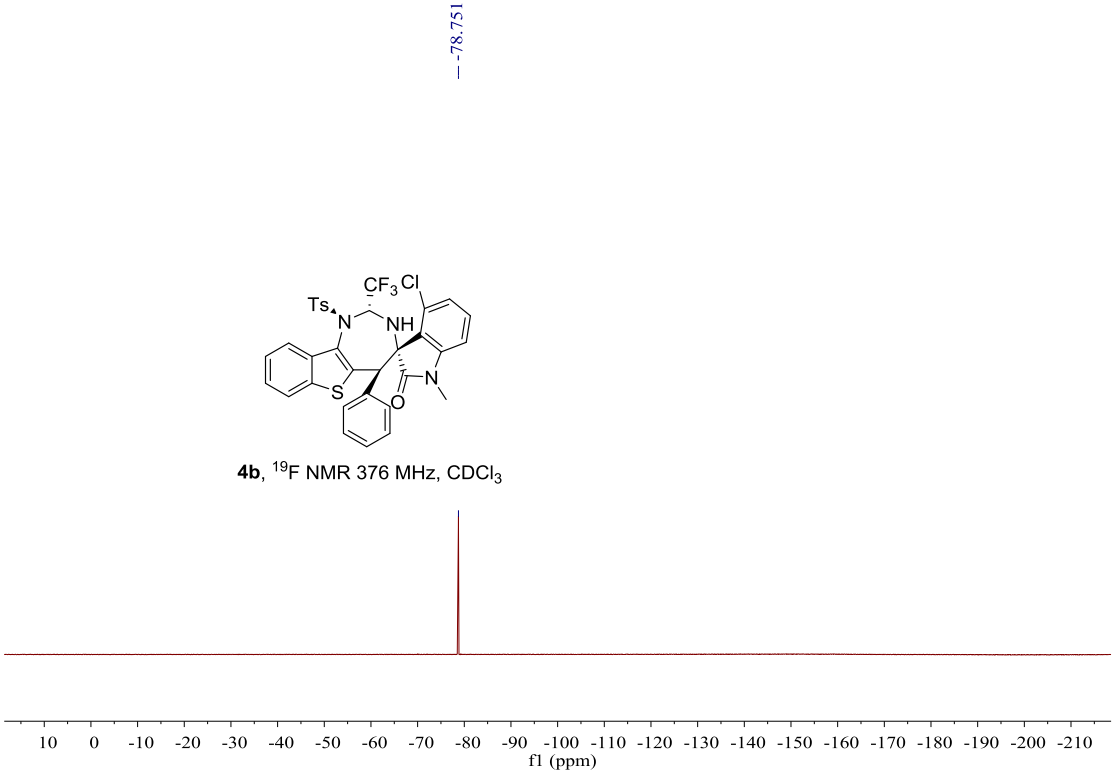

**4a**, $^{19}F$ NMR 376 MHz, $CDCl_3$



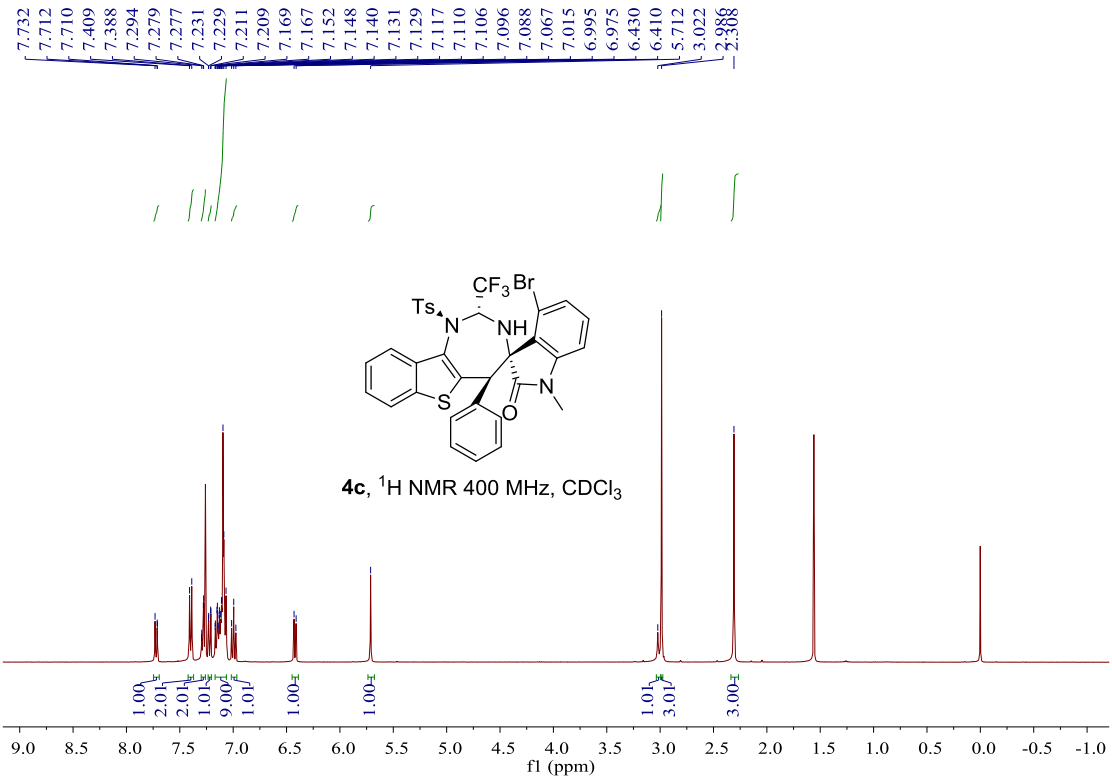

**4b**, $^{1}H$ NMR 400 MHz, $CDCl_3$



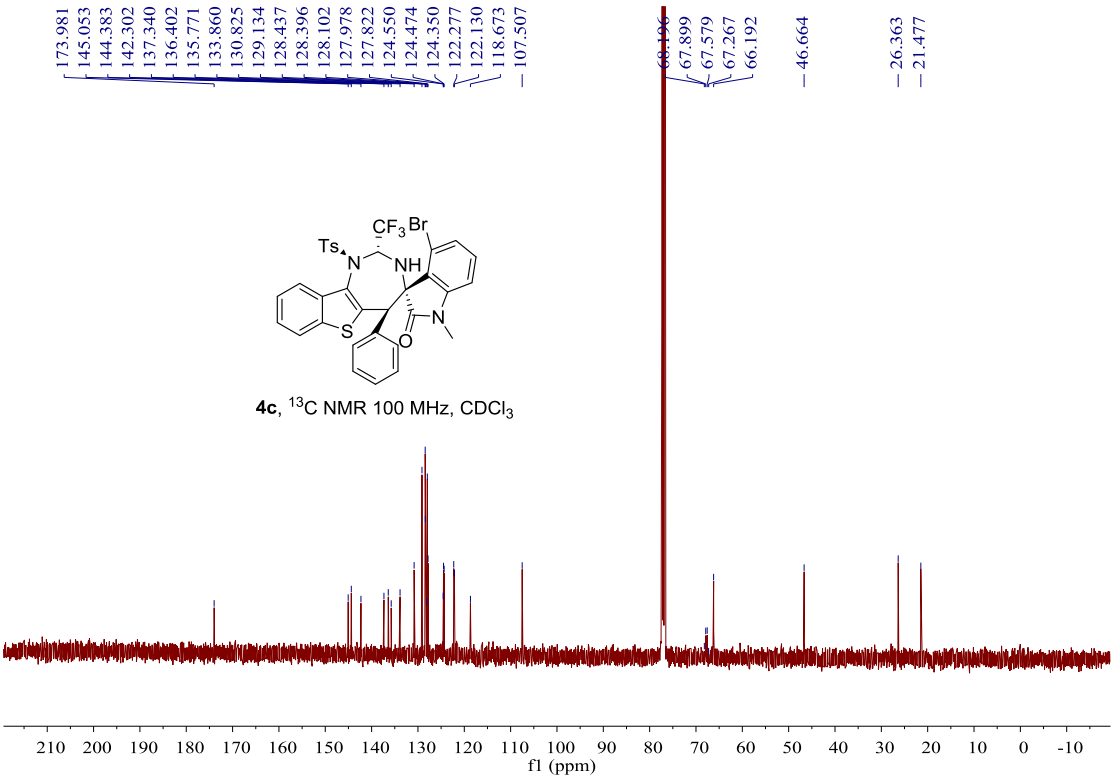

**4b**, $^{13}C$ NMR 100 MHz, $CDCl_3$



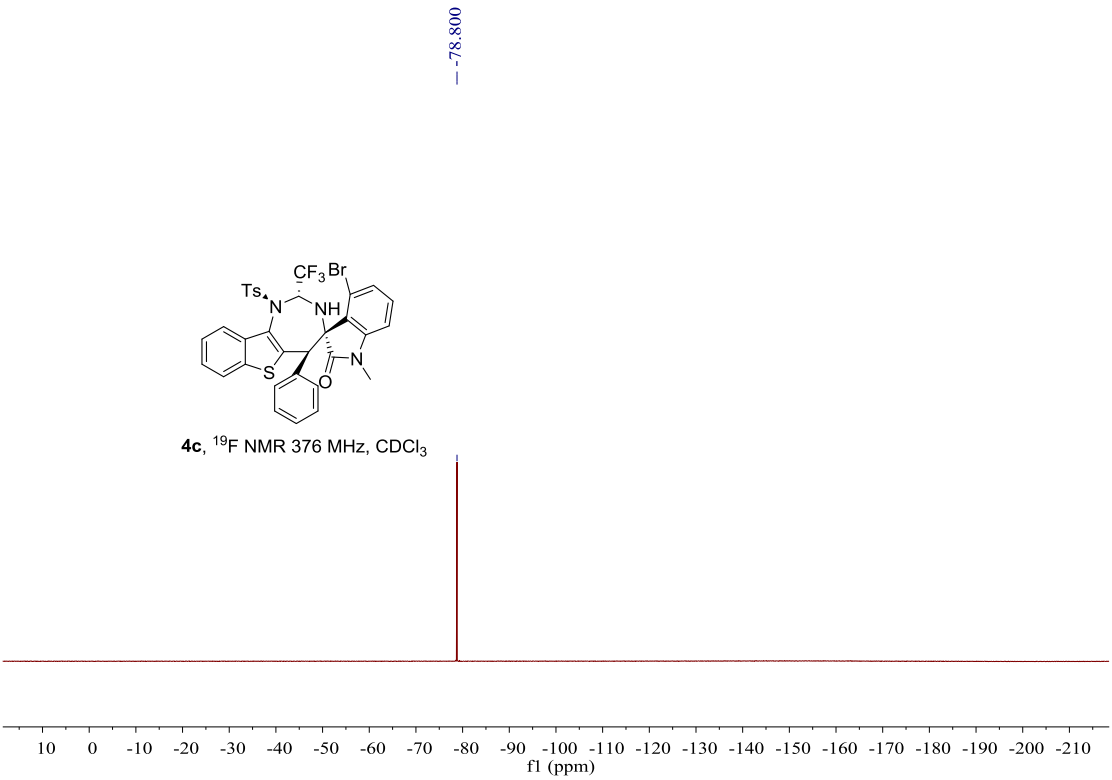

**4b**, $^{19}F$ NMR 376 MHz, $CDCl_3$



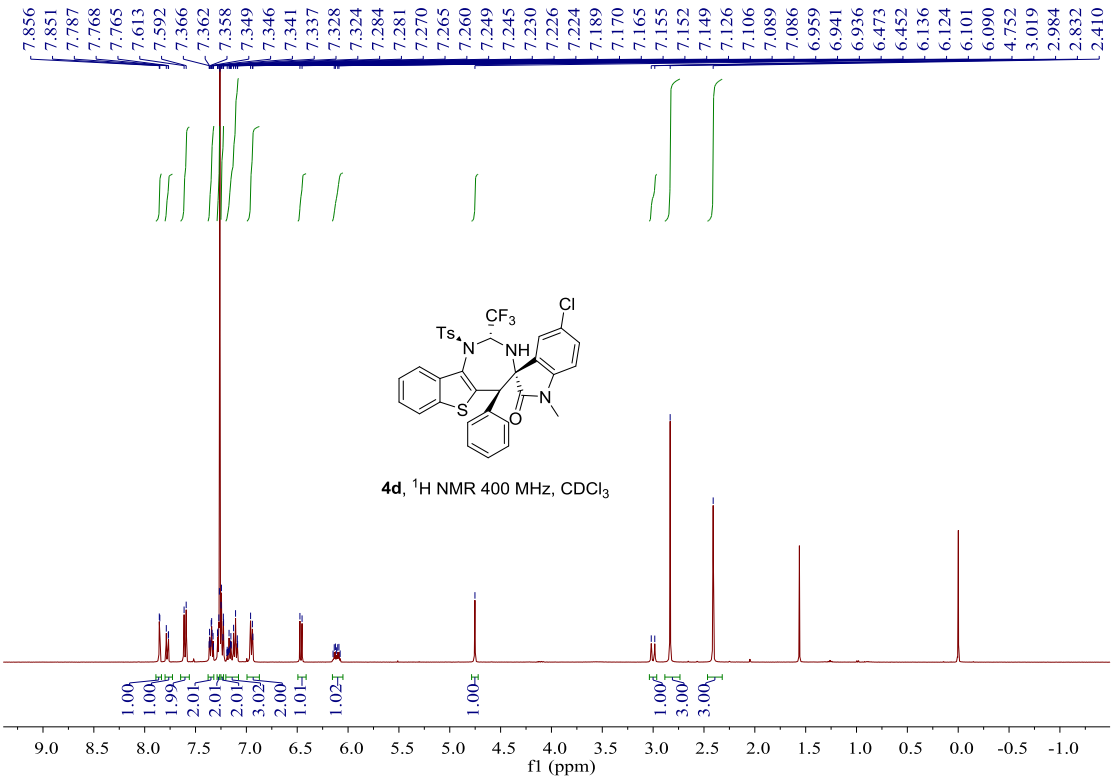

**4c**, $^{1}$H NMR 400 MHz, $CDCl_3$



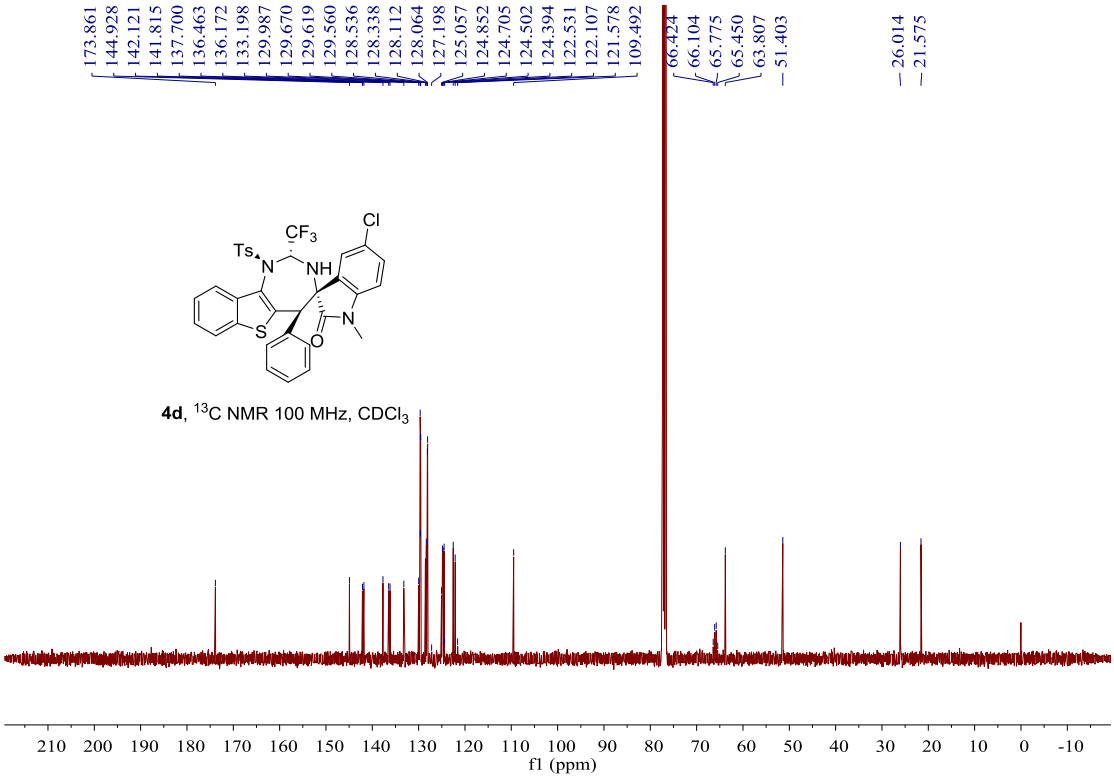

**4c**, $^{13}$C NMR 100 MHz, $CDCl_3$



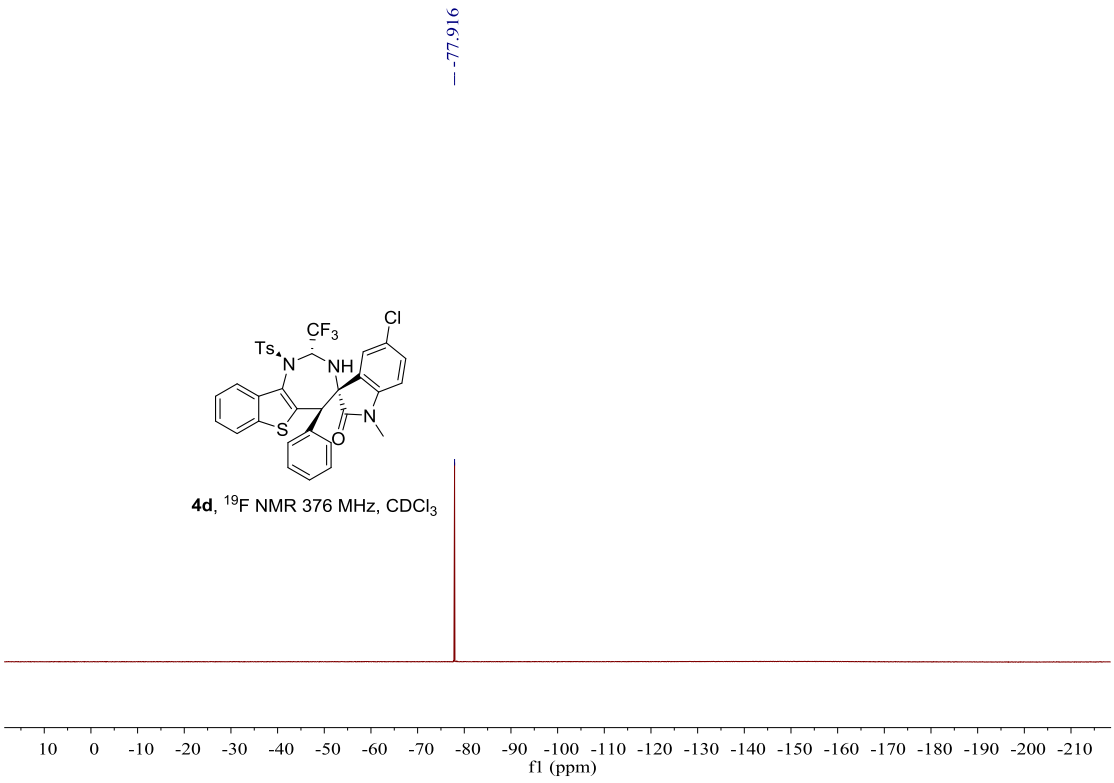

**4c**, $^{19}F$ NMR 376 MHz, $CDCl_3$



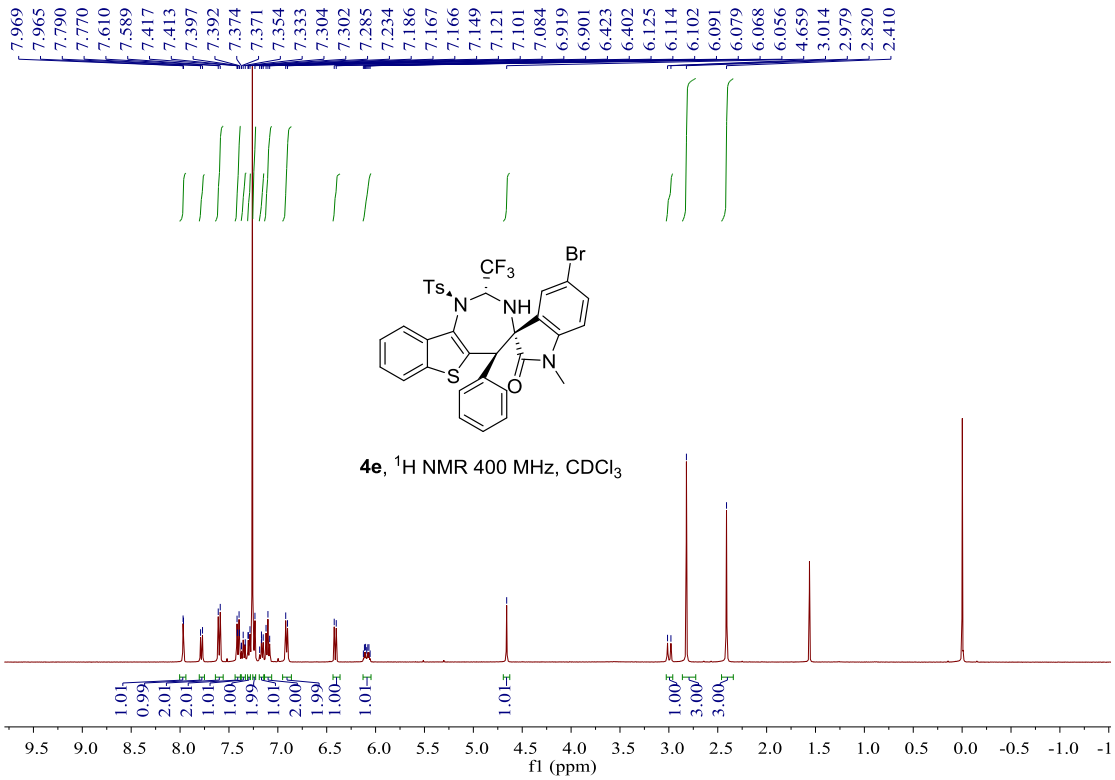

**4d**, $^{1}H$ NMR 400 MHz, $CDCl_3$



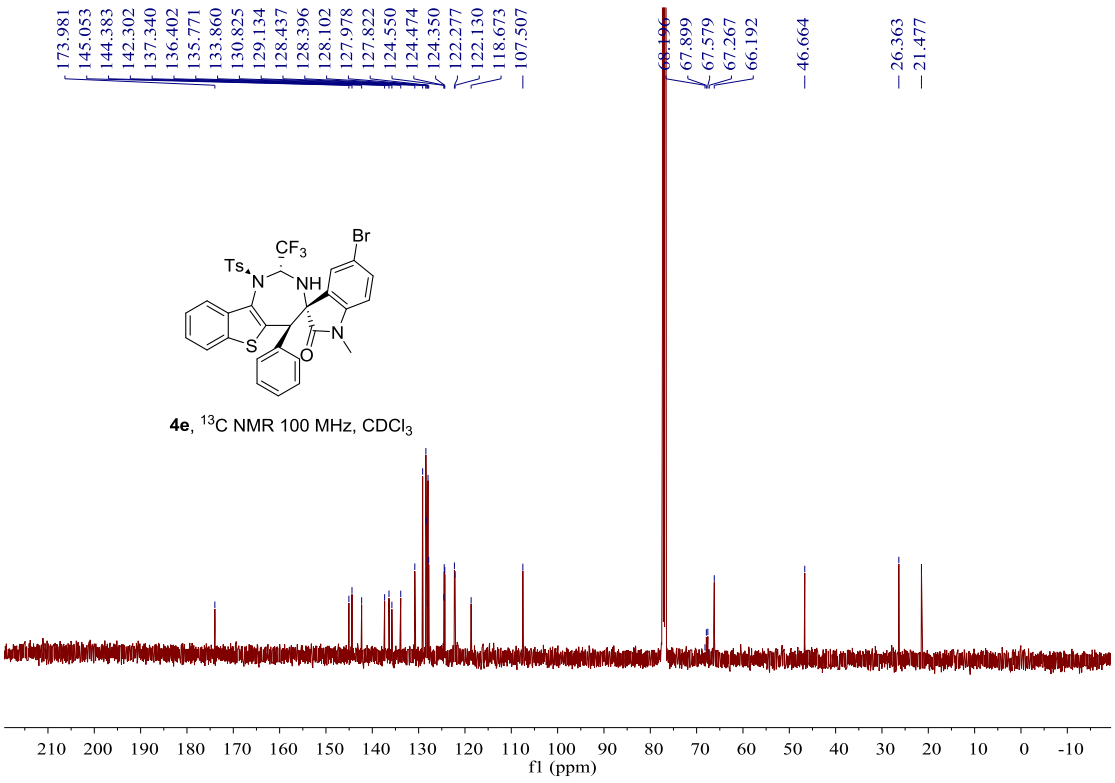

**4d**, $^{13}$C NMR 100 MHz, $CDCl_3$



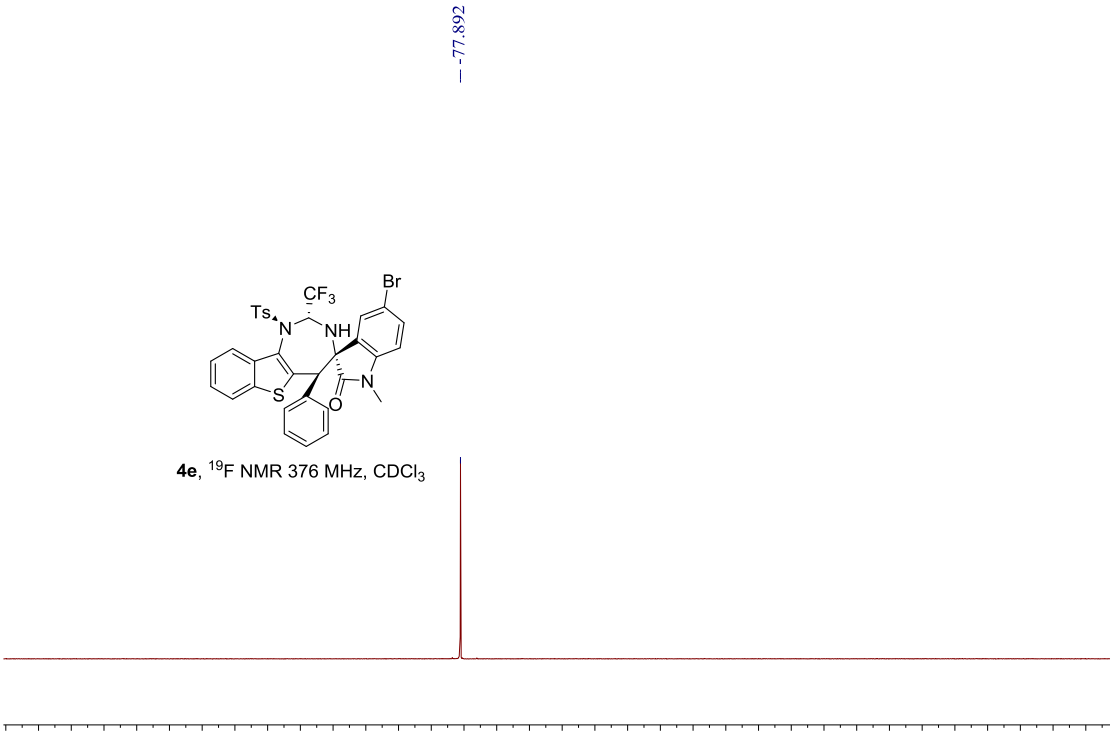

**4d**, $^{19}$F NMR 376 MHz, $CDCl_3$



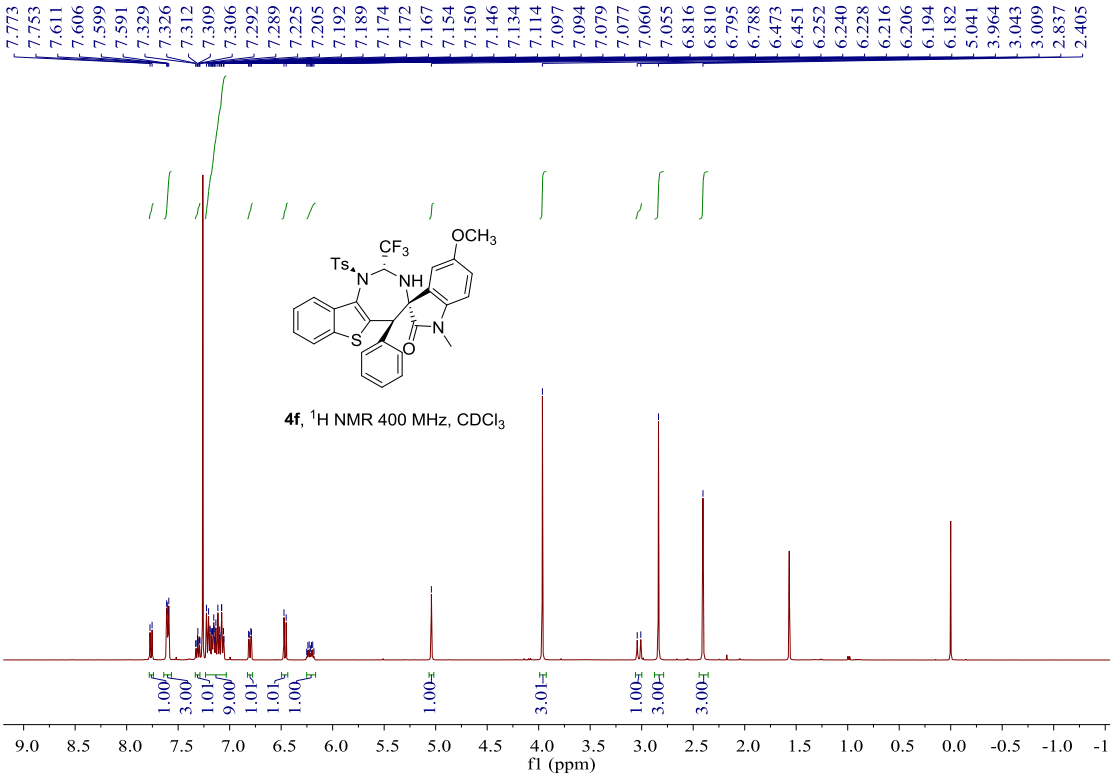

**4e**, $^{1}$H NMR 400 MHz, $CDCl_3$



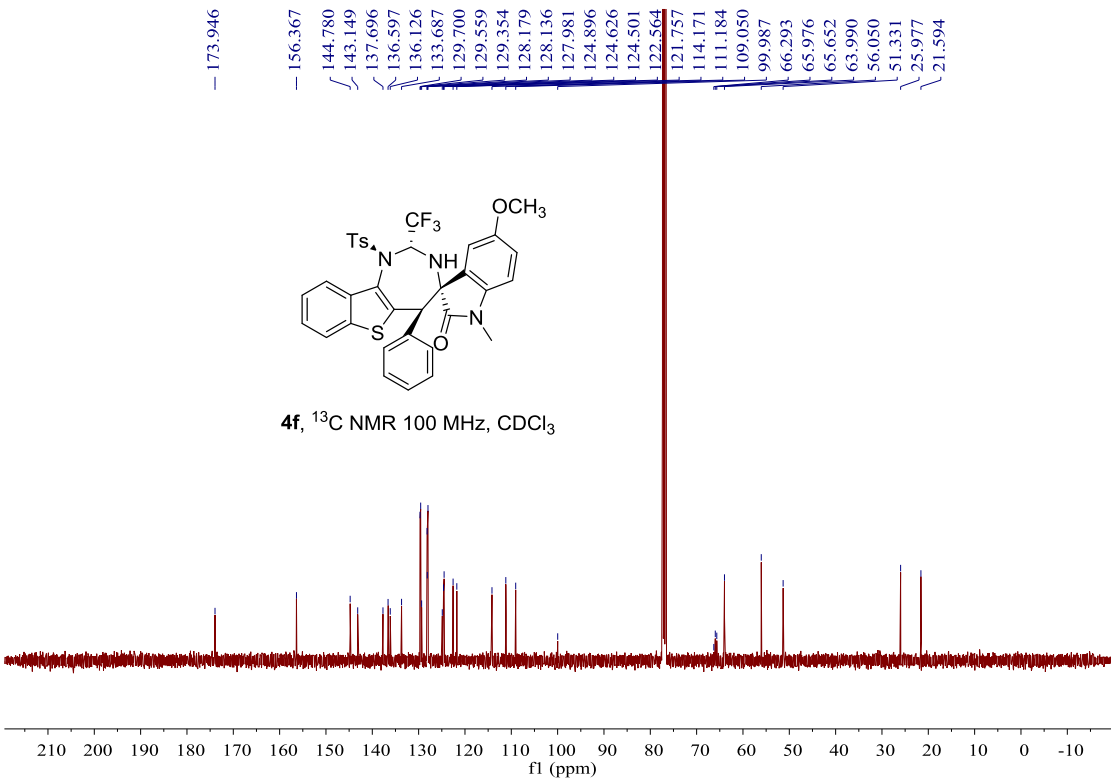

**4e**, $^{13}$C NMR 100 MHz, $CDCl_3$



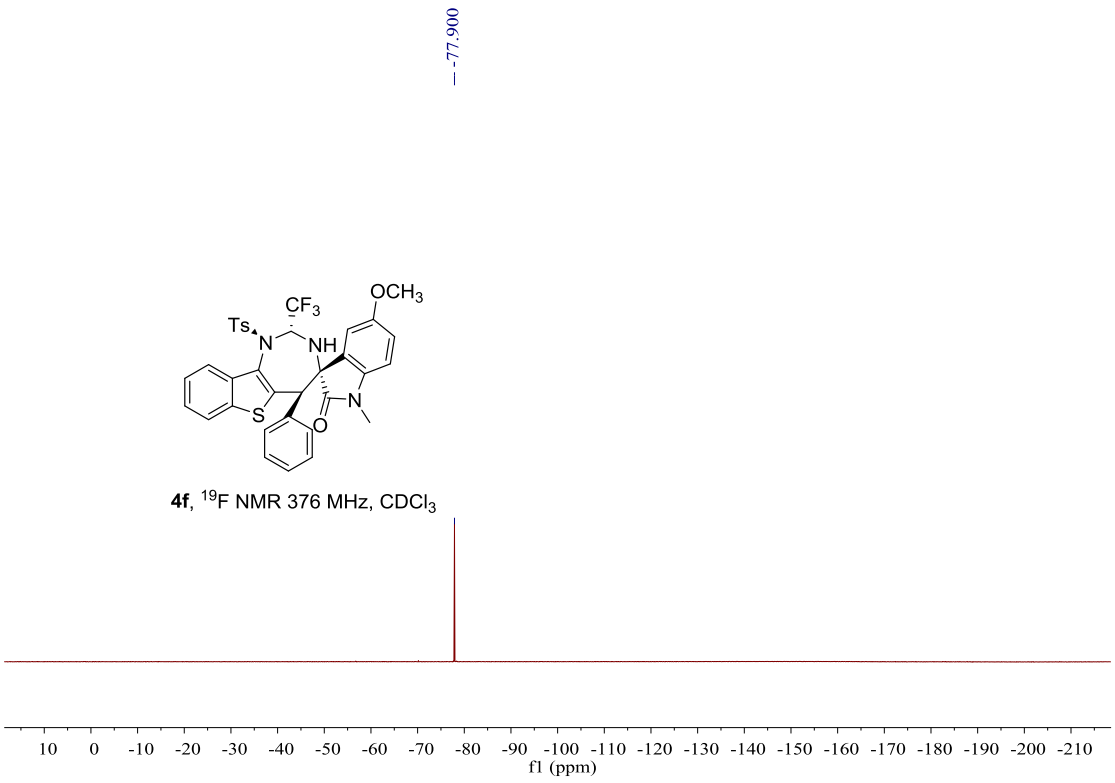

**4e**, $^{19}F$ NMR 376 MHz, $CDCl_3$



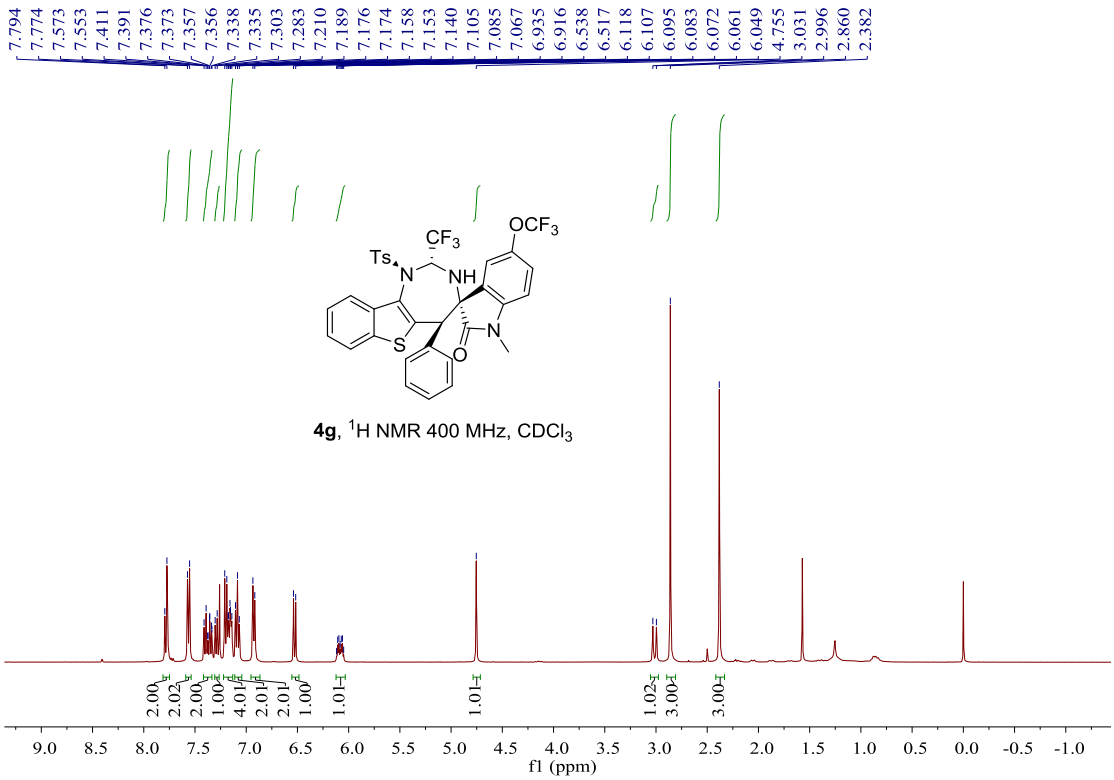

**4f**, $^{1}H$ NMR 400 MHz, $CDCl_3$



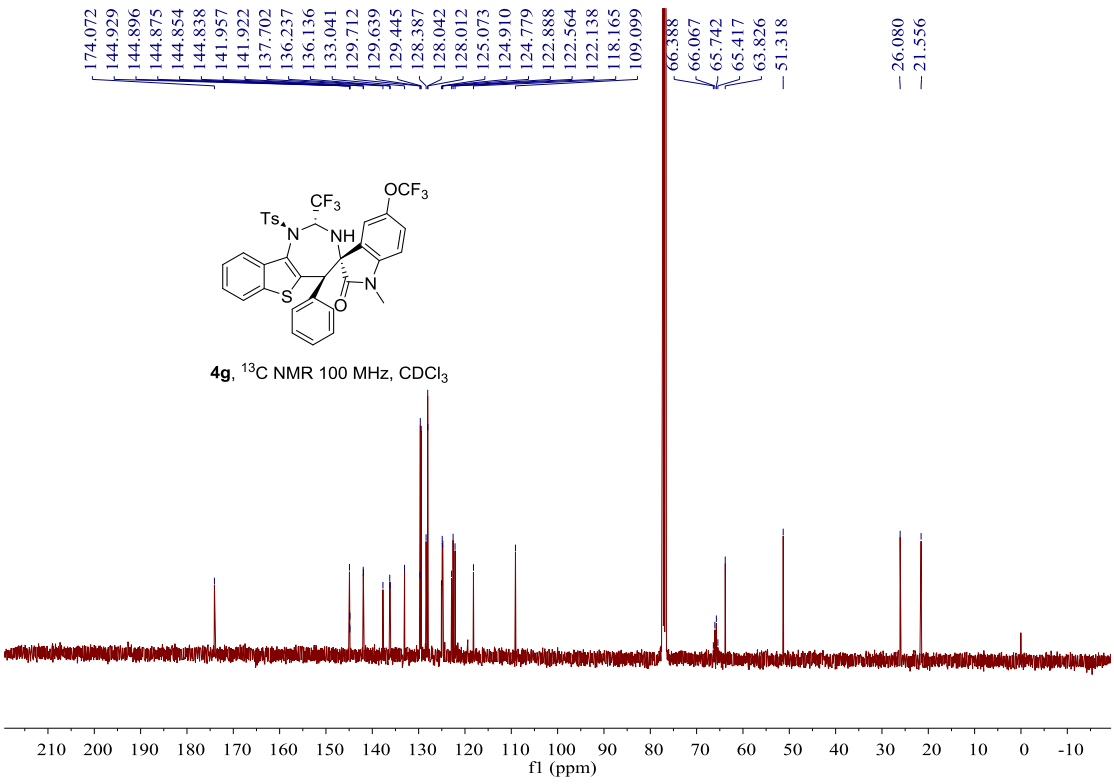

**4f**, $^{13}C$ NMR 100 MHz, $CDCl_3$



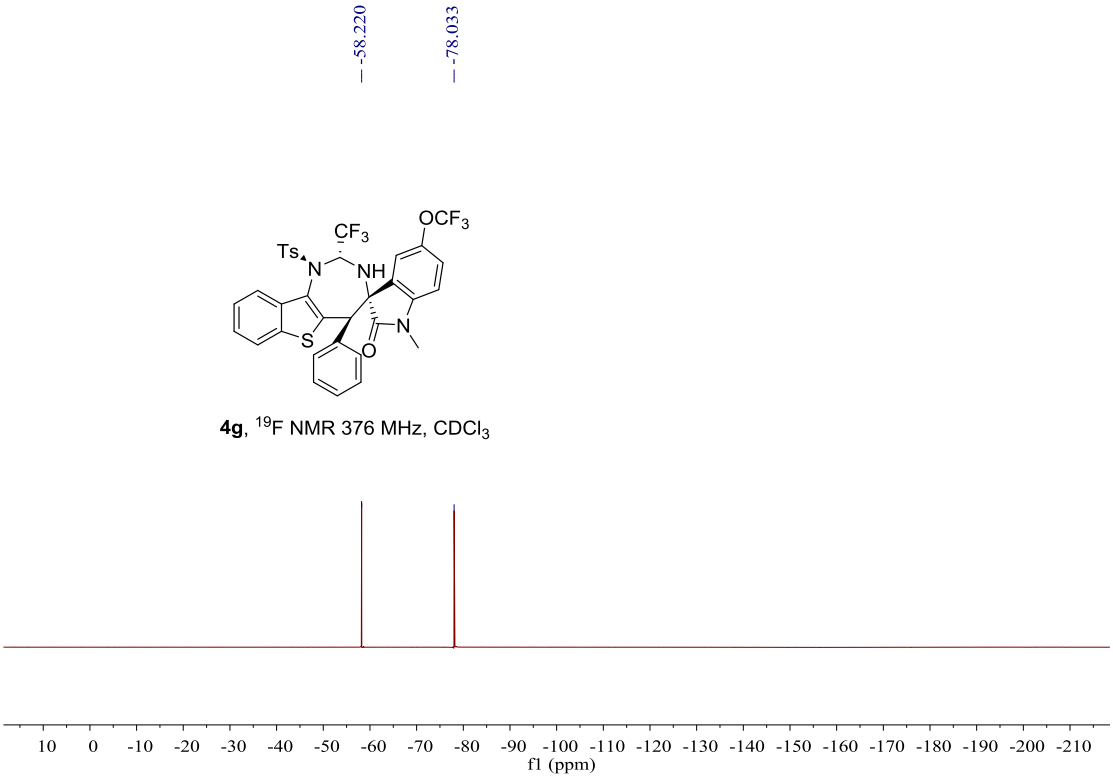

**4f**, $^{19}F$ NMR 376 MHz, $CDCl_3$



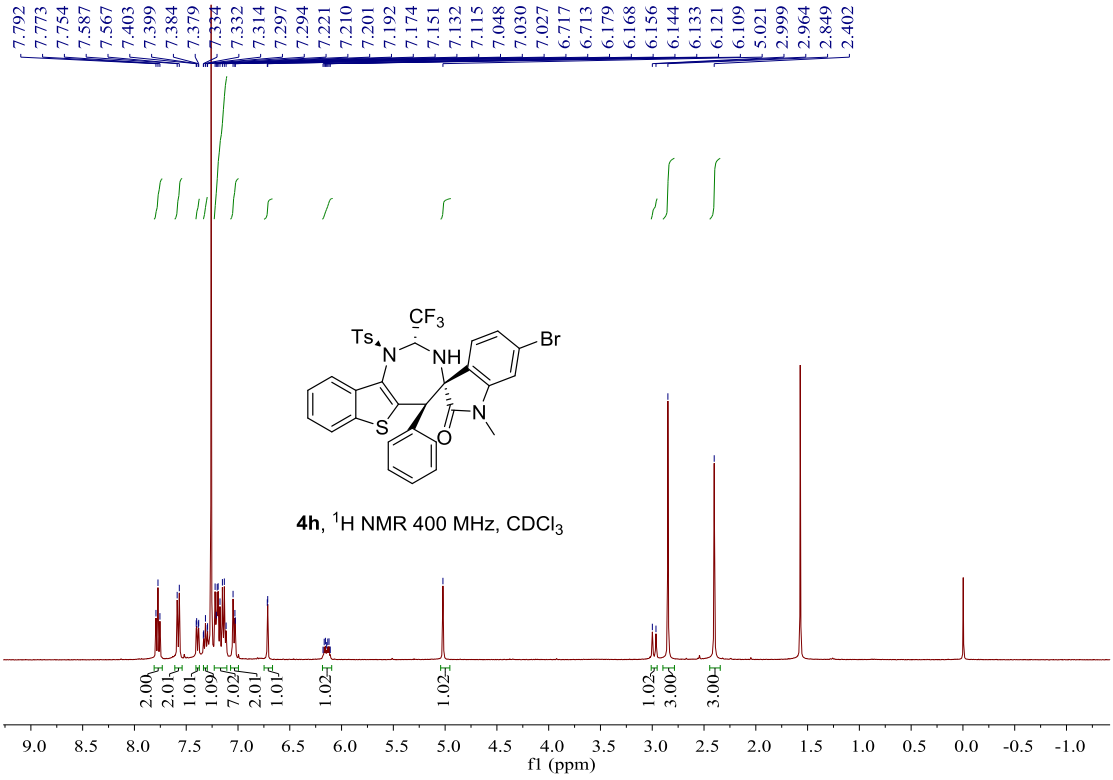

**4g**, $^{1}$H NMR 400 MHz, $CDCl_3$



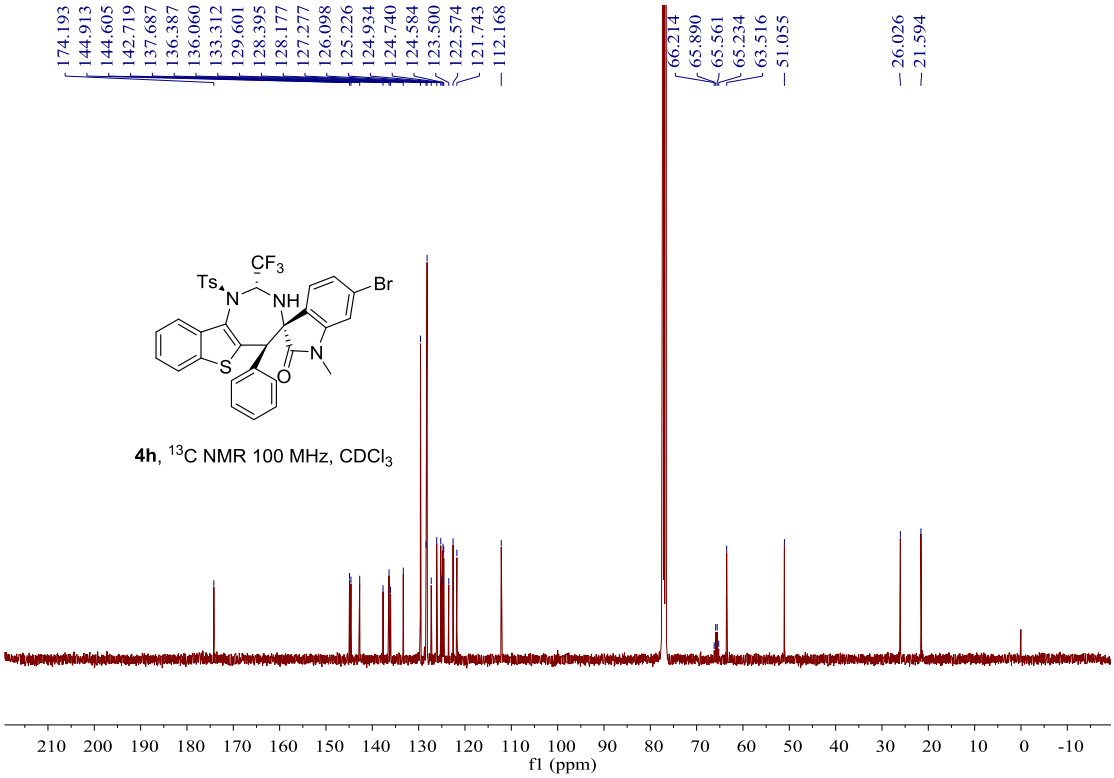

**4g**, $^{13}$C NMR 100 MHz, $CDCl_3$



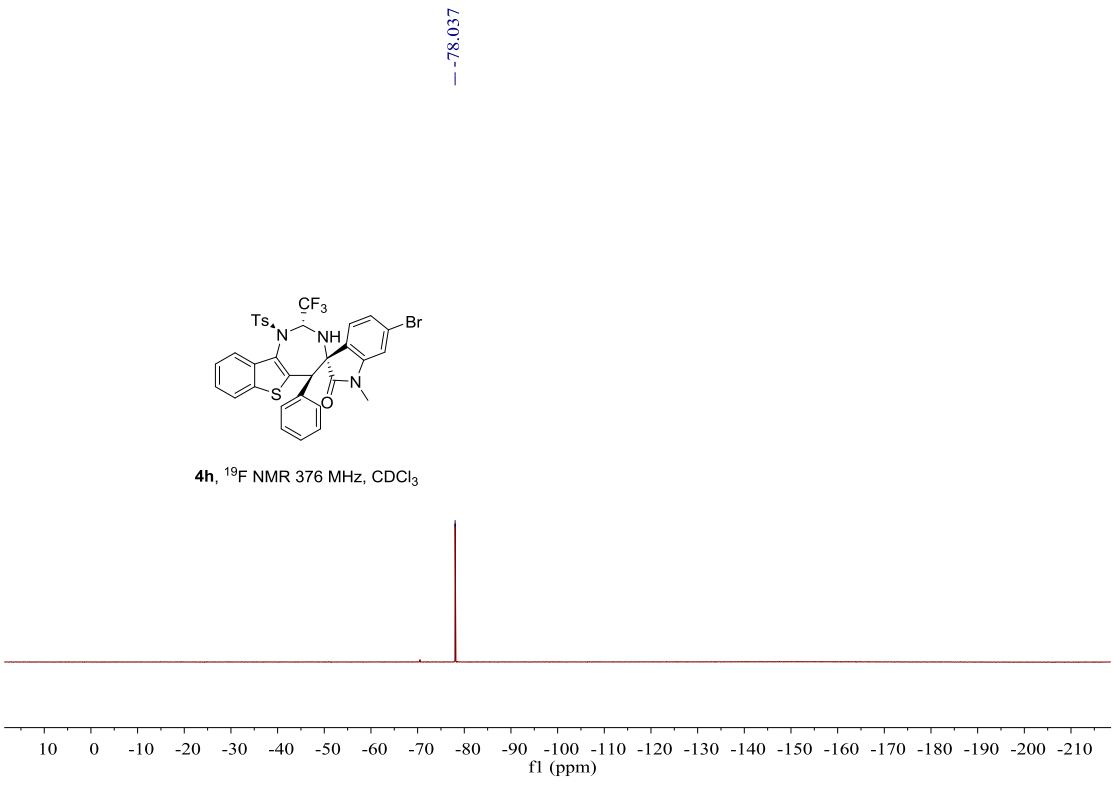

**4g**, $^{19}F$ NMR 376 MHz, $CDCl_3$



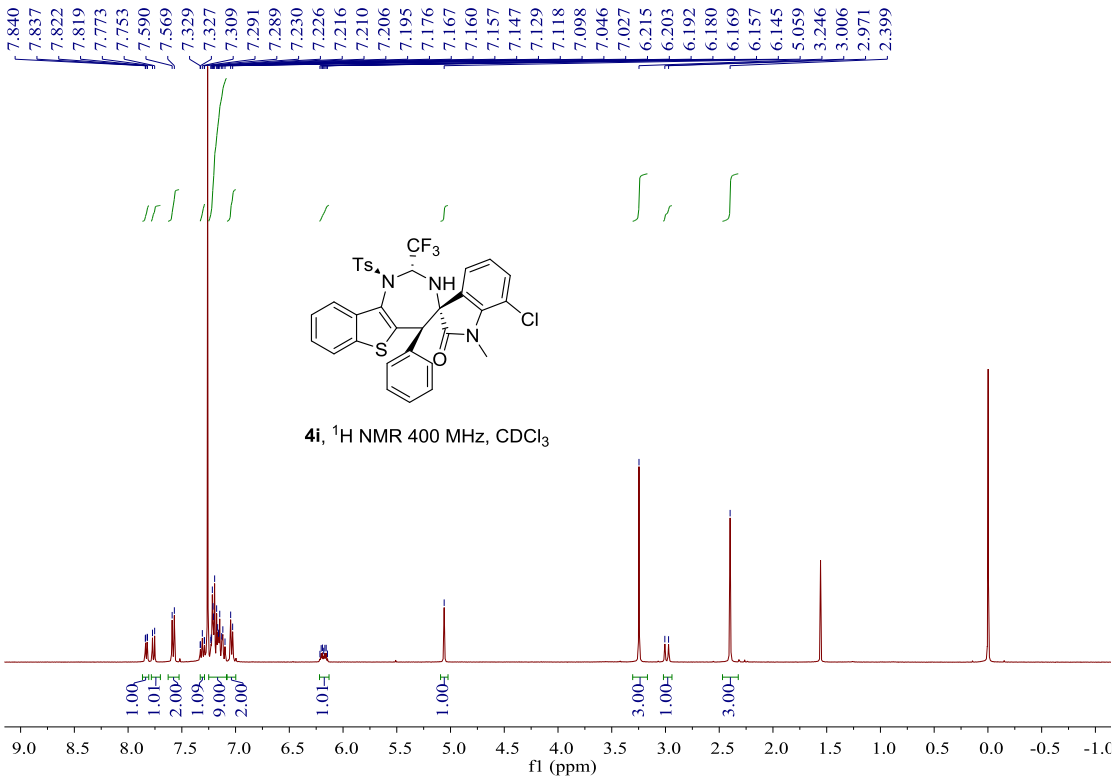

**4h**, $^{1}H$ NMR 400 MHz, $CDCl_3$



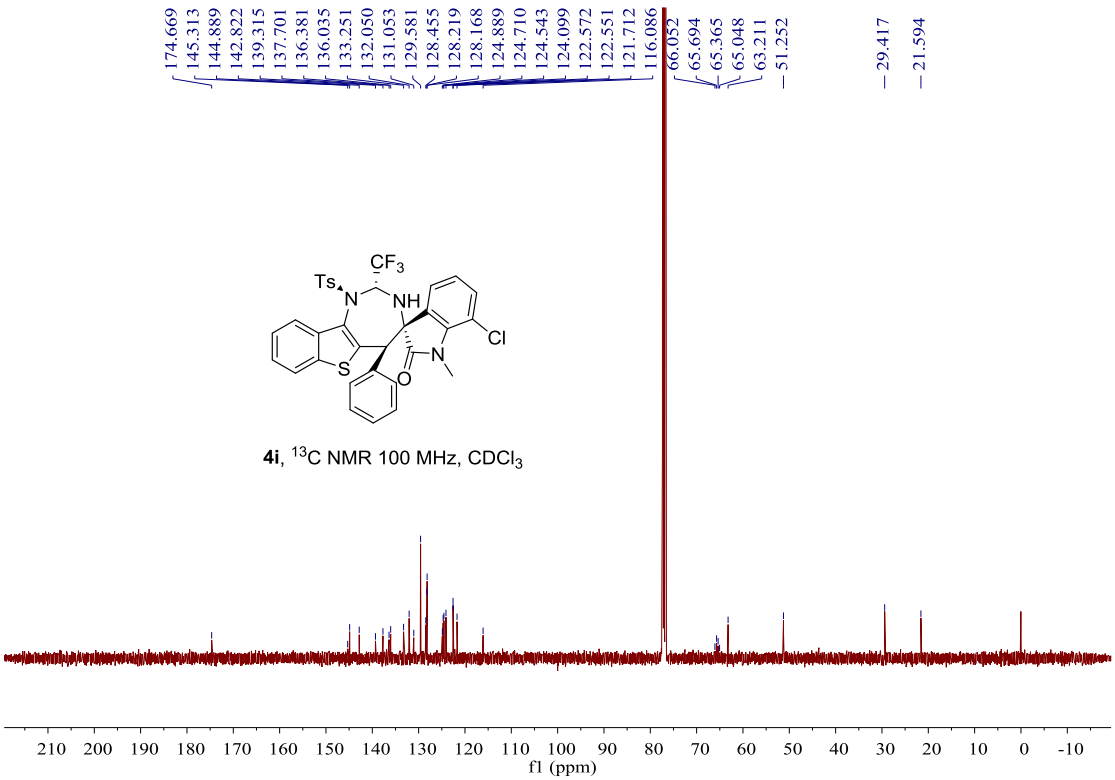

**4h**, $^{13}C$ NMR 100 MHz, $CDCl_3$



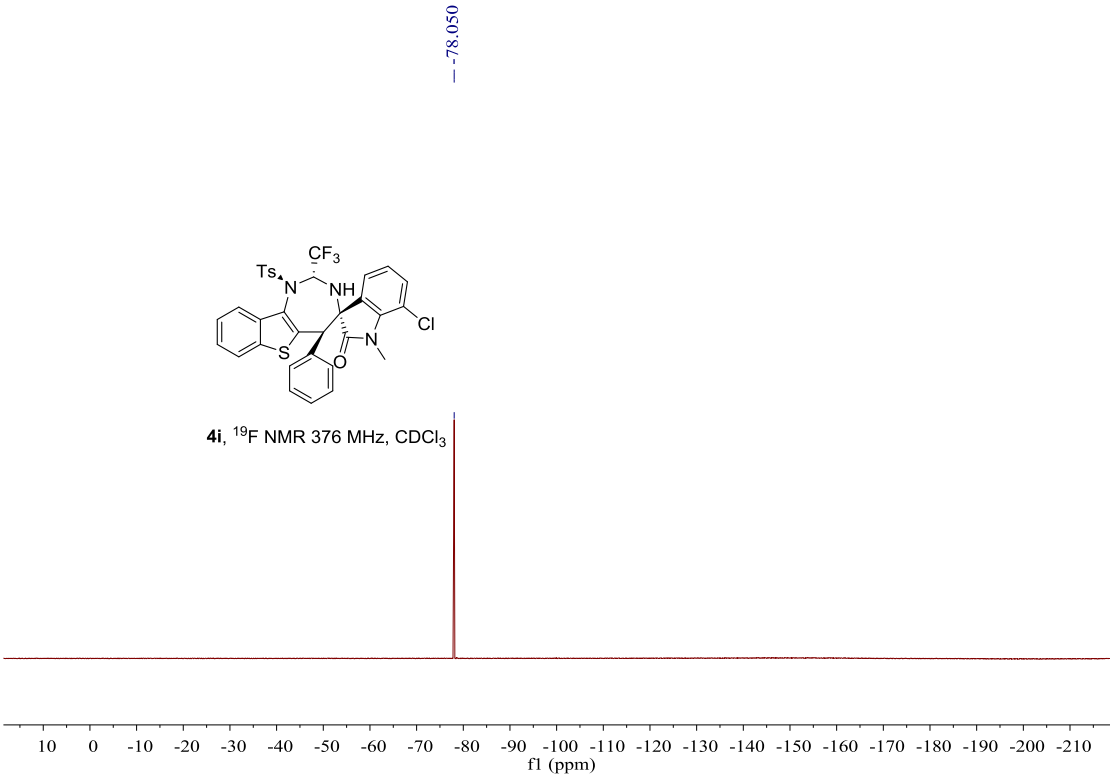

**4h**, $^{19}F$ NMR 376 MHz, $CDCl_3$



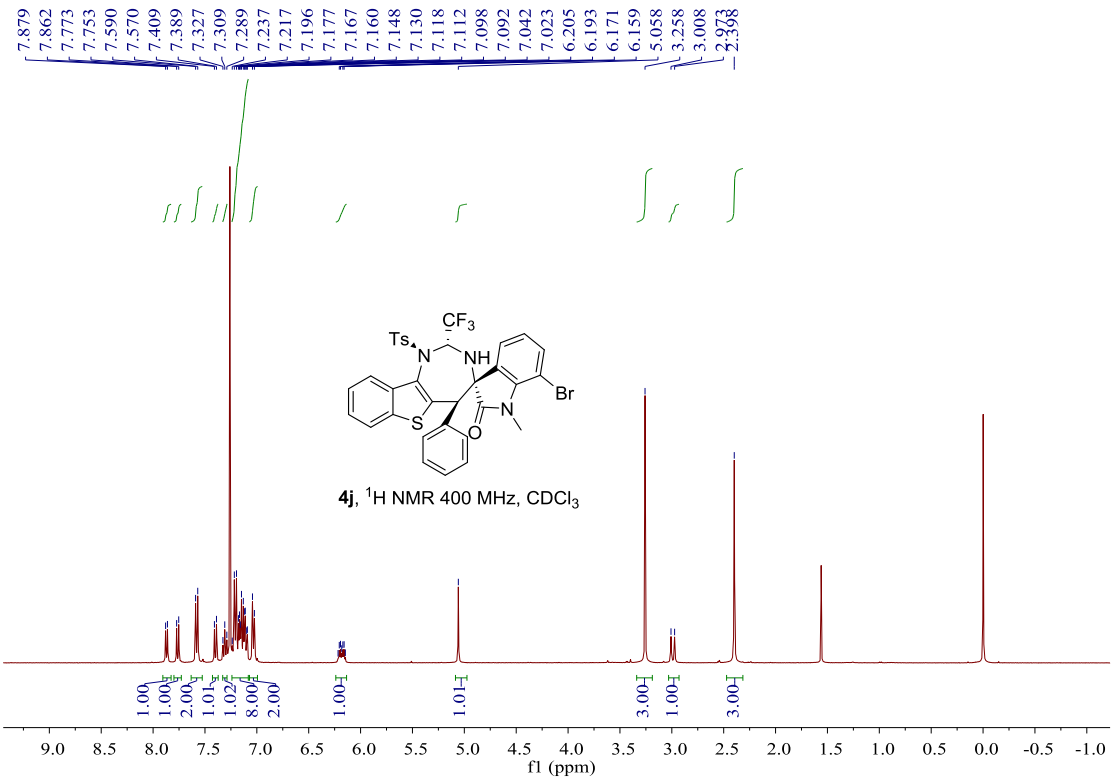

**4i**, $^{1}$H NMR 400 MHz, $CDCl_3$



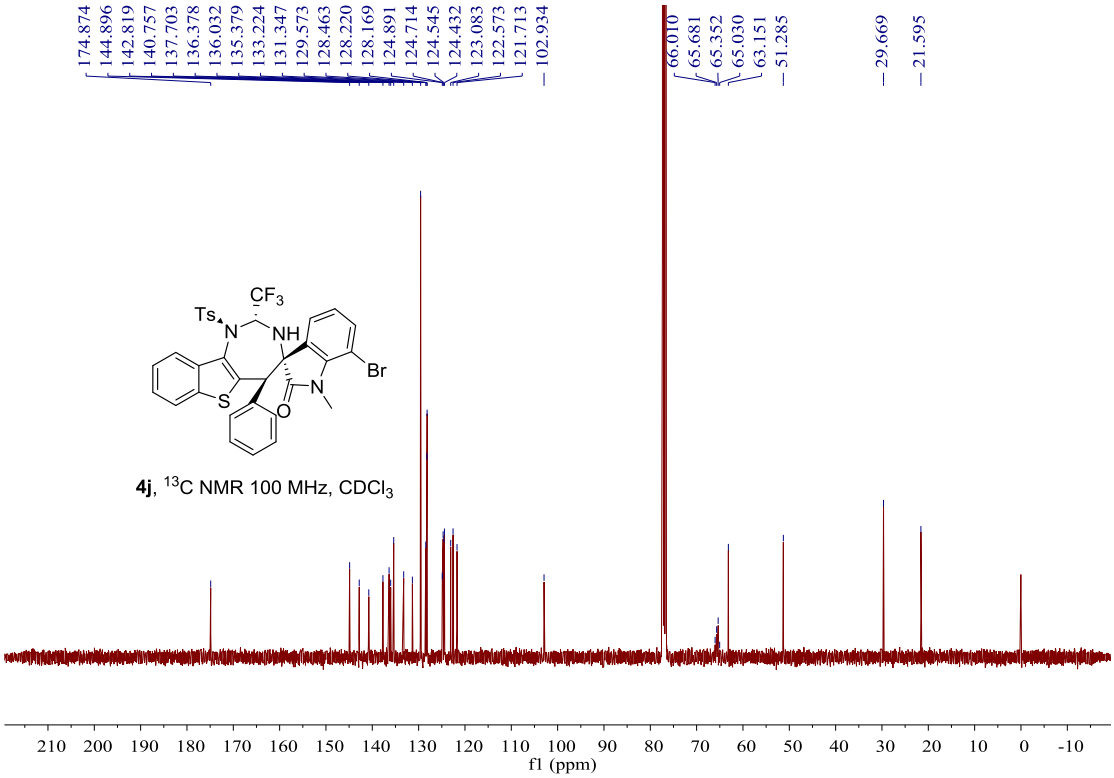

**4i**, $^{13}$C NMR 100 MHz, $CDCl_3$




**4i**, $^{19}F$ NMR 376 MHz, $CDCl_3$




**4j**, $^{1}H$ NMR 400 MHz, $CDCl_3$

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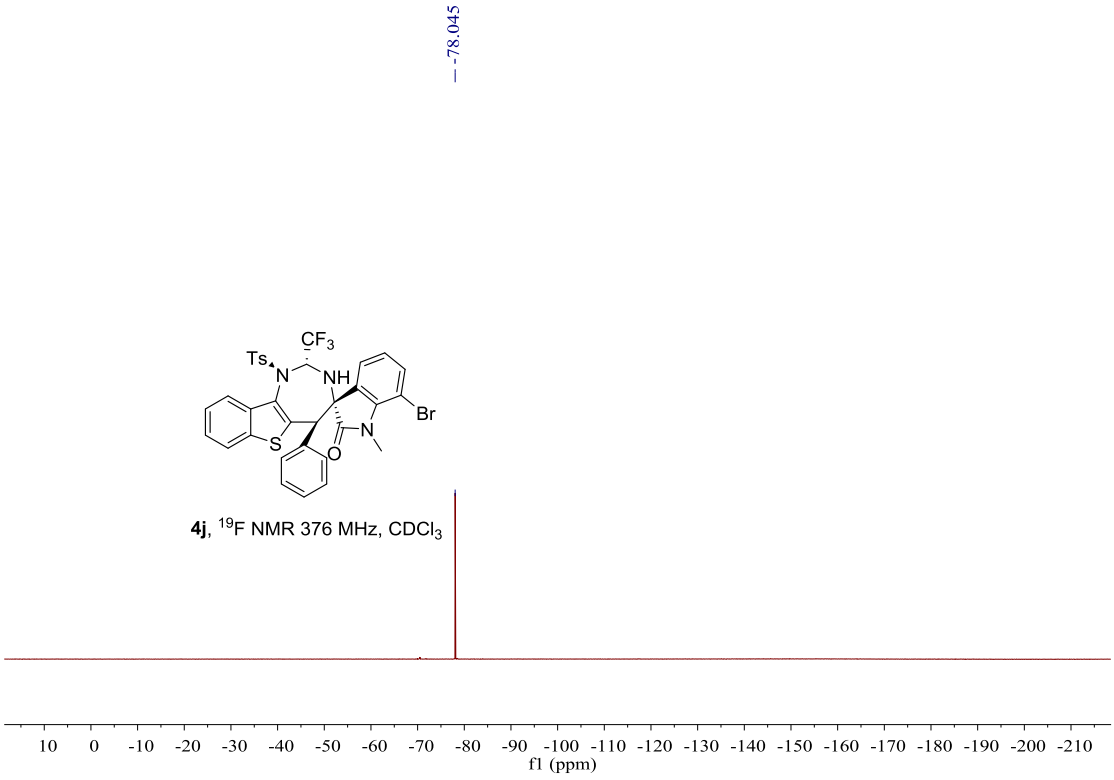


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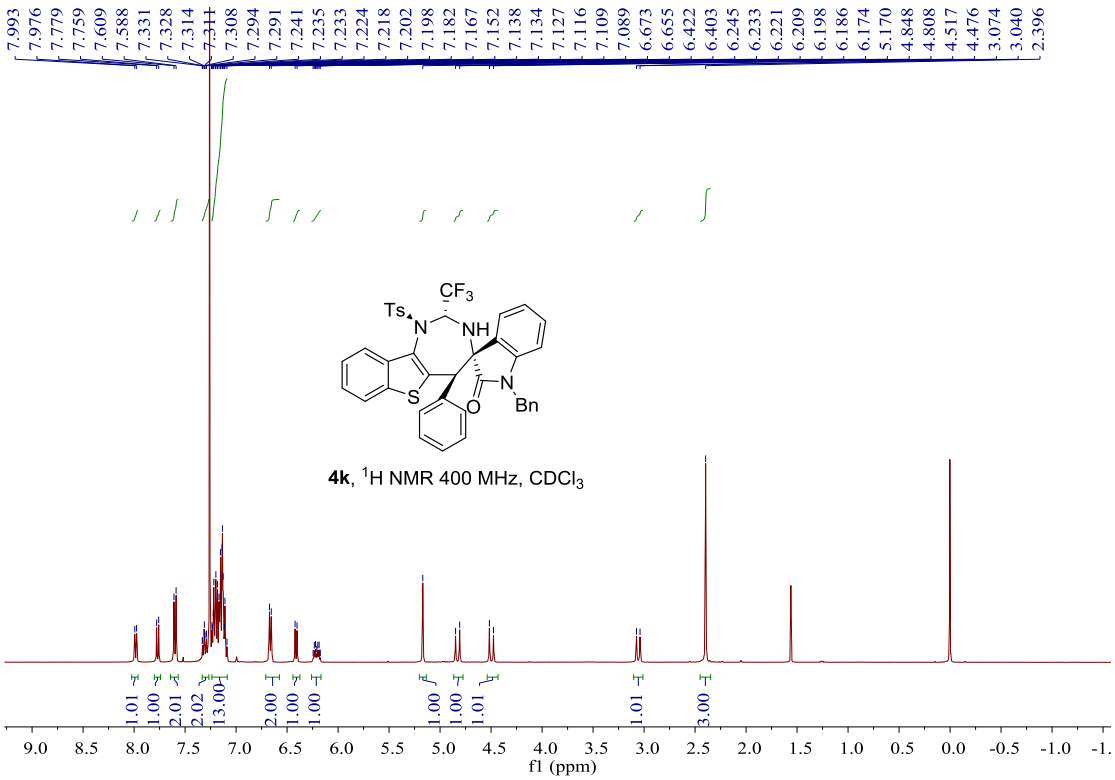
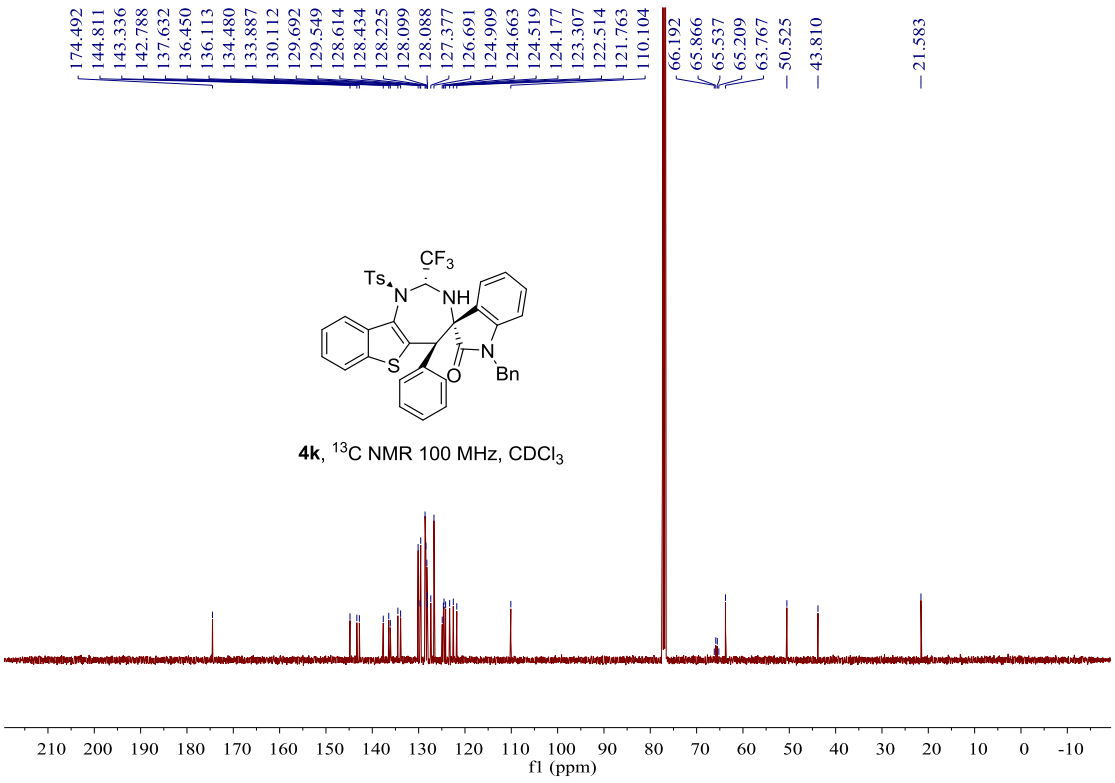
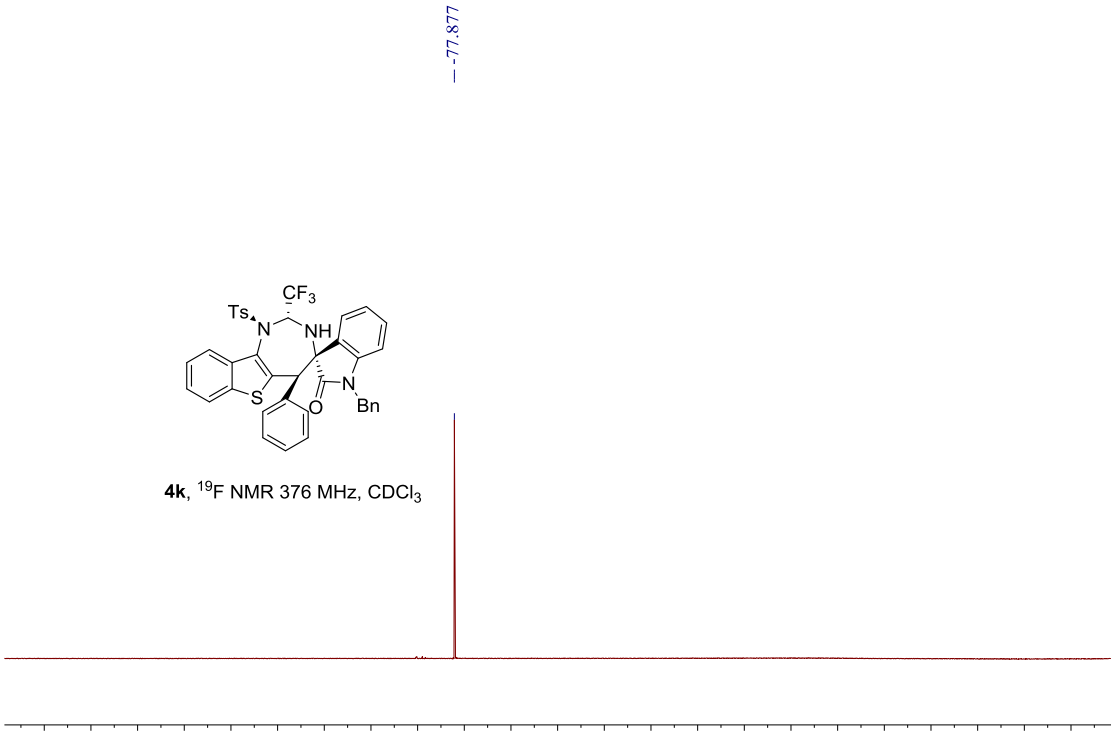


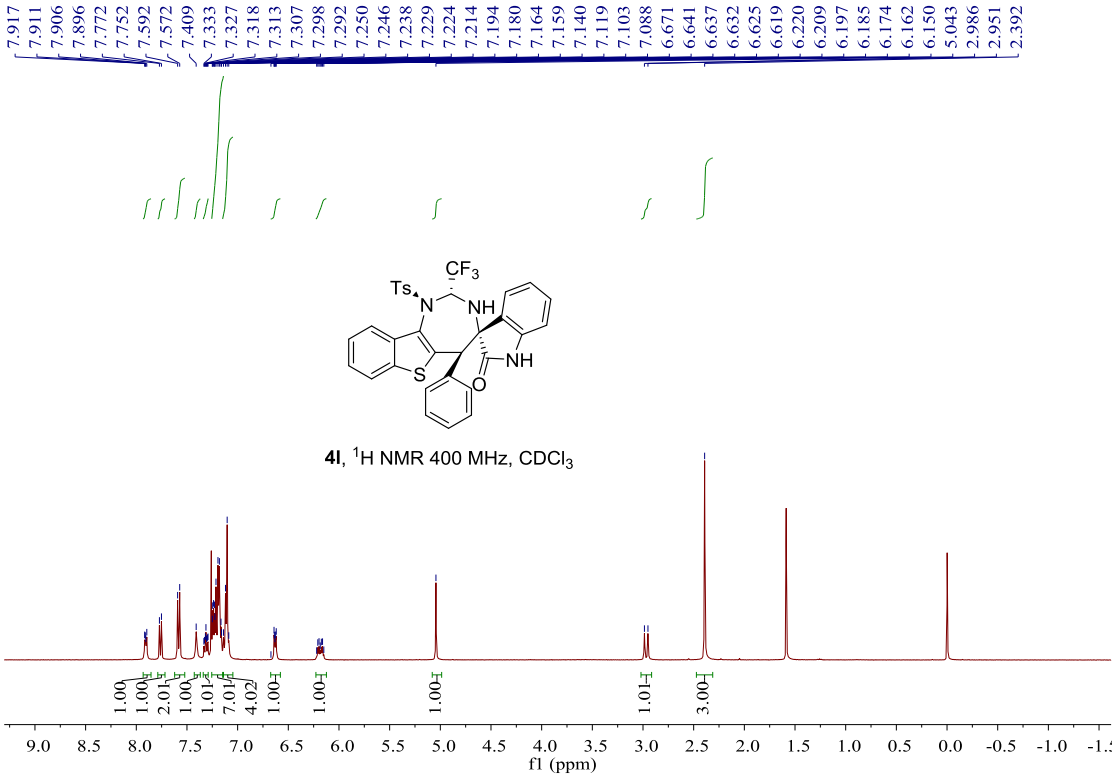

**4k**, $^{1}$H NMR 400 MHz, $CDCl_3$



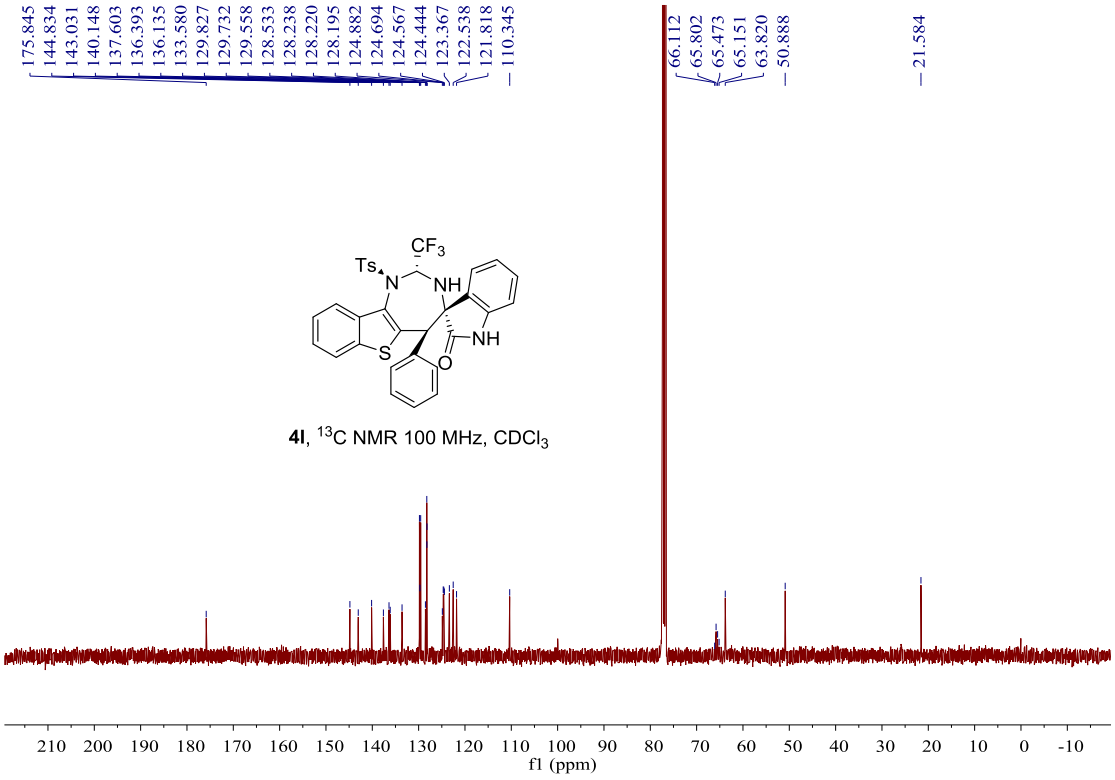

**4k**, $^{13}$C NMR 100 MHz, $CDCl_3$



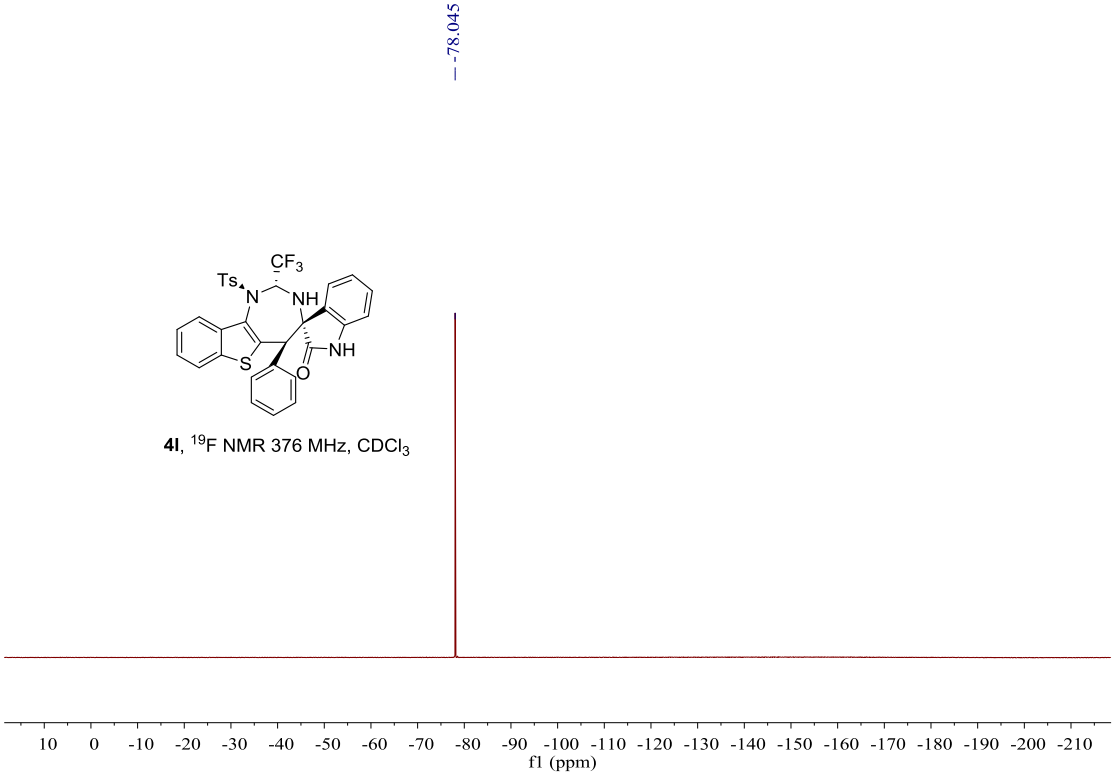

**4k**, $^{19}F$ NMR 376 MHz, $CDCl_3$



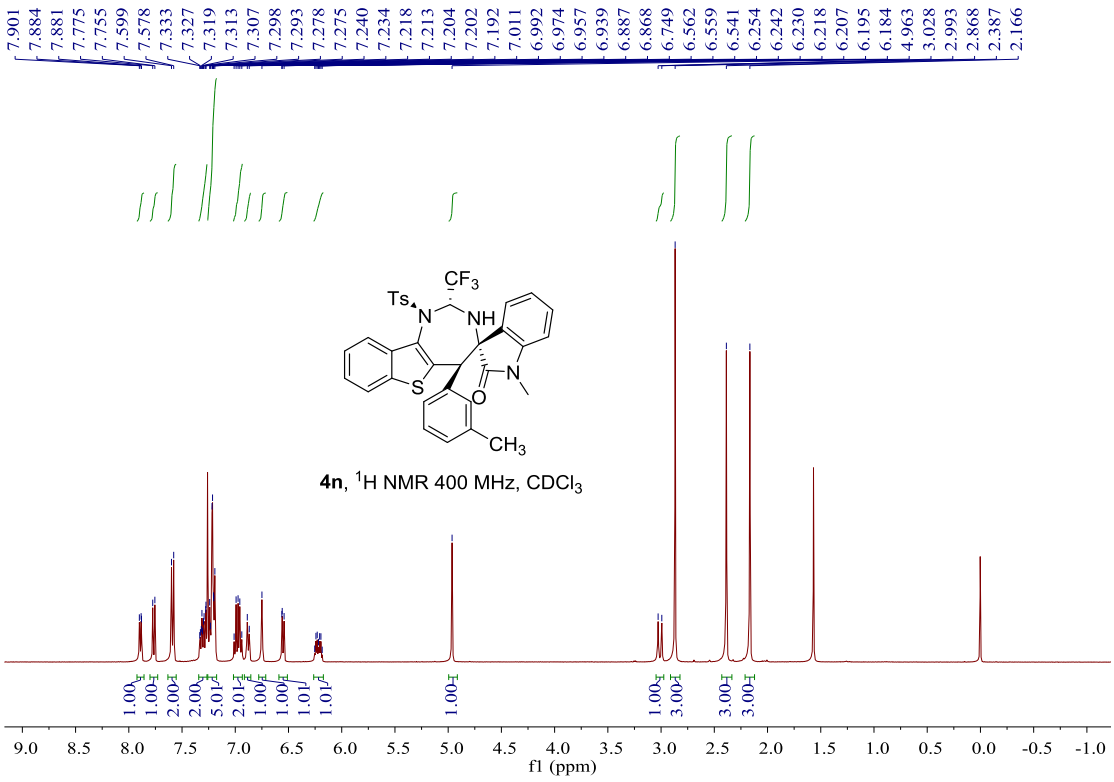

**4l**, $^{1}H$ NMR 400 MHz, $CDCl_3$



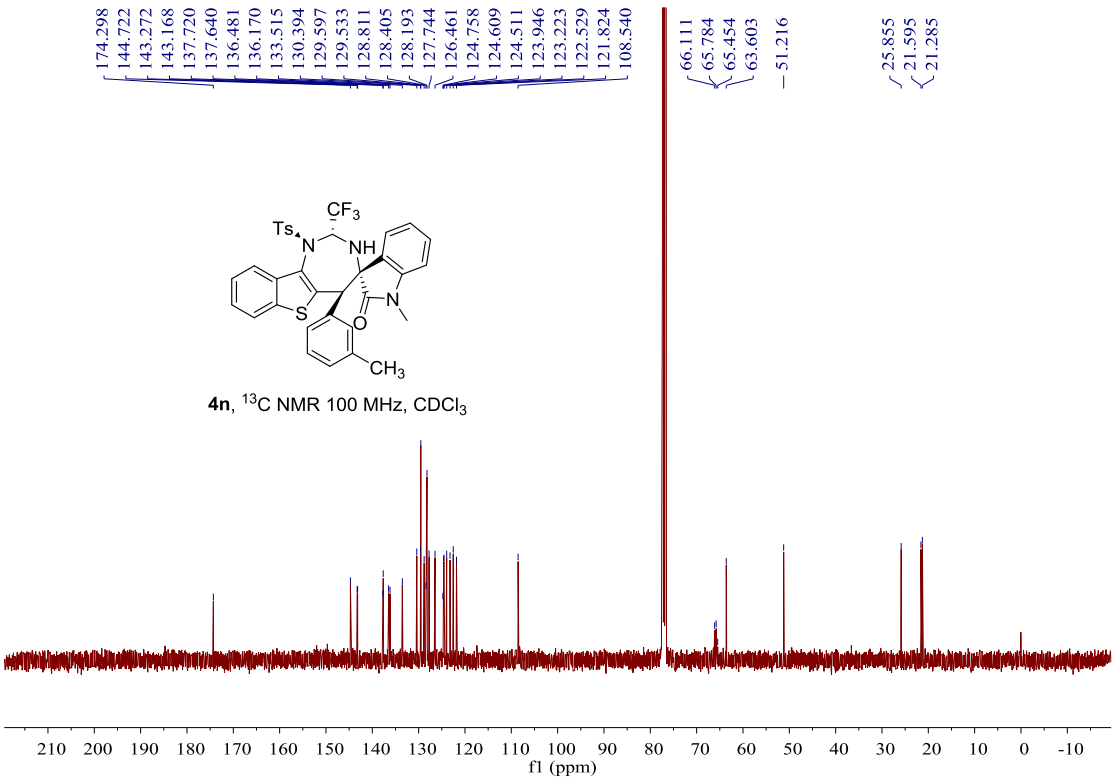

**4l**, $^{13}C$ NMR 100 MHz, $CDCl_3$




**4l**, $^{19}F$ NMR 376 MHz, $CDCl_3$




**4n**, $^{1}$H NMR 400 MHz, $CDCl_3$

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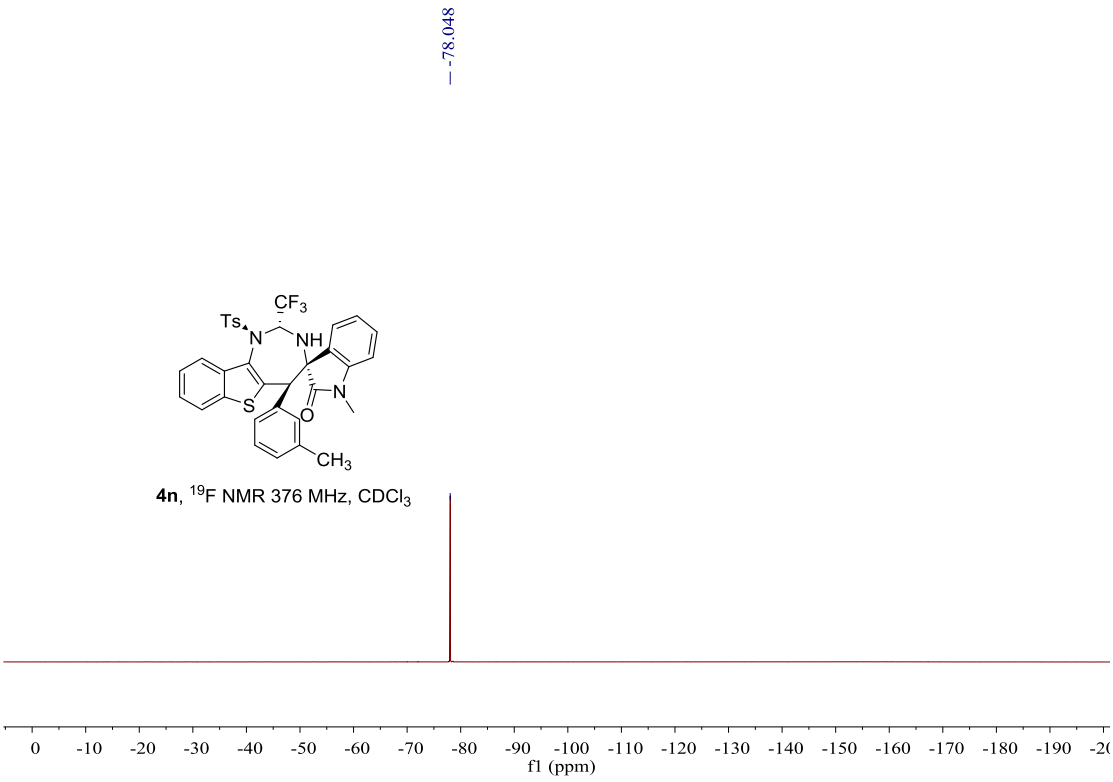
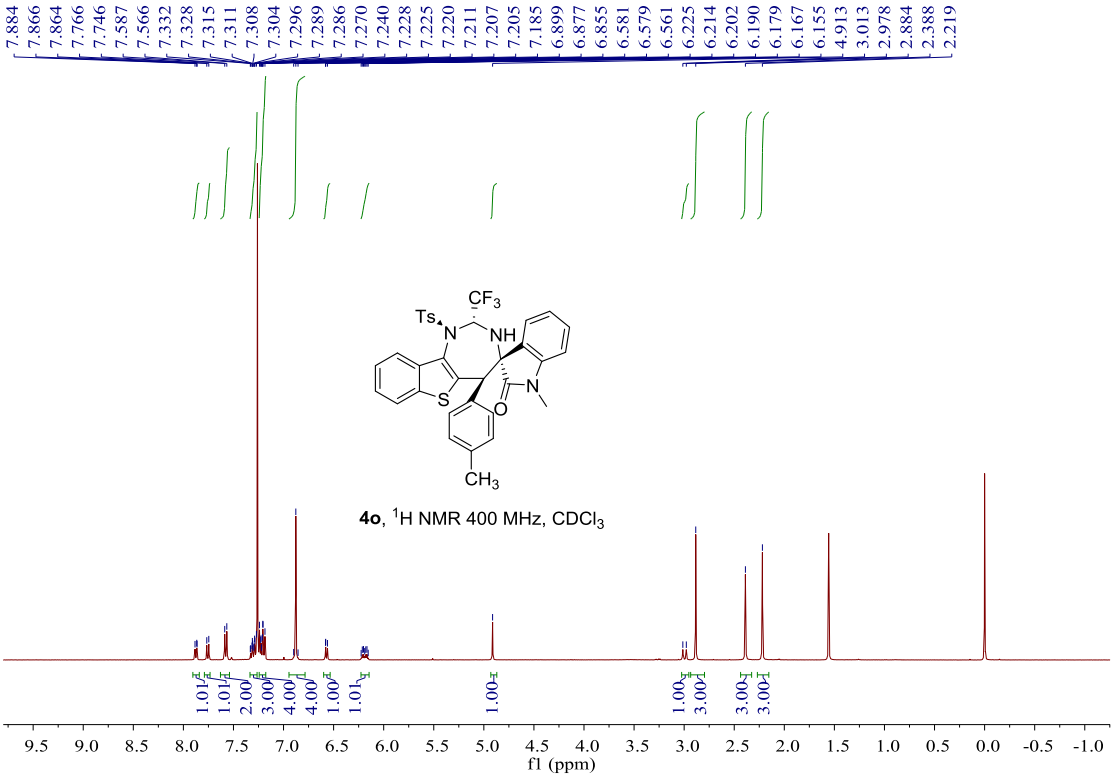
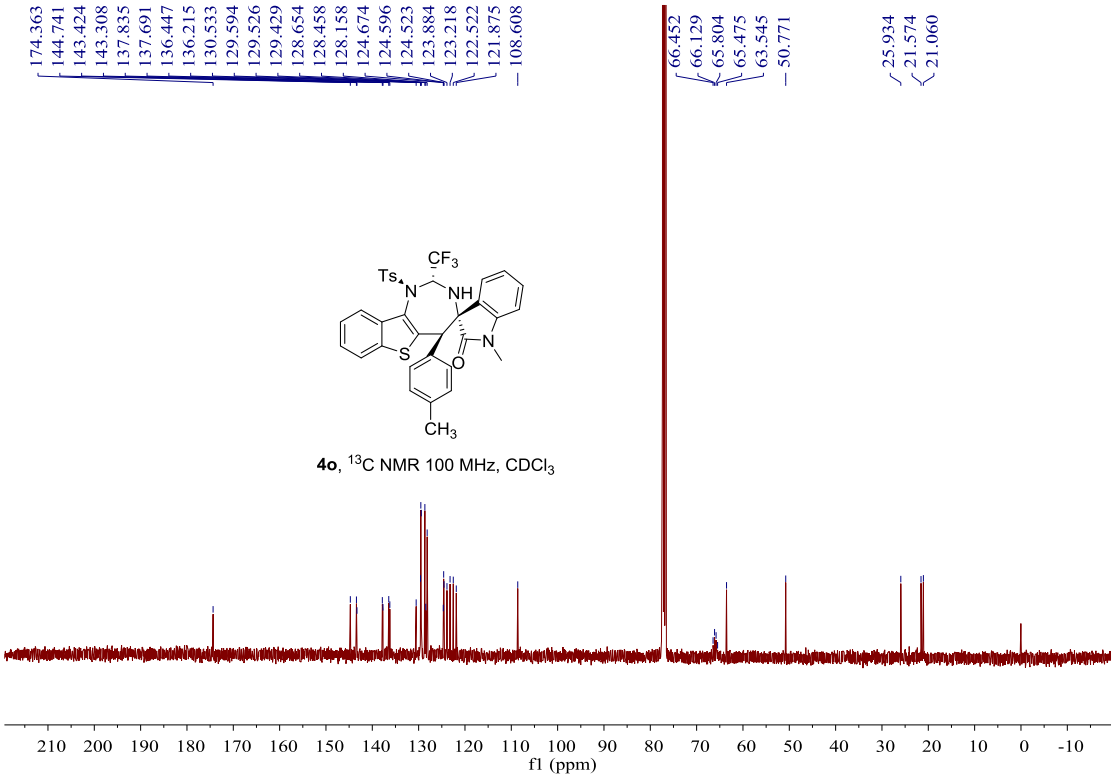


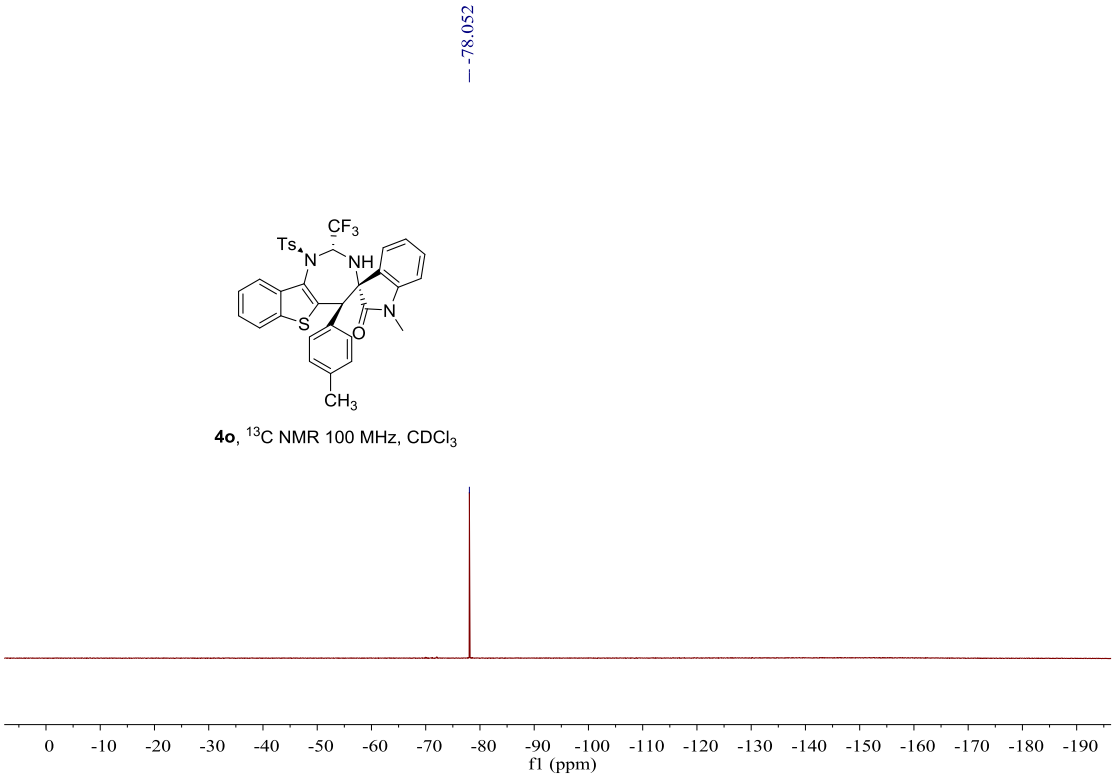

**4n**, $^{19}F$ NMR 376 MHz, $CDCl_3$



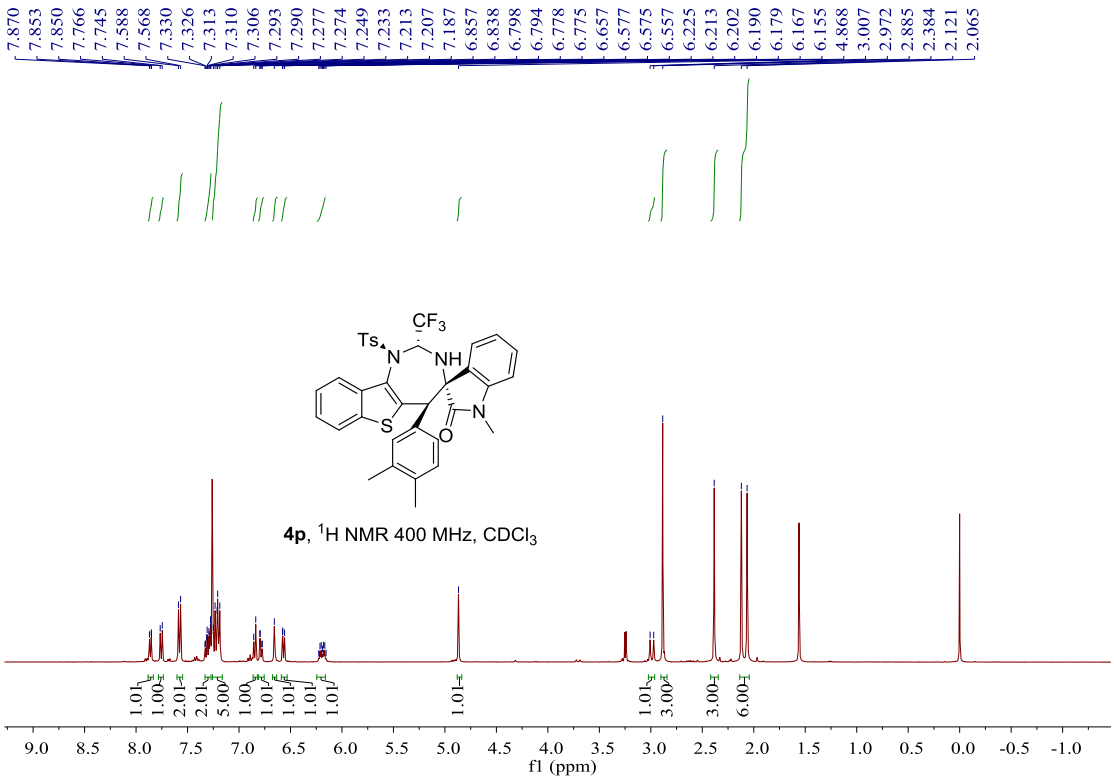

**4o**, $^{1}H$ NMR 400 MHz, $CDCl_3$



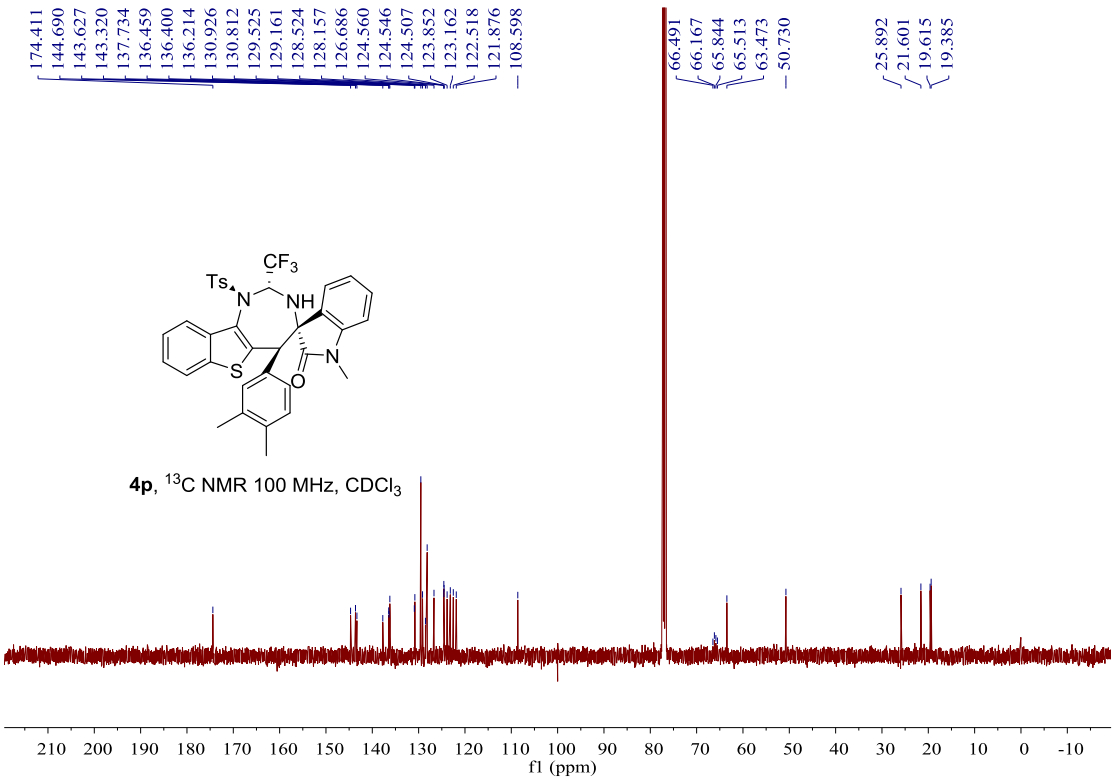

**4o**, $^{13}C$ NMR 100 MHz, $CDCl_3$



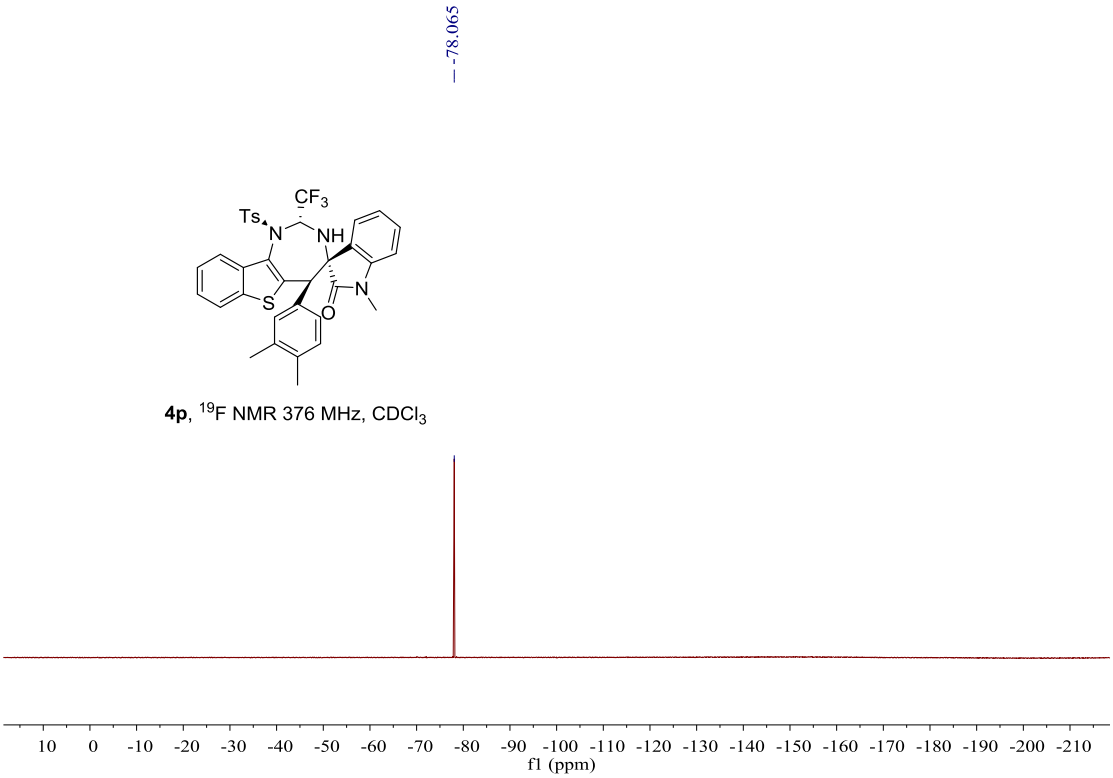

**4o**, $^{13}C$ NMR 100 MHz, $CDCl_3$



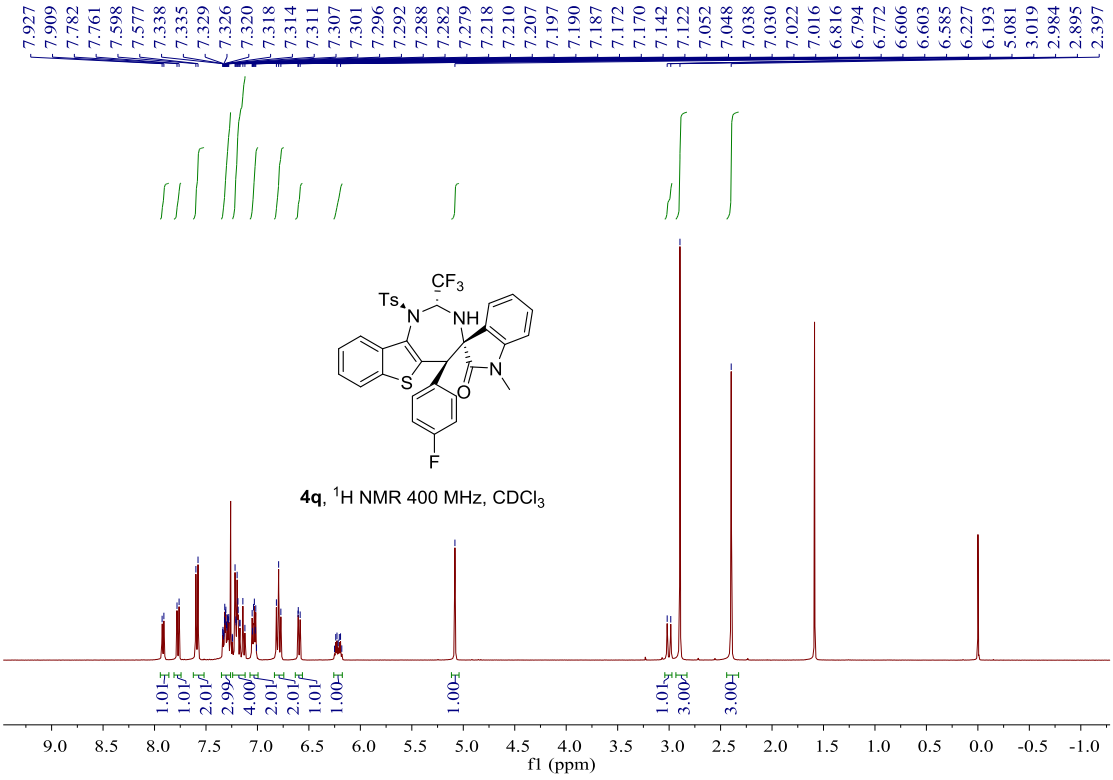

**4p**, $^{1}$H NMR 400 MHz, $CDCl_3$



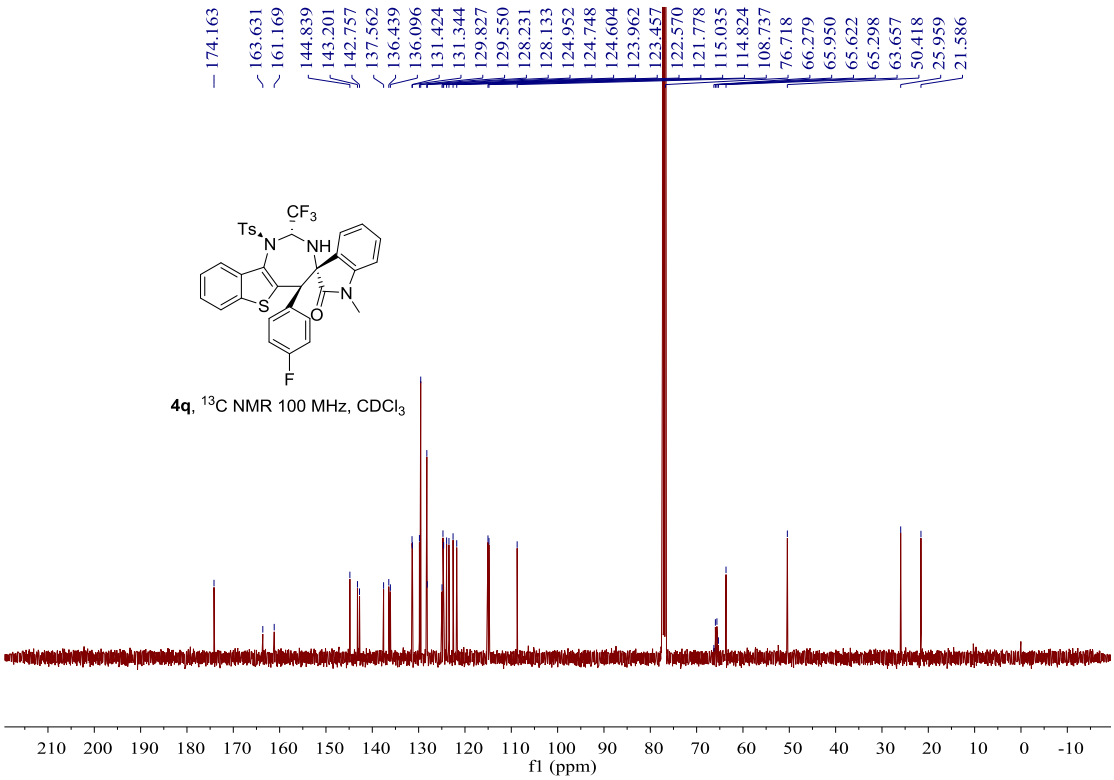

**4p**, $^{13}$C NMR 100 MHz, $CDCl_3$



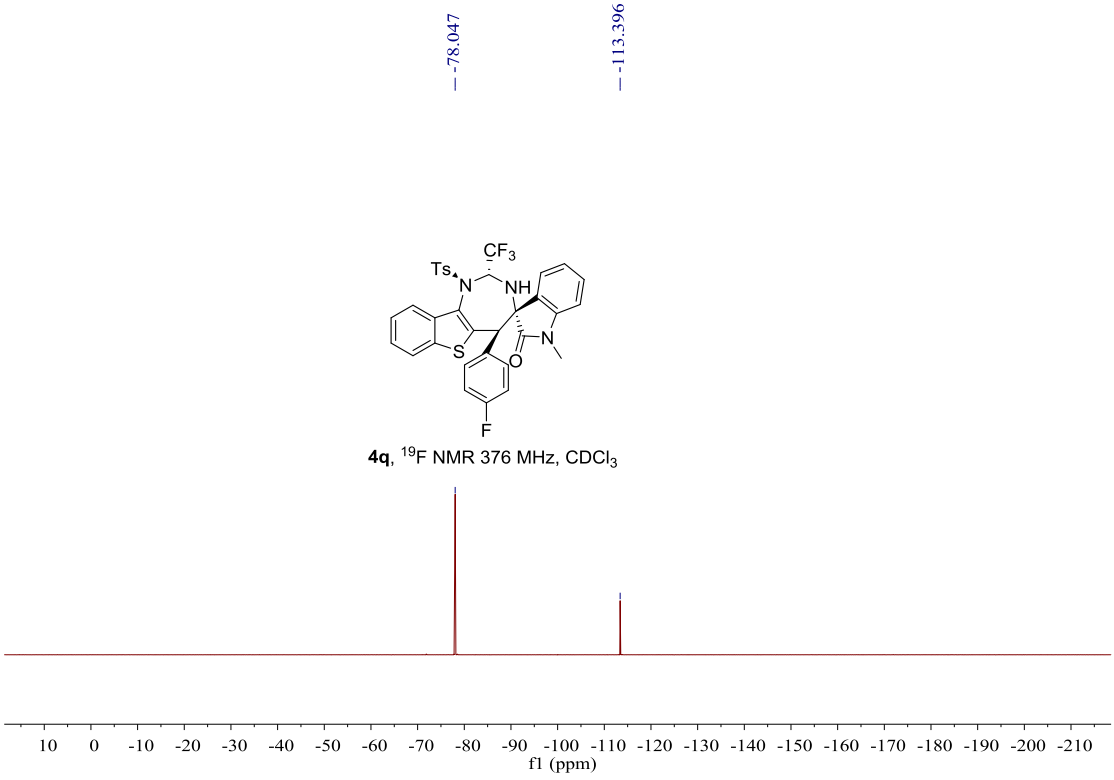

**4p**, $^{19}F$ NMR 376 MHz, $CDCl_3$



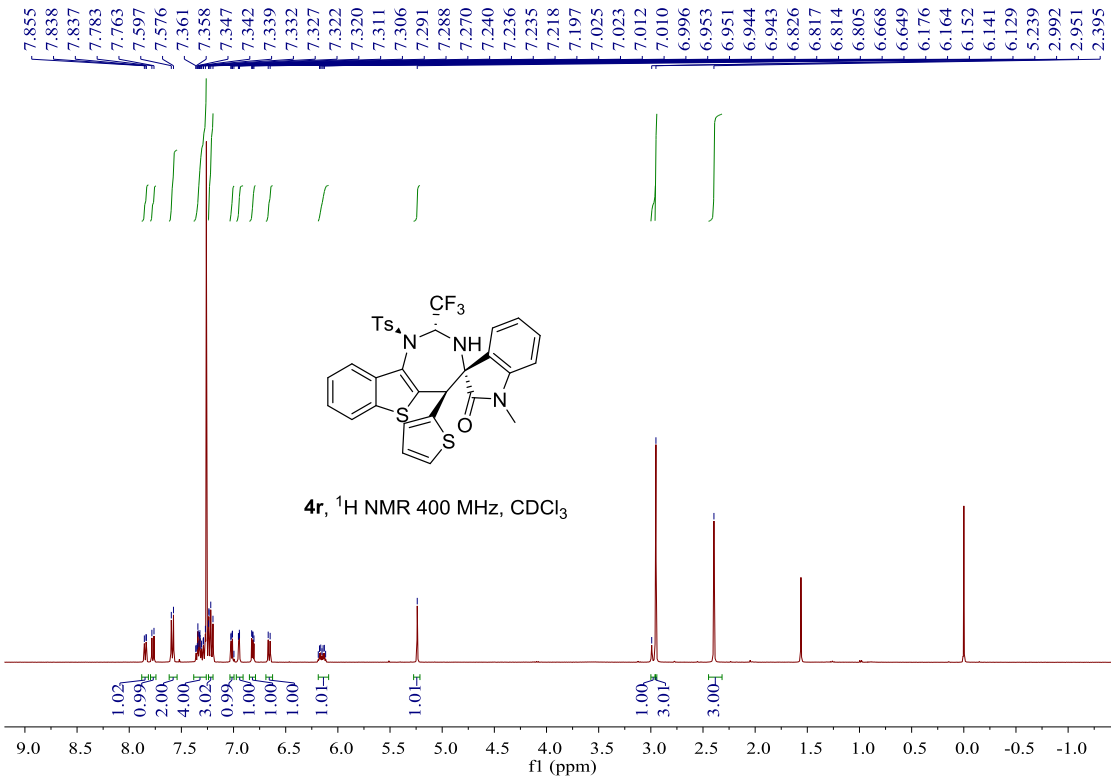

**4q**, $^{1}H$ NMR 400 MHz, $CDCl_3$



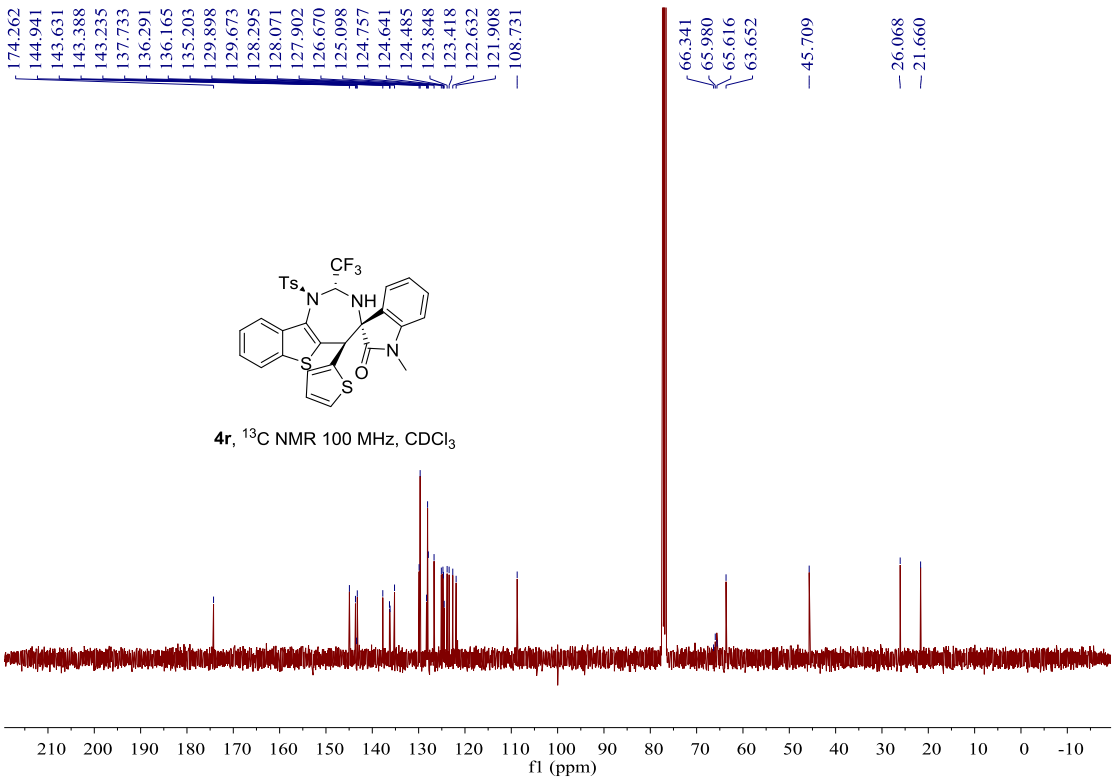

**4q**, $^{13}C$ NMR 100 MHz, $CDCl_3$



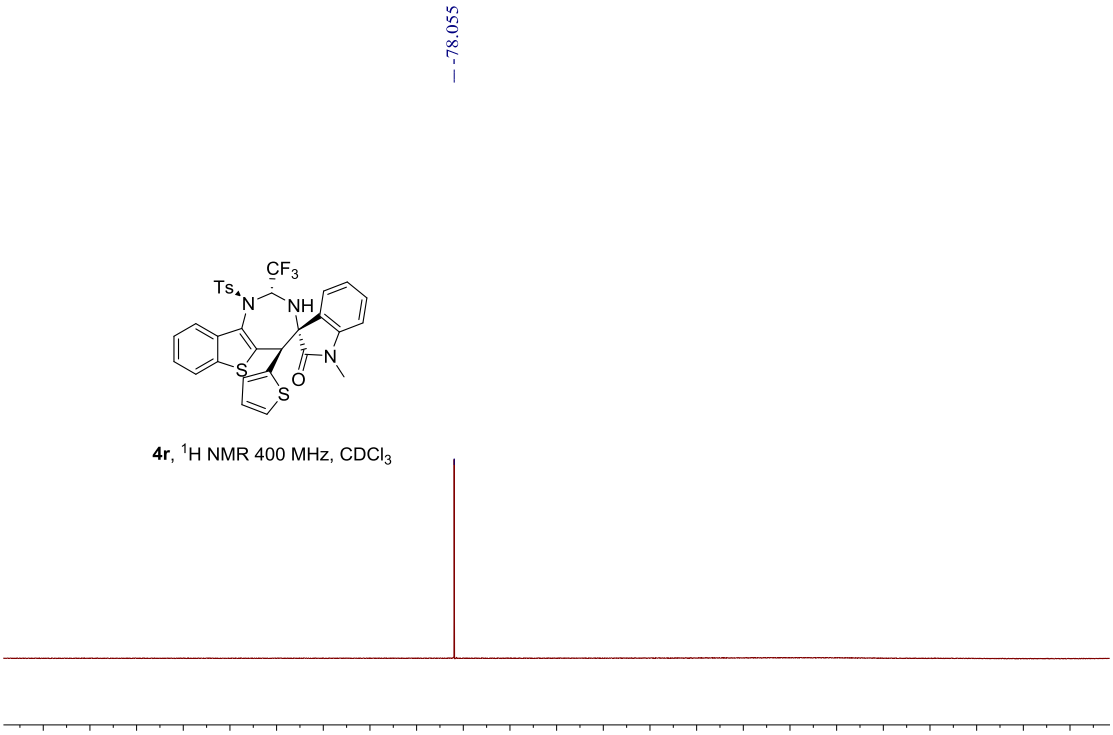

**4q**, $^{19}F$ NMR 376 MHz, $CDCl_3$



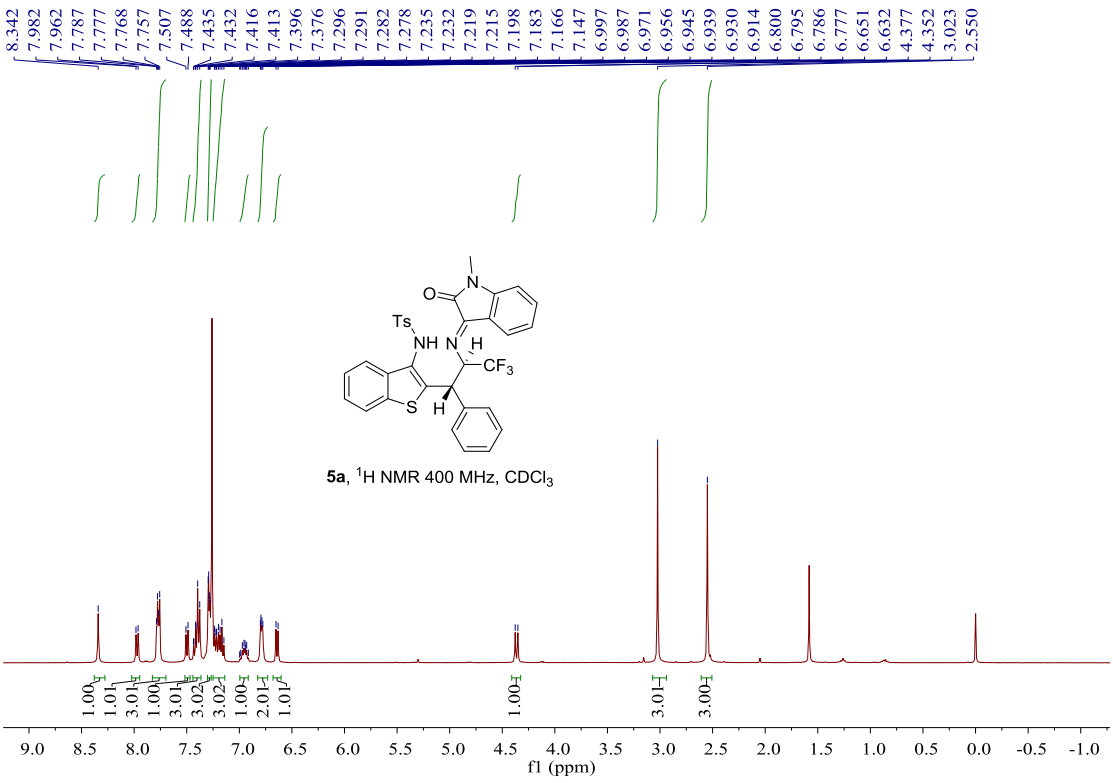

**4r**, $^{1}$H NMR 400 MHz, $CDCl_3$



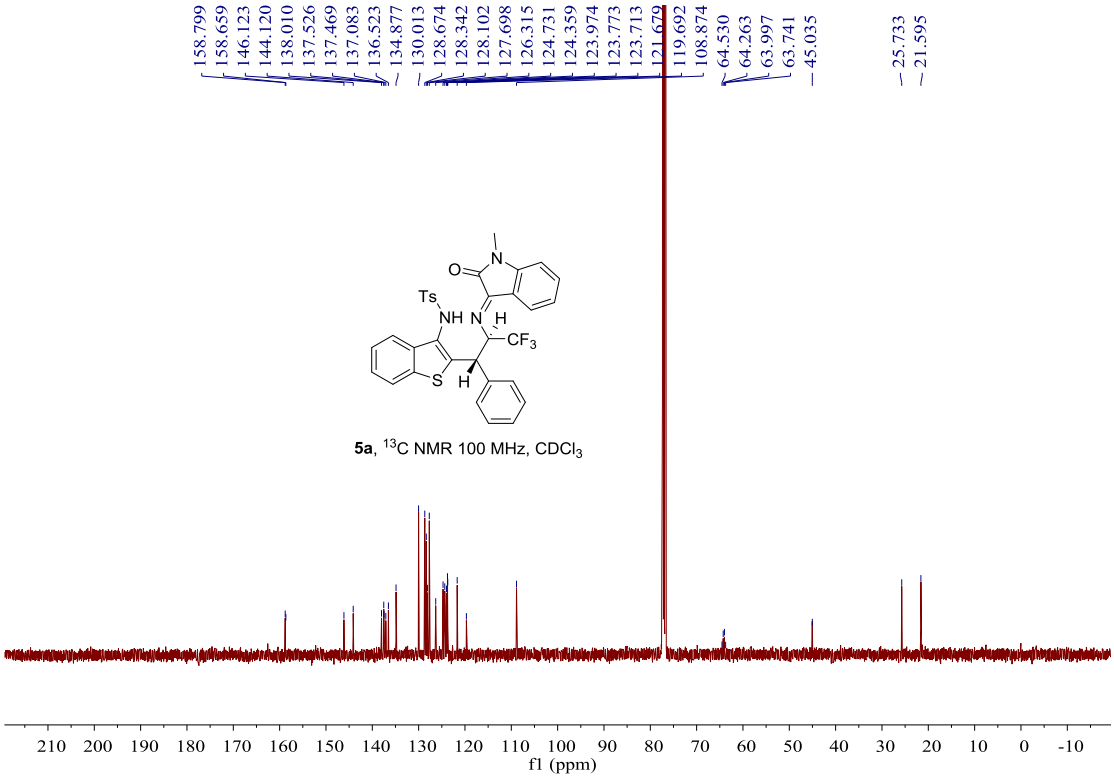

**4r**, $^{13}$C NMR 100 MHz, $CDCl_3$



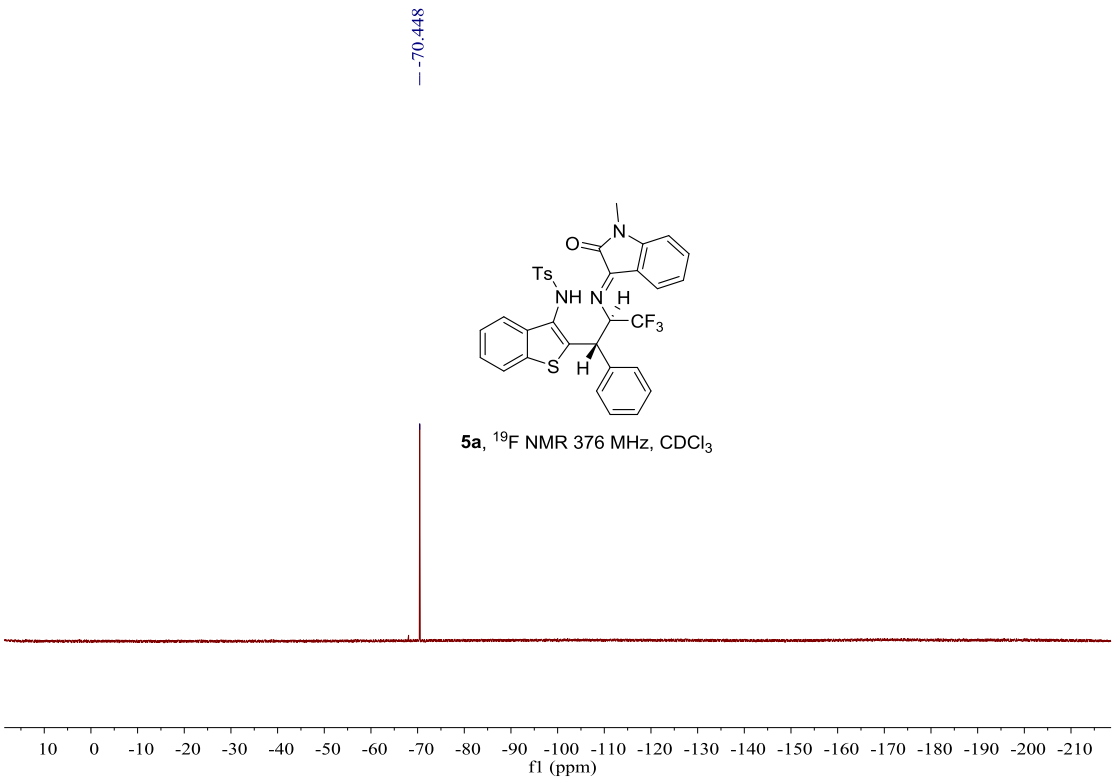

**4r**, $^{1}$H NMR 400 MHz, $CDCl_3$



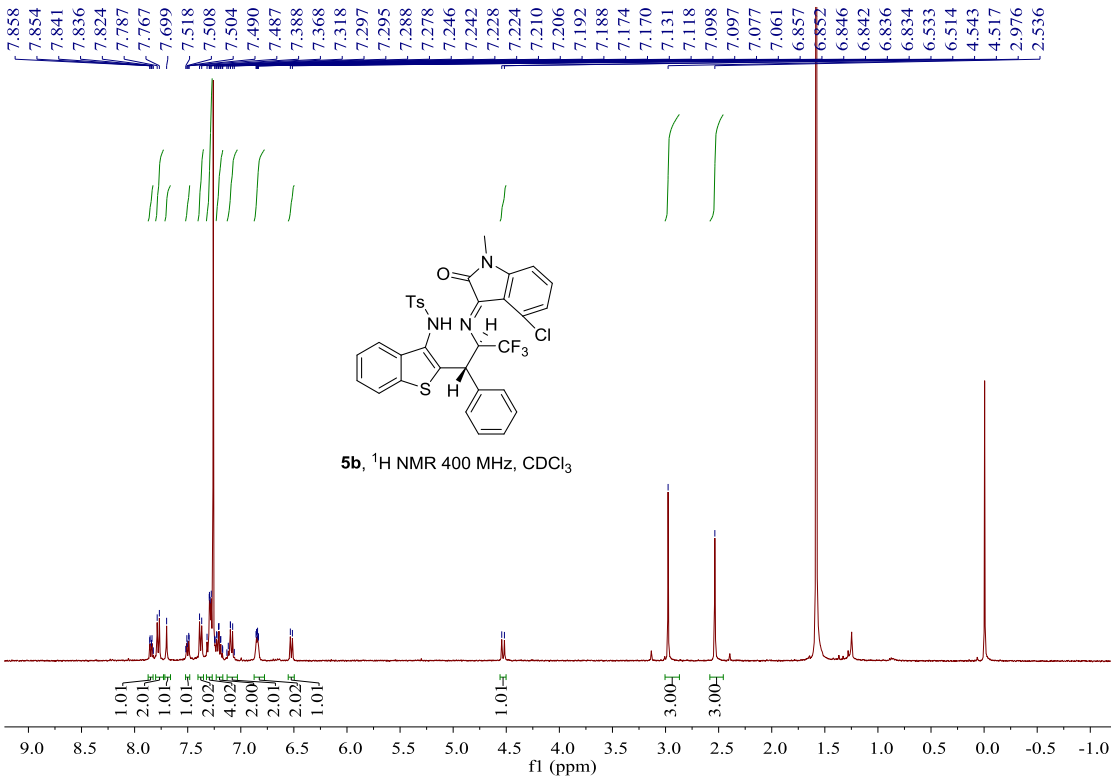

**5a**, $^{1}$H NMR 400 MHz, $CDCl_3$



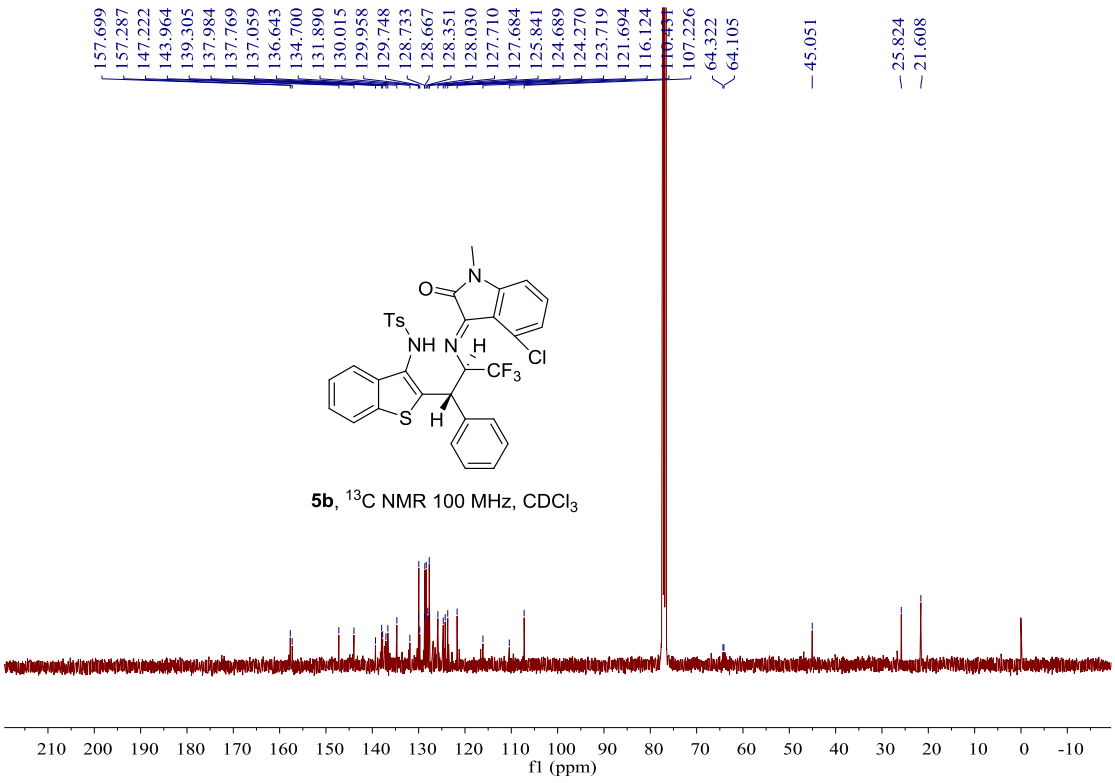

**5a**, $^{13}C$ NMR 100 MHz, $CDCl_3$



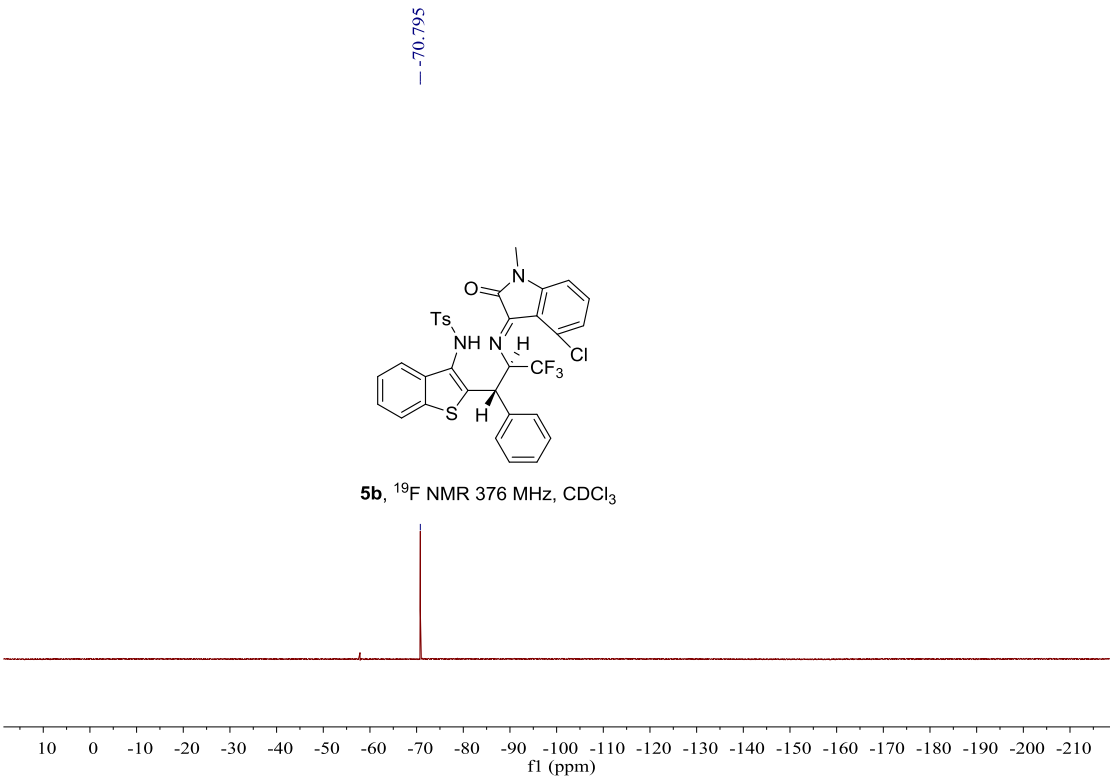

**5a**, $^{19}F$ NMR 376 MHz, $CDCl_3$



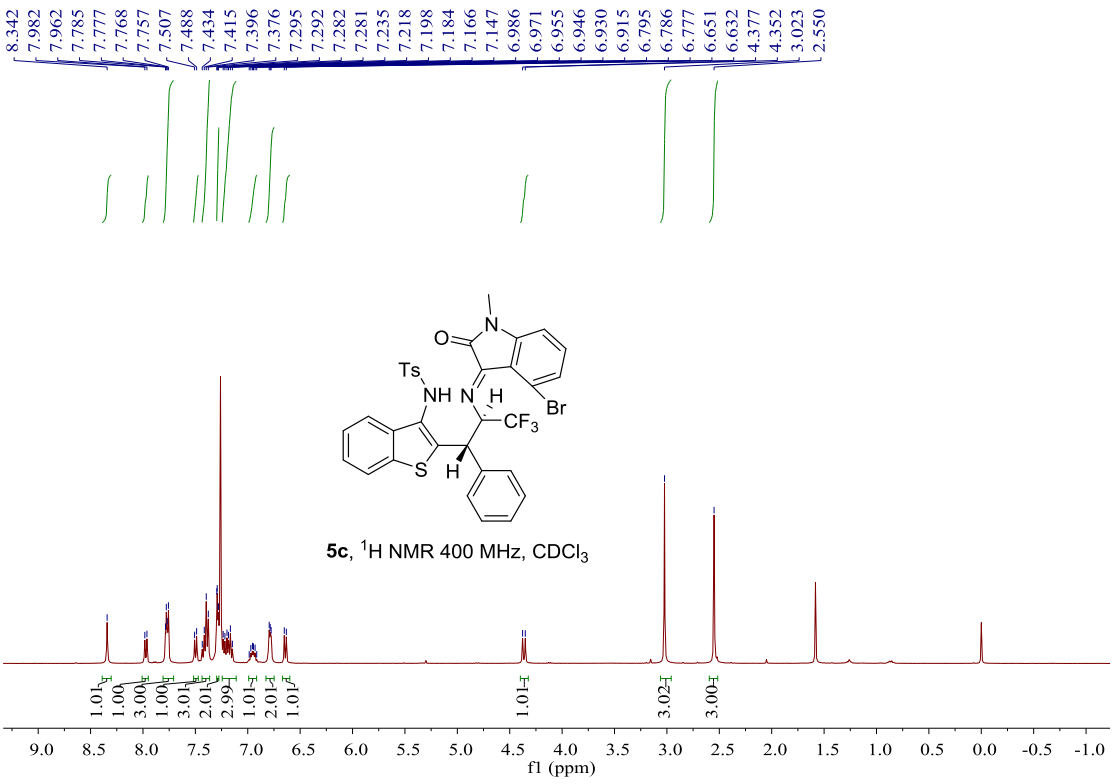

**5b**, $^{1}$H NMR 400 MHz, $CDCl_3$



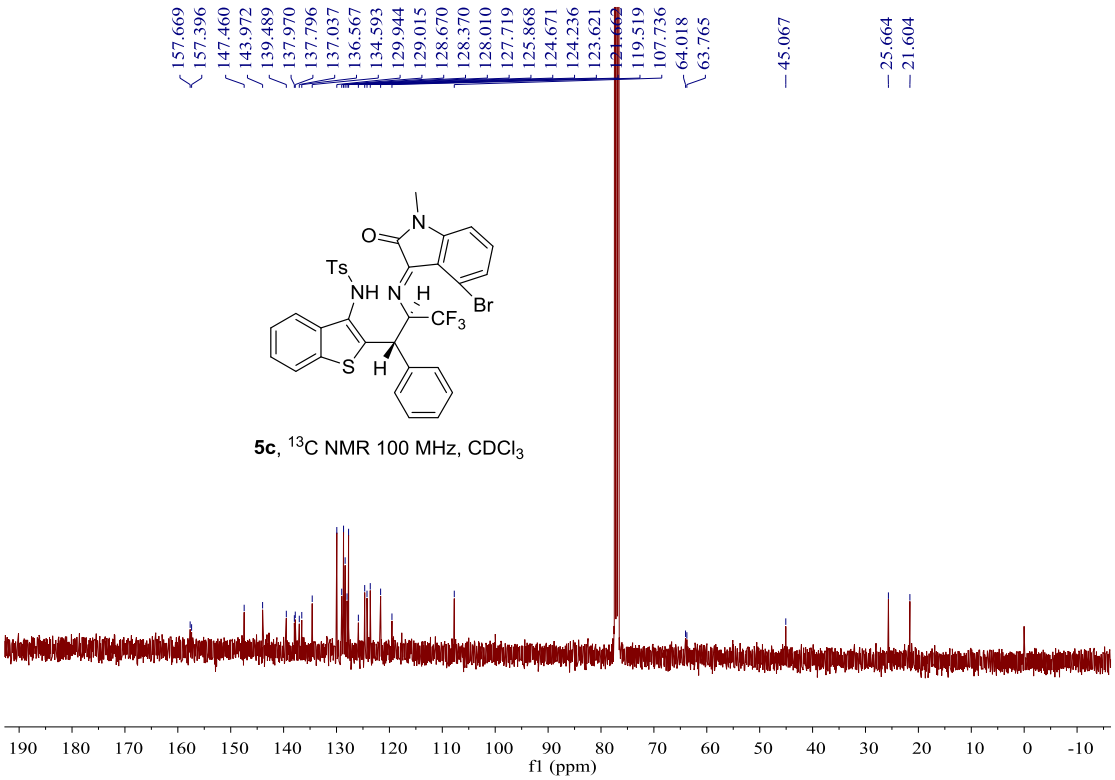

**5b**, $^{13}$C NMR 100 MHz, $CDCl_3$



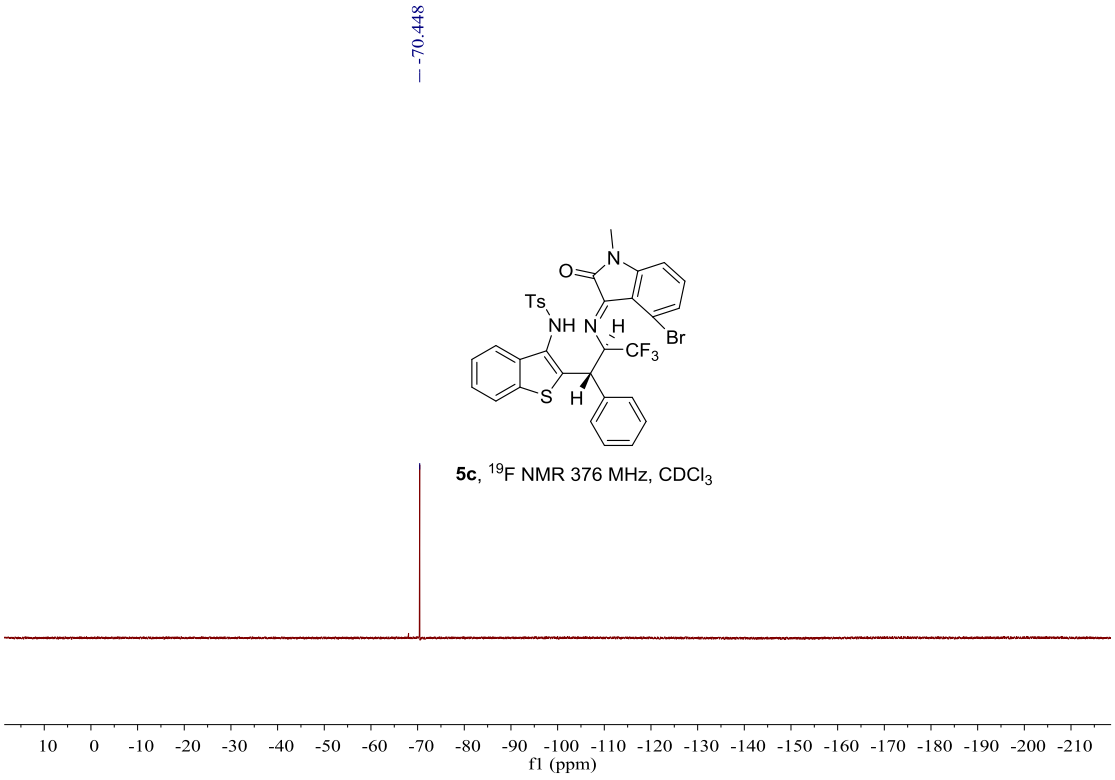

**5b**, $^{19}F$ NMR 376 MHz, $CDCl_3$



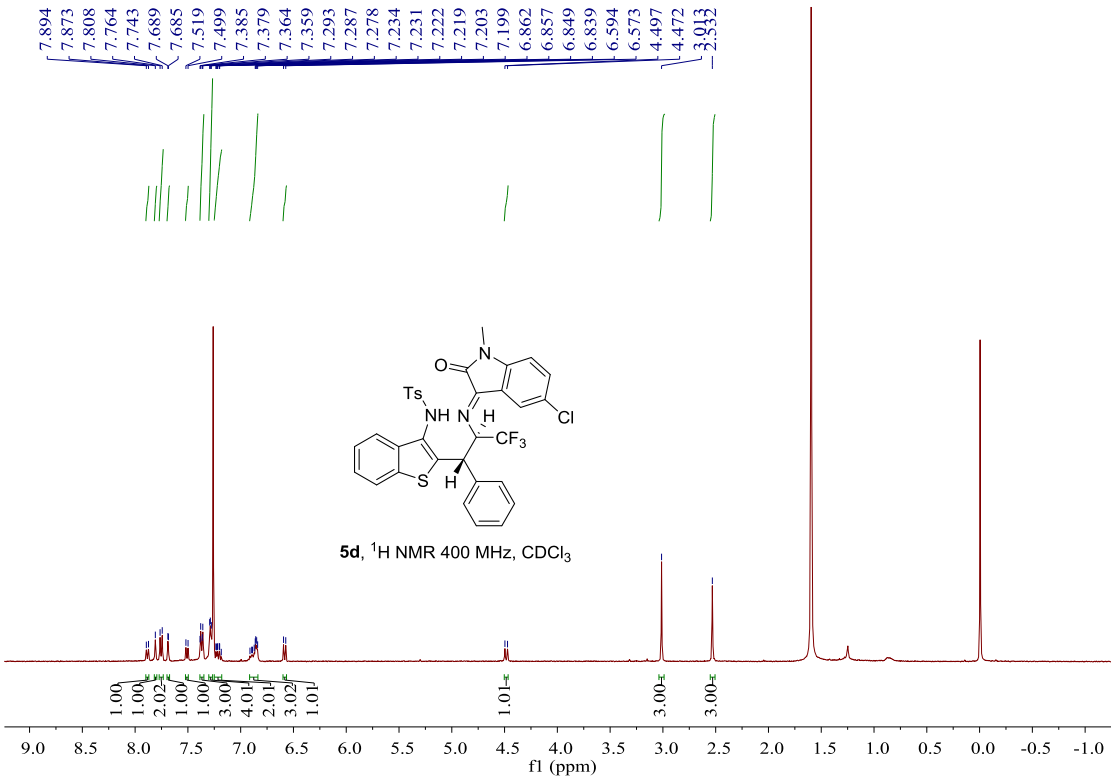

**5c**, $^{1}H$ NMR 400 MHz, $CDCl_3$



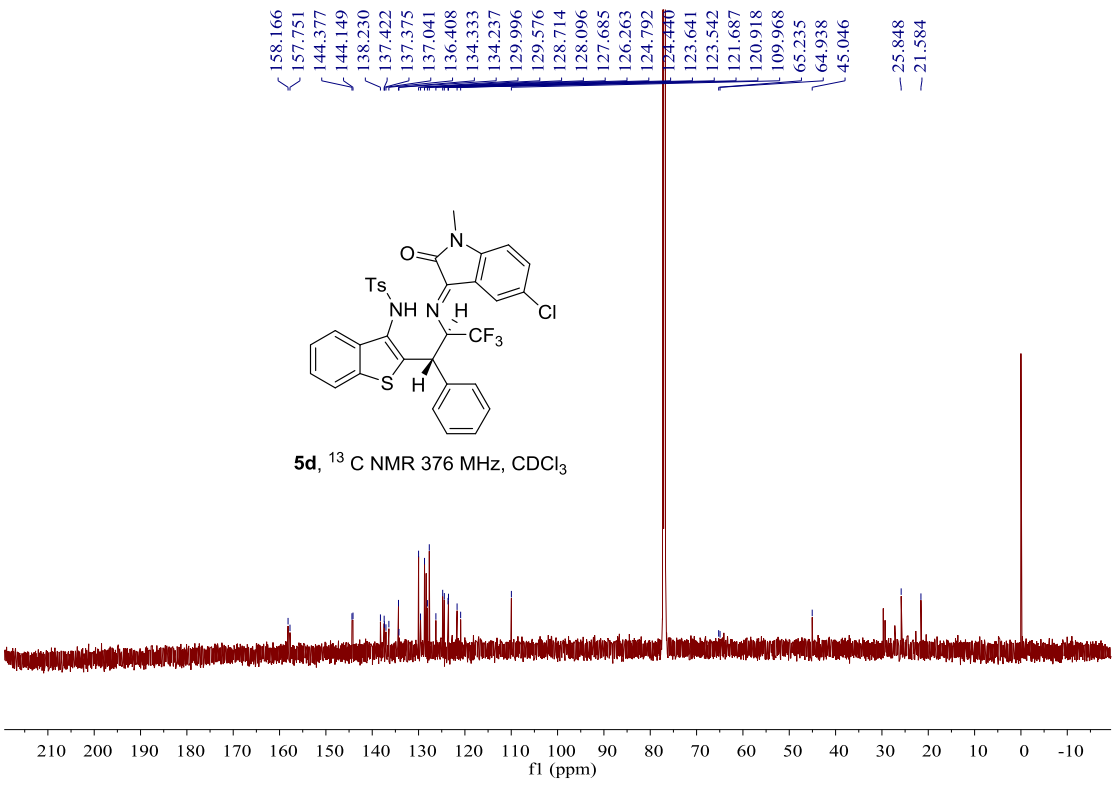

**5c**, $^{13}C$ NMR 100 MHz, $CDCl_3$



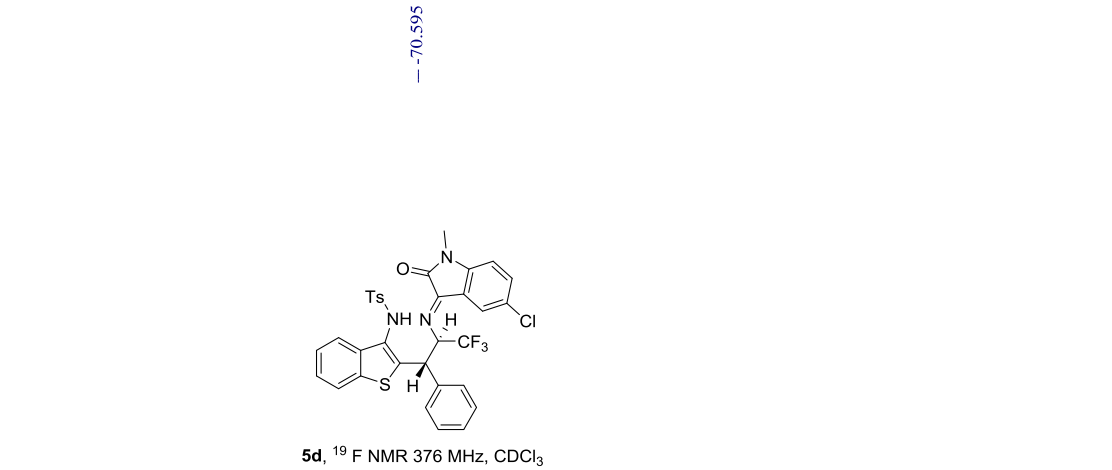

**5c**, $^{19}F$ NMR 376 MHz, $CDCl_3$



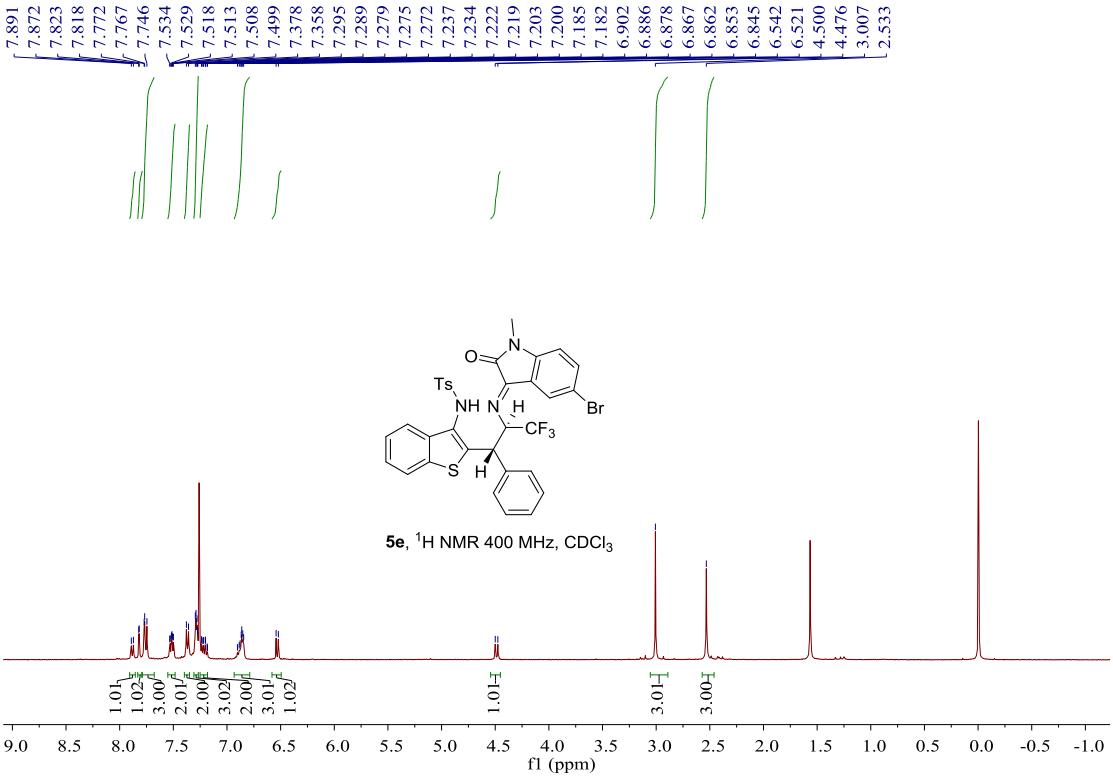

**5d**, $^{1}$H NMR 400 MHz, $CDCl_3$



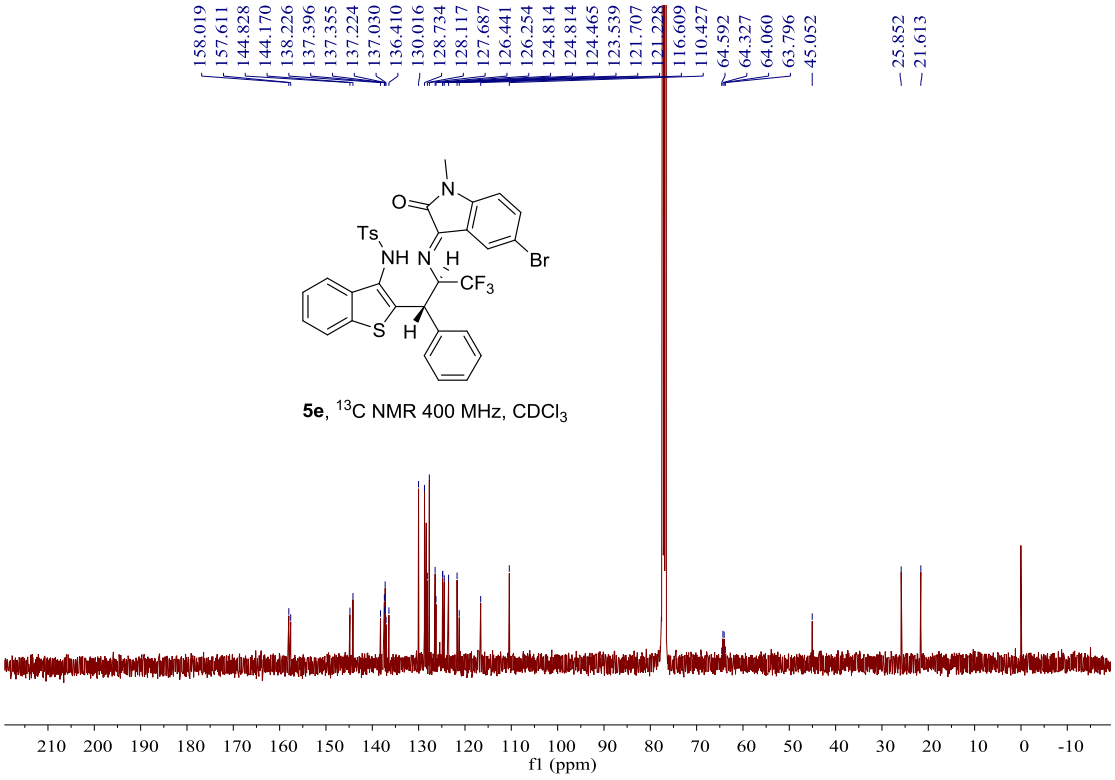

**5d**, $^{13}$ C NMR 376 MHz, $CDCl_3$



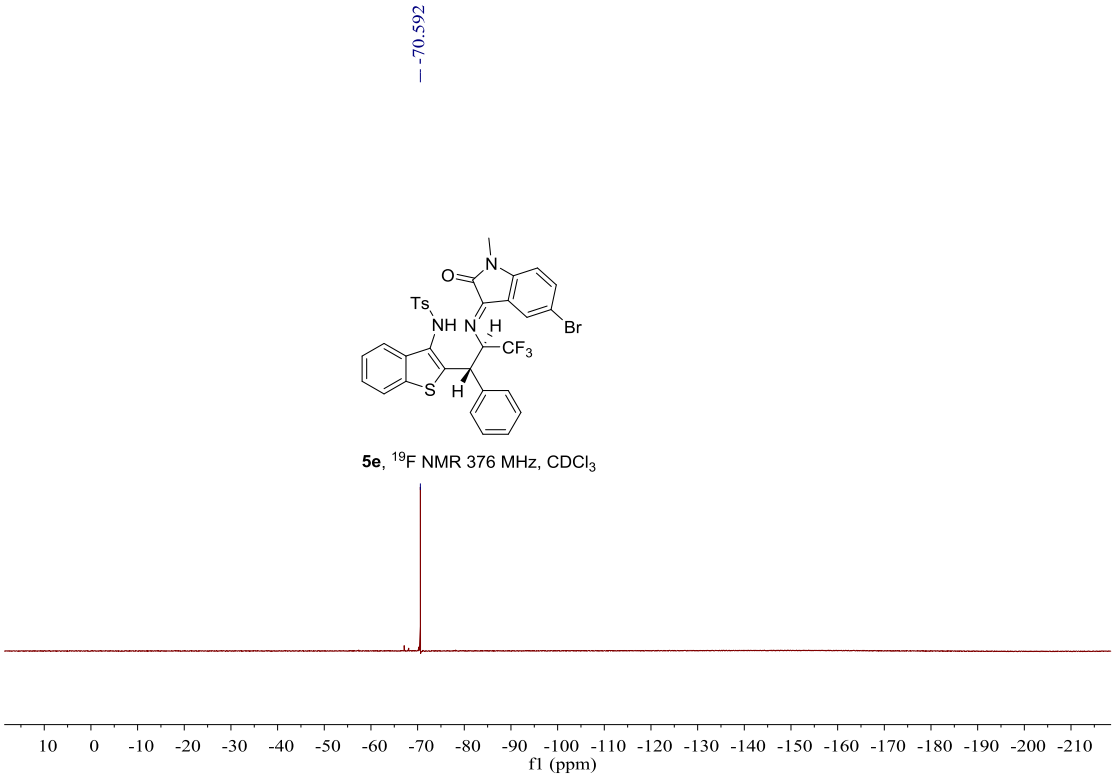

**5d**, $^{19}$F NMR 376 MHz, $CDCl_3$



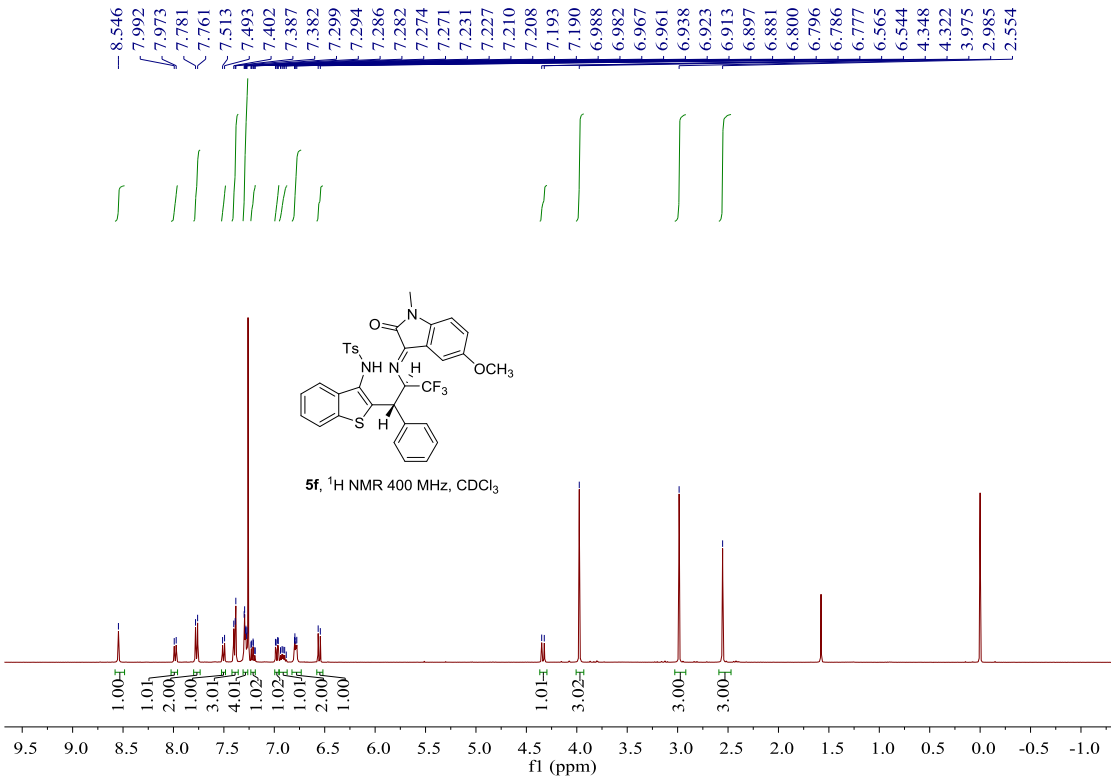

**5e**, $^{1}$H NMR 400 MHz, $CDCl_3$



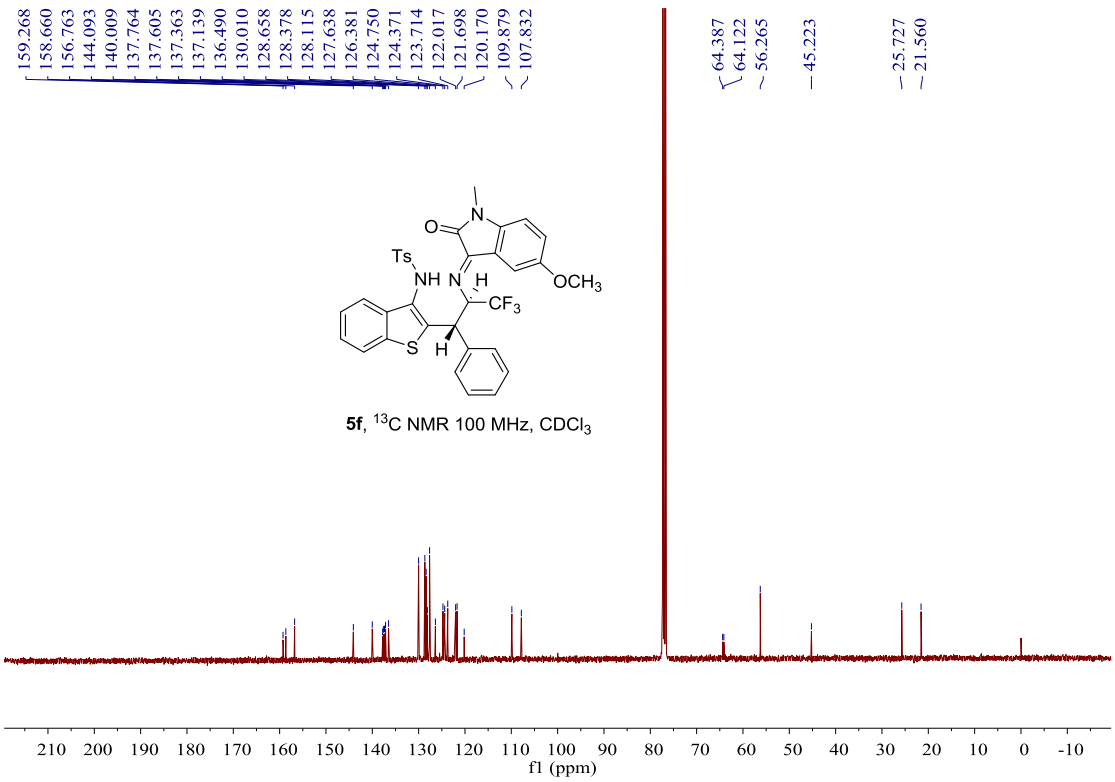

**5e**, $^{13}C$ NMR 400 MHz, $CDCl_3$



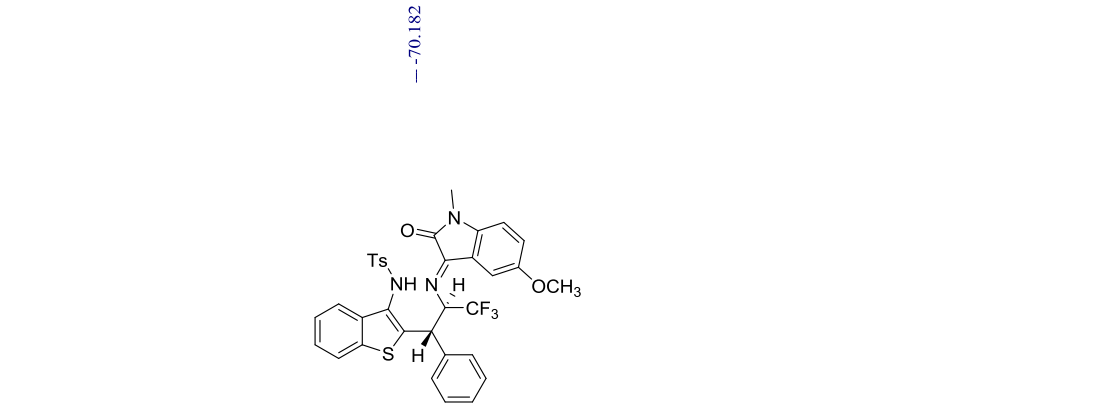

**5e**, $^{19}F$ NMR 376 MHz, $CDCl_3$



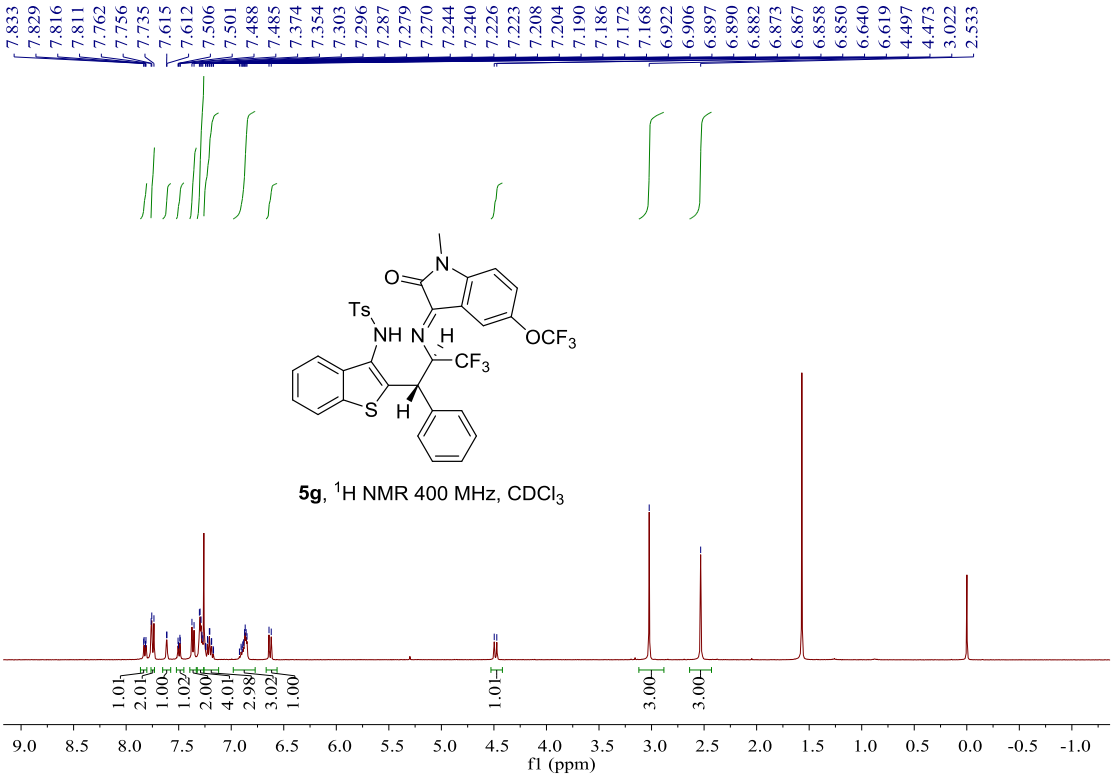

**5f**, $^{1}$H NMR 400 MHz, $CDCl_3$



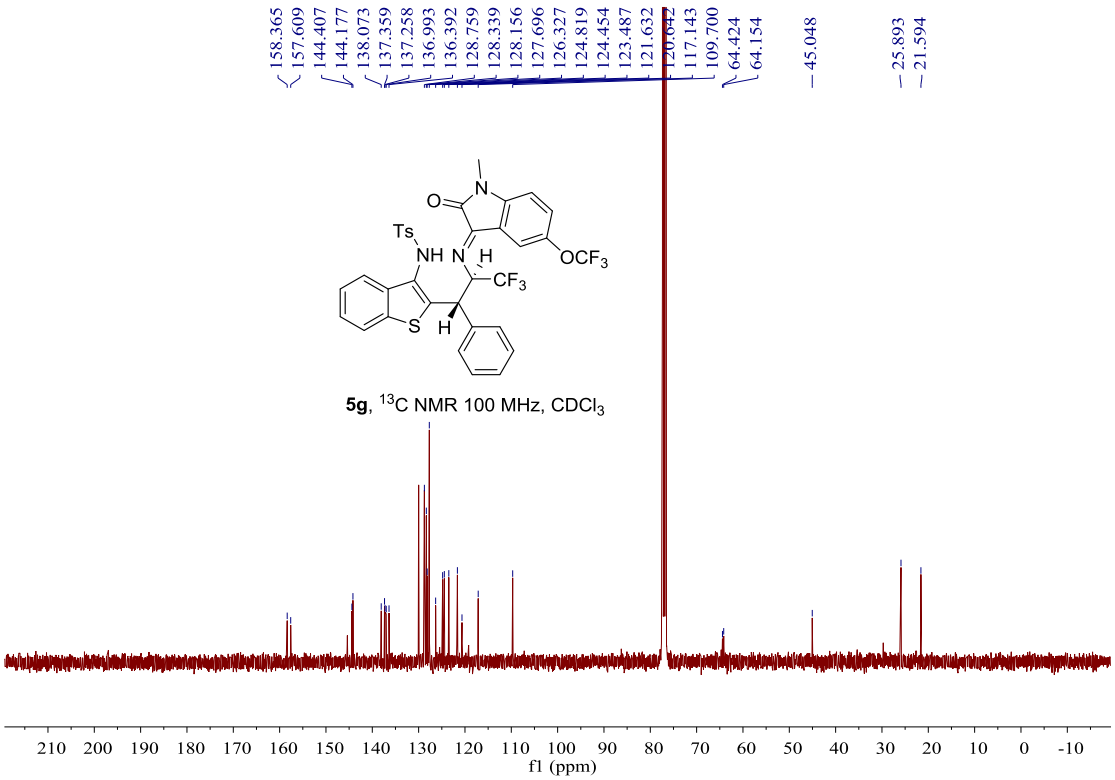

**5f**, $^{13}$C NMR 100 MHz, $CDCl_3$



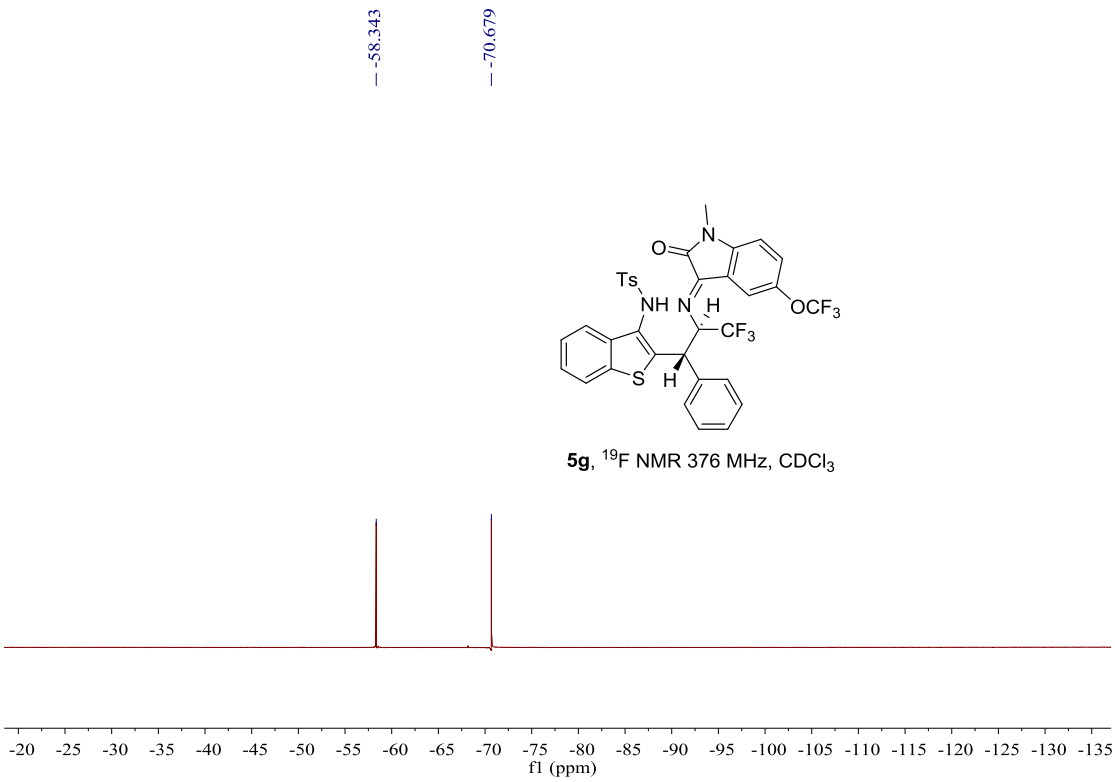

**5f**, $^{19}F$ NMR 376 MHz, $CDCl_3$



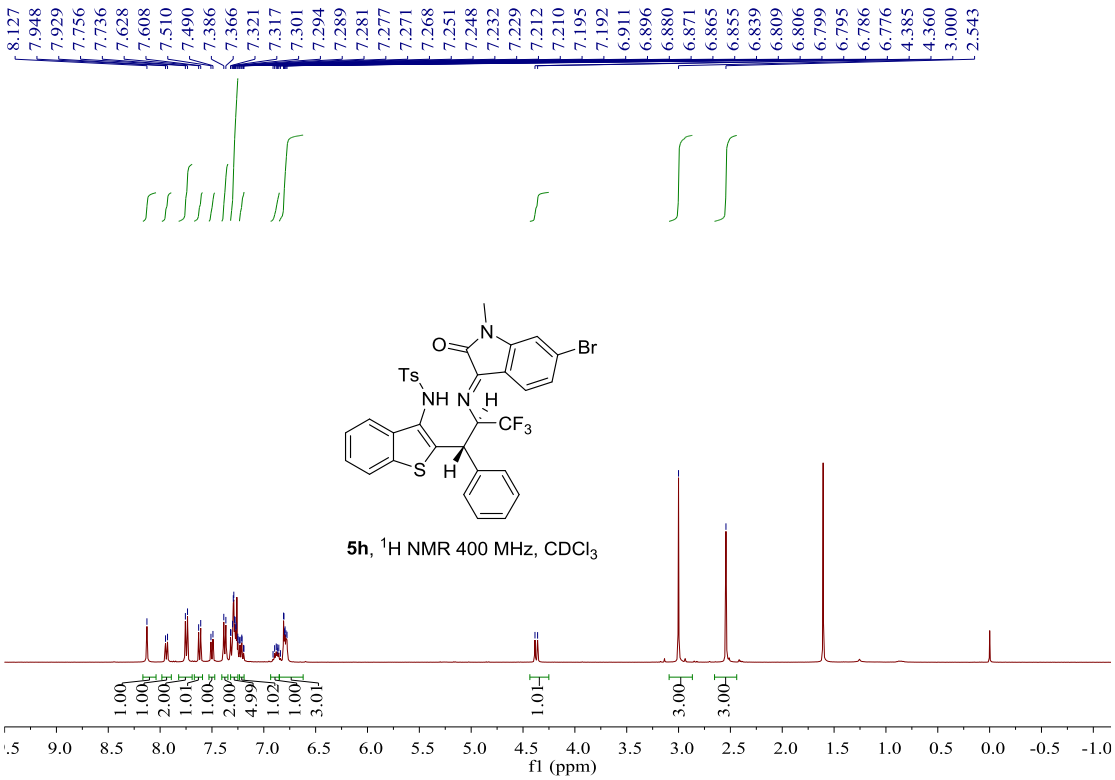

**5g**, $^{1}H$ NMR 400 MHz, $CDCl_3$



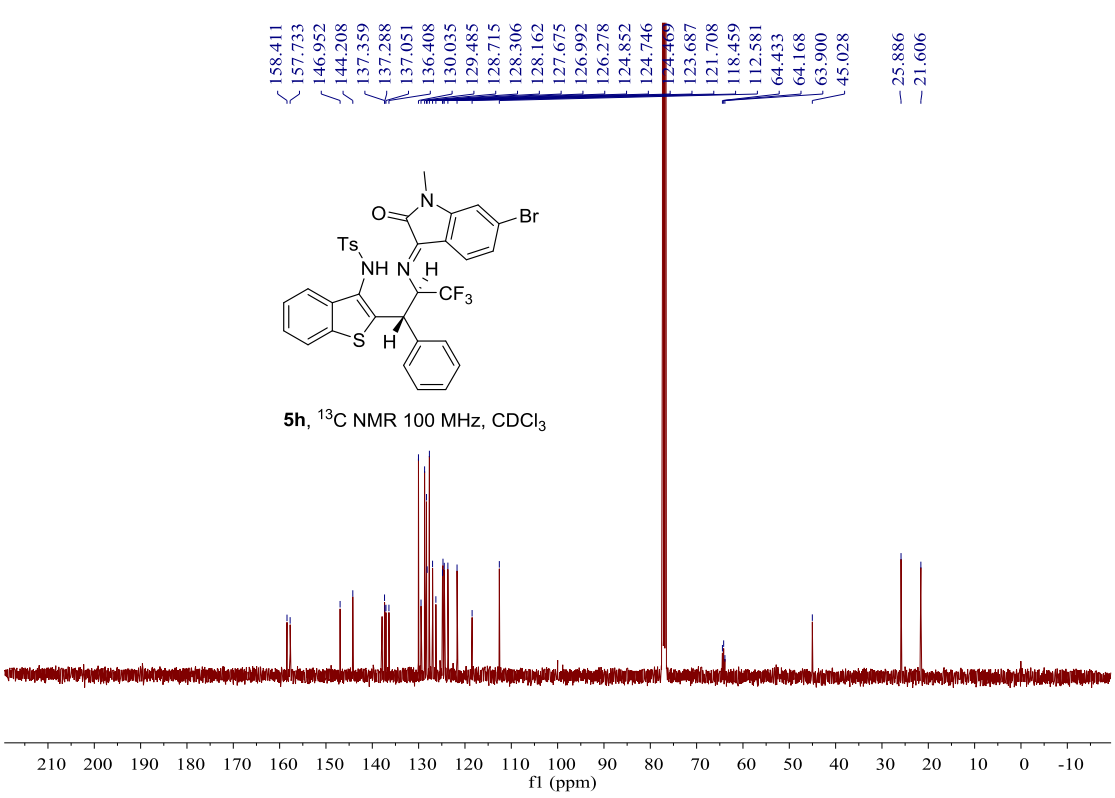

**5g**, $^{13}C$ NMR 100 MHz, $CDCl_3$



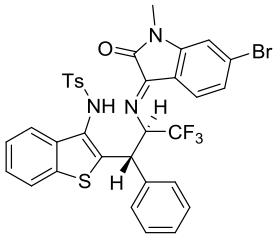

**5g**, $^{19}F$ NMR 376 MHz, $CDCl_3$



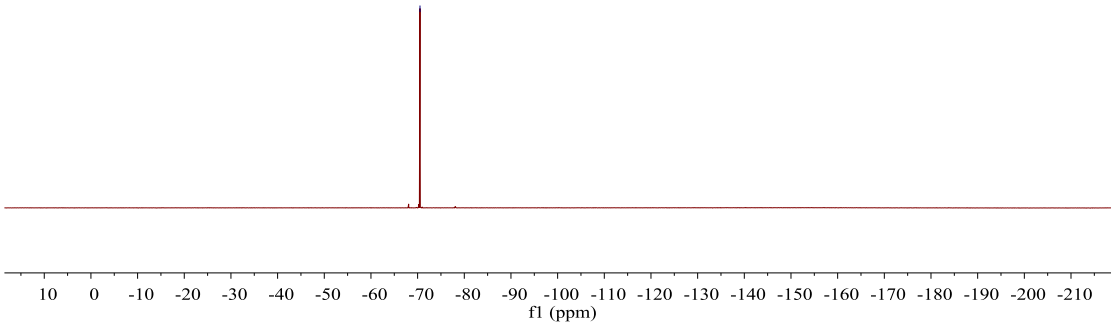

**5h**, $^{1}$H NMR 400 MHz, $CDCl_3$

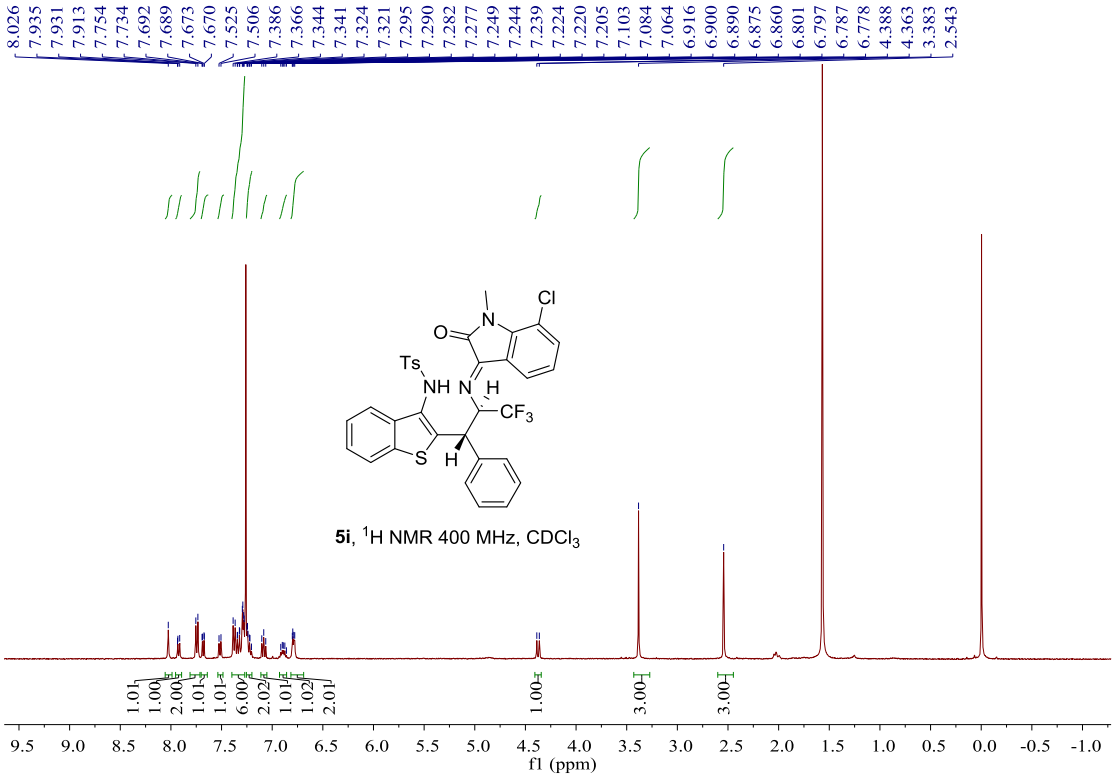



**5h**, $^{13}$C NMR 100 MHz, $CDCl_3$




**5h**, $^{19}F$ NMR 376 MHz, $CDCl_3$

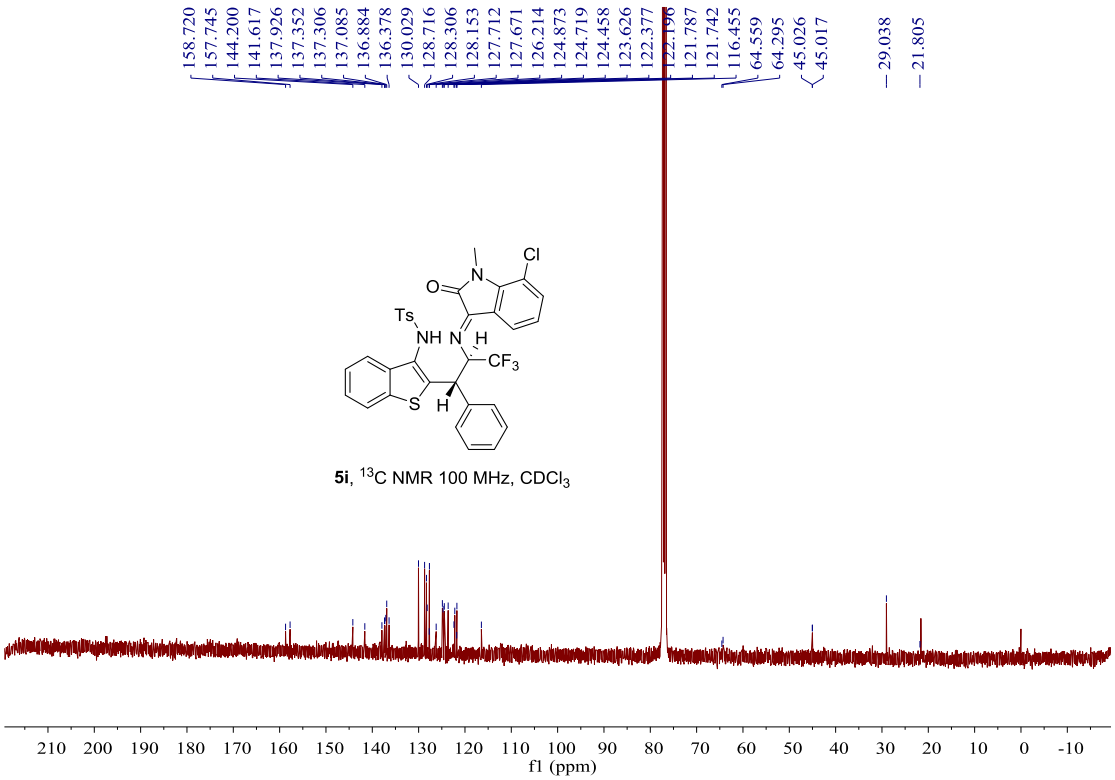


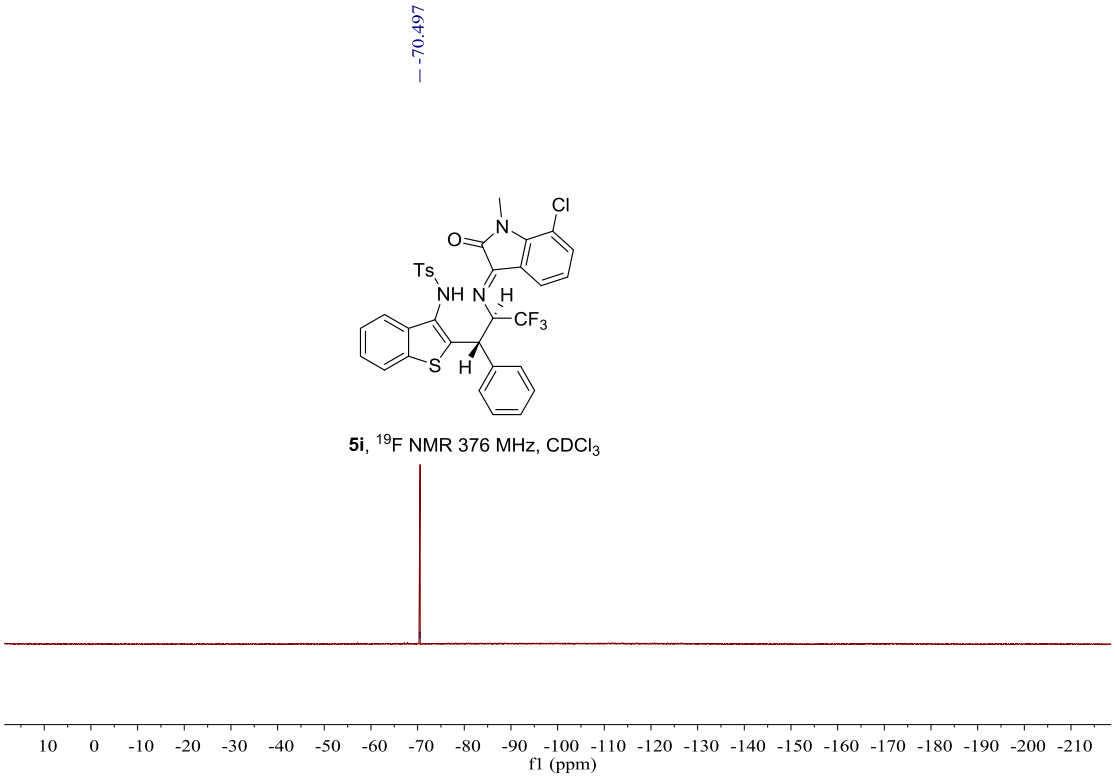




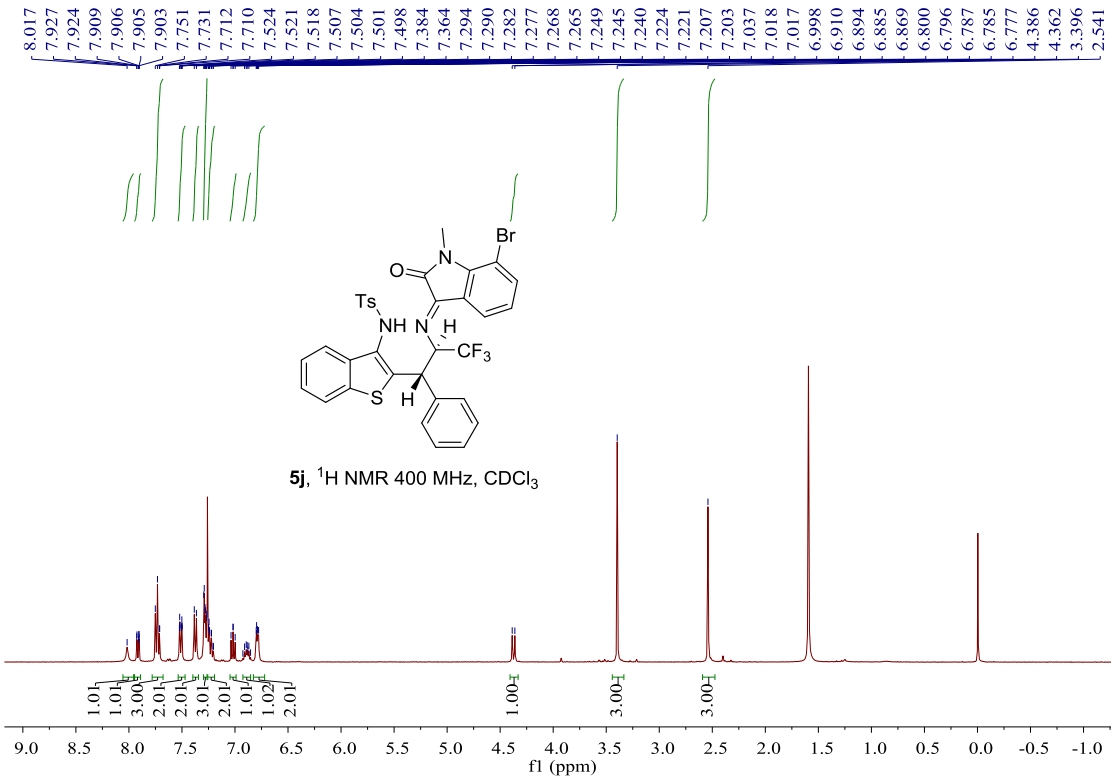
**5i**, $^{1}H$ NMR 400 MHz, $CDCl_3$



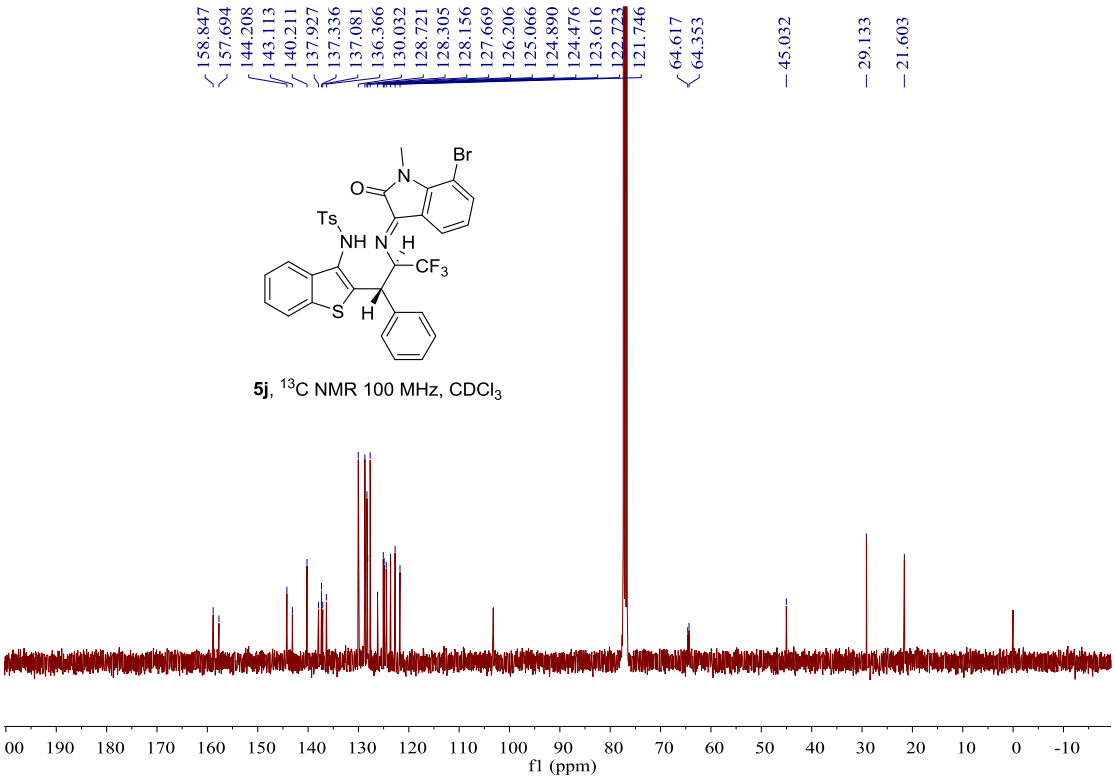

**5i**, $^{13}C$ NMR 100 MHz, $CDCl_3$



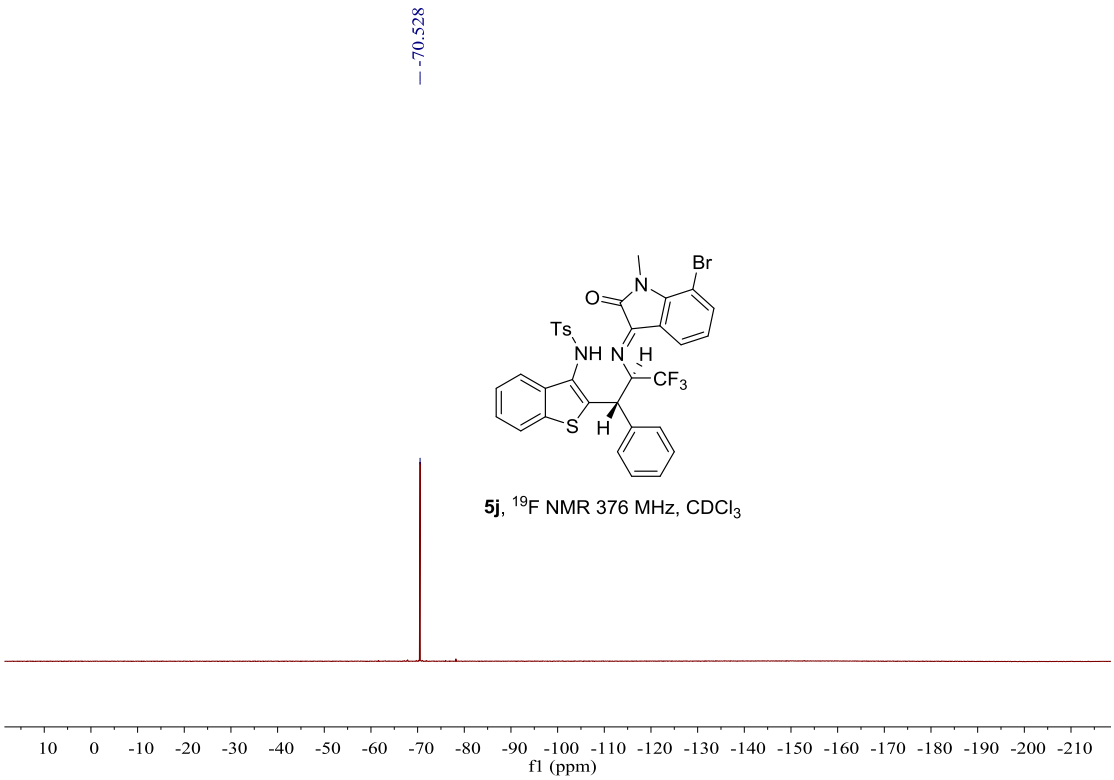

**5i**, $^{19}F$ NMR 376 MHz, $CDCl_3$




**5j**, $^{1}$H NMR 400 MHz, $CDCl_3$




**5j**, $^{13}$C NMR 100 MHz, $CDCl_3$

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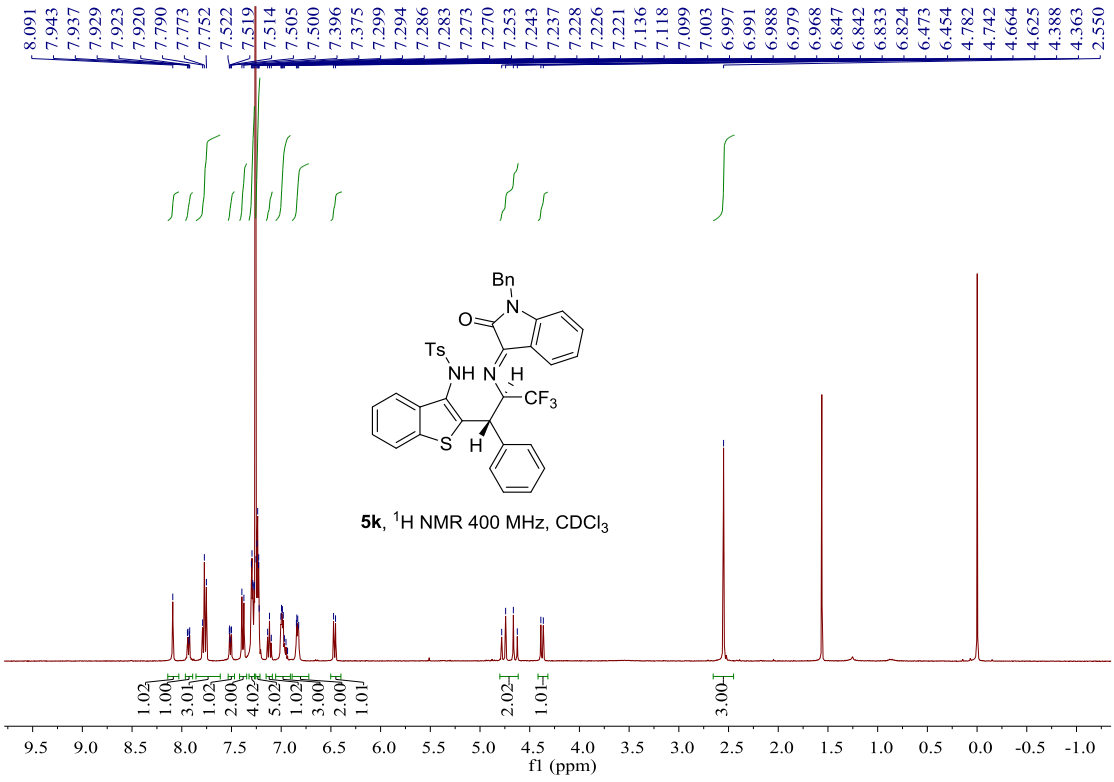
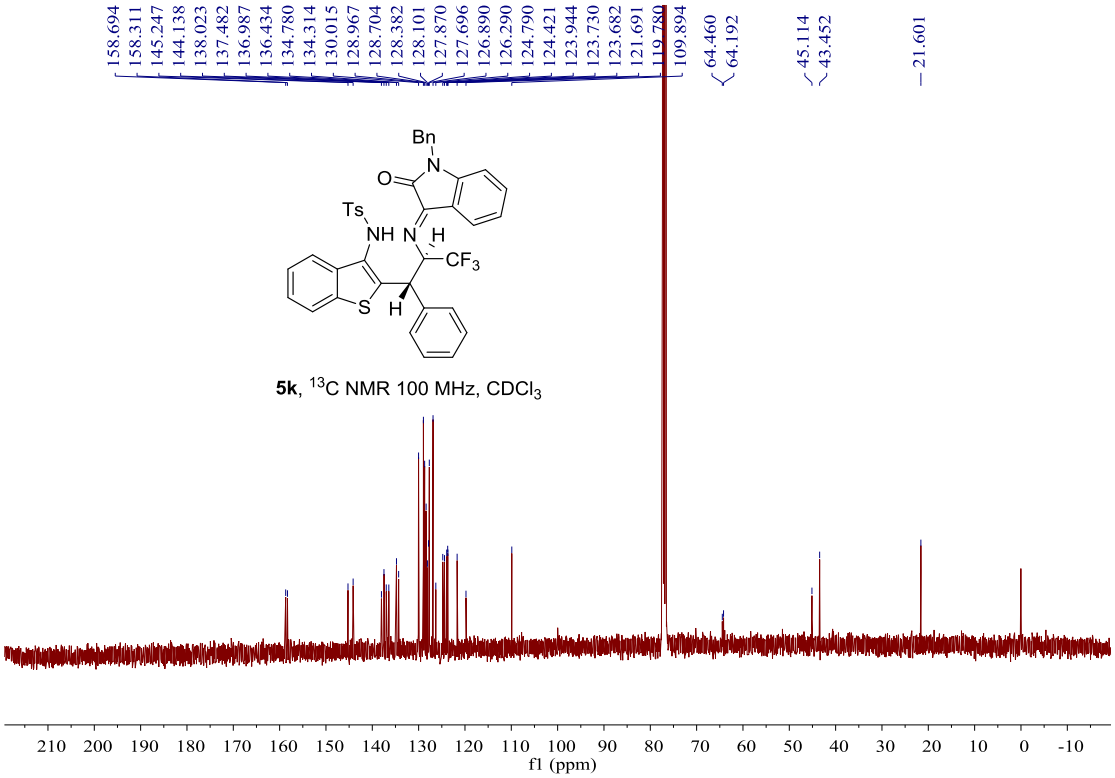
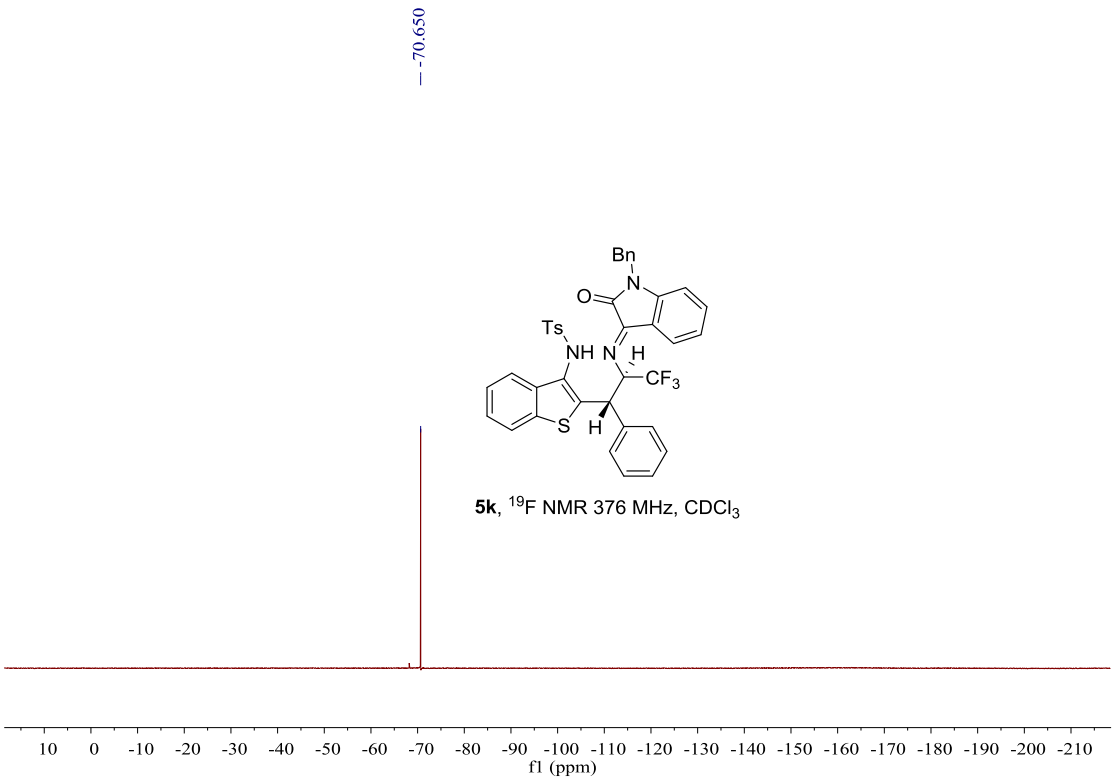


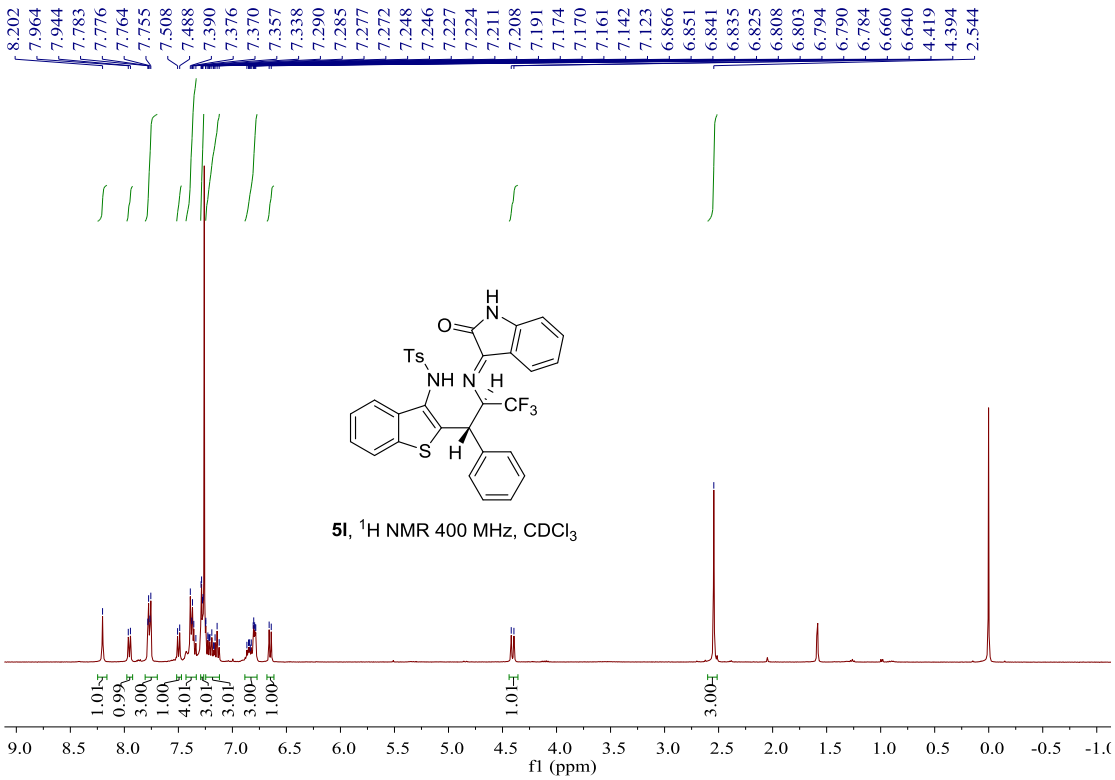

**5k**, $^{1}H$ NMR 400 MHz, $CDCl_3$



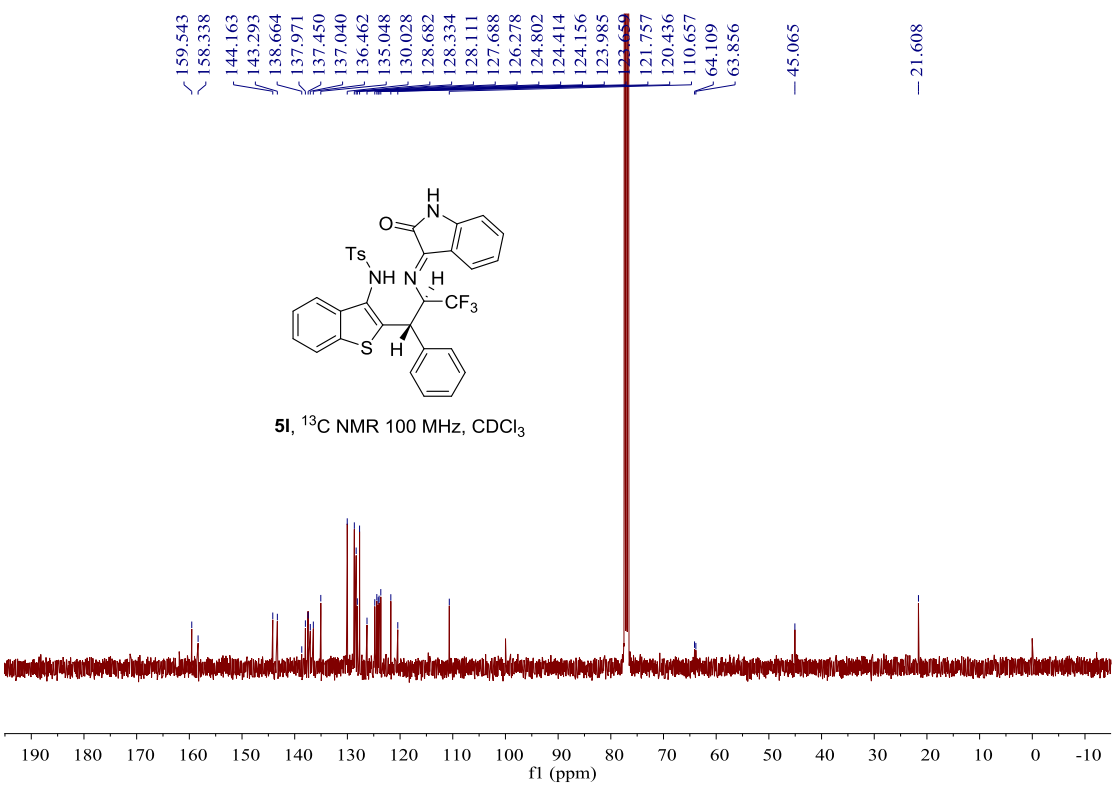

**5k**, $^{13}C$ NMR 100 MHz, $CDCl_3$



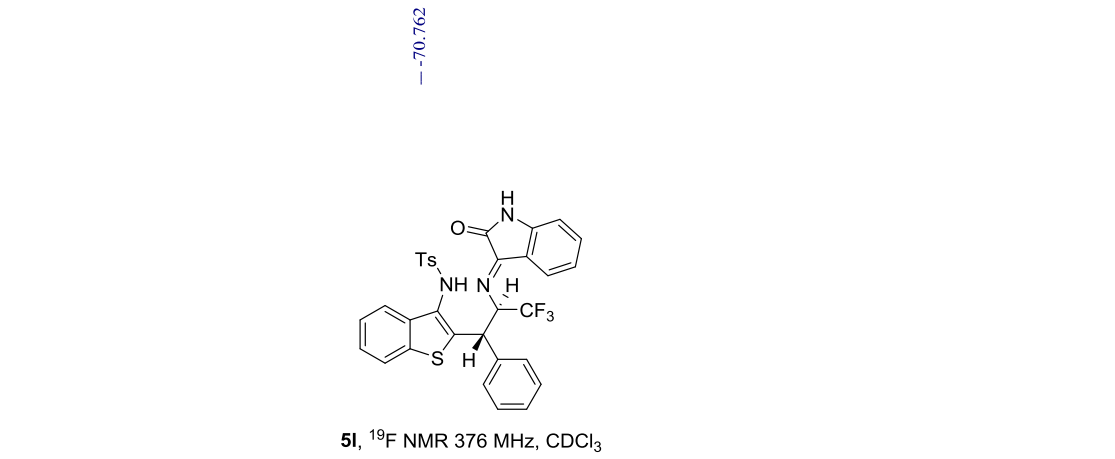

**5k**, $^{19}F$ NMR 376 MHz, $CDCl_3$



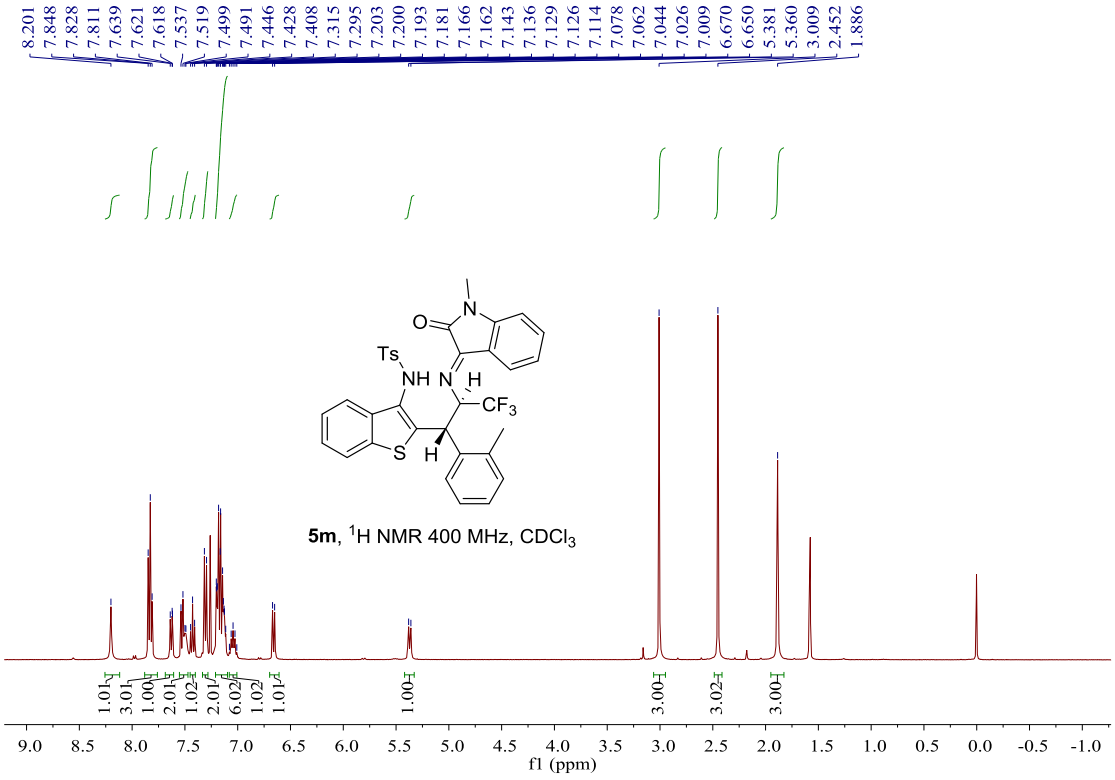

**5l**, $^{1}$H NMR 400 MHz, $CDCl_3$



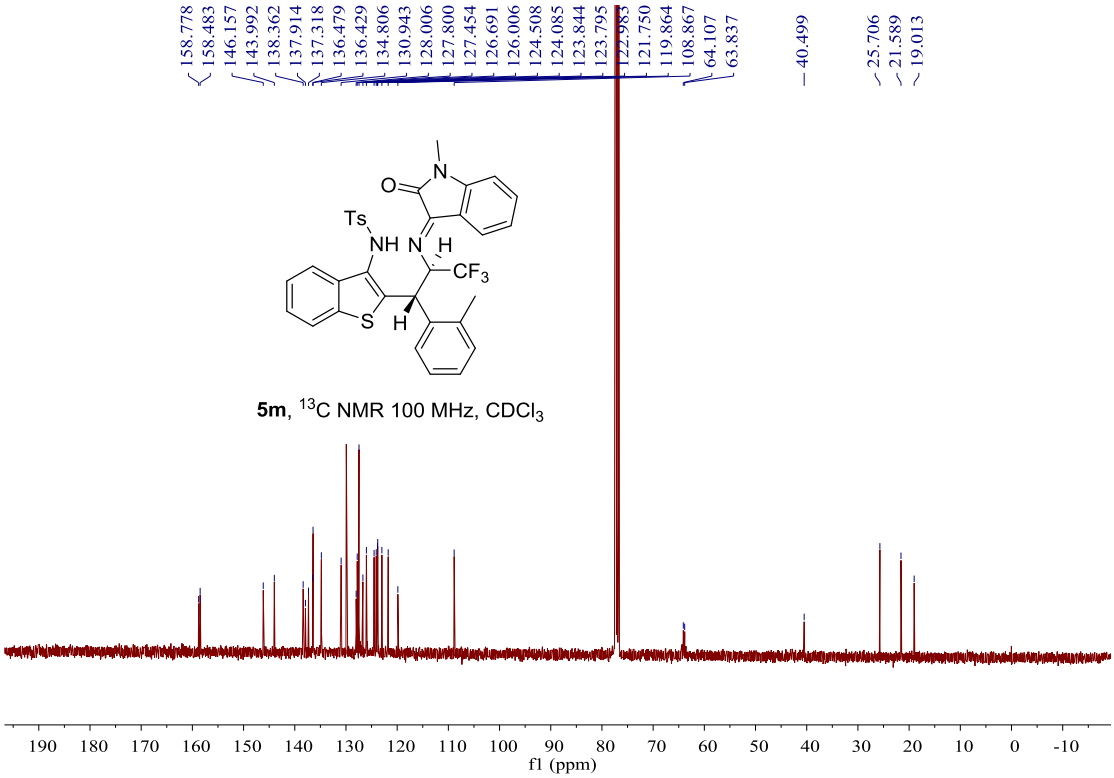

**5l**, $^{13}$C NMR 100 MHz, $CDCl_3$



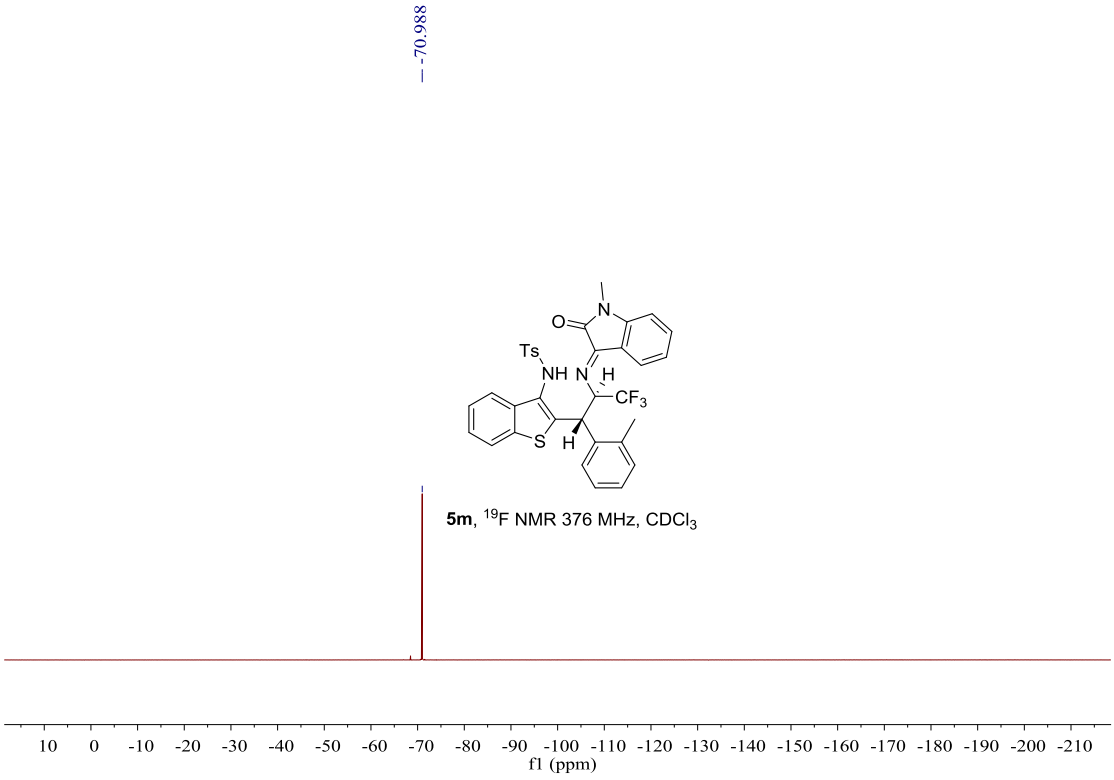

**5l**, $^{19}F$ NMR 376 MHz, $CDCl_3$



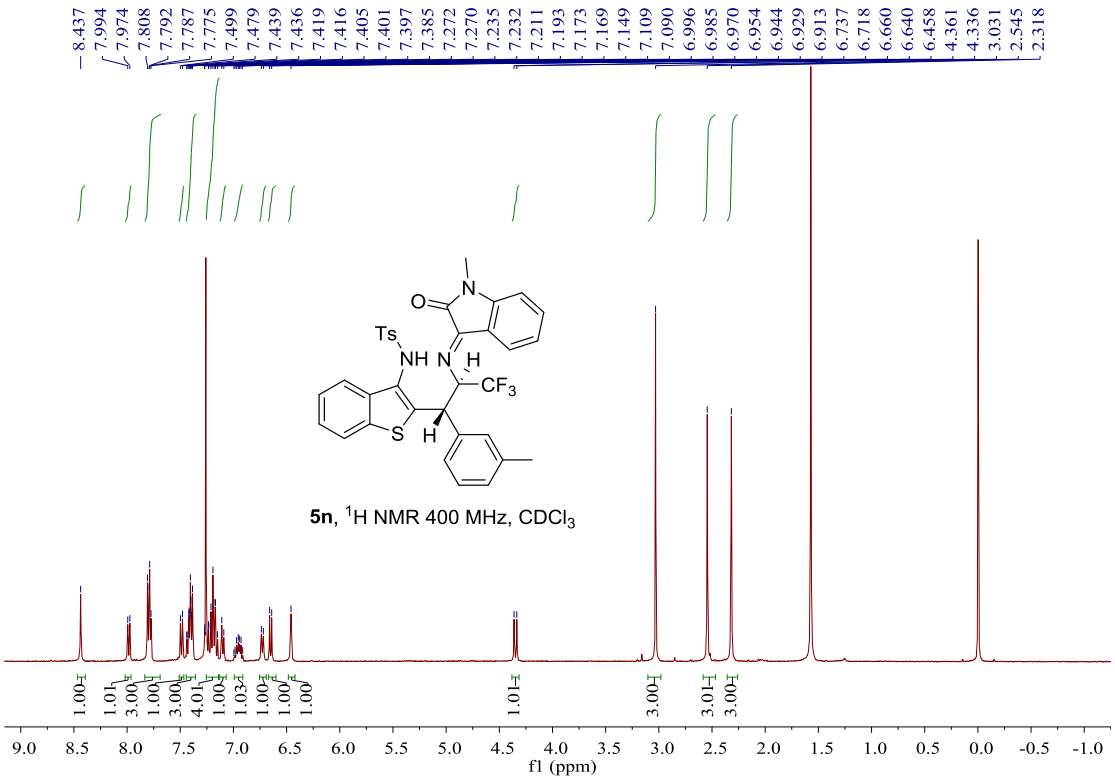

**5m**, $^{1}H$ NMR 400 MHz, $CDCl_3$



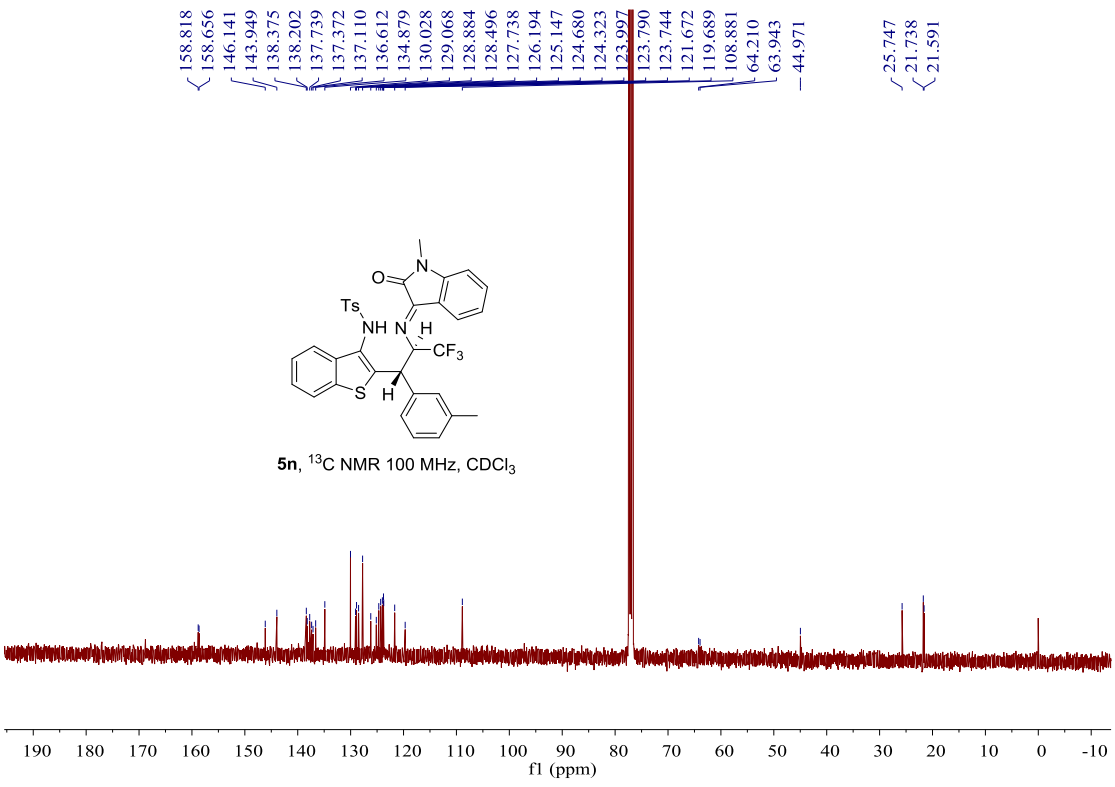

**5m**, $^{13}C$ NMR 100 MHz, $CDCl_3$



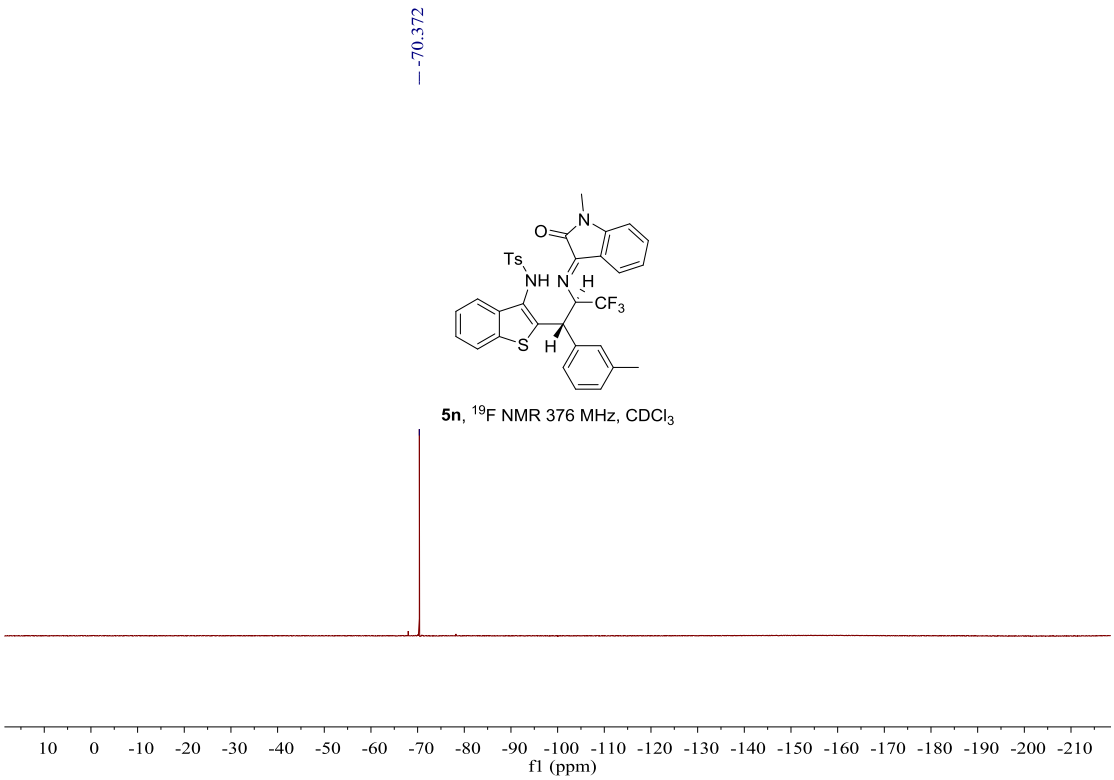

**5m**, $^{19}F$ NMR 376 MHz, $CDCl_3$



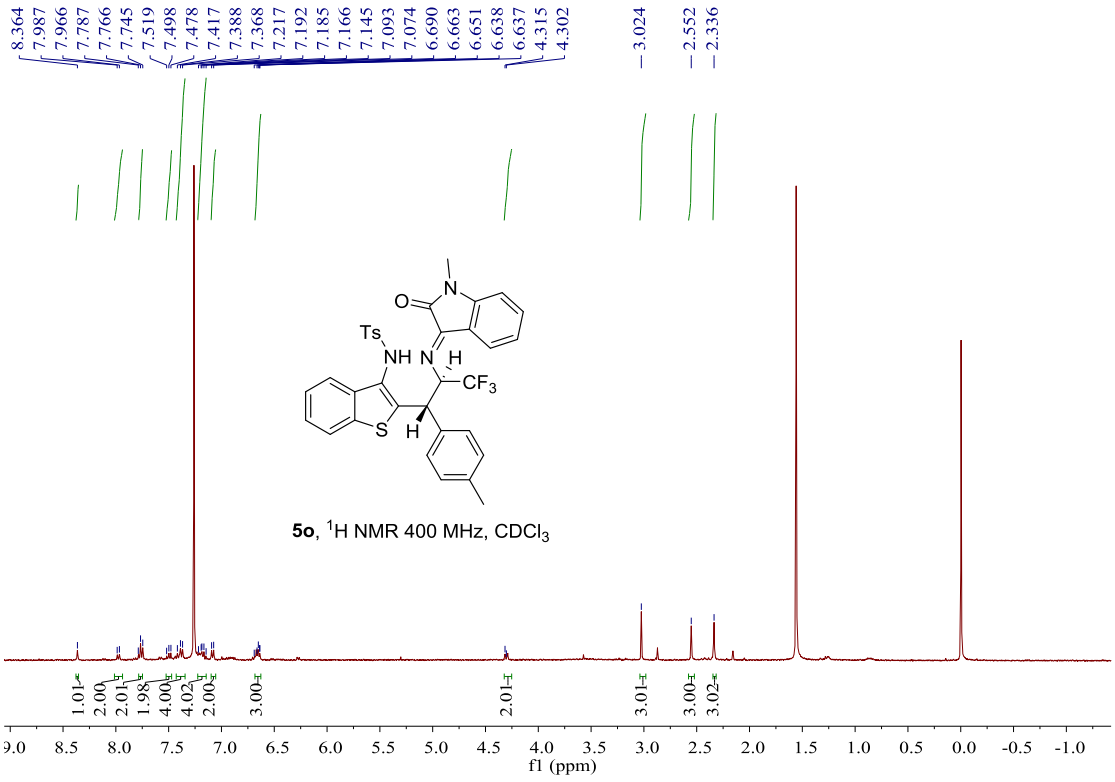

**5n**, $^{1}$H NMR 400 MHz, $CDCl_3$



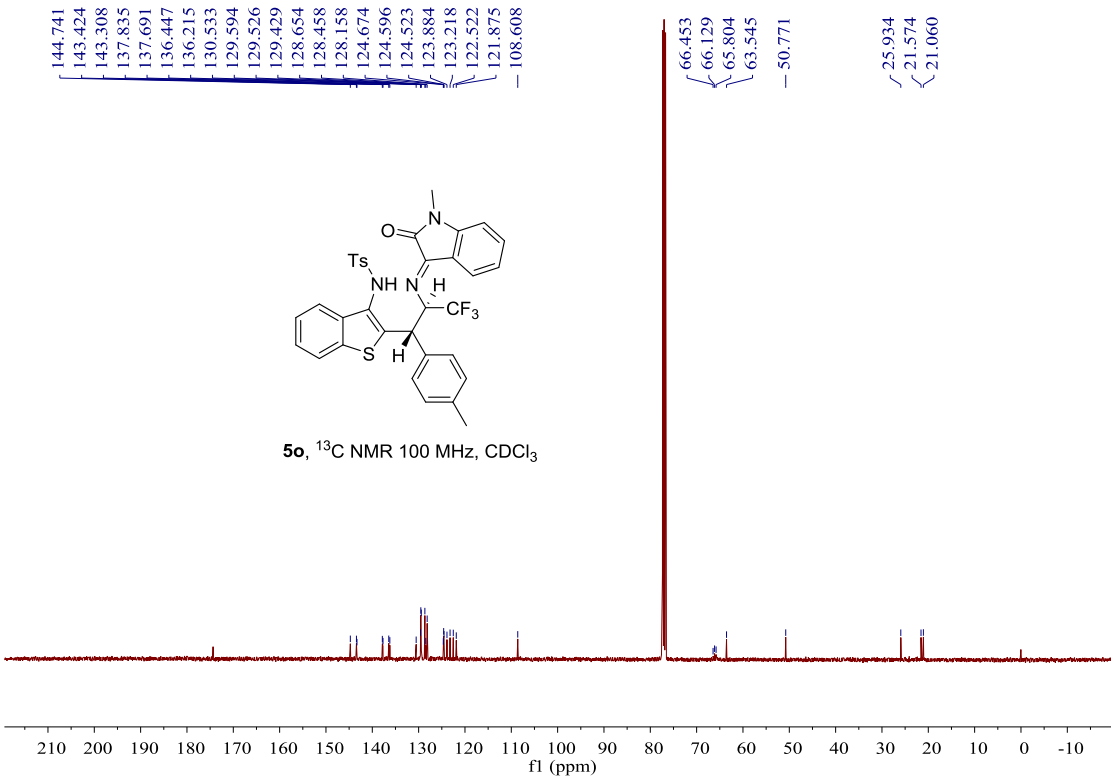

**5n**, $^{13}$C NMR 100 MHz, $CDCl_3$



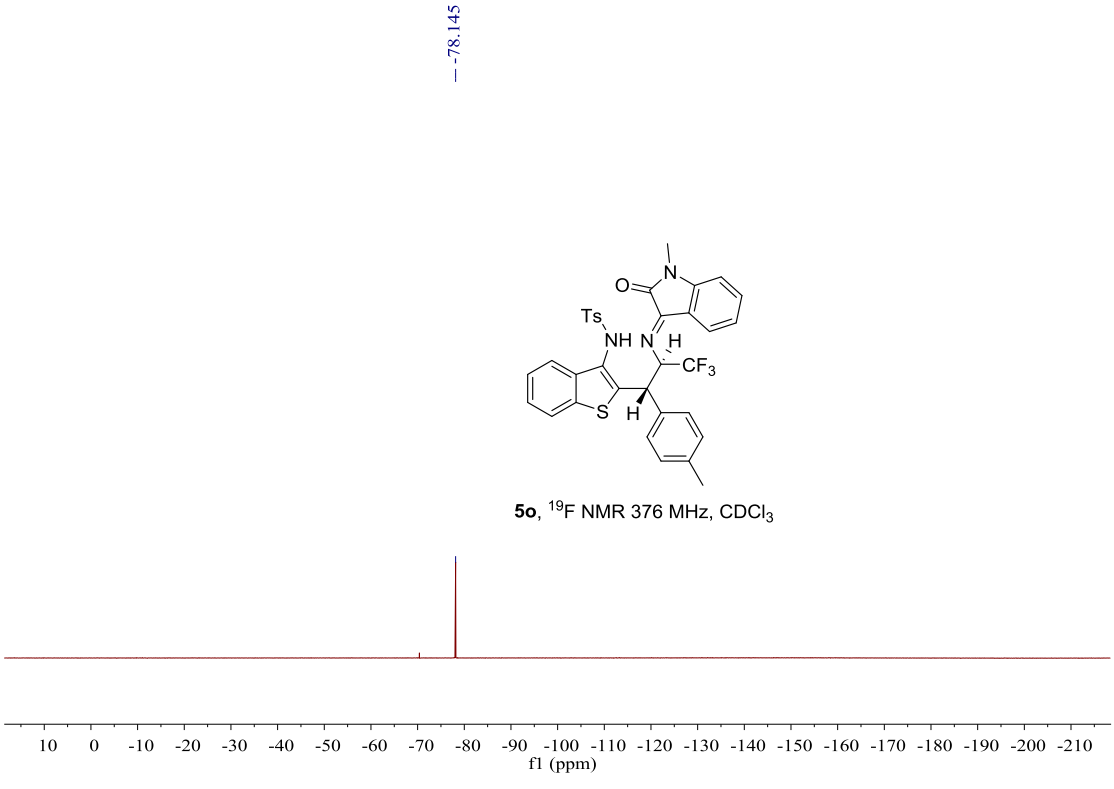

**5n**, $^{19}$F NMR 376 MHz, $CDCl_3$



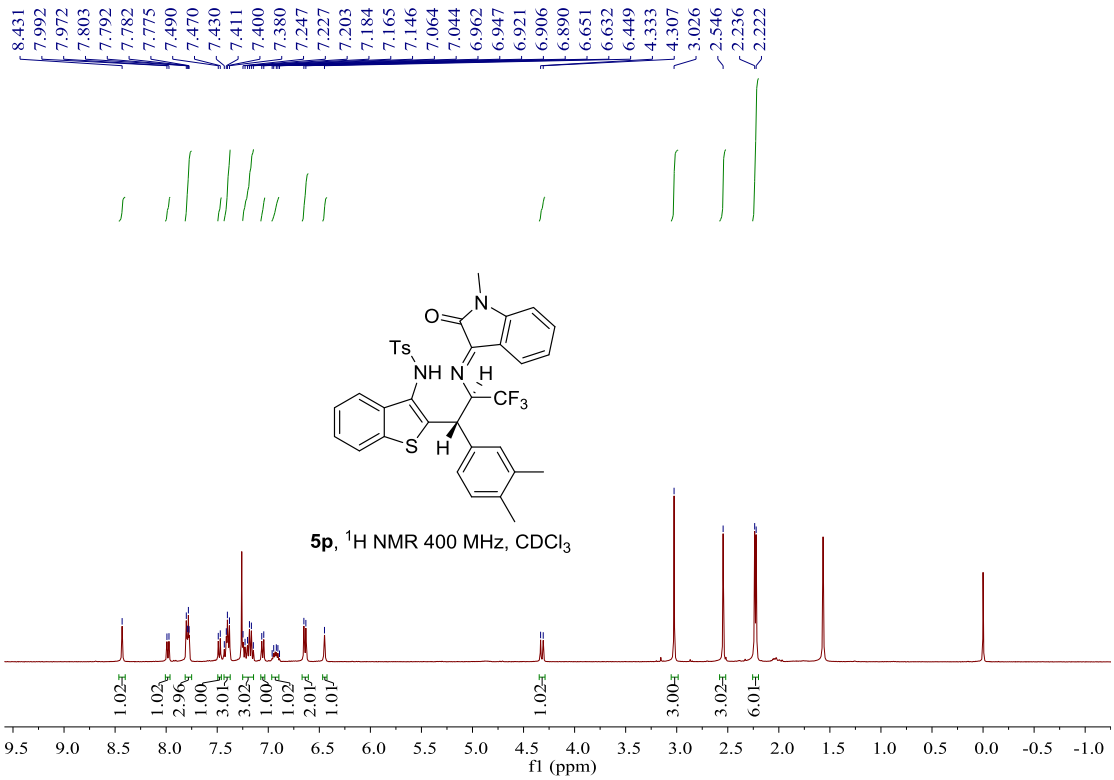

**5o**, $^{1}$H NMR 400 MHz, $CDCl_3$



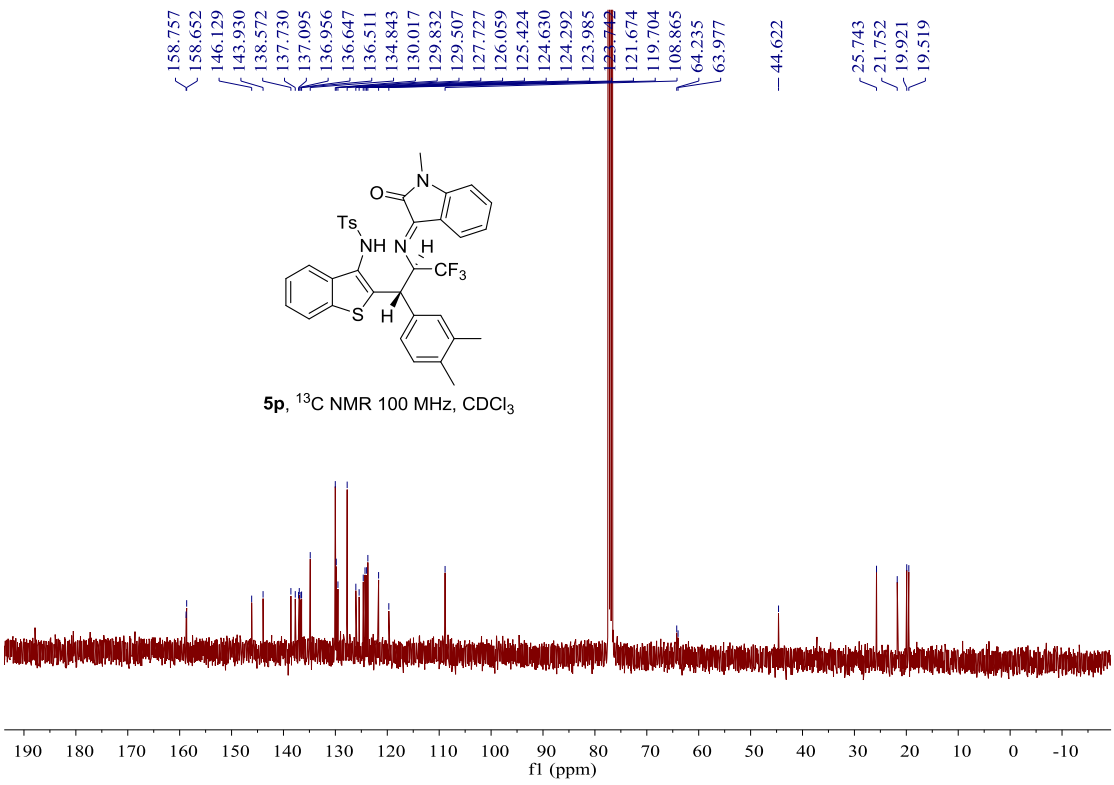

**5o**, $^{13}C$ NMR 100 MHz, $CDCl_3$



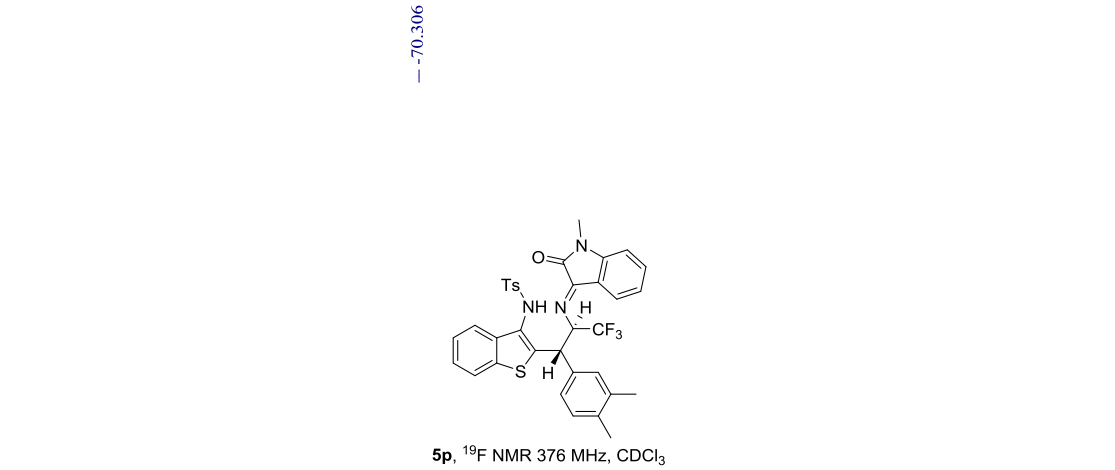

**5o**, $^{19}F$ NMR 376 MHz, $CDCl_3$



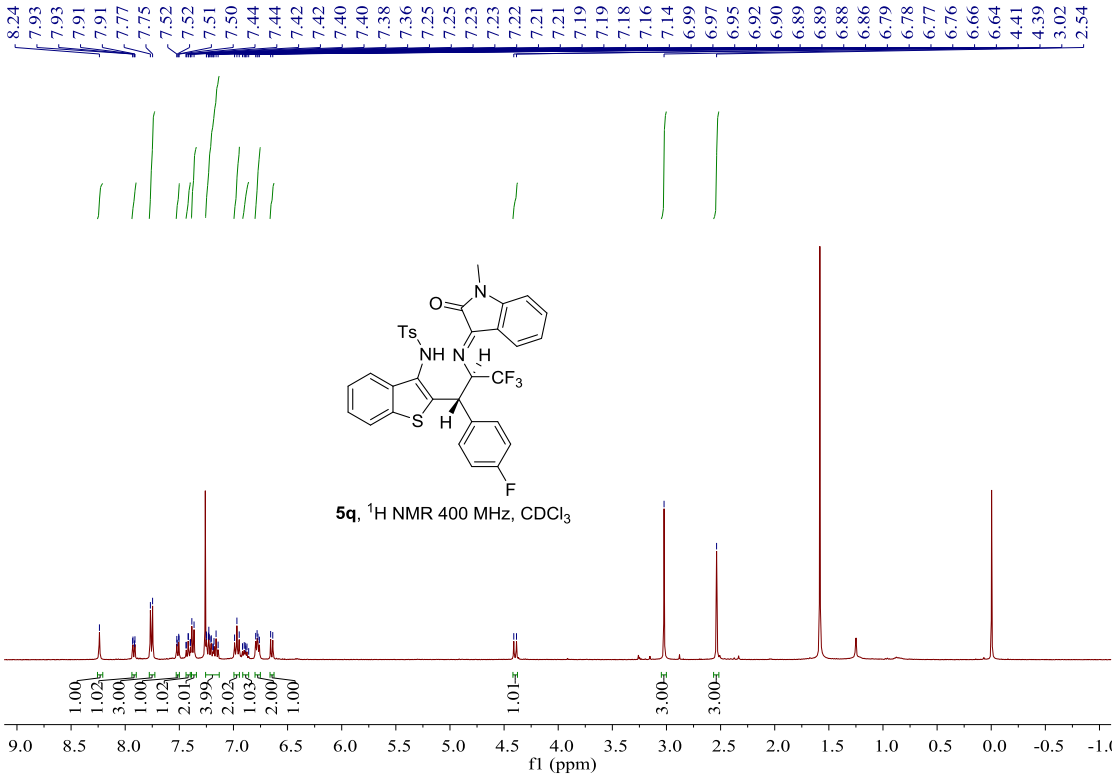

**5p**, $^{1}$H NMR 400 MHz, $CDCl_3$



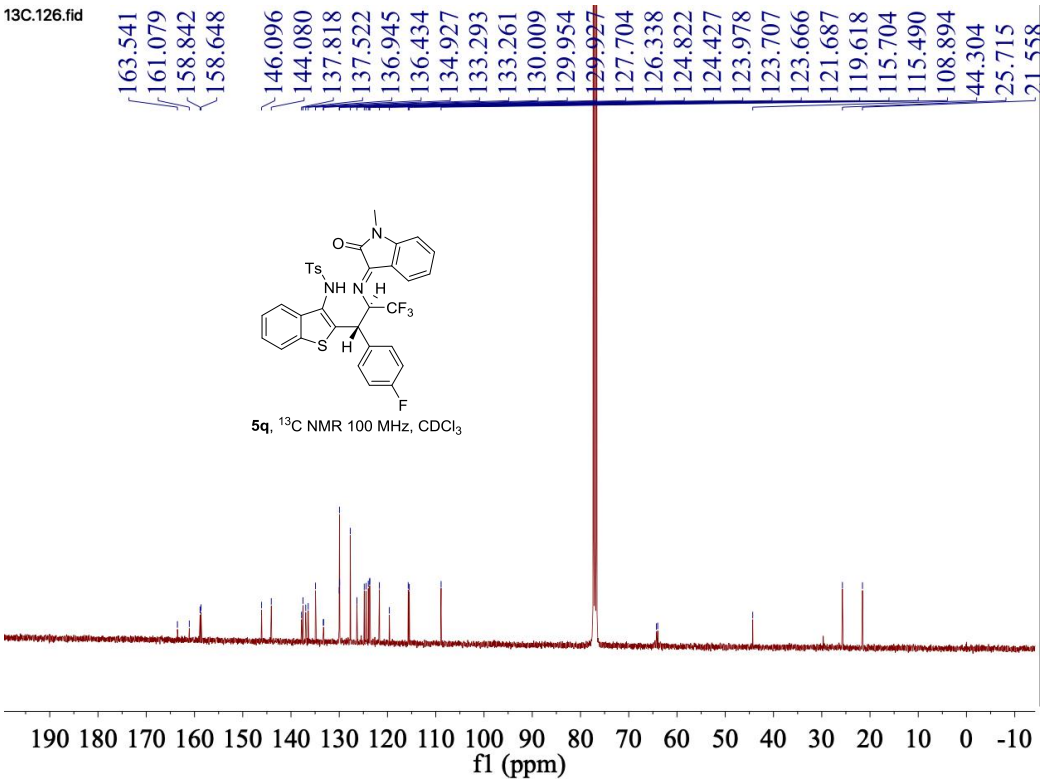

**5p**, $^{13}$C NMR 100 MHz, $CDCl_3$



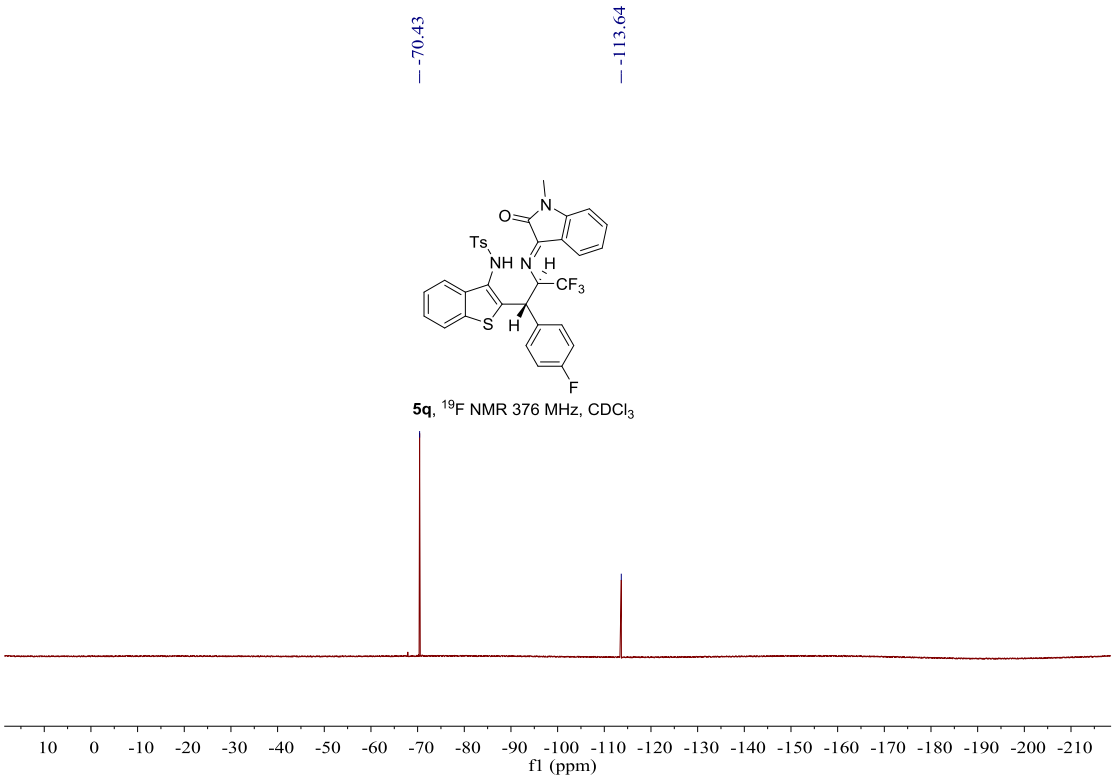

**5p**, $^{19}F$ NMR 376 MHz, $CDCl_3$



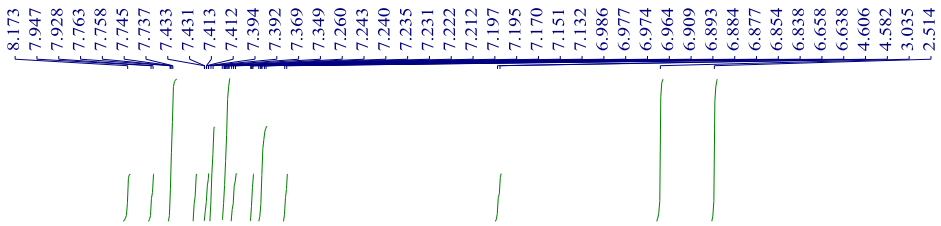

**5q**, $^{1}H$ NMR 400 MHz, $CDCl_3$

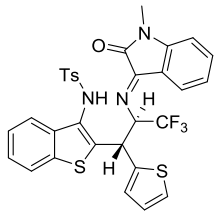



**5q**, $^{13}C$ NMR 100 MHz, $CDCl_3$

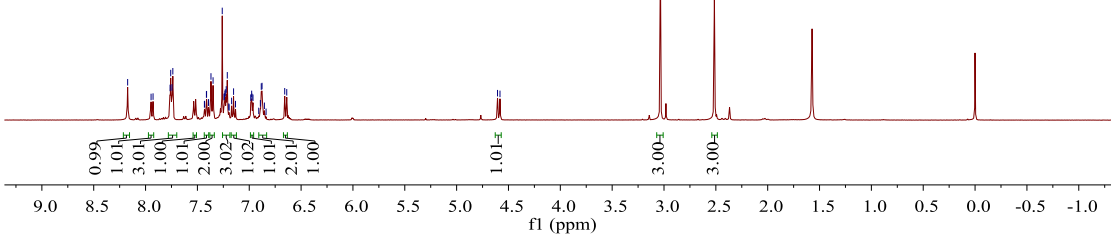


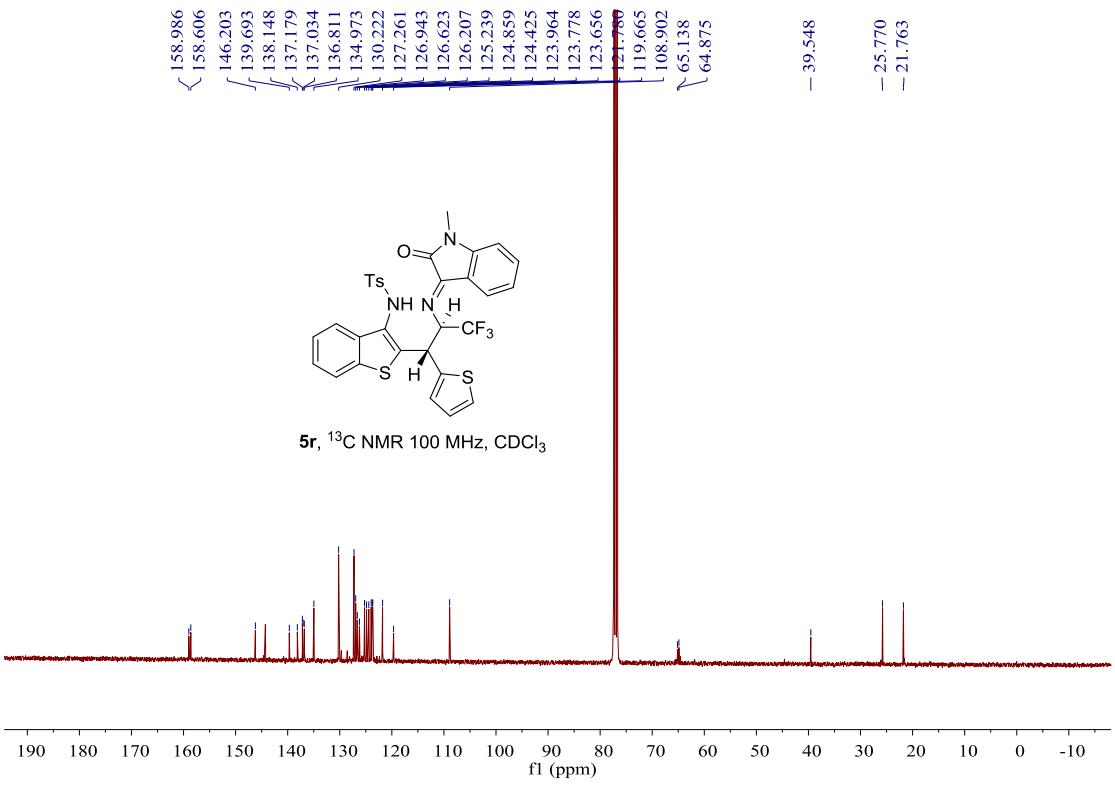

**5q**, $^{19}F$ NMR 376 MHz, $CDCl_3$




**5r**, $^{1}$H NMR 400 MHz, $CDCl_3$

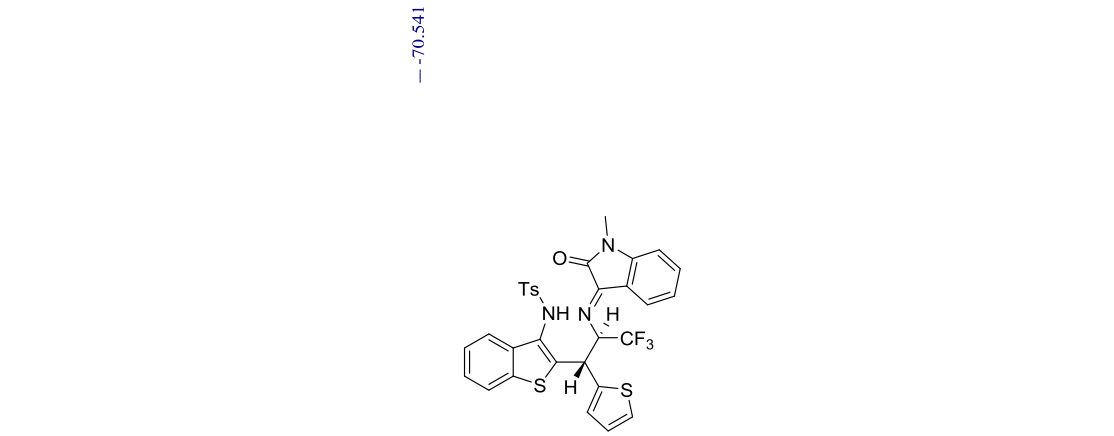


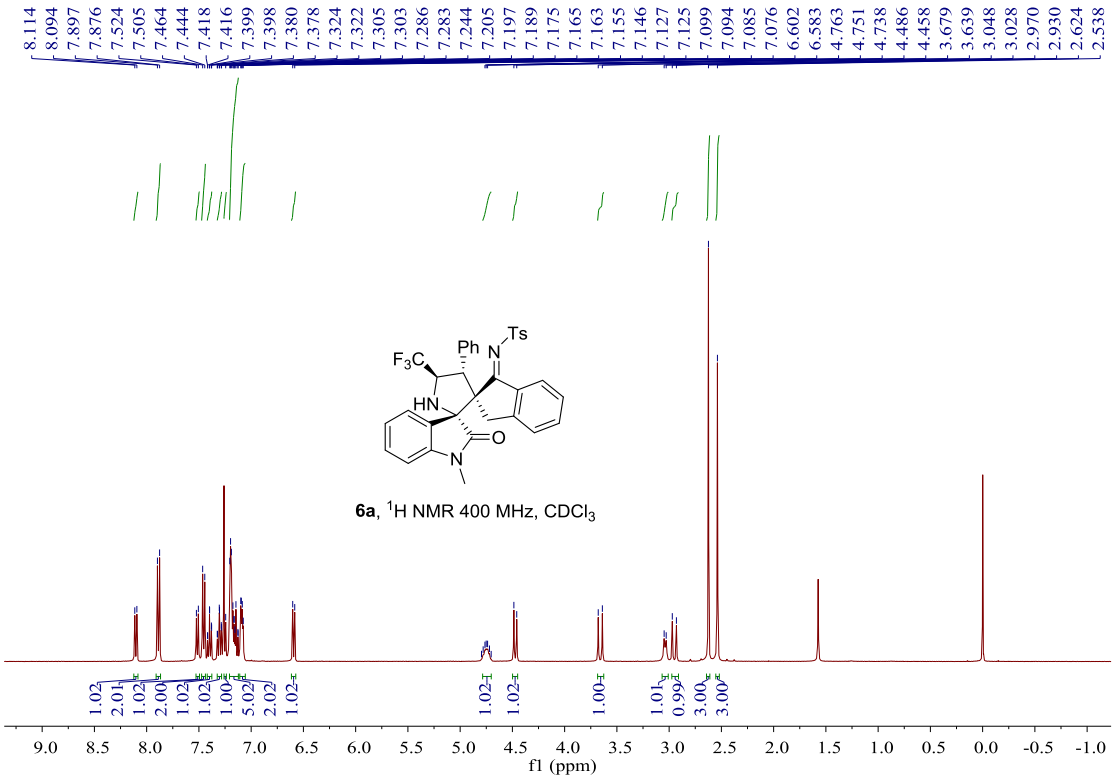




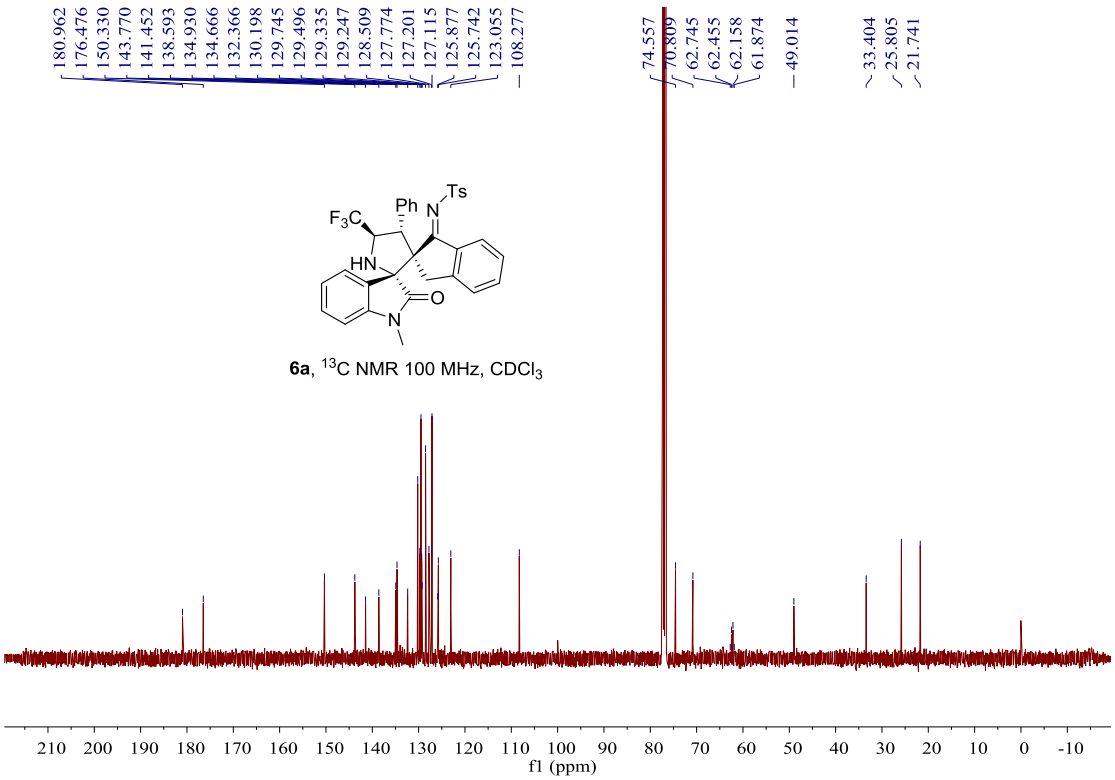
**5r**, $^{13}$C NMR 100 MHz, $CDCl_3$



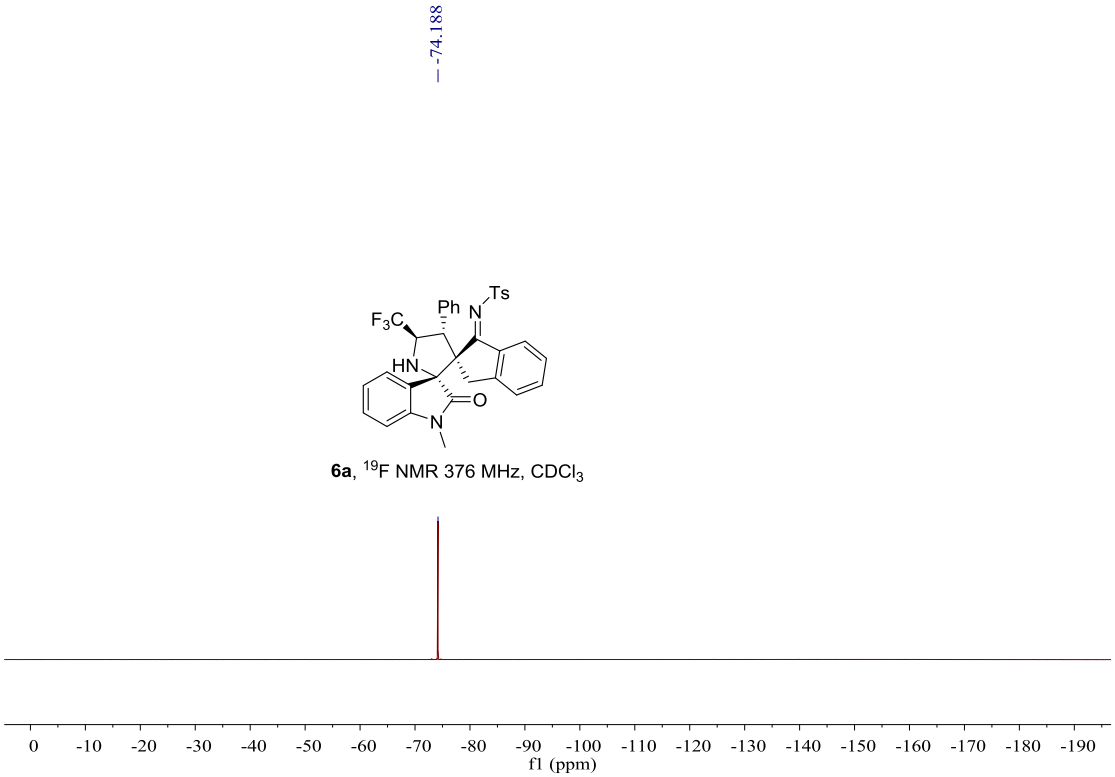

**5r**, $^{19}F$ NMR 376 MHz, $CDCl_3$



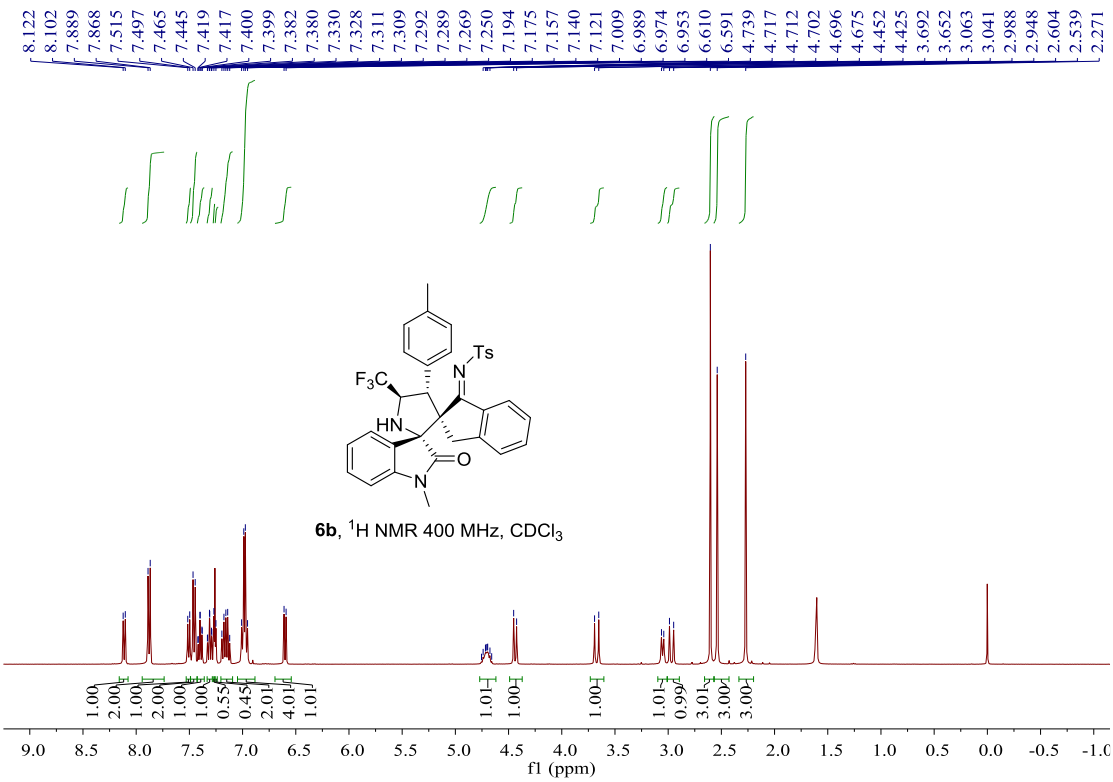

**6a**, $^{1}H$ NMR 400 MHz, $CDCl_3$



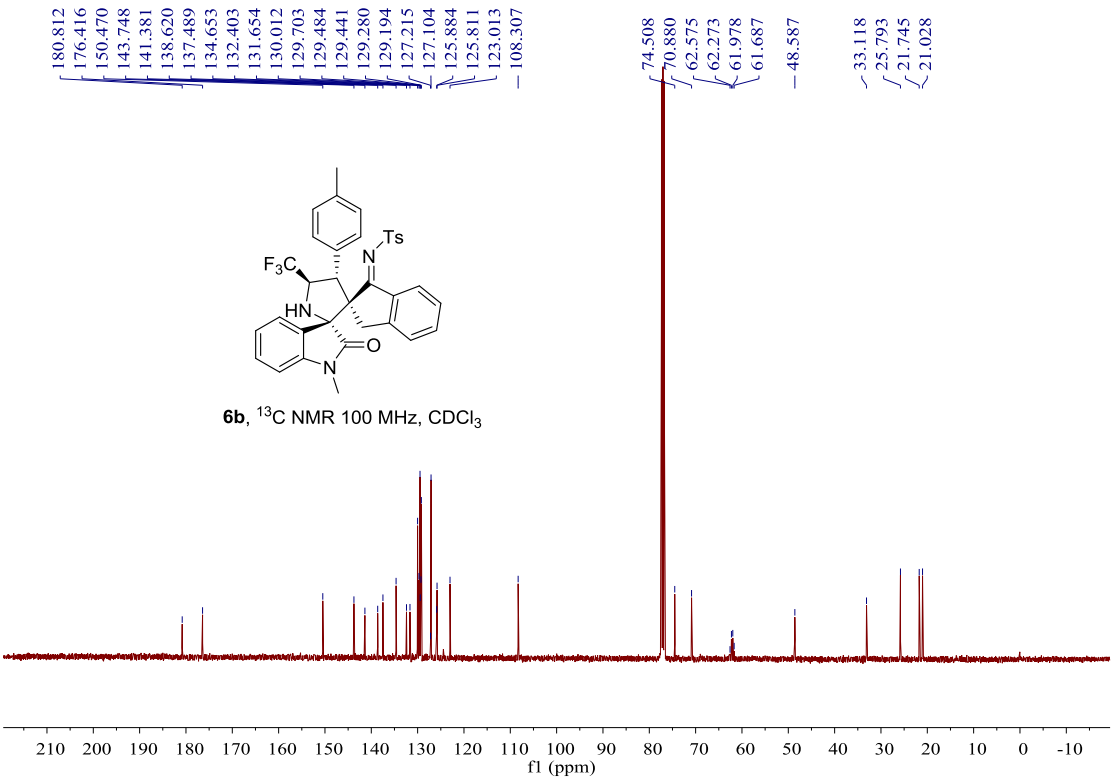

**6a**, $^{13}C$ NMR 100 MHz, $CDCl_3$



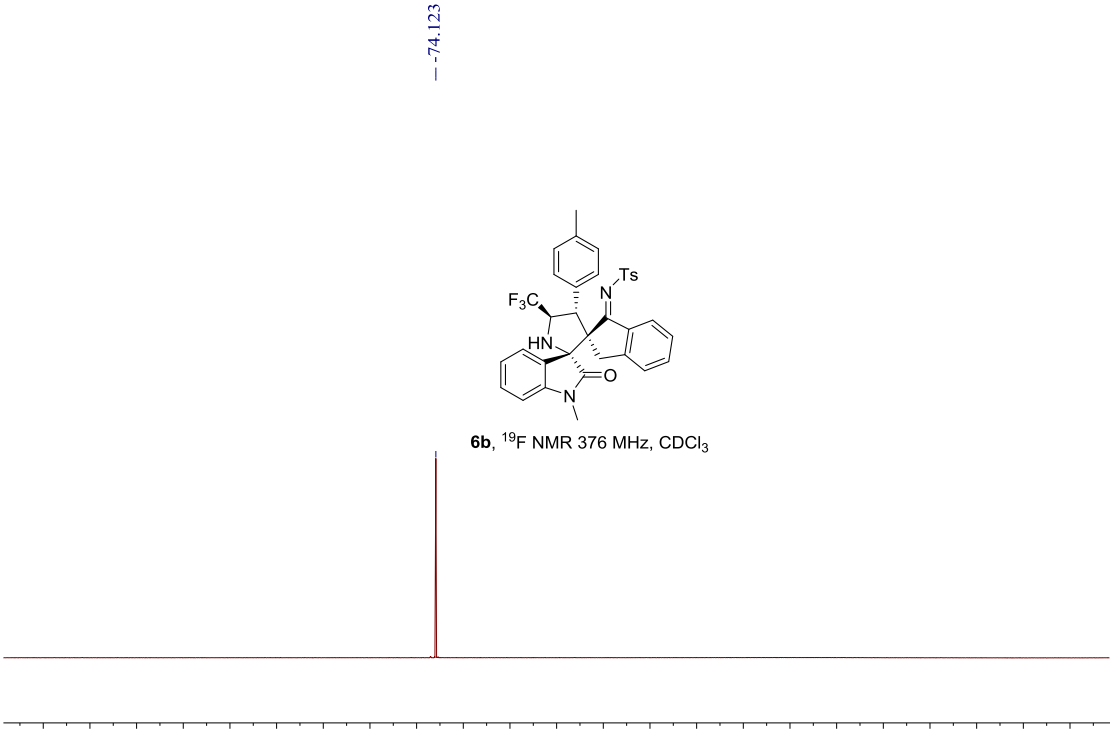

**6a**, $^{19}F$ NMR 376 MHz, $CDCl_3$



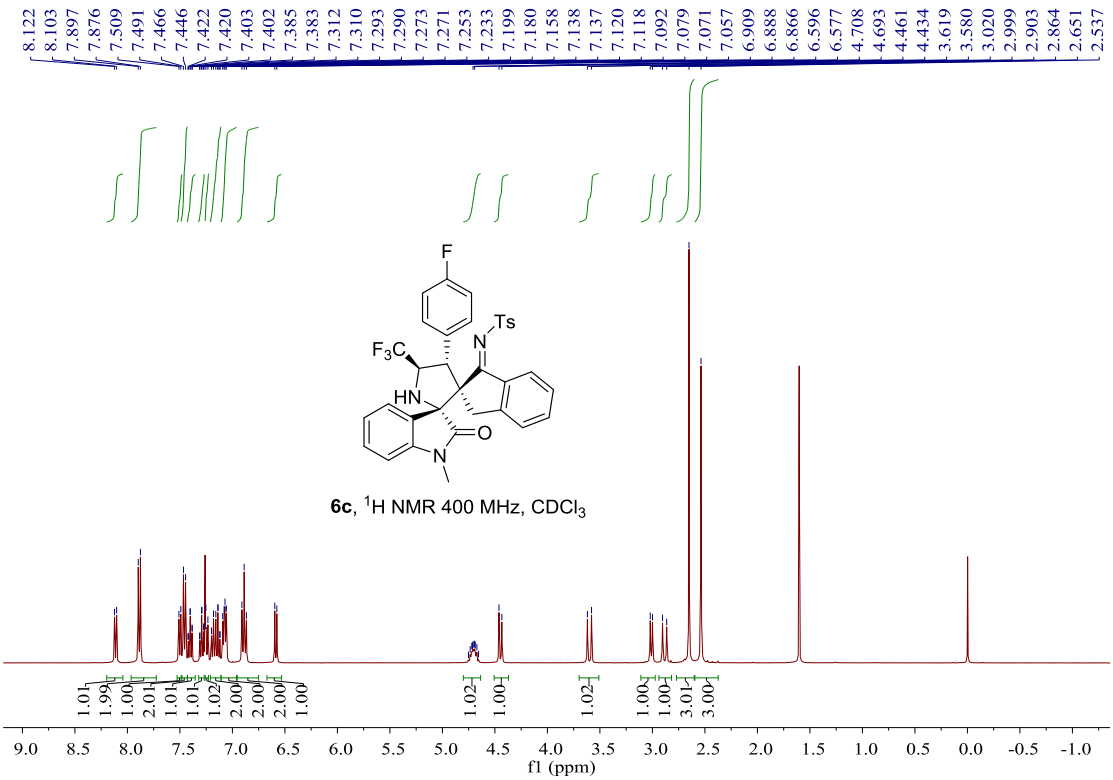

**6b**, $^{1}$H NMR 400 MHz, $CDCl_3$



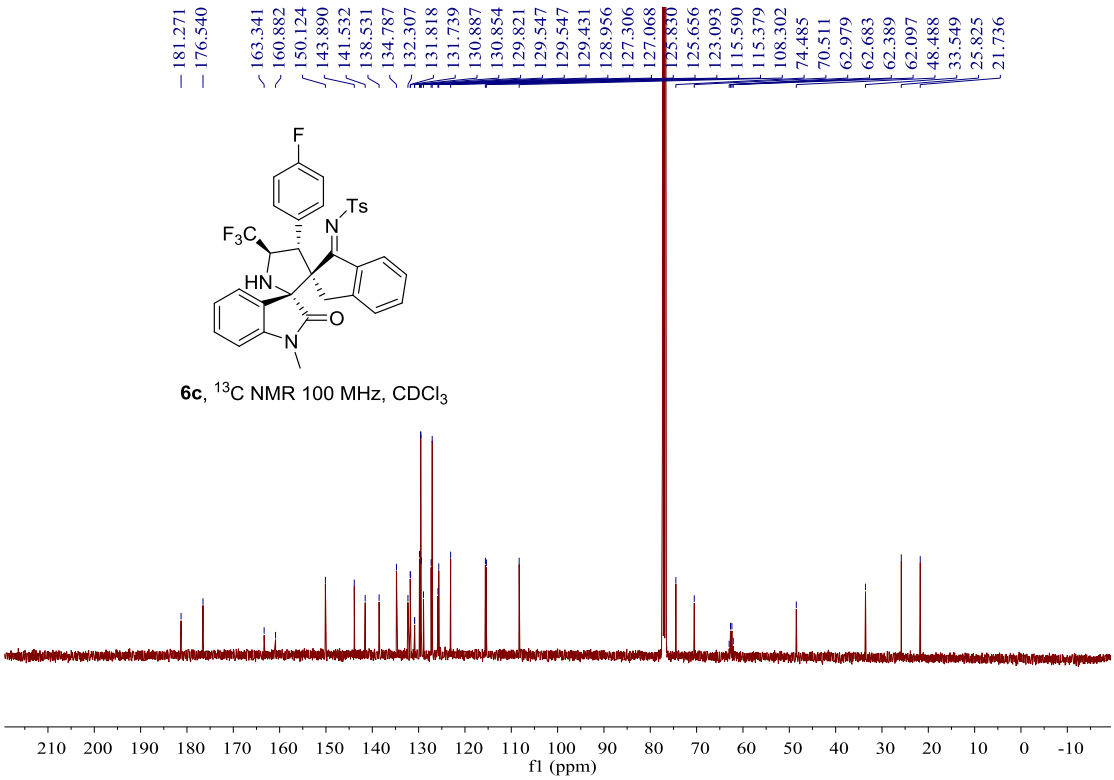

**6b**, $^{13}$C NMR 100 MHz, $CDCl_3$



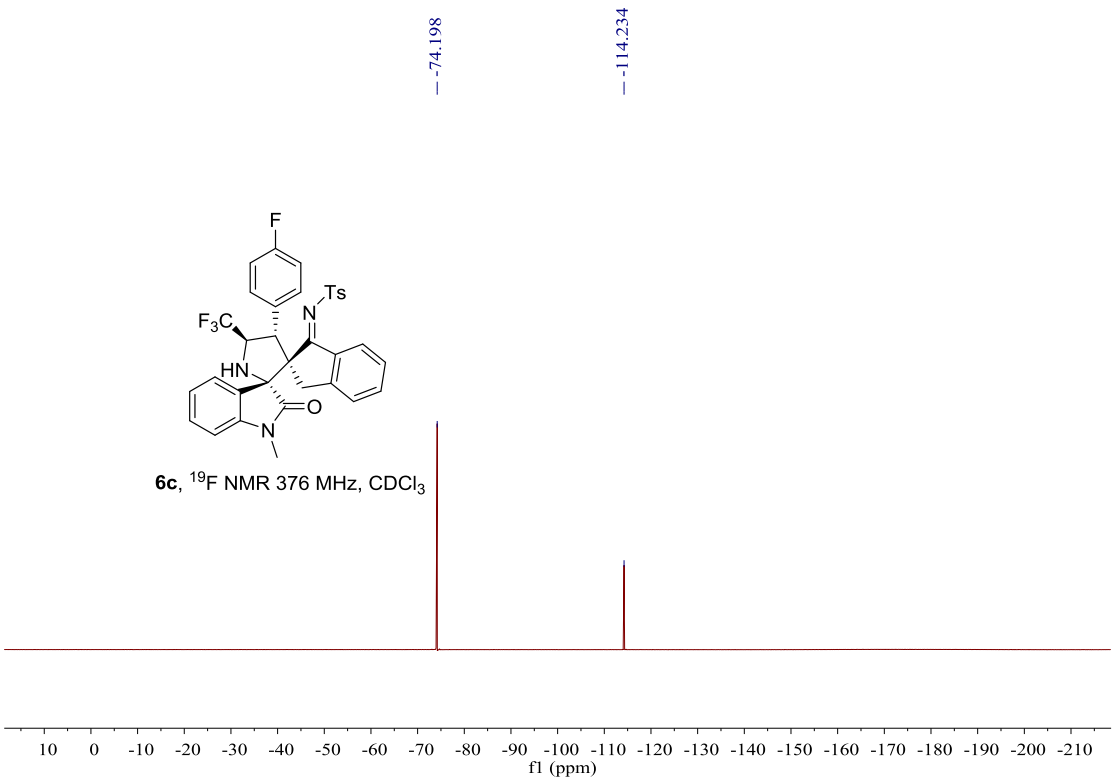

**6b**, $^{19}$F NMR 376 MHz, $CDCl_3$



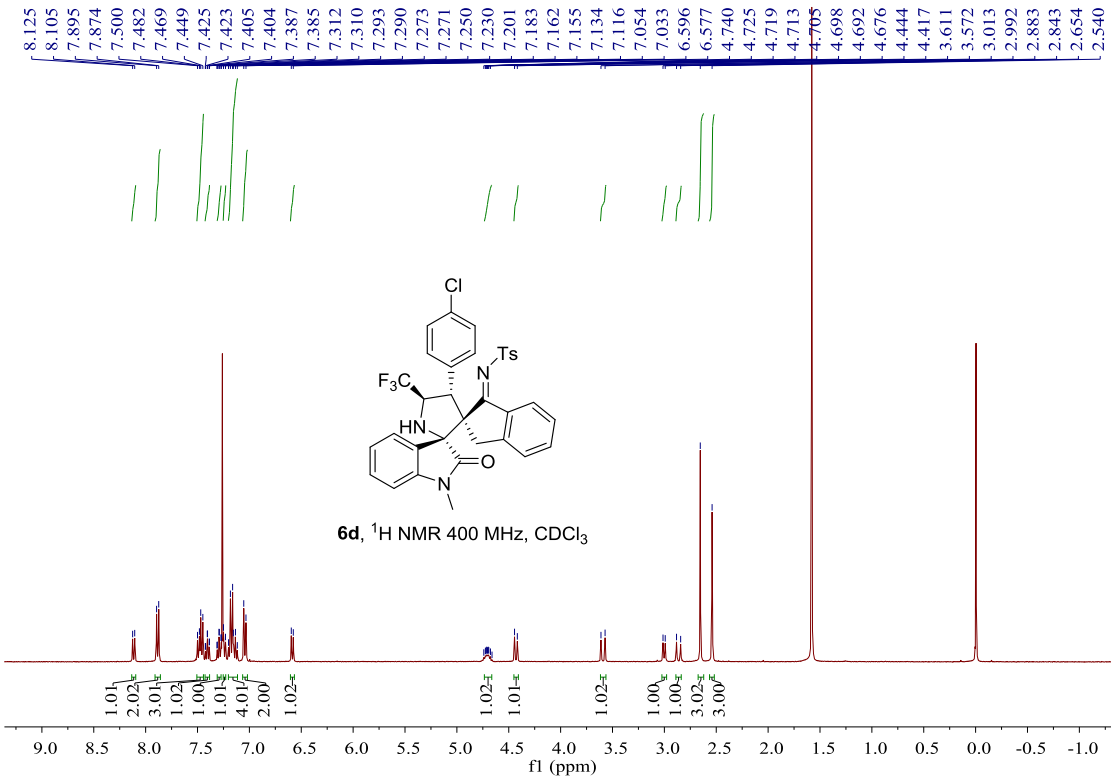

**6c**, $^{1}$H NMR 400 MHz, $CDCl_3$



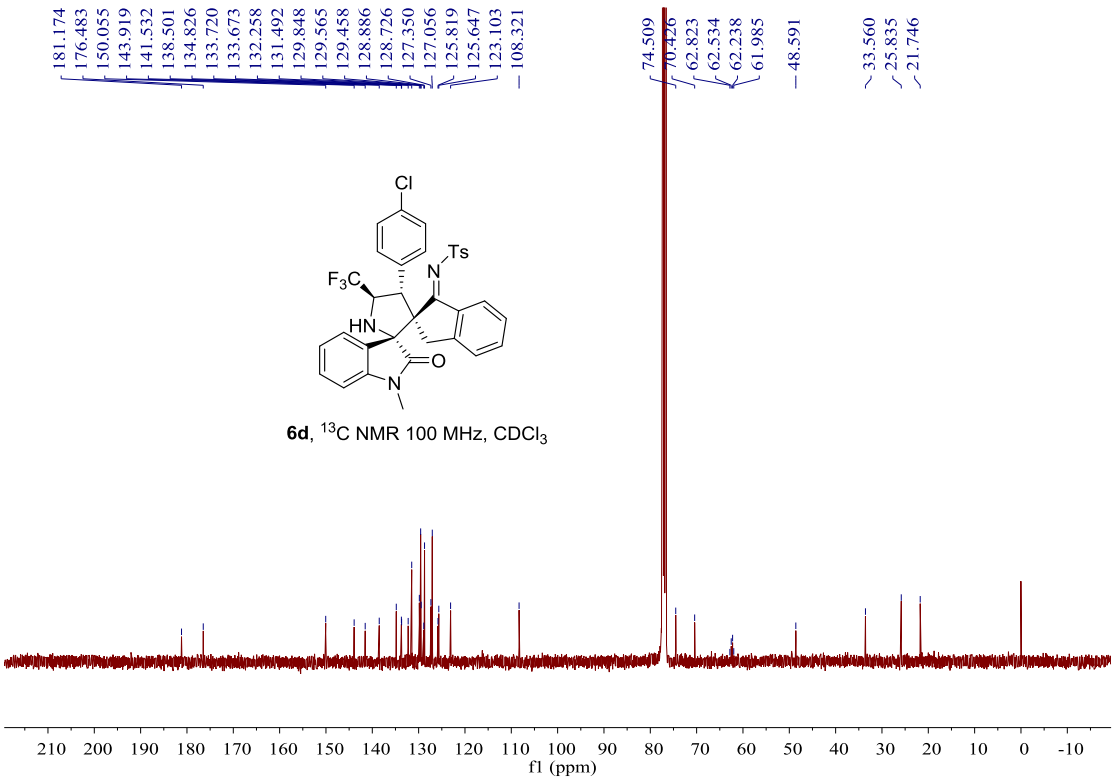

**6c**, $^{13}C$ NMR 100 MHz, $CDCl_3$



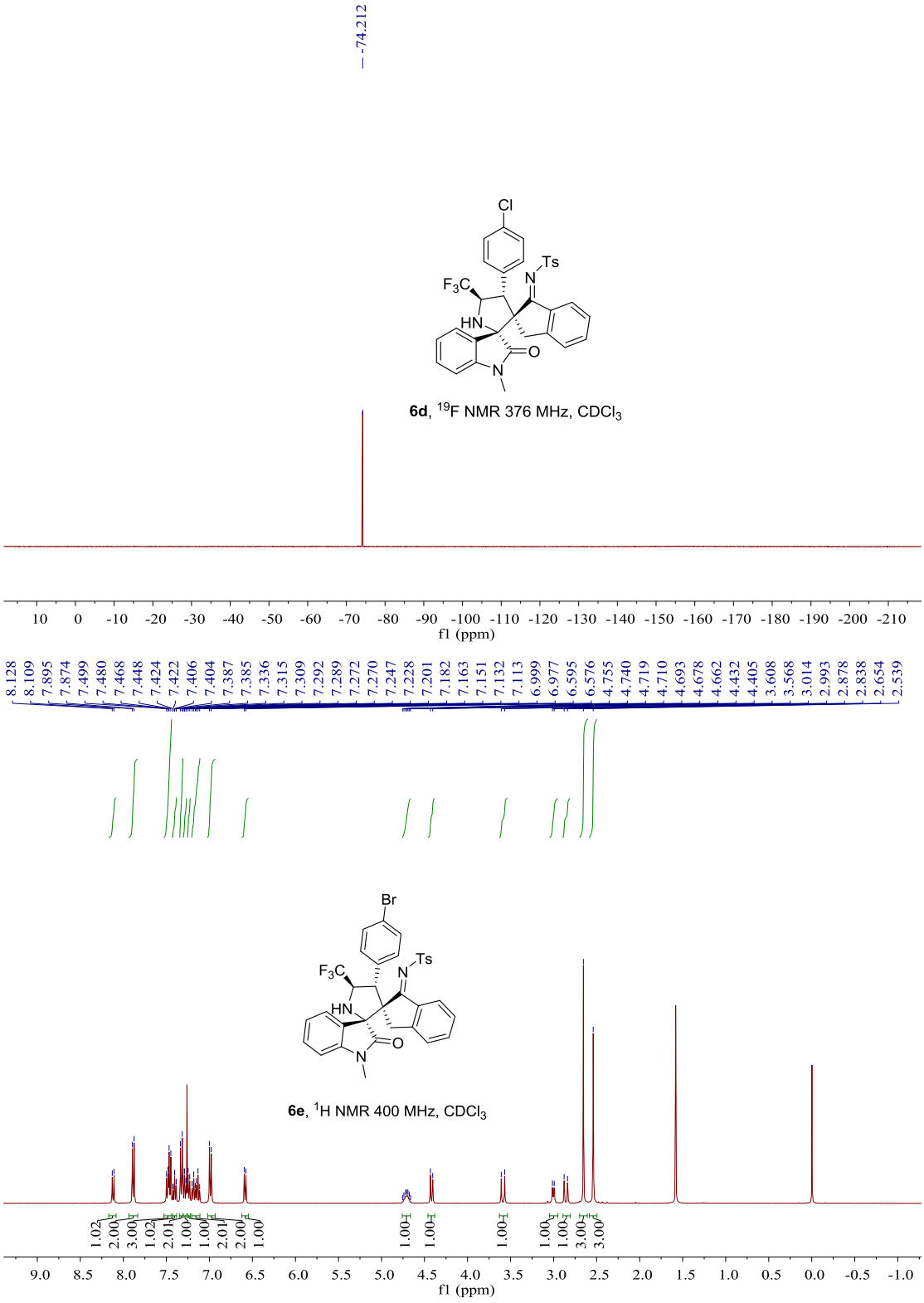

**6c**, $^{19}F$ NMR 376 MHz, $CDCl_3$




**6d**, $^{1}$H NMR 400 MHz, $CDCl_3$

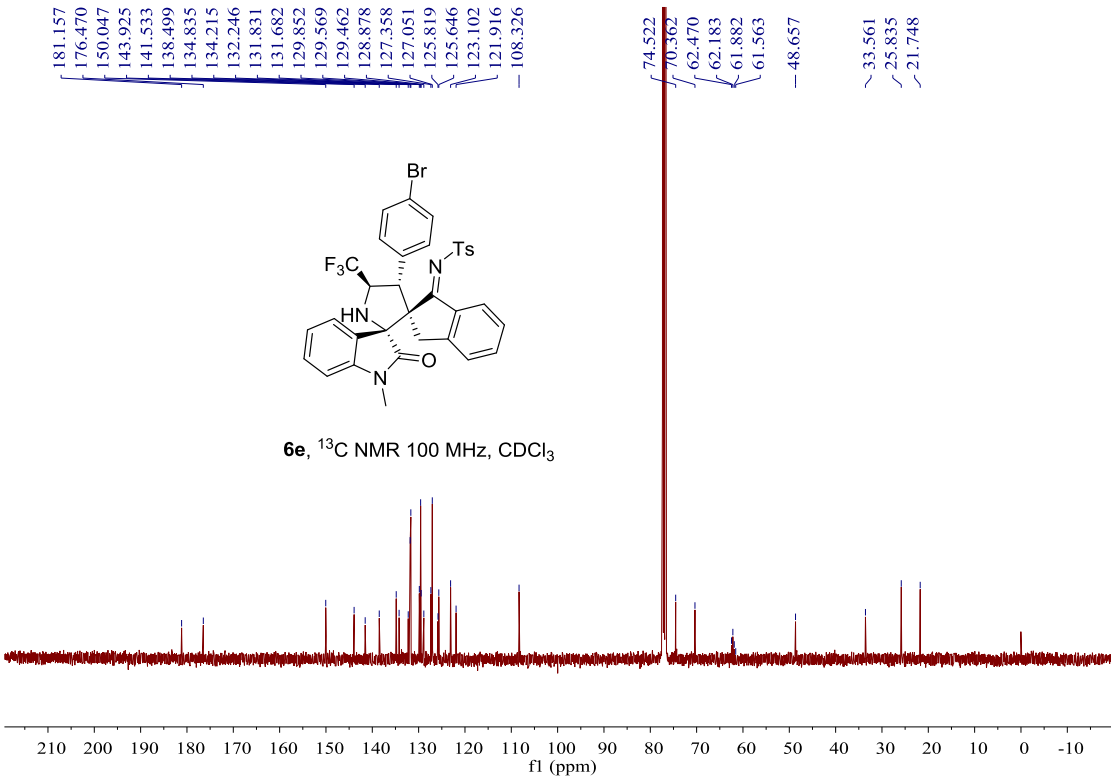



**6d**, $^{13}$C NMR 100 MHz, $CDCl_3$

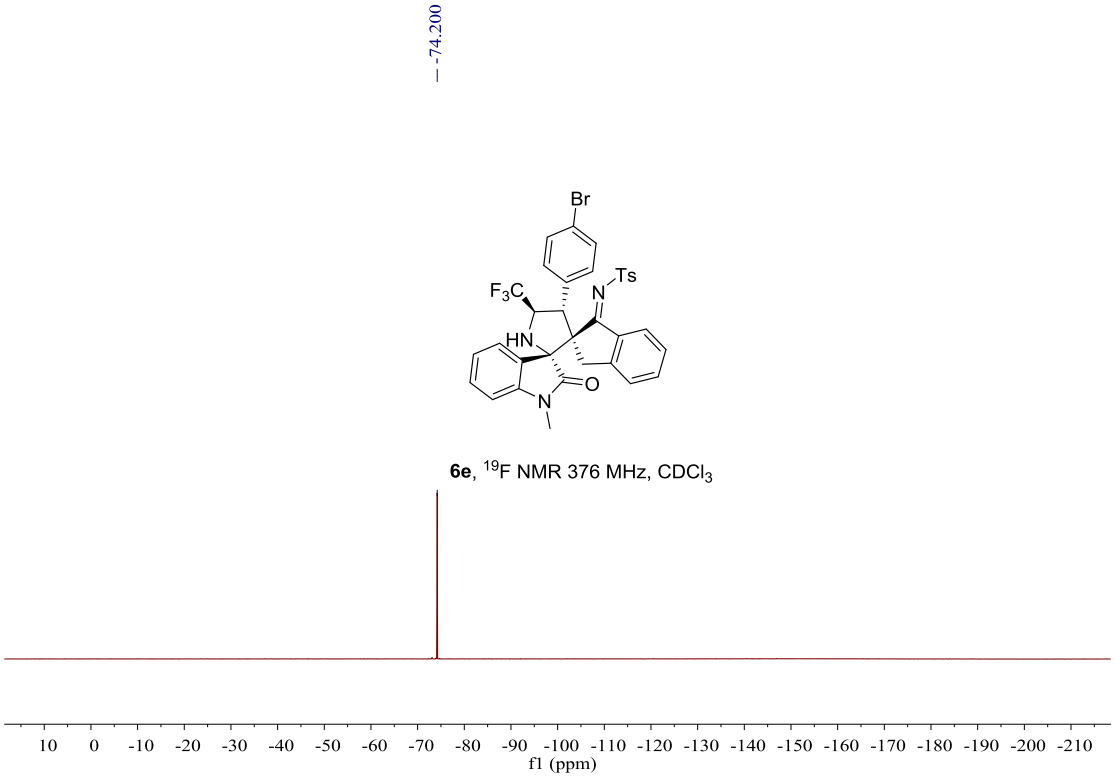



**6d**, $^{19}F$ NMR 376 MHz, $CDCl_3$

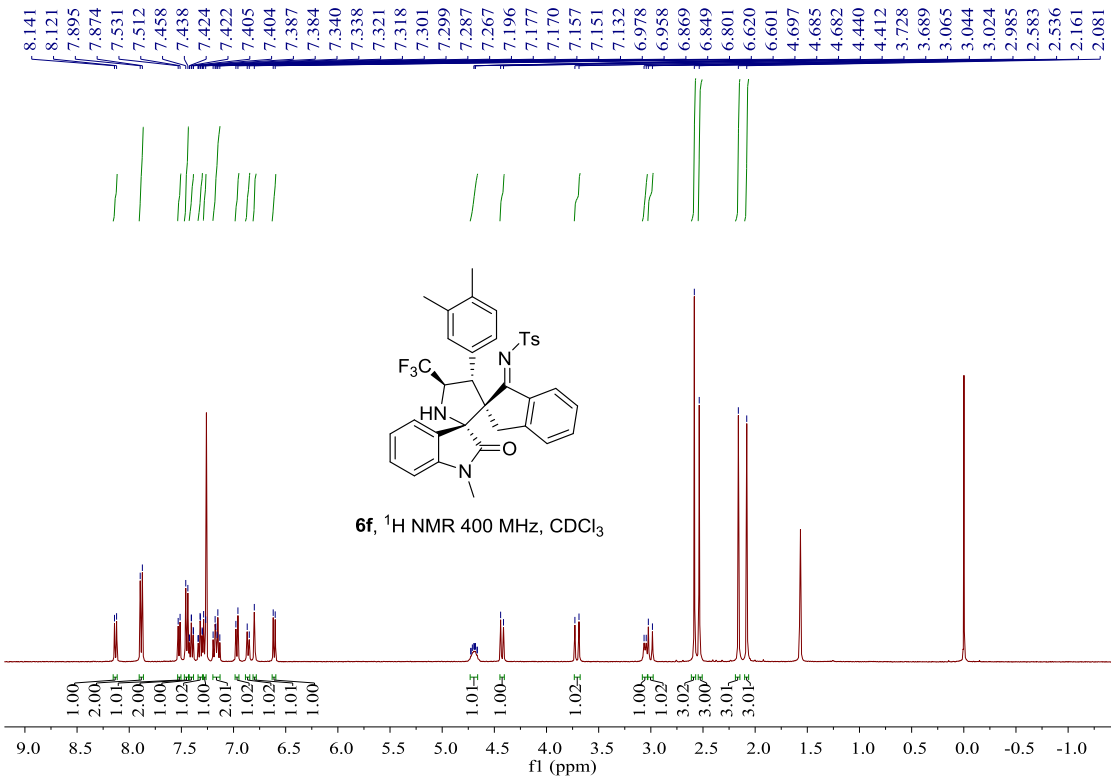
**6e**, $^{1}H$ NMR 400 MHz, $CDCl_3$



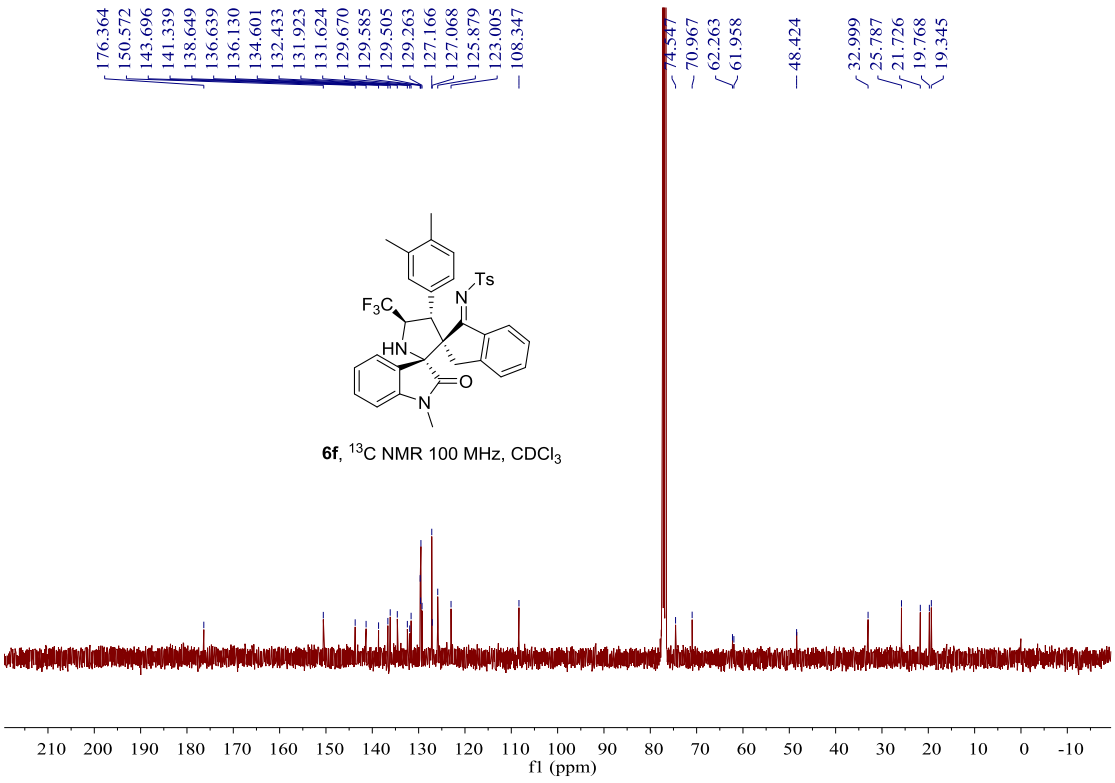

**6e**, $^{13}C$ NMR 100 MHz, $CDCl_3$



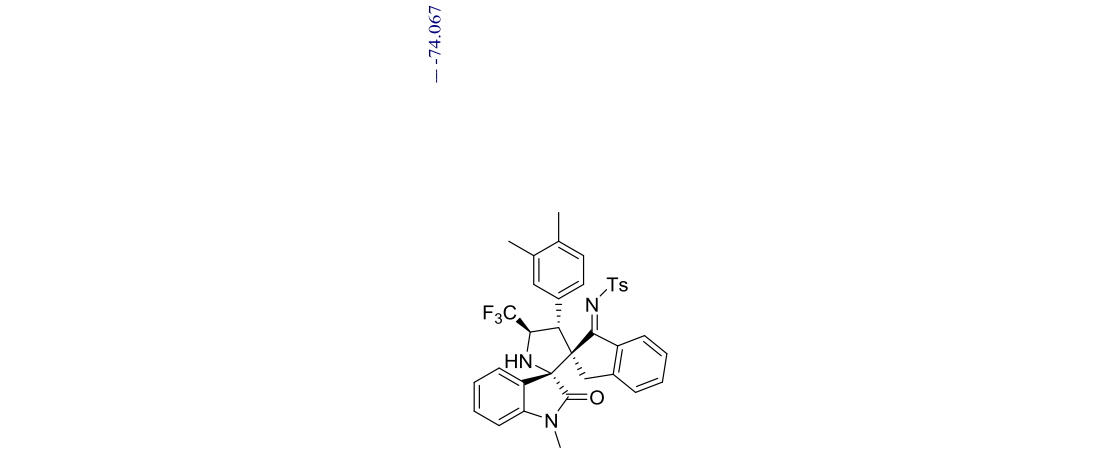

**6e**, $^{19}F$ NMR 376 MHz, $CDCl_3$



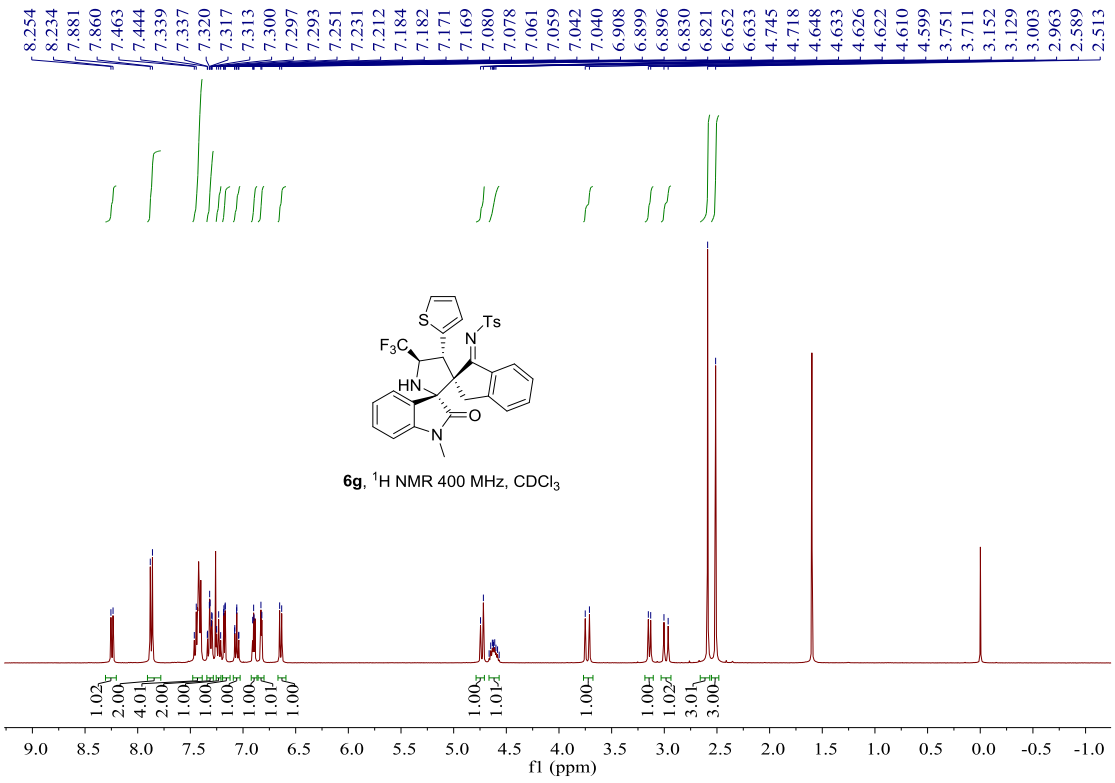

**6f**, $^{1}$H NMR 400 MHz, $CDCl_3$



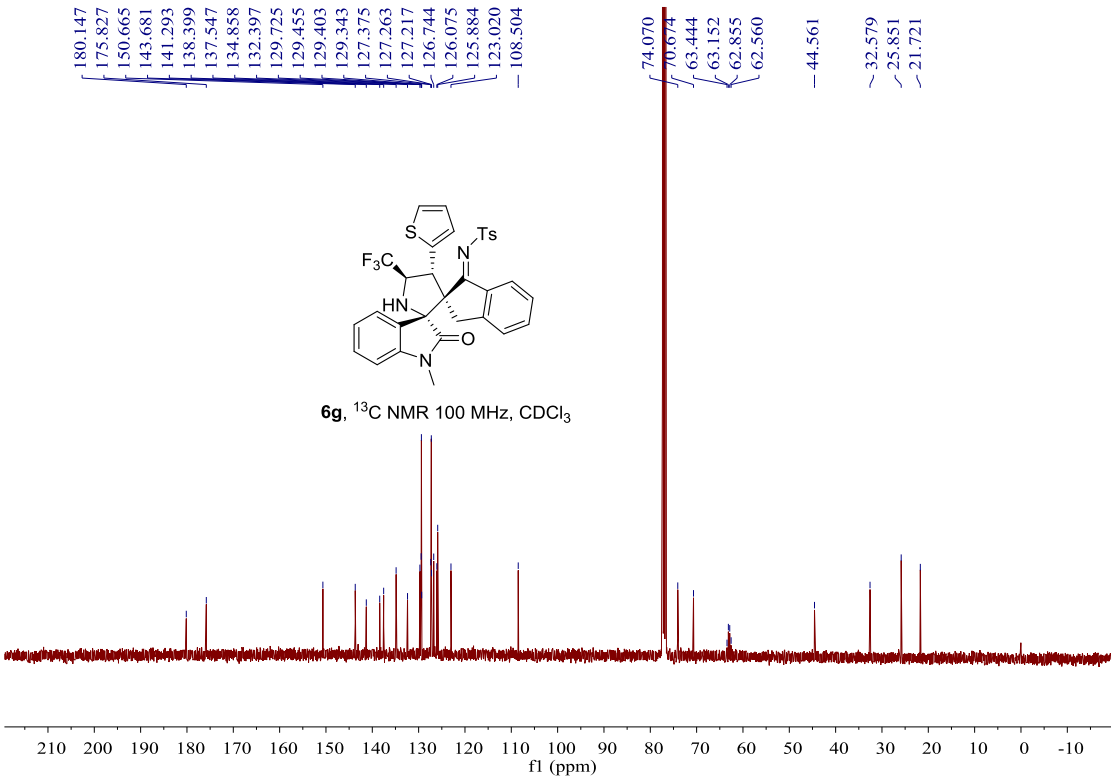

**6f**, $^{13}$C NMR 100 MHz, $CDCl_3$



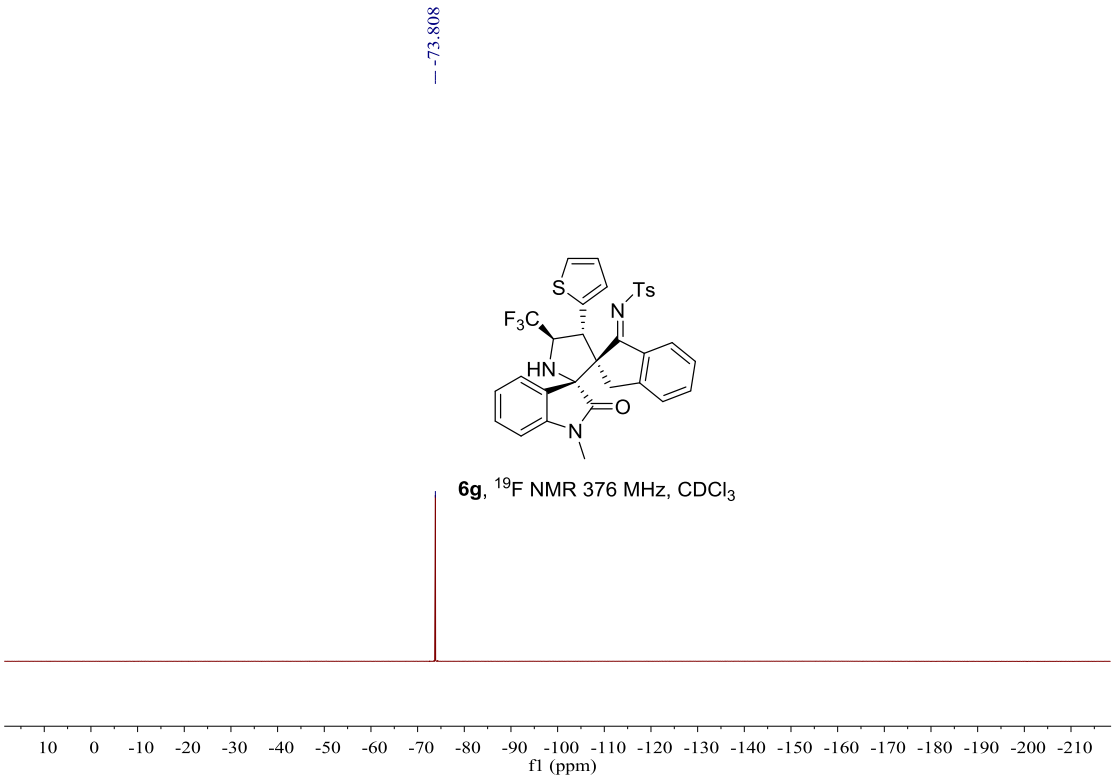

**6f**, $^{19}F$ NMR 376 MHz, $CDCl_3$



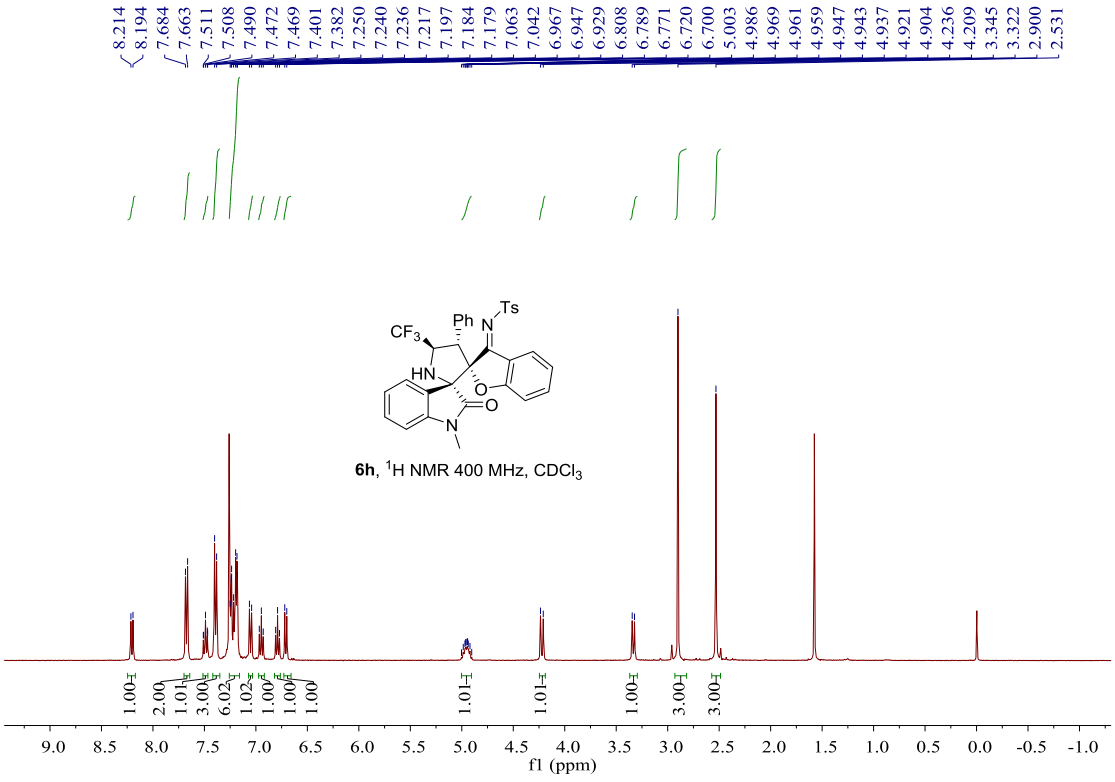

**6g**, $^{1}H$ NMR 400 MHz, $CDCl_3$



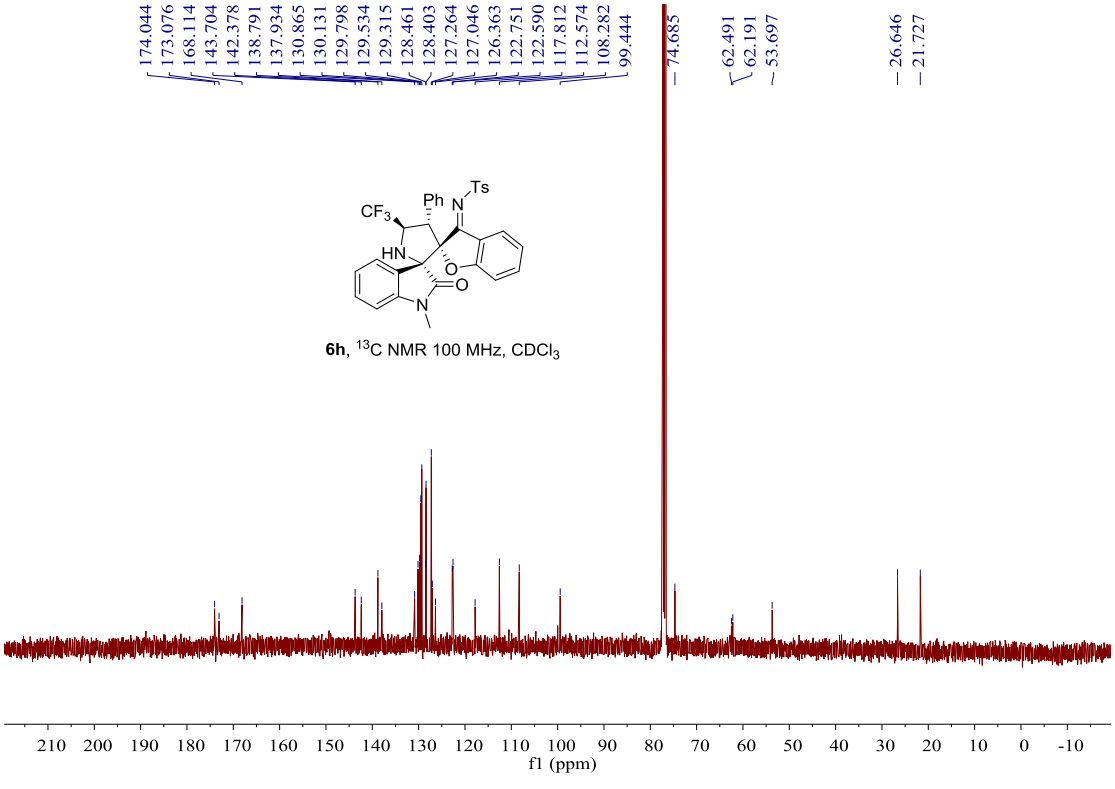

**6g**, $^{13}C$ NMR 100 MHz, $CDCl_3$



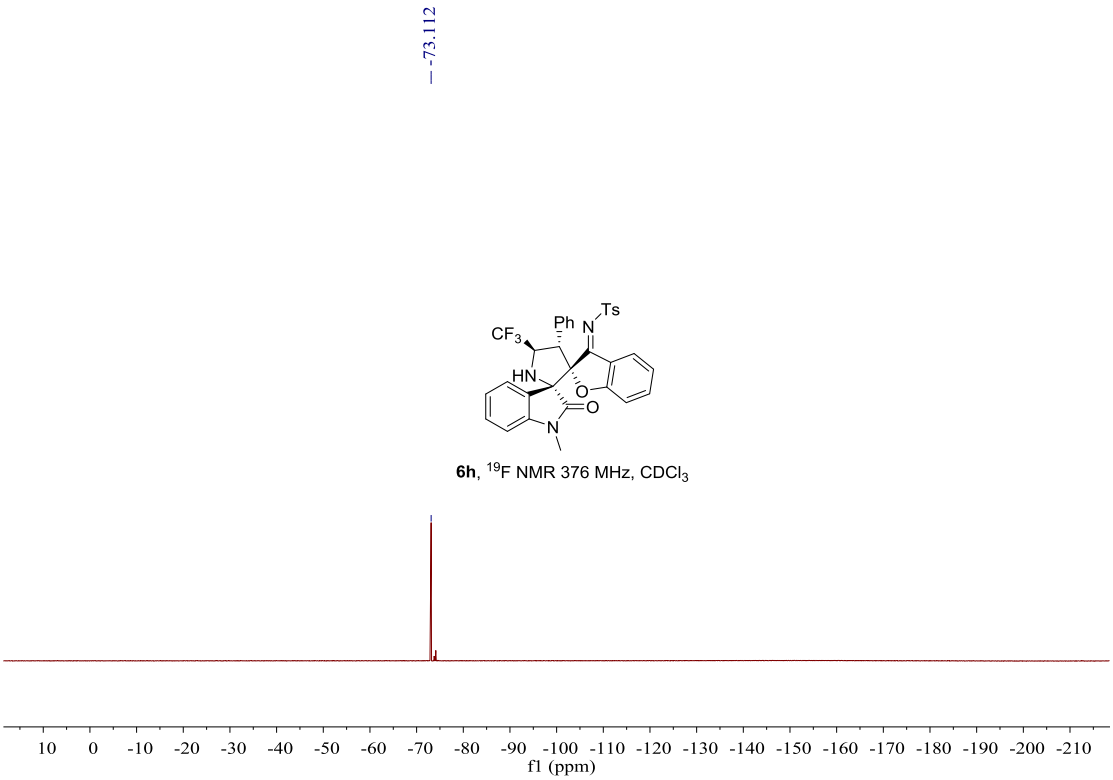

**6g**, $^{19}F$ NMR 376 MHz, $CDCl_3$




**6h**, $^{1}$H NMR 400 MHz, $CDCl_3$




**6h**, $^{13}$C NMR 100 MHz, $CDCl_3$




## 9. Computational details and archive entries

**Table S2.** Cartesian coordinates of the stationary points for the complexation between **1a** and DMAP, optimized at the B3LYP/6-31G* level of theory in $CH_3CN$.

| Species Name | Cartesian Coordinates | | | |
|---|---|---|---|---|
| **1a** | 6 | -2.872236000 | 2.098798000 | -0.002196000 |
| | 6 | -1.466788000 | 2.234696000 | 0.013184000 |
| | 6 | -0.919526000 | 3.532543000 | 0.038128000 |
| | 6 | -1.760564000 | 4.638824000 | 0.046036000 |
| | 6 | -3.153269000 | 4.476935000 | 0.028868000 |
| | 6 | -3.720998000 | 3.204904000 | 0.004589000 |
| | 6 | -1.768725000 | -0.181288000 | -0.014717000 |
| | 6 | -0.781105000 | 0.935104000 | -0.000780000 |
| | 1 | 0.150069000 | 3.683808000 | 0.052501000 |
| | 1 | -1.332493000 | 5.635907000 | 0.065776000 |
| | 1 | -3.799488000 | 5.349762000 | 0.034930000 |
| | 1 | -4.798911000 | 3.078029000 | -0.008273000 |
| | 16 | -3.436158000 | 0.427203000 | -0.029502000 |
| | 6 | -1.379481000 | -1.483038000 | 0.006994000 |
| | 1 | -0.298646000 | -1.603079000 | 0.047651000 |
| | 6 | -2.125553000 | -2.730435000 | 0.001984000 |
| | 6 | -1.381855000 | -3.919199000 | 0.183834000 |
| | 6 | -3.522029000 | -2.845259000 | -0.176241000 |
| | 6 | -2.002619000 | -5.163573000 | 0.203761000 |
| | 1 | -0.305176000 | -3.851711000 | 0.314780000 |
| | 6 | -4.139733000 | -4.092591000 | -0.161233000 |

| | | | | |
|---|---|---|---|---|
| | 1 | -4.133626000 | -1.967380000 | -0.347244000 |
| | 6 | -3.386804000 | -5.254933000 | 0.032218000 |
| | 1 | -1.409027000 | -6.061265000 | 0.349669000 |
| | 1 | -5.214387000 | -4.158472000 | -0.303922000 |
| | 1 | -3.875801000 | -6.224741000 | 0.044547000 |
| | 7 | 0.480918000 | 0.595631000 | -0.006713000 |
| | 16 | 1.789987000 | 1.628062000 | 0.008601000 |
| | 8 | 1.860077000 | 2.404196000 | -1.246712000 |
| | 8 | 1.861669000 | 2.369810000 | 1.284496000 |
| | 6 | 3.121109000 | 0.435620000 | -0.008430000 |
| | 6 | 3.658607000 | -0.010707000 | 1.199462000 |
| | 6 | 3.613202000 | -0.027269000 | -1.230752000 |
| | 6 | 4.698443000 | -0.939075000 | 1.175930000 |
| | 1 | 3.273937000 | 0.366454000 | 2.140911000 |
| | 6 | 4.652286000 | -0.954948000 | -1.234242000 |
| | 1 | 3.193616000 | 0.337237000 | -2.162324000 |
| | 6 | 5.211813000 | -1.424448000 | -0.035551000 |
| | 1 | 5.118987000 | -1.289616000 | 2.114728000 |
| | 1 | 5.037203000 | -1.318484000 | -2.183473000 |
| | 6 | 6.358539000 | -2.405866000 | -0.053787000 |
| | 1 | 7.315021000 | -1.884630000 | -0.190525000 |
| | 1 | 6.421458000 | -2.965634000 | 0.884267000 |
| | 1 | 6.259314000 | -3.120647000 | -0.877212000 |
| **1b** | 6 | 2.550567000 | 2.128109000 | 0.001662000 |
| | 6 | 1.152599000 | 2.273615000 | 0.000176000 |
| | 6 | 0.601490000 | 3.567465000 | -0.000273000 |
| | 6 | 1.465243000 | 4.656845000 | 0.000816000 |
| | 6 | 2.860407000 | 4.474576000 | 0.002370000 |
| | 6 | 3.430396000 | 3.201504000 | 0.002828000 |
| | 6 | 1.796471000 | 0.042381000 | 0.000272000 |
| | 6 | 0.609025000 | 0.917958000 | -0.000837000 |
| | 1 | -0.470179000 | 3.717014000 | -0.001156000 |
| | 1 | 1.058565000 | 5.662951000 | 0.000530000 |
| | 1 | 3.511060000 | 5.344008000 | 0.003252000 |
| | 1 | 4.503795000 | 3.048306000 | 0.004011000 |
| | 8 | 2.946099000 | 0.817095000 | 0.001793000 |
| | 6 | 1.804523000 | -1.309402000 | -0.000191000 |
| | 1 | 0.807751000 | -1.743304000 | -0.001462000 |
| | 6 | 2.912245000 | -2.248918000 | 0.000567000 |
| | 6 | 4.273965000 | -1.870974000 | 0.001874000 |
| | 6 | 2.599098000 | -3.626120000 | -0.000120000 |
| | 6 | 5.272704000 | -2.839990000 | 0.002405000 |
| | 1 | 4.542133000 | -0.821971000 | 0.002444000 |
| | 6 | 3.602355000 | -4.590266000 | 0.000433000 |

| | | | | |
|---|---|---|---|---|
| | 1 | 1.555957000 | -3.931305000 | -0.001105000 |
| | 6 | 4.944395000 | -4.200090000 | 0.001685000 |
| | 1 | 6.314998000 | -2.533804000 | 0.003391000 |
| | 1 | 3.339216000 | -5.644046000 | -0.000130000 |
| | 1 | 5.730249000 | -4.950050000 | 0.002100000 |
| | 7 | -0.585308000 | 0.385425000 | -0.002534000 |
| | 16 | -1.969490000 | 1.328206000 | -0.004589000 |
| | 8 | -2.083053000 | 2.087245000 | 1.258172000 |
| | 8 | -2.082456000 | 2.080328000 | -1.271527000 |
| | 6 | -3.219433000 | 0.051813000 | -0.001248000 |
| | 6 | -3.695554000 | -0.446588000 | -1.215671000 |
| | 6 | -3.708223000 | -0.427134000 | 1.215230000 |
| | 6 | -4.668344000 | -1.443872000 | -1.202942000 |
| | 1 | -3.314736000 | -0.056468000 | -2.153493000 |
| | 6 | -4.681509000 | -1.424883000 | 1.207867000 |
| | 1 | -3.337195000 | -0.022357000 | 2.150725000 |
| | 6 | -5.176640000 | -1.947995000 | 0.004182000 |
| | 1 | -5.040376000 | -1.835793000 | -2.145956000 |
| | 1 | -5.063685000 | -1.801616000 | 2.152910000 |
| | 6 | -6.251445000 | -3.007837000 | 0.005041000 |
| | 1 | -7.247139000 | -2.552827000 | -0.077737000 |
| | 1 | -6.136987000 | -3.693244000 | -0.840855000 |
| | 1 | -6.235160000 | -3.593282000 | 0.929425000 |
| **1c** | 6 | -2.749726000 | 2.226751000 | 0.010161000 |
| | 6 | -1.344550000 | 2.332671000 | -0.001488000 |
| | 6 | -0.734585000 | 3.599236000 | -0.013773000 |
| | 6 | -1.540774000 | 4.733366000 | -0.013797000 |
| | 6 | -2.938723000 | 4.619805000 | -0.001598000 |
| | 6 | -3.550538000 | 3.365384000 | 0.010452000 |
| | 6 | -1.900012000 | 0.014085000 | 0.008590000 |
| | 6 | -0.767755000 | 0.973478000 | 0.000575000 |
| | 1 | 0.341034000 | 3.707979000 | -0.023347000 |
| | 1 | -1.080885000 | 5.716973000 | -0.023468000 |
| | 1 | -3.550637000 | 5.517446000 | -0.001763000 |
| | 1 | -4.633529000 | 3.279147000 | 0.019610000 |
| | 6 | -3.198790000 | 0.788577000 | 0.021820000 |
| | 6 | -1.688246000 | -1.324182000 | -0.001391000 |
| | 1 | -0.639330000 | -1.615913000 | -0.015477000 |
| | 6 | -2.618467000 | -2.447385000 | -0.000253000 |
| | 6 | -2.059062000 | -3.744199000 | -0.036065000 |
| | 6 | -4.026118000 | -2.337537000 | 0.034273000 |
| | 6 | -2.862660000 | -4.880325000 | -0.039568000 |
| | 1 | -0.977557000 | -3.849508000 | -0.061837000 |
| | 6 | -4.828215000 | -3.475776000 | 0.031548000 |

| | | | | |
|---|---|---|---|---|
| | 1 | -4.502039000 | -1.366280000 | 0.065213000 |
| | 6 | -4.253476000 | -4.750022000 | -0.005789000 |
| | 1 | -2.406008000 | -5.865472000 | -0.068170000 |
| | 1 | -5.908837000 | -3.368174000 | 0.058917000 |
| | 1 | -4.885517000 | -5.633502000 | -0.007955000 |
| | 7 | 0.455757000 | 0.513938000 | -0.002798000 |
| | 16 | 1.828868000 | 1.463279000 | -0.011337000 |
| | 8 | 1.949438000 | 2.206954000 | -1.283443000 |
| | 8 | 1.951913000 | 2.228666000 | 1.247559000 |
| | 6 | 3.084457000 | 0.189973000 | -0.001246000 |
| | 6 | 3.574467000 | -0.281997000 | 1.217312000 |
| | 6 | 3.565722000 | -0.311184000 | -1.212434000 |
| | 6 | 4.553408000 | -1.274446000 | 1.215730000 |
| | 1 | 3.200216000 | 0.124730000 | 2.150704000 |
| | 6 | 4.544152000 | -1.302988000 | -1.194516000 |
| | 1 | 3.184629000 | 0.073468000 | -2.152428000 |
| | 6 | 5.053672000 | -1.799556000 | 0.015192000 |
| | 1 | 4.936220000 | -1.645035000 | 2.162999000 |
| | 1 | 4.919962000 | -1.696275000 | -2.135537000 |
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| | 1 | 7.127486000 | -2.393223000 | -0.074221000 |
| | 1 | 6.128940000 | -3.426689000 | 0.953471000 |
| | 1 | 6.018826000 | -3.549770000 | -0.814520000 |
| | 1 | -3.827788000 | 0.560176000 | -0.848764000 |
| | 1 | -3.803700000 | 0.569383000 | 0.911765000 |
| **1a-py-com** | 6 | -3.824606000 | 0.017207000 | -0.907171000 |
| | 6 | -2.889701000 | -1.039106000 | -1.026143000 |
| | 6 | -3.277675000 | -2.196690000 | -1.729520000 |
| | 6 | -4.560885000 | -2.290104000 | -2.254637000 |
| | 6 | -5.482164000 | -1.238569000 | -2.101898000 |
| | 6 | -5.118370000 | -0.074835000 | -1.433426000 |
| | 6 | -1.618722000 | 0.559598000 | 0.142831000 |
| | 6 | -1.601413000 | -0.717833000 | -0.400365000 |
| | 1 | -2.567833000 | -3.003477000 | -1.874561000 |
| | 1 | -4.853845000 | -3.185075000 | -2.796695000 |
| | 1 | -6.482572000 | -1.329607000 | -2.515934000 |
| | 1 | -5.820388000 | 0.747133000 | -1.324777000 |
| | 16 | -3.158278000 | 1.408707000 | -0.071312000 |
| | 6 | -0.469493000 | 1.146544000 | 0.888228000 |
| | 1 | 0.051876000 | 0.300630000 | 1.347269000 |
| | 6 | -0.853687000 | 2.155891000 | 1.960963000 |
| | 6 | -1.079202000 | 3.506889000 | 1.663117000 |
| | 6 | -1.025153000 | 1.710925000 | 3.278272000 |
| | 6 | -1.477898000 | 4.393746000 | 2.665283000 |

| | | | | |
|---|---|---|---|---|
| | 1 | -0.935680000 | 3.874237000 | 0.650663000 |
| | 6 | -1.425626000 | 2.597220000 | 4.279086000 |
| | 1 | -0.847000000 | 0.666046000 | 3.519784000 |
| | 6 | -1.653500000 | 3.941531000 | 3.974752000 |
| | 1 | -1.647724000 | 5.438596000 | 2.421055000 |
| | 1 | -1.552292000 | 2.238389000 | 5.296625000 |
| | 1 | -1.960621000 | 4.633098000 | 4.754188000 |
| | 7 | -0.428607000 | -1.441488000 | -0.359113000 |
| | 16 | -0.373669000 | -3.041077000 | -0.256207000 |
| | 8 | -1.305495000 | -3.626005000 | 0.751741000 |
| | 8 | -0.388194000 | -3.741672000 | -1.577410000 |
| | 6 | 1.296278000 | -3.263721000 | 0.376400000 |
| | 6 | 2.388904000 | -3.204319000 | -0.492729000 |
| | 6 | 1.492217000 | -3.500610000 | 1.736662000 |
| | 6 | 3.677744000 | -3.369209000 | 0.010791000 |
| | 1 | 2.230133000 | -3.037042000 | -1.553134000 |
| | 6 | 2.788273000 | -3.668473000 | 2.227398000 |
| | 1 | 0.635925000 | -3.557184000 | 2.400593000 |
| | 6 | 3.900113000 | -3.605596000 | 1.376675000 |
| | 1 | 4.525996000 | -3.318216000 | -0.667944000 |
| | 1 | 2.936704000 | -3.852779000 | 3.288757000 |
| | 6 | 5.299504000 | -3.814561000 | 1.905712000 |
| | 1 | 5.637321000 | -4.844444000 | 1.730172000 |
| | 1 | 6.017277000 | -3.151932000 | 1.410191000 |
| | 1 | 5.351528000 | -3.632129000 | 2.983597000 |
| | 6 | 2.638506000 | 2.829216000 | -1.644663000 |
| | 6 | 2.805585000 | 2.633147000 | -0.239870000 |
| | 6 | 1.789282000 | 2.108089000 | 0.510548000 |
| | 7 | 0.594193000 | 1.752983000 | -0.032591000 |
| | 6 | 0.406487000 | 1.912379000 | -1.364131000 |
| | 6 | 1.376340000 | 2.438697000 | -2.179189000 |
| | 1 | 3.728691000 | 2.889014000 | 0.261197000 |
| | 1 | 1.891561000 | 1.953767000 | 1.577832000 |
| | 1 | -0.553619000 | 1.590941000 | -1.745142000 |
| | 1 | 1.153168000 | 2.537617000 | -3.232416000 |
| | 7 | 3.615871000 | 3.345375000 | -2.414190000 |
| | 6 | 3.403786000 | 3.529137000 | -3.852111000 |
| | 1 | 4.300872000 | 3.965672000 | -4.288043000 |
| | 1 | 3.208781000 | 2.571544000 | -4.347609000 |
| | 1 | 2.563163000 | 4.205351000 | -4.042328000 |
| | 6 | 4.903959000 | 3.720104000 | -1.824718000 |
| | 1 | 5.551788000 | 4.105399000 | -2.610351000 |
| | 1 | 4.779207000 | 4.501061000 | -1.066505000 |
| | 1 | 5.394755000 | 2.854483000 | -1.366462000 |

| | | | | |
|---|---|---|---|---|
| **1b-py-com** | 6 | -0.516595000 | -3.333565000 | -0.931850000 |
| | 6 | 0.749871000 | -2.749726000 | -1.127649000 |
| | 6 | 1.706463000 | -3.460048000 | -1.873948000 |
| | 6 | 1.367109000 | -4.713970000 | -2.375948000 |
| | 6 | 0.093549000 | -5.272454000 | -2.153767000 |
| | 6 | -0.875797000 | -4.583907000 | -1.426698000 |
| | 6 | -0.570641000 | -1.379419000 | 0.079492000 |
| | 6 | 0.702347000 | -1.448446000 | -0.451686000 |
| | 1 | 2.682810000 | -3.030711000 | -2.066347000 |
| | 1 | 2.097731000 | -5.272191000 | -2.954871000 |
| | 1 | -0.140136000 | -6.253641000 | -2.557399000 |
| | 1 | -1.864668000 | -4.994491000 | -1.248792000 |
| | 8 | -1.333519000 | -2.516169000 | -0.208801000 |
| | 6 | -1.158614000 | -0.321312000 | 0.927056000 |
| | 1 | -0.307864000 | 0.286522000 | 1.247318000 |
| | 6 | -1.909002000 | -0.830440000 | 2.151858000 |
| | 6 | -3.206348000 | -1.352334000 | 2.061273000 |
| | 6 | -1.267980000 | -0.809234000 | 3.396794000 |
| | 6 | -3.848414000 | -1.845161000 | 3.197779000 |
| | 1 | -3.721216000 | -1.373319000 | 1.105143000 |
| | 6 | -1.909104000 | -1.306176000 | 4.533223000 |
| | 1 | -0.262263000 | -0.404279000 | 3.477414000 |
| | 6 | -3.201849000 | -1.824650000 | 4.436490000 |
| | 1 | -4.855034000 | -2.245487000 | 3.114868000 |
| | 1 | -1.400147000 | -1.280807000 | 5.492698000 |
| | 1 | -3.704441000 | -2.207168000 | 5.320426000 |
| | 7 | 1.598887000 | -0.412979000 | -0.316745000 |
| | 16 | 3.166436000 | -0.623944000 | -0.574416000 |
| | 8 | 3.802614000 | -1.656881000 | 0.296428000 |
| | 8 | 3.543454000 | -0.743080000 | -2.016679000 |
| | 6 | 3.789559000 | 0.973570000 | -0.031404000 |
| | 6 | 3.727185000 | 2.074974000 | -0.888851000 |
| | 6 | 4.346181000 | 1.103302000 | 1.240508000 |
| | 6 | 4.211586000 | 3.308986000 | -0.459428000 |
| | 1 | 3.308953000 | 1.964831000 | -1.884204000 |
| | 6 | 4.830564000 | 2.344351000 | 1.657504000 |
| | 1 | 4.401770000 | 0.238229000 | 1.892991000 |
| | 6 | 4.771995000 | 3.465169000 | 0.818261000 |
| | 1 | 4.157590000 | 4.165129000 | -1.127907000 |
| | 1 | 5.261845000 | 2.441782000 | 2.650965000 |
| | 6 | 5.322449000 | 4.800110000 | 1.261713000 |
| | 1 | 6.343601000 | 4.949097000 | 0.886596000 |
| | 1 | 4.715744000 | 5.628940000 | 0.881586000 |
| | 1 | 5.360983000 | 4.874793000 | 2.352976000 |

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|---|---|---|---|---|
| | 6 | -3.667233000 | 2.509468000 | -1.209561000 |
| | 6 | -3.068101000 | 2.809053000 | 0.051730000 |
| | 6 | -2.286669000 | 1.880359000 | 0.683632000 |
| | 7 | -2.039723000 | 0.655791000 | 0.147897000 |
| | 6 | -2.591899000 | 0.337084000 | -1.049329000 |
| | 6 | -3.391760000 | 1.213382000 | -1.736610000 |
| | 1 | -3.210328000 | 3.766908000 | 0.532321000 |
| | 1 | -1.826939000 | 2.081414000 | 1.643731000 |
| | 1 | -2.367091000 | -0.649863000 | -1.429916000 |
| | 1 | -3.800626000 | 0.890415000 | -2.683706000 |
| | 7 | -4.443404000 | 3.396965000 | -1.859611000 |
| | 6 | -5.034597000 | 3.052145000 | -3.155261000 |
| | 1 | -5.612210000 | 3.901490000 | -3.516105000 |
| | 1 | -4.258340000 | 2.823644000 | -3.893667000 |
| | 1 | -5.705519000 | 2.190546000 | -3.065869000 |
| | 6 | -4.703585000 | 4.717832000 | -1.280751000 |
| | 1 | -5.358767000 | 5.272762000 | -1.950111000 |
| | 1 | -5.198837000 | 4.630543000 | -0.307564000 |
| | 1 | -3.774309000 | 5.284946000 | -1.157721000 |
| | 6 | -0.021622000 | -3.725037000 | -0.951624000 |
| | 6 | 1.091580000 | -2.866205000 | -1.062976000 |
| | 6 | 2.235345000 | -3.294087000 | -1.747976000 |
| | 6 | 2.256531000 | -4.582512000 | -2.291060000 |
| | 6 | 1.154927000 | -5.435623000 | -2.164935000 |
| | 6 | 0.003374000 | -5.004422000 | -1.495780000 |
| | 6 | -0.538540000 | -1.679386000 | 0.090158000 |
| | 6 | 0.755139000 | -1.576990000 | -0.390593000 |
| | 1 | 3.088981000 | -2.639255000 | -1.874318000 |
| | 1 | 3.141595000 | -4.922385000 | -2.822979000 |
| | 1 | 1.190496000 | -6.433989000 | -2.593139000 |
| | 1 | -0.859232000 | -5.660890000 | -1.405821000 |
| **1c-py-com** | 6 | -1.171116000 | -0.598481000 | 0.893324000 |
| | 1 | -0.361334000 | -0.004075000 | 1.327776000 |
| | 6 | -2.087776000 | -1.094125000 | 2.001319000 |
| | 6 | -3.396155000 | -1.530311000 | 1.747506000 |
| | 6 | -1.594514000 | -1.161518000 | 3.310926000 |
| | 6 | -4.190806000 | -2.026432000 | 2.782192000 |
| | 1 | -3.800913000 | -1.476917000 | 0.740296000 |
| | 6 | -2.387172000 | -1.661585000 | 4.345947000 |
| | 1 | -0.582741000 | -0.822819000 | 3.520235000 |
| | 6 | -3.688604000 | -2.094967000 | 4.084310000 |
| | 1 | -5.203414000 | -2.358599000 | 2.570196000 |
| | 1 | -1.989401000 | -1.704811000 | 5.356095000 |
| | 1 | -4.308883000 | -2.479446000 | 4.889136000 |

| | | | | |
|---|---|---|---|---|
| | 7 | 1.477601000 | -0.421885000 | -0.245431000 |
| | 16 | 3.069188000 | -0.320623000 | -0.421657000 |
| | 8 | 3.846287000 | -1.267620000 | 0.430048000 |
| | 8 | 3.527735000 | -0.265310000 | -1.843014000 |
| | 6 | 3.352526000 | 1.326628000 | 0.245156000 |
| | 6 | 3.135475000 | 2.451596000 | -0.554526000 |
| | 6 | 3.799560000 | 1.473133000 | 1.557878000 |
| | 6 | 3.355957000 | 3.722676000 | -0.027734000 |
| | 1 | 2.803904000 | 2.331627000 | -1.580916000 |
| | 6 | 4.019572000 | 2.751919000 | 2.072553000 |
| | 1 | 3.977558000 | 0.592556000 | 2.166216000 |
| | 6 | 3.802418000 | 3.895374000 | 1.292104000 |
| | 1 | 3.182525000 | 4.596087000 | -0.652089000 |
| | 1 | 4.367238000 | 2.861385000 | 3.097028000 |
| | 6 | 4.067853000 | 5.276673000 | 1.842917000 |
| | 1 | 5.053396000 | 5.644070000 | 1.527640000 |
| | 1 | 3.326008000 | 5.999045000 | 1.485681000 |
| | 1 | 4.051848000 | 5.280945000 | 2.937256000 |
| | 6 | -3.254065000 | 2.413961000 | -1.478093000 |
| | 6 | -3.112324000 | 2.512332000 | -0.060731000 |
| | 6 | -2.464292000 | 1.530048000 | 0.639146000 |
| | 7 | -1.931003000 | 0.437419000 | 0.032822000 |
| | 6 | -2.029317000 | 0.323616000 | -1.311427000 |
| | 6 | -2.671246000 | 1.261921000 | -2.080350000 |
| | 1 | -3.508192000 | 3.354190000 | 0.490318000 |
| | 1 | -2.349933000 | 1.579804000 | 1.715128000 |
| | 1 | -1.556698000 | -0.551450000 | -1.738760000 |
| | 1 | -2.710375000 | 1.101243000 | -3.148804000 |
| | 7 | -3.895053000 | 3.355485000 | -2.199185000 |
| | 6 | -4.019476000 | 3.214462000 | -3.651638000 |
| | 1 | -4.595382000 | 4.053087000 | -4.039590000 |
| | 1 | -3.036481000 | 3.215764000 | -4.136443000 |
| | 1 | -4.542445000 | 2.288032000 | -3.912906000 |
| | 6 | -4.455811000 | 4.538446000 | -1.541842000 |
| | 1 | -4.926581000 | 5.169665000 | -2.293808000 |
| | 1 | -5.215051000 | 4.256901000 | -0.803851000 |
| | 1 | -3.673974000 | 5.121737000 | -1.042726000 |
| | 6 | -1.138617000 | -3.031738000 | -0.212545000 |
| | 1 | -1.425031000 | -3.581561000 | 0.696121000 |
| | 1 | -2.050333000 | -2.989861000 | -0.829816000 |

**Table S3.** Cartesian coordinates of the main stationary points for the formation of **4** and **5**, optimized at the B3LYP/6-31G* level of theory in $CH_3CN$.

| Species Name | Cartesian Coordinates | | | |
|---|---|---|---|---|
| **2** | 6 | -3.950142000 | -1.687867000 | 0.006595000 |
| | 6 | -3.744759000 | -0.299879000 | 0.008550000 |
| | 6 | -2.431513000 | 0.151014000 | 0.002112000 |
| | 6 | -1.344819000 | -0.745124000 | -0.006023000 |
| | 6 | -1.562000000 | -2.119067000 | -0.007792000 |
| | 6 | -2.879836000 | -2.589408000 | -0.001495000 |
| | 1 | -4.968128000 | -2.066781000 | 0.011459000 |
| | 1 | -4.584357000 | 0.386968000 | 0.014801000 |
| | 1 | -0.719895000 | -2.804576000 | -0.014249000 |
| | 1 | -3.073750000 | -3.657448000 | -0.002926000 |
| | 6 | -0.119491000 | 0.057019000 | -0.011251000 |
| | 6 | -0.589202000 | 1.519051000 | -0.007133000 |
| | 7 | -1.964183000 | 1.480539000 | 0.002289000 |
| | 8 | 0.112664000 | 2.522713000 | -0.011080000 |
| | 7 | 1.075054000 | -0.390449000 | -0.016927000 |
| | 6 | 2.201042000 | 0.526730000 | -0.021209000 |
| | 1 | 2.214163000 | 1.162014000 | -0.913811000 |
| | 1 | 2.198759000 | 1.196265000 | 0.845815000 |
| | 6 | 3.489644000 | -0.271590000 | 0.004584000 |
| | 9 | 3.588217000 | -1.042243000 | 1.109386000 |
| | 9 | 3.604026000 | -1.089218000 | -1.064183000 |
| | 9 | 4.556652000 | 0.560410000 | -0.005559000 |
| | 6 | -2.809094000 | 2.661414000 | 0.009557000 |
| | 1 | -2.156275000 | 3.534866000 | 0.008377000 |
| | 1 | -3.448179000 | 2.683330000 | -0.879141000 |
| | 1 | -3.438770000 | 2.678742000 | 0.905016000 |
| **2'** | 6 | -2.762093000 | -3.810752000 | -0.954290000 |
| | 6 | -3.703748000 | -3.030489000 | -0.265915000 |
| | 6 | -3.405329000 | -1.691342000 | -0.037621000 |
| | 6 | -2.183170000 | -1.099904000 | -0.471384000 |
| | 6 | -1.270632000 | -1.895869000 | -1.174605000 |
| | 6 | -1.563378000 | -3.246520000 | -1.405862000 |
| | 1 | -2.973646000 | -4.859905000 | -1.143080000 |
| | 1 | -4.640980000 | -3.461992000 | 0.074620000 |
| | 1 | -0.346602000 | -1.470388000 | -1.556530000 |
| | 1 | -0.850350000 | -3.861017000 | -1.950026000 |
| | 6 | -2.225195000 | 0.289572000 | -0.071621000 |
| | 6 | -3.501442000 | 0.521146000 | 0.585184000 |
| | 7 | -4.171546000 | -0.717124000 | 0.594448000 |
| | 8 | -3.975268000 | 1.561545000 | 1.083035000 |

| | | | | |
|---|---|---|---|---|
| | 7 | -1.238265000 | 1.197334000 | -0.259781000 |
| | 6 | -1.343580000 | 2.465752000 | 0.032405000 |
| | 1 | -2.234034000 | 2.918618000 | 0.457867000 |
| | 6 | -0.176632000 | 3.348931000 | -0.202115000 |
| | 9 | 0.841389000 | 3.191377000 | 0.704905000 |
| | 9 | 0.420439000 | 3.146304000 | -1.418738000 |
| | 9 | -0.533073000 | 4.651805000 | -0.145928000 |
| | 6 | -5.482763000 | -0.912369000 | 1.170310000 |
| | 1 | -5.804099000 | 0.048356000 | 1.576834000 |
| | 1 | -6.205779000 | -1.243734000 | 0.414734000 |
| | 1 | -5.457483000 | -1.655002000 | 1.977145000 |
| | 6 | 4.057141000 | -0.780868000 | 0.239143000 |
| | 6 | 2.913818000 | -1.384506000 | 0.846963000 |
| | 6 | 1.662745000 | -0.874280000 | 0.618748000 |
| | 7 | 1.475119000 | 0.204852000 | -0.177712000 |
| | 6 | 2.530261000 | 0.815202000 | -0.767726000 |
| | 6 | 3.809187000 | 0.357441000 | -0.587583000 |
| | 1 | 3.006802000 | -2.248112000 | 1.490308000 |
| | 1 | 0.770170000 | -1.307080000 | 1.052951000 |
| | 1 | 2.300224000 | 1.680955000 | -1.373854000 |
| | 1 | 4.615466000 | 0.880930000 | -1.081766000 |
| | 7 | 5.301619000 | -1.258651000 | 0.435883000 |
| | 6 | 6.450922000 | -0.620964000 | -0.211550000 |
| | 1 | 6.345415000 | -0.633764000 | -1.301825000 |
| | 1 | 6.568463000 | 0.416084000 | 0.122249000 |
| | 1 | 7.353159000 | -1.170675000 | 0.051486000 |
| | 6 | 5.520711000 | -2.420872000 | 1.300730000 |
| | 1 | 6.587213000 | -2.636417000 | 1.337981000 |
| | 1 | 5.173073000 | -2.224342000 | 2.320806000 |
| | 1 | 5.003028000 | -3.305258000 | 0.912967000 |
| | 1 | 0.503873000 | 0.574260000 | -0.318432000 |
| **TS-1** | 6 | -3.938653000 | 1.044947000 | -2.373997000 |
| | 6 | -2.660934000 | 1.583874000 | -2.106364000 |
| | 6 | -2.272001000 | 2.759131000 | -2.776104000 |
| | 6 | -3.144826000 | 3.356153000 | -3.676061000 |
| | 6 | -4.414053000 | 2.802115000 | -3.928580000 |
| | 6 | -4.822874000 | 1.642307000 | -3.279569000 |
| | 6 | -2.637369000 | -0.291008000 | -0.684349000 |
| | 6 | -1.916461000 | 0.800751000 | -1.126412000 |
| | 1 | -1.298294000 | 3.189103000 | -2.579743000 |
| | 1 | -2.845749000 | 4.264337000 | -4.191800000 |
| | 1 | -5.082493000 | 3.283834000 | -4.636542000 |
| | 1 | -5.801040000 | 1.210823000 | -3.470563000 |
| | 16 | -4.223733000 | -0.420004000 | -1.452651000 |

| | | | | |
|---|---|---|---|---|
| | 6 | -2.164952000 | -1.358421000 | 0.269754000 |
| | 1 | -1.072655000 | -1.348378000 | 0.218999000 |
| | 6 | -2.662557000 | -2.757966000 | -0.102287000 |
| | 6 | -3.753420000 | -3.369345000 | 0.527429000 |
| | 6 | -2.010819000 | -3.436345000 | -1.141784000 |
| | 6 | -4.190414000 | -4.632417000 | 0.117239000 |
| | 1 | -4.268760000 | -2.876046000 | 1.345767000 |
| | 6 | -2.445899000 | -4.697076000 | -1.548350000 |
| | 1 | -1.152998000 | -2.979785000 | -1.626132000 |
| | 6 | -3.540120000 | -5.299536000 | -0.920928000 |
| | 1 | -5.038084000 | -5.092722000 | 0.617148000 |
| | 1 | -1.920336000 | -5.211596000 | -2.347702000 |
| | 1 | -3.878038000 | -6.283033000 | -1.235342000 |
| | 7 | -0.587124000 | 1.082272000 | -0.757697000 |
| | 16 | -0.289330000 | 1.940517000 | 0.595082000 |
| | 8 | -1.240535000 | 1.603088000 | 1.678799000 |
| | 8 | 1.152997000 | 1.801810000 | 0.880981000 |
| | 6 | -0.570655000 | 3.691161000 | 0.252055000 |
| | 6 | 0.407702000 | 4.437949000 | -0.412067000 |
| | 6 | -1.773297000 | 4.288067000 | 0.635207000 |
| | 6 | 0.171059000 | 5.782412000 | -0.691051000 |
| | 1 | 1.342201000 | 3.974492000 | -0.706490000 |
| | 6 | -1.995046000 | 5.635402000 | 0.348178000 |
| | 1 | -2.522251000 | 3.705853000 | 1.160804000 |
| | 6 | -1.030211000 | 6.404694000 | -0.316163000 |
| | 1 | 0.934258000 | 6.360490000 | -1.206507000 |
| | 1 | -2.933105000 | 6.095758000 | 0.648759000 |
| | 6 | -1.261674000 | 7.870399000 | -0.596062000 |
| | 1 | -0.774356000 | 8.181490000 | -1.525859000 |
| | 1 | -2.329225000 | 8.099444000 | -0.672840000 |
| | 1 | -0.850787000 | 8.493096000 | 0.209618000 |
| | 6 | -3.004856000 | -0.640069000 | 4.441373000 |
| | 6 | -1.822102000 | -1.296570000 | 3.991728000 |
| | 6 | -1.588237000 | -1.482975000 | 2.654514000 |
| | 7 | -2.471024000 | -1.056639000 | 1.710564000 |
| | 6 | -3.598154000 | -0.410097000 | 2.099423000 |
| | 6 | -3.893383000 | -0.193936000 | 3.419598000 |
| | 1 | -1.075037000 | -1.651208000 | 4.688430000 |
| | 1 | -0.677353000 | -1.955688000 | 2.285439000 |
| | 1 | -4.256075000 | -0.068746000 | 1.311758000 |
| | 1 | -4.810288000 | 0.328330000 | 3.654420000 |
| | 7 | -3.264513000 | -0.445772000 | 5.749800000 |
| | 6 | -4.485691000 | 0.246932000 | 6.166681000 |
| | 1 | -4.509405000 | 0.296575000 | 7.254088000 |

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|---|---|---|---|---|
| | 1 | -4.514158000 | 1.269572000 | 5.773875000 |
| | 1 | -5.378843000 | -0.288905000 | 5.826548000 |
| | 6 | -2.318868000 | -0.909110000 | 6.767922000 |
| | 1 | -2.718372000 | -0.673849000 | 7.753158000 |
| | 1 | -2.172422000 | -1.992944000 | 6.705008000 |
| | 1 | -1.347518000 | -0.413376000 | 6.661129000 |
| | 6 | 1.693265000 | -5.339556000 | -3.524382000 |
| | 6 | 1.501090000 | -5.443071000 | -2.137583000 |
| | 6 | 1.450858000 | -4.270950000 | -1.388120000 |
| | 6 | 1.577335000 | -2.981114000 | -1.994913000 |
| | 6 | 1.781260000 | -2.905035000 | -3.381321000 |
| | 6 | 1.837859000 | -4.084420000 | -4.132625000 |
| | 1 | 1.734674000 | -6.243065000 | -4.127149000 |
| | 1 | 1.401406000 | -6.415244000 | -1.661555000 |
| | 1 | 1.904627000 | -1.938374000 | -3.864530000 |
| | 1 | 1.995167000 | -4.023723000 | -5.207134000 |
| | 6 | 1.473874000 | -2.028557000 | -0.930709000 |
| | 6 | 1.311952000 | -2.712416000 | 0.303734000 |
| | 7 | 1.299085000 | -4.093646000 | -0.022408000 |
| | 8 | 1.172838000 | -2.283648000 | 1.481284000 |
| | 7 | 1.687216000 | -0.633960000 | -1.041947000 |
| | 6 | 0.935981000 | 0.159121000 | -1.784165000 |
| | 1 | 0.198854000 | -0.319002000 | -2.419765000 |
| | 6 | 1.640271000 | 1.324468000 | -2.455272000 |
| | 9 | 2.494250000 | 1.970059000 | -1.642896000 |
| | 9 | 2.371802000 | 0.821625000 | -3.486127000 |
| | 9 | 0.801119000 | 2.225797000 | -2.986180000 |
| | 6 | 1.101942000 | -5.140860000 | 0.952420000 |
| | 1 | 1.039771000 | -4.662609000 | 1.931864000 |
| | 1 | 0.174953000 | -5.697536000 | 0.764293000 |
| | 1 | 1.939180000 | -5.849789000 | 0.951321000 |
| | 1 | 2.488278000 | -0.236151000 | -0.505656000 |
| | 6 | 5.679010000 | 1.458896000 | 1.548246000 |
| | 6 | 4.437190000 | 1.142947000 | 1.019883000 |
| | 6 | 5.214057000 | -0.798013000 | 0.104476000 |
| | 6 | 6.496806000 | -0.584946000 | 0.583474000 |
| | 6 | 6.775592000 | 0.583037000 | 1.339029000 |
| | 1 | 5.790865000 | 2.375300000 | 2.114302000 |
| | 1 | 3.591538000 | 1.807965000 | 1.175373000 |
| | 1 | 5.002169000 | -1.693966000 | -0.476070000 |
| | 1 | 7.265415000 | -1.317327000 | 0.370613000 |
| | 7 | 4.176852000 | 0.034702000 | 0.302267000 |
| | 7 | 8.021529000 | 0.847214000 | 1.833089000 |
| | 6 | 8.259796000 | 2.059177000 | 2.607820000 |

| | | | | |
|---|---|---|---|---|
| | 1 | 9.308209000 | 2.091812000 | 2.904340000 |
| | 1 | 8.042634000 | 2.961554000 | 2.021890000 |
| | 1 | 7.646389000 | 2.084794000 | 3.517845000 |
| | 6 | 9.116337000 | -0.085486000 | 1.593364000 |
| | 1 | 8.905605000 | -1.074729000 | 2.020028000 |
| | 1 | 9.313150000 | -0.209442000 | 0.520611000 |
| | 1 | 10.021949000 | 0.300000000 | 2.061717000 |
| **INT-1** | 6 | -2.515628000 | 1.072594000 | 2.919827000 |
| | 6 | -2.408153000 | 0.030655000 | 1.971561000 |
| | 6 | -3.387264000 | -0.983410000 | 1.979116000 |
| | 6 | -4.429665000 | -0.922396000 | 2.892186000 |
| | 6 | -4.526663000 | 0.135938000 | 3.815808000 |
| | 6 | -3.567921000 | 1.140418000 | 3.840959000 |
| | 6 | -0.468610000 | 1.281852000 | 1.466106000 |
| | 6 | -1.230362000 | 0.182136000 | 1.132538000 |
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| | 1 | -5.182095000 | -1.705634000 | 2.895552000 |
| | 1 | -5.353088000 | 0.164458000 | 4.519928000 |
| | 1 | -3.627262000 | 1.953418000 | 4.558159000 |
| | 16 | -1.166987000 | 2.180091000 | 2.808953000 |
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| | 1 | 1.466779000 | 0.844140000 | 0.658181000 |
| | 6 | 1.693836000 | 2.524003000 | 1.936696000 |
| | 6 | 1.644147000 | 3.920412000 | 2.030130000 |
| | 6 | 2.508188000 | 1.811862000 | 2.829032000 |
| | 6 | 2.383126000 | 4.591391000 | 3.008627000 |
| | 1 | 1.040993000 | 4.501142000 | 1.338961000 |
| | 6 | 3.241263000 | 2.481703000 | 3.807536000 |
| | 1 | 2.582206000 | 0.733625000 | 2.736839000 |
| | 6 | 3.179679000 | 3.874822000 | 3.902015000 |
| | 1 | 2.335290000 | 5.675167000 | 3.065927000 |
| | 1 | 3.869486000 | 1.915866000 | 4.489897000 |
| | 1 | 3.755082000 | 4.397257000 | 4.661142000 |
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| | 6 | -4.324909000 | -0.011616000 | -1.267249000 |
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| | 1 | -1.295206000 | 5.149216000 | -4.232340000 |
| | 1 | -0.352968000 | 6.411227000 | -3.396246000 |
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| | 6 | 5.586344000 | -4.040137000 | -0.373421000 |
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| | 6 | 3.264944000 | -3.207731000 | -0.598495000 |
| | 6 | 2.865161000 | -4.478261000 | -1.049816000 |
| | 6 | 3.807973000 | -5.507254000 | -1.154378000 |
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| | 1 | 6.814818000 | -1.141428000 | -0.318712000 |
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| | 6 | 3.020240000 | -1.906267000 | 0.480894000 |
| | 6 | 3.261155000 | -3.118419000 | -0.188295000 |
| | 6 | 4.578120000 | -3.507346000 | -0.420838000 |
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| | 1 | -3.628366000 | -2.970313000 | -0.559854000 |
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| | 1 | -3.644837000 | 1.097341000 | -1.983636000 |
| | 6 | -6.287706000 | -0.900314000 | -1.139635000 |
| | 1 | -6.102266000 | -2.939696000 | -0.464077000 |
| | 1 | -6.114025000 | 1.127423000 | -1.861737000 |
| | 6 | -7.793303000 | -0.872385000 | -1.049886000 |
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| | 1 | 0.422055000 | -2.570852000 | 0.284582000 |
| **4** | 6 | 5.234365000 | -3.183659000 | -0.884453000 |
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| | 6 | -1.305695000 | -2.182451000 | 1.672901000 |
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| | 9 | -1.474587000 | -3.264415000 | 0.882972000 |
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| | 6 | -1.509252000 | 2.326172000 | 0.661100000 |
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| | 6 | -0.728200000 | 1.198913000 | 0.214586000 |
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| | 1 | -4.422620000 | 3.632936000 | 1.820753000 |
| | 1 | -3.061806000 | 5.706521000 | 1.776364000 |
| | 1 | -0.686946000 | 5.643311000 | 1.053309000 |
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| | 6 | 1.619946000 | 0.531012000 | -0.644759000 |
| | 1 | 1.170950000 | 0.124932000 | -1.560933000 |
| | 6 | 2.905491000 | 1.238577000 | -1.071586000 |
| | 6 | 3.240912000 | 1.289231000 | -2.432159000 |
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| | 1 | 2.582247000 | 0.827093000 | -3.163025000 |
| | 6 | 4.938831000 | 2.482438000 | -0.576943000 |
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| | 6 | 5.261923000 | 2.521861000 | -1.934291000 |
| | 1 | 4.644815000 | 1.951021000 | -3.922127000 |
| | 1 | 5.594211000 | 2.947466000 | 0.154253000 |
| | 1 | 6.170638000 | 3.016195000 | -2.266183000 |
| | 7 | -1.248799000 | -0.135442000 | 0.181246000 |
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| | 8 | -1.643949000 | 0.424588000 | -2.296000000 |

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| | 6 | -4.472079000 | 0.287612000 | -1.419933000 |
| | 6 | -5.586626000 | -2.119197000 | -0.543157000 |
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| | 1 | -4.035956000 | 1.213281000 | -1.778312000 |
| | 6 | -6.430911000 | -1.035466000 | -0.829646000 |
| | 1 | -6.016716000 | -3.060863000 | -0.212827000 |
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| | 1 | -8.271853000 | -2.171278000 | -0.845969000 |
| | 1 | -8.209507000 | -0.904716000 | 0.382356000 |
| | 1 | -8.462481000 | -0.467338000 | -1.310411000 |
| | 1 | 0.517486000 | -2.179712000 | -0.356508000 |
| **TS-3** | 6 | 4.938565000 | -2.746656000 | 0.515735000 |
| | 6 | 4.266815000 | -3.202522000 | -0.627705000 |
| | 6 | 2.959348000 | -2.767811000 | -0.821550000 |
| | 6 | 2.321132000 | -1.899532000 | 0.075656000 |
| | 6 | 2.997329000 | -1.457977000 | 1.202925000 |
| | 6 | 4.315524000 | -1.888421000 | 1.423981000 |
| | 1 | 5.959587000 | -3.072433000 | 0.694054000 |
| | 1 | 4.752183000 | -3.873766000 | -1.328864000 |
| | 1 | 2.518111000 | -0.785371000 | 1.908689000 |
| | 1 | 4.852218000 | -1.549409000 | 2.305119000 |
| | 6 | 0.925349000 | -1.582281000 | -0.442498000 |
| | 6 | 0.850088000 | -2.509187000 | -1.691498000 |
| | 7 | 2.083142000 | -3.100450000 | -1.867136000 |
| | 8 | -0.109381000 | -2.667259000 | -2.440261000 |
| | 7 | 0.921840000 | -0.171085000 | -0.894600000 |
| | 6 | -0.170723000 | 0.252506000 | -1.514160000 |
| | 1 | -0.788235000 | -0.457027000 | -2.068776000 |
| | 6 | -0.002897000 | 1.504393000 | -2.369595000 |
| | 9 | -1.164858000 | 2.135420000 | -2.638394000 |
| | 9 | 0.849626000 | 2.420316000 | -1.877674000 |
| | 9 | 0.502545000 | 1.110636000 | -3.571388000 |
| | 6 | 2.406548000 | -3.977855000 | -2.976338000 |
| | 1 | 1.524172000 | -4.041842000 | -3.613835000 |
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| | 6 | -4.057305000 | -2.211923000 | -0.367731000 |
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| | 6 | -4.639481000 | 0.051048000 | -1.025901000 |

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| | 6 | -1.629076000 | -1.771036000 | 0.180295000 |
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| | 1 | -5.626063000 | -3.702164000 | -0.497100000 |
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| | 6 | -0.179536000 | -1.878188000 | 0.652284000 |
| | 1 | -0.057726000 | -1.047920000 | 1.358108000 |
| | 6 | 0.071082000 | -3.163854000 | 1.439266000 |
| | 6 | 0.194125000 | -3.100029000 | 2.834858000 |
| | 6 | 0.167446000 | -4.421326000 | 0.821839000 |
| | 6 | 0.413444000 | -4.251067000 | 3.593427000 |
| | 1 | 0.114727000 | -2.136510000 | 3.332422000 |
| | 6 | 0.388574000 | -5.574898000 | 1.577734000 |
| | 1 | 0.059436000 | -4.510559000 | -0.254754000 |
| | 6 | 0.514197000 | -5.494667000 | 2.965940000 |
| | 1 | 0.505831000 | -4.174847000 | 4.673552000 |
| | 1 | 0.461390000 | -6.537127000 | 1.077998000 |
| | 1 | 0.686820000 | -6.392568000 | 3.552909000 |
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| | 16 | -1.524585000 | 1.623064000 | 0.901373000 |
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| | 8 | -0.413871000 | 2.561584000 | 0.623185000 |
| | 6 | -3.019440000 | 2.628861000 | 0.915162000 |
| | 6 | -3.252445000 | 3.518201000 | -0.141181000 |
| | 6 | -3.921215000 | 2.530188000 | 1.971945000 |
| | 6 | -4.398820000 | 4.305724000 | -0.127923000 |
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| | 1 | -3.725013000 | 1.840317000 | 2.785341000 |
| | 6 | -5.325891000 | 4.225827000 | 0.927027000 |
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| | 1 | -5.770280000 | 3.251990000 | 2.796167000 |
| | 6 | -6.563202000 | 5.091488000 | 0.925650000 |
| | 1 | -7.161758000 | 4.925577000 | 0.021920000 |
| | 1 | -7.196225000 | 4.885564000 | 1.793648000 |
| | 1 | -6.300692000 | 6.156383000 | 0.943927000 |
| | 1 | 2.202554000 | 0.865772000 | -0.487412000 |
| | 6 | 5.188921000 | 3.191753000 | 0.326496000 |
| | 6 | 5.360910000 | 1.973825000 | -0.397073000 |

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| | 6 | 4.277491000 | 1.173793000 | -0.662118000 |
| | 7 | 3.033524000 | 1.508025000 | -0.257006000 |
| | 6 | 2.823316000 | 2.653188000 | 0.429827000 |
| | 6 | 3.858233000 | 3.502398000 | 0.736613000 |
| | 1 | 6.334163000 | 1.657339000 | -0.745370000 |
| | 1 | 4.367956000 | 0.239270000 | -1.202713000 |
| | 1 | 1.793821000 | 2.847799000 | 0.709409000 |
| | 1 | 3.636583000 | 4.405192000 | 1.288667000 |
| | 7 | 6.230245000 | 4.005882000 | 0.606996000 |
| | 6 | 6.018174000 | 5.244451000 | 1.357624000 |
| | 1 | 6.974885000 | 5.749162000 | 1.483519000 |
| | 1 | 5.339698000 | 5.919998000 | 0.824246000 |
| | 1 | 5.603559000 | 5.040094000 | 2.351300000 |
| | 6 | 7.581969000 | 3.655774000 | 0.167960000 |
| | 1 | 8.268373000 | 4.442738000 | 0.476946000 |
| | 1 | 7.914084000 | 2.712677000 | 0.617247000 |
| | 1 | 7.632755000 | 3.564011000 | -0.922904000 |
| **INT-3** | 6 | -4.351828000 | -2.793664000 | -2.222267000 |
| | 6 | -3.904744000 | -3.683208000 | -1.235186000 |
| | 6 | -2.813688000 | -3.292275000 | -0.467788000 |
| | 6 | -2.173274000 | -2.060591000 | -0.655087000 |
| | 6 | -2.613892000 | -1.196543000 | -1.647088000 |
| | 6 | -3.717390000 | -1.567531000 | -2.431224000 |
| | 1 | -5.203417000 | -3.071480000 | -2.836777000 |
| | 1 | -4.393845000 | -4.639779000 | -1.083492000 |
| | 1 | -2.109729000 | -0.251395000 | -1.827173000 |
| | 1 | -4.074324000 | -0.898142000 | -3.207991000 |
| | 6 | -1.018996000 | -1.947442000 | 0.324164000 |
| | 6 | -1.115770000 | -3.308209000 | 1.078296000 |
| | 7 | -2.177692000 | -4.006756000 | 0.563329000 |
| | 8 | -0.399284000 | -3.690518000 | 1.997753000 |
| | 7 | -1.226007000 | -0.815290000 | 1.246202000 |
| | 6 | -0.566756000 | -0.804482000 | 2.333833000 |
| | 1 | 0.073657000 | -1.613034000 | 2.682269000 |
| | 6 | -0.679625000 | 0.353379000 | 3.296518000 |
| | 9 | 0.548484000 | 0.815642000 | 3.606060000 |
| | 9 | -1.404929000 | 1.382152000 | 2.828719000 |
| | 9 | -1.253688000 | -0.064451000 | 4.448757000 |
| | 6 | -2.576560000 | -5.322828000 | 1.030290000 |
| | 1 | -1.902928000 | -5.605726000 | 1.839299000 |
| | 1 | -3.605804000 | -5.301263000 | 1.402802000 |
| | 1 | -2.503611000 | -6.055914000 | 0.220271000 |
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| | 6 | 3.116594000 | 0.068892000 | 1.445359000 |

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| | 6 | 3.758815000 | 1.212609000 | 1.950585000 |
| | 6 | 4.904257000 | 1.071557000 | 2.724038000 |
| | 6 | 5.426222000 | -0.205332000 | 3.007022000 |
| | 6 | 4.803008000 | -1.352004000 | 2.522884000 |
| | 6 | 1.543971000 | -1.299892000 | 0.346355000 |
| | 6 | 1.914837000 | 0.006864000 | 0.621816000 |
| | 1 | 3.346192000 | 2.191078000 | 1.726444000 |
| | 1 | 5.403589000 | 1.953181000 | 3.116826000 |
| | 1 | 6.323799000 | -0.299292000 | 3.612241000 |
| | 1 | 5.202349000 | -2.337643000 | 2.745175000 |
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| | 6 | 0.351600000 | -1.704249000 | -0.481543000 |
| | 1 | 0.122905000 | -0.806548000 | -1.057013000 |
| | 6 | 0.638140000 | -2.805225000 | -1.504187000 |
| | 6 | 0.723252000 | -2.448331000 | -2.859038000 |
| | 6 | 0.849832000 | -4.148946000 | -1.156789000 |
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| | 6 | 1.126266000 | -5.105961000 | -2.136593000 |
| | 1 | 0.808016000 | -4.462215000 | -0.118865000 |
| | 6 | 1.200854000 | -4.738747000 | -3.481197000 |
| | 1 | 1.061887000 | -3.102359000 | -4.880981000 |
| | 1 | 1.285442000 | -6.140339000 | -1.843543000 |
| | 1 | 1.415342000 | -5.484597000 | -4.241806000 |
| | 7 | 1.195667000 | 1.164796000 | 0.311513000 |
| | 16 | 1.226442000 | 1.831890000 | -1.124356000 |
| | 8 | 0.990682000 | 0.901078000 | -2.271928000 |
| | 8 | 0.310643000 | 3.008179000 | -1.078255000 |
| | 6 | 2.870252000 | 2.519943000 | -1.445567000 |
| | 6 | 3.188506000 | 3.805627000 | -0.995409000 |
| | 6 | 3.841331000 | 1.744330000 | -2.081586000 |
| | 6 | 4.474009000 | 4.307321000 | -1.187110000 |
| | 1 | 2.428047000 | 4.409768000 | -0.511141000 |
| | 6 | 5.127342000 | 2.257089000 | -2.263648000 |
| | 1 | 3.588694000 | 0.752739000 | -2.442136000 |
| | 6 | 5.465958000 | 3.542990000 | -1.822733000 |
| | 1 | 4.712064000 | 5.310529000 | -0.840509000 |
| | 1 | 5.877964000 | 1.647599000 | -2.761366000 |
| | 6 | 6.850258000 | 4.106425000 | -2.042708000 |
| | 1 | 7.227418000 | 4.602366000 | -1.141211000 |
| | 1 | 7.560984000 | 3.323382000 | -2.324126000 |
| | 1 | 6.849309000 | 4.856378000 | -2.844462000 |
| | 1 | -2.402998000 | 0.639669000 | 0.745697000 |
| | 6 | -4.978371000 | 3.356759000 | -0.044149000 |

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| | 6 | -5.360182000 | 2.089445000 | 0.494503000 |
| | 6 | -4.408377000 | 1.139841000 | 0.756775000 |
| | 7 | -3.097386000 | 1.372985000 | 0.513209000 |
| | 6 | -2.682369000 | 2.557171000 | 0.001028000 |
| | 6 | -3.584461000 | 3.550035000 | -0.285554000 |
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| | 1 | -4.653783000 | 0.167895000 | 1.166673000 |
| | 1 | -1.615607000 | 2.664473000 | -0.184263000 |
| | 1 | -3.208735000 | 4.475523000 | -0.699150000 |
| | 7 | -5.887334000 | 4.316086000 | -0.310259000 |
| | 6 | -5.462168000 | 5.607885000 | -0.854684000 |
| | 1 | -6.337943000 | 6.241971000 | -0.982441000 |
| | 1 | -4.767141000 | 6.112649000 | -0.174693000 |
| | 1 | -4.978659000 | 5.486013000 | -1.830298000 |
| | 6 | -7.310344000 | 4.079023000 | -0.055989000 |
| | 1 | -7.873116000 | 4.964389000 | -0.347278000 |
| | 1 | -7.679097000 | 3.228712000 | -0.640251000 |
| | 1 | -7.495231000 | 3.886428000 | 1.006776000 |
| **TS-4** | 6 | -1.377467000 | -4.788680000 | 2.300923000 |
| | 6 | -2.372223000 | -4.639378000 | 1.324023000 |
| | 6 | -2.280269000 | -3.544742000 | 0.472075000 |
| | 6 | -1.235234000 | -2.601115000 | 0.567602000 |
| | 6 | -0.270426000 | -2.751574000 | 1.560801000 |
| | 6 | -0.340958000 | -3.858508000 | 2.419181000 |
| | 1 | -1.422470000 | -5.637453000 | 2.977868000 |
| | 1 | -3.181833000 | -5.357405000 | 1.237795000 |
| | 1 | 0.507774000 | -2.006177000 | 1.682859000 |
| | 1 | 0.413018000 | -3.986694000 | 3.190932000 |
| | 6 | -1.483799000 | -1.556228000 | -0.445164000 |
| | 6 | -2.695560000 | -2.030498000 | -1.201366000 |
| | 7 | -3.132232000 | -3.188475000 | -0.580428000 |
| | 8 | -3.223322000 | -1.533567000 | -2.199716000 |
| | 7 | -0.429677000 | -0.957534000 | -1.120865000 |
| | 6 | -0.656311000 | -0.160946000 | -2.111097000 |
| | 1 | -1.635245000 | 0.017172000 | -2.546511000 |
| | 6 | 0.507572000 | 0.406434000 | -2.872194000 |
| | 9 | 0.146877000 | 1.522135000 | -3.538794000 |
| | 9 | 1.568526000 | 0.714595000 | -2.095044000 |
| | 9 | 0.965204000 | -0.477016000 | -3.806917000 |
| | 6 | -4.312362000 | -3.924874000 | -0.985737000 |
| | 1 | -4.728315000 | -3.425775000 | -1.861764000 |
| | 1 | -4.054771000 | -4.957498000 | -1.245129000 |
| | 1 | -5.059256000 | -3.934243000 | -0.184001000 |
| | 6 | -2.864556000 | 3.099604000 | -1.728679000 |

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| | 6 | -0.726830000 | 4.246361000 | -1.746516000 |
| | 6 | -1.240423000 | 5.148896000 | -2.669268000 |
| | 6 | -2.568158000 | 5.029561000 | -3.119768000 |
| | 6 | -3.391690000 | 4.008699000 | -2.653024000 |
| | 6 | -2.242923000 | 1.261744000 | -0.077460000 |
| | 6 | -1.172046000 | 2.183316000 | -0.286589000 |
| | 1 | 0.292714000 | 4.327758000 | -1.384066000 |
| | 1 | -0.615885000 | 5.954214000 | -3.045215000 |
| | 1 | -2.959115000 | 5.743262000 | -3.839718000 |
| | 1 | -4.417456000 | 3.920612000 | -2.998755000 |
| | 16 | -3.707376000 | 1.749037000 | -0.995476000 |
| | 6 | -2.219053000 | 0.099656000 | 0.739090000 |
| | 1 | -1.320959000 | 0.025579000 | 1.338567000 |
| | 6 | -3.401226000 | -0.430158000 | 1.469641000 |
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| | 6 | -4.664303000 | -0.658184000 | 0.892518000 |
| | 6 | -4.312107000 | -1.148705000 | 3.617591000 |
| | 1 | -2.277180000 | -0.524315000 | 3.306794000 |
| | 6 | -5.730812000 | -1.115812000 | 1.666693000 |
| | 1 | -4.812896000 | -0.512308000 | -0.171633000 |
| | 6 | -5.562353000 | -1.358936000 | 3.032405000 |
| | 1 | -4.165494000 | -1.337120000 | 4.677673000 |
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| | 1 | -6.396351000 | -1.712725000 | 3.632207000 |
| | 7 | 0.046822000 | 2.332285000 | 0.277138000 |
| | 16 | 0.592032000 | 1.700243000 | 1.651930000 |
| | 8 | -0.305414000 | 1.917440000 | 2.818562000 |
| | 8 | 1.090016000 | 0.294430000 | 1.525865000 |
| | 6 | 2.051751000 | 2.716835000 | 1.885333000 |
| | 6 | 3.026030000 | 2.780667000 | 0.882035000 |
| | 6 | 2.232519000 | 3.385879000 | 3.092695000 |
| | 6 | 4.179123000 | 3.527670000 | 1.099151000 |
| | 1 | 2.873511000 | 2.262166000 | -0.059304000 |
| | 6 | 3.397456000 | 4.131661000 | 3.295219000 |
| | 1 | 1.469068000 | 3.326800000 | 3.860886000 |
| | 6 | 4.385551000 | 4.215897000 | 2.308079000 |
| | 1 | 4.933729000 | 3.581071000 | 0.317968000 |
| | 1 | 3.535374000 | 4.656447000 | 4.237192000 |
| | 6 | 5.641880000 | 5.025925000 | 2.522904000 |
| | 1 | 5.712920000 | 5.846130000 | 1.797883000 |
| | 1 | 5.670538000 | 5.460830000 | 3.526243000 |
| | 1 | 6.538989000 | 4.408310000 | 2.395044000 |
| | 1 | 1.399635000 | -1.332026000 | -0.640492000 |

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| | 6 | 4.844505000 | -2.995136000 | -0.845703000 |
| | 6 | 3.829228000 | -3.224763000 | -1.824290000 |
| | 6 | 2.612329000 | -2.605386000 | -1.710235000 |
| | 7 | 2.341653000 | -1.770033000 | -0.680849000 |
| | 6 | 3.274793000 | -1.510026000 | 0.264957000 |
| | 6 | 4.513675000 | -2.095774000 | 0.213479000 |
| | 1 | 3.994479000 | -3.882491000 | -2.666074000 |
| | 1 | 1.817995000 | -2.741733000 | -2.433497000 |
| | 1 | 2.970204000 | -0.817564000 | 1.040062000 |
| | 1 | 5.225608000 | -1.857201000 | 0.991235000 |
| | 7 | 6.050530000 | -3.592893000 | -0.920338000 |
| | 6 | 7.069087000 | -3.334687000 | 0.100131000 |
| | 1 | 7.958405000 | -3.917340000 | -0.134539000 |
| | 1 | 7.346528000 | -2.274922000 | 0.123042000 |
| | 1 | 6.715201000 | -3.630449000 | 1.093874000 |
| | 6 | 6.358385000 | -4.506121000 | -2.023427000 |
| | 1 | 7.372582000 | -4.881428000 | -1.897276000 |
| | 1 | 5.672887000 | -5.360798000 | -2.031730000 |
| | 1 | 6.298387000 | -3.993475000 | -2.989978000 |
| **INT-4** | 6 | 1.201599000 | -5.206613000 | 1.672834000 |
| | 6 | 2.281763000 | -4.832903000 | 0.859549000 |
| | 6 | 2.102904000 | -3.771241000 | -0.020577000 |
| | 6 | 0.870883000 | -3.062603000 | -0.121663000 |
| | 6 | -0.187412000 | -3.452266000 | 0.707490000 |
| | 6 | -0.016501000 | -4.521725000 | 1.595797000 |
| | 1 | 1.316960000 | -6.034217000 | 2.367758000 |
| | 1 | 3.230683000 | -5.358735000 | 0.917593000 |
| | 1 | -1.138707000 | -2.931011000 | 0.672587000 |
| | 1 | -0.843450000 | -4.819877000 | 2.235574000 |
| | 6 | 1.060406000 | -2.033548000 | -1.121933000 |
| | 6 | 2.427321000 | -2.146608000 | -1.613664000 |
| | 7 | 3.012290000 | -3.216609000 | -0.915816000 |
| | 8 | 3.029327000 | -1.485280000 | -2.483147000 |
| | 7 | 0.124495000 | -1.152705000 | -1.548503000 |
| | 6 | 0.361872000 | -0.211935000 | -2.424479000 |
| | 1 | 1.322583000 | -0.068285000 | -2.908157000 |
| | 6 | -0.748725000 | 0.660601000 | -2.872861000 |
| | 9 | -1.574760000 | 0.077032000 | -3.802920000 |
| | 9 | -1.589756000 | 1.043733000 | -1.865518000 |
| | 9 | -0.276434000 | 1.789123000 | -3.450565000 |
| | 6 | 4.380591000 | -3.642772000 | -1.103355000 |
| | 1 | 4.823159000 | -2.990219000 | -1.857969000 |
| | 1 | 4.952788000 | -3.557368000 | -0.171486000 |
| | 1 | 4.431656000 | -4.682042000 | -1.450534000 |

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| | 6 | 3.580991000 | -0.496122000 | 2.047781000 |
| | 6 | 2.232631000 | -0.204597000 | 2.354665000 |
| | 6 | 1.608223000 | -0.922494000 | 3.393238000 |
| | 6 | 2.330163000 | -1.866862000 | 4.112820000 |
| | 6 | 3.678436000 | -2.112345000 | 3.814253000 |
| | 6 | 4.313288000 | -1.433173000 | 2.776549000 |
| | 6 | 2.646583000 | 1.190261000 | 0.410785000 |
| | 6 | 1.673448000 | 0.823898000 | 1.471640000 |
| | 1 | 0.567089000 | -0.757631000 | 3.631046000 |
| | 1 | 1.843271000 | -2.420713000 | 4.909098000 |
| | 1 | 4.233619000 | -2.848889000 | 4.387773000 |
| | 1 | 5.350963000 | -1.637619000 | 2.532353000 |
| | 16 | 4.212633000 | 0.386571000 | 0.659014000 |
| | 6 | 2.349643000 | 2.081641000 | -0.570177000 |
| | 1 | 1.361376000 | 2.526844000 | -0.476650000 |
| | 6 | 3.159322000 | 2.579380000 | -1.674882000 |
| | 6 | 2.829098000 | 3.843400000 | -2.209689000 |
| | 6 | 4.235134000 | 1.869232000 | -2.248900000 |
| | 6 | 3.576511000 | 4.401314000 | -3.242603000 |
| | 1 | 1.987893000 | 4.391054000 | -1.792975000 |
| | 6 | 4.971461000 | 2.426070000 | -3.291855000 |
| | 1 | 4.449387000 | 0.855898000 | -1.927460000 |
| | 6 | 4.655393000 | 3.696081000 | -3.784080000 |
| | 1 | 3.314712000 | 5.381611000 | -3.630391000 |
| | 1 | 5.789327000 | 1.861607000 | -3.730615000 |
| | 1 | 5.236102000 | 4.126203000 | -4.595144000 |
| | 7 | 0.531198000 | 1.464704000 | 1.463559000 |
| | 16 | -0.682213000 | 1.351887000 | 2.586564000 |
| | 8 | -1.510383000 | 0.152085000 | 2.312146000 |
| | 8 | -0.206839000 | 1.525085000 | 3.974590000 |
| | 6 | -1.625639000 | 2.809737000 | 2.157534000 |
| | 6 | -2.061211000 | 3.011322000 | 0.843480000 |
| | 6 | -1.969132000 | 3.701160000 | 3.172369000 |
| | 6 | -2.842103000 | 4.125940000 | 0.555430000 |
| | 1 | -1.779857000 | 2.320872000 | 0.056706000 |
| | 6 | -2.755954000 | 4.812462000 | 2.863371000 |
| | 1 | -1.618595000 | 3.532226000 | 4.184304000 |
| | 6 | -3.204937000 | 5.042841000 | 1.557502000 |
| | 1 | -3.174539000 | 4.290635000 | -0.466398000 |
| | 1 | -3.019509000 | 5.511568000 | 3.652497000 |
| | 6 | -4.063425000 | 6.239383000 | 1.225864000 |
| | 1 | -3.672728000 | 6.778594000 | 0.355526000 |
| | 1 | -5.087272000 | 5.931186000 | 0.979131000 |
| | 1 | -4.117715000 | 6.938161000 | 2.065545000 |

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| | 6 | -5.451142000 | -2.004668000 | -1.053264000 |
| | 6 | -4.663517000 | -2.391227000 | -2.180472000 |
| | 6 | -3.312551000 | -2.159868000 | -2.187017000 |
| | 7 | -2.693608000 | -1.572084000 | -1.137796000 |
| | 6 | -3.398670000 | -1.176202000 | -0.051552000 |
| | 6 | -4.753710000 | -1.375264000 | 0.022388000 |
| | 1 | -5.108186000 | -2.866410000 | -3.043496000 |
| | 1 | -2.681039000 | -2.425841000 | -3.025456000 |
| | 1 | -2.831741000 | -0.700344000 | 0.742277000 |
| | 1 | -5.272372000 | -1.044149000 | 0.911162000 |
| | 7 | -6.781662000 | -2.219620000 | -1.008615000 |
| | 6 | -7.558807000 | -1.807921000 | 0.162854000 |
| | 1 | -7.209956000 | -2.318003000 | 1.067626000 |
| | 1 | -7.494871000 | -0.725308000 | 0.318909000 |
| | 1 | -8.603413000 | -2.069968000 | 0.002748000 |
| | 6 | -7.465303000 | -2.870932000 | -2.128387000 |
| | 1 | -8.526755000 | -2.945504000 | -1.897668000 |
| | 1 | -7.353385000 | -2.291087000 | -3.051259000 |
| | 1 | -7.076530000 | -3.881822000 | -2.294641000 |
| | 1 | -1.658487000 | -1.401680000 | -1.187346000 |
| **TS-5** | 6 | 1.028738000 | -5.099287000 | 1.529721000 |
| | 6 | 2.086730000 | -4.824550000 | 0.651342000 |
| | 6 | 1.999568000 | -3.677278000 | -0.127211000 |
| | 6 | 0.888108000 | -2.801126000 | -0.061378000 |
| | 6 | -0.141636000 | -3.081591000 | 0.838762000 |
| | 6 | -0.067777000 | -4.236393000 | 1.626990000 |
| | 1 | 1.070689000 | -5.991806000 | 2.147828000 |
| | 1 | 2.943543000 | -5.487681000 | 0.585201000 |
| | 1 | -0.977819000 | -2.402383000 | 0.953160000 |
| | 1 | -0.869146000 | -4.458964000 | 2.325788000 |
| | 6 | 1.140614000 | -1.716403000 | -1.001245000 |
| | 6 | 2.467715000 | -2.007070000 | -1.628086000 |
| | 7 | 2.918916000 | -3.191026000 | -1.061718000 |
| | 8 | 3.069573000 | -1.390920000 | -2.515277000 |
| | 7 | 0.280623000 | -0.779029000 | -1.371884000 |
| | 6 | 0.665285000 | 0.233717000 | -2.174892000 |
| | 1 | 1.530135000 | 0.120374000 | -2.820734000 |
| | 6 | -0.448563000 | 1.009426000 | -2.800294000 |
| | 9 | -1.142053000 | 0.269173000 | -3.725299000 |
| | 9 | -1.383609000 | 1.433942000 | -1.909533000 |
| | 9 | 0.000319000 | 2.096602000 | -3.460024000 |
| | 6 | 4.168962000 | -3.830714000 | -1.419258000 |
| | 1 | 4.649900000 | -3.211802000 | -2.177652000 |
| | 1 | 4.827426000 | -3.914706000 | -0.547586000 |

| | | | | |
|---|---|---|---|---|
| | 1 | 3.992415000 | -4.832006000 | -1.827869000 |
| | 6 | 3.824368000 | -0.292489000 | 1.763113000 |
| | 6 | 2.490118000 | -0.232153000 | 2.231152000 |
| | 6 | 2.169571000 | -0.923550000 | 3.416234000 |
| | 6 | 3.158568000 | -1.610817000 | 4.109810000 |
| | 6 | 4.483152000 | -1.627313000 | 3.643972000 |
| | 6 | 4.823998000 | -0.972454000 | 2.464594000 |
| | 6 | 2.338626000 | 0.948740000 | 0.150613000 |
| | 6 | 1.625562000 | 0.543008000 | 1.332540000 |
| | 1 | 1.158156000 | -0.916531000 | 3.797546000 |
| | 1 | 2.901239000 | -2.142495000 | 5.021154000 |
| | 1 | 5.247008000 | -2.164137000 | 4.199492000 |
| | 1 | 5.842726000 | -0.997926000 | 2.088994000 |
| | 16 | 4.061859000 | 0.519440000 | 0.225517000 |
| | 6 | 1.746531000 | 1.704321000 | -0.874909000 |
| | 1 | 0.800572000 | 2.141256000 | -0.568308000 |
| | 6 | 2.515686000 | 2.509264000 | -1.851956000 |
| | 6 | 2.170244000 | 3.862855000 | -2.020280000 |
| | 6 | 3.586573000 | 1.994010000 | -2.605059000 |
| | 6 | 2.894127000 | 4.685838000 | -2.881394000 |
| | 1 | 1.334252000 | 4.272124000 | -1.458880000 |
| | 6 | 4.306753000 | 2.818639000 | -3.470400000 |
| | 1 | 3.826169000 | 0.936688000 | -2.543045000 |
| | 6 | 3.969834000 | 4.167541000 | -3.607709000 |
| | 1 | 2.616410000 | 5.731080000 | -2.987560000 |
| | 1 | 5.128325000 | 2.401969000 | -4.047040000 |
| | 1 | 4.532491000 | 4.806351000 | -4.282896000 |
| | 7 | 0.353299000 | 0.944808000 | 1.442400000 |
| | 16 | -0.637775000 | 0.867233000 | 2.718175000 |
| | 8 | -1.529547000 | -0.325135000 | 2.619599000 |
| | 8 | -0.000303000 | 1.063339000 | 4.044036000 |
| | 6 | -1.659258000 | 2.317624000 | 2.431369000 |
| | 6 | -2.192371000 | 2.588611000 | 1.166687000 |
| | 6 | -1.973374000 | 3.130807000 | 3.519650000 |
| | 6 | -3.038183000 | 3.681541000 | 1.002541000 |
| | 1 | -1.929273000 | 1.968329000 | 0.318655000 |
| | 6 | -2.825154000 | 4.222711000 | 3.337805000 |
| | 1 | -1.547787000 | 2.916297000 | 4.493597000 |
| | 6 | -3.372992000 | 4.515078000 | 2.083343000 |
| | 1 | -3.443137000 | 3.895195000 | 0.016221000 |
| | 1 | -3.062867000 | 4.857613000 | 4.187515000 |
| | 6 | -4.303696000 | 5.688059000 | 1.889080000 |
| | 1 | -3.986205000 | 6.312860000 | 1.046266000 |
| | 1 | -5.324058000 | 5.349036000 | 1.669487000 |

| | | | | |
|---|---|---|---|---|
| | 1 | -4.346298000 | 6.317564000 | 2.782795000 |
| | 6 | -5.291099000 | -1.961757000 | -1.203224000 |
| | 6 | -4.431357000 | -2.062939000 | -2.339578000 |
| | 6 | -3.111707000 | -1.709793000 | -2.237959000 |
| | 7 | -2.590234000 | -1.260984000 | -1.071749000 |
| | 6 | -3.365665000 | -1.144303000 | 0.034105000 |
| | 6 | -4.695114000 | -1.479263000 | 0.001727000 |
| | 1 | -4.796633000 | -2.415311000 | -3.293832000 |
| | 1 | -2.428805000 | -1.759666000 | -3.075616000 |
| | 1 | -2.872985000 | -0.782219000 | 0.931957000 |
| | 1 | -5.271917000 | -1.370072000 | 0.909537000 |
| | 7 | -6.593483000 | -2.302806000 | -1.266228000 |
| | 6 | -7.446324000 | -2.190122000 | -0.080441000 |
| | 1 | -7.081385000 | -2.830231000 | 0.730465000 |
| | 1 | -7.490749000 | -1.155410000 | 0.276600000 |
| | 1 | -8.455041000 | -2.506832000 | -0.340370000 |
| | 6 | -7.170374000 | -2.796267000 | -2.519257000 |
| | 1 | -8.224706000 | -3.015644000 | -2.359328000 |
| | 1 | -7.090934000 | -2.045626000 | -3.313392000 |
| | 1 | -6.672609000 | -3.715093000 | -2.848282000 |
| | 1 | -1.576735000 | -1.014379000 | -1.041552000 |
| | 6 | -5.914746000 | 1.357200000 | -1.969369000 |
| | 6 | -6.069941000 | 0.225293000 | -1.155182000 |
| | 6 | -4.915984000 | -0.424667000 | -0.741030000 |
| | 6 | -3.636715000 | 0.027931000 | -1.118850000 |
| | 6 | -3.496931000 | 1.151921000 | -1.929779000 |
| | 6 | -4.651007000 | 1.818207000 | -2.354304000 |
| | 1 | -6.801872000 | 1.885071000 | -2.307027000 |
| | 1 | -7.055960000 | -0.121483000 | -0.865700000 |
| | 1 | -2.513387000 | 1.505401000 | -2.223423000 |
| | 1 | -4.566149000 | 2.696823000 | -2.985674000 |
| | 6 | -2.657942000 | -0.880112000 | -0.521212000 |
| **5** | 6 | -3.492913000 | -1.929587000 | 0.248695000 |
| | 7 | -4.806228000 | -1.572207000 | 0.068503000 |
| | 8 | -3.087670000 | -2.882307000 | 0.901560000 |
| | 7 | -1.386939000 | -0.778883000 | -0.623727000 |
| | 6 | -0.490436000 | -1.753810000 | -0.002607000 |
| | 1 | -0.971221000 | -2.293713000 | 0.814816000 |
| | 6 | -0.163267000 | -2.803865000 | -1.079934000 |
| | 9 | -1.291681000 | -3.313976000 | -1.618181000 |
| | 9 | 0.558232000 | -2.275153000 | -2.094644000 |
| | 9 | 0.540543000 | -3.838585000 | -0.581337000 |
| | 6 | -5.927358000 | -2.298917000 | 0.639611000 |
| | 1 | -5.523268000 | -3.135569000 | 1.209911000 |

| | | | | |
|---|---|---|---|---|
| | 1 | -6.505553000 | -1.649636000 | 1.304637000 |
| | 1 | -6.581106000 | -2.678856000 | -0.151812000 |
| | 6 | 0.093406000 | 1.929194000 | 3.100400000 |
| | 6 | -0.032005000 | 2.475838000 | 1.804231000 |
| | 6 | -0.396310000 | 3.828266000 | 1.667977000 |
| | 6 | -0.605301000 | 4.594472000 | 2.807019000 |
| | 6 | -0.458609000 | 4.037495000 | 4.091611000 |
| | 6 | -0.111139000 | 2.700136000 | 4.250132000 |
| | 6 | 0.505113000 | 0.231655000 | 1.280078000 |
| | 6 | 0.217839000 | 1.479115000 | 0.782429000 |
| | 1 | -0.499625000 | 4.259456000 | 0.679080000 |
| | 1 | -0.887039000 | 5.638782000 | 2.706264000 |
| | 1 | -0.623179000 | 4.655595000 | 4.969558000 |
| | 1 | -0.007273000 | 2.264149000 | 5.239297000 |
| | 16 | 0.493585000 | 0.220036000 | 3.042838000 |
| | 6 | 0.809748000 | -1.025555000 | 0.479488000 |
| | 1 | 1.311115000 | -0.680012000 | -0.430093000 |
| | 6 | 1.779724000 | -1.953252000 | 1.211585000 |
| | 6 | 3.136942000 | -1.933540000 | 0.866002000 |
| | 6 | 1.362697000 | -2.804992000 | 2.245897000 |
| | 6 | 4.058242000 | -2.740567000 | 1.536192000 |
| | 1 | 3.477135000 | -1.280820000 | 0.066672000 |
| | 6 | 2.282847000 | -3.611635000 | 2.917927000 |
| | 1 | 0.316255000 | -2.850800000 | 2.534338000 |
| | 6 | 3.633901000 | -3.582584000 | 2.565783000 |
| | 1 | 5.106261000 | -2.711099000 | 1.250883000 |
| | 1 | 1.940397000 | -4.265624000 | 3.715065000 |
| | 1 | 4.348470000 | -4.212981000 | 3.087612000 |
| | 7 | 0.007671000 | 1.728791000 | -0.602095000 |
| | 16 | 1.076511000 | 2.568282000 | -1.600237000 |
| | 8 | 0.387236000 | 2.599921000 | -2.899091000 |
| | 8 | 1.434501000 | 3.814624000 | -0.911776000 |
| | 6 | 2.585009000 | 1.622388000 | -1.805972000 |
| | 6 | 2.655057000 | 0.649199000 | -2.808974000 |
| | 6 | 3.673976000 | 1.870182000 | -0.967355000 |
| | 6 | 3.833297000 | -0.075156000 | -2.968045000 |
| | 1 | 1.805429000 | 0.470443000 | -3.459245000 |
| | 6 | 4.845993000 | 1.135036000 | -1.144211000 |
| | 1 | 3.611517000 | 2.635501000 | -0.201698000 |
| | 6 | 4.947630000 | 0.157281000 | -2.144806000 |
| | 1 | 3.892084000 | -0.828198000 | -3.749381000 |
| | 1 | 5.696682000 | 1.329682000 | -0.496785000 |
| | 6 | 6.231043000 | -0.608293000 | -2.355123000 |
| | 1 | 6.033643000 | -1.651153000 | -2.623620000 |

| | | | | |
|---|---|---|---|---|
| | 1 | 6.815182000 | -0.167952000 | -3.173596000 |
| | 1 | 6.857647000 | -0.593704000 | -1.458547000 |
| | 1 | -0.426802000 | 0.929535000 | -1.079813000 |

**Table S4** Number and values ($cm^{-1}$) of imaginary frequencies for the stationary points involved in the formation of **4** and **5**, computed at the B3LYP/6-31G* level of theory.

| Name | No. of I.F. | Value of I.F. | Name | No. of I.F. | Value of I.F. |
|---|---|---|---|---|---|
| **2** | 0 | – | **TS-3** | 1 | -165.7 *i* |
| **2'** | 0 | – | **INT-3** | 0 | – |
| **3a** | 0 | – | **TS-4** | 1 | -277.8 *i* |
| **TS-1** | 1 | -142.6 *i* | **INT-4** | 0 | – |
| **INT-1** | 0 | – | **TS-5** | 1 | -260.7 *i* |
| **TS-2** | 1 | -26.4 *i* | **5** | 0 | – |
| **4** | 0 | – | | | |

**Table S5** Electronic energies, Gibbs free-energies, entropies (at 298.15 K in $CH_3CN$ solvent) computed at the B3LYP/6-31G* level of theory, and electronic energies computed at the m06-PCM/6-311++G** level of theory.

| Species | $E^{B3}$ in a.u. | $S^{B3}$ *in cal/mol K* | $G^{B3}$ in a.u. | $E^{M06}$ in a.u. |
|---|---|---|---|---|
| **DMAP** | -382.26509 | 92.654 | -382.13692 | -382.0732376 |
| **1a** | -1850.09977 | 176.052 | -1849.82352 | -1849.578841 |
| **1a-py-com (3a)** | -2232.36622 | 219.147 | -2231.93423 | -2231.670483 |
| **1b** | -1491.22731 | 171.955 | -1490.92192 | -1490.688549 |
| **1b-py-com** | -1873.48235 | 219.425 | -1873.02397 | -1872.767472 |
| **1c** | -1527.13164 | 168.76 | -1526.84933 | -1526.606627 |
| **1c-py-com** | -1909.38978 | 216.491 | -1908.95391 | -1908.68764 |
| **2** | -908.86287 | 124.861 | -908.71734 | -908.6038949 |
| **2'** | -1291.12294 | 177.755 | -1290.82861 | -1290.677694 |
| **3a** | -2232.36622 | 219.147 | -2231.93423 | -2231.670483 |
| **TS-1** | -3523.46657 | 344.579 | -3522.71358 | -3522.346673 |
| **INT-1** | -3141.20257 | 282.685 | -3140.5925 | -3140.274001 |
| **DMAP** | -382.26509 | 92.654 | -382.13692 | -382.0732376 |
| **TS-2** | -2758.92722 | 229.648 | -2758.47 | -2758.179931 |
| **4** | -2758.96839 | 232.155 | -2758.50895 | -2758.225425 |
| **TS-3** | -3141.20947 | 285.183 | -3140.60406 | -3140.278658 |
| **INT-3** | -3141.22607 | 294.744 | -3140.62267 | -3140.293108 |
| **TS-4** | -3141.21199 | 292.053 | -3140.61008 | -3140.274937 |
| **INT-4** | -3141.22769 | 310.181 | -3140.63439 | -3140.275737 |
| **TS-5** | -3141.21867 | 292.056 | -3140.61697 | -3140.273437 |
| **5** | -2758.98133 | 243.919 | -2758.52822 | -2758.225802 |

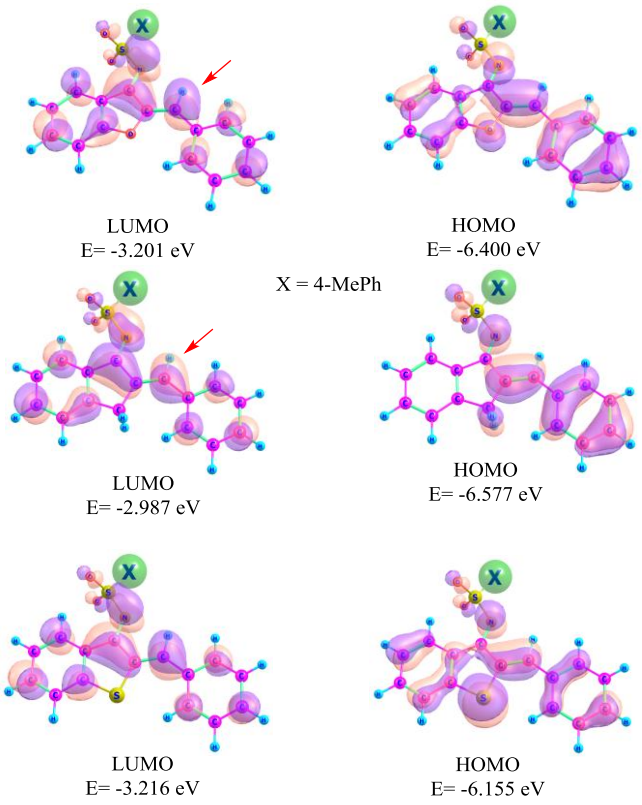



**Figure S1.** Molecular orbitals of **1a**, **1b** and **1c**, computed at the B3LYP/6-311+g* level of theory.

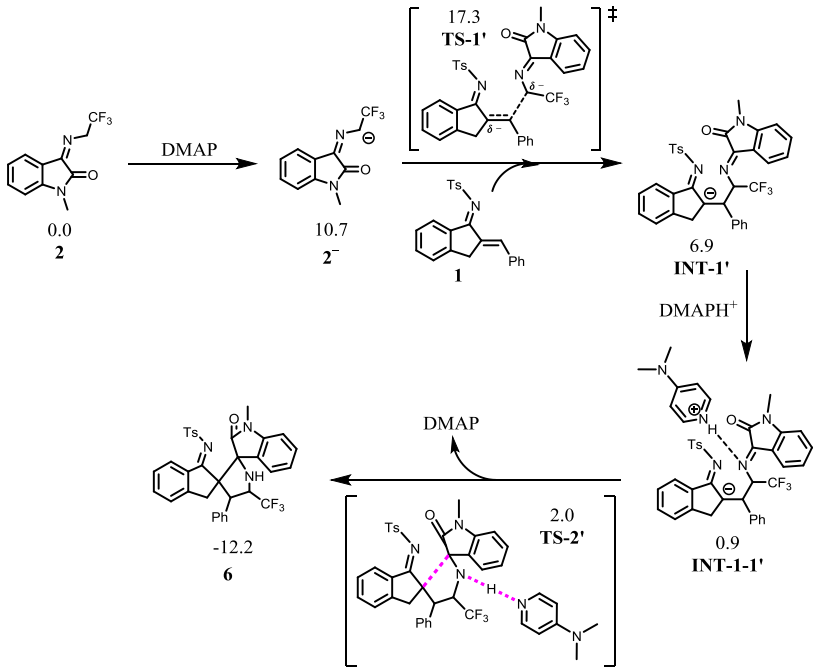



**Figure S2.** Proposed reaction mechanism and free-energy variations (kcal/mol) for the formation of product **6** from the azadiene bearing an indene moiety and **2**.

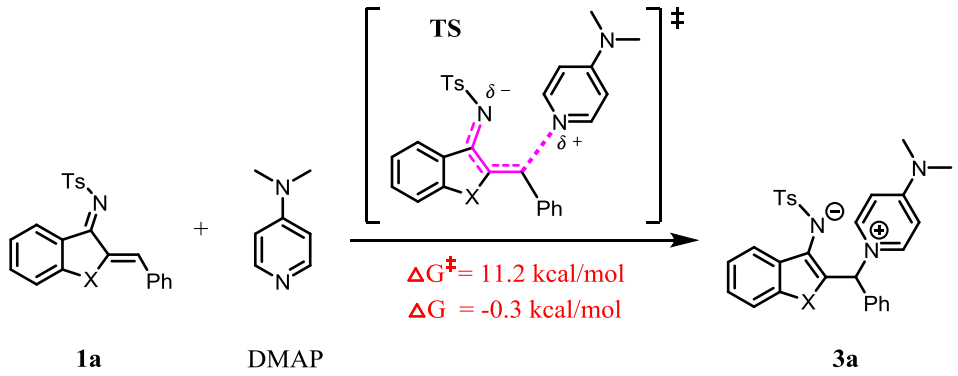



**Figure S3.** Proposed mechanism for the formation of **3a** from **1a** and DMAP.

**Computational Methods**

All calculations were finished using the Gaussian 16 computational program[4]. Geometrical optimizations were performed by the B3LYP density functional method[5] with the 6-31g* basis set for all elements. The default self-consistent reaction field polarizable continuum model[6] was used to consider the implicit solvation effects of $CH_3CN$. All of the resultant stationary point geometries were characterized by vibrational analyses, from which zero point energies and Gibbs free-energies were obtained, in addition to confirming whether all of the structures resided at minima or first-order saddle points on the potential energy surfaces. Then, single point calculations were carried out using the m06 method [7] and the 6-311++G** basis set in $CH_3CN$. Considering the default entropic data obtained from the Gaussian output files are the idea-gas-phase entropies, which would exaggerate the activation entropies for the bimolecular reaction in solution.[8] Hence, the default entropies are scaled by a factor of 0.4 in Gibbs free-energy determinations.

## 10. X-ray data collection and structure determinations

Single crystals of **3a**, **4a, 4c, 5a, 5f, 5l, 6a, 6h** was grown by slow diffusion of *n*-hexane into a dichloromethane solution. X-ray single-crystal diffraction data was collected on a Rigaku XtaLAB P200 diffractometer at 200 K with MoK α radiation ($\lambda$=0.71073 Å) in the $\omega$ scan mode. The program SAINT was used for integration of the diffraction profiles. The structure was solved using direct methods using the SHELXS program of the SHELXTL package and refined using full matrix least-squares methods with SHELXL (semi empirical absorption corrections were applied using the SADABS program). Other non-hydrogen atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters on *F*2. The hydrogen atoms were generated theoretically onto the specific atoms and refined isotopically with fixed thermal factors. Detailed crystallographic data were summarized in Table S3-S10.

**Table S6** Crystal Date and Structure Refinements for （**3a**）

| Empirical formula | $C_{29}H_{27}N_3O_2S_2$ |
|---|---|
| Formula weight | 513.65 |
| Temperature/K | 293 |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ |
| a/Å | 9.1649(3) |
| b/Å | 11.9976(4) |
| c/Å | 23.8507(9) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 2622.55(16) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.301 |
| μ/mm$^{-1}$ | 2.088 |
| F(000) | 1080.0 |
| Crystal size/mm$^3$ | 0.05 ×0.03 ×0.02 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/ ° | 7.412 to 134.918 |
| Index ranges | $-10 \le h \le 10$, $-13 \le k \le 14$, $-28 \le l \le 28$ |
| Reflections collected | 24974 |
| Independent reflections | 4693 [$R_{int}$ = 0.1160, $R_{sigma}$ = 0.0868] |
| Data/restraints/parameters | 4693/384/328 |
| Goodness-of-fit on $F^2$ | 1.032 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0669, $wR_2$ = 0.1558 |
| Final R indexes [all data] | $R_1$ = 0.1158, $wR_2$ = 0.1877 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.23/-0.35 |
| Flack parameter | -0.06(2) |

**Table S7** Crystal Date and Structure Refinements for **4a**

| Empirical formula | $C_{33}H_{26}F_3N_3O_3S_2$ |
|---|---|
| Formula weight | 633.69 |
| Temperature/K | 296(2) |
| Crystal system | monoclinic |
| Space group | C2/c |
| a/Å | 40.85(6) |
| b/Å | 9.365(15) |
| c/Å | 16.24(3) |
| α/° | 90 |
| β/° | 95.12(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 6188(18) |
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.360 |
| μ/mm$^{-1}$ | 0.229 |
| F(000) | 2624.0 |
| Crystal size/mm$^3$ | 0.080 × 0.070 × 0.060 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.08 to 49.994 |
| Index ranges | -48 ≤ h ≤ 48, -11 ≤ k ≤ 11, -19 ≤ l ≤ 19 |
| Reflections collected | 24102 |
| Independent reflections | 5404 [$R_{int}$ = 0.1713, $R_{sigma}$ = 0.1271] |
| Data/restraints/parameters | 5404/0/399 |
| Goodness-of-fit on F$^2$ | 0.917 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0600, w$R_2$ = 0.1218 |
| Final R indexes [all data] | $R_1$ = 0.1566, w$R_2$ = 0.1672 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.40/-0.39 |

**Table S8** Crystal Date and Structure Refinements for **4c**

| Empirical formula | $C_{33}H_{25}BrF_3N_3O_3S_2$ |
|---|---|
| Formula weight | 712.59 |
| Temperature/K | 293 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 9.9808(3) |
| b/Å | 12.3492(4) |
| c/Å | 26.8447(7) |
| α/° | 83.386(2) |
| β/° | 83.439(2) |
| γ/° | 69.273(3) |
| Volume/Å$^3$ | 3064.36(17) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.545 |
| μ/mm$^{-1}$ | 3.609 |
| F(000) | 1448.0 |
| Crystal size/mm$^3$ | 0.05 × 0.04 × 0.04 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/ ° | 3.324 to 133.186 |
| Index ranges | $-11 \le h \le 9$, $-14 \le k \le 14$, $-31 \le l \le 31$ |
| Reflections collected | 31185 |
| Independent reflections | 10506 [$R_{int}$ = 0.0679, $R_{sigma}$ = 0.0782] |
| Data/restraints/parameters | 10506/0/815 |
| Goodness-of-fit on $F^2$ | 1.043 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0581, $wR_2$ = 0.1554 |
| Final R indexes [all data] | $R_1$ = 0.0772, $wR_2$ = 0.1719 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.56/-0.65 |

**Table S9** Crystal Date and Structure Refinements for **5a**

| Empirical formula | $C_{33}H_{25}F_3N_3O_3S_2$ |
|---|---|
| Formula weight | 632.68 |
| Temperature/K | 293(2) |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 10.6708(2) |
| b/Å | 11.2012(2) |
| c/Å | 13.5189(2) |
| α/° | 72.0460(10) |
| β/° | 81.0890(10) |
| γ/° | 79.8810(10) |
| Volume/Å$^3$ | 1504.48(5) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.397 |
| μ/mm$^{-1}$ | 2.107 |
| F(000) | 654.0 |
| Crystal size/mm$^3$ | 0.4 × 0.05 × 0.05 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/ ° | 6.914 to 133.194 |
| Index ranges | $-12 \le h \le 12$, $-13 \le k \le 13$, $-15 \le l \le 16$ |
| Reflections collected | 13816 |
| Independent reflections | 5162 [$R_{int}$ = 0.0305, $R_{sigma}$ = 0.0369] |
| Data/restraints/parameters | 5162/0/399 |
| Goodness-of-fit on $F^2$ | 1.082 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0407, $wR_2$ = 0.1184 |
| Final R indexes [all data] | $R_1$ = 0.0444, $wR_2$ = 0.1220 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.66/-0.32 |

**Table S10** Crystal Date and Structure Refinements for **5f**

| Empirical formula | $C_{34}H_{28}F_3N_3O_4S_2$ |
|---|---|
| Formula weight | 663.71 |
| Temperature/K | 100.00(10) |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 10.2368(7) |
| b/Å | 11.0840(5) |
| c/Å | 14.3042(6) |
| α/° | 89.713(4) |
| β/° | 80.773(4) |
| γ/° | 69.781(5) |
| Volume/Å$^3$ | 1501.07(15) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.468 |
| μ/mm$^{-1}$ | 2.164 |
| F(000) | 688.0 |
| Crystal size/mm$^3$ | 0.2 ×0.2 ×0.2 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 6.27 to 134.136 |
| Index ranges | -12 ≤ h ≤ 11, -13 ≤ k ≤ 13, -17 ≤ l ≤ 16 |
| Reflections collected | 15530 |
| Independent reflections | 5364 [$R_{int}$ = 0.0435, $R_{sigma}$ = 0.0485] |
| Data/restraints/parameters | 5364/0/418 |
| Goodness-of-fit on F$^2$ | 1.076 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0353, w$R_2$ = 0.0910 |
| Final R indexes [all data] | $R_1$ = 0.0387, w$R_2$ = 0.0946 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.36/-0.32 |

**Table S11** Crystal Date and Structure Refinements for **5l**

| Empirical formula | $C_{32}H_{24}F_3N_3O_3S_2$ |
|---|---|
| Formula weight | 619.66 |
| Temperature/K | 293(2) |
| Crystal system | monoclinic |
| Space group | C2/c |
| a/Å | 21.5032(3) |
| b/Å | 9.51180(10) |
| c/Å | 29.3944(4) |
| α/° | 90 |
| β/° | 95.3570(10) |
| γ/° | 90 |
| Volume/Å$^3$ | 5985.90(13) |
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.375 |
| μ/mm$^{-1}$ | 2.106 |
| F(000) | 2560.0 |
| Crystal size/mm$^3$ | 0.100 × 0.080 × 0.040 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/ ° | 6.04 to 135.432 |
| Index ranges | $-25 \le h \le 25$, $-11 \le k \le 7$, $-35 \le l \le 35$ |
| Reflections collected | 26349 |
| Independent reflections | 5362 [$R_{int}$ = 0.0513, $R_{sigma}$ = 0.0283] |
| Data/restraints/parameters | 5362/0/389 |
| Goodness-of-fit on $F^2$ | 1.070 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0546, $wR_2$ = 0.1617 |
| Final R indexes [all data] | $R_1$ = 0.0574, $wR_2$ = 0.1645 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.64/-0.43 |

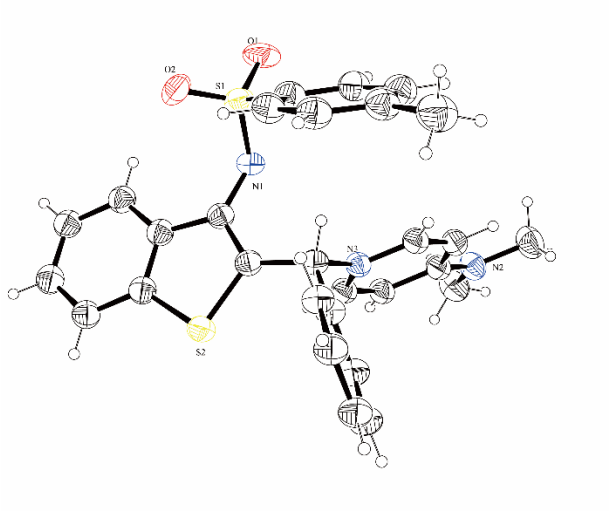
**Table S12** Crystal Date and Structure Refinements for **6a**

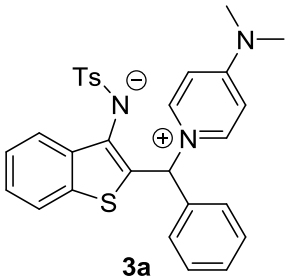
| Empirical formula | $C_{33}H_{25}F_3N_3O_4S$ |
|---|---|
| Formula weight | 616.62 |
| Temperature/K | 293.0 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 10.5671(5) |
| b/Å | 12.1324(4) |
| c/Å | 13.2703(5) |
| α/° | 89.021(3) |
| β/° | 79.487(4) |
| γ/° | 89.424(3) |
| Volume/Å$^3$ | 1672.46(12) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.224 |
| μ/mm$^{-1}$ | 1.337 |
| F(000) | 638.0 |
| Crystal size/mm$^3$ | 0.06 × 0.05 × 0.04 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.288 to 133.2 |
| Index ranges | $-12 \le h \le 12$, $-9 \le k \le 13$, $-15 \le l \le 15$ |
| Reflections collected | 14693 |
| Independent reflections | 5695 [$R_{int}$ = 0.0811, $R_{sigma}$ = 0.0966] |
| Data/restraints/parameters | 5695/301/403 |
| Goodness-of-fit on $F^2$ | 1.143 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.1240, $wR_2$ = 0.3211 |
| Final R indexes [all data] | $R_1$ = 0.1874, $wR_2$ = 0.3916 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.70/-0.87 |

**Table S13** Crystal Date and Structure Refinements for **6h**

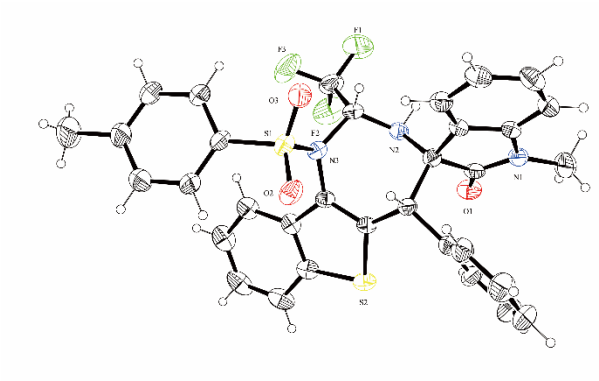
| Empirical formula | $C_{34}H_{30}F_3N_3O_3S$ |
|---|---|
| Formula weight | 617.67 |
| Temperature/K | 293(2) |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 10.8546(8) |
| b/Å | 17.5790(10) |
| c/Å | 18.6479(9) |
| α/° | 113.319(5) |
| β/° | 106.026(6) |
| γ/° | 92.826(5) |
| Volume/Å$^3$ | 3089.5(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.328 |
| μ/mm$^{-1}$ | 1.420 |
| F(000) | 1288.0 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 5.452 to 133.202 |
| Index ranges | $-12 \le h \le 12$, $-20 \le k \le 16$, $-21 \le l \le 22$ |
| Reflections collected | 28409 |
| Independent reflections | 10480 [$R_{int}$ = 0.0654, $R_{sigma}$ = 0.1076] |
| Data/restraints/parameters | 10480/0/806 |
| Goodness-of-fit on $F^2$ | 0.976 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0696, $wR_2$ = 0.1757 |
| Final R indexes [all data] | $R_1$ = 0.1351, $wR_2$ = 0.2178 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.31/-0.28 |

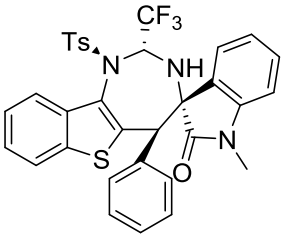
## 11. X-ray crystal structures



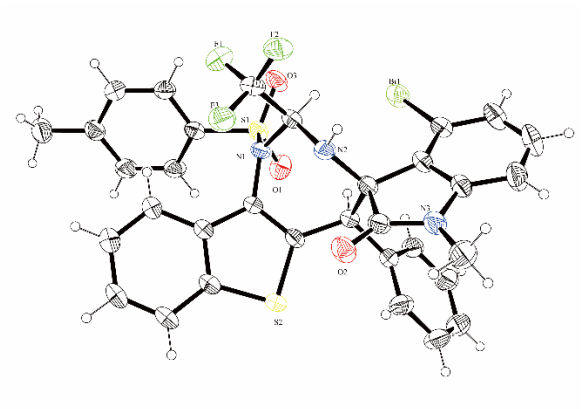


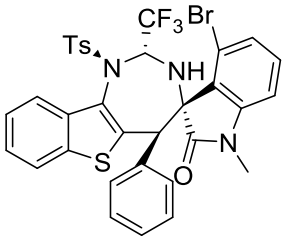

**3a**



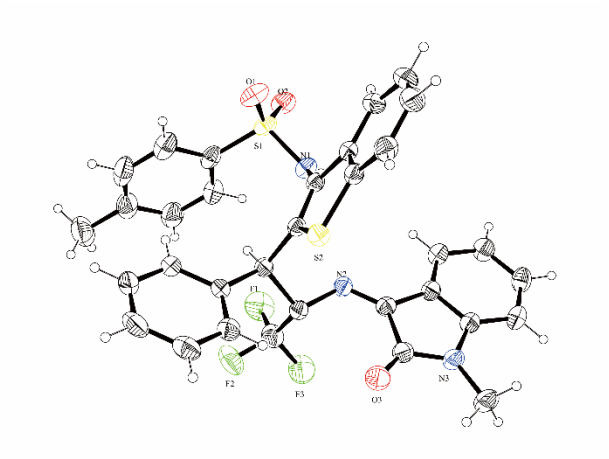


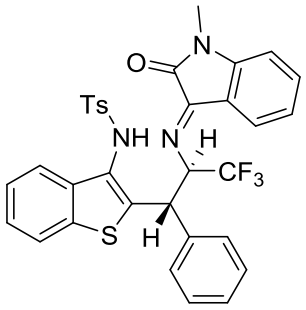

**4a**



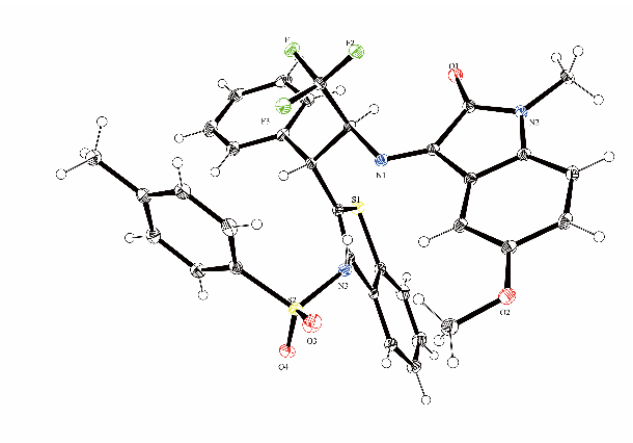


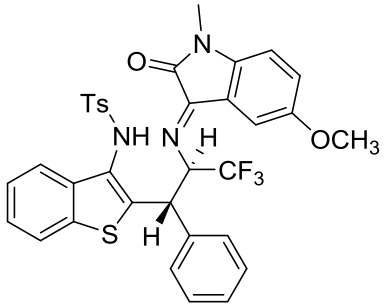

**4c**



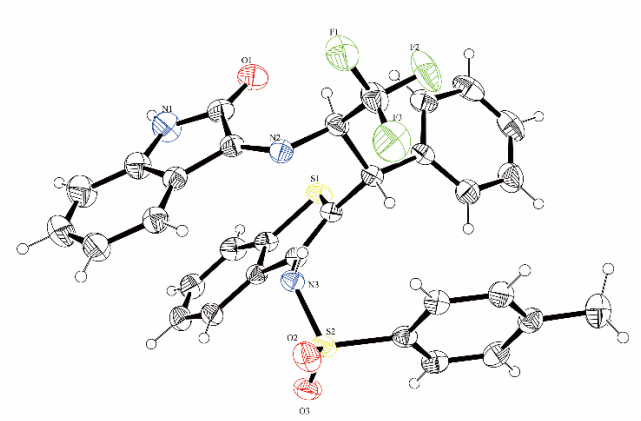


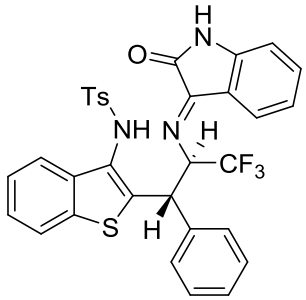

**5a**



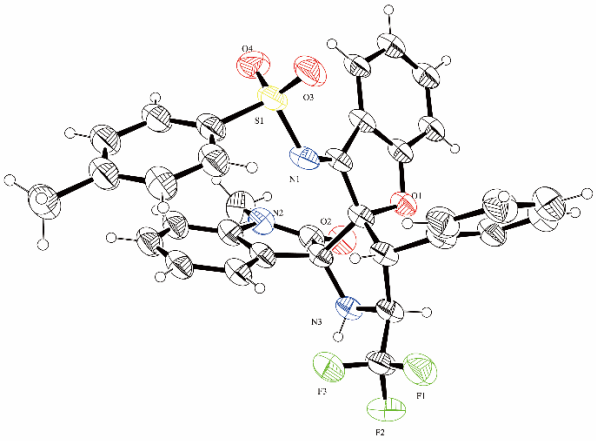


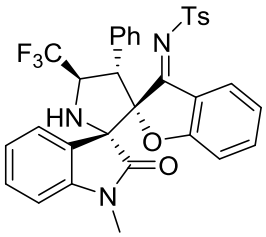

**5f**



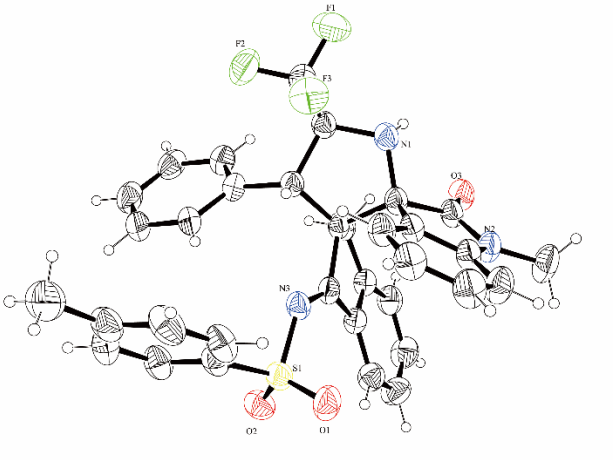


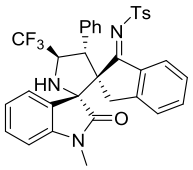

**5l**






**6a**






**6h**

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