Supporting Information

for

Hypervalent Iodine-Triggered Transformation of Homopropargyl Sulfonamides into Dihalo-2,3-Dihydropyrroles

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1. General information

All product mixtures were analyzed by thin layer chromatography glass-backed silica TLC plates with a fluorescent indicator from Branch of Qingdao Haiyang Chemical CO. LTD. For flash column chromatography, silica gel (200-300 mesh) was used as stationary phase. ^{1}H and ^{13}C NMR spectra were recorded on a Varian INOVA-400 in deuterated chloroform at 25 °C with residue solvent peaks as internal standards. Chemical shifts (δ) are reported in ppm, and spin-spin coupling constants (J) are given in Hz, while multiplicities are abbreviated by s (singlet), d (doublet), t (triplet), dd (doublet, doublet),and m (multiplet). High resolution mass spectra (HRMS) were obtained using GCT-TOF instrument with the EI/ESI technique. Melting points were recorded on a national standard melting point apparatus (Model: Taike XT-4) and were uncorrected.

All other reagents were purchased from commercial companies and used without further purification.

2. Experimental Section

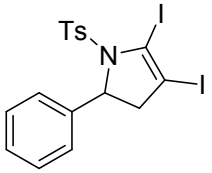
General procedure of Mono/Dihalo-2,3-Dihydropyrroles

A. CuI (0.7 mmol), DBU (0.7 mmol), PhCl (2 ml) and K_2CO_3 (0.2 mmol) were sequentially added to a round-bottom flask (10 ml) and stirred at room temperature for 5 min. Then, PIFA (0.2 mmol) and homopropargyl sulfonamide derivatives **1** (0.2 mmol) were separately dissolved in PhCl (1.0 ml) for sequential addition to the system at room temperature. The reaction mixture was heated with stirring at 100°C for 5 min. Upon completion, the mixture was cooled to room temperature and quenched with an aqueous solution of saturated $Na_2S_2O_3$ (5 ml). After extraction with CH_2Cl_2 (3 × 15 ml), the organic phases were combined and dried over anhydrous Na_2SO_4. The solvent was removed, and the residual crude product was purified by flash column chromatography with a mixture of n-hexane and ethyl acetate to give the desired product in the noted yields.

B. $CuBr_2$/$CuCl_2$ (0.6 mmol), DBU (0.6 mmol), PhCl (2 ml) and K_2CO_3 (0.2 mmol) were sequentially added to a round- bottom flask (10 ml) and stirred at room temperature for 5 min. Then, DIB (0.4 mmol) and homopropargyl sulfonamide derivatives **1** (0.2 mmol) were separately dissolved in PhCl (1.0 ml) for sequential addition to the system at room temperature. The reaction mixture was heated with stirring at 110°C for 10 min. Upon completion, the mixture was cooled to room temperature and quenched with an aqueous solution of saturated $NaHCO_3$ (5 ml). After extraction with CH_2Cl_2 (3 × 15 ml), the organic phases were combined and dried over anhydrous Na_2SO_4. The solvent was removed, and the residual crude product was purified by flash column chromatography with a mixture of n-hexane and ethyl acetate to give the desired product in the noted yields.

3. Spectral data

4,5-diiodo-2-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole(**2a**)



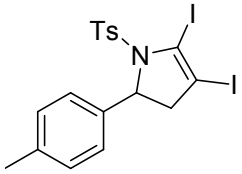
Follow the general procedure A, **2a** was obtained 96.9 mg (88%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.s

Melting point: 150 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.36 ~ 7.28 (m, 7H), 5.39 (d, J = 8.0 Hz, 1H), 2.90 ~ 2.83 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.49 ~ 2.45 (m, 1H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 141.2, 134.1, 129.8, 128.8, 128.0, 127.9, 125.7, 98.1, 95.8, 65.7, 48.6, 21.7.
HRMS (EI): [$C_{17}H_{15}I_2NO_2S$] calcd. For 550.8907; found 550.8888.

4,5-diiodo-2-(p-tolyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**2b**)



Follow the general procedure A, **2b** was obtained 90.3 mg (80%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

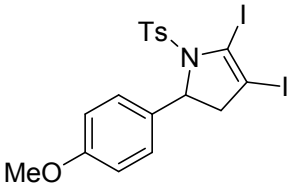
Melting point: 130 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.19 ~ 7.15 (m, 4H), 5.35 (d, J = 8.0 Hz, 1H), 2.87 ~ 2.80 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.48 ~ 2.44 (m, 1H), 2.46 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 138.3, 137.8, 134.2, 129.8, 129.5, 127.9, 125.7, 98.1, 95.9, 65.6, 48.6, 21.7, 21.1.

HRMS (EI): [$C_{18}H_{17}I_2NO_2S$] calcd. For 564.9064; found 564.9063.

4,5-diiodo-2-(4-methoxyphenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**2c**):



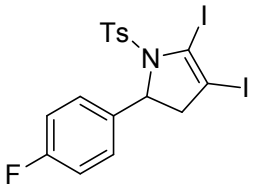
Follow the general procedure A, **2c** was obtained 98.7 mg (85%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 8.0 Hz, 2H), 5.34 (d, J = 8.0 Hz, 1H), 3.80 (s, 3H), 2.86 ~ 2.80 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.48 ~ 2.44 (m, 1H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 144.5, 134.3, 133.4, 129.8, 127.9, 127.1, 114.2, 98.0, 95.8, 65.4, 55.3, 48.5, 21.7.

HRMS (EI): [$C_{18}H_{17}I_2NO_3S$] calcd. For 580.9013; found 580.9003.

2-(4-fluorophenyl)-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2d**):



Follow the general procedure A, **2d** was obtained 83.0 mg (73%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

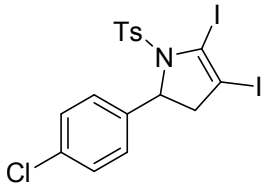
Melting point: 136-138^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.26 (t, J = 4.0 Hz, 2H), 7.04 (t, J = 8.0 Hz, 2H), 5.36 (d, J = 8.0 Hz, 1H), 2.89 ~ 2.82 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.46 (s, 3H), 2.46 ~ 2.41 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 161.1, 144.7, 137.1, 134.0, 129.8, 127.9, 127.6, 115.8, 98.0, 95.5, 65.0, 48.6, 21.7.

HRMS (EI): [$C_{17}H_{14}FI_2NO_2S$] calcd. For 568.8813; found 568.8828.

2-(4-chlorophenyl)-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2e**):



Follow the general procedure A, **2e** was obtained 81.8 mg (70%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

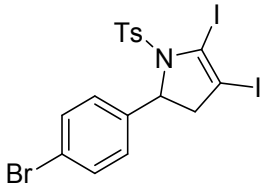
Melting point: 154-156^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.35-7.32 (m, 4H), 7.23 (d, J = 8.0 Hz, 2H), 5.35 (d, J = 8.0 Hz, 1H), 2.89 ~ 2.83 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.46 (s, 3H), 2.42 (d, J = 8.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 139.7, 134.0, 133.9, 129.9, 129.0, 127.9, 127.2, 98.0, 95.4, 65.1, 48.5, 21.7.

HRMS (EI): [$C_{17}H_{14}ClI_2NO_2S$] calcd. For 584.8518; found 584.8516.

2-(4-bromophenyl)-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2f**):



Follow the general procedure A, **2f** was obtained 94.3 mg (75%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

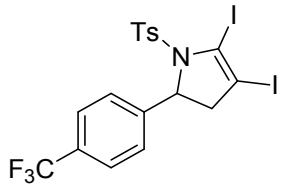
Melting point: 162-164 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 5.33 (d, J = 8.0Hz, 1H), 2.89 ~ 2.83 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.46 (s, 3H), 2.41 (d, J = 8.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 140.2, 134.0, 132.0, 129.9, 127.9, 127.5, 122.0, 98.0, 65.1, 48.5, 21.7.

HRMS (EI): [$C_{17}H_{14}{}^{81}BrI_2NO_2S$] calcd. For 630.7992; found 630.8013.

4,5-diiodo-1-tosyl-2-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrole(**2g**):



Follow the general procedure A, **2g** was obtained 111.3 mg (90%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

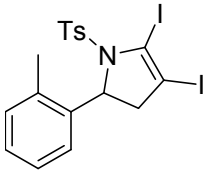
Melting point: 135^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 5.43 (d, J = 12.0 Hz, 1H), 2.94 ~ 2.87 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.46 (s, 3H), 2.46 ~ 2.41 (m, 1H) .

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 144.9, 133.8, 130.4, 129.9, 127.9, 126.1, 125.9, 125.2, 122.5, 98.0, 95.3, 65.1, 48.6, 21.7.

HRMS (EI): [$C_{18}H_{14}F_3I_2NO_2S$] calcd. For 618.8781; found 618.8780.

4,5-diiodo-2-(o-tolyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**2h**):



Follow the general procedure A, **2h** was obtained 87.0 mg (77%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

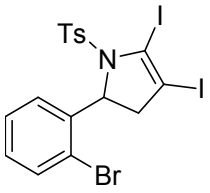
Melting point: 174-176°C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.26 (s, 1H), 7.22 – 7.17 (m, 3H), 5.55 (d, J = 8.0 Hz, 1H), 3.00 ~ 2.94 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.46 (s, 3H), 2.29 (s, 3H), 2.29 ~ 2.24 (m, 1H) .

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 139.6, 134.1, 133.2, 130.7, 129.8, 128.0, 127.8, 126.6, 125.5, 98.3, 95.3, 63.2, 48.7, 21.7, 19.2.

HRMS (EI): [$C_{18}H_{17}I_2NO_2S$] calcd. For 564.9064; found 564.9051.

2-(2-bromophenyl)-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2i**):



Follow the general procedure A, **2i** was obtained 94.3 mg (75%) as white solid with *n*-hexane/ethyl acetate (25/1) used as eluent.

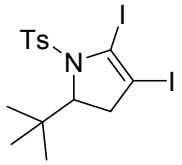
Melting point: 202-204°C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 8.0 Hz, 1H), 7.42 – 7.35 (m, 4H), 7.17 (t, J = 4.0 Hz, 1H), 5.62 (d, J = 12.0 Hz, 1H), 2.98 ~ 2.92 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.47 (s, 3H), 2.26 (d, J = 20.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 140.2, 133.5, 132.9, 129.9, 129.3, 128.05, 128.02, 127.6, 120.8, 98.2, 96.1, 65.4, 48.8, 21.7.

HRMS (EI): [$C_{17}H_{14}{}^{81}BrI_2NO_2S$] calcd. For 630.7992; found 630.7972.

2-(tert-butyl)-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2j**):



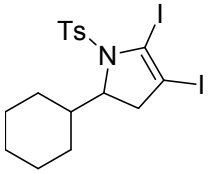
Follow the general procedure A, **2j** was obtained 100.8 mg (95%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.87 (d, *J* = 8.0 Hz, 1H), 2.42 (s, 3H), 2.30 ~ 2.14 (m, 2H), 0.90 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 138.1, 129.6, 127.0, 65.9, 60.6, 59.6, 35.3, 26.7, 21.5, 21.0.

HRMS (EI): [$C_{15}H_{19}I_2NO_2S$] calcd. For 530.9220; found 530.9216.

2-cyclohexyl-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2k**):



Follow the general procedure A, **2k** was obtained 109.1 mg (98%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

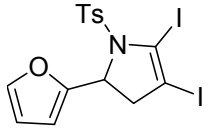
Melting point: 172-174^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.31(d, *J* = 8.0 Hz, 2H), 4.10 ~ 4.07 (m, 1H), 2.44 (s, 3H), 2.20 ~ 2.16 (m, 1H), 2.09 ~ 2.05 (m, 1H), 1.76 (d, *J* = 12.0 Hz, 2H), 1.64 (t, *J* = 16.0 Hz, 3H), 1.44 (d, *J* = 12.0 Hz, 1H), 1.23 ~ 0.93 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 133.7, 129.7, 127.8, 99.4, 68.9, 43.2, 42.9, 27.6, 27.5, 26.2, 25.99, 25.92, 21.7.

HRMS (EI): [$C_{17}H_{21}I_2NO_2S$] calcd. For 556.9377; found 556.9368.

2-(furan-2-yl)-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2l**):



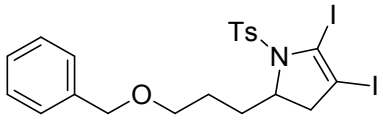
Follow the general procedure A, **2l** was obtained 102.7 mg (95%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.37 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 6.35 (d, *J* = 8.0 Hz, 2H), 5.45 (d, *J* = 8.0 Hz, 1H), 2.68 ~ 2.65(m, 2H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4, 144.7, 142.8, 134.1, 129.8, 127.9, 110.5, 107.7, 97.5, 95.9, 59.7, 45.0, 21.7.

HRMS (EI): [$C_{15}H_{13}I_2NO_3S$] calcd. For 540.8700; found 540.8689.

2-(3-(benzyloxy)propyl)-4,5-diiodo-1-tosyl-2,3-dihydro-1H-pyrrole(**2m**):



Follow the general procedure C, **2m** was obtained 115.8 mg (93%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

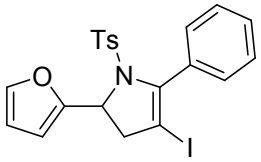
Melting point: 70^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0Hz, 2H), 7.34 (s, 4H), 7.29 (d, *J* = 8.0Hz, 3H), 4.50 (s, 2H), 4.31 ~ 4.27 (m, 1H), 3.54 ~ 3.49 (m , 2H), 2.43 (s, 3H), 2.31 ~ 2.25 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 1.99 (d, *J* = 16.0Hz, 1H), 1.75 ~ 1.64 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 138.4, 133.7, 129.7, 128.3, 127.8, 127.6, 127.5, 98.4, 98.3, 72.8, 69.7, 63.9, 45.8, 32.9, 24.9, 21.6.

HRMS (ESI): [$C_{21}H_{23}I_2NO_3S$+H]$^+$ calcd. For 623.9482; found 623.9372.

2-(furan-2-yl)-4-iodo-5-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole(**2n**):



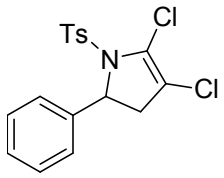
Follow the general procedure A, **2n** was obtained 93.2 mg (95%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (t, *J* = 8.0 Hz, 4H), 7.26 (s, 1H), 7.21 (d, *J* = 4.0 Hz, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.30 (s, 1H), 6.23 (s, 1H), 5.27 (d, *J* = 8.0 Hz, 1H), 2.72 – 2.60 (m, 2H), 2.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.6, 144.2, 143.2, 142.6, 134.5, 132.2, 129.69, 129.62, 129.1, 127.7, 110.5, 106.8, 78.1, 59.0, 45.2, 21.6.

HRMS (EI): [$C_{21}H_{18}INO_3S$] calcd. For 491.0046; found 491.0038.

4,5-dichloro-2-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole(**3a**):



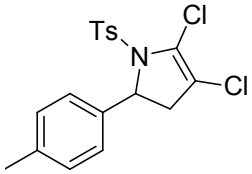
Follow the general procedure B, **3a** was obtained 40.3 mg (55%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.38 ~ 7.32 (m, 7H), 5.30 (d, J = 8.0 Hz, 1H), 2.95 ~ 2.88 (dd, J_1 = 20.0 Hz, J_2 = 12.0 Hz, 1H), 2.47 (s, 3H), 2.47 ~ 2.41(m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 141.1, 133.8, 129.9, 128.9, 128.2, 127.8, 126.0, 125.7, 117.5, 63.0, 40.9, 21.7.

HRMS (EI): [$C_{17}H_{15}Cl_2NO_2S$] calcd. For 367.0195; found 367.0181.

4,5-dichloro-2-(p-tolyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**3b**)



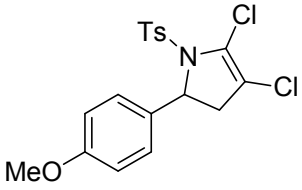
Follow the general procedure B, **3b** was obtained 41.9 mg (55%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 7.18 (d, J = 8.0 Hz, 2H), 5.25 (d, J = 8.0 Hz, 1H), 2.92 ~ 2.86 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.46 (s, 3H), 2.43 ~ 2.39 (m, 1H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 138.2, 138.0, 133.9, 129.9, 129.5, 127.9, 125.9, 125.7, 117.5, 63.0, 40.9, 21.7, 21.1.

HRMS (EI): [$C_{18}H_{17}Cl_2NO_2S$] calcd. For 381.0352; found 381.0342.

4,5-dichloro-2-(4-methoxyphenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**3c**):



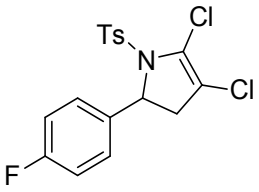
Follow the general procedure B, **3c** was obtained 48.4 mg (61%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 6.90 (d, J = 8.0 Hz, 2H), 5.24 (d, J = 8.0 Hz, 1H), 3.81 (s, 3H), 2.91 ~ 2.84 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H), 2.46 (s, 3H), 2.44 ~ 2.40 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 144.7, 133.9, 133.3, 129.9, 127.8, 127.1, 125.8, 117.5, 114.2, 62.8, 55.3, 40.8, 21.7.

HRMS (EI): [$C_{18}H_{17}Cl_2NO_3S$] calcd. For 397.0301; found 397.0293.

4,5-dichloro-2-(4-fluorophenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**3d**)



Follow the general procedure B, **3d** was obtained 50.0 mg (65%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

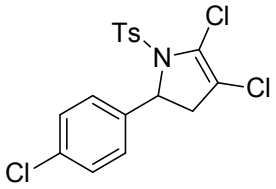
Melting point: 126°C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.37 – 7.31 (m, 4H), 7.06 (t, J = 8.0 Hz, 2H), 5.26 (d, J = 8.0Hz, 1H), 2.95 ~ 2.88 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H), 2.47 (s, 3H), 2.40 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 144.9, 137.0, 133.8, 130.0, 127.8, 127.7, 125.9, 117.2, 115.9, 62.4, 40.9, 21.7.

HRMS (EI): [$C_{17}H_{14}Cl_2FNO_2S$] calcd. For 385.0101; found 385.0099.

4,5-dichloro-2-(4-chlorophenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**3e**):



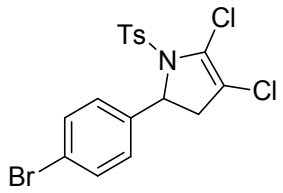
Follow the general procedure B, **3e** was obtained 50.5 mg (63%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.0 Hz, 4H), 7.29 (d, J = 8.0 Hz, 2H), 5.25 (d, J = 8.0 Hz, 1H), 2.95 ~ 2.89 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.47 (s, 3H), 2.38 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 139.7, 134.1, 133.7, 130.0, 129.1, 127.9, 127.2, 126.0, 117.2, 62.4, 40.9, 21.7.

HRMS (EI): [$C_{17}H_{14}Cl_3NO_2S$] calcd. For 400.9805; found 400.9797.

2-(4-bromophenyl)-4,5-dichloro-1-tosyl-2,3-dihydro-1H-pyrrole(**3f**)



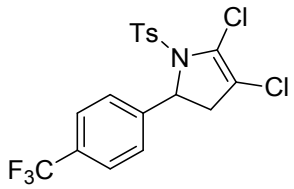
Follow the general procedure B, **3f** was obtained 51.6 mg (58%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 5.24 (d, J = 8.0 Hz, 1H), 2.95 ~ 2.89 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.47 (s, 3H), 2.37 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 140.2, 133.6, 132.0, 130.0, 127.8, 127.5, 125.9, 122.2, 117.2, 62.4, 40.8, 21.7.

HRMS (EI): [$C_{17}H_{14}{}^{81}BrCl_2NO_2S$] calcd. For 446.9280; found 446.9275.

4,5-dichloro-1-tosyl-2-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrole(**3g**)



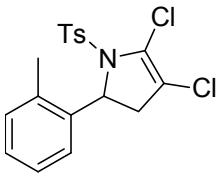
Follow the general procedure B, **3g** was obtained 53.9 mg (62%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 8.0 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 5.33 (d, J = 8.0Hz, 1H), 3.00 ~ 2.94 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.47 (s, 3H), 2.40 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 145.0, 133.5, 130.0, 127.9, 126.2, 126.0, 125.9, 117.1, 62.48, 40.90, 21.71.

HRMS (EI): [$C_{18}H_{14}Cl_2F_3NO_2S$] calcd. For 435.0069; found 435.0065.

4,5-dichloro-2-(o-tolyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**3h**)



Follow the general procedure B, **3h** was obtained 49.5 mg (65%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

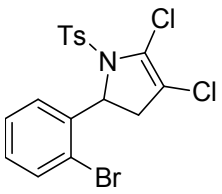
Melting point: 150-152°C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.0 Hz, 2H), 7.37 (t, J = 8.0 Hz, 3H), 7.22 – 7.19 (m,3H), 5.45 (d, J = 12.0 Hz, 1H), 3.04 ~ 2.97 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H), 2.47 (s, 3H), 2.31 (s, 3H), 2.22 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 139.7, 133.9, 133.4, 130.7, 129.9, 127.96, 127.93, 126.6, 126.1, 125.3, 117.0, 60.4, 40.9, 21.7, 19.1.

HRMS (EI): [$C_{18}H_{17}Cl_2NO_2S$] calcd. For 381.0352; found 381.0340.

2-(2-bromophenyl)-4,5-dichloro-1-tosyl-2,3-dihydro-1H-pyrrole(**3i**)



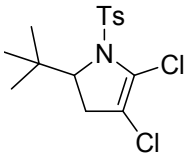
Follow the general procedure B, **3i** was obtained 48.0 mg (54%) as white viscous oil with *n*-hexane/ethyl acetate (25/1) used as eluent

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.0 Hz, 2H), 7.58 ~ 7.52 (m, 2H), 7.40 (d, J = 8.0 Hz, 3H), 7.19 (t, J = 8.0 Hz, 1H), 5.51 (d, J = 8.0 Hz, 1H), 3.04 ~ 2.97 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.48 (s, 3H), 2.22 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 140.3, 133.1, 132.9, 130.1, 129.5, 128.0, 127.4, 126.0, 121.1, 117.7, 62.7, 41.0, 21.7.

HRMS (EI): [$C_{17}H_{14}BrCl^{37}ClNO_2S$] calcd. For 446.9271; found 446.9269.

2-(tert-butyl)-4,5-dichloro-1-tosyl-2,3-dihydro-1H-pyrrole(**3j**)



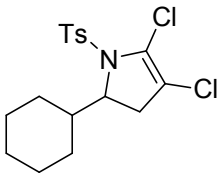
Follow the general procedure B, **3j** was obtained 43.0 mg (62%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 3.91 (d, J = 8.0 Hz, 1H), 2.46 (s, 3H), 2.18 ~ 2.06 (m, 2H), 0.93 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 133.2, 129.7, 128.0, 127.3, 122.0, 70.1, 35.4, 34.0, 25.1, 21.7.

HRMS (EI): [$C_{15}H_{19}Cl_2NO_2S$] calcd. For 347.0508; found 347.0510.

4,5-dichloro-2-cyclohexyl-1-tosyl-2,3-dihydro-1H-pyrrole(**3k**)



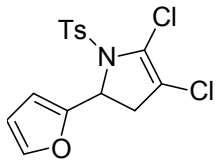
Follow the general procedure B, **3k** was obtained 42.5 mg (57%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 4.03 ~ 3.99 (m, 1H), 2.45 (s, 3H), 2.27 ~ 2.21 (m, 1H), 2.09 ~ 2.05 (m, 1H), 1.78 (d, J = 12.0 Hz, 2H), 1.71 ~ 1.68(m, 3H), 1.25 ~ 0.96 (m , 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 133.4, 129.8, 127.8, 126.3, 120.3, 66.1, 43.2, 35.0, 27.6, 27.3, 26.2, 25.9, 25.8, 21.6.

HRMS (EI): [$C_{17}H_{21}Cl_2NO_2S$] calcd. For 373.0664; found 373.0659.

4,5-dichloro-2-(furan-2-yl)-1-tosyl-2,3-dihydro-1H-pyrrole(**3l**):



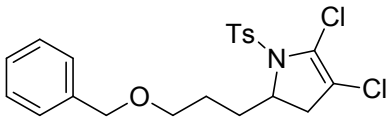
Follow the general procedure B, **3l** was obtained 39.2 mg (55%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.39 (s, 1H), 7.35 (m, J = 8.0 Hz, 2H), 6.42 (s, 1H), 6.36 (s, 1H), 5.38 (d, J = 8.0 Hz, 1H), 2.78 ~ 2.72 (m, 1H), 2.65 ~ 2.61 (m, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 144.9, 142.9, 133.9, 129.9, 127.9, 125.7, 118.0, 110.5, 107.9, 57.4, 37.3, 21.7.

HRMS (EI): [$C_{15}H_{13}Cl_2NO_3S$] calcd. For 356.9988; found 356.9979.

2-(3-(benzyloxy)propyl)-4,5-dichloro-1-tosyl-2,3-dihydro-1H-pyrrole(**3m**)



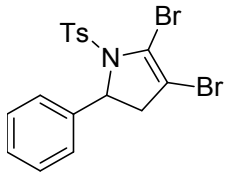
Follow the general procedure B, **3m** was obtained 56.2 mg (64%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.0 Hz, 2H), 7.35 ~ 7.30(m, 7H), 4.51 (s, 2H), 4.24 ~ 4.21 (m, 1H), 3.57 ~ 3.51 (m, 2H), 2.45 (s, 3H), 2.39 ~ 2.33 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 1.96 (d, J = 16.0 Hz, 1H), 1.83 ~ 1.71 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 138.4, 133.4, 129.9, 128.4, 127.8, 127.6, 127.5, 125.8, 119.7, 72.9, 69.7, 61.5, 38.0, 33.3, 24.8, 21.6.

HRMS (ESI): $[C_{21}H_{23}Cl_2NO_3S+H]^+$ calcd. For 440.0770; found 440.0760.

4,5-dibromo-2-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole(**4a**):



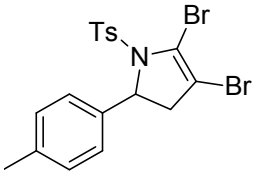
Follow the general procedure B, **4a** was obtained 63.6 mg (70%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.0 Hz, 2H), 7.40 ~ 7.32 (m, 7H), 5.38 (d, J = 12.0 Hz, 1H), 2.94 ~ 2.88 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.48 ~2.44 (m, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 141.1, 134.0, 129.9, 128.9, 128.2, 127.9, 125.8, 117.8, 111.6, 64.6, 43.6, 21.7.

HRMS (EI): $[C_{17}H_{15}Br^{81}BrNO_2S]$ calcd. For 456.9164; found 456.9170.

4,5-dibromo-2-(p-tolyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4b**)



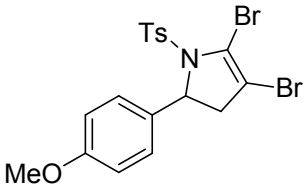
Follow the general procedure B, **4b** was obtained 73.1 mg (78%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.19 ~ 7.15 (m, 4H), 5.35 (d, J = 8.0 Hz, 1H), 2.87 ~ 2.80 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.48 ~ 2.44 (m, 1H), 2.46 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 144.5, 138.3, 137.8, 134.2, 129.8, 129.5, 127.9, 125.7, 98.1, 95.9, 65.6, 48.6, 21.7, 21.1.

HRMS (EI): $[C_{18}H_{17}Br^{81}BrNO_2S]$ calcd. for 470.9321; found 470.9324.

4,5-dibromo-2-(4-methoxyphenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4c**)



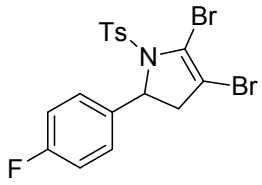
Follow the general procedure B, **4c** was obtained 68.8 mg (71%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H), 6.89 (d, J = 8.0 Hz, 2H), 5.33 (d, J = 8.0 Hz, 1H), 3.81 (s, 3H), 2.91 ~ 2.84 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H), 2.47 ~ 2.43 (m, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 144.7, 134.2, 133.3, 129.8, 127.9, 127.1, 117.6, 114.2, 111.6, 64.3, 55.3, 43.5, 21.7.

HRMS (EI): [$C_{18}H_{17}Br^{81}BrNO_3S$] calcd. For 486.9270; found 486.9268.

4,5-dibromo-2-(4-fluorophenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4d**)



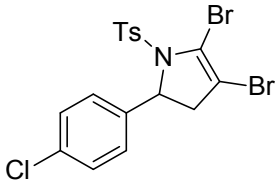
Follow the general procedure B, **4d** was obtained 70.9 mg (75%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.36 ~ 7.29 (m, 4H), 7.06 (t, J = 8.0 Hz, 2H), 5.35 (d, J = 8.0 Hz, 1H), 2.94 ~ 2.87 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H), 2.46 (s, 3H), 2.46 ~ 2.41(m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 161.2, 144.9, 137.0, 133.9, 129.9, 127.9, 127.69, 117.7, 115.9, 111.4, 63.9, 43.6, 21.7.

HRMS (EI): [$C_{17}H_{14}Br^{81}BrFNO_2S$] calcd. for 474.9070; found 474.9061.

4,5-dibromo-2-(4-chlorophenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4e**)



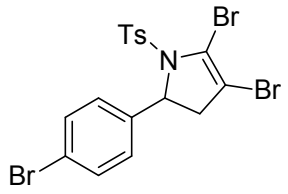
Follow the general procedure B, **4e** was obtained 66.4 mg (68%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 4H), 7.20 (d, J = 8.0 Hz, 2H), 5.27 (d, J = 12.0 Hz, 1H), 2.87 ~ 2.80 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.39 (s, 3H) 2.36 ~ 2.32 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 139.6, 134.0, 133.8, 129.9, 129.1, 127.9, 127.2, 117.7, 111.3, 63.9, 43.5, 21.7.

HRMS (EI): [$C_{17}H_{14}Br^{81}BrClNO_2S$] calcd. for 490.8795; found 490.8789.

4,5-dibromo-2-(4-bromophenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4f**)



Follow the general procedure B, **4f** was obtained 70.3 mg (66%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

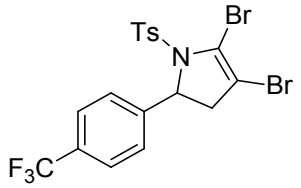
Melting point: 172 - 174 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 8.0 Hz, 2H), 5.32 (d, J = 8.0 Hz, 1H), 2.94 ~ 2.87 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H), 2.46 (s, 3H), 2.41 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 140.1, 133.7, 132.0, 129.9, 127.9, 127.5, 122.1, 117.7, 111.3, 63.9, 43.5, 21.7.

HRMS (EI): [$C_{17}H_{14}Br_2{}^{81}BrNO_2S$] calcd. for 534.8269; found 534.8270.

4,5-dibromo-1-tosyl-2-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrole(**4g**)



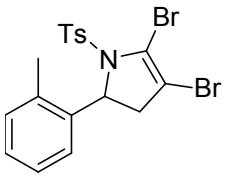
Follow the general procedure B, **4g** was obtained 73.2 mg (70%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 4.0 Hz, 2H), 7.64 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 5.41 (d, J = 12.0 Hz, 1H), 2.99 ~ 2.93 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.47 (s, 3H), 2.45 ~ 2.41 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 145.0, 133.7, 130.0, 127.9, 126.2, 126.0, 125.9, 117.8, 111.2, 64.0, 43.6, 21.7.

HRMS (EI): [$C_{18}H_{14}Br^{81}BrF_3NO_2S$] calcd. for 524.9038; found 524.9030.

4,5-dibromo-2-(o-tolyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4h**)



Follow the general procedure B, **4h** was obtained 66.5 mg (71%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

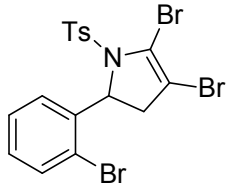
Melting point: 156-158 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.0 Hz, 3H), 7.23 ~ 7.17 (m, 3H), 5.54 (d, J = 8.0 Hz, 1H), 3.04 ~ 2.97 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H), 2.46 (s, 3H), 2.31 (s, 3H), 2.25 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 139.6, 134.0, 133.3, 130.7, 129.8, 128.0, 127.9, 126.6, 125.3, 117.9, 111.2, 62.0, 43.7, 21.7, 19.1.

HRMS (EI): [$C_{18}H_{17}Br^{81}BrNO_2S$] calcd. for 470.9321; found 470.9305.

4,5-dibromo-2-(2-bromophenyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4i**)



Follow the general procedure B, **4i** was obtained 61.8 mg (58%) as white solid with *n*-hexane/ethyl acetate (25/1) used as eluent.

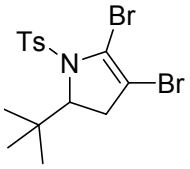
Melting point: 178 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 8.0 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.38 (t, J = 12.0 Hz, 3H), 7.19 (t, J = 8.0 Hz, 1H), 5.59 (d, J = 8.0 Hz, 1H), 3.02 ~ 2.96 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.48 (s, 3H), 2.25 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 140.3, 133.3, 132.9, 130.0, 129.5, 128.09, 128.06, 127.5, 121.0, 117.8, 111.9, 64.3, 43.8, 21.7.

HRMS (EI): [$C_{17}H_{14}Br^{81}Br_2NO_2S$] calcd. for 536.8249; found 536.8247.

4,5-dibromo-2-(tert-butyl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4j**)



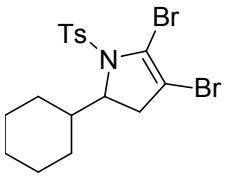
Follow the general procedure B, **4j** was obtained 47.8 mg (55%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 3.97 (t, *J* = 4.0 Hz, 1H), 2.45 (s, 3H), 2.11 (d, *J* = 4.0 Hz, 2H), 0.92 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 133.3, 129.7, 128.1, 119.6, 116.5, 71.8, 36.7, 35.4, 25.1, 21.7.

HRMS (EI): [$C_{15}H_{19}Br^{81}BrNO_2S$] calcd. for 436.9477; found 436.9479.

4,5-dibromo-2-cyclohexyl-1-tosyl-2,3-dihydro-1H-pyrrole(**4k**)



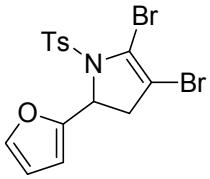
Follow the general procedure B, **4k** was obtained 54.4 mg (59%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 4.09 (t, *J* = 8.0 Hz, 1H), 2.45 (s, 3H), 2.26 ~ 2.19 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.09 (d, *J* = 16.0 Hz, 1H), 1.78 (d, *J* = 12.0 Hz, 2H), 1.67 (d, *J* = 12.0 Hz, 3H), 1.25 ~ 0.96 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 133.5, 129.8, 127.8, 118.4, 114.7, 67.7, 43.2, 37.8, 27.6, 27.3, 26.2, 25.9, 25.8, 21.7.

HRMS (EI): [$C_{17}H_{21}Br^{81}BrNO_2S$] calcd. for 462.9634; found 462.9640.

4,5-dibromo-2-(furan-2-yl)-1-tosyl-2,3-dihydro-1H-pyrrole(**4l**)



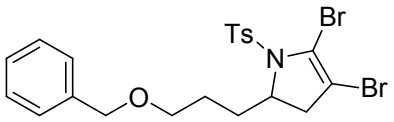
Follow the general procedure B, **4l** was obtained 51.6 mg (58%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.39 (s, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.38(d, *J* = 16.0 Hz, 2H), 5.45 (d, *J* = 12.0 Hz, 1H), 2.77 ~ 2.71 (m, 1H), 2.68 ~ 2.64 (m, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 144.8, 142.9, 134.0, 129.9, 127.9, 117.4, 112.0, 110.5, 107.8, 58.8, 40.0, 21.7.

HRMS (EI): [$C_{15}H_{13}Br^{81}BrNO_3S$] calcd. for 446.8957; found 446.8953.

2-(3-(benzyloxy)propyl)-4,5-dibromo-1-tosyl-2,3-dihydro-1H-pyrrole(**4m**)



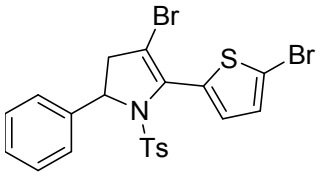
Follow the general procedure B, **4m** was obtained 57.9 mg (55%) as white viscous oil with *n*-hexane/ethyl acetate (10/1) used as eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.0 Hz, 2H), 7.35 ~ 7.30 (m, 7H), 4.52 (s, 2H), 4.34 (d, *J* = 8.0 Hz, 1H), 3.54 (t, *J* = 8.0 Hz, 2H), 2.83 ~ 2.75 (m, 1H), 2.44 (s, 3H), 2.30 (d, *J* = 16.0 Hz, 2H), 2.11 ~ 2.03 (m, 1H), 1.72 ~1.65 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.1, 145.5, 138.3, 135.1, 129.6, 128.5, 128.4, 127.6, 73.0, 69.6, 59.5, 40.2, 33.3, 31.2, 25.9, 21.7.

HRMS (ESI): [$C_{21}H_{23}Br^{81}BrNO_3S$+H]$^+$ calcd. for 529.9759; found 529.9751.

4-bromo-5-(5-bromothiophen-2-yl)-2-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole(**4o**)



Follow the general procedure B, **4o** was obtained 55.8 mg (52%) as white solid with *n*-hexane/ethyl acetate (10/1) used as eluent.

Melting point: 160 ^{o}C.

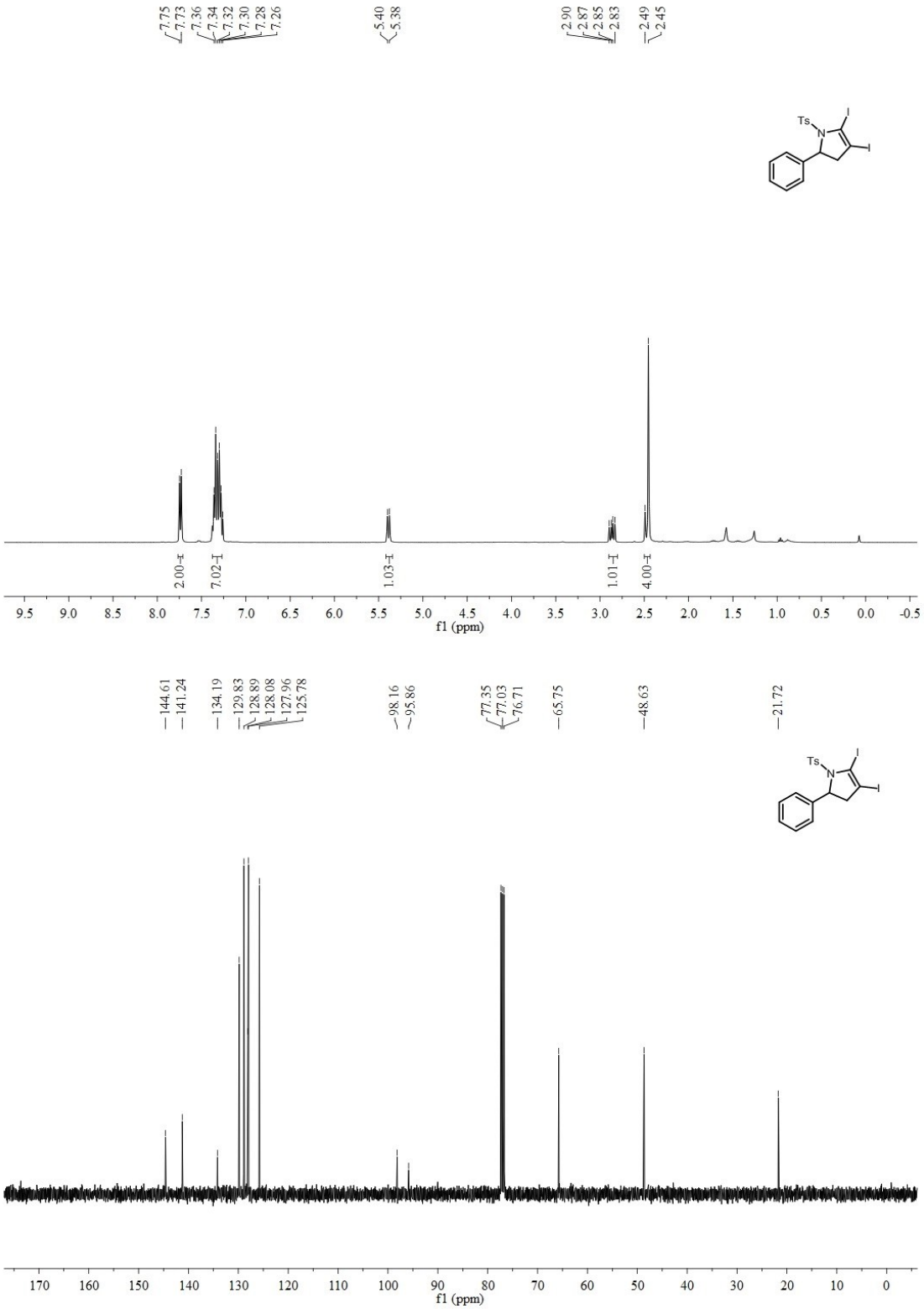
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.37 ~ 7.33 (m, 8H), 7.06 (d, *J* = 4.0 Hz, 1H), 5.28 (d, *J* = 8.0 Hz, 1H), 2.75 ~ 2.69 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 2.48 (s, 3H), 2.48 ~ 2.45 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 141.1, 134.2, 133.7, 133.4, 130.4, 129.8, 129.5, 128.9, 128.0, 127.9, 125.6, 114.9, 109.4, 63.6, 44.5, 21.7.

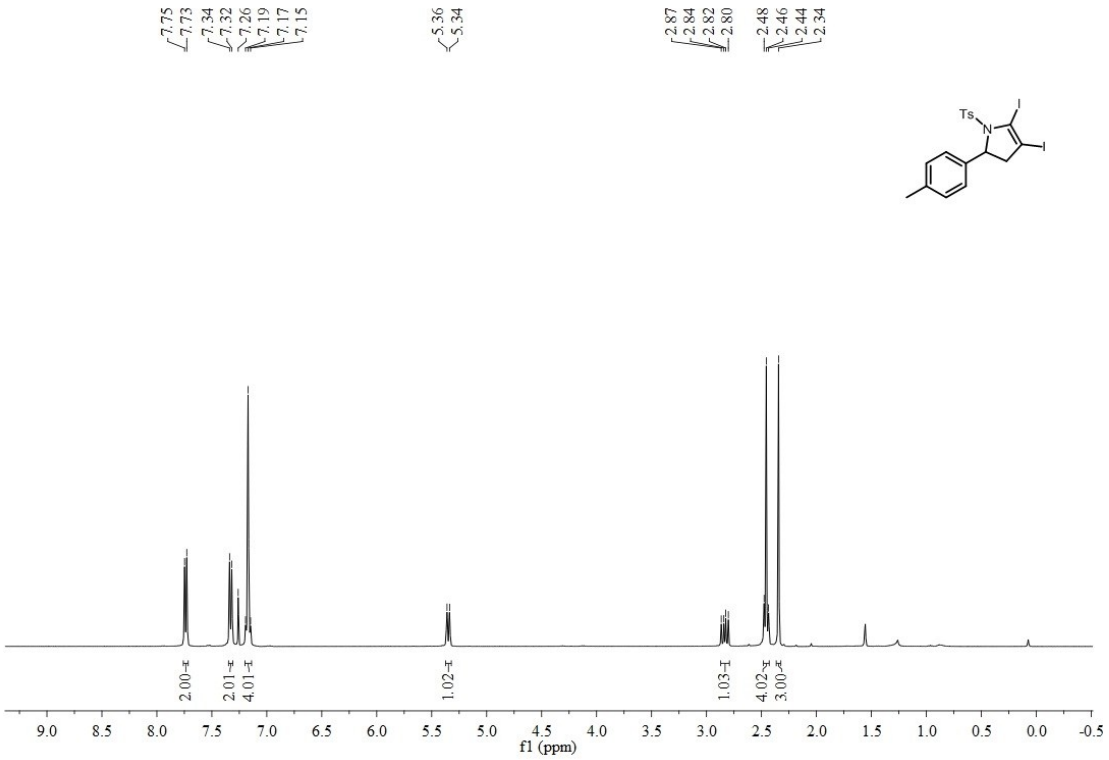
HRMS (EI): [$C_{21}H_{17}Br^{81}BrNO_2S_2$] calcd. for 538.9042; found 538.9028.

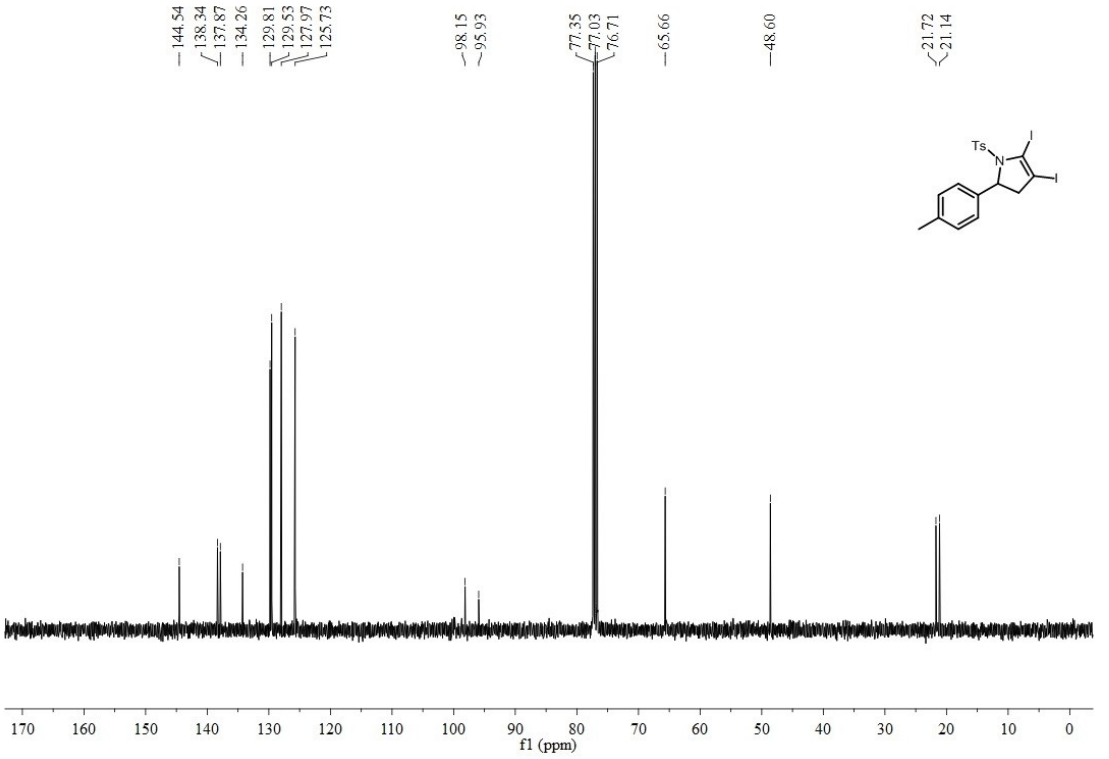
4. ^{1}H and ^{13}C NMR Spectra:

^{1}H, ^{13}C-NMR spectra of **2a**

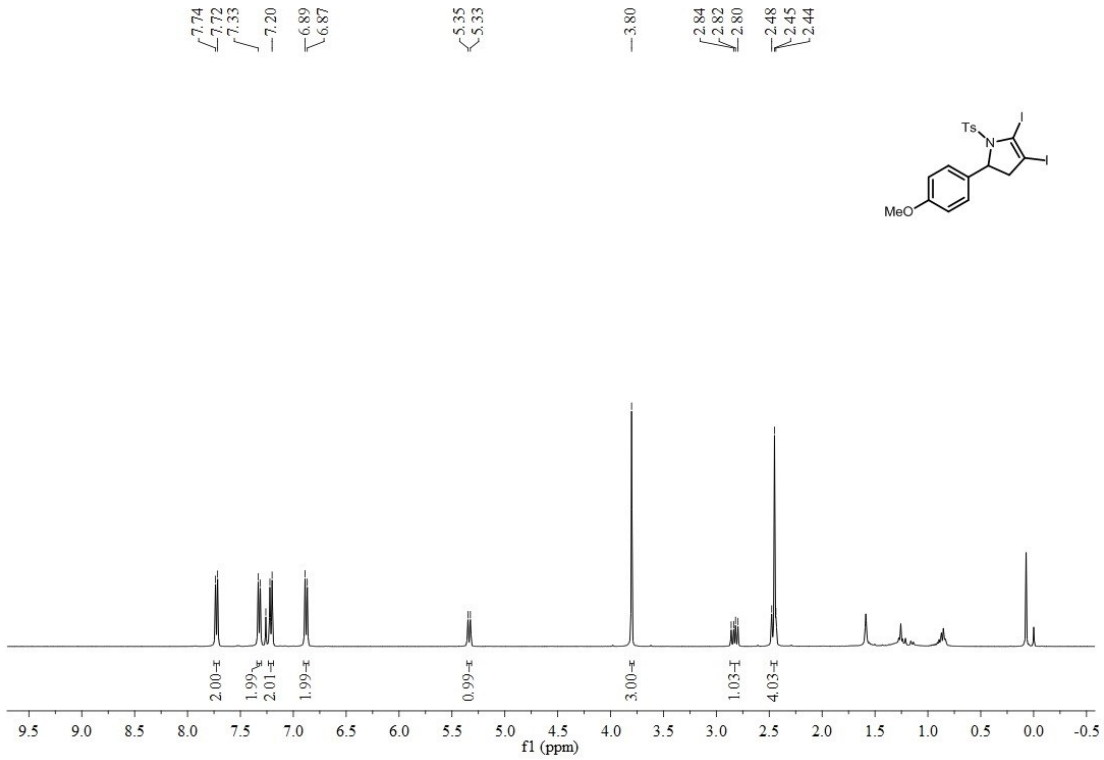


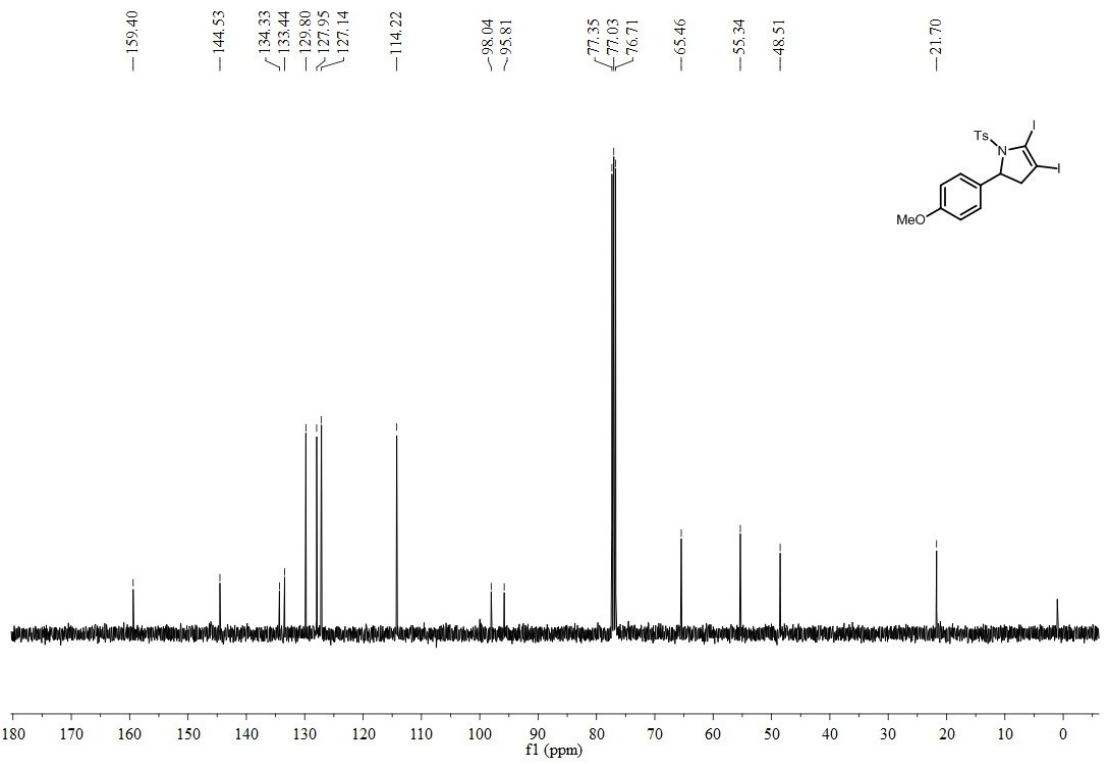
^{1}H, ^{13}C-NMR spectra of **2b**



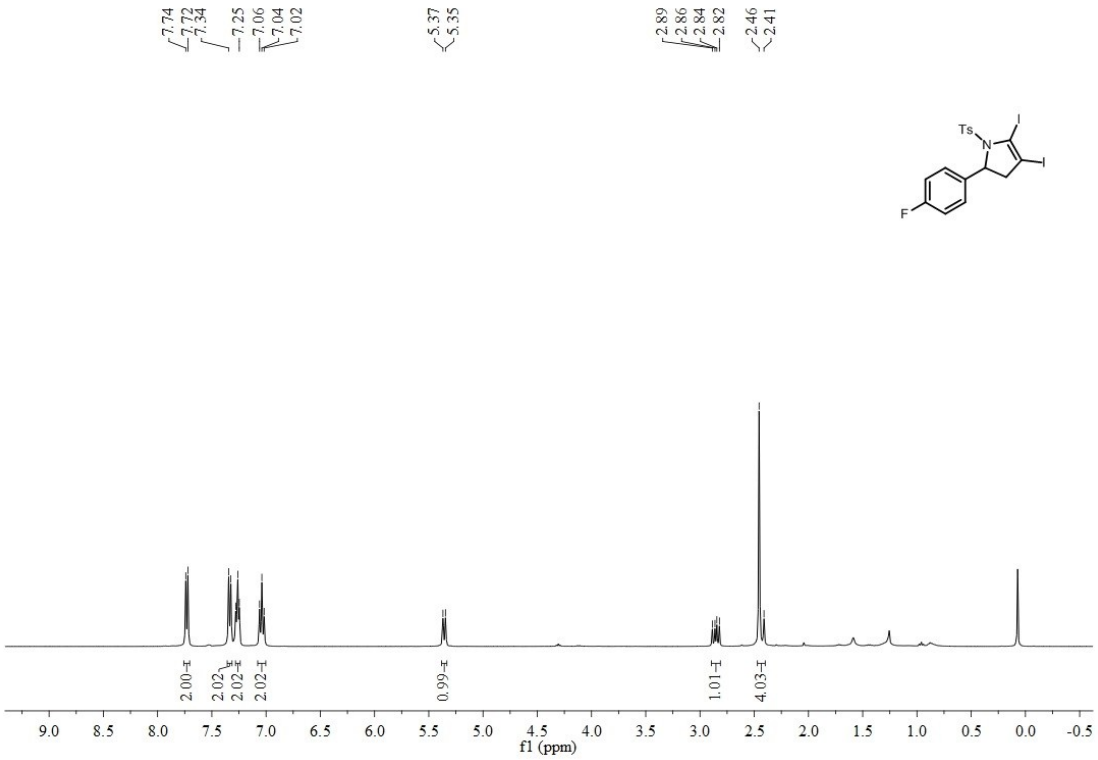


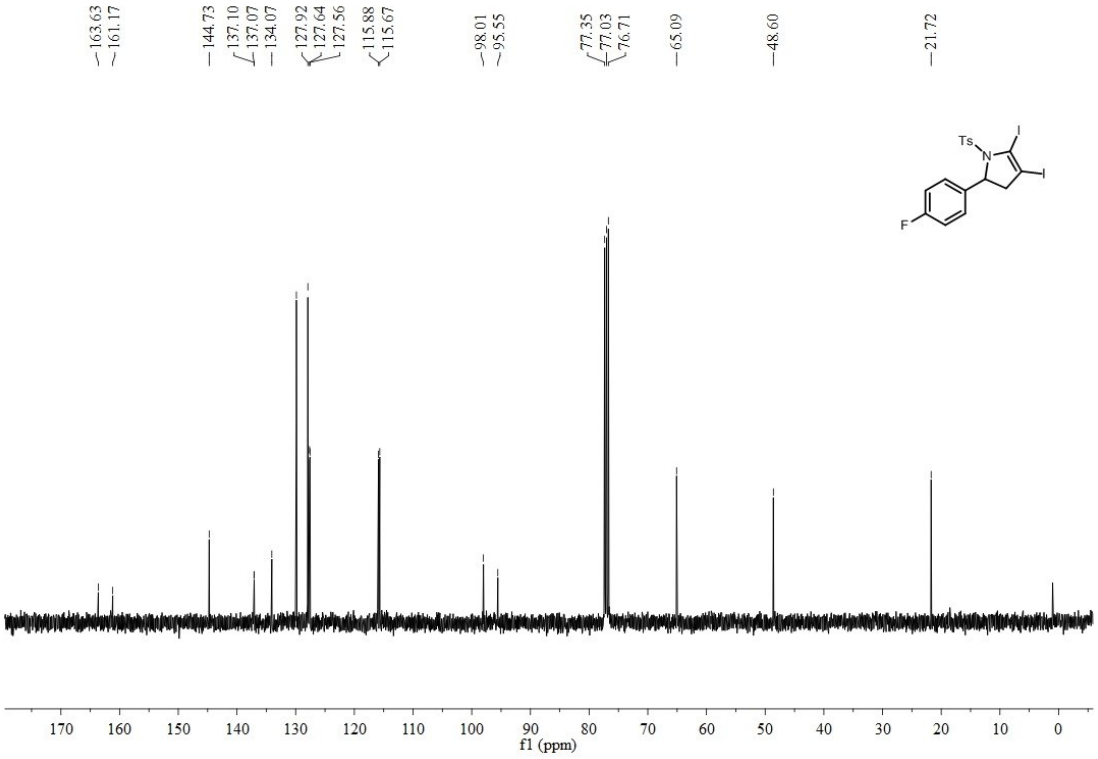
^{1}H, ^{13}C-NMR spectra of **2c**



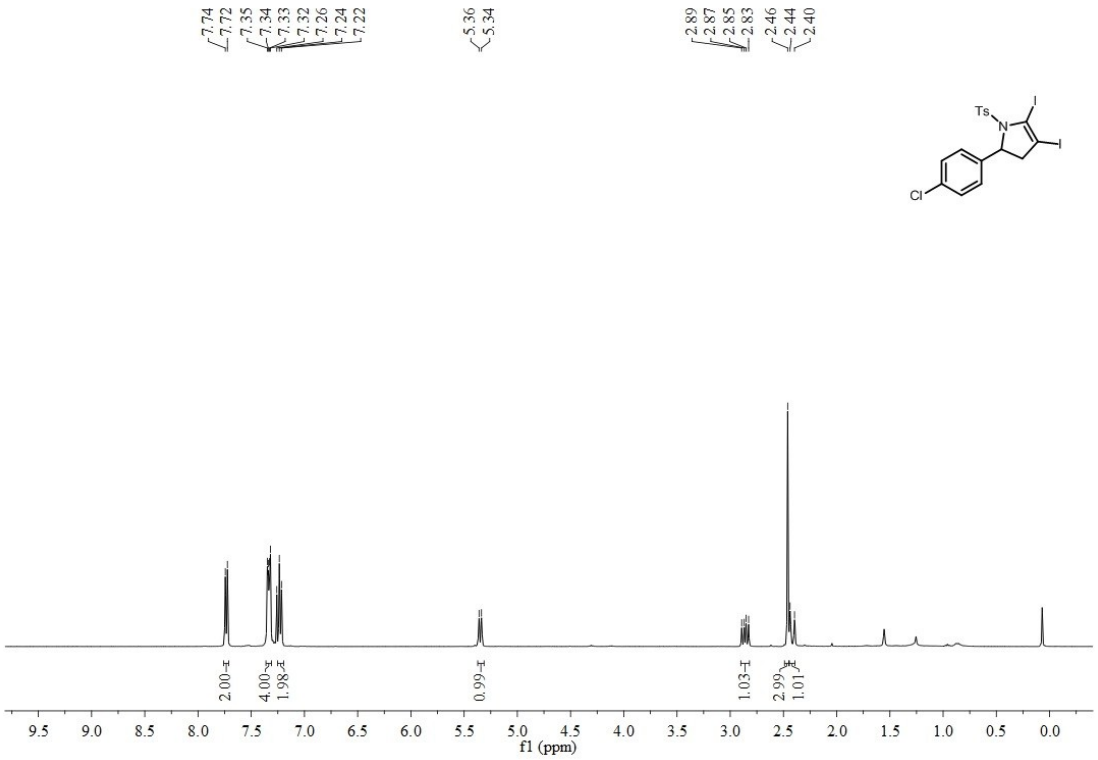


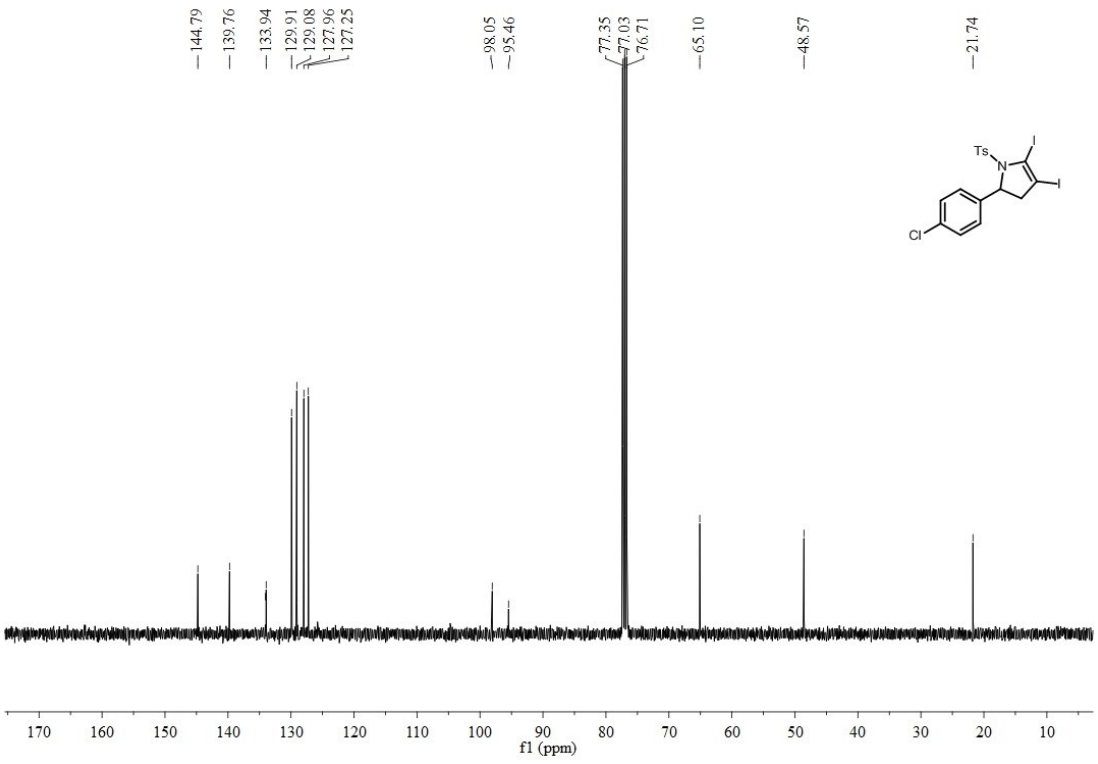
^{1}H, ^{13}C-NMR spectra of **2d**



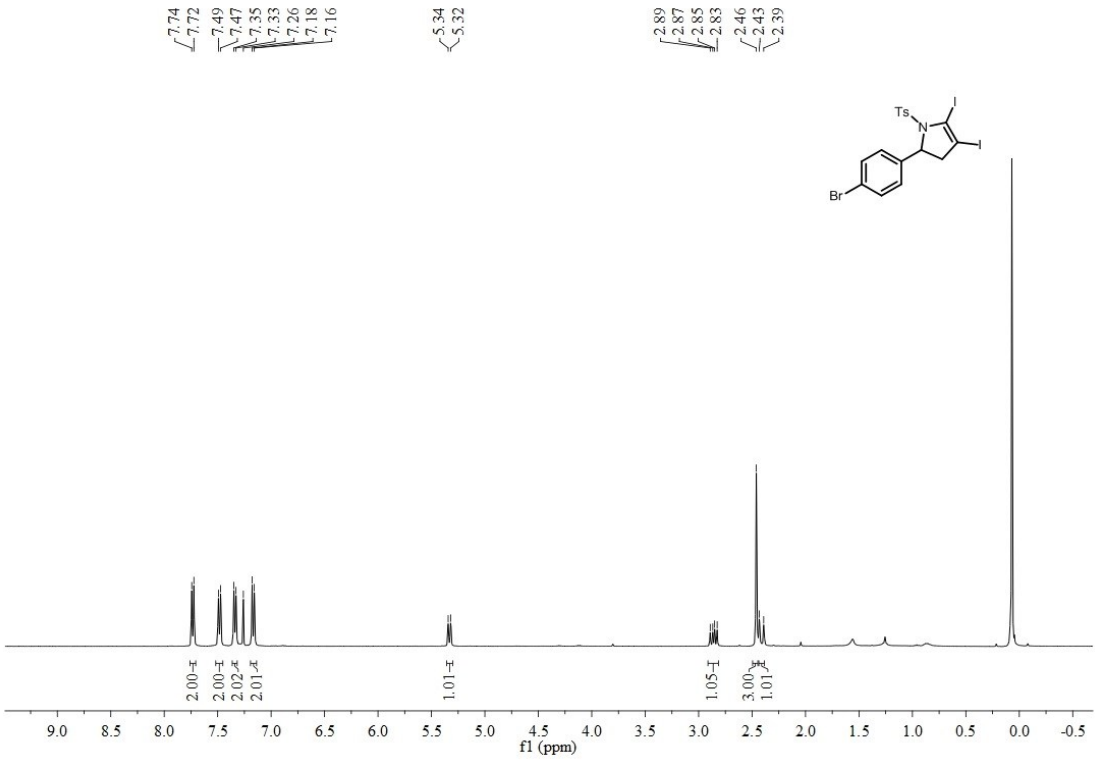


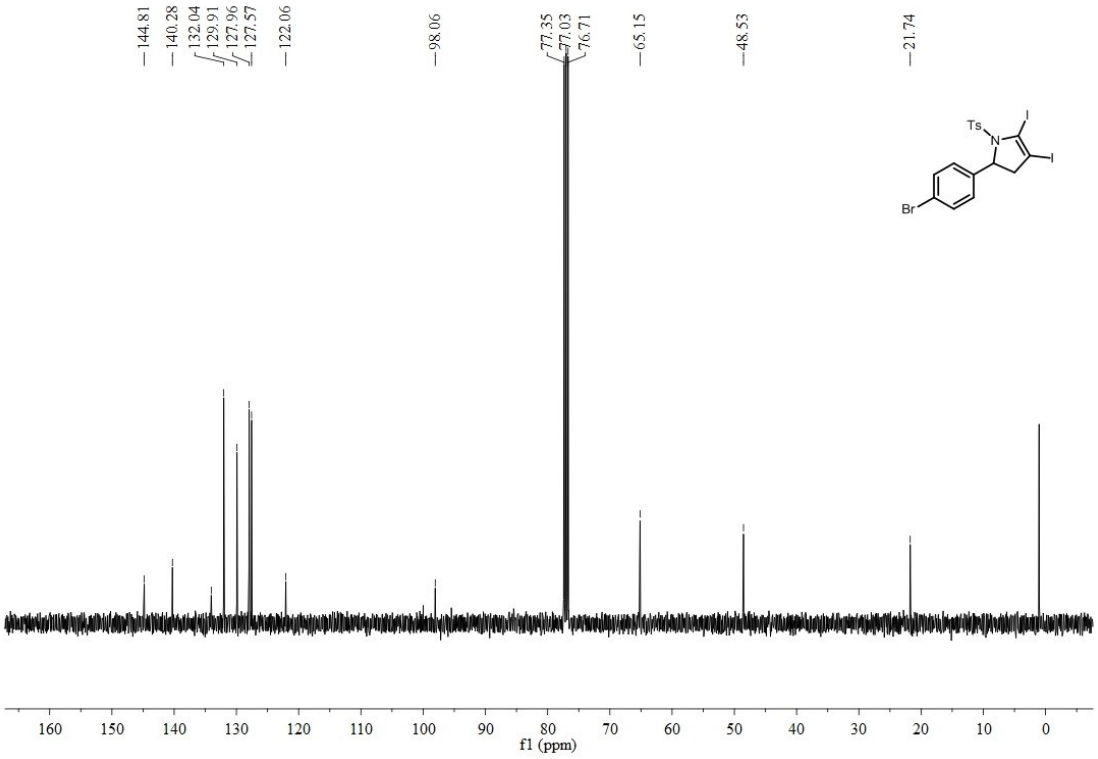
^{1}H, ^{13}C-NMR spectra of **2e**



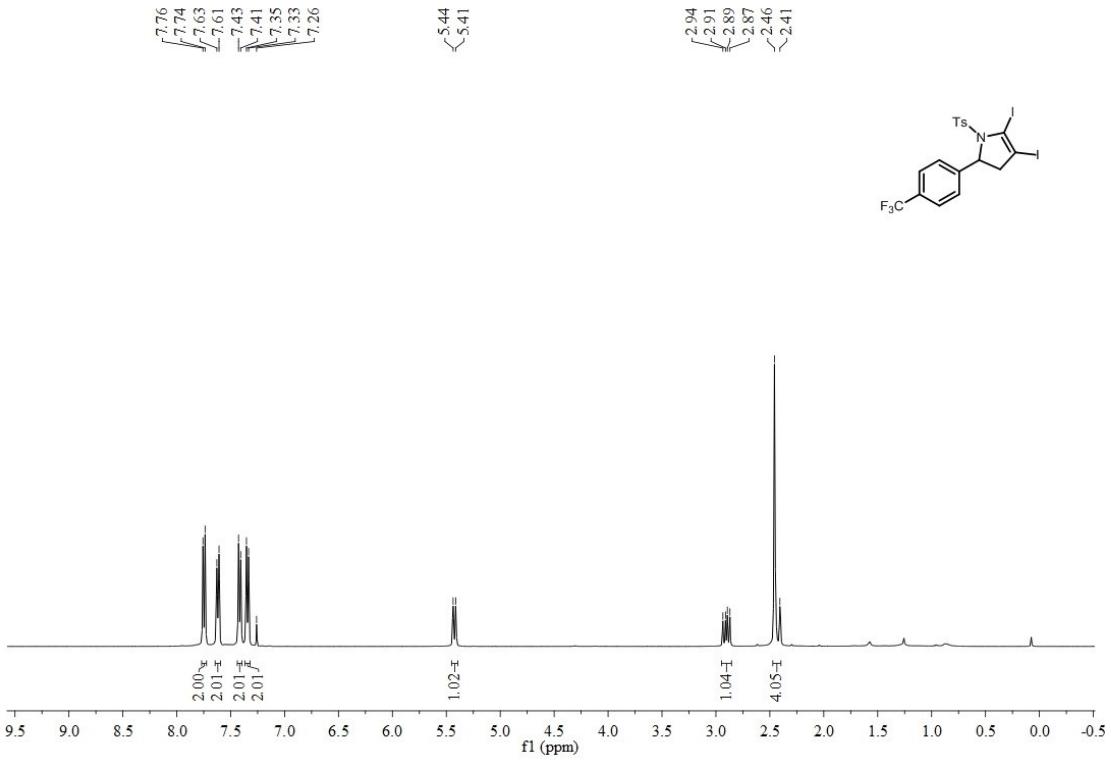


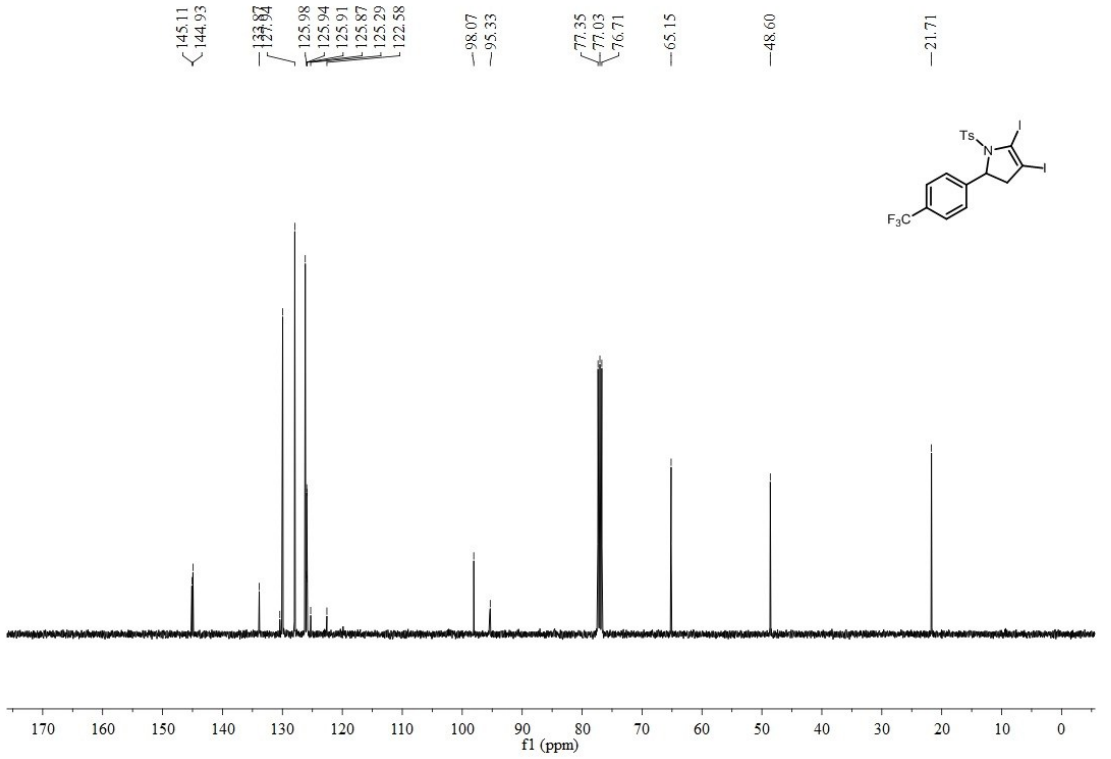
^{1}H, ^{13}C-NMR spectra of **2f**



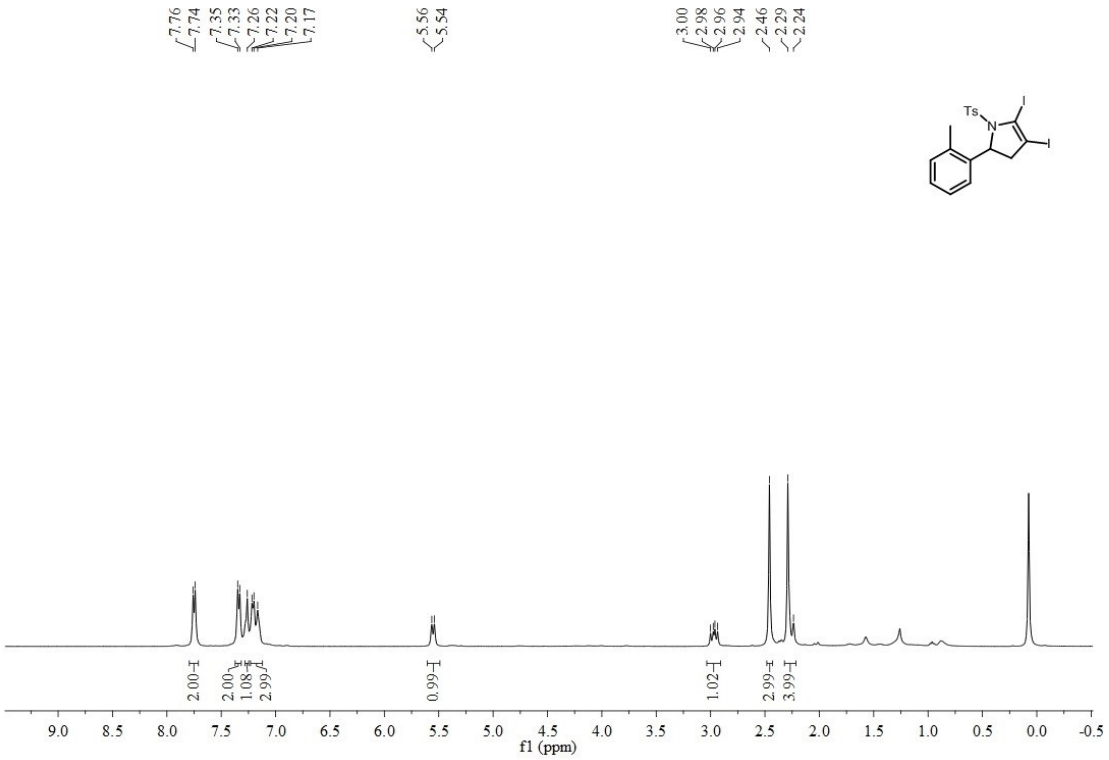


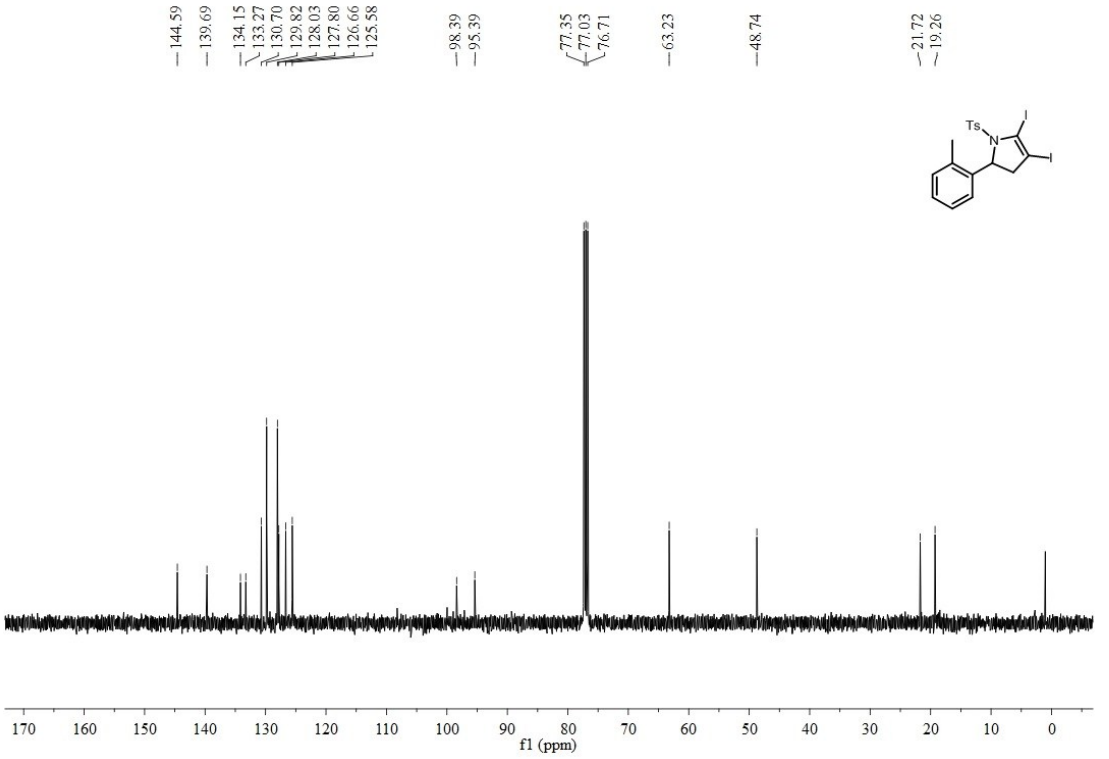
^{1}H, ^{13}C-NMR spectra of **2g**



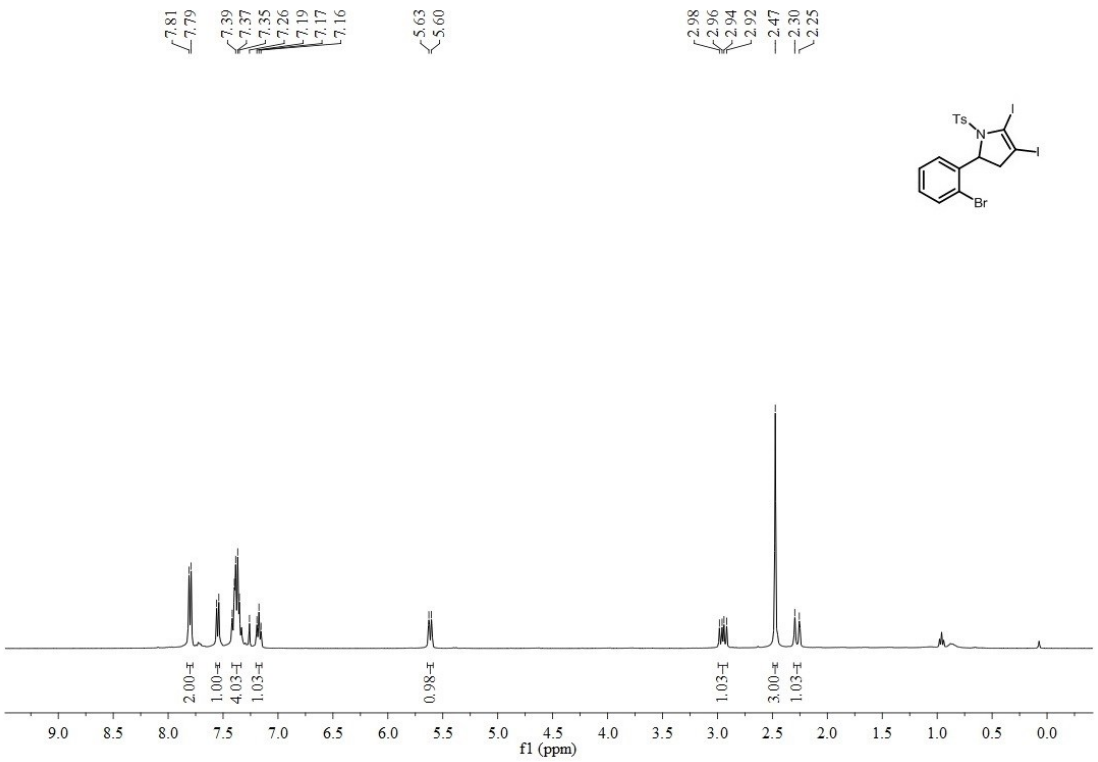


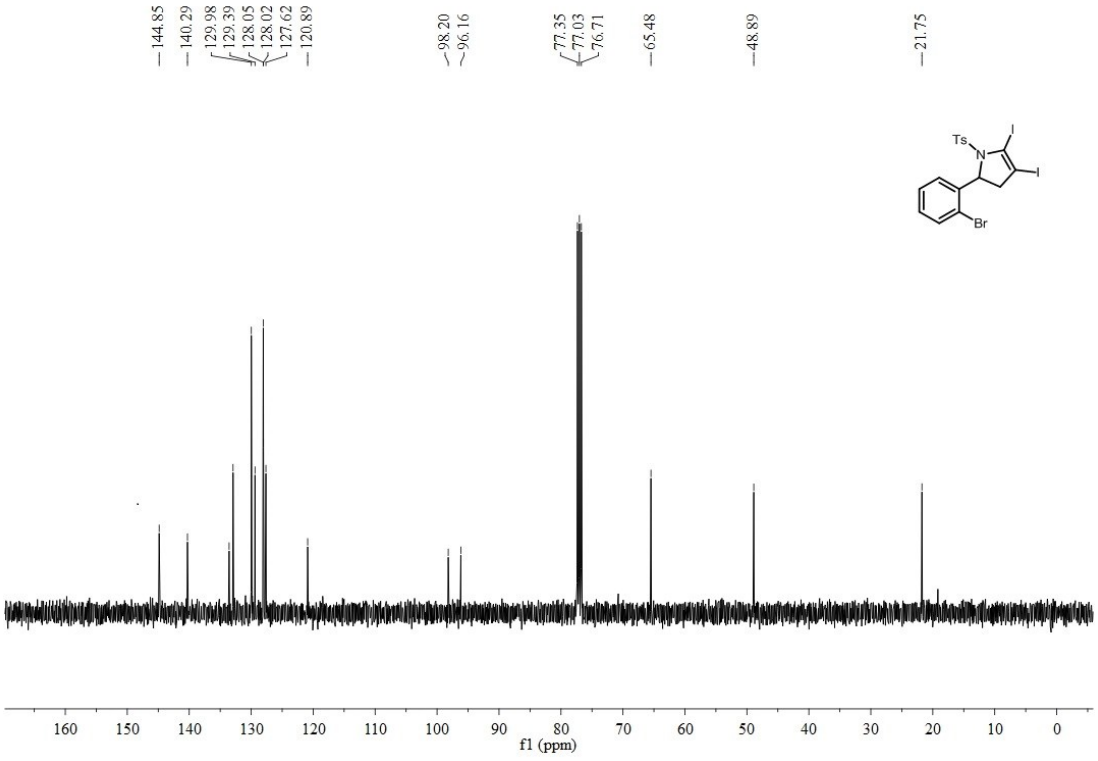
^{1}H, ^{13}C-NMR spectra of **2h**



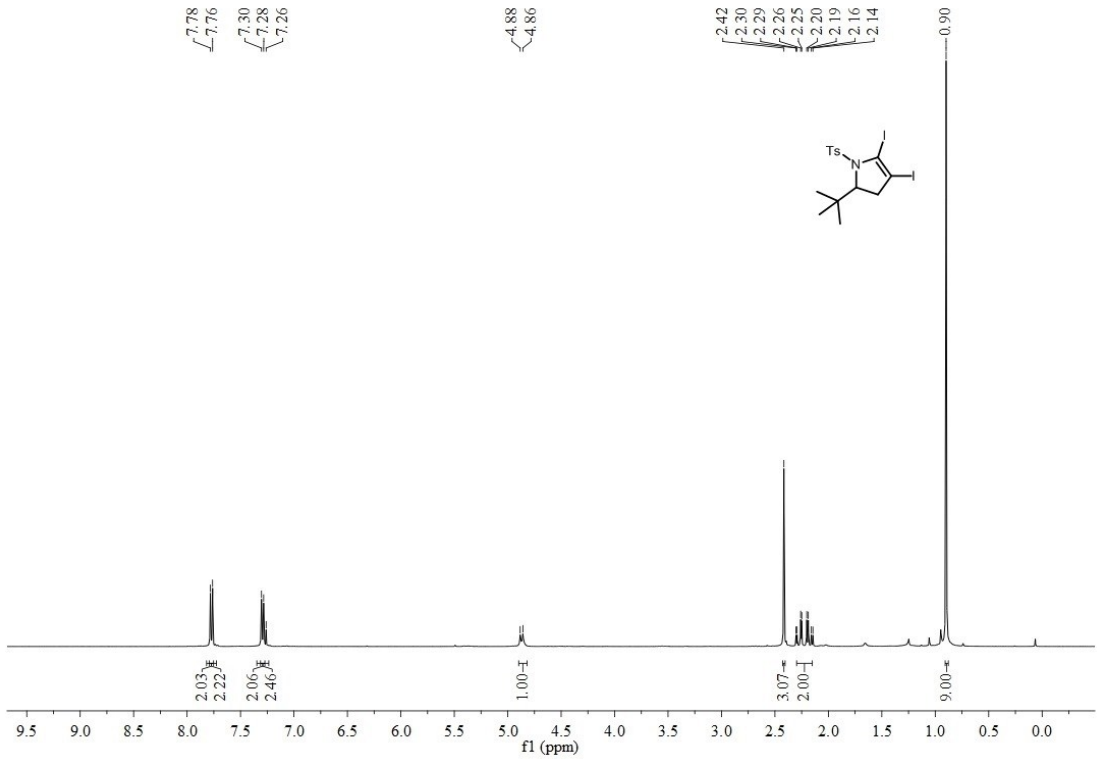


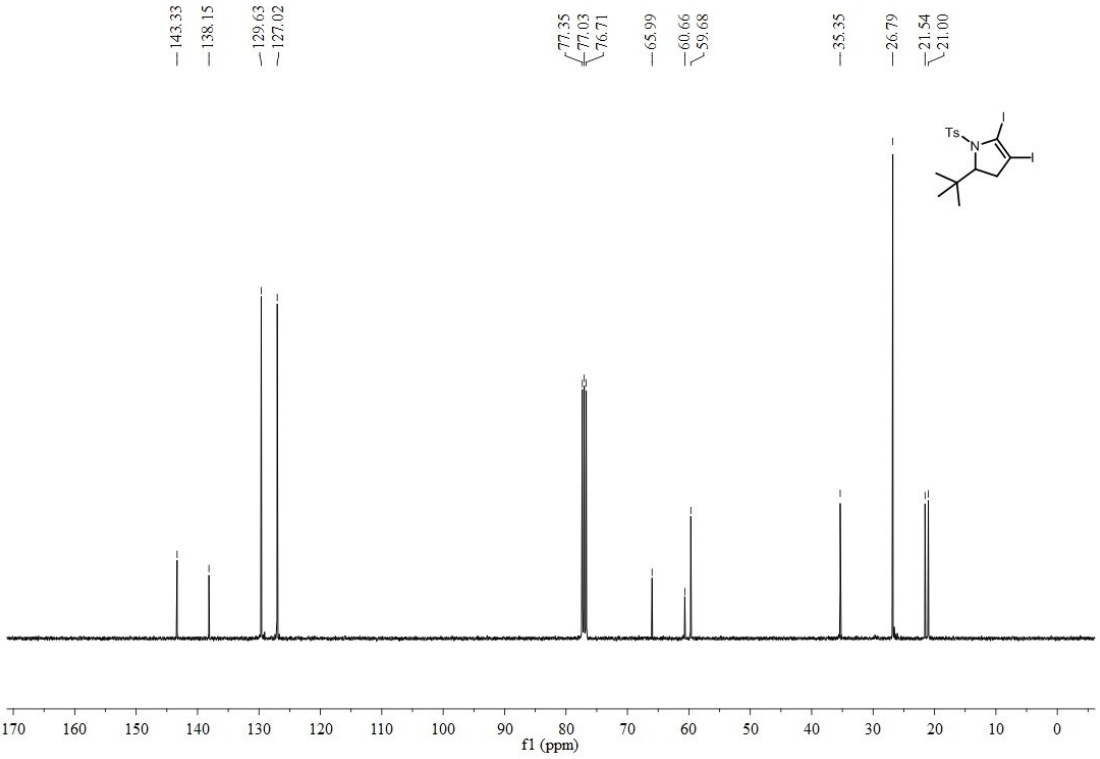
^{1}H, ^{13}C-NMR spectra of **2i**



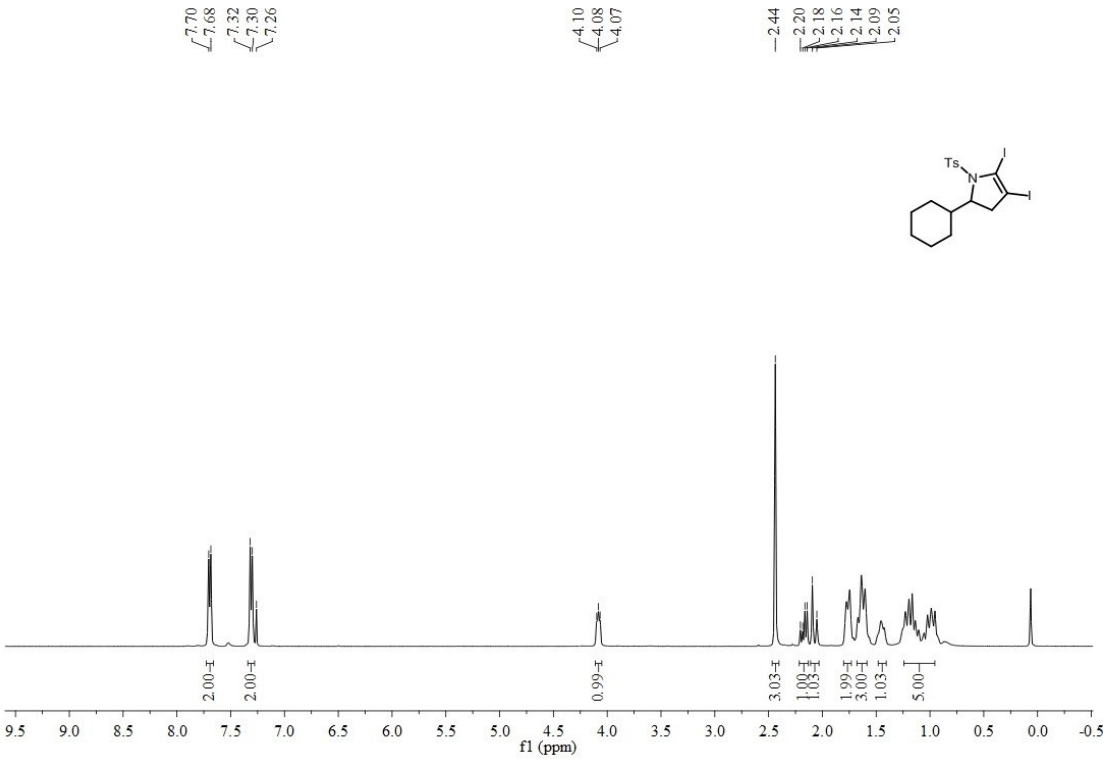


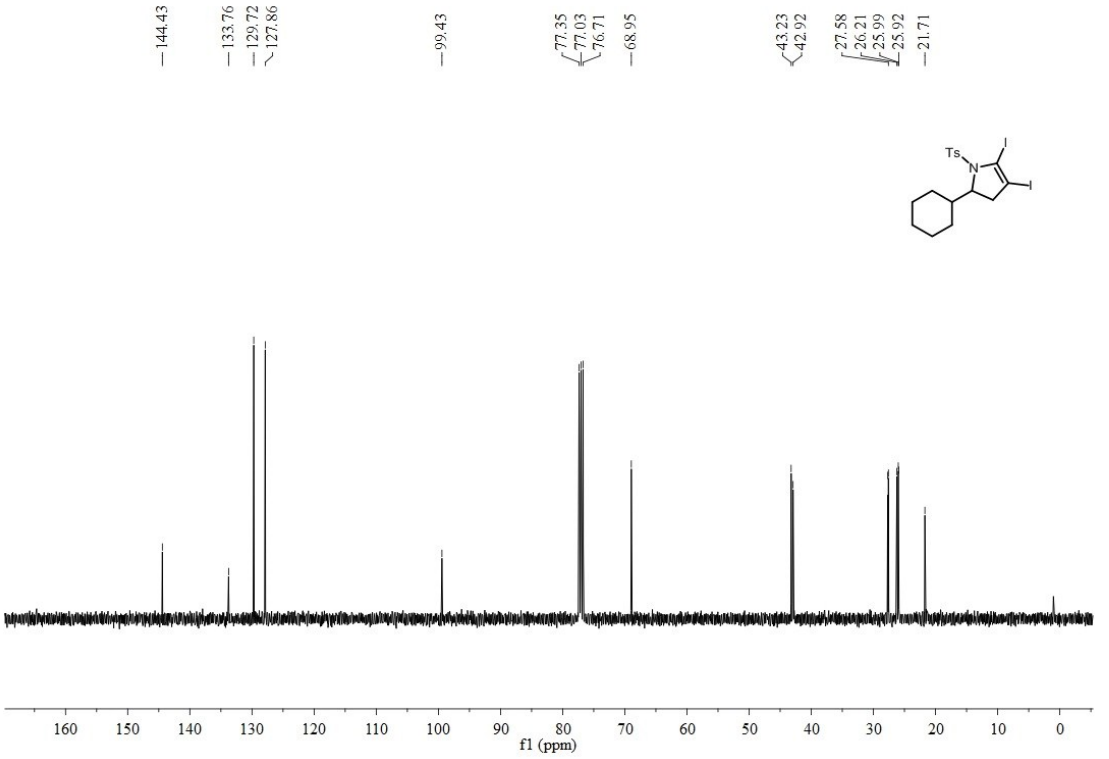
^{1}H, ^{13}C-NMR spectra of **2j**



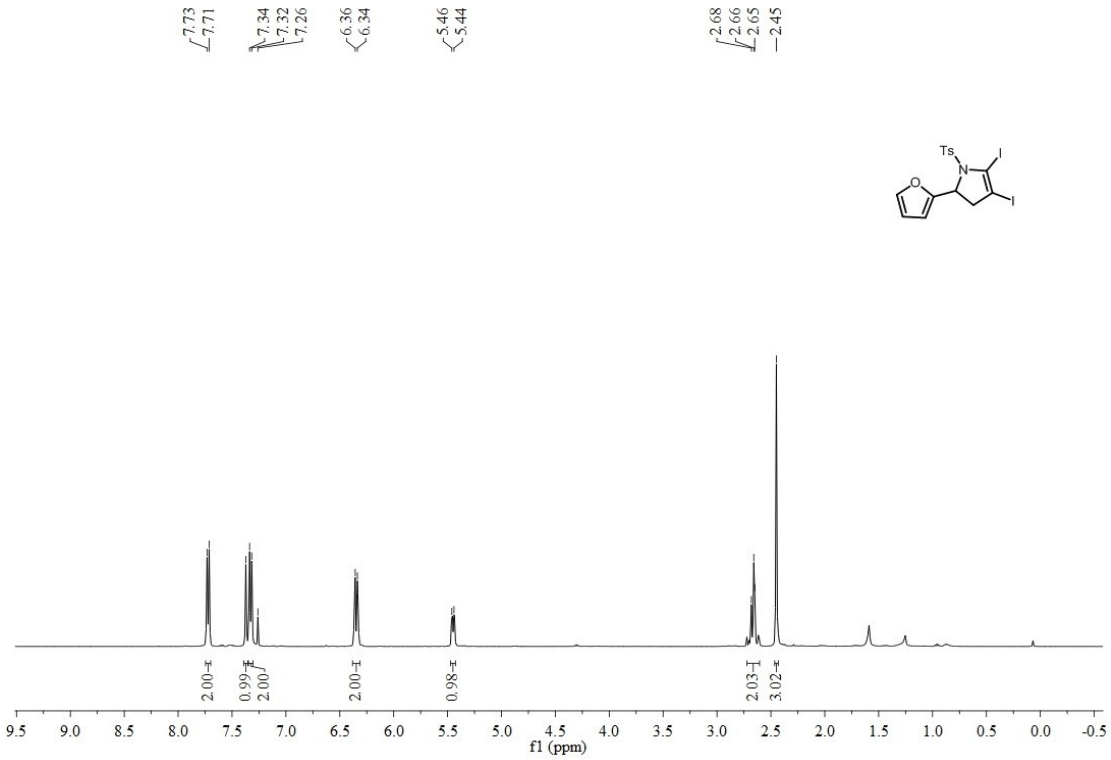


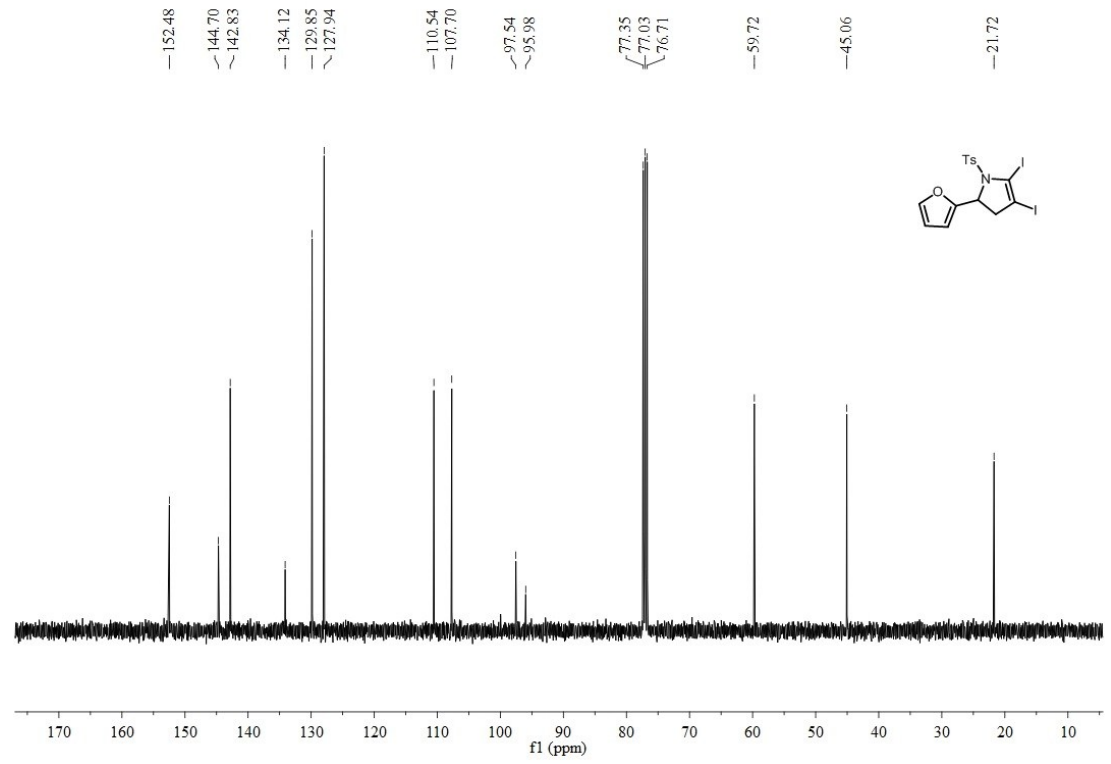
^{1}H, ^{13}C-NMR spectra of **2k**



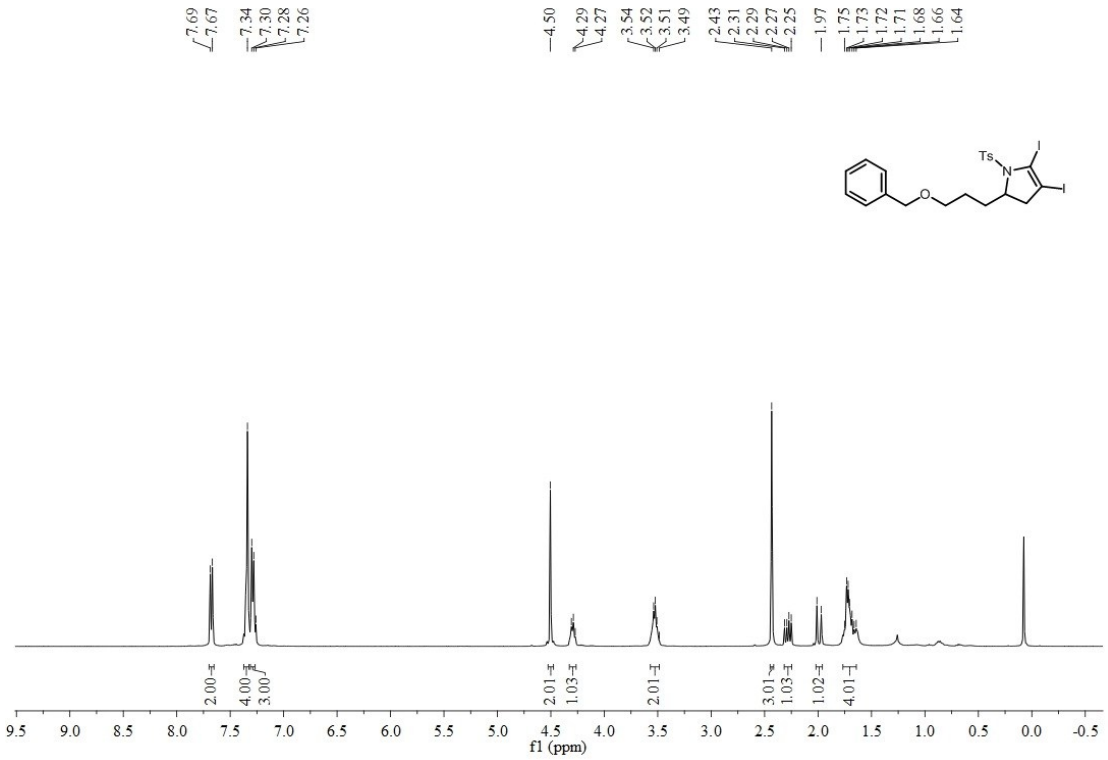


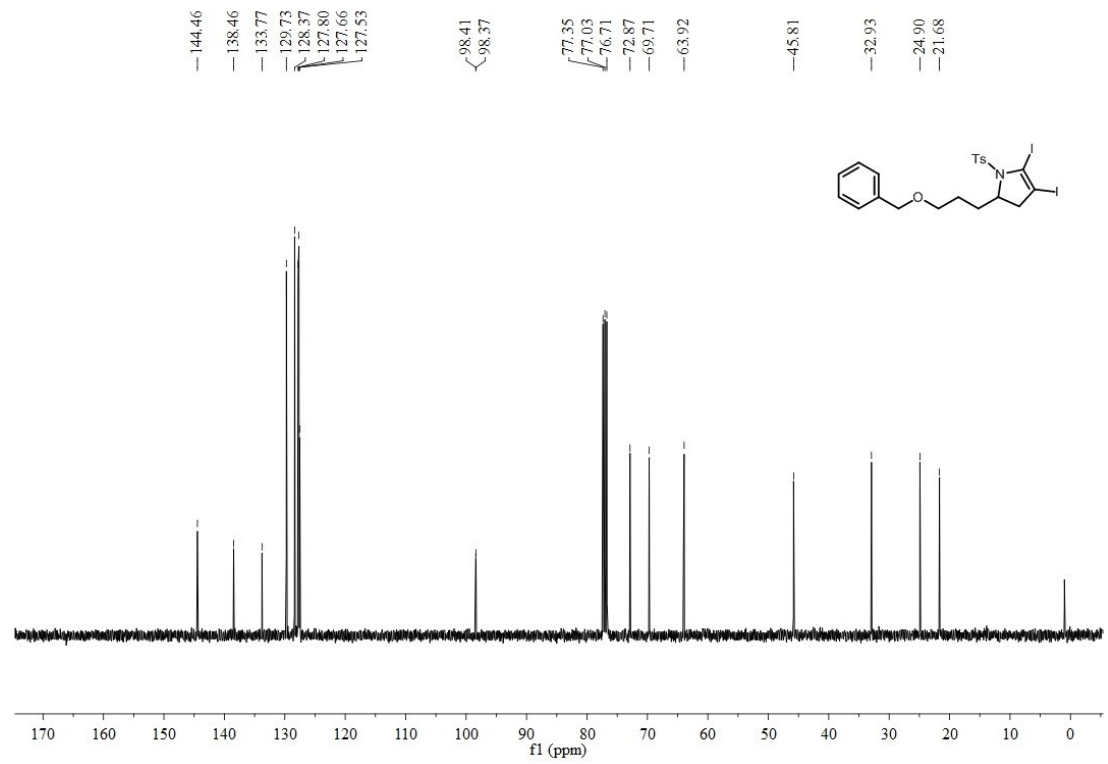
^{1}H, ^{13}C-NMR spectra of **2l**



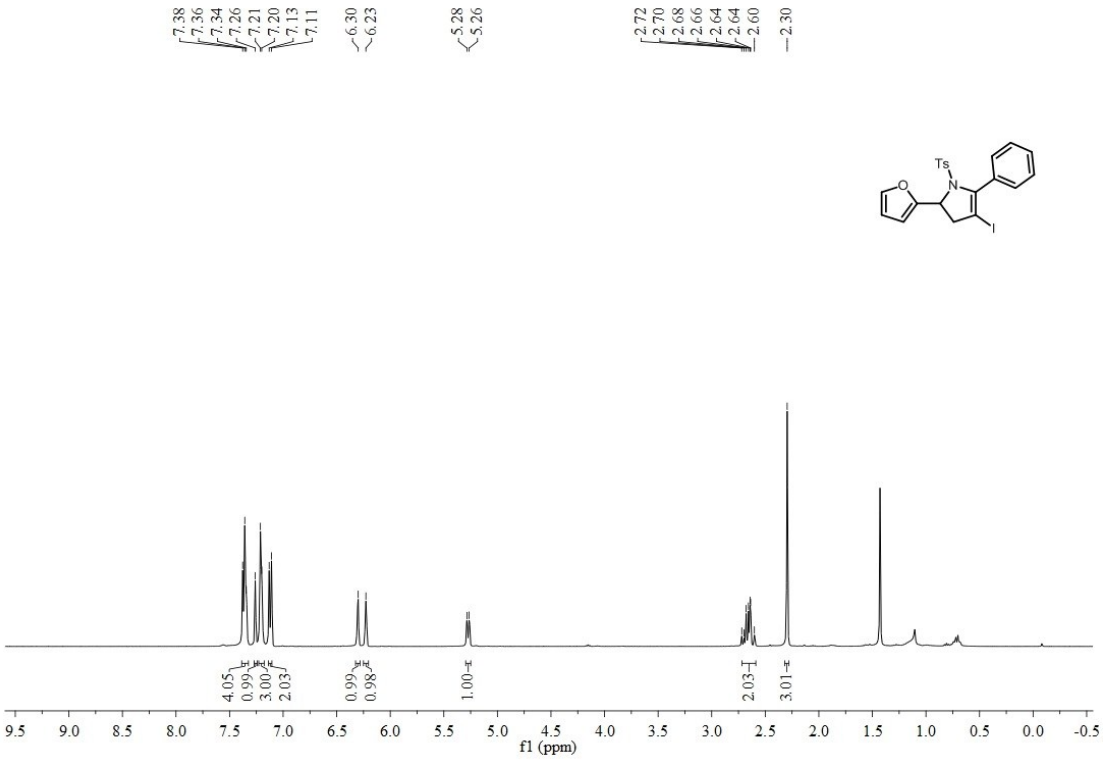


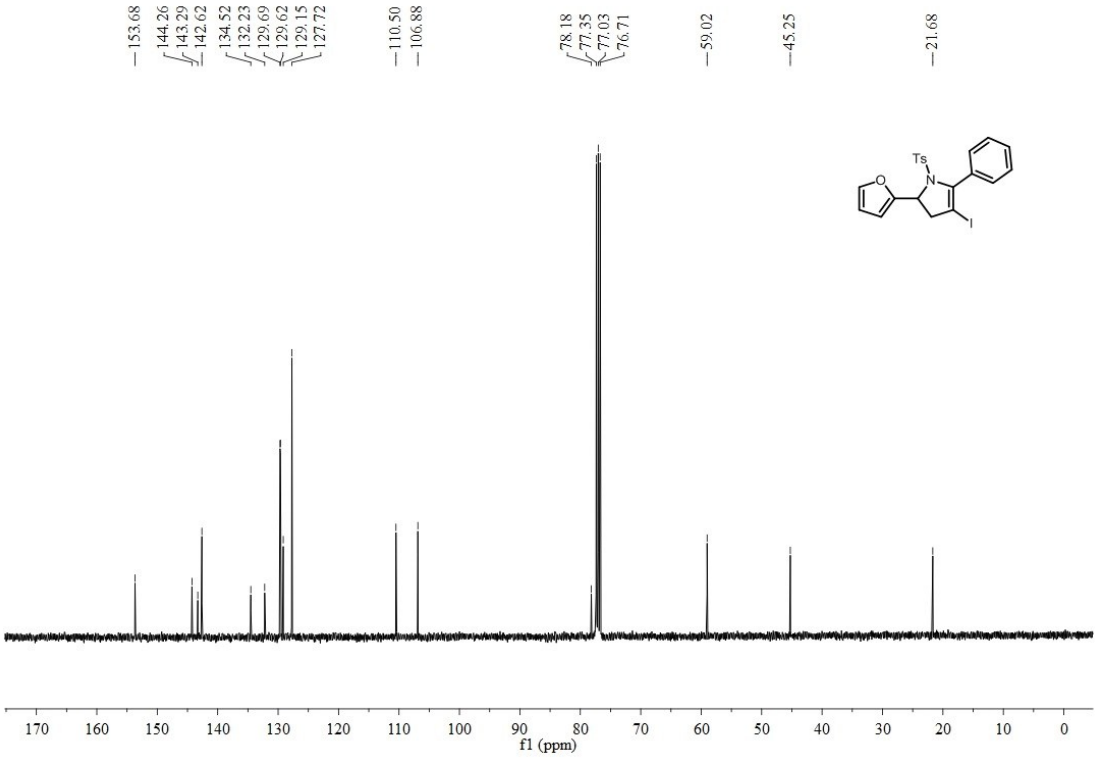
^{1}H, ^{13}C-NMR spectra of **2m**



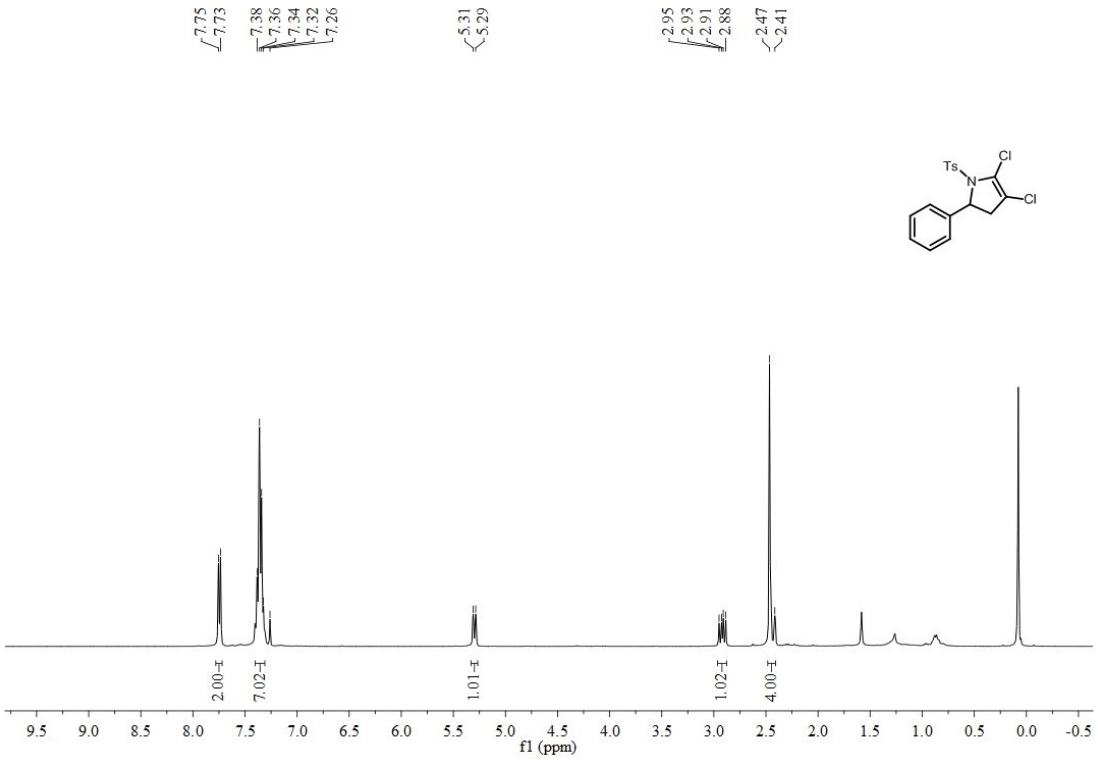


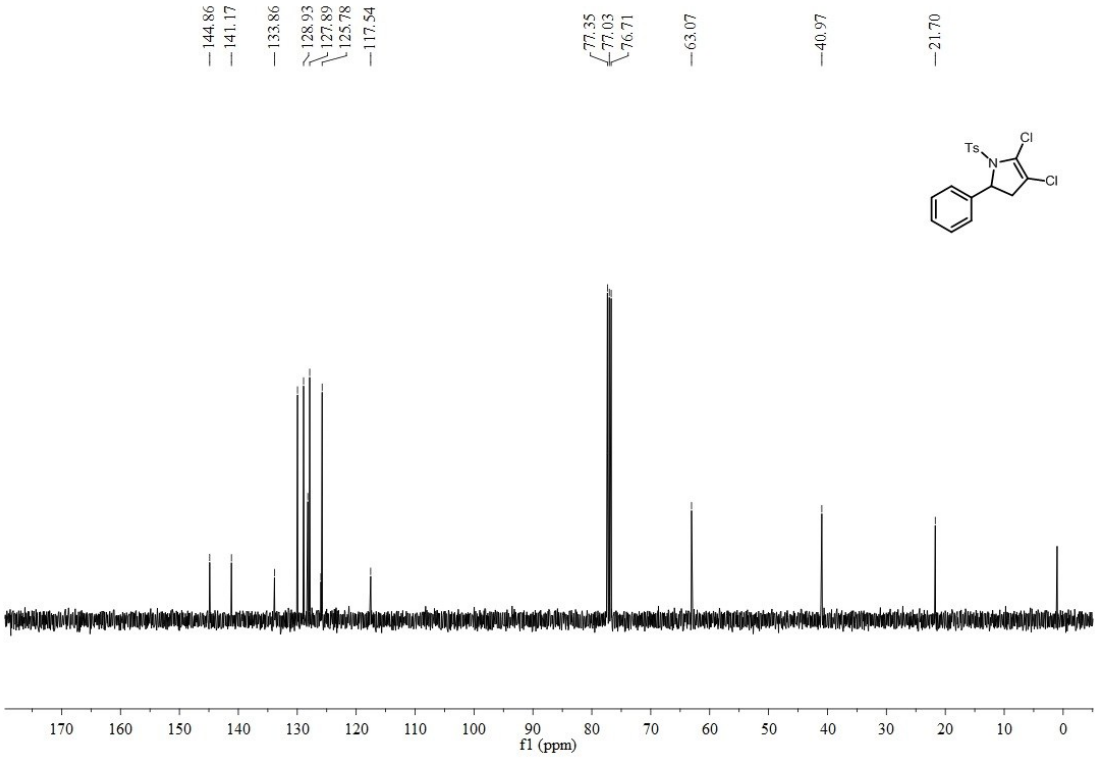
^{1}H, ^{13}C-NMR spectra of **2n**



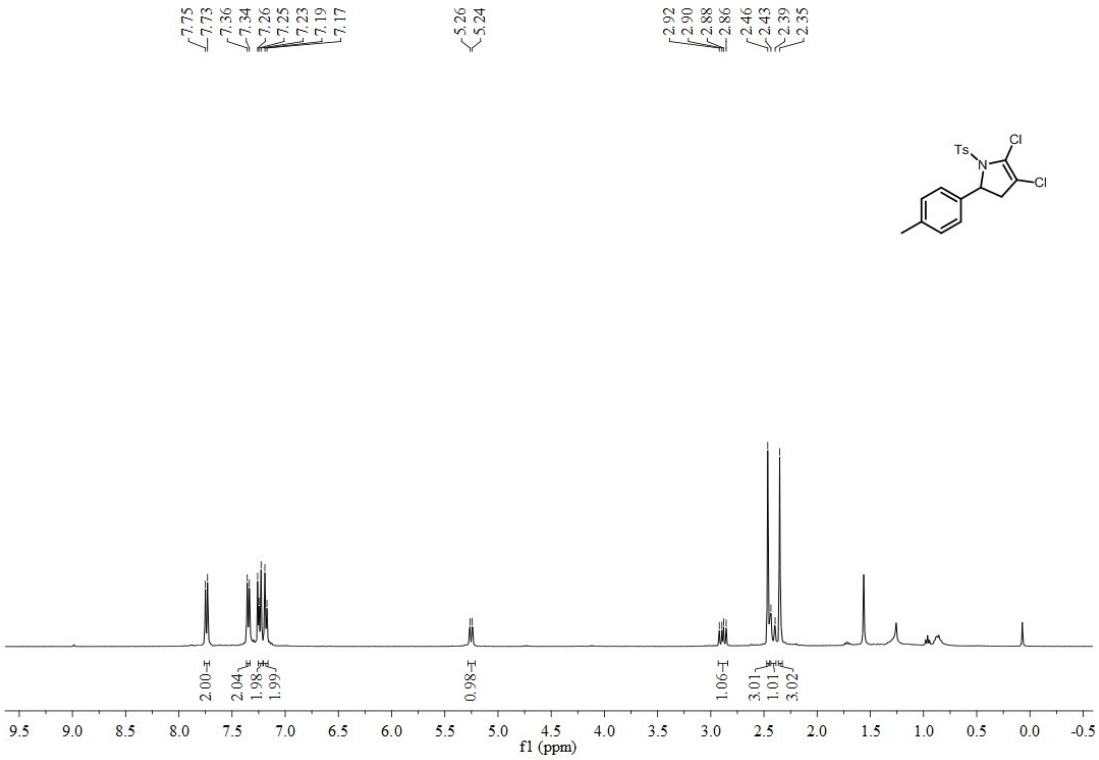


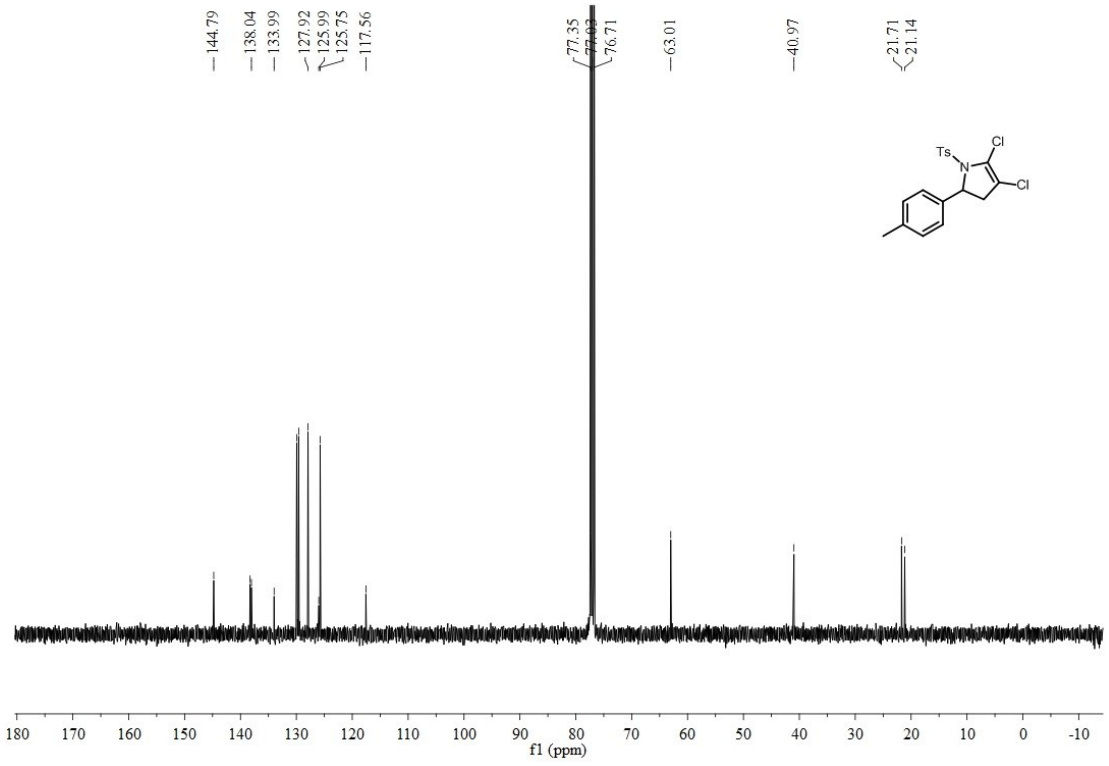
^{1}H, ^{13}C-NMR spectra of **3a**



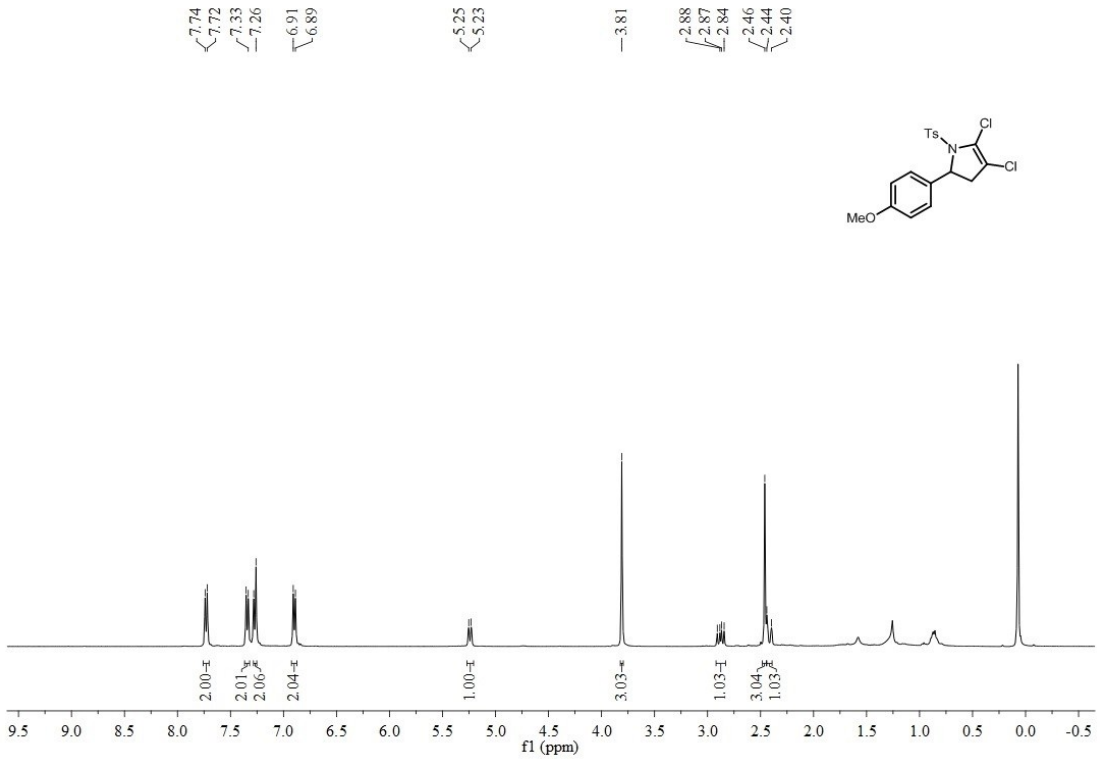


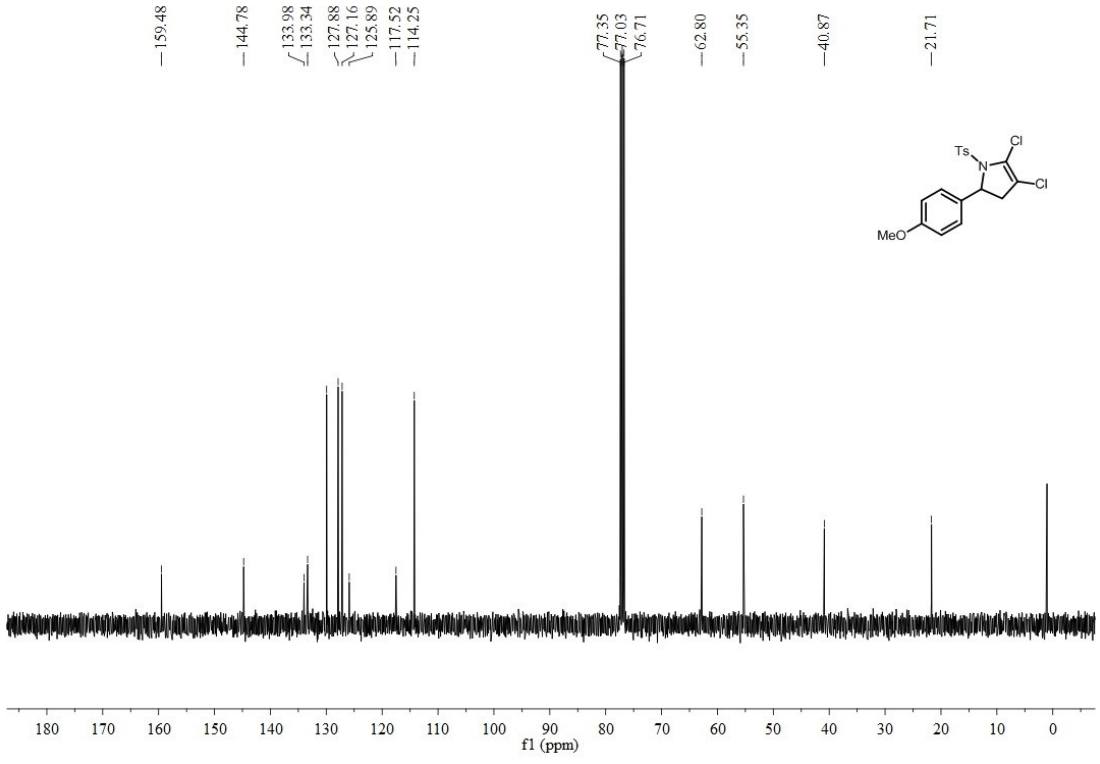
^{1}H, ^{13}C-NMR spectra of **3b**



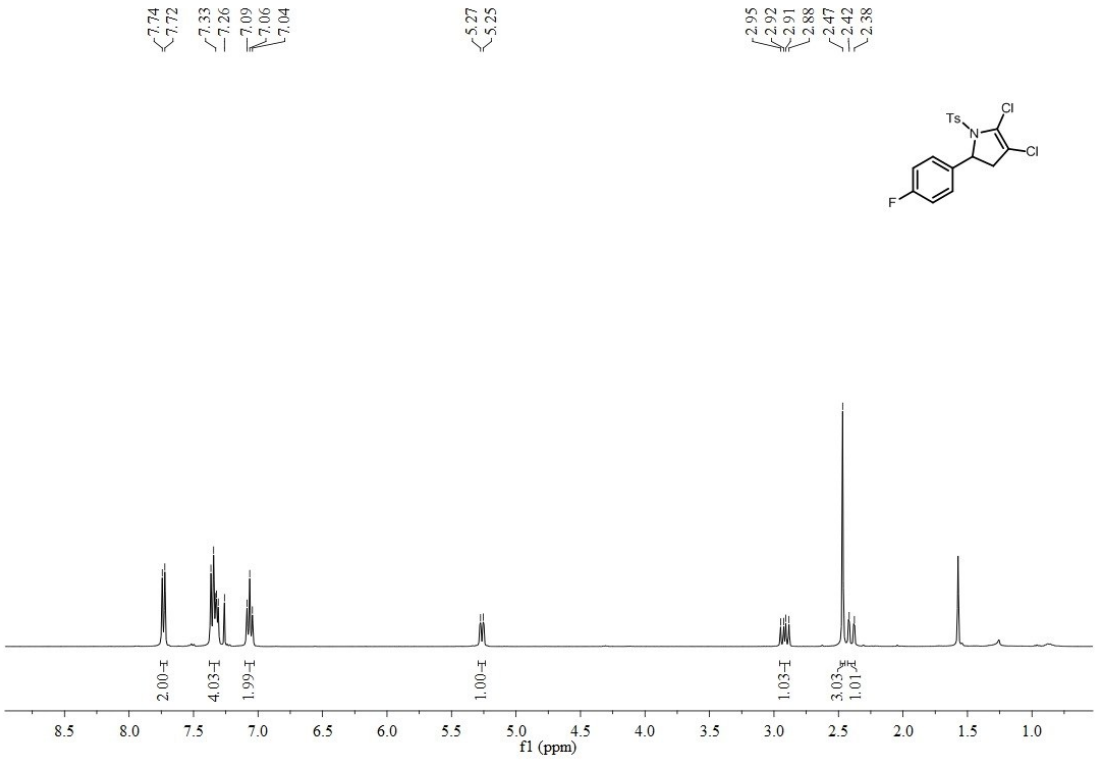


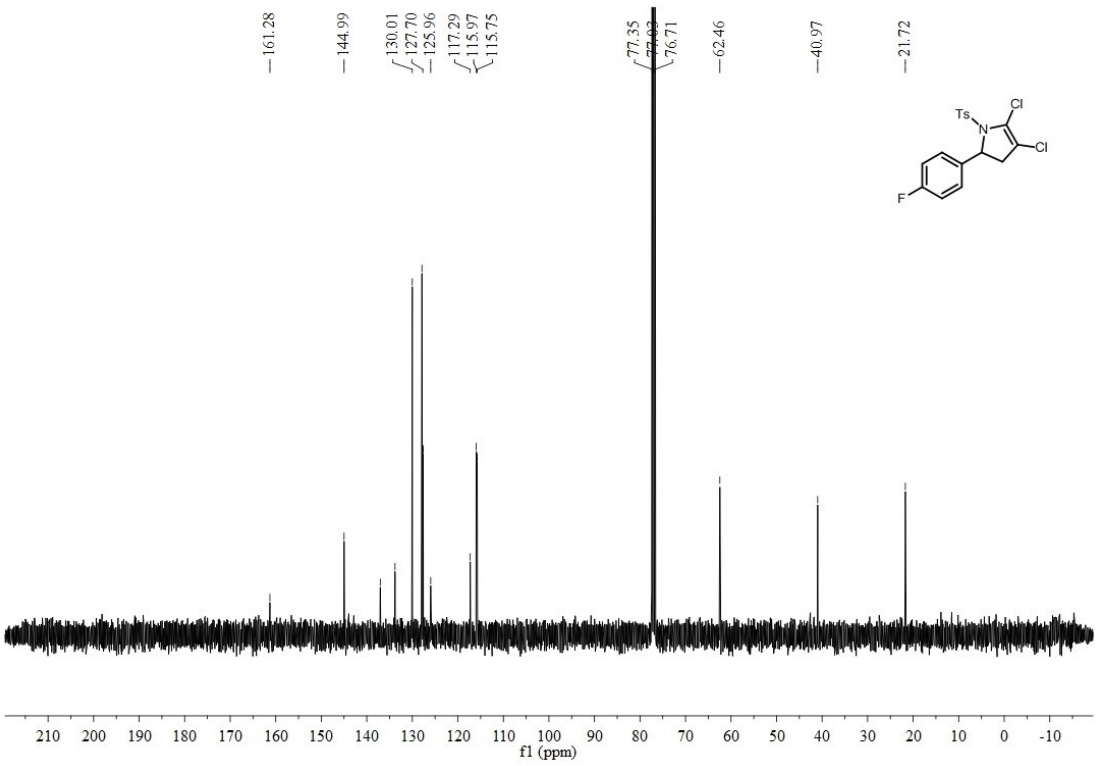
^{1}H, ^{13}C-NMR spectra of **3c**



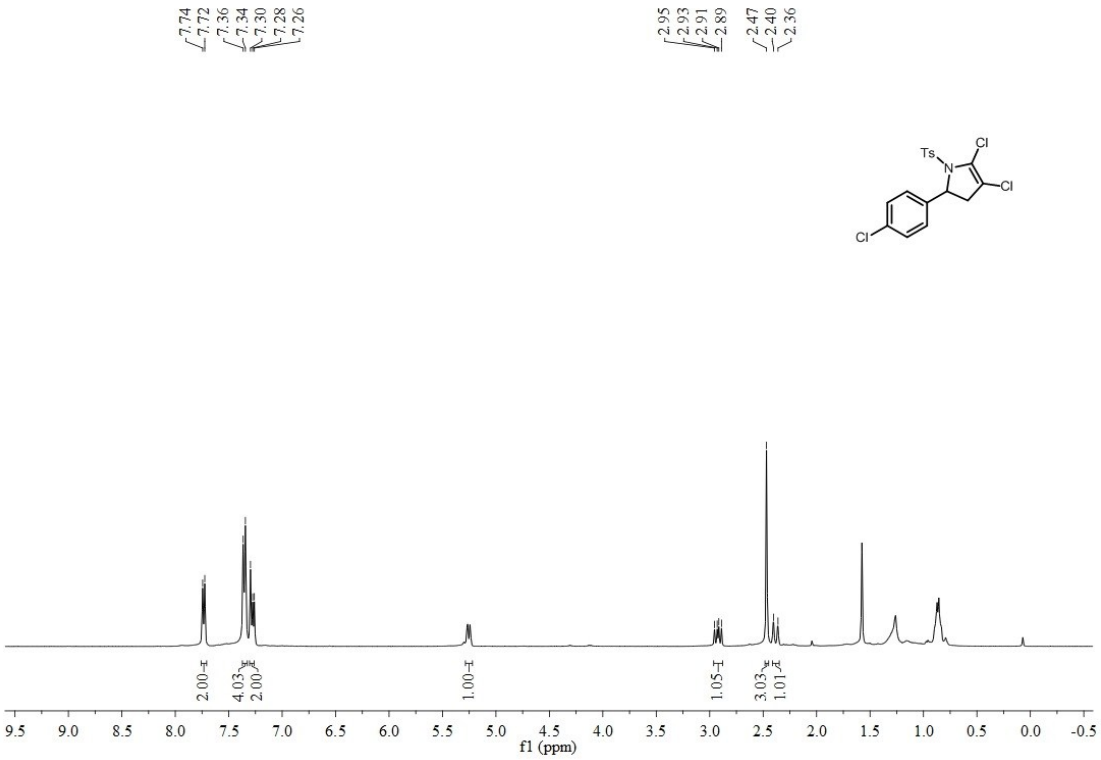


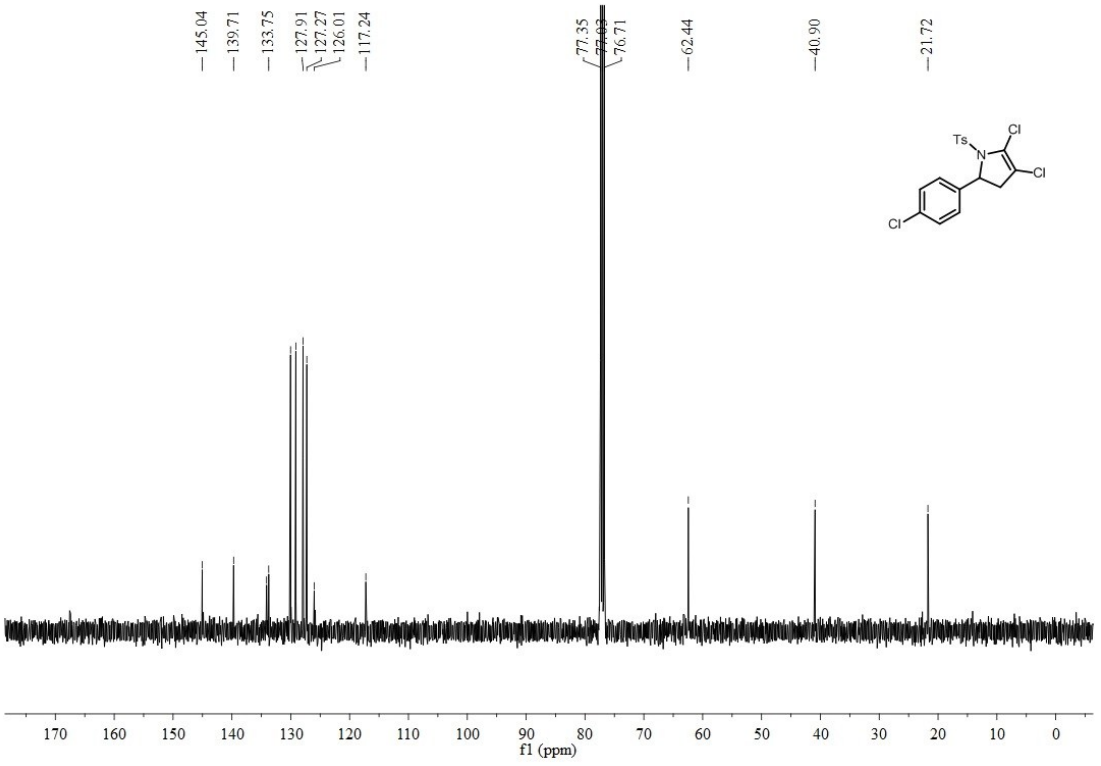
^{1}H, ^{13}C-NMR spectra of **3d**



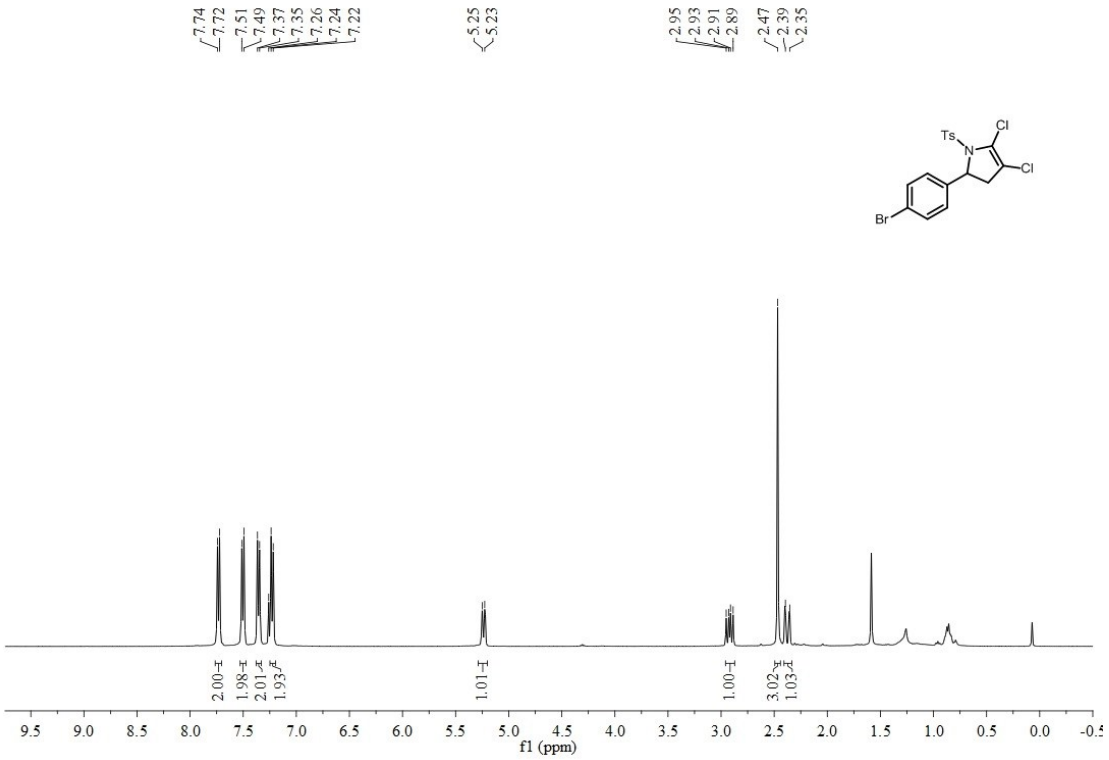


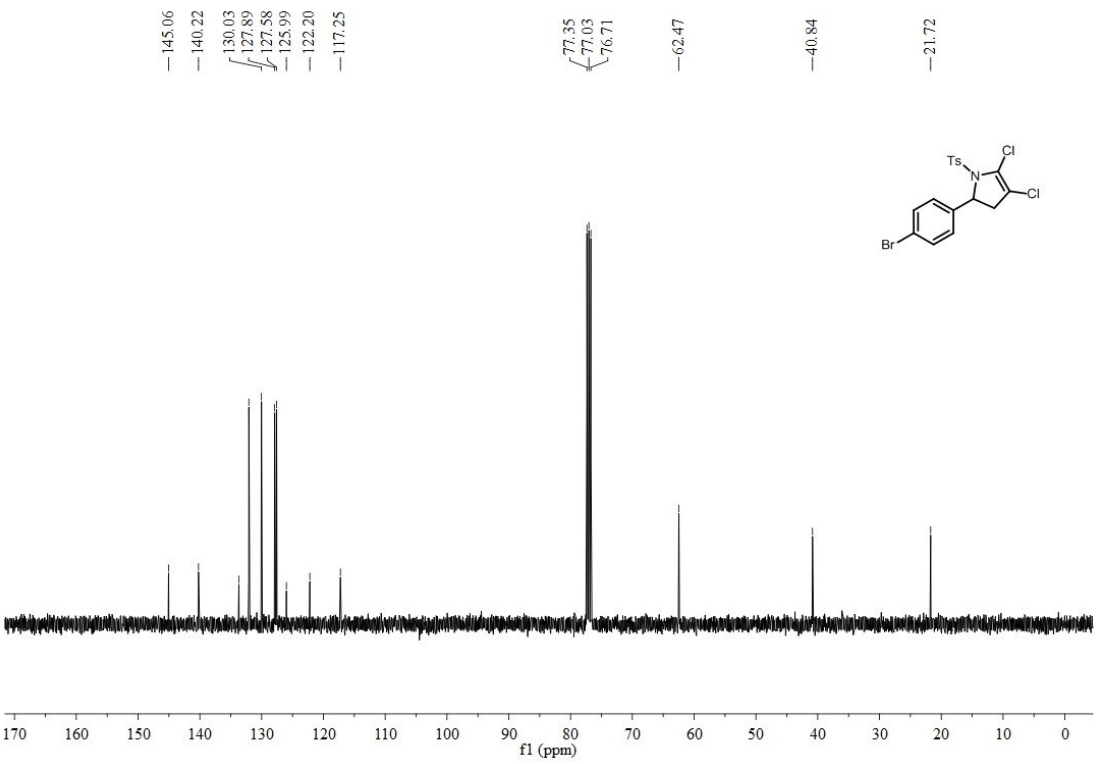
^{1}H, ^{13}C-NMR spectra of **3e**



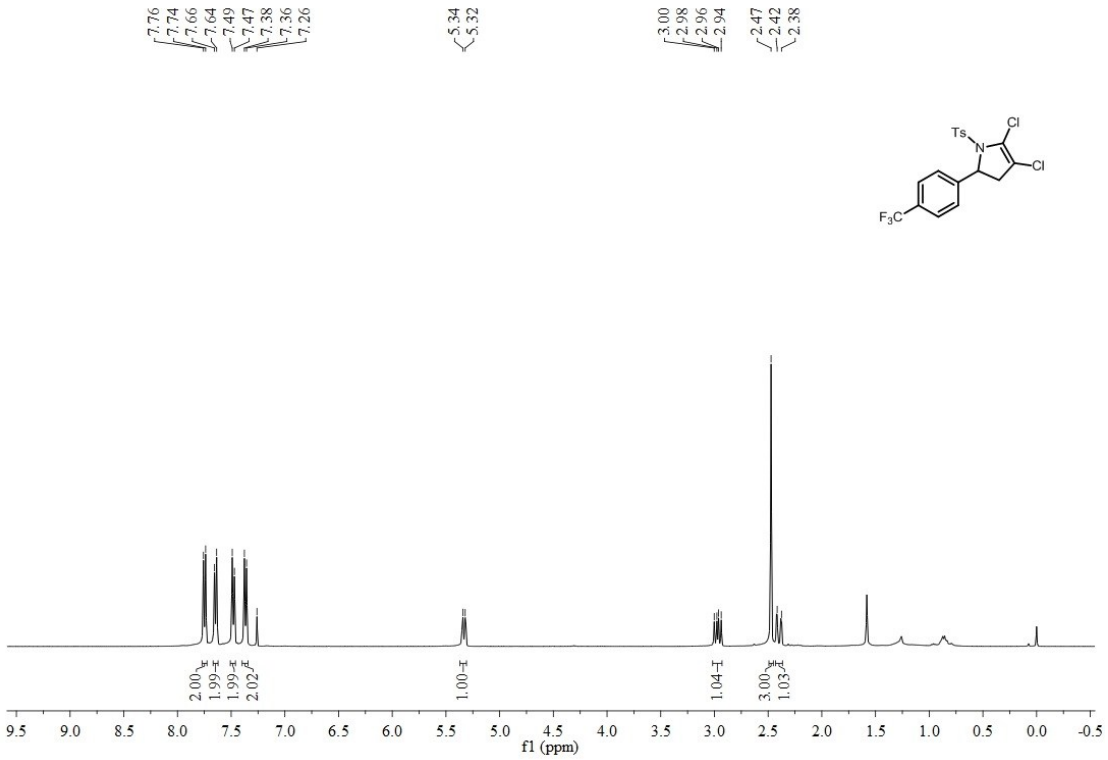


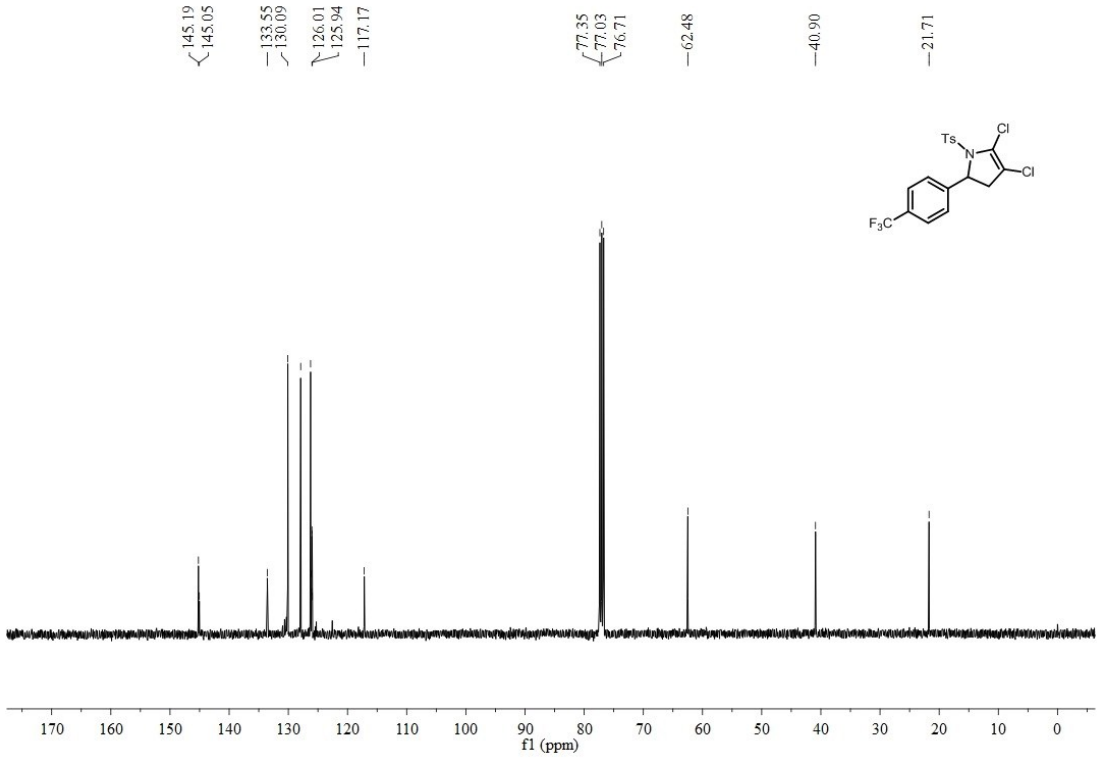
^{1}H, ^{13}C-NMR spectra of **3f**



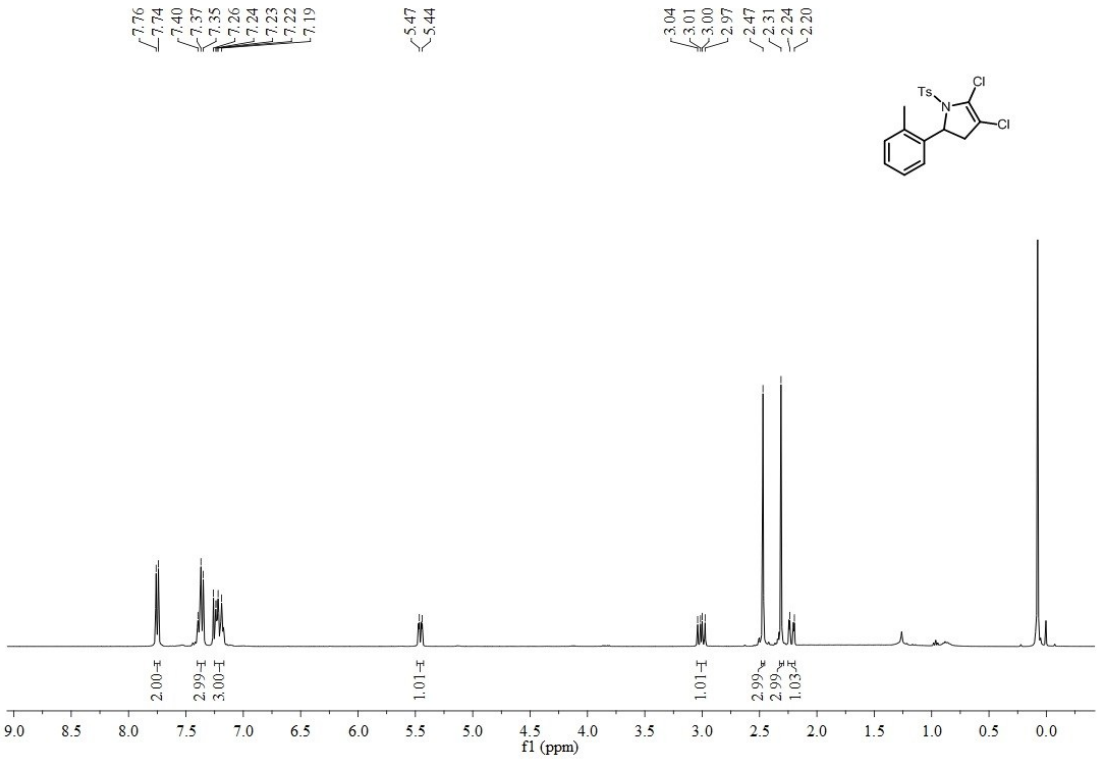


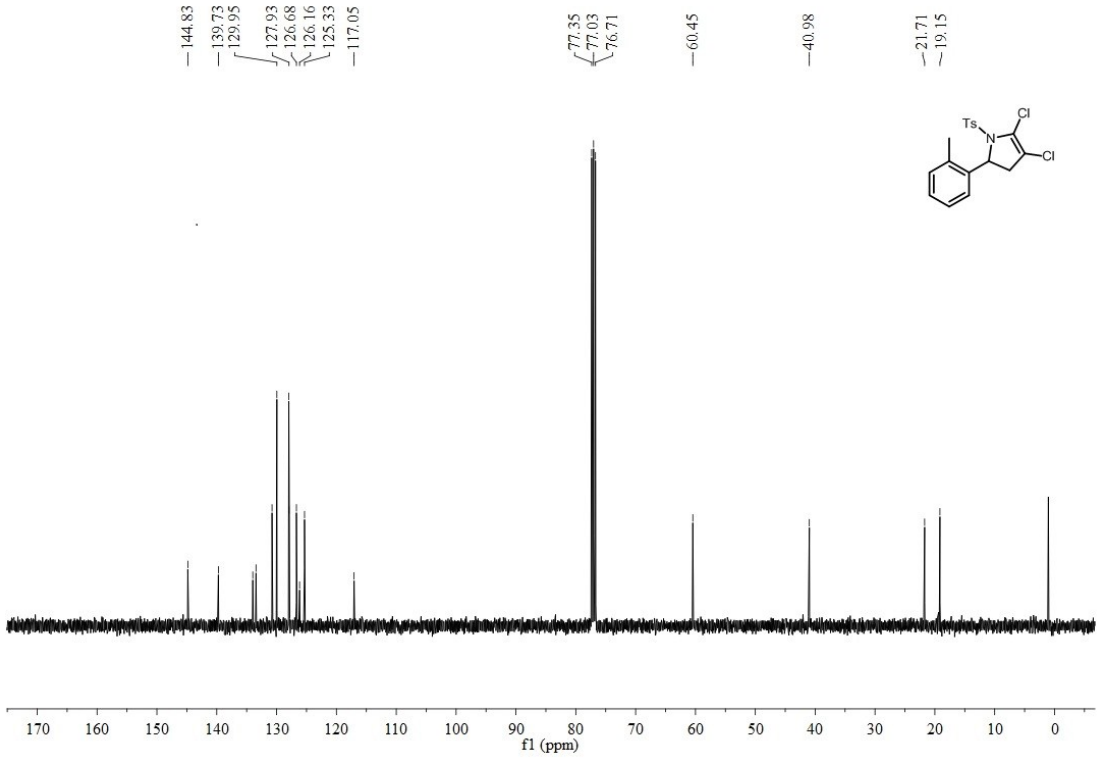
^{1}H, ^{13}C-NMR spectra of **3g**



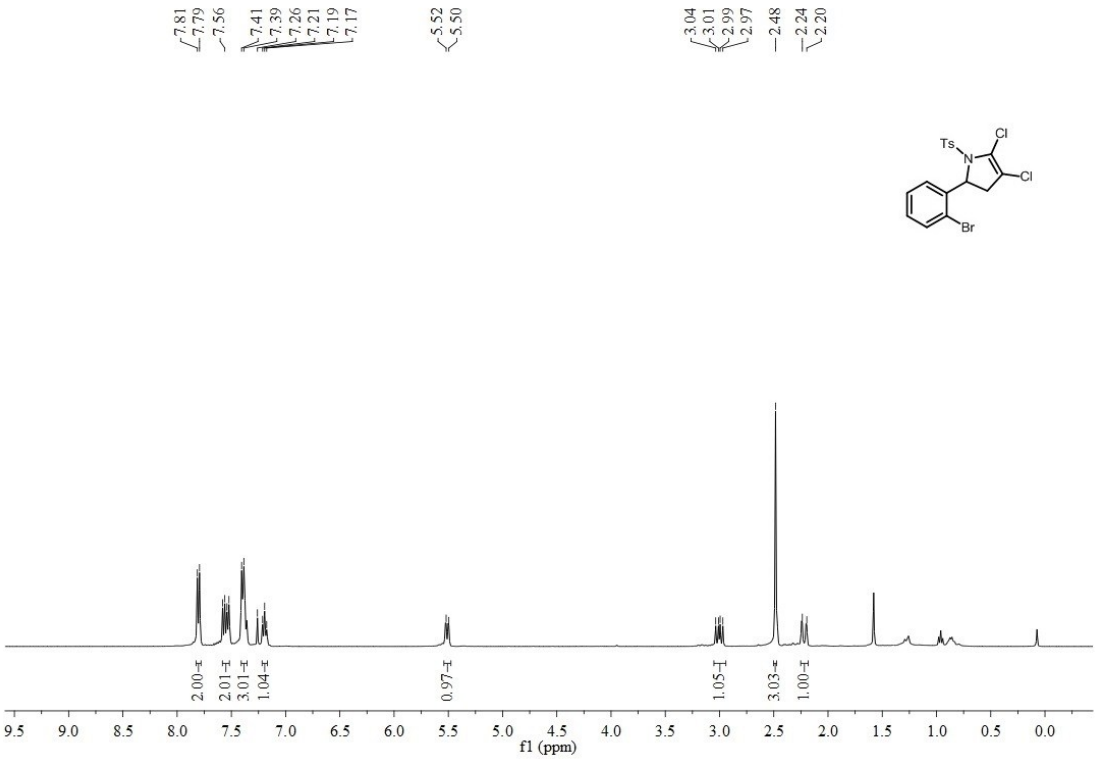


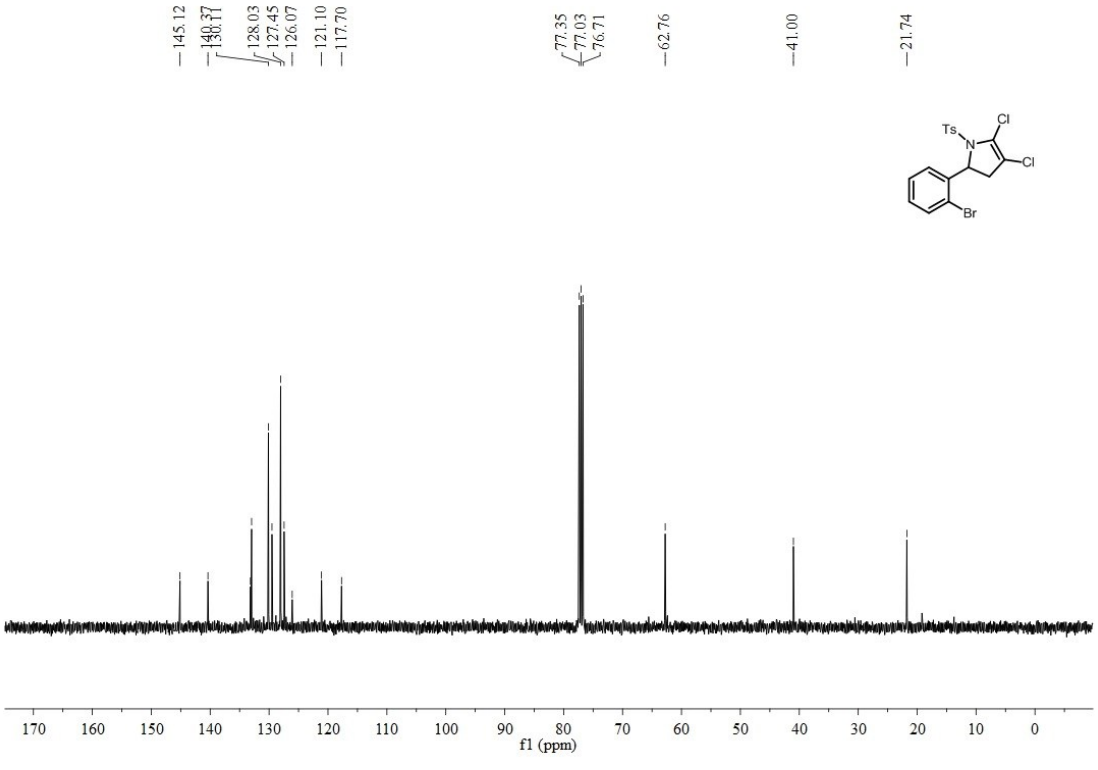
^{1}H, ^{13}C-NMR spectra of **3h**



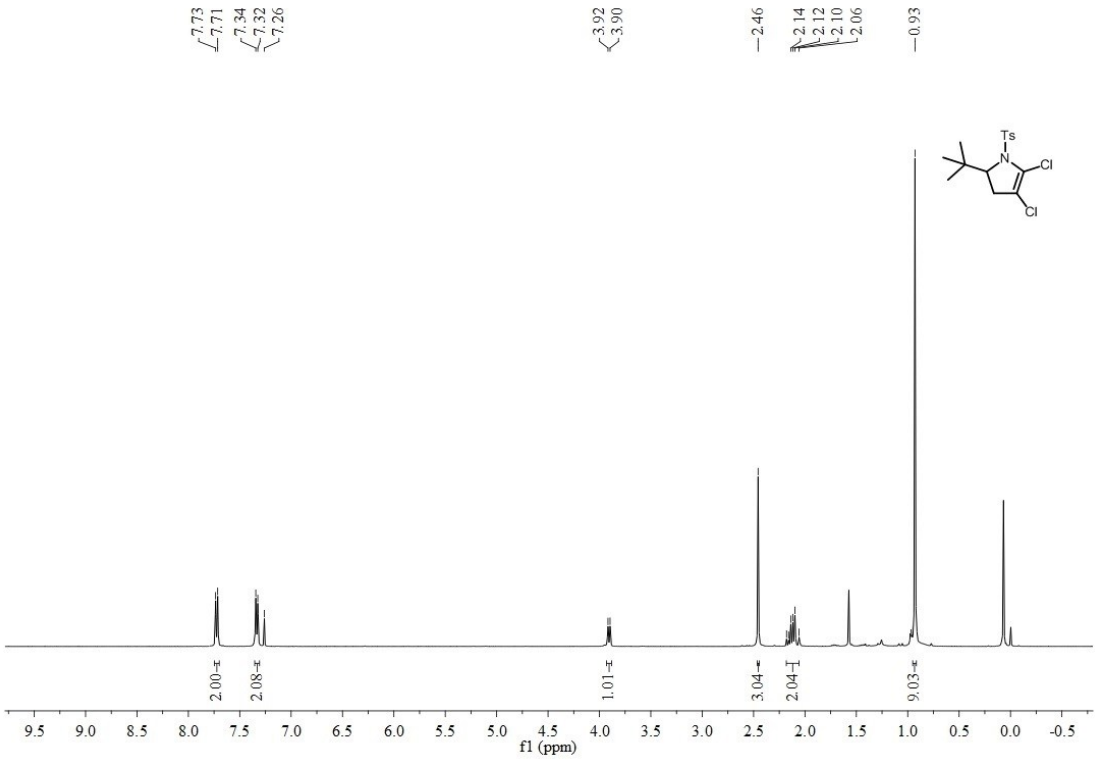


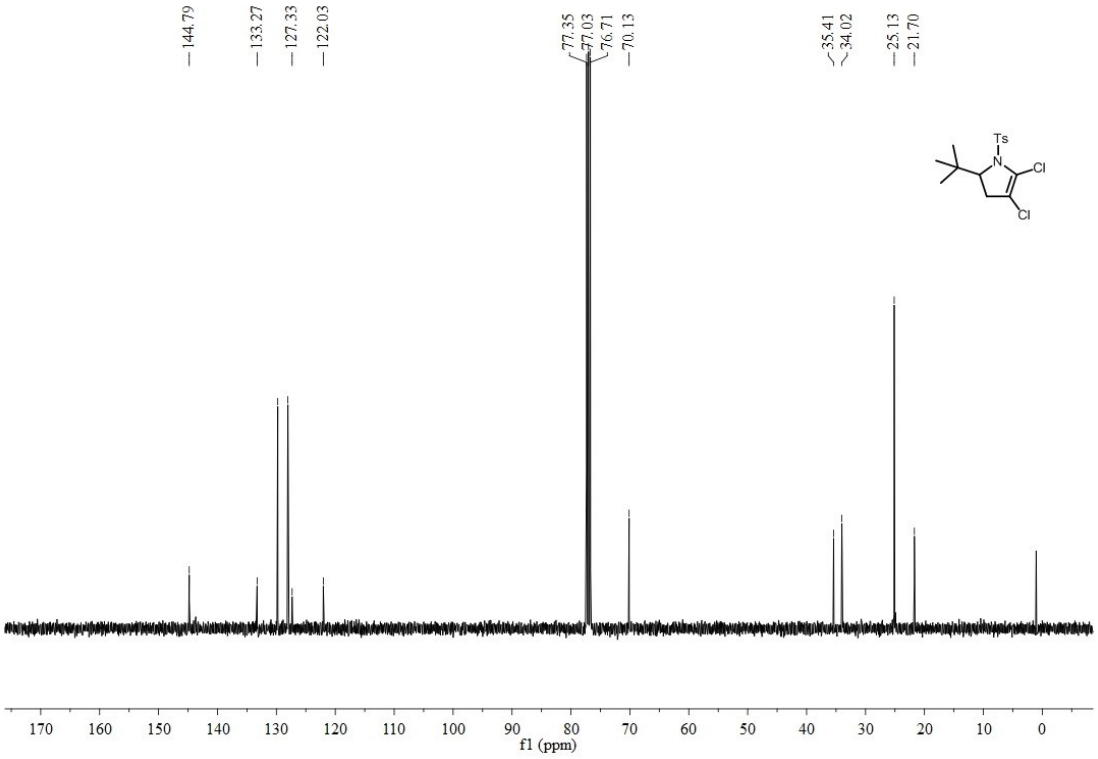
^{1}H, ^{13}C-NMR spectra of **3i**



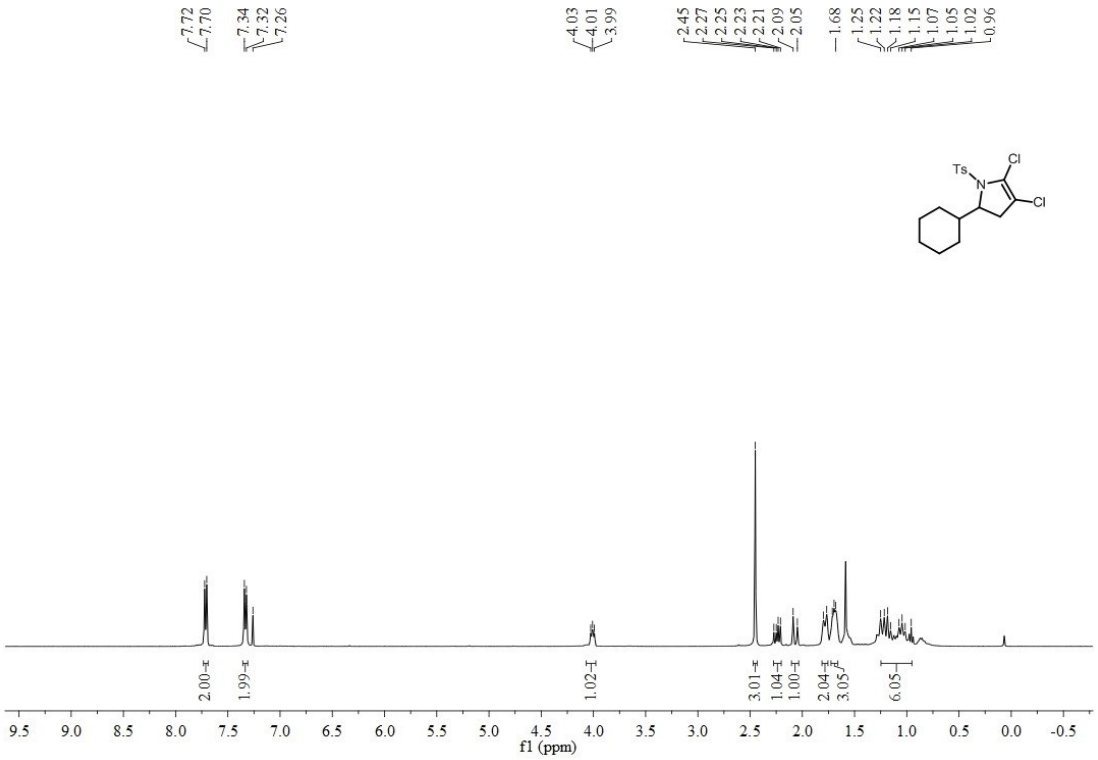


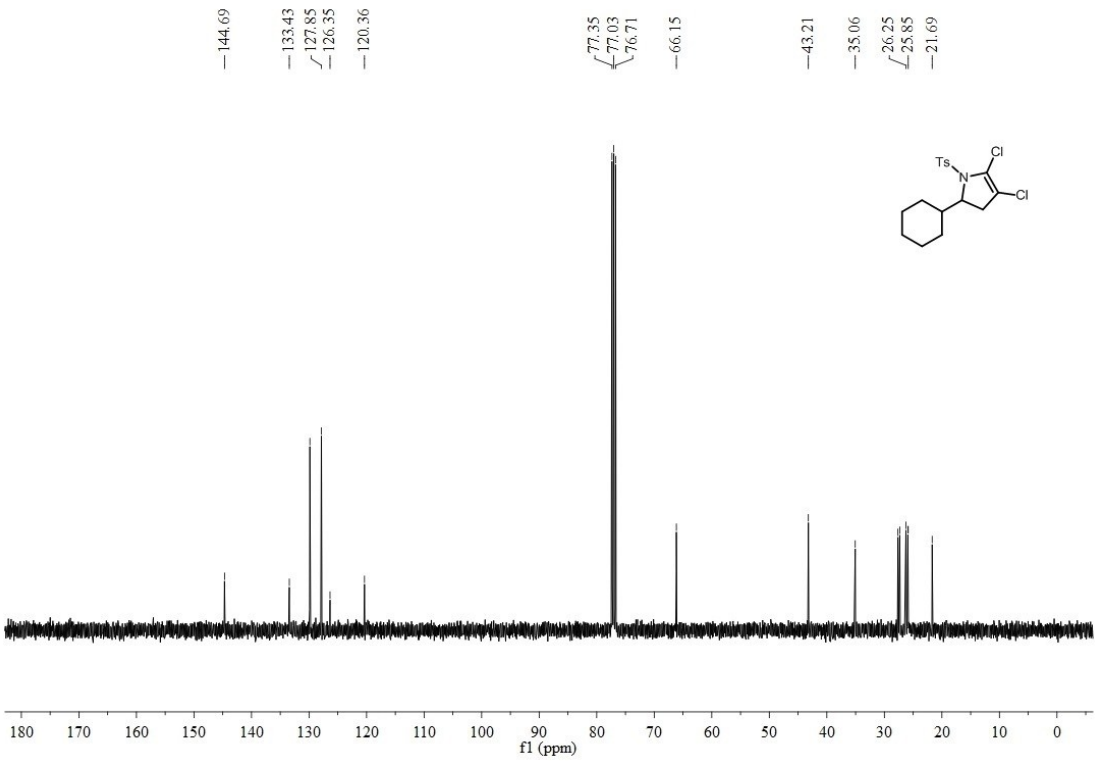
^{1}H, ^{13}C-NMR spectra of **3j**



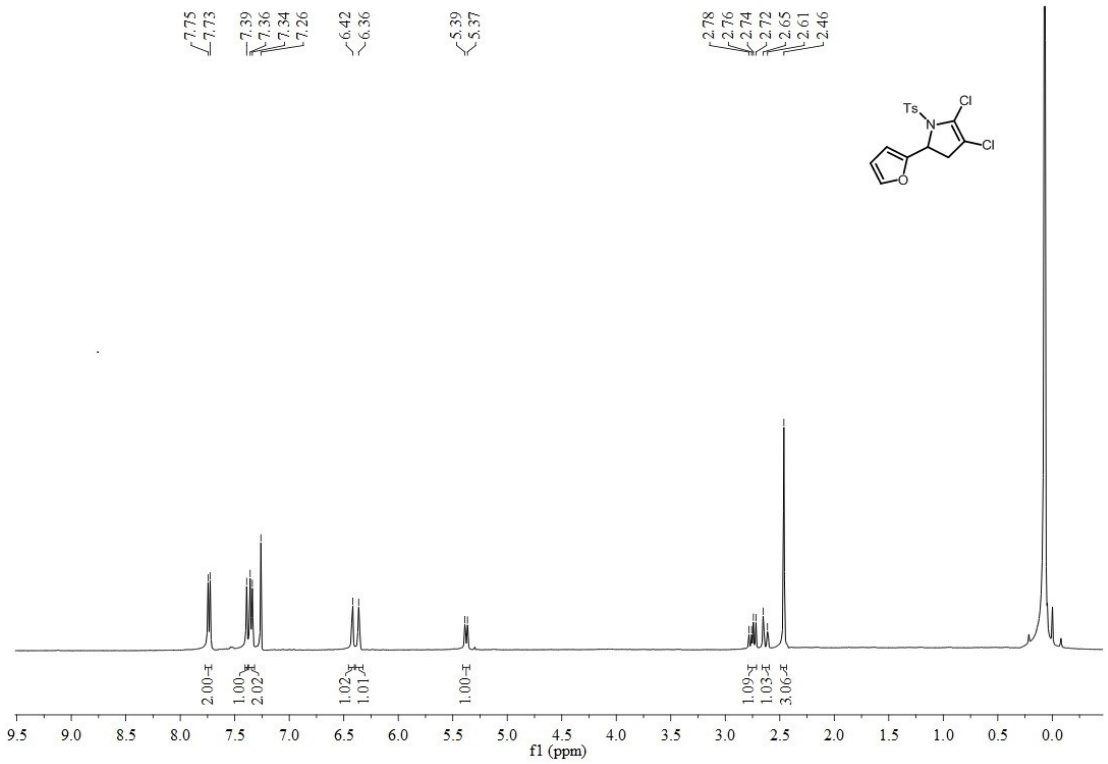


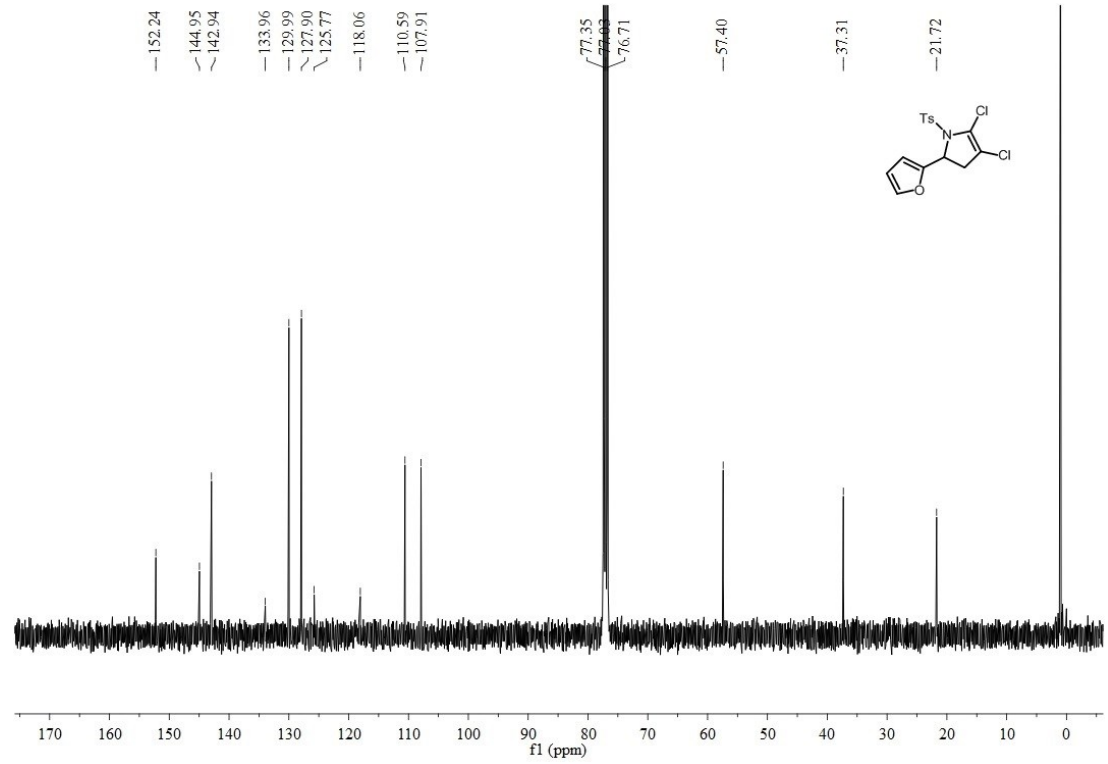
^{1}H, ^{13}C-NMR spectra of **3k**



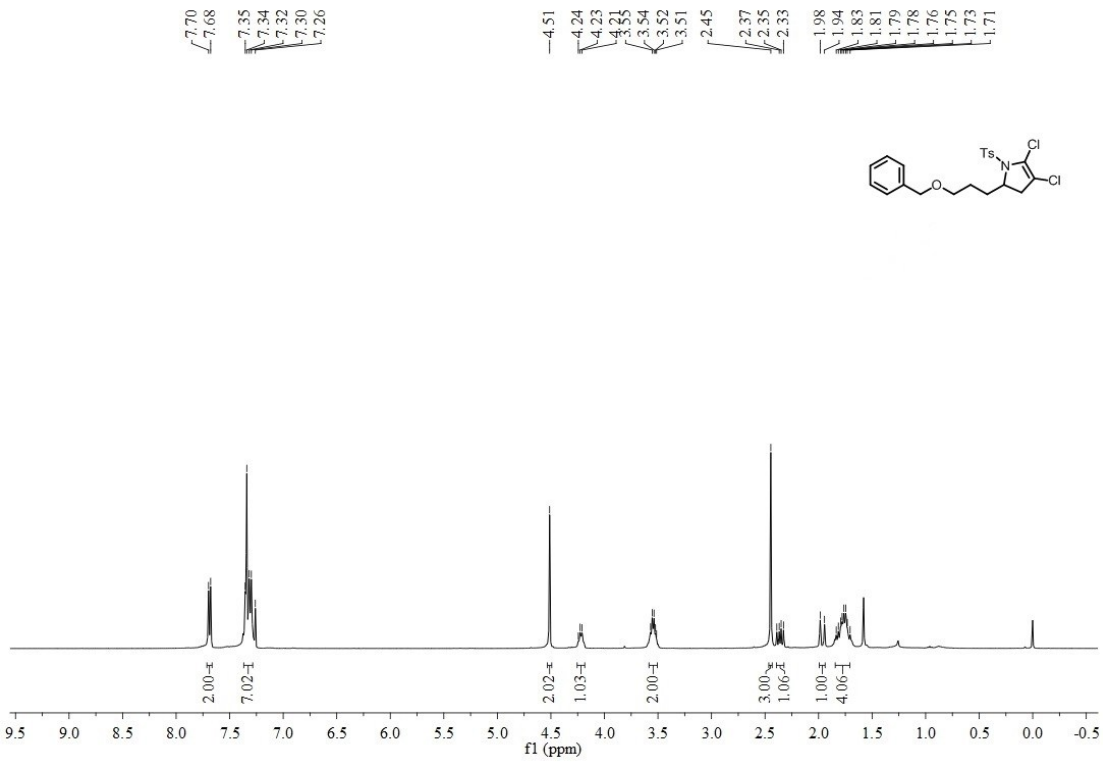


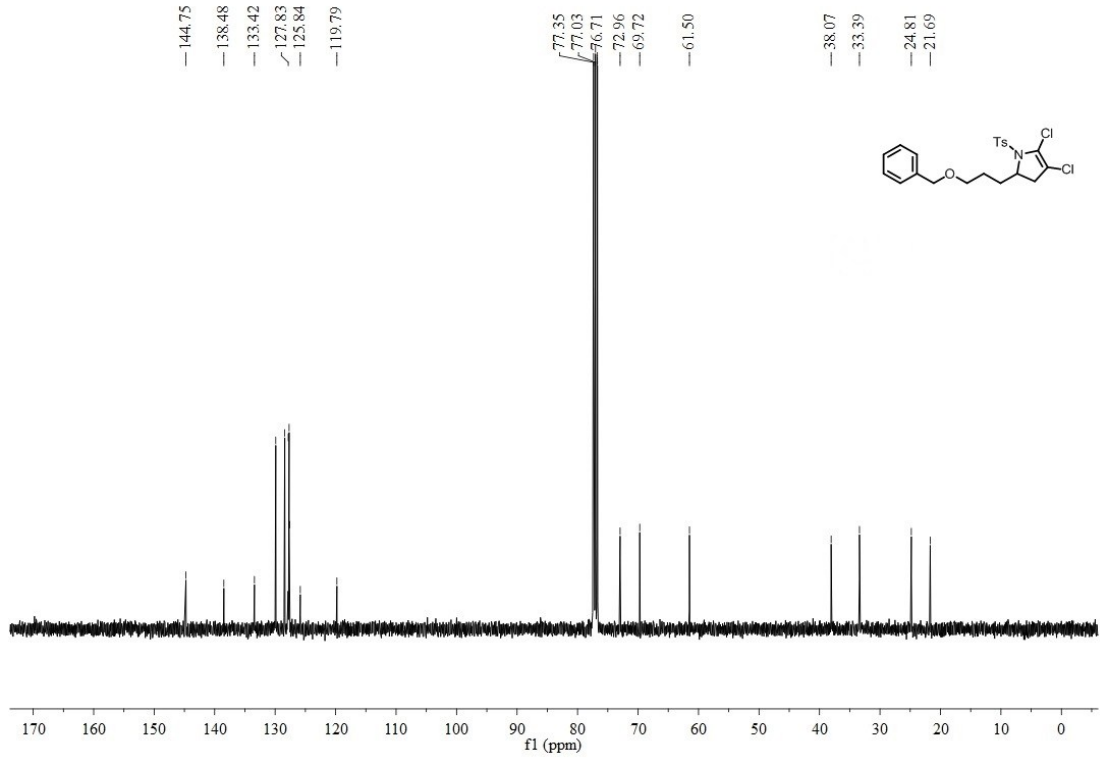
^{1}H, ^{13}C-NMR spectra of **3l**



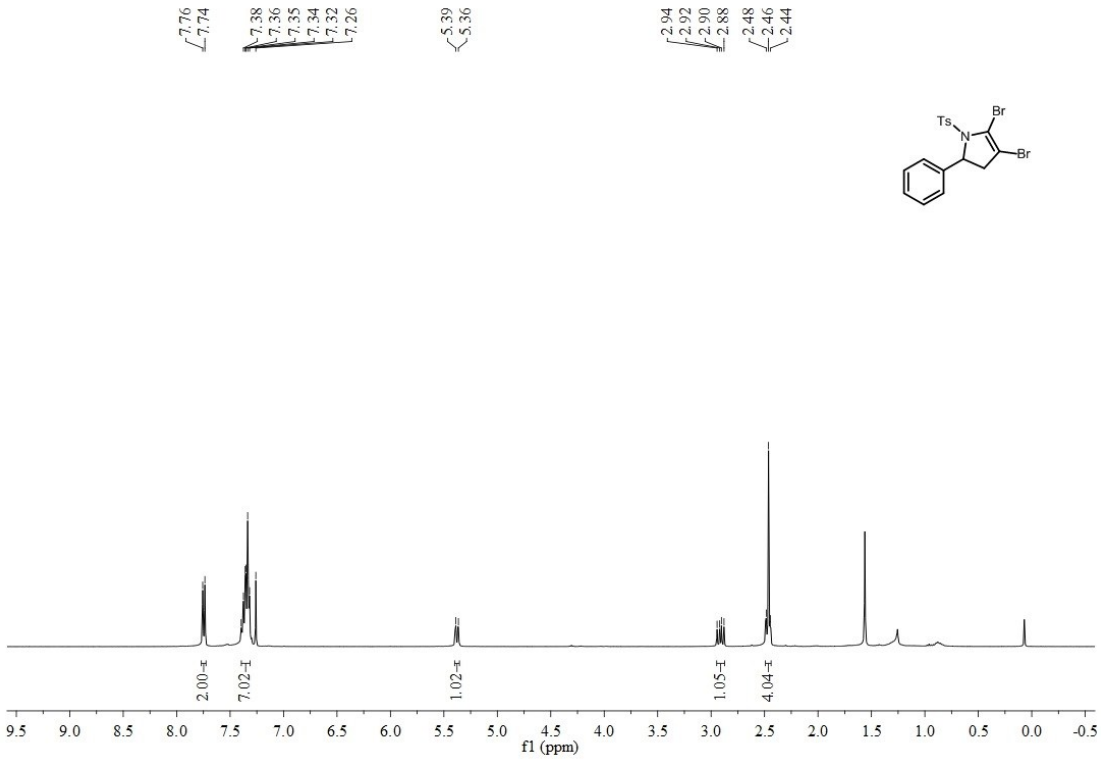


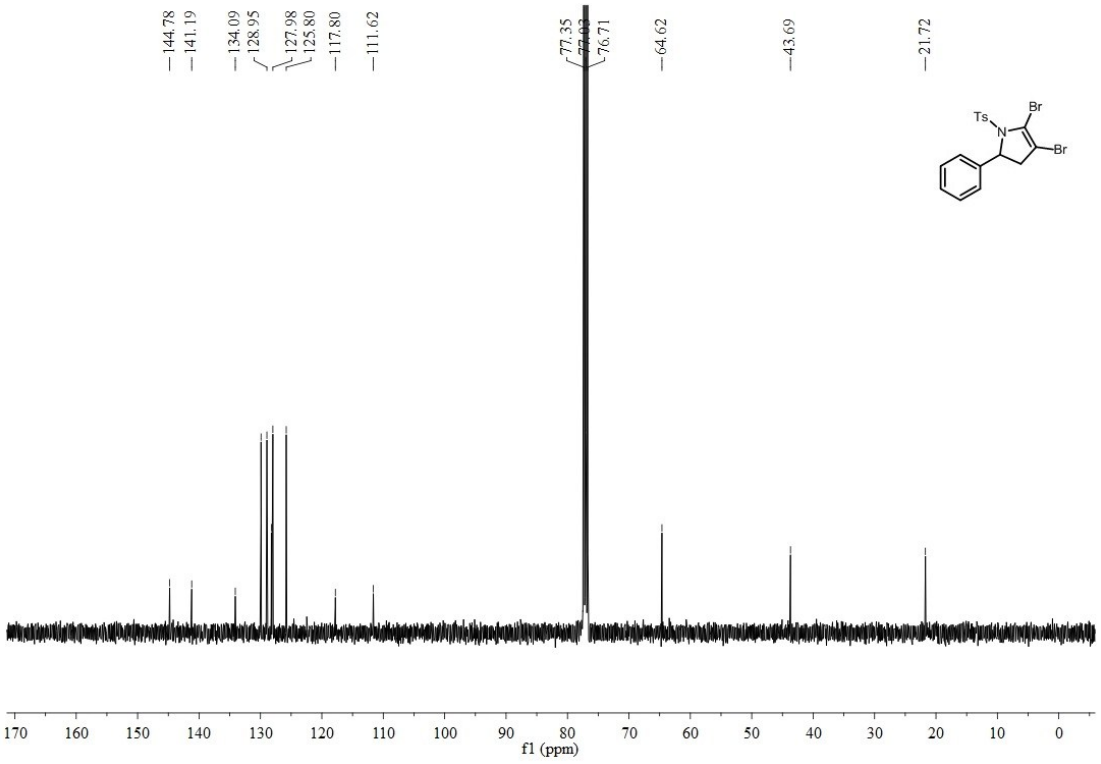
^{1}H, ^{13}C-NMR spectra of **3m**



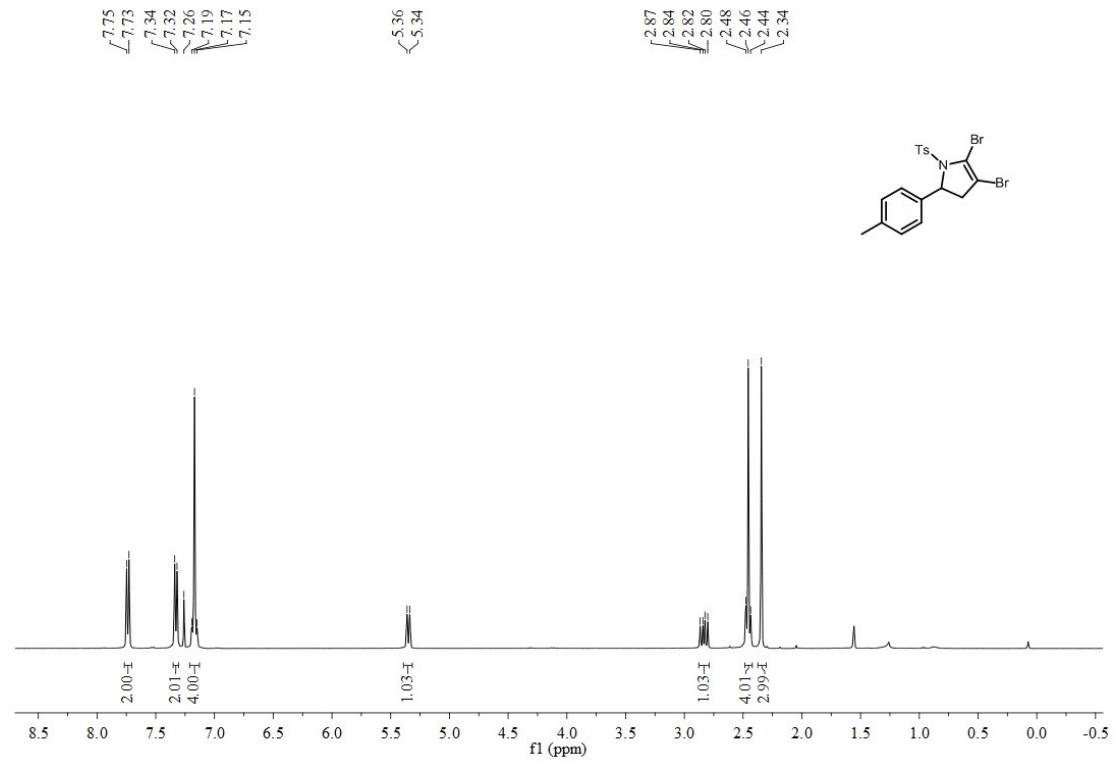


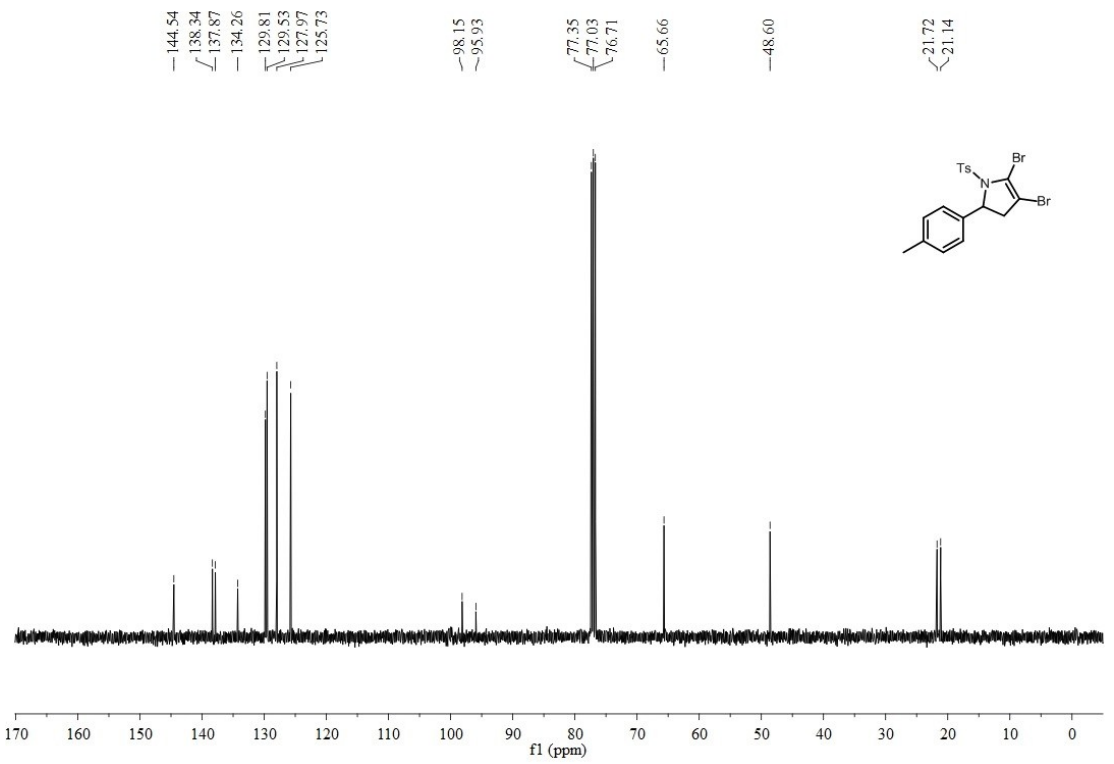
^{1}H, ^{13}C-NMR spectra of **4a**



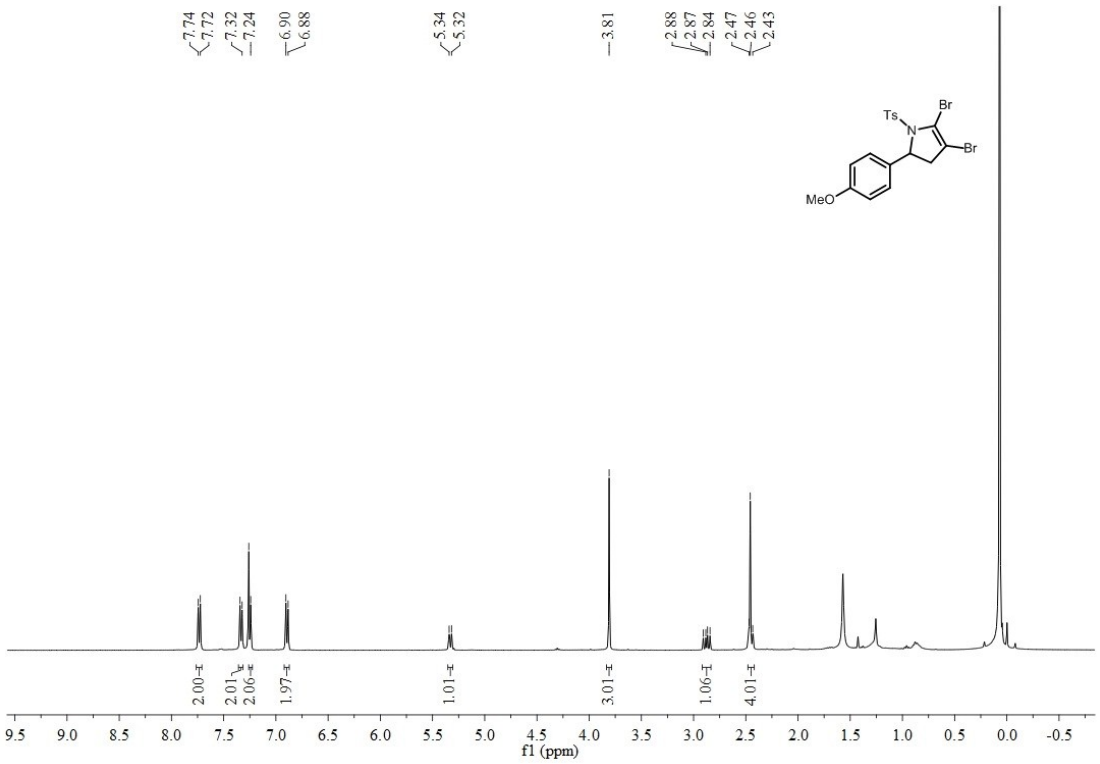


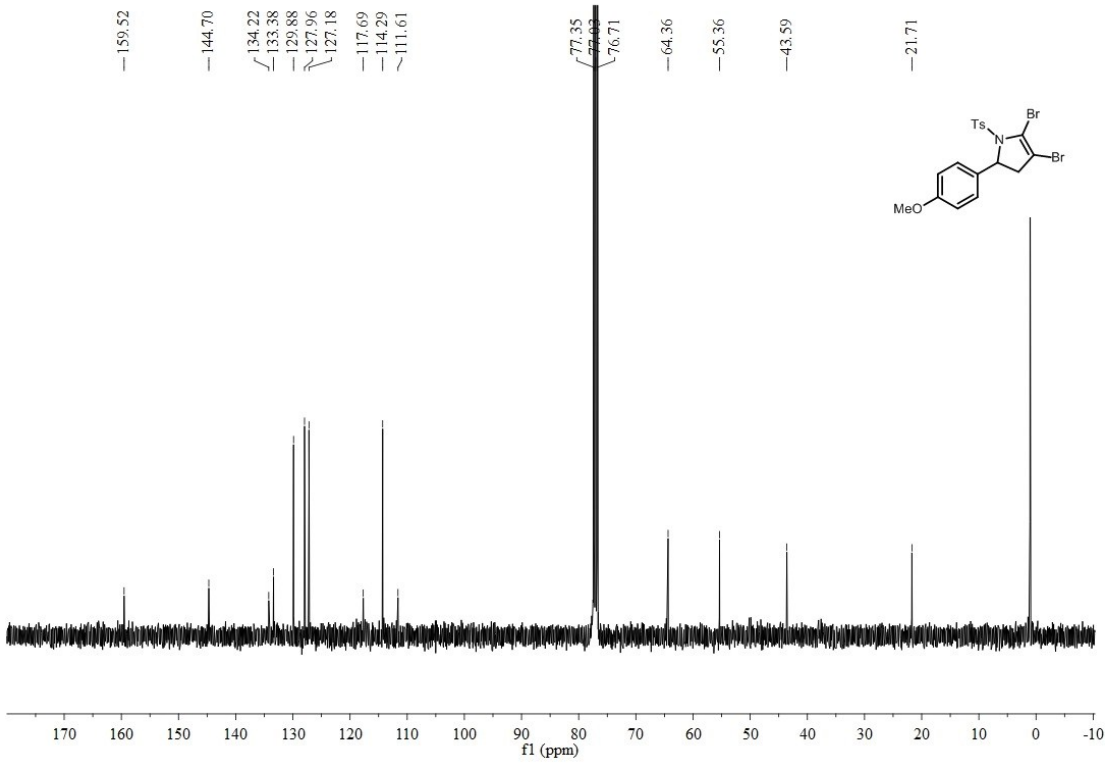
^{1}H, ^{13}C-NMR spectra of **4b**



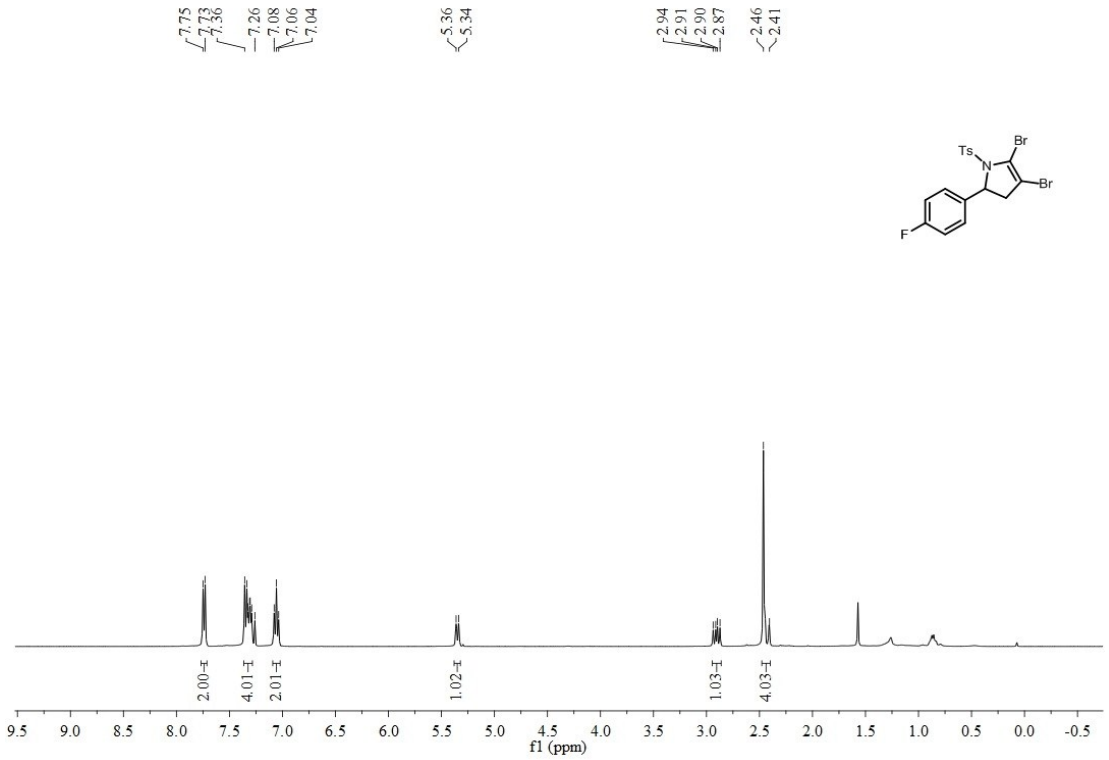


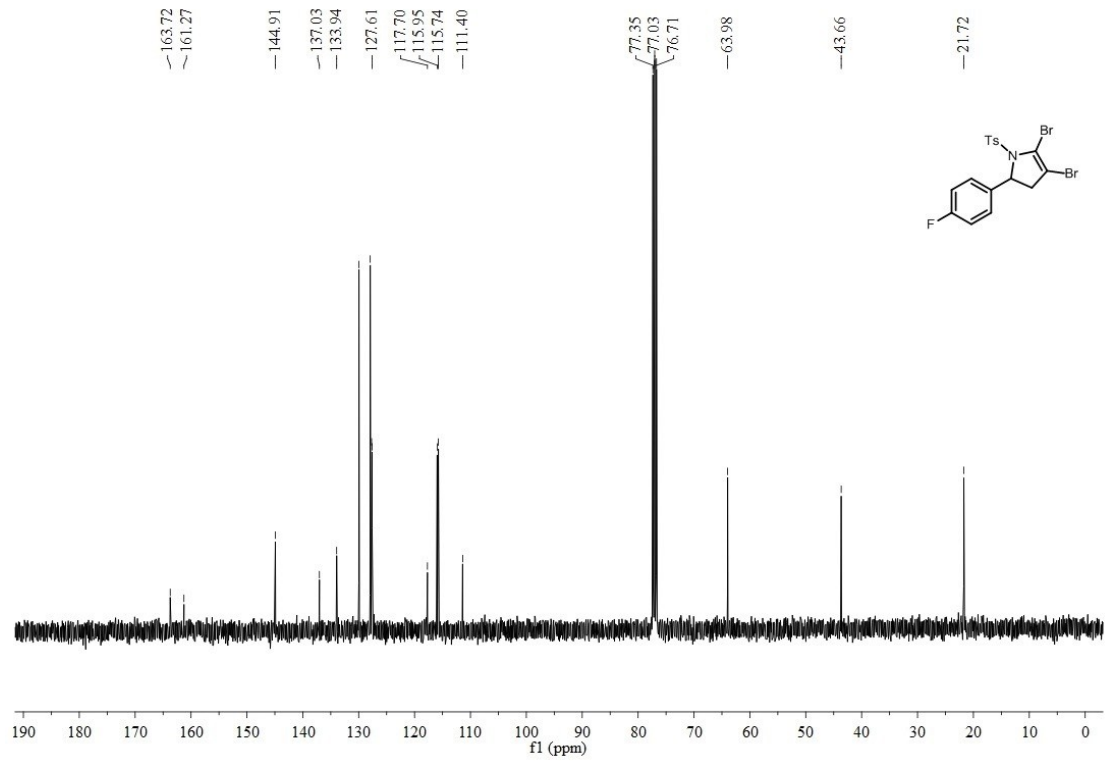
^{1}H, ^{13}C-NMR spectra of **4c**



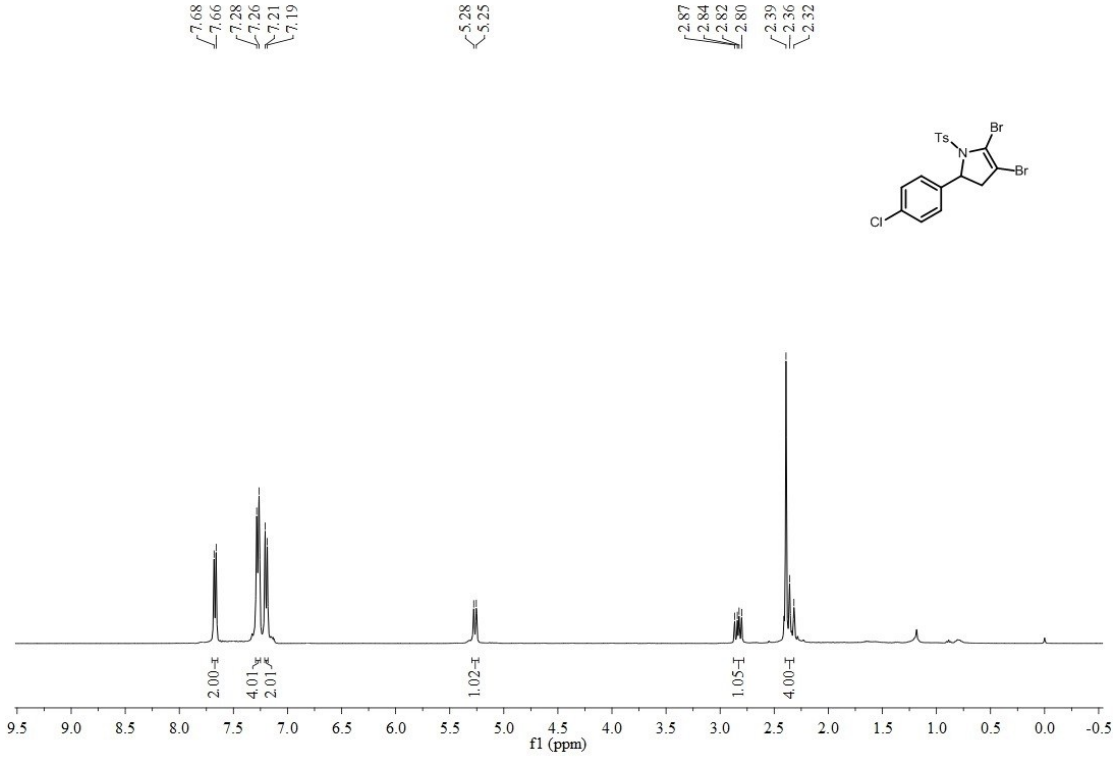


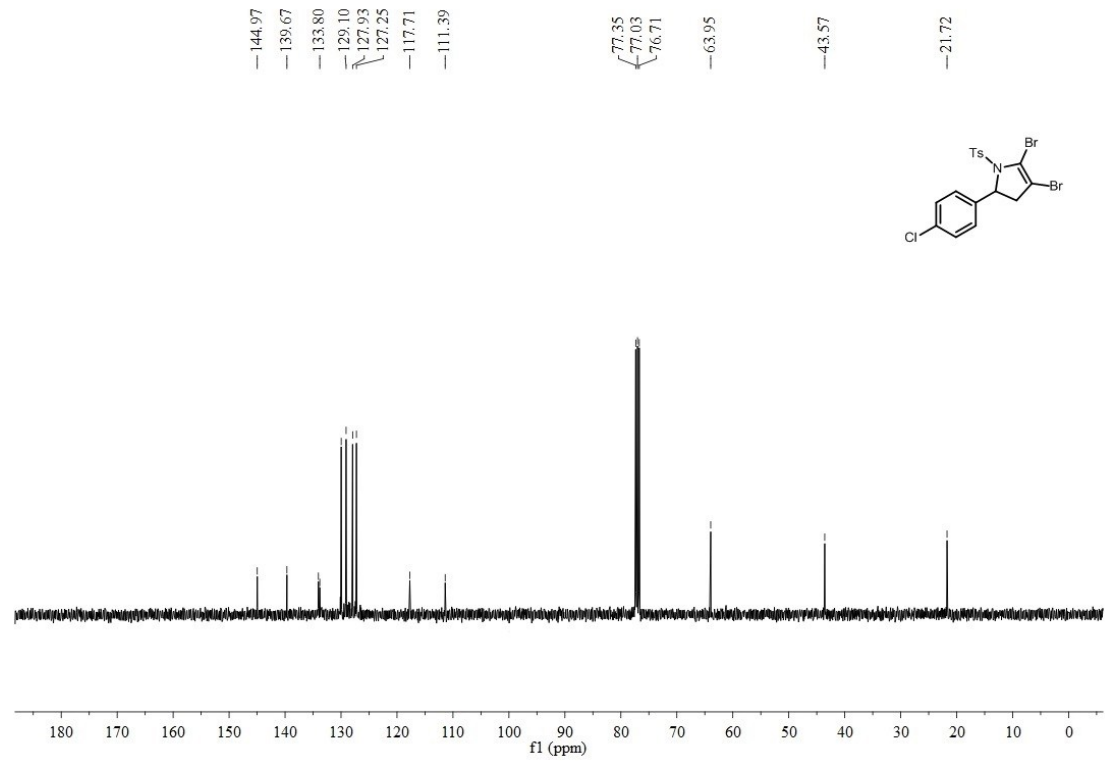
^{1}H, ^{13}C-NMR spectra of **4d**



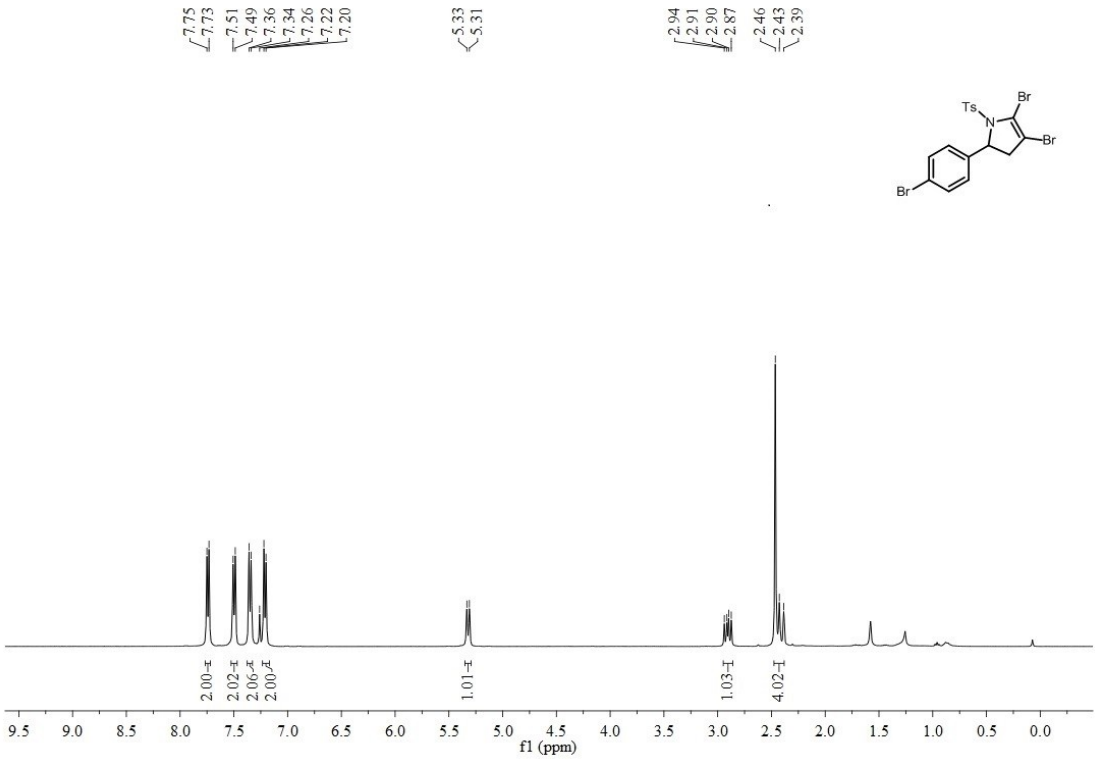


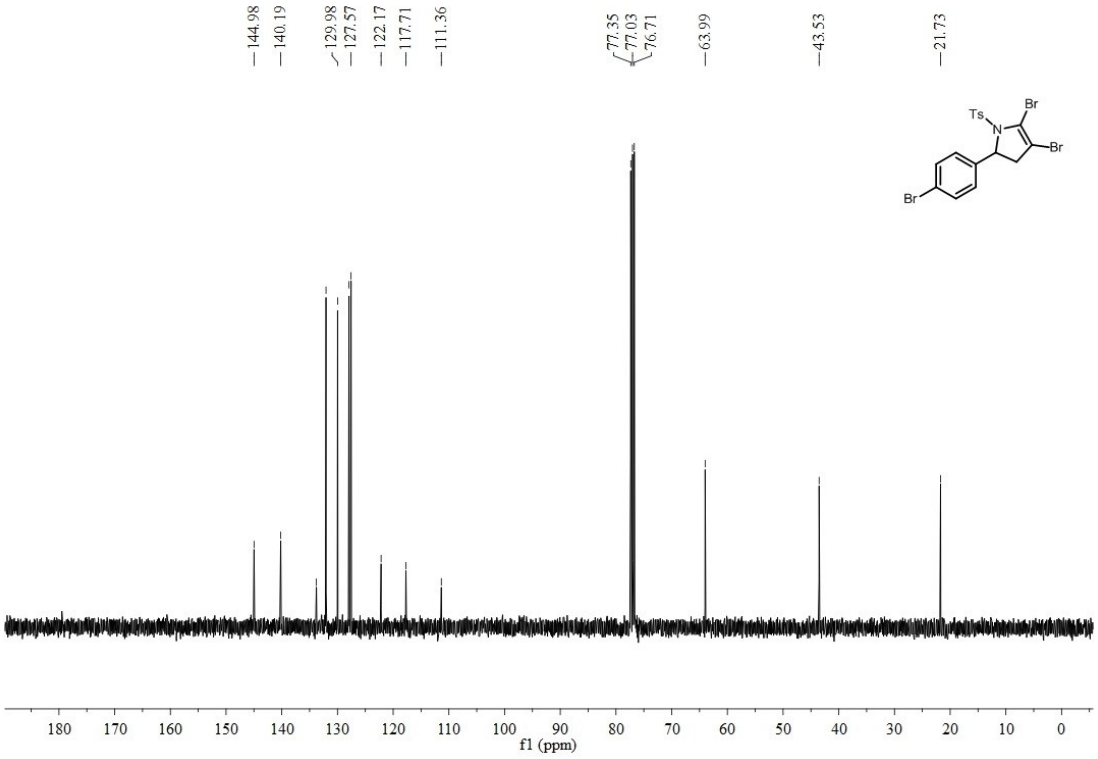
^{1}H, ^{13}C-NMR spectra of **4e**



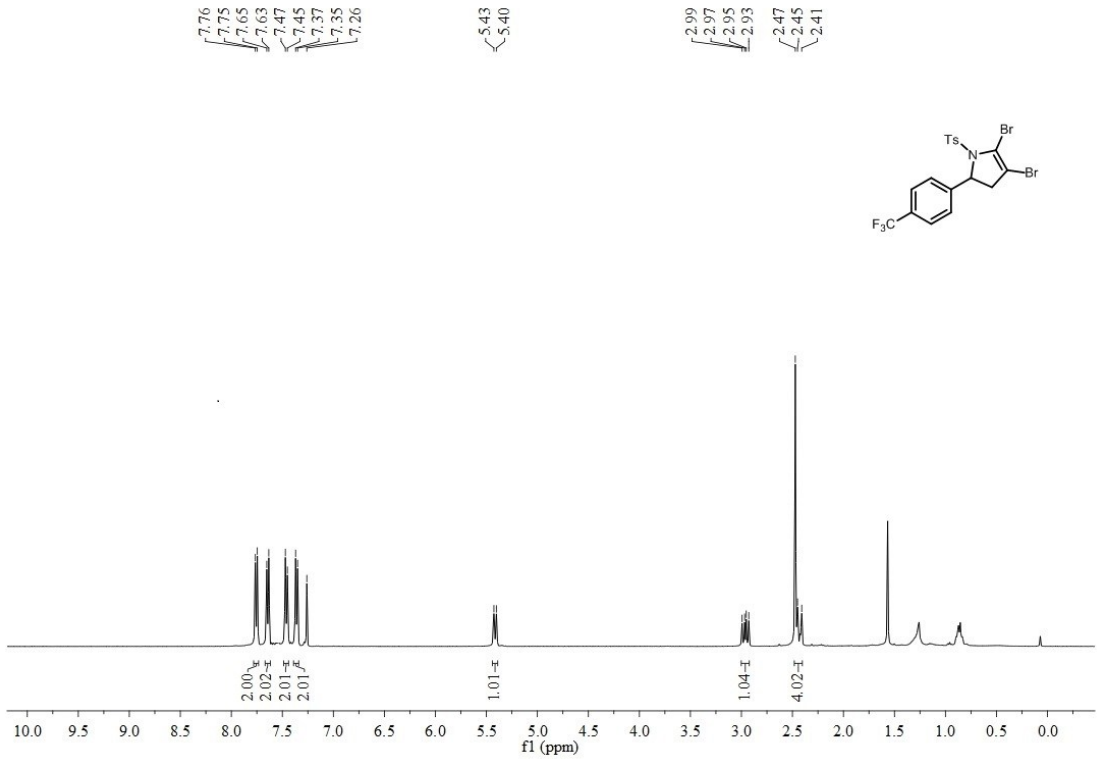


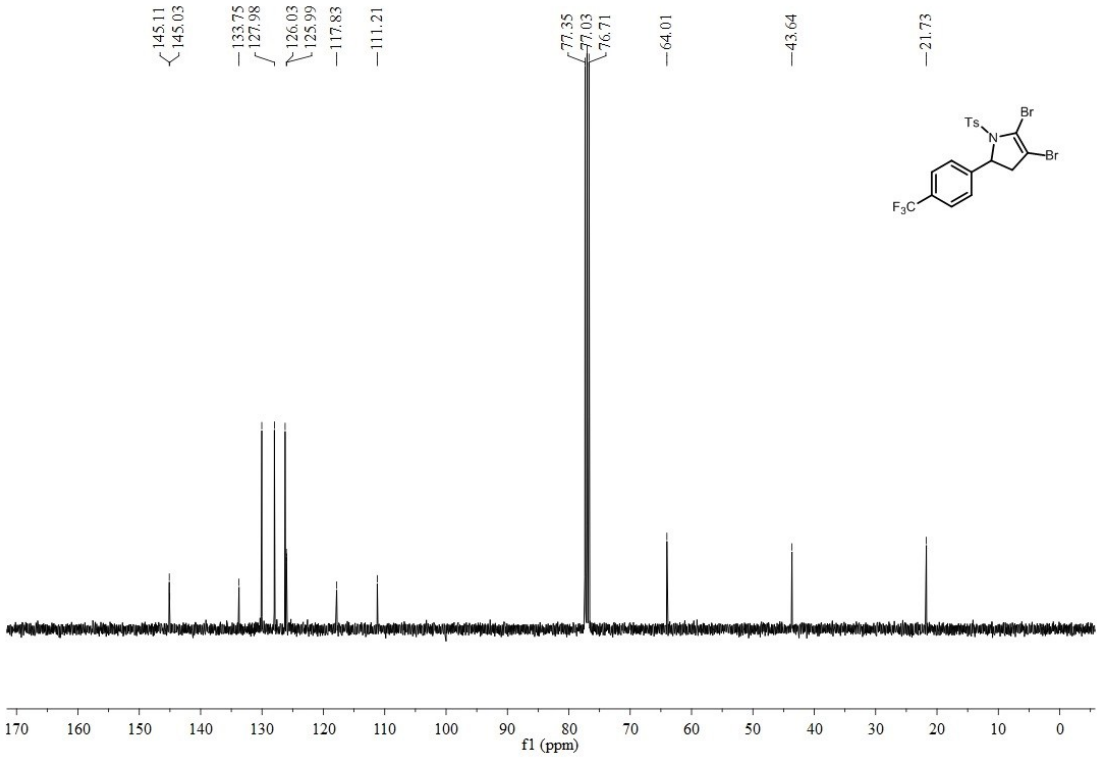
^{1}H, ^{13}C-NMR spectra of **4f**



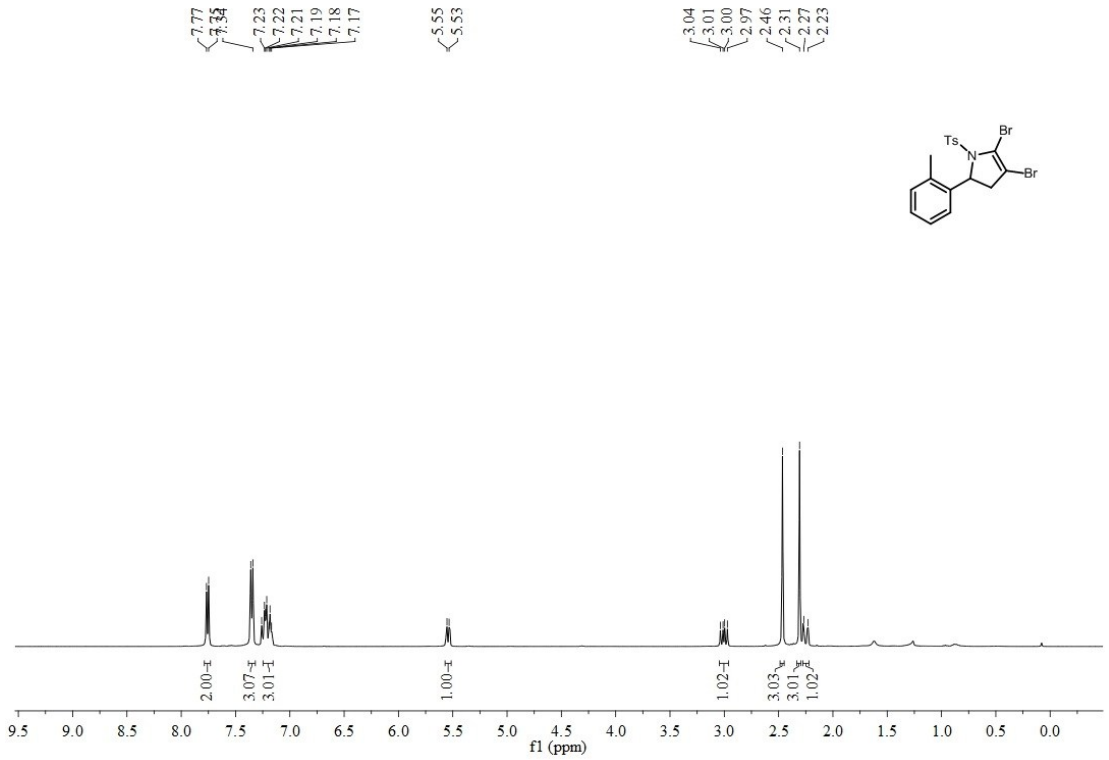


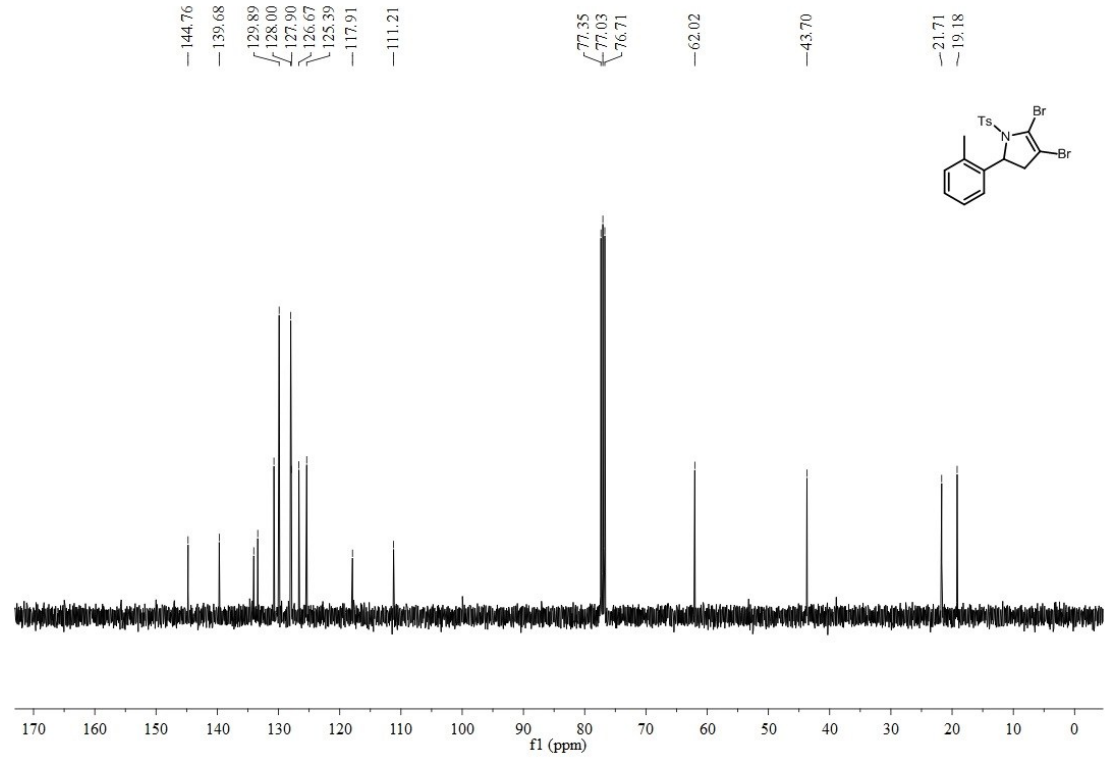
^{1}H, ^{13}C-NMR spectra of **4g**



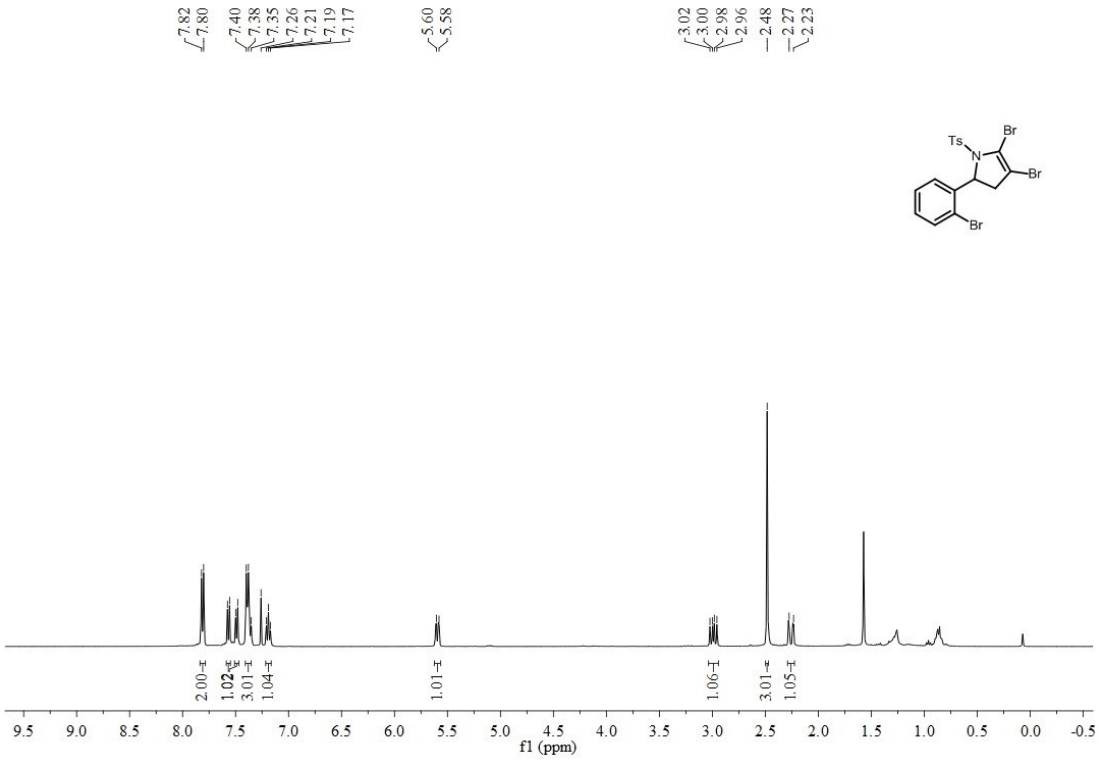


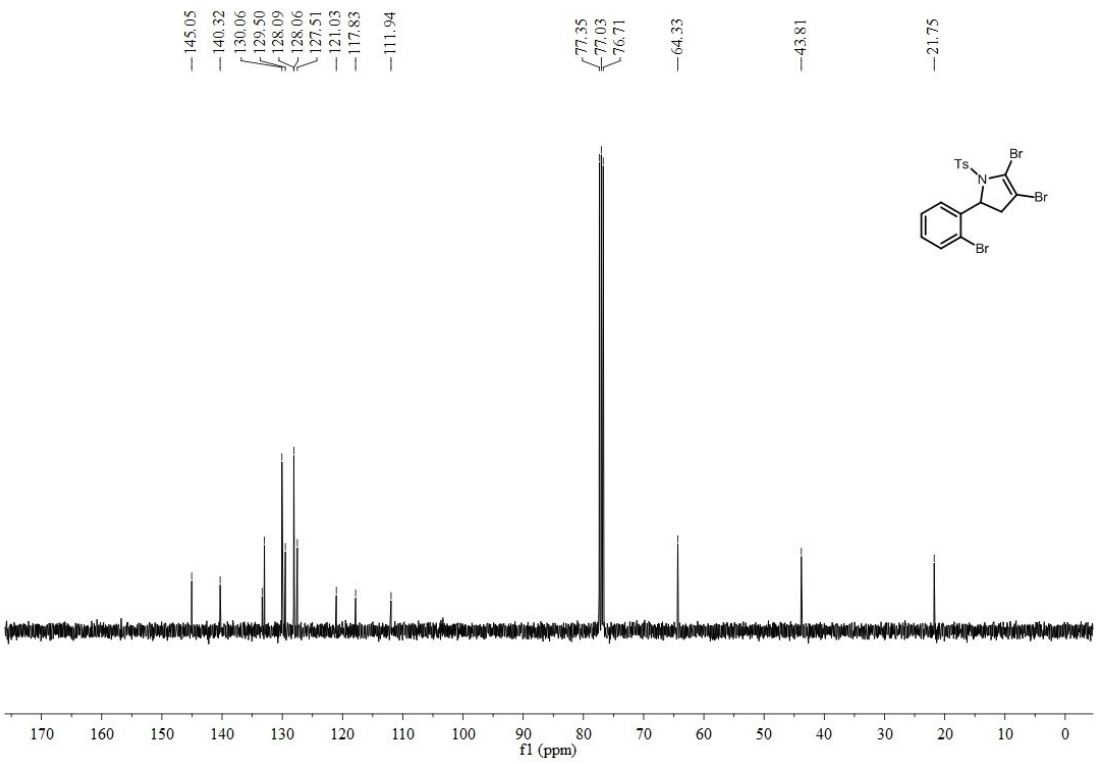
^{1}H, ^{13}C-NMR spectra of **4h**



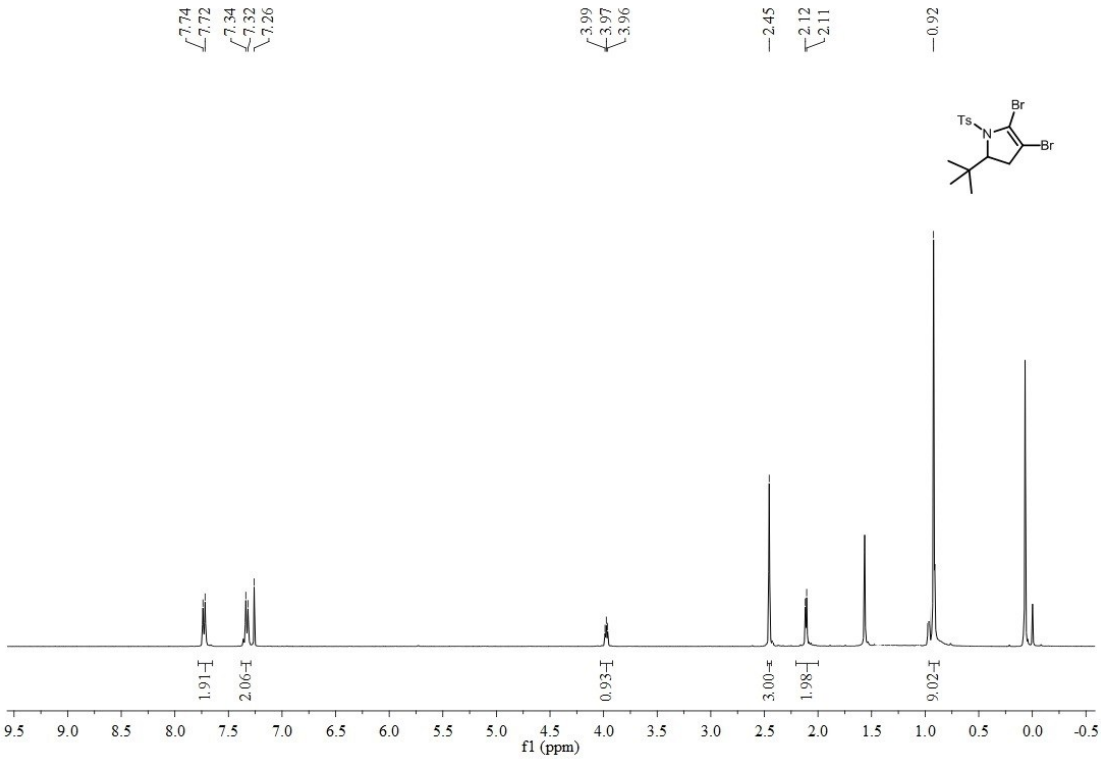


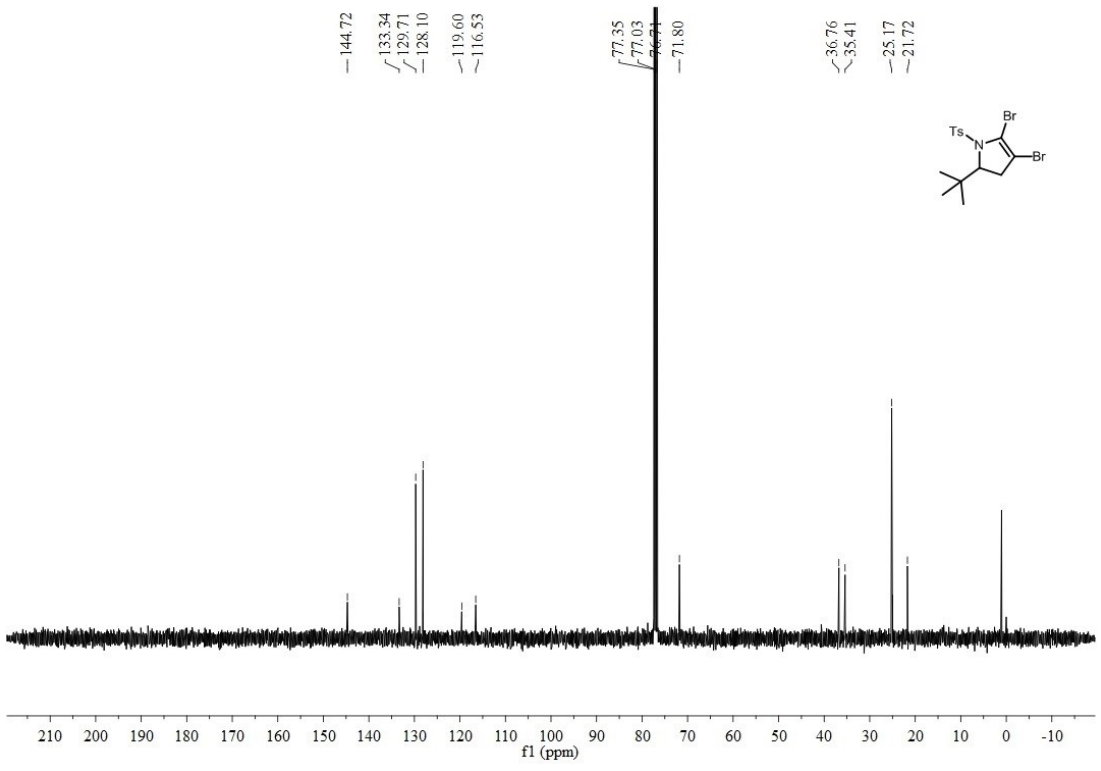
^{1}H, ^{13}C-NMR spectra of **4i**



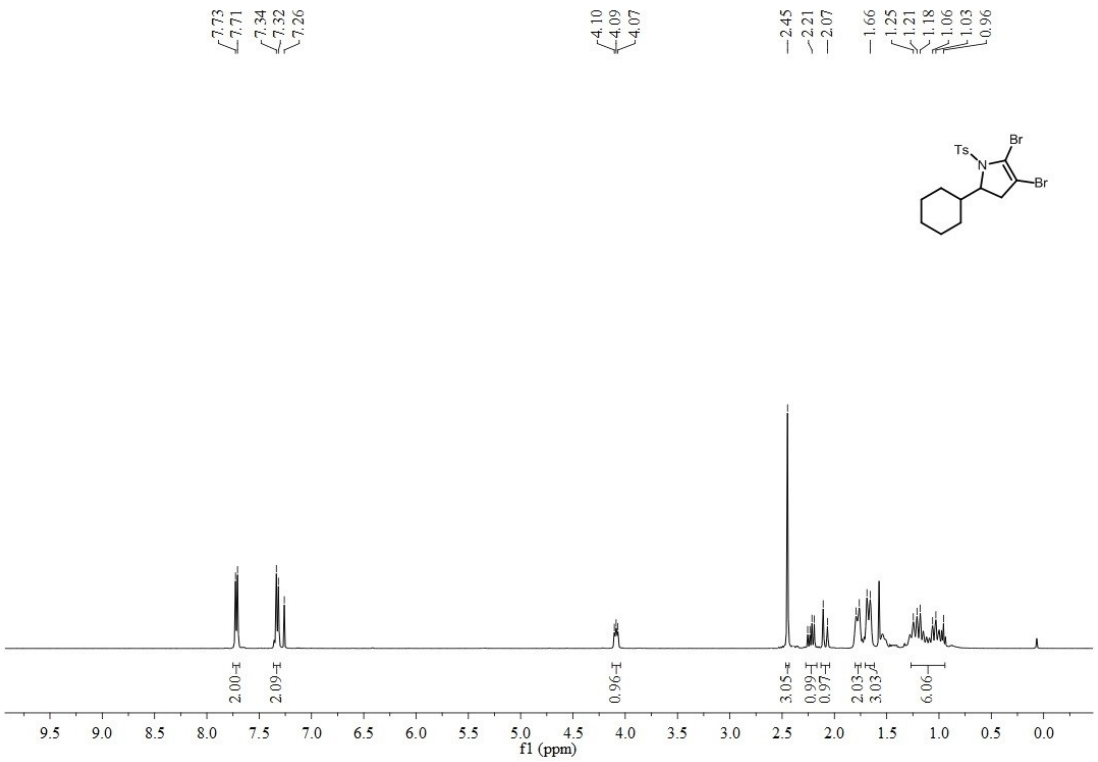


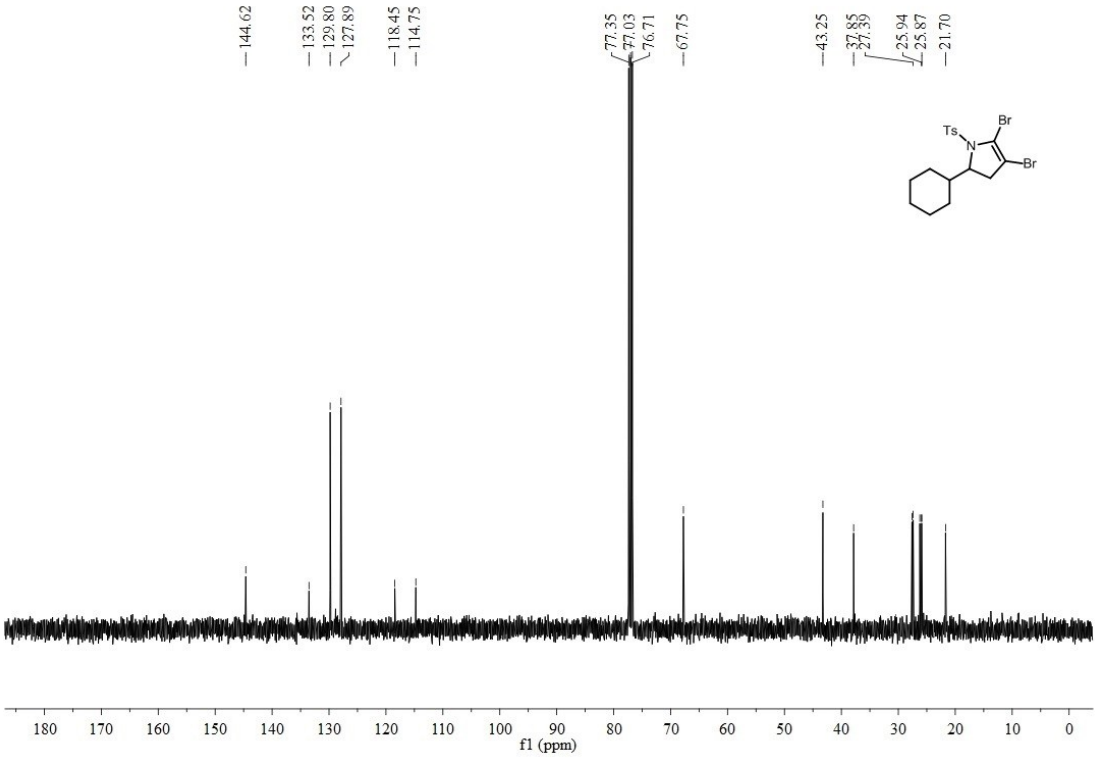
^{1}H, ^{13}C-NMR spectra of **4j**



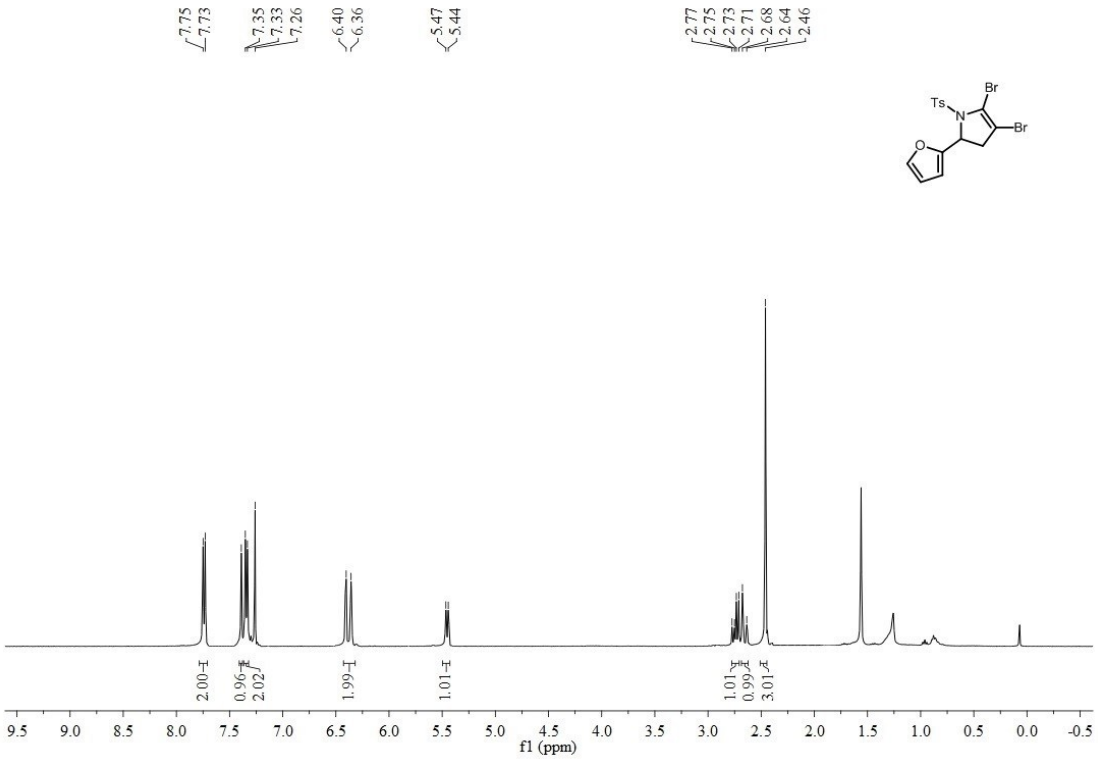


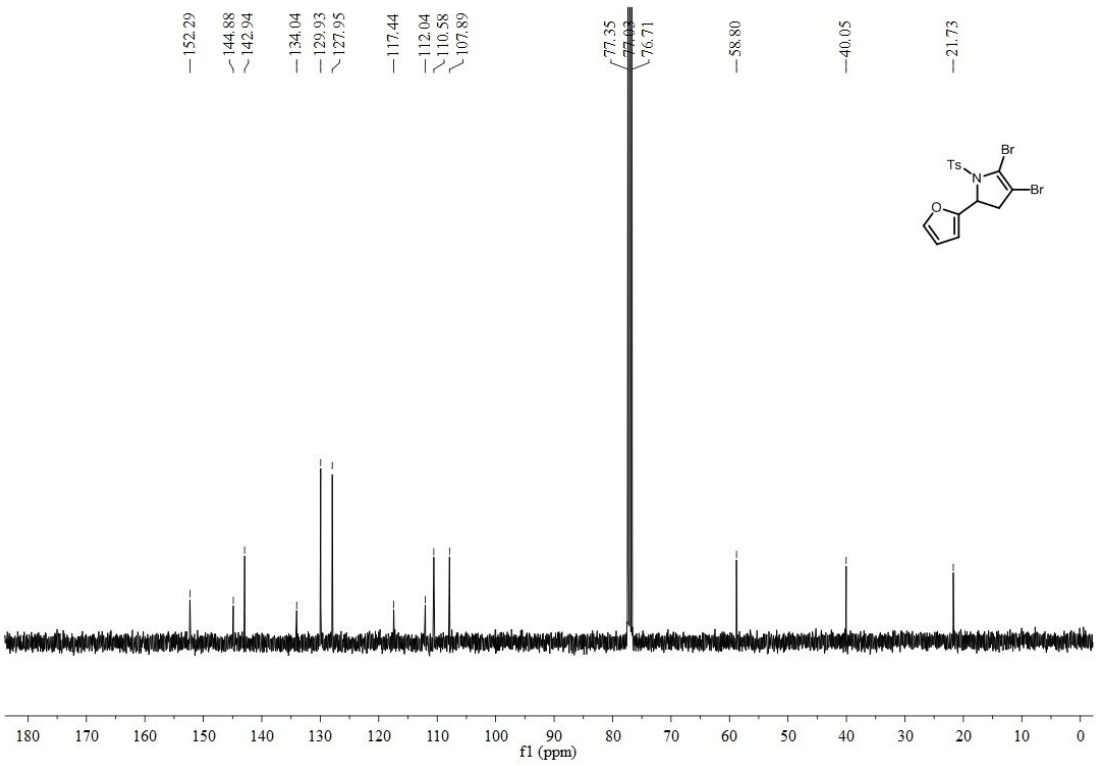
^{1}H, ^{13}C-NMR spectra of **4k**



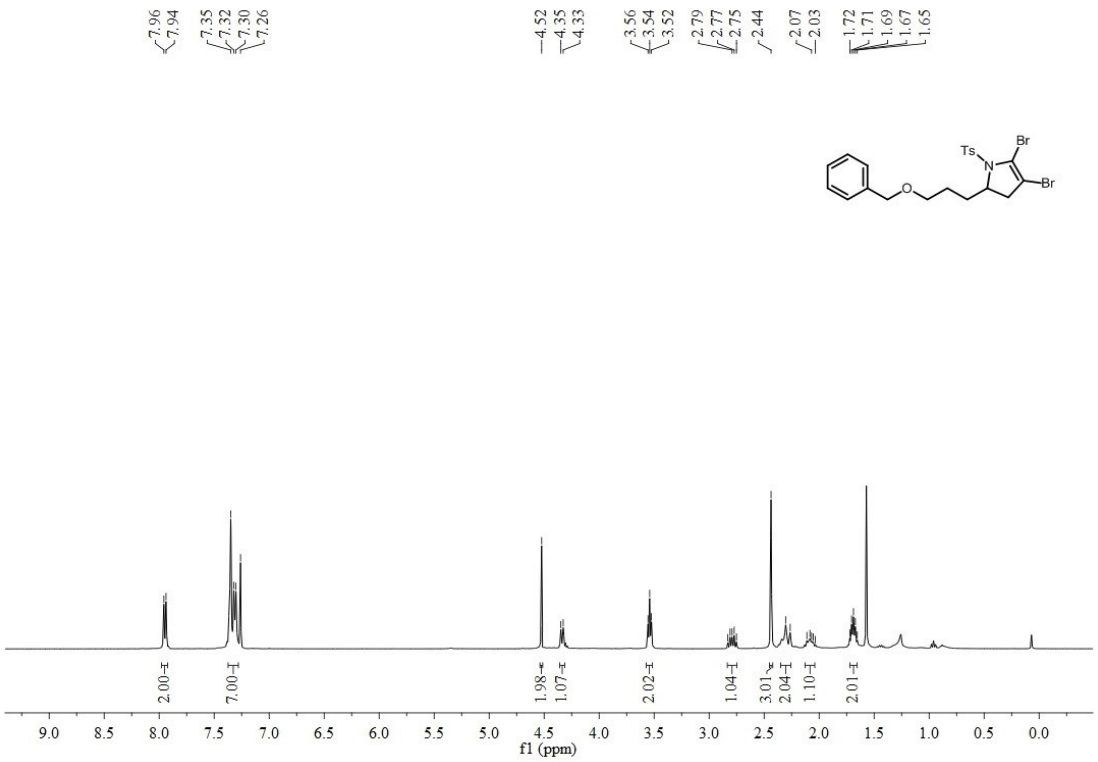


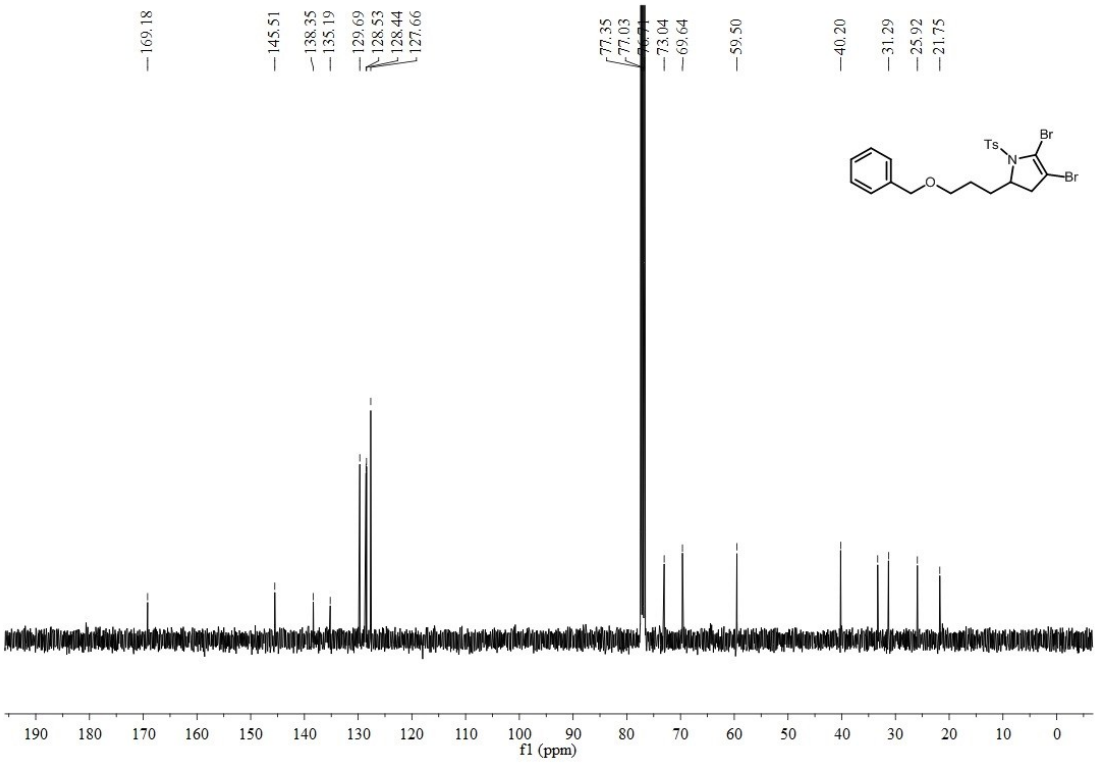
^{1}H, ^{13}C-NMR spectra of **4l**



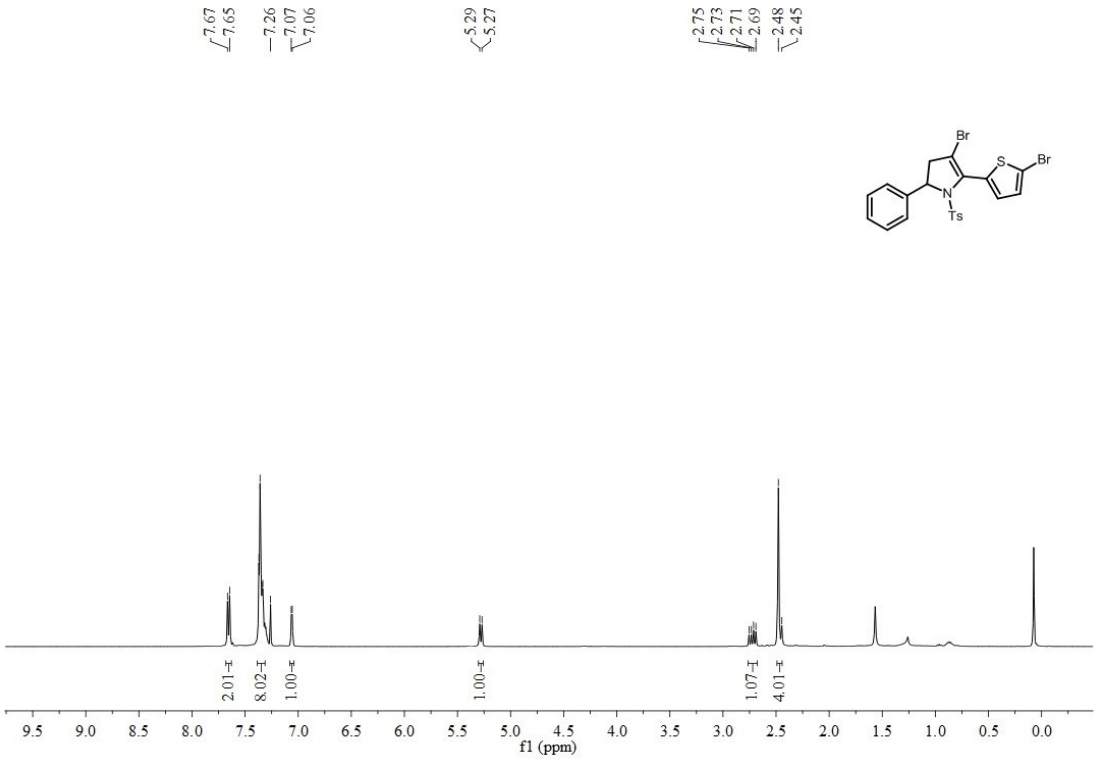


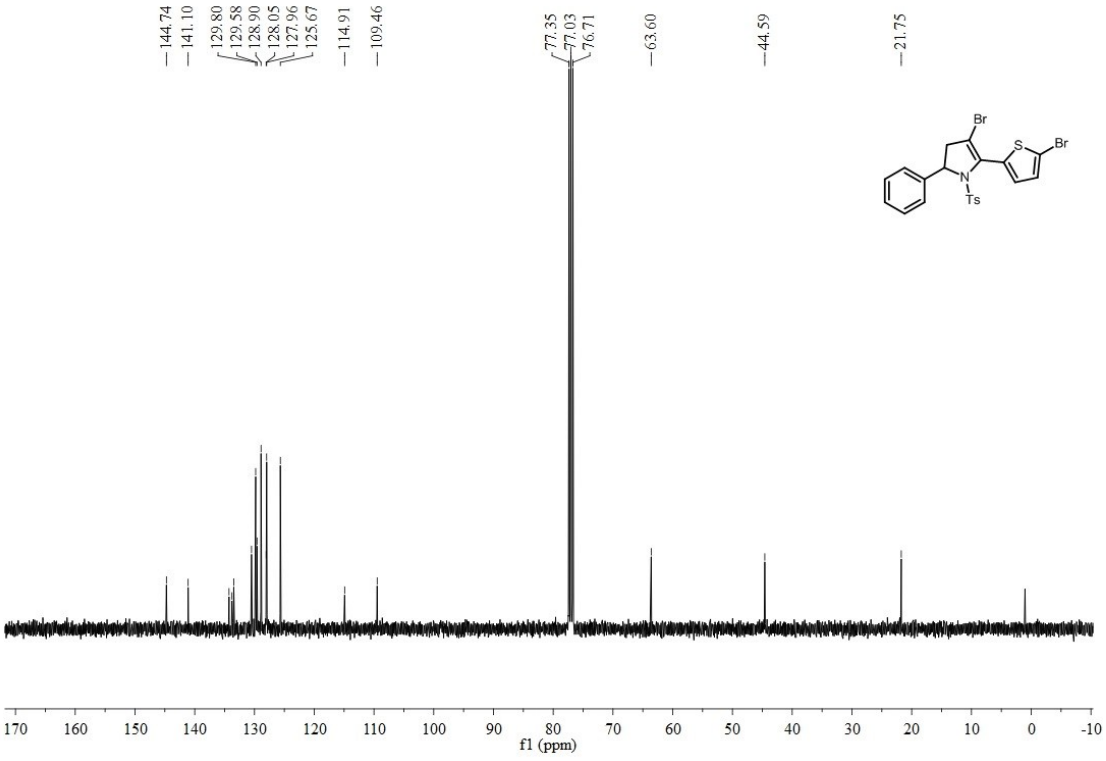
^{1}H, ^{13}C-NMR spectra of **4m**





^{1}H, ^{13}C-NMR spectra of **4o**





5. Crystallographic spectrum for 2j

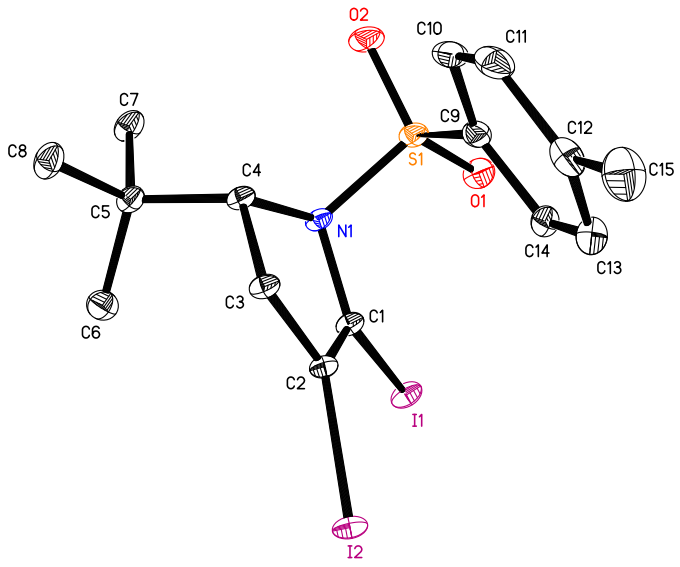


Table 1. Crystal data and structure refinement for **2j**

Identification code	2	
Empirical formula	C15 H19 I2 N O2 S	
Formula weight	531.17	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 9.5678(5) Å	α= 90°.
	b = 12.3013(7) Å	β= 101.7100(10)°.
	c = 15.5374(9) Å	γ = 90°.
Volume	1790.64(17) $Å^3$	
Z	4	
Density (calculated)	1.970 Mg/m^3	
Absorption coefficient	3.632 mm^{-1}	
F(000)	1016	
Crystal size	0.25 x 0.2 x 0.18 mm^3	
Theta range for data collection	2.129 to 30.568°.	
Index ranges	-12<=h<=13, -11<=k<=17, -21<=l<=22	
Reflections collected	17910	
Independent reflections	5504 [R(int) = 0.0199]	
Completeness to theta = 25.242°	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6718
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5504 / 0 / 194
Goodness-of-fit on F^2	1.098
Final R indices [I>2sigma(I)]	R1 = 0.0214, wR2 = 0.0511
R indices (all data)	R1 = 0.0257, wR2 = 0.0527
Extinction coefficient	n/a
Largest diff. peak and hole	0.492 and -1.116 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_dm15079_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	6812(1)	998(1)	2336(1)	24(1)
I(2)	3879(1)	3108(1)	2326(1)	22(1)
S(1)	9640(1)	3196(1)	2896(1)	22(1)
O(1)	9793(2)	2131(1)	3268(1)	30(1)
O(2)	10800(2)	3678(1)	2580(1)	31(1)
N(1)	8265(2)	3146(1)	2030(1)	18(1)
C(1)	6978(2)	2668(2)	2202(1)	19(1)
C(2)	5939(2)	3399(2)	2159(1)	18(1)
C(3)	6424(2)	4506(2)	1940(1)	18(1)
C(4)	7834(2)	4257(2)	1638(1)	18(1)
C(5)	7727(2)	4242(2)	635(2)	21(1)
C(6)	6518(2)	3507(2)	170(2)	29(1)
C(7)	9141(2)	3839(2)	435(2)	27(1)
C(8)	7486(3)	5417(2)	313(2)	30(1)
C(9)	9065(2)	4104(2)	3626(2)	23(1)
C(10)	9435(2)	5199(2)	3633(2)	29(1)
C(11)	8792(3)	5918(2)	4112(2)	31(1)
C(12)	7780(3)	5582(2)	4581(2)	31(1)
C(13)	7446(3)	4478(2)	4581(2)	30(1)
C(14)	8077(2)	3734(2)	4106(2)	25(1)
C(15)	7058(3)	6379(2)	5084(2)	43(1)

Table 3. Bond lengths [Å] and angles [°] for mo_dm15079_0m.

I(1)-C(1)	2.074(2)
I(2)-C(2)	2.0710(19)
S(1)-O(1)	1.4276(16)
S(1)-O(2)	1.4311(16)
S(1)-N(1)	1.6811(19)
S(1)-C(9)	1.757(2)
N(1)-C(1)	1.438(2)
N(1)-C(4)	1.519(2)
C(1)-C(2)	1.331(3)
C(2)-C(3)	1.500(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.546(3)
C(4)-H(4)	1.0000
C(4)-C(5)	1.540(3)
C(5)-C(6)	1.530(3)
C(5)-C(7)	1.531(3)
C(5)-C(8)	1.532(3)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.393(3)
C(9)-C(14)	1.394(3)
C(10)-H(10)	0.9500
C(10)-C(11)	1.379(4)
C(11)-H(11)	0.9500
C(11)-C(12)	1.388(4)
C(12)-C(13)	1.396(3)
C(12)-C(15)	1.506(4)

C(13)-H(13)	0.9500
C(13)-C(14)	1.388(3)
C(14)-H(14)	0.9500
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800

O(1)-S(1)-O(2)	119.81(10)
O(1)-S(1)-N(1)	106.86(10)
O(1)-S(1)-C(9)	109.97(11)
O(2)-S(1)-N(1)	105.98(10)
O(2)-S(1)-C(9)	108.93(11)
N(1)-S(1)-C(9)	104.06(9)
C(1)-N(1)-S(1)	115.25(14)
C(1)-N(1)-C(4)	105.61(15)
C(4)-N(1)-S(1)	113.18(13)
N(1)-C(1)-I(1)	120.61(13)
C(2)-C(1)-I(1)	127.05(15)
C(2)-C(1)-N(1)	111.91(17)
C(1)-C(2)-I(2)	126.62(15)
C(1)-C(2)-C(3)	111.26(17)
C(3)-C(2)-I(2)	122.10(13)
C(2)-C(3)-H(3A)	111.2
C(2)-C(3)-H(3B)	111.2
C(2)-C(3)-C(4)	102.60(15)
H(3A)-C(3)-H(3B)	109.2
C(4)-C(3)-H(3A)	111.2
C(4)-C(3)-H(3B)	111.2
N(1)-C(4)-C(3)	103.83(15)
N(1)-C(4)-H(4)	109.0
N(1)-C(4)-C(5)	110.61(16)
C(3)-C(4)-H(4)	109.0
C(5)-C(4)-C(3)	115.26(17)
C(5)-C(4)-H(4)	109.0
C(6)-C(5)-C(4)	111.91(17)
C(6)-C(5)-C(7)	109.12(19)
C(6)-C(5)-C(8)	110.73(19)
C(7)-C(5)-C(4)	109.27(17)

C(7)-C(5)-C(8)	108.63(18)
C(8)-C(5)-C(4)	107.10(18)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-S(1)	120.51(18)
C(10)-C(9)-C(14)	120.7(2)
C(14)-C(9)-S(1)	118.22(17)
C(9)-C(10)-H(10)	120.5
C(11)-C(10)-C(9)	119.0(2)
C(11)-C(10)-H(10)	120.5
C(10)-C(11)-H(11)	119.1
C(10)-C(11)-C(12)	121.9(2)
C(12)-C(11)-H(11)	119.1
C(11)-C(12)-C(13)	118.3(2)
C(11)-C(12)-C(15)	121.4(2)
C(13)-C(12)-C(15)	120.3(2)
C(12)-C(13)-H(13)	119.4
C(14)-C(13)-C(12)	121.2(2)
C(14)-C(13)-H(13)	119.4
C(9)-C(14)-H(14)	120.5
C(13)-C(14)-C(9)	119.0(2)
C(13)-C(14)-H(14)	120.5

C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_dm15079_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	27(1)	14(1)	35(1)	2(1)	15(1)	0(1)
I(2)	15(1)	21(1)	33(1)	-3(1)	11(1)	-2(1)
S(1)	14(1)	24(1)	30(1)	7(1)	5(1)	3(1)
O(1)	25(1)	25(1)	39(1)	12(1)	6(1)	7(1)
O(2)	14(1)	36(1)	44(1)	7(1)	9(1)	1(1)
N(1)	14(1)	17(1)	26(1)	5(1)	8(1)	1(1)
C(1)	19(1)	15(1)	25(1)	1(1)	9(1)	-1(1)
C(2)	15(1)	19(1)	22(1)	-1(1)	7(1)	-1(1)
C(3)	16(1)	14(1)	26(1)	1(1)	8(1)	1(1)
C(4)	15(1)	14(1)	26(1)	3(1)	7(1)	2(1)
C(5)	19(1)	20(1)	26(1)	4(1)	9(1)	4(1)
C(6)	26(1)	34(1)	27(1)	-4(1)	7(1)	0(1)
C(7)	25(1)	28(1)	32(1)	6(1)	15(1)	6(1)
C(8)	30(1)	30(1)	34(1)	12(1)	12(1)	8(1)
C(9)	18(1)	24(1)	25(1)	4(1)	0(1)	0(1)
C(10)	20(1)	28(1)	35(1)	4(1)	-1(1)	-6(1)
C(11)	31(1)	22(1)	37(1)	-2(1)	-4(1)	-6(1)
C(12)	33(1)	30(1)	25(1)	-3(1)	-3(1)	1(1)
C(13)	34(1)	31(1)	24(1)	2(1)	6(1)	1(1)
C(14)	28(1)	25(1)	22(1)	4(1)	4(1)	-2(1)
C(15)	56(2)	36(1)	35(1)	-7(1)	8(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_dm15079_0m.

	x	y	z	U(eq)
H(3A)	6589	4988	2461	22
H(3B)	5718	4850	1463	22
H(4)	8570	4802	1905	21
H(6A)	6442	3558	-467	43
H(6B)	5617	3739	320	43
H(6C)	6719	2754	359	43
H(7A)	9926	4287	752	41
H(7B)	9108	3892	-198	41
H(7C)	9294	3080	622	41
H(8A)	8289	5869	602	46
H(8B)	6600	5694	455	46
H(8C)	7417	5441	-325	46
H(10)	10120	5447	3312	34
H(11)	9049	6665	4121	38
H(13)	6775	4231	4912	36
H(14)	7838	2985	4107	30
H(15A)	6200	6668	4698	64
H(15B)	7714	6978	5296	64
H(15C)	6791	6010	5586	64

Table 6. Torsion angles [°] for mo_dm15079_0m.

I(1)-C(1)-C(2)-I(2)	6.0(3)
I(1)-C(1)-C(2)-C(3)	-172.18(15)
I(2)-C(2)-C(3)-C(4)	-165.15(14)
S(1)-N(1)-C(1)-I(1)	-75.26(18)
S(1)-N(1)-C(1)-C(2)	111.76(18)
S(1)-N(1)-C(4)-C(3)	-105.92(15)
S(1)-N(1)-C(4)-C(5)	129.88(15)
S(1)-C(9)-C(10)-C(11)	170.09(18)
S(1)-C(9)-C(14)-C(13)	-170.22(17)
O(1)-S(1)-N(1)-C(1)	50.27(16)
O(1)-S(1)-N(1)-C(4)	171.98(13)
O(1)-S(1)-C(9)-C(10)	150.77(17)
O(1)-S(1)-C(9)-C(14)	-38.0(2)
O(2)-S(1)-N(1)-C(1)	179.11(14)
O(2)-S(1)-N(1)-C(4)	-59.18(16)
O(2)-S(1)-C(9)-C(10)	17.6(2)
O(2)-S(1)-C(9)-C(14)	-171.13(17)
N(1)-S(1)-C(9)-C(10)	-95.08(18)
N(1)-S(1)-C(9)-C(14)	76.17(18)
N(1)-C(1)-C(2)-I(2)	178.44(14)
N(1)-C(1)-C(2)-C(3)	0.2(3)
N(1)-C(4)-C(5)-C(6)	65.8(2)
N(1)-C(4)-C(5)-C(7)	-55.1(2)
N(1)-C(4)-C(5)-C(8)	-172.62(16)
C(1)-N(1)-C(4)-C(3)	21.1(2)
C(1)-N(1)-C(4)-C(5)	-103.15(18)
C(1)-C(2)-C(3)-C(4)	13.1(2)
C(2)-C(3)-C(4)-N(1)	-20.3(2)
C(2)-C(3)-C(4)-C(5)	100.85(19)
C(3)-C(4)-C(5)-C(6)	-51.5(2)
C(3)-C(4)-C(5)-C(7)	-172.51(17)
C(3)-C(4)-C(5)-C(8)	70.0(2)
C(4)-N(1)-C(1)-I(1)	159.03(14)
C(4)-N(1)-C(1)-C(2)	-13.9(2)
C(9)-S(1)-N(1)-C(1)	-66.08(16)
C(9)-S(1)-N(1)-C(4)	55.63(15)

C(9)-C(10)-C(11)-C(12)	-0.5(3)
C(10)-C(9)-C(14)-C(13)	1.0(3)
C(10)-C(11)-C(12)-C(13)	1.8(4)
C(10)-C(11)-C(12)-C(15)	-178.5(2)
C(11)-C(12)-C(13)-C(14)	-1.7(4)
C(12)-C(13)-C(14)-C(9)	0.4(3)
C(14)-C(9)-C(10)-C(11)	-0.9(3)
C(15)-C(12)-C(13)-C(14)	178.6(2)

Symmetry transformations used to generate equivalent atoms: