Supporting Information for

Direct Synthesis of Spirooxindoles Enabled by Palladium-Catalyzed Allylic Alkylation and DBU-Mediated Cyclization: Concept, Scope and Applications

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1. General Information

Unless otherwise noted, all vinyl benzoxazinanones[1] **1** and 3-isothiocyanato oxindoles[2] **2** were prepared according to the known literature. 1, 2-Dichloroethane, dichloromethane, chloroform, ethyl ether, tetrahydrofuran, 1,4-dioxane, toluene, acetonitrile, methanol and ethanol were obtained from commercial suppliers and used without further purification. Reactions were monitored by thin layer chromatography (TLC), and column chromatography purifications were performed using 200-300 mesh silica gel.

^{1}H NMR spectra were recorded on Varian-Mercury and Bruker AV 400 MHz or 600 MHz spectrophotometers. Solvents for NMR are $CDCl_3$, DMSO-d_6, or acetone-d_6, unless the otherwise noted. Chemical shifts are reported in delta (δ) units in parts per million (ppm) relative to the singlet (0 ppm) for tetramethylsilane (TMS) and relative to the signal of chloroform (δ 7.26, singlet), DMSO-d_6 (δ 2.50, singlet), acetone-d_6 (δ 2.05, singlet). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets), coupling constants (Hz) and integration. ^{13}C NMR spectra were recorded on Varian Mercury and Bruker AV 400 (100 MHz) or 600 (150 MHz) with complete proton decoupling. Chemical shifts are reported in ppm relative to the central line of the heptalet at 77.0 ppm for $CDCl_3$, 39.5 ppm for DMSO-d_6, 29.8 ppm for acetone-d_6. HRMS was measured on a Bruker microTOF II ESI-TOF, Shimadzu LCMS-IT-TOF and Bruker UltiMate3000 & Compact mass spectrometer and Thermo Fisher Orbitrap Elite LTQ XL mass spectrometer using a positive electrospray ionization (ESI), Melting points were determined using a WRS-2 model apparatus. IR was recorded on Bruker tensor 27 or FTIR-650 as KBr pellets with absorption in cm^{-1}.

CCK-8 assay for the determination of cell cytotoxicity

The in vitro cytotoxicity of synthesized compound was determined by standard WST-8 (2-(2-methoxy-4-nitrophenyl)-3-(4-nitrophenyl)-5-(2,4-disulfophenyl)-2*H*-tetrazolium, monosodium salt) (CCK-8) assay. SK-LU-1 cell line was used to test the cytotoxicity of the compounds. Cells were plated at a density of 3-15 × 10^3 cells/well into 96-well plates and cultured in MEM media supplemented with 10% fetal bovine serum. The cells were allowed to attach to the wells for 24 h at 37 ^{o}C, 5% CO_2. After that the medium was replaced with 100 μL of fresh medium containing different concentrations of **4o** (0, 5, 10, 20, 40, 80 μM), and MEM was used as a vehicle control. After 24 h of incubation, 10 μL of 12 mM CCK-8 stock solution mixed with 100 μL of phosphate buffered saline was added to each well for additional 4 h of incubation. The absorbance was measured at 450 nm using the Spectramax PLUS microplate reader (Molecular Devices). Cell viability (%) was calculated as: (OD450 sample/OD450 control) × 100%. IC_{50} values were calculated with GraphPad Prism 5.0 software.

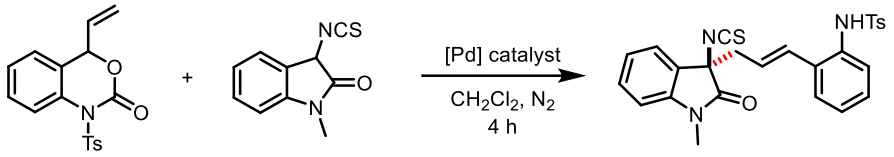
Flow Cytometry Analysis

SK-LU-1 cell line was cultured in 6-well plates at a density of 2 × 10^6 per well and incubated with various concentrations of compound **4o** at 37 °C in a 5% CO_2 humidified incubator for 24 h. The cells were washed with PBS, collected by centrifugation, and resuspended in PBS. Then, the Annexin-V-FITC dye and PI was added to the treated cells and incubated for 15 min, using an Annexin V-FITC/PI Apoptosis Detection Kit (C1062S, Beyotime China). Then the fluorescence of the cells was examined immediately after staining. (NovoCyte, Agilent, USA). Green channel excitation wavelength was 488 nm. Red channel excitation wavelength was 610 nm.

Cellular ROS assay

A fluorescent probe, DCFH-DA was used to measure the intracellular generation of ROS by **4o**. Briefly, the cells were seeded in 12-well plates and allowed to stabilize for 24 h and then incubated with medium containing compound **4o** (0, 2.5, 10, 40 μM) for 24 h at 37 °C. After washing with PBS, the cells were stained with 0.1 μM DCFH-DA (S0033S, Beyotime China) in PBS for 30 min at 37 °C in the dark. The fluorescence signals of DCFH were measured using a fluorescence microscope (OLYMPUS IXplore Standard, Japan).

2. Table S1 Optimization of Palladium Catalysts



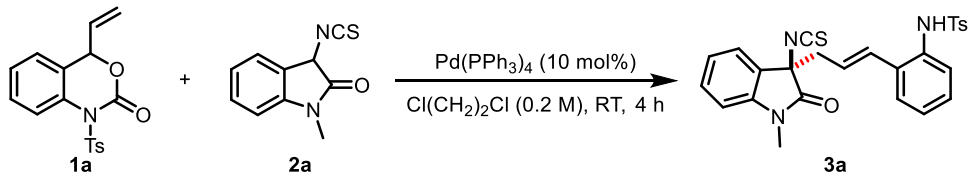
1a **2a** **3a**

Entry[a]	Pd catalyst	T (h)	Yield [%][b]
1	$Pd(PPh_3)_4$	4	89%
2	$Pd_2(dba)_3$	4	ND
3	$Pd(OAc)_2$	4	NR
4	$PdCl_2(PPh_3)_2$	4	NR
5	$Pd(dppf)Cl_2$	4	NR
6	$Pd(dba)_2$	4	ND
7	$Pd(acac)_2$	4	NR
8	$Pd_2(dba)_3{\cdot}CHCl_3$	4	ND

[a] Unless otherwise noted, the reaction was carried out with **1a** (0.10 mmol), **2a** (0.15 mmol) and Pd catalyst (10 mol%) in CH_2Cl_2 (1 mL) at RT under N_2 atmosphere. [b] Yield of isolated product after chromatography. ND: not determined. NR: no reaction.

3. Experimental Procedures and Characterizations

Representative procedure for palladium-catalyzed allylic alkylation reaction of vinyl benzoxazinanone 1a with 3-isothiocyanato oxindole 2a.

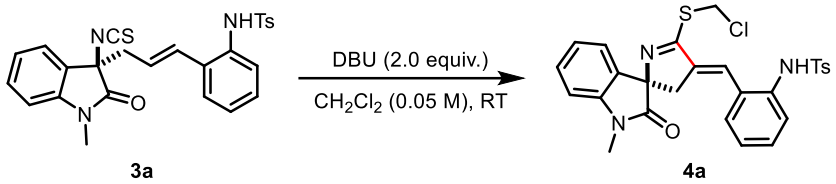


1a **2a** **3a**

The metal catalyst $Pd(PPh_3)_4$ (23.1 mg, 0.02 mmol) and vinyl benzoxazinanone **1a** (65.9 mg, 0.20 mmol) were dissolved in 1.0 mL of $Cl(CH_2)_2Cl$ for 10 minutes at room temperature. 3-Isothiocyanato oxindole **2a**

(61.3 mg, 0.30 mmol) was then added and the reaction mixture was stirred at room temperature for 4 h. After the complete consumption (as monitored by TLC), the reaction mixture was purified directly by flash column chromatography on silica gel (petroleum ether / ethyl acetate = 10:1 to 5:1) to give the corresponding pure product **3a** as a light yellow solid in 92% yield.

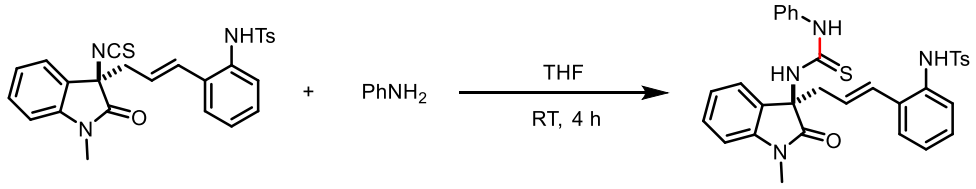
Representative procedure for DBU-mediated cyclization reaction of 3a.



3a **4a**

The allylic alkylated product **3a** (97.9 mg, 0.20 mmol) and DBU (60.9 mg, 0.40 mmol) were dissolved in 4.0 mL of CH_2Cl_2 at room temperature for about 4 h. After the complete consumption (as monitored by TLC), the reaction mixture was purified directly by flash column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1 to 1:1) to give the desired adduct **4a** as a white solid in 74% yield.

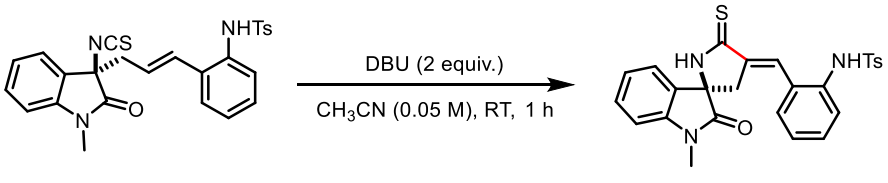
Procedure for addition reaction of 3a with aniline.



3a **5**

The allylic alkylated product **3a** (97.9 mg, 0.20 mmol) and aniline (22.4 mg, 0.24 mmol) were dissolved in 2.0 mL of anhydrous THF at room temperature for about 4 h. After the complete consumption (as monitored by TLC), the reaction mixture was purified directly by flash column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1 to 2:1) to give the addition adduct **5** as a white solid in 90% yield.

Procedure for DBU-mediated reaction of 3a with CH_3CN.

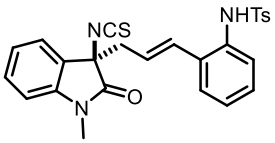


3a **6**

The allylic alkylated product **3a** (48.9 mg, 0.10 mmol) and DBU (30.4 mg, 0.20 mmol) were dissolved in 2.0 mL of CH_3CN at room temperature for about 1 h. After the complete consumption (as monitored by TLC), the reaction mixture was purified directly by flash column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1 to 2:1) to give the novel spirooxindole adduct **6** as a yellow solid in 54% yield.

Spectral data of products

(*E*)-*N*-(2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3a)



Prepared according to the general procedure from **1a** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 92% yield. m.p. 166-168 ℃.

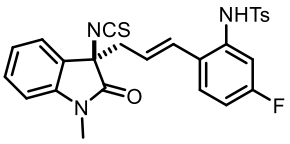
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, J = 8.3 Hz, 2H), 7.42 – 7.38 (m, 1H), 7.35 (dd, J = 7.4, 2.5 Hz, 2H), 7.24 – 7.16 (m, 5H), 7.12 – 7.08 (m, 1H), 6.88 (d, J = 7.8 Hz, 1H), 6.67 (s, 1H), 6.20 (d, J = 15.6 Hz, 1H), 5.81 (dt, J = 15.4, 7.5 Hz, 1H), 3.22 (s, 3H), 2.89 – 2.75 (m, 2H), 2.39 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.7, 143.8, 142.4, 140.0, 136.7, 133.4, 131.7, 131.3, 130.6, 129.6 (2C), 128.7, 127.3, 127.1 (2C), 126.9, 126.1, 125.0, 124.5, 123.7, 123.6, 109.1, 65.7, 42.8, 26.7, 21.5;

HRMS: calculated for $C_{26}H_{24}N_3O_3S_2$ $[M+H]^+$: 490.1254; Found: 490.1255;

IR: 3194, 2938, 2032, 1711, 1611, 1493, 1474, 1452, 1374, 1333, 1164, 1091, 1020, 973, 942, 813, 762, 714, 690, 666, 553, 539 cm^{-1}.

(*E*)-*N*-(5-fluoro-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3b)



Prepared according to the general procedure from **1b** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 95% yield. m.p. 68-70 ℃.

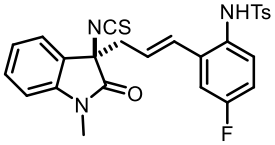
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, J = 8.1 Hz, 2H), 7.34 (t, J = 7.7 Hz, 1H), 7.28 (d, J = 7.4 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.13 – 7.08 (m, 2H), 7.03 (dd, J = 8.6, 6.2 Hz, 1H), 6.91 – 6.79 (m, 2H), 6.73 – 6.68 (m, 1H), 6.09 (d, J = 15.6 Hz, 1H), 5.72 (dt, J = 15.4, 7.5 Hz, 1H), 3.16 (s, 3H), 2.75 (d, J = 7.5 Hz, 2H), 2.32 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 163.6, 161.2, 144.1, 142.4, 140.2, 136.4, 135.1, 135.0, 130.9, 130.6, 129.8 (2C), 128.9, 128.8, 127.1 (2C), 127.0, 126.1 (2C), 125.7 (2C), 123.6, 112.6, 112.4, 110.1, 109.9, 109.1, 65.7, 42.8, 26.8, 21.6;

HRMS: calculated for $C_{26}H_{22}FN_3NaO_3S_2$ $[M+Na]^+$: 530.0979; Found: 530.0973;

IR: 3436, 3258, 2922, 2022, 1727, 1614, 1494, 1471, 1372, 1335, 1186, 1169, 1091, 983, 894, 813, 753, 665, 544 cm^{-1}.

(*E*)-*N*-(4-fluoro-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3c)



Prepared according to the general procedure from **1c** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 85% yield. m.p. 169-172 ℃.

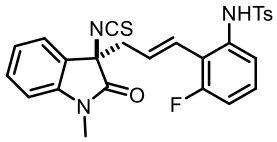
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, J = 8.3 Hz, 2H), 7.36 – 7.32 (m, 1H), 6.83 (dd, J = 6.4, 3.1 Hz, 2H), 6.81 (t, J = 2.5 Hz, 1H), 6.59 (s, 1H), 6.09 (d, J = 15.6 Hz, 1H), 5.76 (dt, J = 15.3, 7.5 Hz, 1H), 3.15 (s, 3H), 2.79 – 2.64 (m, 2H), 2.33 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 162.2, 159.7, 144.0, 142.4, 140.1, 136.4, 134.5, 134.4, 130.9, 130.6, 129.7 (2C), 129.1, 128.2, 128.1, 127.1 (2C), 126.8, 125.7, 123.7, 123.6, 115.6, 115.4, 113.5, 113.3, 109.1, 65.6, 42.6, 26.7, 21.6;

HRMS: calculated for $C_{26}H_{22}FN_3NaO_3S_2$ $[M+Na]^+$: 530.0979; Found: 530.0971;

IR: 3201, 2041, 1715, 1610, 1493, 1474, 1443, 1374, 1331, 1273, 1162, 1092, 973, 811, 761, 691, 543 cm^{-1}.

(*E*)-*N*-(3-fluoro-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3d)



Prepared according to the general procedure from **1d** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 80% yield. m.p. 153-155 ℃.

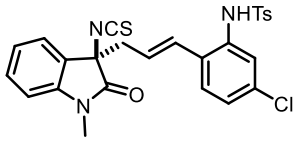
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 7.6 Hz, 2H), 7.23 (d, J = 8.3 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H), 7.13 – 7.08 (m, 2H), 7.08 – 7.02 (m, 1H), 6.83 (d, J = 7.8 Hz, 1H), 6.72 (t, J = 8.9 Hz, 1H), 5.90 (d, J = 16.1 Hz, 1H), 5.79 – 5.70 (m, 1H), 3.19 (s, 3H), 2.89 – 2.71 (m, 2H), 2.32 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.5, 161.2, 158.8, 144.0, 142.4, 139.9, 136.4, 135.7 (2C), 130.6, 130.0, 129.7 (2C), 128.9, 128.8, 127.1 (2C), 127.0, 125.0, 123.7, 123.5, 117.9, 117.7, 117.6 (2C), 112.1, 111.9, 109.3, 65.6, 43.2, 26.8, 21.6;

HRMS: calculated for $C_{26}H_{22}FN_3NaO_3S_2$ $[M+Na]^+$: 530.0979; Found: 530.0970;

IR: 3464, 3279, 2924, 2020, 1741, 1614, 1464, 1388, 1368, 1333, 1245, 1191, 1092, 1021, 893, 842, 754, 682, 563 cm^{-1}.

(*E*)-*N*-(5-chloro-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3e)



Prepared according to the general procedure from **1e** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 84% yield. m.p. 76-78 ℃.

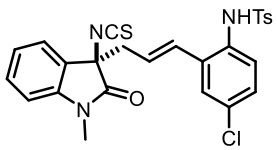
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.3 Hz, 2H), 7.36 – 7.30 (m, 2H), 7.26 (d, J = 7.4 Hz, 1H), 7.18 (d, J = 8.1 Hz, 2H), 7.09 (t, J = 7.5 Hz, 1H), 7.03 – 6.95 (m, 2H), 6.90 (s, 1H), 6.81 (d, J = 7.8 Hz, 1H), 6.10 (d, J = 15.6 Hz, 1H), 5.74 (dt, J = 15.4, 7.5 Hz, 1H), 3.14 (s, 3H), 2.79 – 2.69 (m, 2H), 2.32 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 144.1, 142.3, 140.1, 136.3, 134.5, 134.0, 130.7, 130.6, 129.7 (2C), 129.1, 128.3, 127.1 (2C), 126.8, 126.0, 125.8, 123.7, 123.6 (2C), 109.1, 65.6, 42.7, 26.7, 21.6;

HRMS: calculated for $C_{26}H_{22}ClN_3NaO_3S_2$ $[M+Na]^+$: 546.0683; Found: 546.0681;

IR: 3243, 2921, 2020, 1728, 1614, 1596, 1492, 1471, 1334, 1305, 1253, 1164, 1120, 1091, 888, 813, 753, 671, 569, 544 cm^{-1}.

(*E*)-*N*-(4-chloro-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3f)

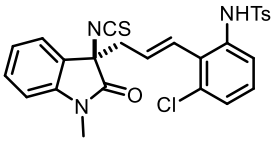


Prepared according to the general procedure from **1f** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 80% yield. m.p. 73-76 ℃.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, J = 8.2 Hz, 2H), 7.34 (t, J = 7.8 Hz, 1H), 7.28 (d, J = 7.1 Hz, 1H), 7.23 (d, J = 8.5 Hz, 1H), 7.18 (d, J = 8.4 Hz, 2H), 7.14 – 7.05 (m, 3H), 6.82 (d, J = 7.8 Hz, 1H), 6.75 (s, 1H), 6.06 (d, J = 15.7 Hz, 1H), 5.76 (dt, J = 15.3, 7.5 Hz, 1H), 3.16 (s, 3H), 2.78 – 2.69 (m, 2H), 2.33 (s, 3H);

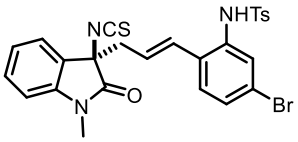
^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 144.0, 142.4, 140.2, 136.4, 132.9, 132.0, 131.7, 130.7 (2C), 129.7 (2C), 128.6, 127.1 (2C), 126.8, 126.3, 126.0, 123.7 (2C), 109.2, 65.6, 42.7, 26.8, 21.6;
HRMS: calculated for $C_{26}H_{22}ClN_3NaO_3S_2$ $[M+Na]^+$: 546.0683; Found: 546.0683;
IR: 3244, 2921, 2020, 1727, 1614, 1493, 1471, 1372, 1333, 1163, 1119, 1091, 969, 886, 814, 753, 665, 577, 547 cm^{-1}.

(*E*)-*N*-(3-chloro-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3g)



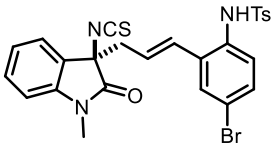
Prepared according to the general procedure from **1g** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 84% yield, m.p. 115-116 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, J = 8.2 Hz, 2H), 7.52 – 7.45 (m, 2H), 7.37 – 7.33 (m, 2H), 7.18 (d, J = 7.6 Hz, 2H), 7.13 (t, J = 7.6 Hz, 1H), 7.05 (t, J = 8.1 Hz, 1H), 6.99 (d, J = 7.9 Hz, 1H), 6.86 (d, J = 8.0 Hz, 1H), 5.99 (d, J = 16.3 Hz, 1H), 5.64 – 5.55 (m, 1H), 3.23 (s, 3H), 3.03 (dd, J = 13.8, 6.3 Hz, 1H), 2.70 (dd, J = 13.8, 8.4 Hz, 1H), 2.32 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 171.4, 144.0, 142.4, 136.5, 136.1, 133.6, 130.7, 129.9, 129.7 (3C), 129.2, 128.8, 127.3, 127.2 (2C), 127.1, 125.0, 123.8, 123.4, 118.7, 109.4, 65.6, 42.9, 26.9, 21.6;
HRMS: calculated for $C_{26}H_{23}ClN_3O_3S_2$ $[M+H]^+$: 524.0864; Found: 524.0863;
IR: 3195, 2915, 2010, 1709, 1615, 1568, 1471, 1446, 1377, 1334, 1166, 1093, 940, 752, 662, 567, 540 cm^{-1}.

(*E*)-*N*-(5-bromo-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3h)



Prepared according to the general procedure from **1h** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 86% yield. m.p. 79-81 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.3 Hz, 2H), 7.48 (d, J = 1.9 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.29 – 7.25 (m, 1H), 7.20 (s, 1H), 7.19 (d, J = 3.4 Hz, 1H), 7.16 – 7.08 (m, 2H), 6.94 (d, J = 8.3 Hz, 1H), 6.81 (d, J = 7.2 Hz, 2H), 6.06 (d, J = 15.7 Hz, 1H), 5.75 (dt, J = 15.4, 7.5 Hz, 1H), 3.15 (s, 3H), 2.74 (d, J = 7.5 Hz, 2H), 2.33 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 144.1, 142.4, 140.3, 136.4, 134.7, 130.8, 130.7, 129.8 (2C), 129.7, 129.0, 128.6, 127.1 (2C), 126.9, 126.7, 125.9, 123.7, 123.6, 122.0, 109.1, 65.6, 42.8, 26.7, 21.6;
HRMS: calculated for $C_{26}H_{22}BrN_3NaO_3S_2$ $[M+Na]^+$: 590.0178; Found: 590.0176;
IR: 3239, 2922, 2016, 1716, 1614, 1561, 1492, 1471, 1332, 1305, 1246, 1163, 1120, 1091, 969, 921, 813, 752, 665, 567, 542 cm^{-1}.

(*E*)-*N*-(4-bromo-2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3i)



Prepared according to the general procedure from **1i** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 93% yield. m.p. 68-70 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, J = 8.3 Hz, 2H), 7.46 – 7.41 (m, 1H), 7.37 (d, J = 7.4 Hz, 1H), 7.33 (dd, J = 8.5, 2.2 Hz, 1H), 7.31 – 7.26 (m, 4H),

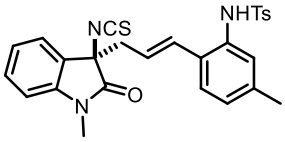
7.21 (t, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 6.82 (s, 1H), 6.16 (d, *J* = 15.6 Hz, 1H), 5.86 (dt, *J* = 15.4, 7.5 Hz, 1H), 3.26 (s, 3H), 2.89 – 2.77 (m, 2H), 2.42 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 144.1, 142.4, 140.2, 136.4, 133.1, 132.6, 131.5, 130.7, 130.6, 130.1, 129.7 (2C), 127.1 (2C), 126.8, 126.5, 125.9, 123.7, 123.6, 119.4, 109.1, 65.6, 42.7, 26.7, 21.5;

HRMS: calculated for $C_{26}H_{23}BrN_3O_3S_2$ $[M+H]^+$: 568.0359; Found: 568.0360;

IR: 3240, 2910, 2037, 1717, 1613, 1597, 1492, 1472, 1389, 1375, 1331, 1292, 1163, 1121, 1091, 989, 870, 815, 754, 665, 574, 547 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)-5-methylphenyl)-4-methylbenzenesulfonamide (3j)



Prepared according to the general procedure from **1j** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light orange solid with 87% yield. m.p. 81-83 ℃.

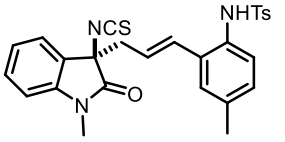
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.35 – 7.31 (m, 1H), 7.26 (d, *J* = 6.8 Hz, 1H), 7.20 – 7.14 (m, 2H), 7.13 – 7.07 (m, 2H), 6.98 (d, *J* = 7.9 Hz, 1H), 6.85 (d, *J* = 7.9 Hz, 1H), 6.80 (d, *J* = 7.8 Hz, 1H), 6.48 (s, 1H), 6.01 (d, *J* = 15.6 Hz, 1H), 5.66 (dt, *J* = 15.3, 7.5 Hz, 1H), 3.14 (s, 3H), 2.82 – 2.61 (m, 2H), 2.32 (s, 3H), 2.21 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.7, 143.8, 142.5, 140.0, 138.9, 136.8, 133.2, 131.6, 130.6, 129.6 (2C), 128.4, 127.1 (3C), 127.0, 126.9, 125.3, 124.0, 123.7, 123.5, 109.1, 65.8, 42.8, 26.7, 21.5, 21.2;

HRMS: calculated for $C_{27}H_{25}N_3NaO_3S_2$ $[M+Na]^+$: 526.1230; Found: 526.1229;

IR: 3251, 2921, 2023, 1728, 1614, 1493, 1471, 1372, 1331, 1251, 1185, 1120, 1091, 968, 898, 814, 753, 664, 570, 540 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)-4-methylphenyl)-4-methylbenzenesulfonamide (3k)



Prepared according to the general procedure from **1k** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 97% yield. m.p. 78-80 ℃.

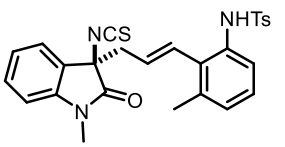
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.3 Hz, 2H), 7.37 – 7.30 (m, 1H), 7.27 (d, *J* = 6.9 Hz, 1H), 7.20 – 7.13 (m, 2H), 7.13 – 7.08 (m, 2H), 6.93 (d, *J* = 6.1 Hz, 2H), 6.80 (d, *J* = 7.8 Hz, 1H), 6.43 (s, 1H), 6.06 (d, *J* = 15.6 Hz, 1H), 5.74 (dt, *J* = 15.4, 7.5 Hz, 1H), 3.14 (s, 3H), 2.82 – 2.61 (m, 2H), 2.32 (s, 3H), 2.20 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.7, 143.7, 142.4, 139.9, 136.7, 136.3, 131.9, 131.6, 130.7, 130.6, 129.6 (2C), 129.4, 127.6, 127.1 (2C), 126.9, 125.4, 124.4, 123.8, 123.6, 109.0, 65.7, 42.8, 26.7, 21.5, 20.9;

HRMS: calculated for $C_{27}H_{25}N_3NaO_3S_2$ $[M+Na]^+$: 526.1230; Found: 526.1220;

IR: 3254, 2921, 2021, 1727, 1614, 1493, 1471, 1422, 1372, 1332, 1250, 1161, 1120, 1091, 970, 905, 814, 753, 665, 551, 538 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)-3-methylphenyl)-4-methylbenzenesulfonamide (3l)

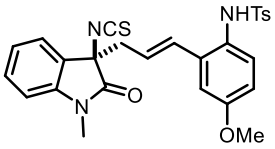


Prepared according to the general procedure from **1l** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 98% yield. m.p. 70-72 ℃.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.44 – 7.36 (m, 3H),

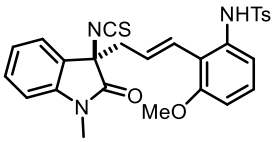
7.24 – 7.16 (m, 3H), 7.10 (s, 1H), 7.07 (t, *J* = 7.9 Hz, 1H), 6.89 (dd, *J* = 17.2, 7.6 Hz, 2H), 6.00 (d, *J* = 16.2 Hz, 1H), 5.42 (dt, *J* = 16.1, 7.4 Hz, 1H), 3.28 (s, 3H), 3.10 – 2.80 (m, 2H), 2.38 (s, 3H), 2.02 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): *δ* 171.4, 143.7, 142.4, 139.9, 136.8, 136.7, 134.1, 131.2, 130.7, 129.5 (2C), 128.6, 128.4, 127.8, 127.1 (2C), 127.0, 126.1, 123.7, 123.3, 118.4, 109.4, 65.6, 42.9, 26.8, 21.5, 20.4;
HRMS: calculated for $C_{27}H_{25}N_3NaO_3S_2$ $[M+Na]^+$: 526.1230; Found: 526.1221;
IR: 3247, 2920, 2021, 1726, 1614, 1493, 1470, 1422, 1371, 1352, 1328, 1248, 1164, 1120, 1092, 970, 868, 814, 753, 663, 571, 541 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)-4-methoxyphenyl)-4-methyl benzenesulfonamide (3m)



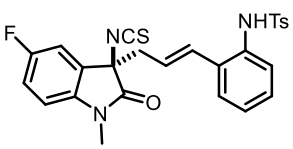
Prepared according to the general procedure from **1m** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 91% yield. m.p. 75-77 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.49 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.29 (m, 1H), 7.26 (d, *J* = 7.2 Hz, 1H), 7.20 – 7.13 (m, 2H), 7.13 – 7.05 (m, 2H), 6.79 (d, *J* = 7.8 Hz, 1H), 6.69 – 6.64 (m, 2H), 6.35 (s, 1H), 6.05 (d, *J* = 15.7 Hz, 1H), 5.73 (dt, *J* = 15.4, 7.5 Hz, 1H), 3.69 (s, 3H), 3.13 (s, 3H), 2.80 – 2.56 (m, 2H), 2.33 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): *δ* 171.6, 158.2, 143.6, 142.4, 139.9, 136.6, 134.4, 131.8, 130.5, 129.5 (2C), 128.6, 127.2 (2C), 126.8, 125.9, 124.3, 123.8, 123.5, 114.0, 111.7, 109.0, 65.7, 55.4, 42.6, 26.7, 21.5;
HRMS: calculated for $C_{27}H_{25}N_3NaO_4S_2$ $[M+Na]^+$: 542.1179; Found: 542.1180;
IR: 3251, 2921, 2020, 1726, 1614, 1493, 1470, 1372, 1331, 1292, 1209, 1160, 1091, 1037, 970, 900, 814, 753, 691, 540 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)-3-methoxyphenyl)-4-methyl benzenesulfonamide (3n)



Prepared according to the general procedure from **1n** (0.20 mmol), **2a** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 72% yield. m.p. 96-99 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.57 (d, *J* = 8.2 Hz, 2H), 7.35 (t, *J* = 7.2 Hz, 2H), 7.20 – 7.13 (m, 3H), 7.13 – 7.09 (m, 1H), 7.09 – 7.03 (m, 2H), 6.86 (d, *J* = 7.8 Hz, 1H), 6.52 (d, *J* = 8.2 Hz, 1H), 6.01 (d, *J* = 16.2 Hz, 1H), 5.68 – 5.59 (m, 1H), 3.65 (s, 3H), 3.22 (s, 3H), 2.91 – 2.74 (m, 2H), 2.30 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): *δ* 171.6, 157.3, 143.7, 142.5, 139.7, 136.6, 135.2, 130.5, 129.6 (2C), 128.6, 128.2, 127.7, 127.3, 127.2 (2C), 123.6 (2C), 117.6, 113.5, 109.4, 106.7, 65.8, 55.6, 43.3, 26.8, 21.5;
HRMS: calculated for $C_{27}H_{26}N_3O_4S_2$ $[M+H]^+$: 520.1359; Found: 520.1357;
IR: 3261, 2026, 1732, 1613, 1492, 1393, 1371, 1334, 1251, 1167, 1090, 1076, 966, 813, 753, 667, 560, 543 cm^{-1}.

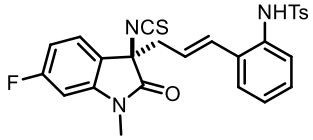
(*E*)-*N*-(2-(3-(5-fluoro-3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbe nzenesulfonamide (3o)



Prepared according to the general procedure from **1a** (0.20 mmol), **2b** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 88% yield. m.p. 147-150 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.56 (d, *J* = 8.3 Hz, 2H), 7.27 – 7.23 (m, 1H),

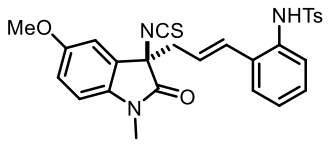
7.17 (dd, *J* = 12.0, 4.0 Hz, 3H), 7.14 – 7.09 (m, 2H), 7.08 – 7.01 (m, 3H), 6.79 – 6.72 (m, 1H), 6.63 (s, 1H), 6.22 (d, *J* = 15.7 Hz, 1H), 5.74 (dt, *J* = 15.4, 7.5 Hz, 1H), 3.16 (s, 3H), 2.83 – 2.66 (m, 2H), 2.33 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 171.5, 160.6, 158.1, 143.9, 141.0, 138.4, 136.7, 133.5, 132.1, 131.2, 129.7 (2C), 128.8, 128.4, 128.3, 127.4, 127.2 (2C), 126.2, 117.1, 116.8, 112.2, 111.9, 109.9, 109.8, 65.8, 42.7, 26.9, 21.6;
HRMS: calculated for $C_{26}H_{22}FN_3NaO_3S_2$ $[M+Na]^+$: 530.0979; Found: 530.0973;
IR: 3196, 2922, 2028, 1712, 1619, 1599, 1497, 1470, 1452, 1365, 1338, 1274, 1166, 1158, 1111, 1091, 974, 816, 759, 713, 692, 564 cm^{-1}.

(*E*)-*N*-(2-(3-(6-fluoro-3-isothiocyanato-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3p)



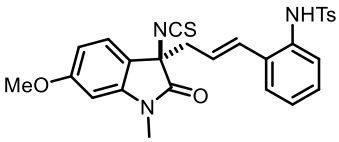
Prepared according to the general procedure from **1a** (0.20 mmol), **2c** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 91% yield. m.p. 68-69 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.24 – 7.17 (m, 2H), 7.15 (d, *J* = 7.8 Hz, 2H), 7.13 – 7.08 (m, 2H), 7.05 – 7.01 (m, 1H), 6.84 (s, 1H), 6.75 – 6.70 (m, 1H), 6.53 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.28 (d, *J* = 15.6 Hz, 1H), 5.75 (dt, *J* = 15.4, 7.6 Hz, 1H), 3.12 (s, 3H), 2.82 – 2.64 (m, 2H), 2.31 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 171.9, 165.3, 162.8, 144.2, 144.0, 143.7, 140.3, 136.6, 133.4, 131.9, 131.5, 129.6, 128.6, 127.1 (2C), 126.2, 125.2, 125.1, 124.7, 124.3, 122.3, 122.2, 109.8, 109.5, 98.1, 97.8, 65.2, 42.6, 26.8, 21.5;
HRMS: calculated for $C_{26}H_{22}FN_3NaO_3S_2$ $[M+Na]^+$: 530.0979; Found: 530.0978;
IR: 3437, 3256, 2922, 2021, 1731, 1615, 1503, 1453, 1376, 1331, 1242, 1161, 1089, 939, 917, 812, 756, 664, 565, 545 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-5-methoxy-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3q)



Prepared according to the general procedure from **1a** (0.20 mmol), **2d** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 80% yield. m.p. 70-72 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.13 – 7.07 (m, 2H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.89 – 6.81 (m, 2H), 6.71 (d, *J* = 8.4 Hz, 1H), 6.63 (s, 1H), 6.08 (d, *J* = 15.7 Hz, 1H), 5.72 (dt, *J* = 15.3, 7.5 Hz, 1H), 3.75 (s, 3H), 3.12 (s, 3H), 2.80 – 2.65 (m, 2H), 2.32 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 171.4, 156.4, 143.8, 140.0, 136.7, 135.6, 133.4, 131.8, 131.3, 129.6 (2C), 128.7, 128.0, 127.3, 127.1 (2C), 126.2, 125.0, 124.7, 114.4, 111.2, 109.5, 66.0, 55.9, 42.8, 26.8, 21.5;
HRMS: calculated for $C_{27}H_{25}N_3NaO_4S_2$ $[M+Na]^+$: 542.1179; Found: 542.1177;
IR: 3243, 2921, 2020, 1722, 1601, 1498, 1471, 1333, 1289, 1230, 1161, 1091, 1031, 968, 917, 813, 755, 693, 565 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-6-methoxy-1-methyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3r)



Prepared according to the general procedure from **1a** (0.20 mmol), **2e** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light orange solid with 92% yield. m.p. 72-74 ℃.

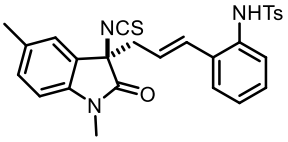
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, J = 8.3 Hz, 2H), 7.27 (dd, J = 8.0, 1.3 Hz, 1H), 7.19 - 7.14 (m, 3H), 7.14 - 7.07 (m, 2H), 7.05 - 7.00 (m, 1H), 6.58 (dd, J = 8.3, 2.3 Hz, 1H), 6.48 (s, 1H), 6.36 (d, J = 2.2 Hz, 1H), 6.09 (d, J = 15.6 Hz, 1H), 5.73 (dt, J = 15.4, 7.5 Hz, 1H), 3.78 (s, 3H), 3.12 (s, 3H), 2.80 – 2.65 (m, 2H), 2.32 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 172.1, 161.8, 143.8, 139.6, 136.7, 133.4, 131.6, 131.2, 129.6 (2C), 128.7, 127.3, 127.1 (2C), 126.1, 125.4, 124.6, 124.4, 118.7, 107.0, 97.1, 65.5, 55.7, 42.9, 26.7, 21.5;

HRMS: calculated for $C_{27}H_{25}N_3NaO_4S_2$ $[M+Na]^+$: 542.1179; Found: 542.1187;

IR: 3088, 2028, 1727, 1683, 1625, 1507, 1457, 1375, 1332, 1161, 1090, 564 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-1,5-dimethyl-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3s)



Prepared according to the general procedure from **1a** (0.20 mmol), **2f** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 89% yield. m.p. 71-74 ℃.

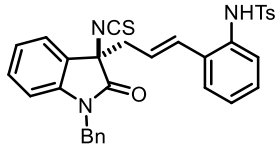
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 8.0 Hz, 1H), 7.18 – 7.14 (m, 2H), 7.10 (dd, J = 11.5, 8.2 Hz, 4H), 7.02 (t, J = 7.1 Hz, 1H), 6.74 – 6.66 (m, 2H), 6.15 (d, J = 15.7 Hz, 1H), 5.72 (dt, J = 15.4, 7.5 Hz, 1H), 3.12 (s, 3H), 2.80 – 2.67 (m, 2H), 2.31 (s, 3H), 2.31 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.6, 143.8, 140.0, 139.5, 136.6, 133.4 (2C), 131.6, 131.2, 130.8, 129.6 (2C), 128.6, 127.3, 127.1 (2C), 126.8, 126.0, 125.2, 124.3, 108.8, 65.8, 42.8, 26.7, 21.5, 21.1;

HRMS: calculated for $C_{27}H_{25}N_3NaO_3S_2$ $[M+Na]^+$: 526.1230; Found: 526.1225;

IR: 3252, 2920, 2025, 1727, 1622, 1604, 1499, 1361, 1334, 1291, 1161, 1091, 969, 914, 813, 756, 664, 566, 551 cm^{-1}.

(*E*)-*N*-(2-(3-(1-benzyl-3-isothiocyanato-2-oxoindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3t)



Prepared according to the general procedure from **1a** (0.20 mmol), **2g** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light orange solid with 96% yield. m.p. 67-69 ℃.

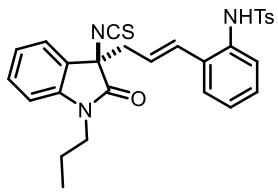
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, J = 8.3 Hz, 2H), 7.40 – 7.27 (m, 3H), 7.24 – 7.10 (m, 7H), 7.07 (t, J = 7.4 Hz, 4H), 6.72 (d, J = 7.8 Hz, 1H), 6.25 (d, J = 6.5 Hz, 1H), 6.09 (d, J = 15.6 Hz, 1H), 5.73 (dt, J = 15.4, 7.5 Hz, 1H), 5.08 (d, J = 15.7 Hz, 1H), 4.68 (d, J = 15.7 Hz, 1H), 2.91 (s, 2H), 2.36 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.7, 143.8, 141.7, 140.3, 136.5, 134.5, 133.3, 131.6, 131.1, 130.5, 129.6 (2C), 128.8 (2C), 128.7, 127.8, 127.0 (2C), 126.9, 126.7, 126.3, 125.0, 124.4, 123.7, 123.6, 110.0, 65.8, 44.2, 42.7, 21.5;

HRMS: calculated for $C_{32}H_{27}N_3NaO_3S_2$ $[M+Na]^+$: 588.1386; Found: 588.1392;

IR: 3252, 2921, 2019, 1726, 1613, 1488, 1468, 1455, 1366, 1333, 1291, 1161, 1091, 969, 913, 814, 753, 697, 664, 565 cm^{-1}.

(*E*)-*N*-(2-(3-(3-isothiocyanato-2-oxo-1-propylindolin-3-yl)prop-1-en-1-yl)phenyl)-4-methylbenzenesulfonamide (3u)



Prepared according to the general procedure from **1a** (0.20 mmol), **2h** (0.30 mmol), $Cl(CH_2)_2Cl$ (1.0 mL) at room temperature for 4 h to provide the title compound as a light yellow solid with 97% yield. m.p. 62-65 ℃.

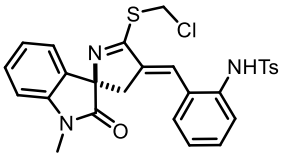
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.54 (d, J = 8.3 Hz, 2H), 7.33 – 7.30 (m, 1H), 7.29 – 7.27 (m, 1H), 7.16 (d, J = 8.1 Hz, 2H), 7.14 – 7.10 (m, 2H), 7.08 (d, J = 7.2 Hz, 2H), 7.02 (t, J = 7.2 Hz, 1H), 6.80 (d, J = 7.8 Hz, 1H), 6.46 (s, 1H), 6.08 (d, J = 15.6 Hz, 1H), 5.73 (dt, J = 15.4, 7.5 Hz, 1H), 3.66 – 3.50 (m, 2H), 2.80 – 2.69 (m, 2H), 2.32 (s, 3H), 1.62 – 1.52 (m, 2H), 0.83 (t, J = 7.4 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.5, 143.7, 141.9, 139.8, 136.5, 133.2, 131.5, 131.4, 130.4 (2C), 129.5, 128.6, 127.0 (2C), 126.9, 126.2, 124.8, 123.8, 123.3, 109.2, 65.6, 42.7, 41.9, 21.5, 20.5, 11.2;

HRMS: calculated for $C_{28}H_{28}N_3O_3S_2$ $[M+H]^+$: 518.1567; Found: 518.1569;

IR: 3266, 2964, 2021, 1725, 1609, 1487, 1467, 1367, 1332, 1274, 1160, 1125, 1091, 908, 813, 752, 664, 564, 551 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)phenyl)-4-methylbenzenesulfonamide (4a)



Prepared according to the general procedure from **3a** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 4 h to provide the title compound as a white solid with 74% yield. m.p. 163-165 ℃.

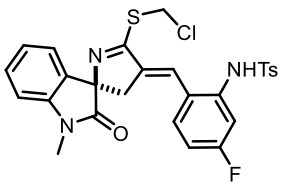
^{1}H NMR (400 MHz, DMSO-d_6): δ 10.10 (s, 1H), 7.58 (d, J = 8.1 Hz, 2H), 7.53 (d, J = 6.2 Hz, 1H), 7.38 (dd, J = 11.8, 8.5 Hz, 3H), 7.30- 7.20 (m, 2H), 7.12 – 7.04 (m, 4H), 6.90 (s, 1H), 5.38 (s, 2H), 3.28 (dd, J = 17.6, 2.7 Hz, 1H), 3.18 (s, 3H), 3.13 (dd, J = 17.6, 2.7 Hz, 1H), 2.38 (s, 3H);

^{13}C NMR (100 MHz, DMSO-d_6): δ 175.0, 171.0, 143.4, 143.2, 140.5, 137.3, 135.2, 131.9, 130.6, 129.9 (2C), 129.5, 129.4, 128.5, 127.7, 126.9, 126.6 (2C), 123.5, 122.9, 122.1, 108.9, 78.5, 44.5, 26.4, 21.1;

HRMS: calculated for $C_{27}H_{24}ClN_3NaO_3S_2$ $[M+Na]^+$: 560.0840; Found: 560.0847;

IR: 3146, 3064, 2254, 1710, 1692, 1647, 1617, 1495, 1471, 1452, 1380, 1338, 1262, 1164, 1092, 916, 810, 758, 730, 575, 538 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-5-fluorophenyl)-4-methylbenzenesulfonamide (4b)



Prepared according to the general procedure from **3b** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 25 h to provide the title compound as a white solid with 57% yield. m.p.197-198 ℃.

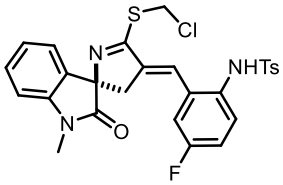
^{1}H NMR (400 MHz, DMSO-d_6): δ 10.41 (s, 1H), 7.62 (d, J = 8.3 Hz, 2H), 7.57 (dd, J = 8.9, 6.4 Hz, 1H), 7.41 (d, J = 8.1 Hz, 2H), 7.40 – 7.34 (m, 1H), 7.08 (t, J = 5.9 Hz, 4H), 6.93 (dd, J = 10.1, 2.7 Hz, 1H), 6.74 (s, 1H), 5.38 (s, 2H), 3.25 (dd, J = 17.5, 2.7 Hz, 1H), 3.18 (s, 3H), 3.10 (dd, J = 17.5, 2.7 Hz, 1H), 2.38 (s, 3H);

^{13}C NMR (100 MHz, DMSO-d_6): δ 175.0, 170.9, 162.7, 160.3, 143.5, 143.4, 140.6 (2C), 137.1, 137.0 (2C), 130.6, 130.5, 130.4, 130.0, 129.6, 127.8, 127.7, 126.6, 123.5, 122.9, 120.9, 114.0, 113.8 (2C), 113.6, 108.9, 78.4, 44.5, 26.3, 21.1;

HRMS: calculated for $C_{27}H_{24}ClFN_3O_3S_2$ $[M+H]^+$: 556.0926; Found: 556.0926;

IR: 3108, 2986, 2923, 1703, 1614, 1537, 1493, 1468, 1416, 1375, 1337, 1264, 1167, 1089, 982, 877, 808, 751, 554, 539 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-4-fluorophenyl)-4-methylbenzenesulfonamide (4c)



Prepared according to the general procedure from **3c** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 25 h to provide the title compound as a white solid with 55% yield. m.p. 194-196 ℃.

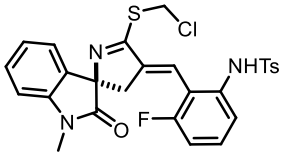
^{1}H NMR (400 MHz, DMSO-d_6): δ 10.05 (s, 1H), 7.57 (d, J = 8.2 Hz, 2H), 7.40 (d, J = 8.0 Hz, 2H), 7.38 – 7.31 (m, 2H), 7.18 – 7.13 (m, 1H), 7.11 – 7.03 (m, 4H), 6.82 (s, 1H), 5.37 (s, 2H), 3.29 (d, J = 2.4 Hz, 1H), 3.23 (d, J = 2.4 Hz, 1H), 3.17 (s, 3H), 2.38 (s, 3H);

^{13}C NMR (100 MHz, DMSO-d_6): δ 174.8, 170.8, 161.6, 159.1, 143.5, 143.3, 141.9, 137.0, 134.4 (2C), 131.5, 131.4, 130.5, 130.2, 130.1, 129.9, 129.5, 126.6, 123.6, 122.8, 121.0, 116.3, 116.1, 114.9, 114.6, 108.8, 78.7, 59.8, 44.4, 26.3, 21.1;

HRMS: calculated for $C_{27}H_{24}ClFN_3O_3S_2$ $[M+H]^+$: 556.0926; Found: 556.0928;

IR: 3148, 2977, 1727, 1697, 1614, 1538, 1488, 1472, 1377, 1340, 1237, 1160, 1091, 992, 880, 810, 751, 692, 664, 591, 540 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-3-fluorophenyl)-4-methylbenzenesulfonamide (4d)



Prepared according to the general procedure from **3d** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 75 h to provide the title compound as a white solid with 50% yield. m.p.167-169 ℃.

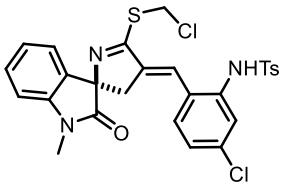
^{1}H NMR (400 MHz, acetone-d_6): δ 8.98 (s, 1H), 7.70 (d, J = 8.3 Hz, 2H), 7.40 (d, J = 7.9 Hz, 2H), 7.37 – 7.32 (m, 2H), 7.26 (d, J = 8.0 Hz, 1H), 7.19 – 7.13 (m, 1H), 7.06 (dd, J = 7.6, 1.0 Hz, 1H), 7.04 – 6.98 (m, 2H), 6.44 (t, J = 2.8 Hz, 1H), 5.34 (q, J = 11.1 Hz, 2H), 3.22 (s, 3H), 3.00 – 2.95 (m, 1H), 2.89 (s, 1H), 2.84 – 2.79 (m, 1H), 2.41 (s, 3H);

^{13}C NMR (100 MHz, acetone-d_6): δ 175.8, 170.7, 161.4, 159.0, 147.1 (2C), 144.8, 144.7, 138.4, 137.8, 137.7, 131.7, 131.0, 130.9, 130.7, 130.3, 127.8, 124.3, 123.6, 121.7, 121.6, 119.6, 119.4, 116.5, 114.0, 113.7, 109.3, 79.1 (2C), 44.7, 40.3, 40.2, 26.6, 21.4;

HRMS: calculated for $C_{27}H_{24}Cl_2FN_3O_3S_2$ $[M+H]^+$: 556.0926; Found: 556.0925;

IR: 3269, 2389, 1702, 1614, 1541, 1492, 1464, 1373, 1336, 1162, 1090, 1010, 752, 662, 563, 542 cm^{-1}.

(*E*)-*N*-(5-chloro-2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene) methyl)phenyl)-4-methylbenzenesulfonamide (4e)

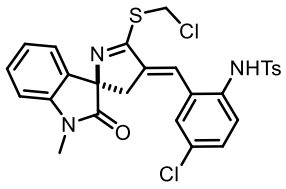


Prepared according to the general procedure from **3e** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 19 h to provide the title compound as a white solid with 47% yield. m.p. 197-200 ℃.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.38 (s, 1H), 7.57 (dd, J = 22.6, 8.3 Hz, 3H), 7.44 – 7.34 (m, 3H), 7.27 (dd, J = 8.5, 2.3 Hz, 1H), 7.12 (d, J = 2.2 Hz, 1H), 7.08 (t, J = 6.4 Hz, 3H), 6.74 (s, 1H), 5.37 (s, 2H), 3.25 (dd, J = 17.7, 2.7 Hz, 1H), 3.17 (s, 3H), 3.12 (dd, J = 17.6, 2.7 Hz, 1H), 2.38 (s, 3H);

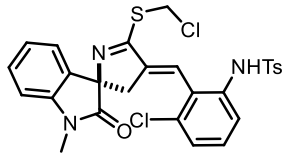
^{13}C NMR (100 MHz, DMSO-d_6): δ 174.8, 170.8, 143.5, 143.4, 141.4, 136.9, 136.5, 133.0, 130.5, 130.4, 130.1, 130.0 (2C), 129.6, 127.0, 126.7, 126.6 (2C), 123.5, 122.8, 120.7, 108.9, 78.5, 44.5, 30.7, 26.3, 21.1;
HRMS: calculated for $C_{27}H_{24}Cl_2N_3O_3S_2$ $[M+H]^+$: 572.0631; Found: 572.0631;
IR: 3065, 2918, 2849, 1703, 1614, 1538, 1469, 1376, 1337, 1182, 1161, 1083, 937, 752, 672, 567, 541, 534 cm^{-1}.

(*E*)-*N*-(4-chloro-2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene) methyl)phenyl)-4-methylbenzenesulfonamide (4f)



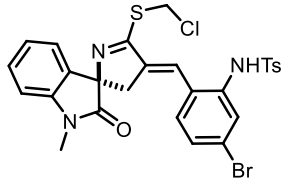
Prepared according to the general procedure from **3f** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 24 h to provide the title compound as a white solid with 46% yield. m.p. 185-187 ℃.
^{1}H NMR (400 MHz, DMSO-d_6): δ 10.20 (s, 1H), 7.59 (d, J = 7.9 Hz, 2H), 7.52 (s, 1H), 7.40 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.3 Hz, 2H), 7.12 – 7.05 (m, 4H), 6.76 (d, J = 2.9 Hz, 1H), 5.37 (s, 2H), 3.31 – 3.22 (m, 2H), 3.17 (s, 3H), 2.38 (s, 3H);
^{13}C NMR (100 MHz, DMSO-d_6): δ 174.7, 170.8, 143.6, 143.4, 142.1, 137.0, 134.1, 133.7, 131.4, 130.5, 130.0 (2C), 129.5, 129.3, 129.1, 127.8, 126.6 (2C), 123.7, 122.8, 120.6, 108.8, 78.7, 44.5, 26.3, 21.1;
HRMS: calculated for $C_{27}H_{24}Cl_2N_3O_3S_2$ $[M+H]^+$: 572.0631; Found: 572.0628;
IR: 3118, 2923, 1698, 1613, 1540, 1472, 1376, 1332, 1260, 1164, 1092, 995, 879, 813, 752, 729, 579, 548 cm^{-1}.

(*E*)-*N*-(3-chloro-2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene) methyl)phenyl)-4-methylbenzenesulfonamide (4g)



Prepared according to the general procedure from **3g** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 48 h to provide the title compound as a white solid with 51% yield. m.p.123-125 ℃.
^{1}H NMR (400 MHz, acetone-d_6): δ 8.69 (s, 1H), 7.70 (d, J = 8.4 Hz, 2H), 7.41 – 7.36 (m, 3H), 7.35 (dd, J = 7.8, 1.3 Hz, 1H), 7.33 – 7.26 (m, 2H), 7.21 – 7.16 (m, 1H), 7.09 – 7.05 (m, 1H), 7.02 (d, J = 7.8 Hz, 1H), 6.41 (t, J = 2.7 Hz, 1H), 5.36 (q, J = 11.1 Hz, 2H), 3.23 (s, 3H), 2.83 (d, J = 2.8 Hz, 1H), 2.76 (dd, J = 17.2, 2.8 Hz, 1H), 2.40 (s, 3H);
^{13}C NMR (100 MHz, acetone-d_6): δ 175.9, 170.4, 147.2, 144.8 (2C), 138.4, 137.5, 133.9, 131.6, 130.7, 130.5, 130.3, 129.5, 127.9, 127.1, 124.5, 123.6, 123.1, 120.2, 109.4, 79.1, 44.7, 39.6, 26.6, 21.4;
HRMS: calculated for $C_{27}H_{24}Cl_2N_3O_3S_2$ $[M+H]^+$: 572.0631; Found: 572.0638;
IR: 3360, 1709, 1614, 1569, 1470, 1445, 1373, 1332, 1258, 1163, 1124, 1090, 944, 752, 661, 565, 541 cm^{-1}.

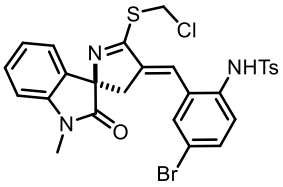
(*E*)-*N*-(5-bromo-2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)phenyl)-4-methylbenzenesulfonamide (4h)



Prepared according to the general procedure from **3h** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 11 h to provide the title compound as a white solid with 47% yield. m.p.215-217 ℃.
^{1}H NMR (400 MHz, acetone-d_6): δ 9.29 (s, 1H), 7.69 (d, J = 8.3 Hz, 2H), 7.57 (d, J = 2.0 Hz, 1H), 7.50 (d, J = 8.5 Hz, 1H), 7.43 (dd, J = 8.2, 2.3 Hz, 3H), 7.39 – 7.35 (m, 1H), 7.18 – 7.14 (m, 1H), 7.08 – 7.03 (m, 2H), 6.65 (t, J = 2.7 Hz, 1H), 5.40 – 5.28 (m, 2H), 3.28 – 3.23 (m, 1H), 3.22 (s, 3H), 3.20 – 3.17 (m, 1H), 2.43 (s, 3H);

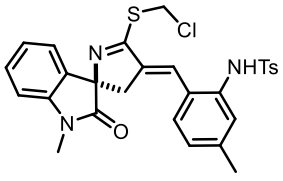
^{13}C NMR (100 MHz, DMSO-d_6): δ 174.8, 170.8, 143.5, 143.4, 141.4, 136.9, 136.6, 130.8, 130.5, 130.2, 130.0 (3C), 129.6, 129.5, 126.6 (2C), 123.5, 122.8, 121.4, 120.8, 108.9, 78.5, 44.5, 30.7, 26.3, 21.1;
HRMS: calculated for $C_{27}H_{24}BrClN_3O_3S_2$ $[M+H]^+$: 616.0125; Found: 616.0125;
IR: 3147, 1726, 1698, 1614, 1538, 1488, 1471, 1376, 1339, 1238, 1161, 1091, 992, 880, 810, 751, 692, 665, 591, 540, 521 cm^{-1}.

(*E*)-*N*-(4-bromo-2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)phenyl)-4-methylbenzenesulfonamide (4i)



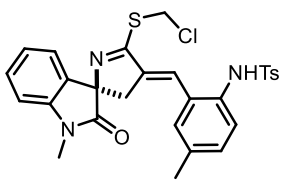
Prepared according to the general procedure from **3h** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 23 h to provide the title compound as a white solid with 52% yield. m.p.195-197 ℃.
^{1}H NMR (400 MHz, DMSO-d_6): δ 10.20 (s, 1H), 7.64 (s, 1H), 7.59 (d, J = 7.9 Hz, 2H), 7.49 (d, J = 8.4 Hz, 1H), 7.38 (dd, J = 16.1, 7.8 Hz, 3H), 7.10 (dd, J = 14.7, 8.1 Hz, 3H), 7.02 (d, J = 8.6 Hz, 1H), 6.76 (s, 1H), 5.37 (s, 2H), 3.26 (t, J = 15.6 Hz, 2H), 3.17 (s, 3H), 2.38 (s, 3H);
^{13}C NMR (100 MHz, DMSO-d_6): δ 174.7, 170.7, 143.6, 143.4, 142.1, 137.0, 134.5, 134.0, 132.1, 130.6, 130.5, 130.0 (2C), 129.5 (2C), 126.6 (2C), 123.7, 122.7, 120.5, 119.7, 108.8, 78.7, 59.8, 44.5, 26.4, 21.1;
HRMS: calculated for $C_{27}H_{24}BrClN_3O_3S_2$ $[M+H]^+$: 616.0125; Found: 616.0125;
IR: 3134, 1722, 1698, 1613, 1538, 1472, 1377, 1332, 1260, 1165, 1091, 994, 876, 753, 730, 662, 575, 547 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-5-methylphenyl)-4-methylbenzenesulfonamide (4j)



Prepared according to the general procedure from **3j** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 4 h to provide the title compound as a white solid with 41% yield. m.p. 209-211 ℃.
^{1}H NMR (400 MHz, DMSO-d_6): δ 10.06 (s, 1H), 7.58 (d, J = 8.5 Hz, 2H), 7.42 – 7.35 (m, 4H), 7.10 – 7.03 (m, 4H), 6.92 (s, 1H), 6.81 (s, 1H), 5.37 (s, 2H), 3.26 (dd, J = 17.5, 2.6 Hz, 1H), 3.17 (s, 3H), 3.09 (dd, J = 17.5, 2.6 Hz, 1H), 2.37 (s, 3H), 2.22 (s, 3H);
^{13}C NMR (100 MHz, DMSO-d_6): δ 175.0, 171.0, 143.4, 143.1, 139.5, 139.2, 137.3, 135.1, 130.7, 129.8 (2C), 129.5, 129.0, 128.5, 128.3, 127.7, 126.6 (2C), 123.4, 122.8, 122.0, 108.9, 78.4, 44.5, 30.7, 26.3, 21.1, 20.8;
HRMS: calculated for $C_{28}H_{27}ClN_3O_3S_2$ $[M+H]^+$: 552.1177; Found: 552.1173;
IR: 3113, 2918, 1704, 1612, 1537, 1494, 1468, 1336, 1244, 1161, 1090, 995, 880, 808, 753, 692, 669, 571, 554, 537 cm^{-1}.

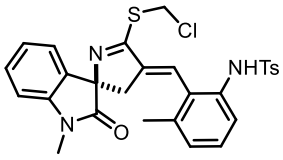
(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-4-methylphenyl)-4-methylbenzenesulfonamide (4k)



Prepared according to the general procedure from **3k** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 2 h to provide the title compound as a white solid with 66% yield. m.p. 214-216 ℃.
^{1}H NMR (400 MHz, DMSO-d_6): δ 9.95 (s, 1H), 7.57 (d, J = 8.1 Hz, 2H), 7.38 (t, J = 8.2 Hz, 3H), 7.34 (s, 1H), 7.11 – 7.06 (m, 4H), 6.90 (d, J = 8.0 Hz, 2H), 5.37 (s, 2H), 3.31 (d, J = 2.7 Hz, 1H), 3.18 (s, 3H), 3.13 (d, J = 2.7 Hz, 1H), 2.37 (s, 3H), 2.23 (s, 3H);

^{13}C NMR (100 MHz, DMSO-d_6): δ 175.0, 171.1, 143.5, 143.0, 140.1, 137.3, 136.6, 132.7, 132.0, 130.7, 130.0, 129.8 (2C), 129.5, 128.6, 128.0, 126.7 (2C), 123.5, 122.8, 122.1, 108.8, 78.5, 44.5, 26.3, 21.0, 20.5;
HRMS: calculated for $C_{28}H_{27}ClN_3O_3S_2$ $[M+H]^+$: 552.1177; Found: 552.1174;
IR: 3150, 1722, 1696, 1614, 1536, 1492, 1470, 1377, 1333, 1234, 1161, 1090, 995, 884, 809, 750, 664, 590, 550, 536 cm^{-1}.

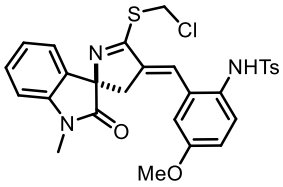
(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-3-methylphenyl)-4-methylbenzenesulfonamide (4l)



Prepared according to the general procedure from **3l** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 4 h to provide the title compound as a white solid with 61% yield. m.p.187-188 ℃.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.65 (s, 1H), 7.62 (d, J = 8.0 Hz, 2H), 7.36 (t, J = 8.7 Hz, 3H), 7.14 (d, J = 7.0 Hz, 1H), 7.12 – 7.03 (m, 4H), 6.79 (d, J = 7.7 Hz, 1H), 6.56 (s, 1H), 5.39 (s, 2H), 3.16 (s, 3H), 2.69 (dd, J = 17.1, 2.7 Hz, 1H), 2.59 (dd, J = 17.1, 2.7 Hz, 1H), 2.37 (s, 3H), 2.18 (s, 3H);
^{13}C NMR (100 MHz, DMSO-d_6): δ 175.0, 169.8, 143.4, 143.3, 143.1, 137.7, 136.8, 134.3, 130.9, 130.6, 129.7 (2C), 129.5, 128.1, 127.5, 126.6 (2C), 123.4, 122.8, 122.5, 122.1, 108.8, 77.7, 44.5, 38.4, 26.3, 21.0, 19.7;
HRMS: calculated for $C_{28}H_{27}ClN_3O_3S_2$ $[M+H]^+$: 552.1177; Found: 552.1179;
IR: 3258, 1715, 1613, 1533, 1464, 1400, 1372, 1332, 1255, 1188, 1166, 1094, 988, 973, 780, 760, 664, 568, 543 cm^{-1}.

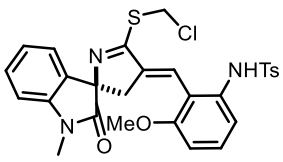
(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-4-methoxyphenyl)-4-methylbenzenesulfonamide (4m)



Prepared according to the general procedure from **3m** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 2 h to provide the title compound as a white solid with 75% yield. m.p. 189-192 ℃.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.84 (s, 1H), 7.56 (d, J = 8.2 Hz, 2H), 7.39 (d, J = 8.2 Hz, 3H), 7.08 (t, J = 6.3 Hz, 3H), 6.98 (d, J = 2.8 Hz, 1H), 6.92 - 6.84 (m, 3H), 5.37 (s, 2H), 3.70 (s, 3H), 3.33 (d, J = 2.7 Hz, 1H), 3.23 (d, J = 2.7 Hz, 1H), 3.18 (s, 3H), 2.38 (s, 3H);
^{13}C NMR (100 MHz, DMSO-d_6): δ 174.9, 170.9, 157.8, 143.5, 143.0, 140.7, 137.2, 133.8, 130.6, 129.8 (3C), 129.5, 127.9, 126.7 (2C), 123.5, 122.8, 122.2, 115.4, 112.5, 108.8, 78.6, 55.3, 44.4, 26.3, 21.1;
HRMS: calculated for $C_{28}H_{27}ClN_3O_4S_2$ $[M+H]^+$: 568.1126; Found: 568.1132;
IR: 3141, 2951, 1697, 1613, 1538, 1494, 1471, 1377, 1336, 1208, 1161, 1091, 1035, 995, 880, 811, 753, 693, 662, 549 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)-3-methoxyphenyl)-4-methylbenzenesulfonamide (4n)



Prepared according to the general procedure from **3n** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 2 h to provide the title compound as a white solid with 30% yield. m.p. 142-143 ℃.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.85 (s, 1H), 7.62 (d, J = 8.2 Hz, 2H), 7.35 (dd, J = 18.8, 7.9 Hz, 3H), 7.20 (t, J = 8.2 Hz, 1H), 7.11 (d, J = 6.9 Hz, 1H), 7.05 (t, J = 7.6 Hz, 2H), 6.86

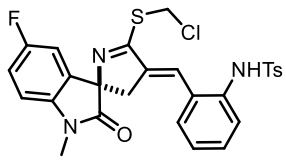
(d, *J* = 8.4 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 6.55 (t, *J* = 2.3 Hz, 1H), 5.36 (s, 2H), 3.71 (s, 3H), 3.17 (s, 3H), 2.82 (dd, *J* = 17.2, 2.8 Hz, 1H), 2.65 (dd, *J* = 17.2, 2.3 Hz, 1H), 2.37 (s, 3H);

^{13}C NMR (100 MHz, DMSO-d_6): δ 175.2, 170.2, 156.7, 143.3, 137.7, 135.8, 130.8, 129.8 (2C), 129.6, 129.4, 126.6 (2C), 123.3, 122.8, 119.8, 119.3, 117.5, 109.1, 108.8, 77.8, 55.6, 44.5, 26.3, 21.0;

HRMS: calculated for $C_{28}H_{27}ClN_3O_4S_2$ $[M+H]^+$: 568.1126; Found: 568.1124;

IR: 3254, 2933, 1709, 1614, 1578, 1546, 1493, 1467, 1375, 1326, 1257, 1161, 1091, 1072, 991, 815, 750, 732, 663, 559, 542 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-5-fluoro-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene) methyl)phenyl)-4-methylbenzenesulfonamide (4o)



Prepared according to the general procedure from **3o** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 24 h to provide the title compound as a white solid with 40% yield. m.p.196-198 ℃.

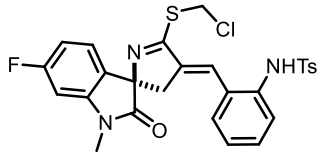
^{1}H NMR (400 MHz, acetone-d_6): δ 9.02 (s, 1H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.54 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.36 – 7.30 (m, 2H), 7.25 – 7.29 (m, 1H), 7.16 – 7.11 (m, 1H), 7.07 – 7.00 (m, 2H), 6.78 (t, *J* = 2.7 Hz, 1H), 5.40 – 5.29 (m, 2H), 3.30 (dd, *J* = 17.3, 2.7 Hz, 1H), 3.24 (d, *J* = 2.7 Hz, 1H), 3.22 (s, 3H), 2.42 (s, 3H);

^{13}C NMR (100 MHz, acetone-d_6): δ 175.8, 172.4, 161.4, 159.0, 144.4, 142.1, 141.0, 140.9, 138.6, 136.4, 133.7, 133.6, 132.5, 130.7 (2C), 130.2, 129.4, 128.4, 127.8 (2C), 127.5, 123.0, 116.4, 116.1, 112.6, 112.3, 110.2, 110.1, 79.7, 79.6, 44.7, 40.3, 26.7, 21.5;

HRMS: calculated for $C_{27}H_{24}ClFN_3O_3S_2$ $[M+H]^+$: 556.0926; Found: 556.0923;

IR: 2923, 2852, 1704, 1615, 1539, 1495, 1453, 1368, 1332, 1273, 1162, 1092, 812, 729, 699, 662, 562, 532 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-6-fluoro-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene) methyl)phenyl)-4-methylbenzenesulfonamide (4p)



Prepared according to the general procedure from **3p** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 24 h to provide the title compound as a white solid with 64% yield. m.p. 126-127 ℃.

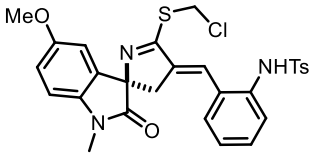
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.3 Hz, 2H), 7.47 – 7.44 (m, 1H), 7.30 – 7.26 (m, 3H), 7.26 – 7.23 (m, 1H), 7.18 – 7.14 (m, 1H), 7.05 – 6.99 (m, 2H), 6.74 – 6.71 (m, 1H), 6.60 (dd, *J* = 8.7, 2.3 Hz, 1H), 6.44 (t, *J* = 2.3 Hz, 1H), 5.22 (d, *J* = 11.0 Hz, 1H), 5.04 (d, *J* = 11.0 Hz, 1H), 3.26 (dd, *J* = 17.2, 2.5 Hz, 1H), 3.21 (s, 3H), 2.96 (dd, *J* = 17.1, 2.7 Hz, 1H), 2.42 (s, 3H);

^{13}C NMR (150 MHz, $CDCl_3$): δ 176.1, 171.2, 164.7, 163.1, 145.2, 144.0, 142.4, 136.7, 134.6, 130.4, 129.9 (2C), 129.64, 128.2, 127.1 (2C), 126.5 (2C), 126.0 (2C), 121.6, 109.4, 109.3, 97.6, 97.4, 78.1, 43.5, 39.9, 26.7, 21.6;

HRMS: calculated for $C_{27}H_{24}ClFN_3O_3S_2$ $[M+H]^+$: 556.0926; Found: 556.0925;

IR: 3131, 3024, 2976, 1717, 1614, 1532, 1488, 1454, 1161, 1084, 1047, 998, 925, 847, 765, 724, 663, 564, 550 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-5-methoxy-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylide ne)methyl)phenyl)-4-methylbenzenesulfonamide (4q)



Prepared according to the general procedure from **3q** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 3 h to provide the title compound as a white solid with 56% yield. m.p. 210-212 ℃.

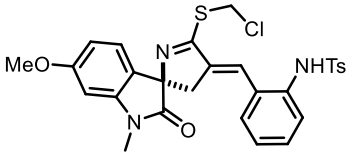
^{1}H NMR (400 MHz, acetone-d_6): δ 9.03 (s, 1H), 7.72 – 7.62 (m, 2H), 7.55 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 2H), 7.37 – 7.30 (m, 2H), 7.29 – 7.25 (m, 1H), 6.96 - 6.89 (m, 2H), 6.85 (dd, *J* = 2.3, 0.7 Hz, 1H), 6.77 (t, *J* = 2.7 Hz, 1H), 5.40 – 5.31 (m, 2H), 3.74 (s, 3H), 3.27 (dd, *J* = 17.3, 2.7 Hz, 1H), 3.21 (d, *J* = 2.8 Hz, 1H), 3.19 (s, 3H), 2.42 (s, 3H);

^{13}C NMR (150 MHz, acetone-d_6): δ 206.1, 175.7, 171.8, 157.3, 144.4, 142.4, 138.6, 138.1, 136.4, 133.2, 132.6, 130.7, 130.1, 129.4, 128.4, 127.8, 127.5, 122.7, 114.4, 112.0, 109.7, 79.9, 56.0, 44.8, 40.5, 26.6, 21.5;

HRMS: calculated for $C_{28}H_{27}ClN_3O_4S_2$ $[M+H]^+$: 568.1126; Found: 568.1121;

IR: 3143, 2835, 1693, 1602, 1536, 1498, 1372, 1335, 1287, 1216, 1164, 1091, 1032, 918, 804, 765, 733, 664, 560, 548 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-6-methoxy-1-methyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)phenyl)-4-methylbenzenesulfonamide (4r)



Prepared according to the general procedure from **3r** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 3 h to provide the title compound as a white solid with 51% yield. m.p. 218-220 ℃.

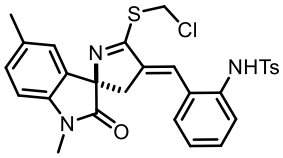
^{1}H NMR (400 MHz, acetone-d_6): δ 9.02 (s, 1H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.53 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.37 – 7.33 (m, 1H), 7.33 – 7.23 (m, 2H), 7.06 (d, *J* = 8.2 Hz, 1H), 6.75 (t, *J* = 2.7 Hz, 1H), 6.65 (d, *J* = 2.3 Hz, 1H), 6.58 (dd, *J* = 8.2, 2.3 Hz, 1H), 5.34 (q, *J* = 11.1 Hz, 2H), 3.83 (s, 3H), 3.26 (dd, *J* = 17.3, 2.7 Hz, 1H), 3.21 (s, 3H), 3.12 (dd, *J* = 17.3, 2.7 Hz, 1H), 2.42 (s, 3H);

^{13}C NMR (100 MHz, DMSO-d_6) δ 175.6, 170.5, 160.9, 144.8, 143.1, 140.6, 137.3, 135.2, 131.9, 129.8 (2C), 129.3, 128.5, 127.7, 126.9, 126.6 (2C), 124.3, 122.4, 121.9, 107.1, 96.5, 78.2, 55.6, 44.5, 26.4, 21.1;

HRMS: calculated for $C_{28}H_{27}ClN_3O_4S_2$ $[M+H]^+$: 568.1126; Found: 568.1130;

IR: 3116, 2932, 1701, 1624, 1532, 1508, 1455, 1419, 1377, 1331, 1226, 1158, 1087, 1062, 817, 761, 727, 656, 565, 550 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-1,5-dimethyl-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)phenyl)-4-methylbenzenesulfonamide (4s)



Prepared according to the general procedure from **3s** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 3 h to provide the title compound as a white solid with 47% yield. m.p. 203-205 ℃.

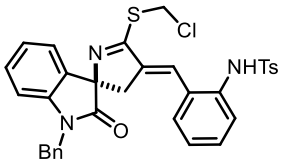
^{1}H NMR (400 MHz, acetone-d_6): δ 9.02 (s, 1H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.55 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.37 – 7.30 (m, 2H), 7.30 – 7.24 (m, 1H), 7.18 – 7.13 (m, 1H), 7.04 – 6.98 (m, 1H), 6.91 (d, *J* = 7.9 Hz, 1H), 6.78 (t, *J* = 2.7 Hz, 1H), 5.40 – 5.30 (m, 2H), 3.27 (dd, *J* = 17.3, 2.7 Hz, 1H), 3.19 (s, 3H), 3.16 (dd, *J* = 17.3, 2.8 Hz, 1H), 2.42 (s, 3H), 2.27 (s, 3H);

^{13}C NMR (100 MHz, acetone-d_6): δ 176.9, 171.3, 144.3, 142.1, 138.5, 136.8, 133.4, 132.6, 131.6, 131.3, 130.7, 130.4 (2C), 129.9, 129.8, 128.0 (2C), 126.8, 126.5 (2C), 125.0, 109.2, 62.0, 38.6, 26.6, 21.4, 21.0;

HRMS: calculated for $C_{28}H_{27}ClN_3O_3S_2$ $[M+H]^+$: 552.1177; Found: 552.1172;

IR: 3199, 2918, 1686, 1602, 1539, 1497, 1481, 1367, 1336, 1291, 1156, 1093, 1060, 996, 919, 811, 727, 698, 659, 551, 530 cm^{-1}.

(*E*)-*N*-(2-((1-benzyl-5'-((chloromethyl)thio)-2-oxospiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)phenyl)-4-methylbenzenesulfonamide (4t)



Prepared according to the general procedure from **3t** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 3 h to provide the title compound as a white solid with 64% yield. m.p. 174-175 ℃.

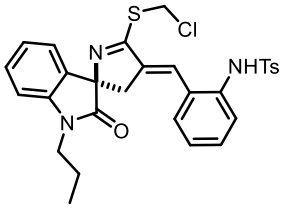
^{1}H NMR (600 MHz, acetone-d_6) δ 9.05 (s, 1H), 7.67 (d, J = 8.3 Hz, 2H), 7.59 – 7.56 (m, 1H), 7.40 (t, J = 6.9 Hz, 4H), 7.38 – 7.36 (m, 1H), 7.33 (t, J = 7.6 Hz, 3H), 7.29 – 7.26 (m, 2H), 7.25 – 7.23 (m, 1H), 7.21 – 7.18 (m, 1H), 7.04 – 7.02 (m, 1H), 6.92 (d, J = 7.9 Hz, 1H), 6.81 (t, J = 2.7 Hz, 1H), 5.40 – 5.33 (m, 2H), 5.01 (d, J = 15.7 Hz, 1H), 4.95 (d, J = 15.8 Hz, 1H), 3.38 (dd, J = 17.3, 2.7 Hz, 1H), 3.26 (dd, J = 17.3, 2.8 Hz, 1H), 2.41 (s, 3H);

^{13}C NMR (150 MHz, DMSO-d_6): δ 175.2, 171.1, 143.2, 142.4, 140.5, 137.3, 136.1, 135.2, 131.9, 130.7, 129.8 (2C), 129.4 (2C), 128.7 (2C), 128.6, 127.7, 127.5, 127.3 (2C), 126.9, 126.6, 123.8, 123.0, 122.2, 109.5, 78.6, 44.5, 43.0, 21.1;

HRMS: calculated for $C_{33}H_{29}ClN_3O_3S_2$ $[M+H]^+$: 614.1333; Found: 614.1335;

IR: 3260, 2920, 1702, 1613, 1538, 1485, 1466, 1335, 1189, 1162, 1091, 753, 732, 665, 563, 548 cm^{-1}.

(*E*)-*N*-(2-((5'-((chloromethyl)thio)-2-oxo-1-propylspiro[indoline-3,2'-pyrrol]-4'(3'H)-ylidene)methyl)phenyl)-4-methylbenzenesulfonamide (4u)



Prepared according to the general procedure from **3u** (0.20 mmol), DBU (0.40 mmol), CH_2Cl_2 (4.0 mL) at room temperature for 4 h to provide the title compound as a white solid with 50% yield. m.p. 222-224 ℃.

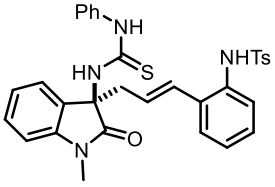
^{1}H NMR (400 MHz, acetone-d_6): δ 9.04 (s, 1H), 7.71 – 7.64 (m, 2H), 7.55 (d, J = 7.4 Hz, 1H), 7.42 – 7.32 (m, 5H), 7.31 – 7.25 (m, 1H), 7.18 (t, J = 6.8 Hz, 1H), 7.11 – 7.03 (m, 2H), 6.79 (s, 1H), 5.42 – 5.28 (m, 2H), 3.72 (q, J = 6.4 Hz, 2H), 3.33 – 3.16 (m, 2H), 2.43 (d, J = 6.4 Hz, 3H), 1.77 – 1.68 (m, 2H), 0.98 – 0.93 (m, 3H);

^{13}C NMR (100 MHz, DMSO-d_6): δ 175.0, 170.9, 143.1, 142.8, 140.5, 137.3, 135.2, 131.9, 130.7, 129.8 (2C), 129.5, 129.3, 128.6, 127.6, 126.9, 126.6 (2C), 123.7, 122.7, 122.0, 109.1, 78.5, 44.5, 41.1, 21.1, 20.3, 11.2;

HRMS: calculated for $C_{29}H_{29}ClN_3O_3S_2$ $[M+H]^+$: 556.1333; Found: 556.1329;

IR: 3147, 2958, 1692, 1614, 1540, 1485, 1465, 1379, 1363, 1333, 1212, 1164, 1091, 922, 812, 748, 692, 661, 562, 548 cm^{-1}.

(*E*)-4-methyl-*N*-(2-(3-(1-methyl-2-oxo-3-(3-phenylthioureido)indolin-3-yl)prop-1-en-1-yl)phenyl)benzenesulfonamide (5)



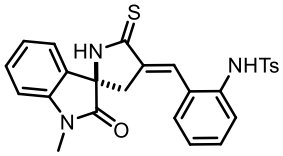
Prepared according to the procedure from **3a** (0.20 mmol), aniline (0.24 mmol), THF (2 mL) at room temperature for 4 h to provide the title compound as a white solid with 90% yield. m.p. 99-101 ℃.

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.82 (s, 1H), 9.50 (s, 1H), 8.01 (s, 1H), 7.46 (dd, J = 18.1, 8.0 Hz, 4H), 7.31 – 7.24 (m, 4H), 7.23 – 7.14 (m, 5H), 7.03 – 6.99 (m, 2H), 6.94 (dd, J = 8.6, 4.1 Hz, 2H), 6.51 (d, J = 15.6 Hz, 1H), 5.78 – 5.67 (m, 1H), 3.11 (s, 3H), 2.58 (dd, J = 13.2, 6.6 Hz, 1H), 2.40 (dd, J = 13.7, 7.6 Hz, 1H), 2.33 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 178.8, 174.8, 143.6, 143.1, 139.3, 137.2, 133.5, 133.4, 130.4, 129.9, 129.5, 128.6, 128.1 (2C), 126.7, 126.1, 124.0, 123.4, 122.1, 121.8, 108.1, 63.4, 41.5, 26.4, 21.0;

HRMS: calculated for $C_{32}H_{31}N_4O_3S_2$ $[M+H]^+$: 583.1832; Found: 583.1826;
IR: 3339, 3058, 2921, 1722, 1613, 1529, 1494, 1470, 1371, 1330, 1254, 1162, 1123, 1091, 927, 814, 752, 697, 666, 566 cm^{-1}.

(*E*)-4-methyl-*N*-(2-((1-methyl-2-oxo-5'-thioxospiro[indoline-3,2'-pyrrolidin]-4'-ylidene)methyl)phenyl)benzenesulfonamide (6)



Prepared according to the procedure from **3a** (0.10 mmol), DBU (0.20 mmol), CH_3CN (2.0 mL) at room temperature for 1 h to provide the title compound as a yellow solid with 54% yield. m.p. 244-245 ℃.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.81 (s, 1H), 10.14 (s, 1H), 7.83 (s, 1H), 7.68 (d, J = 7.8 Hz, 2H), 7.46 (d, J = 8.1 Hz, 1H), 7.38 (t, J = 6.5 Hz, 3H), 7.31 (d, J = 7.2 Hz, 1H), 7.23 (d, J = 7.6 Hz, 1H), 7.19 (d, J = 7.5 Hz, 1H), 7.09 (d, J = 8.0 Hz, 2H), 6.98 (d, J = 7.8 Hz, 1H), 3.39 (d, J = 18.1 Hz, 1H), 3.24 (s, 1H), 3.15 (s, 3H), 2.37 (s, 3H);
^{13}C NMR (100 MHz, DMSO-d_6): δ 197.2, 174.4, 143.2, 143.0, 138.6, 137.6, 135.8, 132.0, 130.1, 129.9, 129.7 (2C), 129.3, 129.0, 128.9, 126.8 (2C), 126.4, 126.3, 123.5, 123.0, 109.1, 67.3, 26.4, 21.1;
HRMS: calculated for $C_{26}H_{24}N_3O_3S_2$ $[M+H]^+$: 490.1254; Found: 490.1253;
IR: 3059, 2918, 2822, 1726, 1612, 1491, 1469, 1444, 1349, 1331, 1217, 1161, 1092, 1022, 990, 817, 761, 661, 563, 539 cm^{-1}.

4. DFT calculations

Computational Details

The DFT calculations presented herein were accomplished with the B3LYP-D3 functional (with the default D3 dispersion correction proposed by Grimme)[3,4] as implemented in the Gaussian 16 program package.[5] All geometries were optimized in dichloroethane using the implicit SMD continuum solvation model.[6] The 6-31G(d,p) basis sets for the S, C, N, O, H elements were used. Based on the optimized geometries, the final energies in DMA were obtained by single-point calculations employing the larger basis sets (6-311+G(2df,2p)) for all elements. Frequency calculations were carried out at the same level of theory as the geometry optimizations to identify the nature of all stationary points and to obtain the Gibbs free energy corrections at 298.15 K.

The pK_as were calculated using the standard methodology as applied in previous studies in water oxidation,[7] proton reduction,[8] and CO_2 reduction,[9] which were also summarized in recent reviews.[7b,10,11] The Gibbs free energy of a proton (contribution from translational entropy) is –6.3 kcal mol^{-1} in the gas phase. The experimental value of -251.3 kcal mol^{-1} was used for a proton's solvation free energy in dichloroethane.[12] Taken together, the total Gibbs free energy of a proton in the mixed solvent becomes –257.6 kcal mol^{-1}, which was used as the reference for the calculations of the pK_as. For all species, a concentration correction of 1.9 kcal mol^{-1} at 298.15 K was added, which originates from the free energy change from 1 atm (24.5 L mol^{-1} for ideal gas) to 1 M (1 mol L^{-1} in dichloroethane solution).

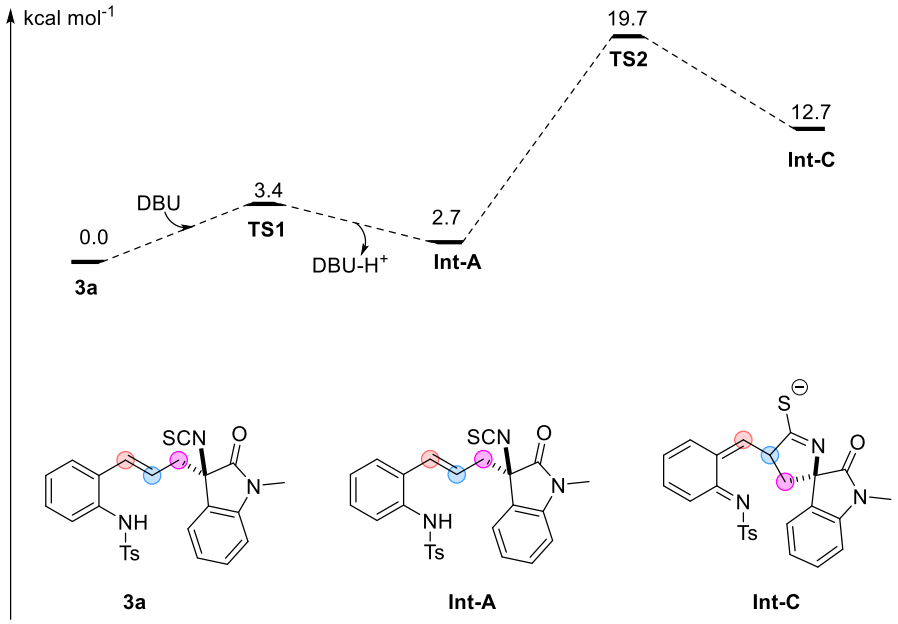


Figure S1. Gibbs free energy diagram (in kcal mol^{-1}) for the reaction of **3a** to **Int-C**.

Cartesian coordinates for all stationary points.

3a E_{opt}= -2190.97857820 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.190246	5.313219	0.432988

2	6	0	-1.776942	4.055235	0.566113
3	6	0	-1.117824	2.921880	0.082751
4	6	0	0.136454	3.029669	-0.558866
5	6	0	0.721584	4.303536	-0.652547
6	6	0	0.067652	5.434066	-0.165046
7	1	0	-1.706923	6.192292	0.806288
8	1	0	-2.737538	3.932207	1.054131
9	1	0	1.682894	4.402829	-1.147757
10	1	0	0.533500	6.410235	-0.263500
11	6	0	0.786714	1.828643	-1.110398
12	6	0	2.099580	1.560482	-1.059217
13	6	0	2.681331	0.279660	-1.574209
14	7	0	-1.726911	1.637570	0.298253
15	6	0	3.008713	-0.739668	-0.430350
16	6	0	3.538310	-2.035586	-1.116890
17	8	0	4.569201	-2.128942	-1.760382
18	7	0	2.598811	-3.016582	-0.913313
19	6	0	2.710849	-4.364716	-1.439749
20	1	0	3.609548	-4.411285	-2.055368
21	1	0	1.835985	-4.607562	-2.050440
22	1	0	2.790590	-5.089037	-0.622748
23	6	0	1.575687	-2.577896	-0.054936
24	6	0	0.489863	-3.300987	0.427757
25	6	0	-0.379941	-2.648337	1.313180
26	6	0	-0.160921	-1.325239	1.706689
27	6	0	0.938036	-0.609338	1.203752
28	6	0	1.789146	-1.240877	0.309924
29	1	0	0.324925	-4.333256	0.138494
30	1	0	-1.238127	-3.185723	1.702547
31	1	0	-0.844874	-0.846545	2.399890
32	1	0	1.123116	0.414082	1.512282
33	1	0	0.125408	1.098030	-1.573809
34	1	0	2.780239	2.255247	-0.569777
35	1	0	1.981388	-0.219613	-2.251797
36	1	0	3.618576	0.447598	-2.116012
37	7	0	4.014189	-0.194060	0.437769
38	6	0	4.293337	0.600338	1.280819
39	16	0	4.778425	1.617862	2.412170
40	1	0	-1.048170	0.876882	0.351982
41	16	0	-2.939379	1.193532	-0.821894
42	6	0	-3.317693	-0.438308	-0.213960
43	6	0	-3.087075	-1.540456	-1.037686
44	6	0	-3.847576	-0.584266	1.071911
45	6	0	-3.394151	-2.812604	-0.558319

46	1	0	-2.674168	-1.401437	-2.030547
47	6	0	-4.139931	-1.864097	1.534116
48	1	0	-4.025034	0.284260	1.697401
49	6	0	-3.917796	-2.994733	0.729711
50	1	0	-3.217694	-3.677203	-1.191831
51	1	0	-4.549091	-1.990031	2.532579
52	8	0	-2.392062	1.074592	-2.187220
53	8	0	-4.065500	2.112904	-0.604604
54	6	0	-4.193831	-4.378073	1.259482
55	1	0	-5.034480	-4.378832	1.959657
56	1	0	-3.318369	-4.760677	1.800085
57	1	0	-4.412152	-5.080978	0.450419

Int-A E_{opt}= -2190.48327476 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.572501	5.187329	-0.121589
2	6	0	-2.135938	3.917702	-0.040013
3	6	0	-1.411192	2.757844	-0.423714
4	6	0	-0.070471	2.949270	-0.903382
5	6	0	0.466452	4.244213	-0.974297
6	6	0	-0.264633	5.366644	-0.589323
7	1	0	-2.163475	6.048429	0.183018
8	1	0	-3.144620	3.807834	0.343205
9	1	0	1.474527	4.367581	-1.363185
10	1	0	0.169430	6.359767	-0.661319
11	6	0	0.701880	1.768548	-1.301171
12	6	0	2.038195	1.621329	-1.275619
13	6	0	2.708452	0.327988	-1.628252
14	7	0	-1.860903	1.454936	-0.348129
15	6	0	3.075525	-0.534802	-0.369316
16	6	0	3.742828	-1.844868	-0.885541
17	8	0	4.799603	-1.915100	-1.491943
18	7	0	2.893468	-2.880361	-0.587447
19	6	0	3.138293	-4.260388	-0.961150
20	1	0	4.057717	-4.292341	-1.546612
21	1	0	2.308316	-4.644062	-1.562670
22	1	0	3.252291	-4.885299	-0.069341
23	6	0	1.799821	-2.443545	0.183628
24	6	0	0.765966	-3.205574	0.714048
25	6	0	-0.204320	-2.535420	1.475389
26	6	0	-0.132229	-1.159021	1.697539

27	6	0	0.920223	-0.406037	1.153671
28	6	0	1.874690	-1.057625	0.388311
29	1	0	0.710650	-4.276412	0.549213
30	1	0	-1.031782	-3.100581	1.891404
31	1	0	-0.900501	-0.663059	2.281010
32	1	0	0.980668	0.662693	1.320883
33	1	0	0.102487	0.909279	-1.595224
34	1	0	2.678429	2.424794	-0.914674
35	1	0	2.055925	-0.295329	-2.248662
36	1	0	3.645904	0.483894	-2.174188
37	7	0	3.996468	0.185232	0.463001
38	6	0	4.235588	1.121770	1.156460
39	16	0	4.671408	2.329622	2.110617
40	16	0	-3.378660	1.118848	0.042602
41	6	0	-3.299587	-0.680011	0.023970
42	6	0	-2.777415	-1.354565	-1.084667
43	6	0	-3.828986	-1.396313	1.095564
44	6	0	-2.777431	-2.745999	-1.105501
45	1	0	-2.361623	-0.792095	-1.913711
46	6	0	-3.830242	-2.793683	1.059998
47	1	0	-4.227870	-0.859036	1.949493
48	6	0	-3.303900	-3.489243	-0.035221
49	1	0	-2.359548	-3.268275	-1.962811
50	1	0	-4.241410	-3.348956	1.899400
51	8	0	-4.374296	1.517598	-0.996778
52	8	0	-3.767164	1.509870	1.430654
53	6	0	-3.263335	-4.997234	-0.061409
54	1	0	-3.874457	-5.431102	0.735357
55	1	0	-2.236471	-5.361478	0.069848
56	1	0	-3.621326	-5.389211	-1.019831

DBU E_{opt}= -462.147988800 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.576071	-0.852692	0.501827
2	6	0	2.788792	0.549387	-0.071155
3	6	0	1.527939	1.375902	0.159167
4	7	0	1.333489	-1.483641	0.058899
5	1	0	1.595852	2.335155	-0.364528
6	1	0	3.413319	-1.506182	0.224890
7	1	0	3.651135	1.042293	0.390286
8	6	0	0.350450	-0.724438	-0.309505

9	6	0	-0.937575	-1.424993	-0.702842
10	6	0	-2.059906	-1.291169	0.350186
11	6	0	-2.818997	0.041260	0.310434
12	6	0	-0.856634	1.443895	-0.581358
13	6	0	-1.947798	1.290472	0.492634
14	1	0	-1.298783	-1.065638	-1.675036
15	1	0	-1.629258	-1.450437	1.347629
16	1	0	-3.336037	0.120121	-0.656885
17	1	0	-1.276616	1.207642	-1.567559
18	1	0	-0.675777	-2.478555	-0.821514
19	1	0	-2.778316	-2.104197	0.190160
20	1	0	-3.601739	0.030415	1.079349
21	1	0	-0.536953	2.487912	-0.626992
22	1	0	-2.593462	2.176986	0.454080
23	1	0	-1.471657	1.287882	1.482066
24	7	0	0.357077	0.654734	-0.349827
25	1	0	2.581117	-0.804598	1.602108
26	1	0	2.980959	0.480477	-1.148813
27	1	0	1.408204	1.597334	1.230923

DBU-pt E_{opt}= -462.639656730 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.645328	0.784918	0.499566
2	6	0	-2.783815	-0.605060	-0.106893
3	6	0	-1.518228	-1.413236	0.154086
4	7	0	-1.374360	1.362995	0.054124
5	1	0	-1.542312	-2.348369	-0.408528
6	1	0	-3.448789	1.448977	0.174408
7	1	0	-3.641071	-1.122322	0.330137
8	6	0	-0.303236	0.658400	-0.298388
9	6	0	0.935622	1.423016	-0.685918
10	6	0	2.073677	1.301867	0.354096
11	6	0	2.860295	-0.011097	0.271707
12	6	0	0.904237	-1.466239	-0.554217
13	6	0	2.023787	-1.279411	0.477275
14	1	0	1.281178	1.070716	-1.664333
15	1	0	1.658426	1.438081	1.360146
16	1	0	3.345366	-0.068152	-0.712300
17	1	0	1.261412	-1.234421	-1.563307
18	1	0	0.657323	2.473153	-0.805720
19	1	0	2.759653	2.137667	0.182057

20	1	0	3.664805	0.011820	1.015687
21	1	0	0.577367	-2.506012	-0.562663
22	1	0	2.682811	-2.151976	0.403909
23	1	0	1.585046	-1.296634	1.482964
24	7	0	-0.312180	-0.669181	-0.274473
25	1	0	-2.656710	0.741141	1.594528
26	1	0	-2.950541	-0.521185	-1.185826
27	1	0	-1.415068	-1.658763	1.217289
28	1	0	-1.295180	2.370626	0.016108

TS1 Eopt= -2653.14430447 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.147455	5.390802	-0.100025
2	6	0	0.774663	4.258832	-0.614072
3	6	0	0.369331	2.959549	-0.242920
4	6	0	-0.697462	2.824938	0.694308
5	6	0	-1.284974	3.990350	1.221644
6	6	0	-0.886522	5.263951	0.830161
7	1	0	0.487350	6.374340	-0.413383
8	1	0	1.595895	4.374326	-1.309608
9	1	0	-2.068717	3.882455	1.965850
10	1	0	-1.363918	6.142091	1.254926
11	6	0	-1.190537	1.502172	1.104095
12	6	0	-2.425055	1.209276	1.544818
13	6	0	-2.834008	-0.189572	1.892819
14	7	0	1.001766	1.800470	-0.760480
15	6	0	-3.680589	-0.877214	0.769722
16	6	0	-3.976886	-2.332390	1.243103
17	8	0	-4.638600	-2.642407	2.219614
18	7	0	-3.304919	-3.180562	0.398550
19	6	0	-3.288493	-4.623870	0.545588
20	1	0	-3.850549	-4.876812	1.445106
21	1	0	-2.259888	-4.984871	0.643844
22	1	0	-3.754008	-5.102726	-0.321729
23	6	0	-2.694781	-2.478683	-0.657314
24	6	0	-1.964150	-2.995072	-1.721472
25	6	0	-1.464669	-2.082435	-2.663517
26	6	0	-1.695080	-0.709820	-2.542653
27	6	0	-2.430898	-0.207536	-1.458193
28	6	0	-2.918303	-1.101048	-0.516897
29	1	0	-1.790658	-4.060993	-1.822811

30	1	0	-0.885026	-2.456659	-3.501941
31	1	0	-1.282319	-0.016065	-3.266530
32	1	0	-2.606562	0.856939	-1.356009
33	1	0	-0.485568	0.683730	1.031016
34	1	0	-3.196063	1.975133	1.603612
35	1	0	-1.955130	-0.822550	2.053488
36	1	0	-3.444810	-0.222653	2.802030
37	7	0	-4.912521	-0.163678	0.581036
38	6	0	-5.465110	0.823177	0.207937
39	16	0	-6.313634	2.092356	-0.263429
40	16	0	1.586446	1.783386	-2.302318
41	6	0	2.368694	0.174192	-2.353193
42	6	0	3.532399	-0.042996	-1.608070
43	6	0	1.847517	-0.822078	-3.174474
44	6	0	4.148387	-1.288294	-1.661415
45	1	0	3.941468	0.747716	-0.988583
46	6	0	2.485947	-2.063384	-3.229460
47	1	0	0.957957	-0.627731	-3.760485
48	6	0	3.633787	-2.319264	-2.468583
49	1	0	5.044682	-1.467846	-1.073142
50	1	0	2.081176	-2.843679	-3.868010
51	8	0	2.663075	2.782712	-2.515991
52	8	0	0.486976	1.804877	-3.296618
53	6	0	4.319977	-3.661402	-2.510103
54	1	0	3.769315	-4.377244	-3.126343
55	1	0	4.419163	-4.081716	-1.502659
56	1	0	5.333014	-3.569994	-2.919455
57	1	0	1.254414	0.826852	-0.060651
58	6	0	0.865831	-1.499404	0.221697
59	6	0	0.708743	-2.496746	1.359183
60	1	0	1.466728	-1.934419	-0.584809
61	1	0	-0.098320	-1.226123	-0.213384
62	6	0	2.058087	-2.664673	2.044746
63	1	0	0.360507	-3.464438	0.986384
64	1	0	-0.028065	-2.129540	2.082967
65	1	0	1.958272	-3.278729	2.943801
66	1	0	2.767719	-3.170706	1.375123
67	7	0	1.511206	-0.273147	0.685014
68	6	0	2.324233	-0.257700	1.710807
69	7	0	2.615047	-1.360469	2.453090
70	6	0	2.913039	1.104854	2.039795
71	1	0	2.691490	1.741459	1.183065
72	1	0	2.364222	1.531894	2.887922
73	6	0	4.425390	1.122473	2.321057

74	1	0	4.919828	0.387778	1.673840
75	6	0	3.698172	-1.473614	3.453845
76	6	0	4.758806	0.842627	3.792583
77	1	0	5.818399	0.573342	3.879398
78	6	0	3.889452	-0.274883	4.386668
79	1	0	4.351074	-0.643089	5.309432
80	1	0	2.901766	0.105843	4.669970
81	1	0	3.436167	-2.344046	4.060036
82	1	0	4.642080	-1.718246	2.945684
83	1	0	4.616024	1.755423	4.383525
84	1	0	4.825879	2.099254	2.030646

TS2 E_{opt}= -2190.46171383 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.404669	-4.203175	-0.125166
2	6	0	3.472571	-2.824769	-0.076620
3	6	0	2.323183	-2.015912	-0.332154
4	6	0	1.081003	-2.715794	-0.642771
5	6	0	1.066498	-4.139884	-0.675378
6	6	0	2.201587	-4.880842	-0.427589
7	1	0	4.305532	-4.779694	0.072476
8	1	0	4.413639	-2.345736	0.167053
9	1	0	0.137524	-4.642554	-0.920652
10	1	0	2.177171	-5.965273	-0.465417
11	6	0	-0.080465	-1.948314	-0.881471
12	6	0	-1.404530	-2.374729	-1.015608
13	6	0	-2.456386	-1.366762	-1.415082
14	7	0	2.278485	-0.662508	-0.298397
15	6	0	-3.022539	-0.697480	-0.111196
16	6	0	-4.491780	-0.276956	-0.390785
17	8	0	-5.411751	-1.025763	-0.684544
18	7	0	-4.560963	1.095172	-0.316064
19	6	0	-5.770343	1.859260	-0.548020
20	1	0	-6.554129	1.163168	-0.849011
21	1	0	-5.611549	2.595664	-1.342433
22	1	0	-6.078392	2.381419	0.364269
23	6	0	-3.337545	1.646155	0.104083
24	6	0	-3.044814	2.981316	0.361509
25	6	0	-1.756724	3.281350	0.831245
26	6	0	-0.813559	2.274188	1.047359
27	6	0	-1.130970	0.933163	0.779174

28	6	0	-2.388002	0.627422	0.279534
29	1	0	-3.786569	3.759883	0.216341
30	1	0	-1.495756	4.315162	1.039998
31	1	0	0.173885	2.525661	1.418561
32	1	0	-0.397926	0.155704	0.965363
33	1	0	0.082740	-0.874548	-0.884805
34	1	0	-1.595141	-3.409755	-1.285907
35	1	0	-2.075428	-0.599330	-2.094164
36	1	0	-3.290692	-1.877516	-1.903632
37	7	0	-2.941693	-1.675041	0.952796
38	6	0	-2.082241	-2.590802	0.876813
39	16	0	-1.449433	-3.857112	1.727459
40	16	0	3.608473	0.226092	-0.019857
41	6	0	2.871777	1.863926	-0.057441
42	6	0	2.166743	2.284284	-1.190778
43	6	0	3.057127	2.724178	1.021827
44	6	0	1.637874	3.569879	-1.227303
45	1	0	2.021086	1.604715	-2.024024
46	6	0	2.522588	4.015453	0.969724
47	1	0	3.605208	2.380954	1.892711
48	6	0	1.805272	4.456074	-0.148701
49	1	0	1.076028	3.892862	-2.100136
50	1	0	2.660250	4.684141	1.815387
51	8	0	4.587596	0.155096	-1.138138
52	8	0	4.185652	0.033241	1.337140
53	6	0	1.206461	5.839444	-0.205471
54	1	0	1.666373	6.435893	-1.002708
55	1	0	1.341102	6.376437	0.737692
56	1	0	0.132898	5.791069	-0.420993

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6. X-Ray Single Crystal Diffraction Structure and Data of 3a, 4a, 4o and 3f

Table S2. Crystal data and structure refinement for mo_190715A_0m (**3a**).

Identification code	mo_190715a_0m
Empirical formula	C26 H23 N3 O3 S2
Formula weight	489.59
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 9.1025(13) Å = 90°.
	b = 18.318(3) Å = 91.066(2)°.
	c = 14.719(2) Å = 90°.
Volume	2453.9(6) Å3
Z	4
Density (calculated)	1.325 Mg/m3
Absorption coefficient	0.250 mm-1
F(000)	1024
Crystal size	0.15 x 0.12 x 0.1 mm3
Theta range for data collection	1.775 to 27.697°.
Index ranges	-10<=h<=11, -23<=k<=23, -19<=l<=17
Reflections collected	18550
Independent reflections	5514 [R(int) = 0.0438]
Completeness to theta = 25.242°	97.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6606
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	5514 / 0 / 309
Goodness-of-fit on F2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0580, wR2 = 0.1468
R indices (all data)	R1 = 0.0972, wR2 = 0.1663
Extinction coefficient	n/a
Largest diff. peak and hole	0.615 and -0.571 e.Å-3

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_190715A_0m (**3a**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)

C(1)	4330(6)	9733(2)	-1389(3)	101(1)
C(2)	4119(4)	9048(2)	-846(2)	63(1)
C(3)	3144(4)	9025(2)	-143(2)	66(1)
C(4)	2937(3)	8405(2)	367(2)	58(1)
C(5)	3699(3)	7777(1)	154(2)	45(1)
C(6)	4675(3)	7781(2)	-550(2)	58(1)
C(7)	4878(4)	8409(2)	-1040(2)	66(1)
C(8)	6020(3)	7405(1)	1633(2)	40(1)
C(9)	7141(3)	6896(1)	1488(2)	42(1)
C(10)	8540(3)	7173(2)	1330(2)	55(1)
C(11)	8812(3)	7906(2)	1327(2)	65(1)
C(12)	7716(3)	8399(2)	1505(2)	64(1)
C(13)	6307(3)	8146(2)	1658(2)	52(1)
C(14)	6871(3)	6104(1)	1534(2)	46(1)
C(15)	7741(3)	5586(2)	1229(2)	52(1)
C(16)	7450(3)	4785(1)	1325(2)	55(1)
C(17)	8565(3)	4394(1)	1955(2)	46(1)
C(18)	8176(3)	3565(1)	1960(2)	49(1)
C(19)	10486(3)	3674(1)	1395(2)	45(1)
C(20)	10120(3)	4385(1)	1626(2)	46(1)
C(21)	11155(3)	4932(2)	1553(2)	55(1)
C(22)	12534(3)	4749(2)	1214(2)	66(1)
C(23)	12858(4)	4046(2)	974(2)	72(1)
C(24)	11823(3)	3478(2)	1061(2)	62(1)
C(25)	8687(4)	5155(2)	3367(2)	61(1)
C(26)	9323(4)	2418(2)	1474(3)	70(1)
N(1)	4530(2)	7156(1)	1754(2)	45(1)
N(2)	9282(3)	3205(1)	1586(2)	51(1)
N(3)	8479(3)	4674(1)	2868(2)	58(1)
O(1)	2053(2)	6943(1)	1147(2)	76(1)
O(2)	4176(2)	6398(1)	364(2)	60(1)
O(3)	7032(2)	3318(1)	2242(2)	70(1)
S(1)	3531(1)	6996(1)	839(1)	50(1)
S(2)	8863(2)	5761(1)	4125(1)	126(1)

Table S4. Bond lengths [Å] and angles [°] for mo_190715A_0m (**3a**).

C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(1)-C(2)	1.502(5)
C(2)-C(3)	1.376(5)
C(2)-C(7)	1.393(4)
C(3)-H(3)	0.9300
C(3)-C(4)	1.376(4)
C(4)-H(4)	0.9300
C(4)-C(5)	1.382(4)
C(5)-C(6)	1.378(4)
C(5)-S(1)	1.759(3)
C(6)-H(6)	0.9300
C(6)-C(7)	1.372(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.402(3)
C(8)-C(13)	1.382(4)
C(8)-N(1)	1.445(3)
C(9)-C(10)	1.395(4)
C(9)-C(14)	1.473(4)
C(10)-H(10)	0.9300
C(10)-C(11)	1.365(4)
C(11)-H(11)	0.9300
C(11)-C(12)	1.374(4)
C(12)-H(12)	0.9300
C(12)-C(13)	1.386(4)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(14)-C(15)	1.321(4)
C(15)-H(15)	0.9300
C(15)-C(16)	1.498(4)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(16)-C(17)	1.539(4)
C(17)-C(18)	1.559(4)
C(17)-C(20)	1.505(4)
C(17)-N(3)	1.441(4)
C(18)-N(2)	1.332(3)

C(18)-O(3)	1.215(3)
C(19)-C(20)	1.390(3)
C(19)-C(24)	1.368(4)
C(19)-N(2)	1.424(3)
C(20)-C(21)	1.380(4)
C(21)-H(21)	0.9300
C(21)-C(22)	1.400(4)
C(22)-H(22)	0.9300
C(22)-C(23)	1.370(5)
C(23)-H(23)	0.9300
C(23)-C(24)	1.410(5)
C(24)-H(24)	0.9300
C(25)-N(3)	1.160(4)
C(25)-S(2)	1.581(4)
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(26)-N(2)	1.453(3)
N(1)-H(1)	0.9784
N(1)-S(1)	1.638(2)
O(1)-S(1)	1.431(2)
O(2)-S(1)	1.431(2)
H(1A)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
C(3)-C(2)-C(1)	121.2(3)
C(3)-C(2)-C(7)	117.2(3)
C(7)-C(2)-C(1)	121.6(3)
C(2)-C(3)-H(3)	118.9
C(2)-C(3)-C(4)	122.2(3)
C(4)-C(3)-H(3)	118.9
C(3)-C(4)-H(4)	120.4
C(3)-C(4)-C(5)	119.2(3)
C(5)-C(4)-H(4)	120.4
C(4)-C(5)-S(1)	119.8(2)

C(6)-C(5)-C(4)	120.0(3)
C(6)-C(5)-S(1)	120.0(2)
C(5)-C(6)-H(6)	120.1
C(7)-C(6)-C(5)	119.7(3)
C(7)-C(6)-H(6)	120.1
C(2)-C(7)-H(7)	119.2
C(6)-C(7)-C(2)	121.6(3)
C(6)-C(7)-H(7)	119.2
C(9)-C(8)-N(1)	119.7(2)
C(13)-C(8)-C(9)	121.3(2)
C(13)-C(8)-N(1)	119.0(2)
C(8)-C(9)-C(14)	121.7(2)
C(10)-C(9)-C(8)	116.9(2)
C(10)-C(9)-C(14)	121.4(2)
C(9)-C(10)-H(10)	119.2
C(11)-C(10)-C(9)	121.7(3)
C(11)-C(10)-H(10)	119.2
C(10)-C(11)-H(11)	119.6
C(10)-C(11)-C(12)	120.9(3)
C(12)-C(11)-H(11)	119.6
C(11)-C(12)-H(12)	120.4
C(11)-C(12)-C(13)	119.2(3)
C(13)-C(12)-H(12)	120.4
C(8)-C(13)-C(12)	119.9(3)
C(8)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(9)-C(14)-H(14)	116.9
C(15)-C(14)-C(9)	126.2(3)
C(15)-C(14)-H(14)	116.9
C(14)-C(15)-H(15)	117.8
C(14)-C(15)-C(16)	124.3(3)
C(16)-C(15)-H(15)	117.8
C(15)-C(16)-H(16A)	108.9
C(15)-C(16)-H(16B)	108.9
C(15)-C(16)-C(17)	113.3(2)
H(16A)-C(16)-H(16B)	107.7
C(17)-C(16)-H(16A)	108.9
C(17)-C(16)-H(16B)	108.9

C(16)-C(17)-C(18)	108.0(2)
C(20)-C(17)-C(16)	115.2(2)
C(20)-C(17)-C(18)	101.9(2)
N(3)-C(17)-C(16)	110.5(2)
N(3)-C(17)-C(18)	109.0(2)
N(3)-C(17)-C(20)	111.8(2)
N(2)-C(18)-C(17)	107.8(2)
O(3)-C(18)-C(17)	124.1(2)
O(3)-C(18)-N(2)	128.0(3)
C(20)-C(19)-N(2)	109.1(2)
C(24)-C(19)-C(20)	123.5(3)
C(24)-C(19)-N(2)	127.4(3)
C(19)-C(20)-C(17)	108.7(2)
C(21)-C(20)-C(17)	131.7(2)
C(21)-C(20)-C(19)	119.6(2)
C(20)-C(21)-H(21)	120.9
C(20)-C(21)-C(22)	118.2(3)
C(22)-C(21)-H(21)	120.9
C(21)-C(22)-H(22)	119.5
C(23)-C(22)-C(21)	121.0(3)
C(23)-C(22)-H(22)	119.5
C(22)-C(23)-H(23)	119.2
C(22)-C(23)-C(24)	121.5(3)
C(24)-C(23)-H(23)	119.2
C(19)-C(24)-C(23)	116.1(3)
C(19)-C(24)-H(24)	121.9
C(23)-C(24)-H(24)	121.9
N(3)-C(25)-S(2)	173.5(3)
H(26A)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(2)-C(26)-H(26A)	109.5
N(2)-C(26)-H(26B)	109.5
N(2)-C(26)-H(26C)	109.5
C(8)-N(1)-H(1)	111.2
C(8)-N(1)-S(1)	117.59(17)
S(1)-N(1)-H(1)	103.1
C(18)-N(2)-C(19)	112.0(2)

C(18)-N(2)-C(26)	124.0(3)
C(19)-N(2)-C(26)	123.7(2)
C(25)-N(3)-C(17)	148.1(3)
N(1)-S(1)-C(5)	105.79(12)
O(1)-S(1)-C(5)	109.23(13)
O(1)-S(1)-N(1)	105.22(14)
O(1)-S(1)-O(2)	119.98(13)
O(2)-S(1)-C(5)	107.58(13)
O(2)-S(1)-N(1)	108.19(11)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2x10^3$) for mo_190715A_0m (**3a**). The anisotropicdisplacement factor exponent takes the form: [$h^2 a^{*2} U_{11}$ + ... + 2 h k a* b* U_{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	136(4)	73(2)	93(3)	23(2)	7(3)	11(2)
C(2)	79(2)	55(2)	55(2)	0(1)	-8(2)	9(2)
C(3)	69(2)	50(2)	80(2)	-6(2)	-1(2)	21(1)
C(4)	47(2)	55(2)	71(2)	-5(2)	5(2)	14(1)
C(5)	35(1)	46(1)	55(2)	-5(1)	-5(1)	5(1)
C(6)	58(2)	55(2)	59(2)	-9(1)	3(2)	16(1)
C(7)	80(2)	66(2)	51(2)	0(2)	10(2)	10(2)
C(8)	34(1)	45(1)	42(2)	1(1)	2(1)	6(1)
C(9)	35(1)	47(1)	43(2)	1(1)	1(1)	9(1)
C(10)	32(1)	57(2)	74(2)	-4(1)	1(1)	6(1)
C(11)	36(2)	74(2)	86(2)	1(2)	-2(2)	-11(1)
C(12)	58(2)	49(2)	84(2)	-3(2)	-10(2)	-9(1)
C(13)	47(2)	47(2)	63(2)	-6(1)	-6(1)	6(1)
C(14)	40(1)	45(1)	54(2)	4(1)	4(1)	10(1)
C(15)	46(2)	47(1)	64(2)	9(1)	8(1)	12(1)
C(16)	53(2)	44(1)	69(2)	0(1)	5(2)	11(1)
C(17)	49(2)	37(1)	52(2)	2(1)	10(1)	6(1)
C(18)	51(2)	42(1)	54(2)	6(1)	4(1)	0(1)
C(19)	47(2)	45(1)	44(2)	1(1)	0(1)	6(1)
C(20)	43(1)	44(1)	51(2)	5(1)	6(1)	5(1)
C(21)	49(2)	48(2)	69(2)	9(1)	5(1)	-1(1)

C(22)	54(2)	72(2)	73(2)	13(2)	6(2)	-8(2)
C(23)	49(2)	90(3)	77(2)	6(2)	17(2)	12(2)
C(24)	53(2)	66(2)	66(2)	-6(2)	6(2)	17(1)
C(25)	70(2)	50(2)	63(2)	9(2)	10(2)	-14(1)
C(26)	80(2)	39(2)	91(3)	-10(2)	-15(2)	6(1)
N(1)	36(1)	44(1)	57(1)	0(1)	13(1)	9(1)
N(2)	53(1)	37(1)	64(2)	-2(1)	2(1)	4(1)
N(3)	74(2)	45(1)	57(2)	-1(1)	18(1)	2(1)
O(1)	30(1)	77(2)	121(2)	8(1)	12(1)	-4(1)
O(2)	54(1)	42(1)	85(2)	-11(1)	-1(1)	1(1)
O(3)	64(1)	53(1)	95(2)	7(1)	22(1)	-11(1)
S(1)	30(1)	44(1)	77(1)	-2(1)	5(1)	1(1)
S(2)	207(2)	73(1)	97(1)	-18(1)	2(1)	-57(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2x10^3$) for mo_190715A_0m (**3a**).

	x	y	z	U(eq)
H(1A)	3608	9753	-1872	151
H(1B)	5296	9734	-1641	151
H(1C)	4222	10151	-1002	151
H(3)	2606	9441	-8	80
H(4)	2292	8408	850	69
H(6)	5193	7360	-693	69
H(7)	5540	8407	-1514	79
H(10)	9308	6851	1225	66
H(11)	9751	8074	1203	78
H(12)	7918	8896	1524	77
H(13)	5556	8474	1777	63
H(14)	6004	5955	1802	55
H(15)	8592	5727	936	63
H(16A)	7472	4560	728	66
H(16B)	6471	4717	1561	66
H(21)	10942	5408	1724	66
H(22)	13241	5111	1150	80

H(23)	13782	3940	749	86
H(24)	12037	3000	901	74
H(26A)	10117	2220	1834	106
H(26B)	9468	2302	845	106
H(26C)	8411	2211	1667	106
H(1)	3951	7519	2078	54

Table S7. Torsion angles [°] for mo_190715A_0m (**3a**).

C(1)-C(2)-C(3)-C(4)	-179.7(3)
C(1)-C(2)-C(7)-C(6)	-179.3(3)
C(2)-C(3)-C(4)-C(5)	-1.9(5)
C(3)-C(2)-C(7)-C(6)	-0.4(5)
C(3)-C(4)-C(5)-C(6)	1.3(4)
C(3)-C(4)-C(5)-S(1)	176.3(2)
C(4)-C(5)-C(6)-C(7)	-0.4(5)
C(4)-C(5)-S(1)-N(1)	-76.3(2)
C(4)-C(5)-S(1)-O(1)	36.5(3)
C(4)-C(5)-S(1)-O(2)	168.3(2)
C(5)-C(6)-C(7)-C(2)	-0.1(5)
C(6)-C(5)-S(1)-N(1)	98.7(2)
C(6)-C(5)-S(1)-O(1)	-148.5(2)
C(6)-C(5)-S(1)-O(2)	-16.8(3)
C(7)-C(2)-C(3)-C(4)	1.4(5)
C(8)-C(9)-C(10)-C(11)	0.7(5)
C(8)-C(9)-C(14)-C(15)	164.9(3)
C(8)-N(1)-S(1)-C(5)	-50.2(2)
C(8)-N(1)-S(1)-O(1)	-165.78(18)
C(8)-N(1)-S(1)-O(2)	64.8(2)
C(9)-C(8)-C(13)-C(12)	2.4(4)
C(9)-C(8)-N(1)-S(1)	-84.1(3)
C(9)-C(10)-C(11)-C(12)	1.8(5)
C(9)-C(14)-C(15)-C(16)	177.4(3)
C(10)-C(9)-C(14)-C(15)	-17.4(5)
C(10)-C(11)-C(12)-C(13)	-2.3(5)
C(11)-C(12)-C(13)-C(8)	0.2(5)
C(13)-C(8)-C(9)-C(10)	-2.8(4)

C(13)-C(8)-C(9)-C(14)	174.9(3)
C(13)-C(8)-N(1)-S(1)	95.6(3)
C(14)-C(9)-C(10)-C(11)	-177.0(3)
C(14)-C(15)-C(16)-C(17)	-113.3(3)
C(15)-C(16)-C(17)-C(18)	-177.6(2)
C(15)-C(16)-C(17)-C(20)	-64.5(3)
C(15)-C(16)-C(17)-N(3)	63.3(3)
C(16)-C(17)-C(18)-N(2)	114.9(3)
C(16)-C(17)-C(18)-O(3)	-63.3(4)
C(16)-C(17)-C(20)-C(19)	-111.2(3)
C(16)-C(17)-C(20)-C(21)	70.6(4)
C(16)-C(17)-N(3)-C(25)	-69.9(6)
C(17)-C(18)-N(2)-C(19)	5.9(3)
C(17)-C(18)-N(2)-C(26)	179.8(3)
C(17)-C(20)-C(21)-C(22)	-179.9(3)
C(18)-C(17)-C(20)-C(19)	5.3(3)
C(18)-C(17)-C(20)-C(21)	-172.8(3)
C(18)-C(17)-N(3)-C(25)	171.6(5)
C(19)-C(20)-C(21)-C(22)	2.2(4)
C(20)-C(17)-C(18)-N(2)	-6.8(3)
C(20)-C(17)-C(18)-O(3)	175.0(3)
C(20)-C(17)-N(3)-C(25)	59.7(6)
C(20)-C(19)-C(24)-C(23)	1.1(5)
C(20)-C(19)-N(2)-C(18)	-2.4(3)
C(20)-C(19)-N(2)-C(26)	-176.3(3)
C(20)-C(21)-C(22)-C(23)	-1.0(5)
C(21)-C(22)-C(23)-C(24)	-0.2(5)
C(22)-C(23)-C(24)-C(19)	0.1(5)
C(24)-C(19)-C(20)-C(17)	179.3(3)
C(24)-C(19)-C(20)-C(21)	-2.3(4)
C(24)-C(19)-N(2)-C(18)	175.9(3)
C(24)-C(19)-N(2)-C(26)	2.0(5)
N(1)-C(8)-C(9)-C(10)	176.9(2)
N(1)-C(8)-C(9)-C(14)	-5.4(4)
N(1)-C(8)-C(13)-C(12)	-177.3(3)
N(2)-C(19)-C(20)-C(17)	-2.3(3)
N(2)-C(19)-C(20)-C(21)	176.0(3)
N(2)-C(19)-C(24)-C(23)	-177.0(3)

N(3)-C(17)-C(18)-N(2)	-125.0(3)
N(3)-C(17)-C(18)-O(3)	56.7(4)
N(3)-C(17)-C(20)-C(19)	121.6(2)
N(3)-C(17)-C(20)-C(21)	-56.5(4)
O(3)-C(18)-N(2)-C(19)	-176.0(3)
O(3)-C(18)-N(2)-C(26)	-2.1(5)
S(1)-C(5)-C(6)-C(7)	-175.3(2)

Symmetry transformations used to generate equivalent atoms:

Table S8. Hydrogen bonds for mo_190715A_0m [Å and °] (**3a**).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3)#1	0.98	1.99	2.969(3)	173.9

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z+1/2

Table S9. Crystal data and structure refinement for T_pl (**4a**).

Identification code	t_pl	
Empirical formula	C27 H24 Cl N3 O3 S2	
Formula weight	538.06	
Temperature	200(1) K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 14.872(5) Å	a= 90°.
	b = 16.485(6) Å	b= 93.106(8)°.
	c = 21.295(10) Å	g = 90°.
Volume	5213(4) $Å^3$	
Z	8	
Density (calculated)	1.371 Mg/m^3	
Absorption coefficient	2.028 mm^{-1}	
F(000)	2240	
Crystal size	0.3 x 0.2 x 0.1 mm^3	
Theta range for data collection	2.589 to 65.639°.	
Index ranges	-19<=h<=18, -18<=k<=22, -28<=l<=27	
Reflections collected	70140	
Independent reflections	12154 [R(int) = 0.1228]	
Completeness to theta = 53.594°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7521 and 0.5339	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12154 / 0 / 653	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0610, wR2 = 0.1510	
R indices (all data)	R1 = 0.0739, wR2 = 0.1596	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.739 and -0.615 $e.Å^{-3}$	

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for T_pl (**4a**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	136(1)	-1678(1)	2875(1)	39(1)

S(1)	3354(1)	1137(1)	4035(1)	28(1)
S(2)	566(1)	-909(1)	4125(1)	23(1)
O(1)	3857(1)	1874(1)	3988(1)	36(1)
O(2)	3818(1)	372(1)	4050(1)	38(1)
O(3)	-2325(1)	334(1)	4791(1)	31(1)
N(1)	2824(1)	1164(1)	4685(1)	27(1)
N(2)	-1018(1)	-179(1)	3821(1)	24(1)
N(3)	-3061(1)	599(1)	3838(1)	25(1)
C(1)	623(2)	1078(2)	1820(1)	44(1)
C(2)	1260(2)	1103(1)	2397(1)	34(1)
C(3)	1738(2)	1811(2)	2553(1)	42(1)
C(4)	2365(2)	1831(1)	3055(1)	38(1)
C(5)	2528(1)	1138(1)	3411(1)	28(1)
C(6)	2045(2)	434(1)	3273(1)	31(1)
C(7)	1413(2)	420(1)	2771(1)	34(1)
C(8)	2198(1)	1808(1)	4793(1)	24(1)
C(9)	1258(1)	1692(1)	4709(1)	22(1)
C(10)	707(1)	2357(1)	4832(1)	28(1)
C(11)	1058(1)	3108(1)	5011(1)	33(1)
C(12)	1988(2)	3210(1)	5077(1)	35(1)
C(13)	2550(1)	2561(1)	4976(1)	32(1)
C(14)	894(1)	904(1)	4502(1)	22(1)
C(15)	55(1)	714(1)	4283(1)	21(1)
C(16)	-205(1)	-100(1)	4058(1)	21(1)
C(17)	-788(1)	1223(1)	4182(1)	23(1)
C(18)	-1474(1)	622(1)	3858(1)	22(1)
C(19)	-2326(1)	496(1)	4234(1)	24(1)
C(20)	-2816(1)	826(1)	3232(1)	24(1)
C(21)	-1877(1)	873(1)	3226(1)	23(1)
C(22)	-1473(2)	1128(1)	2698(1)	32(1)
C(23)	-2018(2)	1326(2)	2167(1)	38(1)
C(24)	-2944(2)	1252(1)	2174(1)	35(1)
C(25)	-3365(1)	1006(1)	2709(1)	30(1)
C(26)	-44(1)	-1686(1)	3703(1)	26(1)
C(27)	-3989(1)	546(2)	4026(1)	34(1)
Cl(1A)	4060(1)	3725(1)	7133(1)	63(1)
S(1A)	1599(1)	6489(1)	4775(1)	33(1)
S(2A)	4000(1)	4278(1)	5798(1)	28(1)

O(1A)	1035(1)	5812(1)	4604(1)	46(1)
O(2A)	1281(1)	7300(1)	4653(1)	47(1)
O(3A)	7076(1)	5289(1)	5695(1)	38(1)
N(1A)	2523(1)	6371(1)	4402(1)	26(1)
N(2A)	5440(1)	4946(1)	6398(1)	32(1)
N(3A)	7528(1)	5738(1)	6685(1)	30(1)
C(1A)	2951(2)	6265(2)	7492(1)	44(1)
C(2A)	2612(2)	6318(1)	6817(1)	33(1)
C(3A)	2611(2)	7052(1)	6498(1)	37(1)
C(4A)	2282(2)	7113(1)	5882(1)	34(1)
C(5A)	1935(1)	6428(1)	5576(1)	32(1)
C(6A)	1935(2)	5686(1)	5882(1)	36(1)
C(7A)	2279(2)	5635(2)	6494(1)	38(1)
C(8A)	3223(1)	6968(1)	4488(1)	25(1)
C(9A)	3990(1)	6831(1)	4894(1)	24(1)
C(10A)	4618(1)	7464(1)	4954(1)	29(1)
C(11A)	4496(2)	8193(1)	4638(1)	34(1)
C(12A)	3740(2)	8315(1)	4243(1)	37(1)
C(13A)	3110(2)	7699(1)	4167(1)	34(1)
C(14A)	4100(1)	6055(1)	5233(1)	22(1)
C(15A)	4719(1)	5853(1)	5687(1)	24(1)
C(16A)	5479(2)	6334(1)	5999(1)	36(1)
C(17A)	4783(1)	5052(1)	5990(1)	25(1)
C(18A)	5967(1)	5708(1)	6444(1)	31(1)
C(19A)	6913(1)	5542(1)	6216(1)	29(1)
C(20A)	7105(1)	5974(1)	7230(1)	28(1)
C(21A)	6172(1)	5967(1)	7111(1)	31(1)
C(22A)	5621(2)	6163(2)	7584(1)	42(1)
C(23A)	6011(2)	6365(2)	8175(1)	49(1)
C(24A)	6933(2)	6364(2)	8283(1)	43(1)
C(25A)	7501(2)	6167(1)	7810(1)	35(1)
C(26A)	4372(2)	3526(1)	6357(1)	36(1)
C(27A)	8496(2)	5696(2)	6624(1)	42(1)

Table S11. Bond lengths [Å] and angles [°] for T_pl (**4a**).

Cl(1)-C(26)	1.798(2)
S(1)-O(1)	1.4331(15)
S(1)-O(2)	1.4372(16)
S(1)-N(1)	1.6299(19)
S(1)-C(5)	1.760(2)
S(2)-C(16)	1.7608(19)
S(2)-C(26)	1.785(2)
O(3)-C(19)	1.216(2)
N(1)-H(1)	0.8800
N(1)-C(8)	1.439(3)
N(2)-C(16)	1.291(2)
N(2)-C(18)	1.489(2)
N(3)-C(19)	1.355(2)
N(3)-C(20)	1.410(3)
N(3)-C(27)	1.460(2)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(1)-C(2)	1.511(4)
C(2)-C(3)	1.397(3)
C(2)-C(7)	1.391(3)
C(3)-H(3)	0.9500
C(3)-C(4)	1.381(4)
C(4)-H(4)	0.9500
C(4)-C(5)	1.386(3)
C(5)-C(6)	1.389(3)
C(6)-H(6)	0.9500
C(6)-C(7)	1.383(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.413(3)
C(8)-C(13)	1.394(3)
C(9)-C(10)	1.402(3)
C(9)-C(14)	1.465(3)
C(10)-H(10)	0.9500
C(10)-C(11)	1.388(3)
C(11)-H(11)	0.9500

C(11)-C(12)	1.393(3)
C(12)-H(12)	0.9500
C(12)-C(13)	1.380(3)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(14)-C(15)	1.345(3)
C(15)-C(16)	1.470(3)
C(15)-C(17)	1.514(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(17)-C(18)	1.556(3)
C(18)-C(19)	1.549(3)
C(18)-C(21)	1.502(3)
C(20)-C(21)	1.400(3)
C(20)-C(25)	1.377(3)
C(21)-C(22)	1.369(3)
C(22)-H(22)	0.9500
C(22)-C(23)	1.394(3)
C(23)-H(23)	0.9500
C(23)-C(24)	1.384(3)
C(24)-H(24)	0.9500
C(24)-C(25)	1.388(3)
C(25)-H(25)	0.9500
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
Cl(1A)-C(26A)	1.772(3)
S(1A)-O(1A)	1.4310(19)
S(1A)-O(2A)	1.4356(19)
S(1A)-N(1A)	1.6359(18)
S(1A)-C(5A)	1.756(2)
S(2A)-C(17A)	1.759(2)
S(2A)-C(26A)	1.786(2)
O(3A)-C(19A)	1.222(3)
N(1A)-H(1AA)	0.8800
N(1A)-C(8A)	1.436(3)

N(2A)-C(17A)	1.283(3)
N(2A)-C(18A)	1.482(3)
N(3A)-C(19A)	1.356(3)
N(3A)-C(20A)	1.405(3)
N(3A)-C(27A)	1.454(3)
C(1A)-H(1AB)	0.9800
C(1A)-H(1AC)	0.9800
C(1A)-H(1AD)	0.9800
C(1A)-C(2A)	1.499(3)
C(2A)-C(3A)	1.387(3)
C(2A)-C(7A)	1.396(3)
C(3A)-H(3A)	0.9500
C(3A)-C(4A)	1.379(3)
C(4A)-H(4A)	0.9500
C(4A)-C(5A)	1.389(3)
C(5A)-C(6A)	1.385(3)
C(6A)-H(6A)	0.9500
C(6A)-C(7A)	1.378(3)
C(7A)-H(7A)	0.9500
C(8A)-C(9A)	1.412(3)
C(8A)-C(13A)	1.391(3)
C(9A)-C(10A)	1.402(3)
C(9A)-C(14A)	1.472(3)
C(10A)-H(10A)	0.9500
C(10A)-C(11A)	1.385(3)
C(11A)-H(11A)	0.9500
C(11A)-C(12A)	1.382(3)
C(12A)-H(12A)	0.9500
C(12A)-C(13A)	1.385(3)
C(13A)-H(13A)	0.9500
C(14A)-H(14A)	0.9500
C(14A)-C(15A)	1.342(3)
C(15A)-C(16A)	1.507(3)
C(15A)-C(17A)	1.470(3)
C(16A)-H(16A)	0.9900
C(16A)-H(16B)	0.9900
C(16A)-C(18A)	1.555(3)
C(18A)-C(19A)	1.538(3)

C(18A)-C(21A)	1.498(3)
C(20A)-C(21A)	1.396(3)
C(20A)-C(25A)	1.378(3)
C(21A)-C(22A)	1.371(3)
C(22A)-H(22A)	0.9500
C(22A)-C(23A)	1.398(4)
C(23A)-H(23A)	0.9500
C(23A)-C(24A)	1.378(4)
C(24A)-H(24A)	0.9500
C(24A)-C(25A)	1.387(4)
C(25A)-H(25A)	0.9500
C(26A)-H(26C)	0.9900
C(26A)-H(26D)	0.9900
C(27A)-H(27D)	0.9800
C(27A)-H(27E)	0.9800
C(27A)-H(27F)	0.9800
O(1)-S(1)-O(2)	119.57(10)
O(1)-S(1)-N(1)	108.31(9)
O(1)-S(1)-C(5)	106.97(10)
O(2)-S(1)-N(1)	105.03(10)
O(2)-S(1)-C(5)	109.41(10)
N(1)-S(1)-C(5)	106.93(9)
C(16)-S(2)-C(26)	101.02(9)
S(1)-N(1)-H(1)	119.9
C(8)-N(1)-S(1)	120.17(14)
C(8)-N(1)-H(1)	119.9
C(16)-N(2)-C(18)	107.98(15)
C(19)-N(3)-C(20)	111.32(16)
C(19)-N(3)-C(27)	124.38(18)
C(20)-N(3)-C(27)	124.14(17)
H(1A)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
C(3)-C(2)-C(1)	120.3(2)
C(7)-C(2)-C(1)	121.3(2)

C(7)-C(2)-C(3)	118.3(2)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-C(2)	121.2(2)
C(4)-C(3)-H(3)	119.4
C(3)-C(4)-H(4)	120.2
C(3)-C(4)-C(5)	119.6(2)
C(5)-C(4)-H(4)	120.2
C(4)-C(5)-S(1)	120.55(17)
C(4)-C(5)-C(6)	120.0(2)
C(6)-C(5)-S(1)	119.46(17)
C(5)-C(6)-H(6)	120.0
C(7)-C(6)-C(5)	119.9(2)
C(7)-C(6)-H(6)	120.0
C(2)-C(7)-H(7)	119.6
C(6)-C(7)-C(2)	120.9(2)
C(6)-C(7)-H(7)	119.6
C(9)-C(8)-N(1)	121.59(18)
C(13)-C(8)-N(1)	117.73(17)
C(13)-C(8)-C(9)	120.67(18)
C(8)-C(9)-C(14)	120.32(18)
C(10)-C(9)-C(8)	117.02(18)
C(10)-C(9)-C(14)	122.65(17)
C(9)-C(10)-H(10)	118.9
C(11)-C(10)-C(9)	122.24(18)
C(11)-C(10)-H(10)	118.9
C(10)-C(11)-H(11)	120.3
C(10)-C(11)-C(12)	119.5(2)
C(12)-C(11)-H(11)	120.3
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-C(11)	119.8(2)
C(13)-C(12)-H(12)	120.1
C(8)-C(13)-H(13)	119.6
C(12)-C(13)-C(8)	120.76(19)
C(12)-C(13)-H(13)	119.6
C(9)-C(14)-H(14)	115.4
C(15)-C(14)-C(9)	129.15(18)
C(15)-C(14)-H(14)	115.4
C(14)-C(15)-C(16)	123.30(17)

C(14)-C(15)-C(17)	131.70(18)
C(16)-C(15)-C(17)	104.96(15)
N(2)-C(16)-S(2)	123.19(15)
N(2)-C(16)-C(15)	116.40(17)
C(15)-C(16)-S(2)	120.40(13)
C(15)-C(17)-H(17A)	111.1
C(15)-C(17)-H(17B)	111.1
C(15)-C(17)-C(18)	103.17(15)
H(17A)-C(17)-H(17B)	109.1
C(18)-C(17)-H(17A)	111.1
C(18)-C(17)-H(17B)	111.1
N(2)-C(18)-C(17)	107.40(14)
N(2)-C(18)-C(19)	107.21(15)
N(2)-C(18)-C(21)	110.99(15)
C(19)-C(18)-C(17)	113.03(16)
C(21)-C(18)-C(17)	116.22(16)
C(21)-C(18)-C(19)	101.66(15)
O(3)-C(19)-N(3)	126.34(18)
O(3)-C(19)-C(18)	125.21(17)
N(3)-C(19)-C(18)	108.45(16)
C(21)-C(20)-N(3)	109.27(16)
C(25)-C(20)-N(3)	128.80(18)
C(25)-C(20)-C(21)	121.91(19)
C(20)-C(21)-C(18)	109.08(16)
C(22)-C(21)-C(18)	130.46(17)
C(22)-C(21)-C(20)	120.46(18)
C(21)-C(22)-H(22)	120.8
C(21)-C(22)-C(23)	118.4(2)
C(23)-C(22)-H(22)	120.8
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-C(22)	120.4(2)
C(24)-C(23)-H(23)	119.8
C(23)-C(24)-H(24)	119.1
C(23)-C(24)-C(25)	121.9(2)
C(25)-C(24)-H(24)	119.1
C(20)-C(25)-C(24)	116.90(19)
C(20)-C(25)-H(25)	121.6
C(24)-C(25)-H(25)	121.6

Cl(1)-C(26)-H(26A)	109.0
Cl(1)-C(26)-H(26B)	109.0
S(2)-C(26)-Cl(1)	112.92(11)
S(2)-C(26)-H(26A)	109.0
S(2)-C(26)-H(26B)	109.0
H(26A)-C(26)-H(26B)	107.8
N(3)-C(27)-H(27A)	109.5
N(3)-C(27)-H(27B)	109.5
N(3)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(1A)-S(1A)-O(2A)	119.78(11)
O(1A)-S(1A)-N(1A)	106.24(10)
O(1A)-S(1A)-C(5A)	109.53(11)
O(2A)-S(1A)-N(1A)	107.50(10)
O(2A)-S(1A)-C(5A)	107.65(11)
N(1A)-S(1A)-C(5A)	105.22(9)
C(17A)-S(2A)-C(26A)	99.85(10)
S(1A)-N(1A)-H(1AA)	120.7
C(8A)-N(1A)-S(1A)	118.57(14)
C(8A)-N(1A)-H(1AA)	120.7
C(17A)-N(2A)-C(18A)	108.13(17)
C(19A)-N(3A)-C(20A)	111.05(18)
C(19A)-N(3A)-C(27A)	123.7(2)
C(20A)-N(3A)-C(27A)	125.21(18)
H(1AB)-C(1A)-H(1AC)	109.5
H(1AB)-C(1A)-H(1AD)	109.5
H(1AC)-C(1A)-H(1AD)	109.5
C(2A)-C(1A)-H(1AB)	109.5
C(2A)-C(1A)-H(1AC)	109.5
C(2A)-C(1A)-H(1AD)	109.5
C(3A)-C(2A)-C(1A)	120.7(2)
C(3A)-C(2A)-C(7A)	118.2(2)
C(7A)-C(2A)-C(1A)	121.1(2)
C(2A)-C(3A)-H(3A)	119.3
C(4A)-C(3A)-C(2A)	121.4(2)
C(4A)-C(3A)-H(3A)	119.3

C(3A)-C(4A)-H(4A)	120.3
C(3A)-C(4A)-C(5A)	119.3(2)
C(5A)-C(4A)-H(4A)	120.3
C(4A)-C(5A)-S(1A)	119.16(18)
C(6A)-C(5A)-S(1A)	120.00(18)
C(6A)-C(5A)-C(4A)	120.5(2)
C(5A)-C(6A)-H(6A)	120.4
C(7A)-C(6A)-C(5A)	119.2(2)
C(7A)-C(6A)-H(6A)	120.4
C(2A)-C(7A)-H(7A)	119.3
C(6A)-C(7A)-C(2A)	121.4(2)
C(6A)-C(7A)-H(7A)	119.3
C(9A)-C(8A)-N(1A)	121.61(18)
C(13A)-C(8A)-N(1A)	117.63(18)
C(13A)-C(8A)-C(9A)	120.74(19)
C(8A)-C(9A)-C(14A)	120.25(18)
C(10A)-C(9A)-C(8A)	116.70(18)
C(10A)-C(9A)-C(14A)	123.05(17)
C(9A)-C(10A)-H(10A)	118.9
C(11A)-C(10A)-C(9A)	122.2(2)
C(11A)-C(10A)-H(10A)	118.9
C(10A)-C(11A)-H(11A)	119.9
C(12A)-C(11A)-C(10A)	120.2(2)
C(12A)-C(11A)-H(11A)	119.9
C(11A)-C(12A)-H(12A)	120.4
C(11A)-C(12A)-C(13A)	119.2(2)
C(13A)-C(12A)-H(12A)	120.4
C(8A)-C(13A)-H(13A)	119.5
C(12A)-C(13A)-C(8A)	121.0(2)
C(12A)-C(13A)-H(13A)	119.5
C(9A)-C(14A)-H(14A)	115.7
C(15A)-C(14A)-C(9A)	128.58(18)
C(15A)-C(14A)-H(14A)	115.7
C(14A)-C(15A)-C(16A)	131.02(18)
C(14A)-C(15A)-C(17A)	124.44(18)
C(17A)-C(15A)-C(16A)	104.54(16)
C(15A)-C(16A)-H(16A)	111.1
C(15A)-C(16A)-H(16B)	111.1

C(15A)-C(16A)-C(18A)	103.47(17)
H(16A)-C(16A)-H(16B)	109.0
C(18A)-C(16A)-H(16A)	111.1
C(18A)-C(16A)-H(16B)	111.1
N(2A)-C(17A)-S(2A)	121.90(16)
N(2A)-C(17A)-C(15A)	116.58(17)
C(15A)-C(17A)-S(2A)	121.52(14)
N(2A)-C(18A)-C(16A)	107.13(16)
N(2A)-C(18A)-C(19A)	108.55(17)
N(2A)-C(18A)-C(21A)	112.72(18)
C(19A)-C(18A)-C(16A)	109.23(19)
C(21A)-C(18A)-C(16A)	116.91(19)
C(21A)-C(18A)-C(19A)	101.96(16)
O(3A)-C(19A)-N(3A)	126.2(2)
O(3A)-C(19A)-C(18A)	125.25(19)
N(3A)-C(19A)-C(18A)	108.49(19)
C(21A)-C(20A)-N(3A)	109.48(18)
C(25A)-C(20A)-N(3A)	128.0(2)
C(25A)-C(20A)-C(21A)	122.5(2)
C(20A)-C(21A)-C(18A)	108.87(19)
C(22A)-C(21A)-C(18A)	131.6(2)
C(22A)-C(21A)-C(20A)	119.5(2)
C(21A)-C(22A)-H(22A)	120.6
C(21A)-C(22A)-C(23A)	118.8(2)
C(23A)-C(22A)-H(22A)	120.6
C(22A)-C(23A)-H(23A)	119.7
C(24A)-C(23A)-C(22A)	120.6(2)
C(24A)-C(23A)-H(23A)	119.7
C(23A)-C(24A)-H(24A)	119.3
C(23A)-C(24A)-C(25A)	121.3(2)
C(25A)-C(24A)-H(24A)	119.3
C(20A)-C(25A)-C(24A)	117.2(2)
C(20A)-C(25A)-H(25A)	121.4
C(24A)-C(25A)-H(25A)	121.4
Cl(1A)-C(26A)-S(2A)	113.95(14)
Cl(1A)-C(26A)-H(26C)	108.8
Cl(1A)-C(26A)-H(26D)	108.8
S(2A)-C(26A)-H(26C)	108.8

S(2A)-C(26A)-H(26D)	108.8
H(26C)-C(26A)-H(26D)	107.7
N(3A)-C(27A)-H(27D)	109.5
N(3A)-C(27A)-H(27E)	109.5
N(3A)-C(27A)-H(27F)	109.5
H(27D)-C(27A)-H(27E)	109.5
H(27D)-C(27A)-H(27F)	109.5
H(27E)-C(27A)-H(27F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for T_pl (**4a**). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	46(1)	41(1)	31(1)	-7(1)	-2(1)	-7(1)
S(1)	16(1)	24(1)	45(1)	0(1)	7(1)	-3(1)
S(2)	17(1)	23(1)	28(1)	-2(1)	-5(1)	2(1)
O(1)	24(1)	31(1)	54(1)	2(1)	9(1)	-11(1)
O(2)	22(1)	30(1)	63(1)	0(1)	10(1)	5(1)
O(3)	28(1)	33(1)	30(1)	6(1)	1(1)	-3(1)
N(1)	17(1)	29(1)	36(1)	4(1)	0(1)	-1(1)
N(2)	17(1)	23(1)	30(1)	-2(1)	-5(1)	0(1)
N(3)	16(1)	28(1)	32(1)	-1(1)	-1(1)	-1(1)
C(1)	41(1)	53(2)	39(1)	1(1)	3(1)	1(1)
C(2)	28(1)	40(1)	36(1)	-3(1)	10(1)	2(1)
C(3)	36(1)	30(1)	59(2)	9(1)	3(1)	4(1)
C(4)	30(1)	23(1)	62(2)	2(1)	4(1)	-3(1)
C(5)	22(1)	27(1)	36(1)	-2(1)	10(1)	-2(1)
C(6)	39(1)	26(1)	30(1)	-1(1)	10(1)	-7(1)
C(7)	40(1)	32(1)	32(1)	-6(1)	9(1)	-9(1)
C(8)	17(1)	28(1)	28(1)	-1(1)	1(1)	-3(1)
C(9)	18(1)	26(1)	22(1)	-1(1)	0(1)	-3(1)
C(10)	18(1)	32(1)	32(1)	-7(1)	0(1)	-2(1)
C(11)	26(1)	29(1)	43(1)	-9(1)	4(1)	-2(1)
C(12)	28(1)	30(1)	48(1)	-12(1)	4(1)	-10(1)
C(13)	20(1)	34(1)	41(1)	-6(1)	2(1)	-7(1)

C(14)	17(1)	25(1)	24(1)	-2(1)	0(1)	-2(1)
C(15)	16(1)	24(1)	21(1)	0(1)	-1(1)	-1(1)
C(16)	16(1)	23(1)	22(1)	0(1)	-2(1)	-1(1)
C(17)	18(1)	24(1)	27(1)	-1(1)	-4(1)	-1(1)
C(18)	16(1)	22(1)	26(1)	-1(1)	-3(1)	1(1)
C(19)	20(1)	21(1)	30(1)	1(1)	-2(1)	-1(1)
C(20)	20(1)	22(1)	28(1)	-2(1)	-4(1)	0(1)
C(21)	18(1)	24(1)	27(1)	-2(1)	-5(1)	0(1)
C(22)	25(1)	42(1)	29(1)	0(1)	-1(1)	-3(1)
C(23)	39(1)	48(1)	27(1)	4(1)	-4(1)	-6(1)
C(24)	38(1)	37(1)	28(1)	-1(1)	-14(1)	0(1)
C(25)	24(1)	28(1)	37(1)	-3(1)	-10(1)	1(1)
C(26)	25(1)	23(1)	30(1)	-2(1)	-4(1)	0(1)
C(27)	17(1)	40(1)	47(1)	-4(1)	4(1)	-3(1)
Cl(1A)	62(1)	86(1)	43(1)	17(1)	10(1)	-14(1)
S(1A)	19(1)	48(1)	32(1)	-4(1)	-3(1)	7(1)
S(2A)	22(1)	25(1)	37(1)	3(1)	-5(1)	-7(1)
O(1A)	22(1)	69(1)	46(1)	-13(1)	-2(1)	-8(1)
O(2A)	35(1)	59(1)	45(1)	0(1)	-2(1)	26(1)
O(3A)	46(1)	30(1)	38(1)	-2(1)	-7(1)	-5(1)
N(1A)	22(1)	32(1)	23(1)	-4(1)	-3(1)	5(1)
N(2A)	26(1)	24(1)	45(1)	7(1)	-13(1)	-5(1)
N(3A)	23(1)	30(1)	36(1)	1(1)	-8(1)	-3(1)
C(1A)	48(1)	51(2)	32(1)	1(1)	1(1)	-5(1)
C(2A)	32(1)	38(1)	31(1)	-4(1)	5(1)	1(1)
C(3A)	41(1)	31(1)	38(1)	-8(1)	-1(1)	2(1)
C(4A)	37(1)	28(1)	38(1)	-1(1)	0(1)	8(1)
C(5A)	23(1)	40(1)	32(1)	-7(1)	4(1)	5(1)
C(6A)	40(1)	36(1)	34(1)	-7(1)	10(1)	-10(1)
C(7A)	47(1)	34(1)	35(1)	1(1)	11(1)	-7(1)
C(8A)	26(1)	28(1)	23(1)	-2(1)	0(1)	5(1)
C(9A)	21(1)	26(1)	24(1)	1(1)	1(1)	4(1)
C(10A)	27(1)	27(1)	32(1)	2(1)	0(1)	0(1)
C(11A)	39(1)	27(1)	35(1)	3(1)	4(1)	-3(1)
C(12A)	53(1)	25(1)	32(1)	6(1)	1(1)	6(1)
C(13A)	38(1)	33(1)	29(1)	1(1)	-5(1)	9(1)
C(14A)	17(1)	23(1)	27(1)	2(1)	-1(1)	-2(1)
C(15A)	18(1)	22(1)	32(1)	2(1)	-4(1)	-2(1)

C(16A)	28(1)	26(1)	52(1)	9(1)	-17(1)	-4(1)
C(17A)	19(1)	23(1)	34(1)	3(1)	-4(1)	-4(1)
C(18A)	26(1)	22(1)	43(1)	5(1)	-14(1)	-3(1)
C(19A)	30(1)	20(1)	35(1)	4(1)	-11(1)	-7(1)
C(20A)	28(1)	21(1)	36(1)	3(1)	-9(1)	-2(1)
C(21A)	26(1)	23(1)	42(1)	5(1)	-10(1)	-3(1)
C(22A)	34(1)	32(1)	61(2)	2(1)	3(1)	1(1)
C(23A)	62(2)	36(1)	50(2)	-2(1)	14(1)	1(1)
C(24A)	62(2)	29(1)	38(1)	3(1)	-5(1)	-7(1)
C(25A)	38(1)	29(1)	38(1)	3(1)	-14(1)	-5(1)
C(26A)	37(1)	26(1)	45(1)	9(1)	-3(1)	-9(1)
C(27A)	24(1)	48(2)	52(1)	-1(1)	-5(1)	-4(1)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for T_pl (**4a**).

	x	y	z	U(eq)
H(1)	2921	784	4971	33
H(1A)	324	548	1794	67
H(1B)	962	1163	1444	67
H(1C)	170	1506	1848	67
H(3)	1628	2287	2310	50
H(4)	2683	2318	3156	46
H(6)	2148	-39	3522	38
H(7)	1079	-61	2682	41
H(10)	72	2292	4791	33
H(11)	668	3548	5088	39
H(12)	2236	3724	5190	42
H(13)	3183	2628	5033	38
H(14)	1310	466	4525	26
H(17A)	-681	1694	3908	28
H(17B)	-1002	1419	4587	28
H(22)	-836	1169	2694	39
H(23)	-1752	1512	1798	46
H(24)	-3303	1373	1803	42
H(25)	-4002	964	2713	36

H(26A)	-695	-1617	3764	31
H(26B)	140	-2221	3879	31
H(27A)	-3993	360	4463	52
H(27B)	-4324	161	3752	52
H(27C)	-4273	1082	3989	52
H(1AA)	2590	5951	4154	31
H(1AB)	2447	6332	7764	65
H(1AC)	3396	6694	7581	65
H(1AD)	3232	5734	7570	65
H(3A)	2841	7522	6709	44
H(4A)	2293	7619	5669	41
H(6A)	1701	5217	5671	44
H(7A)	2289	5124	6701	46
H(10A)	5145	7390	5221	34
H(11A)	4934	8610	4692	40
H(12A)	3653	8815	4027	44
H(13A)	2593	7777	3892	40
H(14A)	3677	5644	5113	27
H(16A)	5248	6796	6240	43
H(16B)	5889	6543	5685	43
H(22A)	4985	6161	7511	51
H(23A)	5637	6505	8506	59
H(24A)	7185	6500	8688	52
H(25A)	8137	6165	7884	43
H(26C)	4120	2994	6221	43
H(26D)	5037	3485	6358	43
H(27D)	8621	5451	6219	63
H(27E)	8770	5365	6966	63
H(27F)	8751	6244	6647	63

Table S14. Torsion angles [°] for T_pl (**4a**).

S(1)-N(1)-C(8)-C(9)	101.5(2)
S(1)-N(1)-C(8)-C(13)	-77.7(2)
S(1)-C(5)-C(6)-C(7)	-178.10(16)
O(1)-S(1)-N(1)-C(8)	58.55(17)
O(1)-S(1)-C(5)-C(4)	-10.7(2)
O(1)-S(1)-C(5)-C(6)	168.62(16)
O(2)-S(1)-N(1)-C(8)	-172.62(15)
O(2)-S(1)-C(5)-C(4)	-141.58(18)
O(2)-S(1)-C(5)-C(6)	37.72(19)
N(1)-S(1)-C(5)-C(4)	105.17(18)
N(1)-S(1)-C(5)-C(6)	-75.52(18)
N(1)-C(8)-C(9)-C(10)	179.47(18)
N(1)-C(8)-C(9)-C(14)	-0.6(3)
N(1)-C(8)-C(13)-C(12)	178.8(2)
N(2)-C(18)-C(19)-O(3)	68.3(2)
N(2)-C(18)-C(19)-N(3)	-111.97(17)
N(2)-C(18)-C(21)-C(20)	109.28(18)
N(2)-C(18)-C(21)-C(22)	-71.5(3)
N(3)-C(20)-C(21)-C(18)	3.0(2)
N(3)-C(20)-C(21)-C(22)	-176.32(19)
N(3)-C(20)-C(25)-C(24)	177.0(2)
C(1)-C(2)-C(3)-C(4)	-175.8(2)
C(1)-C(2)-C(7)-C(6)	175.3(2)
C(2)-C(3)-C(4)-C(5)	0.1(4)
C(3)-C(2)-C(7)-C(6)	-2.2(3)
C(3)-C(4)-C(5)-S(1)	177.65(18)
C(3)-C(4)-C(5)-C(6)	-1.7(3)
C(4)-C(5)-C(6)-C(7)	1.2(3)
C(5)-S(1)-N(1)-C(8)	-56.42(17)
C(5)-C(6)-C(7)-C(2)	0.8(3)
C(7)-C(2)-C(3)-C(4)	1.8(3)
C(8)-C(9)-C(10)-C(11)	1.8(3)
C(8)-C(9)-C(14)-C(15)	-166.1(2)
C(9)-C(8)-C(13)-C(12)	-0.3(3)
C(9)-C(10)-C(11)-C(12)	-0.5(3)
C(9)-C(14)-C(15)-C(16)	176.53(18)

C(9)-C(14)-C(15)-C(17)	-0.7(3)
C(10)-C(9)-C(14)-C(15)	13.8(3)
C(10)-C(11)-C(12)-C(13)	-1.3(4)
C(11)-C(12)-C(13)-C(8)	1.7(4)
C(13)-C(8)-C(9)-C(10)	-1.4(3)
C(13)-C(8)-C(9)-C(14)	178.53(18)
C(14)-C(9)-C(10)-C(11)	-178.11(19)
C(14)-C(15)-C(16)-S(2)	5.4(3)
C(14)-C(15)-C(16)-N(2)	-175.32(18)
C(14)-C(15)-C(17)-C(18)	174.7(2)
C(15)-C(17)-C(18)-N(2)	2.62(19)
C(15)-C(17)-C(18)-C(19)	120.67(16)
C(15)-C(17)-C(18)-C(21)	-122.32(17)
C(16)-S(2)-C(26)-Cl(1)	88.16(12)
C(16)-N(2)-C(18)-C(17)	-1.2(2)
C(16)-N(2)-C(18)-C(19)	-123.00(17)
C(16)-N(2)-C(18)-C(21)	126.78(17)
C(16)-C(15)-C(17)-C(18)	-2.92(19)
C(17)-C(15)-C(16)-S(2)	-176.76(13)
C(17)-C(15)-C(16)-N(2)	2.5(2)
C(17)-C(18)-C(19)-O(3)	-49.9(3)
C(17)-C(18)-C(19)-N(3)	129.87(17)
C(17)-C(18)-C(21)-C(20)	-127.63(18)
C(17)-C(18)-C(21)-C(22)	51.6(3)
C(18)-N(2)-C(16)-S(2)	178.47(13)
C(18)-N(2)-C(16)-C(15)	-0.8(2)
C(18)-C(21)-C(22)-C(23)	179.9(2)
C(19)-N(3)-C(20)-C(21)	0.1(2)
C(19)-N(3)-C(20)-C(25)	-178.1(2)
C(19)-C(18)-C(21)-C(20)	-4.5(2)
C(19)-C(18)-C(21)-C(22)	174.7(2)
C(20)-N(3)-C(19)-O(3)	176.65(19)
C(20)-N(3)-C(19)-C(18)	-3.1(2)
C(20)-C(21)-C(22)-C(23)	-1.0(3)
C(21)-C(18)-C(19)-O(3)	-175.18(19)
C(21)-C(18)-C(19)-N(3)	4.6(2)
C(21)-C(20)-C(25)-C(24)	-1.1(3)
C(21)-C(22)-C(23)-C(24)	-1.0(4)

C(22)-C(23)-C(24)-C(25)	2.0(4)
C(23)-C(24)-C(25)-C(20)	-0.9(3)
C(25)-C(20)-C(21)-C(18)	-178.62(18)
C(25)-C(20)-C(21)-C(22)	2.1(3)
C(26)-S(2)-C(16)-N(2)	7.48(18)
C(26)-S(2)-C(16)-C(15)	-173.28(15)
C(27)-N(3)-C(19)-O(3)	1.2(3)
C(27)-N(3)-C(19)-C(18)	-178.52(18)
C(27)-N(3)-C(20)-C(21)	175.57(18)
C(27)-N(3)-C(20)-C(25)	-2.7(3)
S(1A)-N(1A)-C(8A)-C(9A)	101.1(2)
S(1A)-N(1A)-C(8A)-C(13A)	-77.5(2)
S(1A)-C(5A)-C(6A)-C(7A)	174.06(18)
O(1A)-S(1A)-N(1A)-C(8A)	-179.76(15)
O(1A)-S(1A)-C(5A)-C(4A)	-163.27(17)
O(1A)-S(1A)-C(5A)-C(6A)	23.0(2)
O(2A)-S(1A)-N(1A)-C(8A)	50.88(17)
O(2A)-S(1A)-C(5A)-C(4A)	-31.5(2)
O(2A)-S(1A)-C(5A)-C(6A)	154.70(18)
N(1A)-S(1A)-C(5A)-C(4A)	82.91(19)
N(1A)-S(1A)-C(5A)-C(6A)	-90.87(19)
N(1A)-C(8A)-C(9A)-C(10A)	-178.37(17)
N(1A)-C(8A)-C(9A)-C(14A)	1.3(3)
N(1A)-C(8A)-C(13A)-C(12A)	177.71(19)
N(2A)-C(18A)-C(19A)-O(3A)	58.5(3)
N(2A)-C(18A)-C(19A)-N(3A)	-122.59(18)
N(2A)-C(18A)-C(21A)-C(20A)	118.08(19)
N(2A)-C(18A)-C(21A)-C(22A)	-60.2(3)
N(3A)-C(20A)-C(21A)-C(18A)	0.2(2)
N(3A)-C(20A)-C(21A)-C(22A)	178.7(2)
N(3A)-C(20A)-C(25A)-C(24A)	-178.4(2)
C(1A)-C(2A)-C(3A)-C(4A)	-178.5(2)
C(1A)-C(2A)-C(7A)-C(6A)	177.5(2)
C(2A)-C(3A)-C(4A)-C(5A)	0.8(3)
C(3A)-C(2A)-C(7A)-C(6A)	-1.7(3)
C(3A)-C(4A)-C(5A)-S(1A)	-175.05(17)
C(3A)-C(4A)-C(5A)-C(6A)	-1.3(3)
C(4A)-C(5A)-C(6A)-C(7A)	0.4(3)

C(5A)-S(1A)-N(1A)-C(8A)	-63.66(17)
C(5A)-C(6A)-C(7A)-C(2A)	1.1(4)
C(7A)-C(2A)-C(3A)-C(4A)	0.7(3)
C(8A)-C(9A)-C(10A)-C(11A)	0.5(3)
C(8A)-C(9A)-C(14A)-C(15A)	-171.4(2)
C(9A)-C(8A)-C(13A)-C(12A)	-0.8(3)
C(9A)-C(10A)-C(11A)-C(12A)	-0.5(3)
C(9A)-C(14A)-C(15A)-C(16A)	0.6(4)
C(9A)-C(14A)-C(15A)-C(17A)	-178.77(19)
C(10A)-C(9A)-C(14A)-C(15A)	8.2(3)
C(10A)-C(11A)-C(12A)-C(13A)	-0.3(3)
C(11A)-C(12A)-C(13A)-C(8A)	0.9(3)
C(13A)-C(8A)-C(9A)-C(10A)	0.1(3)
C(13A)-C(8A)-C(9A)-C(14A)	179.77(18)
C(14A)-C(9A)-C(10A)-C(11A)	-179.11(19)
C(14A)-C(15A)-C(16A)-C(18A)	-175.8(2)
C(14A)-C(15A)-C(17A)-S(2A)	-2.7(3)
C(14A)-C(15A)-C(17A)-N(2A)	177.0(2)
C(15A)-C(16A)-C(18A)-N(2A)	-3.7(2)
C(15A)-C(16A)-C(18A)-C(19A)	113.66(19)
C(15A)-C(16A)-C(18A)-C(21A)	-131.3(2)
C(16A)-C(15A)-C(17A)-S(2A)	177.77(16)
C(16A)-C(15A)-C(17A)-N(2A)	-2.5(3)
C(16A)-C(18A)-C(19A)-O(3A)	-58.0(3)
C(16A)-C(18A)-C(19A)-N(3A)	120.92(19)
C(16A)-C(18A)-C(21A)-C(20A)	-117.1(2)
C(16A)-C(18A)-C(21A)-C(22A)	64.6(3)
C(17A)-S(2A)-C(26A)-Cl(1A)	76.04(14)
C(17A)-N(2A)-C(18A)-C(16A)	2.4(3)
C(17A)-N(2A)-C(18A)-C(19A)	-115.4(2)
C(17A)-N(2A)-C(18A)-C(21A)	132.4(2)
C(17A)-C(15A)-C(16A)-C(18A)	3.6(2)
C(18A)-N(2A)-C(17A)-S(2A)	179.75(15)
C(18A)-N(2A)-C(17A)-C(15A)	0.0(3)
C(18A)-C(21A)-C(22A)-C(23A)	178.2(2)
C(19A)-N(3A)-C(20A)-C(21A)	-2.6(2)
C(19A)-N(3A)-C(20A)-C(25A)	175.7(2)
C(19A)-C(18A)-C(21A)-C(20A)	1.9(2)

C(19A)-C(18A)-C(21A)-C(22A)	-176.4(2)
C(20A)-N(3A)-C(19A)-O(3A)	-177.4(2)
C(20A)-N(3A)-C(19A)-C(18A)	3.8(2)
C(20A)-C(21A)-C(22A)-C(23A)	0.1(3)
C(21A)-C(18A)-C(19A)-O(3A)	177.7(2)
C(21A)-C(18A)-C(19A)-N(3A)	-3.4(2)
C(21A)-C(20A)-C(25A)-C(24A)	-0.4(3)
C(21A)-C(22A)-C(23A)-C(24A)	-0.4(4)
C(22A)-C(23A)-C(24A)-C(25A)	0.3(4)
C(23A)-C(24A)-C(25A)-C(20A)	0.1(3)
C(25A)-C(20A)-C(21A)-C(18A)	-178.17(19)
C(25A)-C(20A)-C(21A)-C(22A)	0.4(3)
C(26A)-S(2A)-C(17A)-N(2A)	5.3(2)
C(26A)-S(2A)-C(17A)-C(15A)	-174.96(18)
C(27A)-N(3A)-C(19A)-O(3A)	1.9(3)
C(27A)-N(3A)-C(19A)-C(18A)	-176.92(19)
C(27A)-N(3A)-C(20A)-C(21A)	178.1(2)
C(27A)-N(3A)-C(20A)-C(25A)	-3.6(4)

Symmetry transformations used to generate equivalent atoms:

Table S15. Hydrogen bonds for T_pl [Å and °] (**4a**).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3)#1	0.88	2.12	2.826(2)	136.9
N(1A)-H(1AA)...O(3A)#2	0.88	2.12	2.811(3)	134.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1 #2 -x+1,-y+1,-z+1

Table S16. Crystal data and structure refinement for 20221230-HXY456_auto (**4f**).

Identification code	20221230-HXY456_auto
Empirical formula	C27H23ClFN3O3S2
Formula weight	556.05
Temperature/K	299.75(10)
Crystal system	monoclinic
Space group	P21/n
a/Å	12.59755(19)
b/Å	15.5528(2)
c/Å	14.0293(2)
/°	90
/°	99.4784(14)
γ/°	90
Volume/Å3	2711.20(7)
Z	4
ρcalcg/cm^3	1.362
μ/mm 1	3.032
F(000)	1152.0
Crystal size/mm3	? × ? × ?
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.554 to 151.978
Index ranges	-15 ≤ h ≤ 15, -19 ≤ k ≤ 19, -14 ≤ l ≤ 17
Reflections collected	37327
Independent reflections	5535 [Rint = 0.0322, Rsigma = 0.0166]
Data/restraints/parameters	5535/0/337
Goodness-of-fit on F2	1.095
Final R indexes [I>=2σ (I)]	R1 = 0.0372, wR2 = 0.1104
Final R indexes [all data]	R1 = 0.0398, wR2 = 0.1126
Largest diff. peak/hole / e Å-3	0.29/-0.34

Table S17. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å2×10^3) for 20221230-HXY456_auto (**4f**). Ueq is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
S25	5430.8(3)	4060.6(2)	3570.2(3)	49.83(12)
S22	2692.9(4)	6323.3(3)	1383.0(4)	75.12(17)

Cl27	7249.1(4)	3292.7(4)	2728.9(4)	82.20(17)
O28	7482.9(10)	5312.3(8)	6589.2(9)	65.2(3)
N10	7190.4(10)	4848.7(8)	4486.7(10)	52.4(3)
N8	9081.0(10)	5722.0(8)	6137.4(9)	50.9(3)
N21	2675.6(11)	6334.0(9)	2536.3(11)	59.8(3)
F30	9879.1(13)	6736.8(12)	2607.2(12)	121.6(6)
O24	2006.2(13)	5623.7(11)	1010.7(13)	97.1(5)
C12	5716.6(11)	5782.8(9)	4179.8(10)	42.5(3)
C11	6195.4(11)	4926.0(9)	4118.5(10)	43.4(3)
C15	4183.2(12)	6836.6(9)	3774.7(11)	47.2(3)
C7	9427.0(11)	5990.8(9)	5281.1(11)	47.3(3)
C14	4713.2(11)	5994.4(9)	3775.5(10)	44.7(3)
C16	3202.9(12)	6988.7(10)	3154.7(12)	51.9(4)
O23	2471.6(18)	7173.4(11)	1029.4(13)	111.2(6)
C2	8560.2(12)	5992.1(10)	4529.0(11)	49.4(3)
C9	8014.2(12)	5547.1(9)	5981.2(12)	49.4(3)
C13	6599.0(11)	6307.7(9)	4749.6(12)	49.6(3)
C1	7572.6(11)	5690.8(9)	4904.1(11)	48.1(3)
C20	4610.1(14)	7515.4(10)	4370.6(13)	58.0(4)
C6	10446.2(13)	6221.2(12)	5147.7(14)	60.5(4)
C26	6441.5(14)	3249.2(10)	3659.0(13)	59.2(4)
C19	4114.1(17)	8308.1(11)	4342.3(16)	68.6(5)
C17	2714.0(15)	7792.0(12)	3129.1(15)	66.9(5)
C3	8694.7(15)	6251.8(14)	3622.0(14)	67.3(5)
C36	4372.9(17)	5232.4(12)	1307.6(14)	69.4(5)
C31	4019.6(18)	6072.8(12)	1244.3(13)	68.3(5)

C29	9765.8(15)	5671.9(15)	7072.8(13)	71.0(5)
C5	10587.8(15)	6473.7(13)	4232.5(17)	73.2(5)
C18	3172.5(17)	8447.7(12)	3714.3(17)	73.9(5)
C35	5423.4(18)	5040.6(15)	1248.5(14)	76.5(5)
C4	9720.8(18)	6489.5(15)	3504.0(16)	77.0(6)
C34	6159(2)	5675.2(19)	1126.0(15)	87.8(7)
C32	4738(3)	6712.5(16)	1113(2)	112.3(10)
C33	5788(3)	6507(2)	1057(3)	121.8(11)
C37	7310(2)	5454(3)	1067(2)	126.1(12)

Table S18. Anisotropic Displacement Parameters ($Å^2×10^3$) for 20221230-HXY456_auto (**4f**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
S25	44.4(2)	41.6(2)	60.8(2)	-8.09(15)	0.84(15)	-1.07(13)
S22	86.3(3)	58.3(3)	70.5(3)	15.0(2)	-17.5(2)	7.9(2)
Cl27	73.6(3)	84.5(4)	91.8(4)	-19.5(3)	23.5(3)	11.6(2)
O28	65.7(7)	59.5(7)	72.0(7)	9.1(6)	15.7(6)	-10.9(6)
N10	41.7(6)	43.0(6)	69.1(8)	-8.4(6)	-0.3(5)	3.1(5)
N8	42.5(6)	52.0(7)	55.5(7)	-0.9(6)	0.4(5)	2.5(5)
N21	48.1(7)	50.5(7)	76.7(9)	14.6(6)	-2.2(6)	0.8(6)
F30	103.1(10)	170.4(16)	102.5(10)	62.9(10)	49.9(8)	35.2(10)
O24	83.5(10)	89.0(10)	101.7(11)	-6.5(9)	-35.4(9)	-2.7(8)
C12	40.6(7)	38.4(7)	48.2(7)	-2.5(5)	6.5(5)	0.0(5)
C11	39.9(7)	40.2(7)	49.0(7)	-3.1(5)	4.4(5)	0.4(5)
C15	44.9(7)	40.6(7)	57.7(8)	4.2(6)	13.7(6)	5.1(6)
C7	39.3(7)	40.7(7)	61.0(8)	-3.4(6)	5.7(6)	3.5(5)
C14	42.3(7)	38.9(7)	51.5(7)	-1.0(6)	3.8(6)	2.3(5)

C16	45.1(8)	44.3(8)	67.7(9)	12.1(7)	13.3(7)	6.0(6)
O23	160.8(17)	73.8(10)	89.1(10)	33.7(8)	-8.4(10)	34.2(11)
C2	42.0(7)	46.4(8)	58.4(8)	-0.2(6)	4.4(6)	3.9(6)
C9	46.3(8)	38.9(7)	62.0(9)	-0.5(6)	5.9(6)	-2.7(6)
C13	41.1(7)	41.4(7)	64.6(9)	-6.3(6)	3.1(6)	-0.4(6)
C1	39.1(7)	42.9(7)	60.3(8)	-4.2(6)	2.1(6)	-0.7(6)
C20	60.3(9)	46.4(8)	67.6(10)	-4.4(7)	12.0(7)	6.7(7)
C6	39.1(8)	58.4(9)	83.1(12)	-4.4(8)	7.8(7)	3.4(7)
C26	62.0(10)	41.9(8)	71.7(10)	-6.9(7)	5.2(8)	5.1(7)
C19	79.0(12)	45.6(9)	85.8(13)	-7.7(8)	27.2(10)	6.4(8)
C17	56.2(9)	53.8(10)	92.4(13)	16.8(9)	17.0(9)	17.1(8)
C3	57.7(10)	80.4(12)	63.2(10)	9.9(9)	8.1(8)	14.4(9)
C36	78.3(12)	57.8(10)	70.5(11)	9.3(8)	7.3(9)	-12.4(9)
C31	92.9(14)	54.1(9)	55.4(9)	8.2(7)	4.4(9)	-12.8(9)
C29	58.4(10)	87.7(13)	61.0(10)	-2.4(9)	-7.0(8)	9.7(9)
C5	49.7(9)	71.5(12)	104.2(15)	9.4(10)	29.6(10)	5.5(8)
C18	77.0(12)	46.3(9)	103.8(15)	8.2(9)	31.2(11)	21.6(9)
C35	82.4(13)	82.2(14)	65.5(11)	4.3(10)	13.9(9)	-7.1(11)
C4	73.5(12)	83.6(13)	80.9(13)	24.6(10)	33.2(10)	18.5(10)
C34	87.9(15)	116(2)	61.7(11)	-13.5(12)	19.1(10)	-30.4(14)
C32	142(3)	60.1(14)	143(3)	4.2(14)	47(2)	-28.7(15)
C33	126(3)	95(2)	155(3)	-10.5(19)	54(2)	-52.0(19)
C37	90.2(18)	198(4)	96.7(18)	-34(2)	33.3(15)	-37(2)

Table S19 Bond Lengths for 20221230-HXY456_auto (**4f**).

Atom	Atom	Length/Å	Atom	Atom	Length/Å

S25	C11	1.7569(14)	C7	C2	1.388(2)
S25	C26	1.7825(16)	C7	C6	1.375(2)
S22	N21	1.6218(17)	C16	C17	1.391(2)
S22	O24	1.4340(16)	C2	C1	1.503(2)
S22	O23	1.4234(15)	C2	C3	1.372(2)
S22	C31	1.758(2)	C9	C1	1.538(2)
Cl27	C26	1.7831(19)	C13	C1	1.544(2)
O28	C9	1.224(2)	C20	C19	1.380(2)
N10	C11	1.2803(18)	C6	C5	1.382(3)
N10	C1	1.4824(18)	C19	C18	1.373(3)
N8	C7	1.407(2)	C17	C18	1.375(3)
N8	C9	1.3532(19)	C3	C4	1.380(3)
N8	C29	1.449(2)	C36	C31	1.379(3)
N21	C16	1.428(2)	C36	C35	1.372(3)
F30	C4	1.361(2)	C31	C32	1.378(3)
C12	C11	1.4711(19)	C5	C4	1.368(3)
C12	C14	1.3386(19)	C35	C34	1.384(3)
C12	C13	1.4996(19)	C34	C33	1.374(4)
C15	C14	1.4701(19)	C34	C37	1.506(4)
C15	C16	1.408(2)	C32	C33	1.375(4)
C15	C20	1.398(2)			

Table S20 Bond Angles for 20221230-HXY456_auto (**4f**).

Atom	**Atom**	**Atom**	**Angle/**°	**Atom**	**Atom**	**Atom**	**Angle/**°
C11	S25	C26	100.25(7)	O28	C9	N8	126.14(15)
N21	S22	C31	106.37(8)	O28	C9	C1	125.27(14)

O24	S22	N21	105.35(10)	N8	C9	C1	108.59(13)
O24	S22	C31	108.61(10)	C12	C13	C1	103.80(11)
O23	S22	N21	107.70(10)	N10	C1	C2	111.77(13)
O23	S22	O24	120.40(11)	N10	C1	C9	107.52(12)
O23	S22	C31	107.61(12)	N10	C1	C13	107.14(11)
C11	N10	C1	108.01(12)	C2	C1	C9	101.71(11)
C7	N8	C29	124.56(14)	C2	C1	C13	116.18(13)
C9	N8	C7	111.13(12)	C9	C1	C13	112.25(13)
C9	N8	C29	124.27(15)	C19	C20	C15	121.98(17)
C16	N21	S22	122.13(12)	C7	C6	C5	117.82(17)
C11	C12	C13	104.43(11)	S25	C26	Cl27	114.15(10)
C14	C12	C11	124.45(13)	C18	C19	C20	119.93(18)
C14	C12	C13	131.10(13)	C18	C17	C16	120.66(17)
N10	C11	S25	122.30(11)	C2	C3	C4	116.82(17)
N10	C11	C12	116.43(12)	C35	C36	C31	120.43(19)
C12	C11	S25	121.26(10)	C36	C31	S22	120.38(15)
C16	C15	C14	120.13(14)	C32	C31	S22	120.84(19)
C20	C15	C14	122.85(14)	C32	C31	C36	118.7(2)
C20	C15	C16	117.02(14)	C4	C5	C6	119.34(17)
C2	C7	N8	109.51(13)	C19	C18	C17	119.95(16)
C6	C7	N8	128.39(15)	C36	C35	C34	121.6(2)
C6	C7	C2	122.11(16)	F30	C4	C3	118.0(2)
C12	C14	C15	128.06(14)	F30	C4	C5	118.37(19)
C15	C16	N21	121.88(13)	C5	C4	C3	123.64(19)
C17	C16	N21	117.71(15)	C35	C34	C37	121.0(3)
C17	C16	C15	120.42(16)	C33	C34	C35	117.0(2)

C7	C2	C1	109.05(13)	C33	C34	C37	122.0(3)
C3	C2	C7	120.25(15)	C33	C32	C31	120.0(3)
C3	C2	C1	130.70(15)	C34	C33	C32	122.3(2)

Table S21 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 20221230-HXY456_auto (**4f**).

Atom	***x***	***y***	***z***	**U(eq)**
H21	2338.13	5932.57	2783.64	72
H14	4299.94	5554	3455.42	54
H13A	6409.27	6485.13	5362.75	60
H13B	6750.34	6814.6	4392.09	60
H20	5247.68	7430.08	4799.03	70
H6	11021.31	6207.65	5656.73	73
H26A	6096.72	2690.38	3640.12	71
H26B	6906.62	3302.63	4279.92	71
H19	4417.07	8747.37	4748.02	82
H17	2070.54	7886.69	2712.01	80
H3	8121.82	6266.91	3111.04	81
H36	3896.27	4792.77	1390.76	83
H29A	10420.37	5377.82	7008.76	106
H29B	9399.47	5362.71	7514.14	106
H29C	9931.23	6241.83	7315.26	106
H5	11265.9	6631.32	4113.15	88
H18	2845.16	8985.14	3684.87	89
H35	5646.54	4469.93	1291.93	92
H32	4513.76	7282.64	1061.55	135
H33	6262.74	6946.65	968.56	146

H37A	7609.89	5119.86	1621.23	189
H37B	7717.89	5974.05	1051.74	189
H37C	7335.46	5128.48	490.02	189

Table S22. Crystal data and structure refinement for 20221214-ZYQ-2 (**3f**).

Identification code	20221214-ZYQ-2
Empirical formula	$C_{26}H_{22}ClN_3O_3S_2$
Formula weight	524.03
Temperature/K	99.98(11)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.73770(10)
b/Å	22.4707(2)
c/Å	10.42080(10)
α/°	90
β/°	95.8570(10)
γ/°	90
Volume/Å^3	2501.24(4)
Z	4
ρ_{calc}g/cm^3	1.392
μ/mm^{-1}	3.192
F(000)	1088.0
Crystal size/mm^3	? × ? × ?
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.868 to 151.862
Index ranges	$-13 \leq h \leq 12$, $-25 \leq k \leq 27$, $-13 \leq l \leq 12$
Reflections collected	15026
Independent reflections	4891 [R_{int} = 0.0270, R_{sigma} = 0.0173]
Data/restraints/parameters	4891/0/319
Goodness-of-fit on F^2	1.048

Final R indexes [I>=2σ (I)]	R_1 = 0.0353, wR_2 = 0.0973
Final R indexes [all data]	R_1 = 0.0357, wR_2 = 0.0977
Largest diff. peak/hole / e Å^{-3}	0.49/-0.61

Table S23. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 20221214-ZYQ-2 (**3f**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S20	671.8(3)	6268.0(2)	2447.5(4)	26.15(12)
Cl23	4123.6(4)	8661.7(2)	4823.5(4)	32.86(13)
S26	6878.8(4)	5933.6(2)	3054.9(4)	34.42(13)
O27	6572.0(11)	4718.4(5)	7437.6(10)	28.1(3)
O22	-76.6(10)	6776.2(6)	2050.5(11)	32.2(3)
O21	463.9(12)	5712.0(6)	1785.6(12)	37.1(3)
N9	7146.5(11)	5466.3(5)	8892.8(11)	19.2(3)
N24	6896.4(12)	5715.8(6)	5652.4(12)	26.4(3)
N19	2143.0(12)	6432.9(6)	2324.5(12)	24.4(3)
C1	7222.1(12)	6091.8(6)	8860.8(13)	17.6(3)
C8	6698.9(13)	5242.0(6)	7729.3(13)	19.7(3)
C6	6785.3(13)	6299.2(6)	7636.3(13)	18.7(3)
C13	3521.7(13)	6930.7(6)	4053.2(13)	20.2(3)
C12	3938.6(13)	6361.1(6)	4654.8(14)	20.4(3)
C10	4863.1(13)	5752.8(6)	6533.2(13)	20.0(3)
C2	7699.5(13)	6468.3(7)	9837.5(14)	22.4(3)
C7	6309.8(13)	5772.0(6)	6831.7(13)	18.4(3)
C34	2.3(14)	6592.5(7)	4804.5(15)	24.4(3)
C11	4373.2(13)	6312.3(6)	5890.1(14)	19.2(3)
C14	2660.0(13)	6958.5(7)	2939.5(14)	21.6(3)

C18	3974.4(13)	7467.7(7)	4597.9(14)	22.9(3)
C32	361.0(13)	5980.6(7)	6720.4(16)	25.7(3)
C29	544.0(13)	6157.0(7)	4100.3(15)	22.6(3)
C9	6836.6(14)	5823.3(6)	4541.6(14)	21.7(3)
C17	3551.4(14)	8005.9(7)	4087.3(15)	24.9(3)
C33	-87.7(14)	6501.4(7)	6111.0(15)	25.7(3)
C28	7615.4(16)	5103.6(7)	9994.3(14)	26.9(3)
C16	2695.9(15)	8031.9(7)	2997.9(16)	28.9(3)
C15	2274.5(15)	7506.7(7)	2421.3(15)	27.3(3)
C30	1010.7(15)	5635.2(7)	4693.9(16)	28.2(3)
C5	6856.2(14)	6896.7(7)	7352.0(15)	25.1(3)
C3	7748.3(15)	7071.4(7)	9542.4(16)	28.3(3)
C31	914.4(15)	5553.4(7)	5995.3(17)	29.1(3)
C4	7342.4(15)	7285.5(7)	8322.3(17)	30.6(3)
C35	267.2(16)	5883.9(8)	8138.6(17)	35.3(4)

Table S24. Anisotropic Displacement Parameters ($Å^2×10^3$) for 20221214-ZYQ-2 (**3f**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
S20	22.8(2)	31.0(2)	22.4(2)	-5.14(14)	-8.61(14)	3.22(14)
Cl23	32.4(2)	18.15(19)	49.5(3)	1.11(15)	11.24(17)	-0.97(13)
S26	45.4(3)	41.5(3)	17.2(2)	2.44(15)	7.21(16)	-2.37(18)
O27	37.2(6)	17.6(5)	26.8(5)	-3.8(4)	-9.8(5)	3.7(4)
O22	26.2(6)	40.2(7)	27.4(6)	0.8(5)	-10.3(5)	8.9(5)
O21	35.9(6)	39.3(7)	33.1(6)	-15.8(5)	-11.4(5)	0.0(5)
N9	24.0(6)	17.8(6)	14.6(5)	0.5(4)	-3.5(4)	-0.1(4)
N24	28.5(7)	34.0(7)	16.4(6)	-0.2(5)	1.3(5)	7.4(5)

N19	24.4(6)	29.3(7)	18.6(6)	-3.0(5)	-2.3(5)	6.5(5)
C1	16.7(6)	18.7(7)	17.5(6)	-0.7(5)	1.6(5)	-1.4(5)
C8	21.8(7)	18.8(7)	17.5(6)	-0.6(5)	-2.6(5)	2.3(5)
C6	17.9(6)	19.6(7)	18.2(7)	0.2(5)	-0.4(5)	-0.7(5)
C13	19.3(7)	21.7(7)	19.9(7)	1.3(5)	2.9(5)	3.5(5)
C12	20.5(7)	18.6(7)	21.2(7)	-1.2(5)	-1.9(5)	1.6(5)
C10	21.5(7)	19.4(7)	17.9(6)	-0.1(5)	-3.0(5)	-0.7(5)
C2	21.4(7)	26.2(7)	19.4(7)	-4.9(6)	0.9(5)	-3.7(6)
C7	22.4(7)	19.2(7)	13.1(6)	-0.1(5)	-0.7(5)	2.0(5)
C34	20.2(7)	22.8(7)	29.0(8)	1.0(6)	-3.2(6)	2.6(5)
C11	19.2(7)	17.9(7)	20.1(7)	-2.1(5)	-0.5(5)	1.0(5)
C14	19.9(7)	25.9(7)	19.2(7)	1.4(5)	2.9(5)	4.6(5)
C18	20.9(7)	22.0(7)	25.7(7)	1.8(6)	2.3(6)	1.5(5)
C32	16.3(7)	28.5(8)	32.1(8)	5.1(6)	0.7(6)	-4.2(6)
C29	16.4(6)	23.4(7)	26.7(7)	-2.9(6)	-3.7(5)	-1.6(5)
C9	24.6(7)	19.2(7)	21.0(7)	-2.6(5)	1.3(6)	-0.4(5)
C17	23.3(7)	19.7(7)	33.2(8)	3.0(6)	10.4(6)	1.7(5)
C33	20.0(7)	26.9(8)	30.0(8)	-0.7(6)	1.5(6)	2.3(6)
C28	38.4(9)	23.0(7)	17.3(7)	4.7(6)	-7.0(6)	-1.7(6)
C16	26.0(8)	24.9(8)	37.1(9)	10.9(6)	8.6(6)	7.8(6)
C15	25.0(8)	31.5(8)	25.2(7)	8.2(6)	2.0(6)	6.5(6)
C30	26.7(8)	21.4(7)	35.5(8)	-3.0(6)	-0.9(6)	2.5(6)
C5	23.5(7)	22.0(7)	29.1(8)	5.9(6)	-1.4(6)	-2.6(6)
C3	25.2(7)	24.4(8)	35.0(8)	-9.6(6)	1.8(6)	-6.0(6)
C31	25.6(8)	21.3(7)	39.7(9)	6.3(6)	-0.3(6)	-0.2(6)
C4	28.0(8)	18.0(7)	45.1(9)	-0.2(7)	-0.1(7)	-4.5(6)

C35	27.8(8)	43.0(10)	35.8(9)	13.0(7)	7.5(7)	-0.3(7)

Table S25. Bond Lengths for 20221214-ZYQ-2 (**3f**).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S20	O22	1.4330(12)	C13	C14	1.410(2)
S20	O21	1.4334(12)	C13	C18	1.399(2)
S20	N19	1.6403(14)	C12	C11	1.328(2)
S20	C29	1.7595(16)	C10	C7	1.5535(19)
Cl23	C17	1.7441(16)	C10	C11	1.4949(19)
S26	C9	1.5742(15)	C2	C3	1.392(2)
O27	C8	1.2193(18)	C34	C29	1.386(2)
N9	C1	1.4084(18)	C34	C33	1.390(2)
N9	C8	1.3551(17)	C14	C15	1.391(2)
N9	C28	1.4551(17)	C18	C17	1.379(2)
N24	C7	1.4425(18)	C32	C33	1.394(2)
N24	C9	1.178(2)	C32	C31	1.392(2)
N19	C14	1.4287(19)	C32	C35	1.507(2)
C1	C6	1.3940(19)	C29	C30	1.395(2)
C1	C2	1.3813(19)	C17	C16	1.387(2)
C8	C7	1.5453(18)	C16	C15	1.380(2)
C6	C7	1.5099(19)	C30	C31	1.383(2)
C6	C5	1.379(2)	C5	C4	1.397(2)
C13	C12	1.4747(19)	C3	C4	1.387(2)

Table S26. Bond Angles for 20221214-ZYQ-2 (**3f**).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O22	S20	O21	120.03(7)	N24	C7	C10	109.98(11)

O22	S20	N19	108.28(7)	C8	C7	C10	107.63(11)
O22	S20	C29	107.34(7)	C6	C7	C8	102.32(10)
O21	S20	N19	105.26(7)	C6	C7	C10	114.05(11)
O21	S20	C29	108.88(8)	C29	C34	C33	119.30(14)
N19	S20	C29	106.29(6)	C12	C11	C10	125.21(13)
C1	N9	C28	124.16(12)	C13	C14	N19	121.67(13)
C8	N9	C1	111.47(11)	C15	C14	N19	118.12(13)
C8	N9	C28	124.06(12)	C15	C14	C13	120.20(14)
C9	N24	C7	146.57(14)	C17	C18	C13	120.83(14)
C14	N19	S20	119.00(10)	C33	C32	C35	120.88(15)
C6	C1	N9	109.90(12)	C31	C32	C33	118.60(15)
C2	C1	N9	127.71(13)	C31	C32	C35	120.51(14)
C2	C1	C6	122.32(13)	C34	C29	S20	119.81(12)
O27	C8	N9	127.04(13)	C34	C29	C30	120.66(14)
O27	C8	C7	125.19(12)	C30	C29	S20	119.53(12)
N9	C8	C7	107.71(11)	N24	C9	S26	174.49(14)
C1	C6	C7	108.01(12)	C18	C17	Cl23	118.93(12)
C5	C6	C1	120.10(13)	C18	C17	C16	121.16(14)
C5	C6	C7	131.89(13)	C16	C17	Cl23	119.90(12)
C14	C13	C12	122.25(13)	C34	C33	C32	120.97(14)
C18	C13	C12	119.88(12)	C15	C16	C17	118.73(14)
C18	C13	C14	117.86(13)	C16	C15	C14	121.15(14)
C11	C12	C13	123.02(13)	C31	C30	C29	119.16(15)
C11	C10	C7	111.43(11)	C6	C5	C4	118.58(14)
C1	C2	C3	116.94(14)	C4	C3	C2	121.66(14)
N24	C7	C8	109.49(11)	C30	C31	C32	121.30(14)

N24	C7	C6	112.92(12)		C3	C4	C5	120.38(14)	

Table S27. Torsion Angles for 20221214-ZYQ-2 (**3f**).

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
S20	N19	C14	C13	107.80(14)	C12	C13	C14	C15	178.69(13)
S20	N19	C14	C15	-71.17(16)	C12	C13	C18	C17	-176.87(13)
S20	C29	C30	C31	179.54(12)	C2	C1	C6	C7	-178.76(13)
Cl23	C17	C16	C15	178.90(12)	C2	C1	C6	C5	2.0(2)
O27	C8	C7	N24	-55.02(19)	C2	C3	C4	C5	0.7(3)
O27	C8	C7	C6	-175.03(14)	C7	C6	C5	C4	179.44(15)
O27	C8	C7	C10	64.50(18)	C7	C10	C11	C12	107.31(16)
O22	S20	N19	C14	52.93(12)	C34	C29	C30	C31	0.7(2)
O22	S20	C29	C34	-11.66(14)	C11	C10	C7	N24	-72.10(15)
O22	S20	C29	C30	169.51(12)	C11	C10	C7	C8	168.69(11)
O21	S20	N19	C14	-177.54(11)	C11	C10	C7	C6	55.92(15)
O21	S20	C29	C34	-143.03(12)	C14	C13	C12	C11	-155.79(15)
O21	S20	C29	C30	38.14(14)	C14	C13	C18	C17	2.5(2)
N9	C1	C6	C7	3.91(16)	C18	C13	C12	C11	23.5(2)
N9	C1	C6	C5	-175.29(13)	C18	C13	C14	N19	-179.57(13)
N9	C1	C2	C3	175.77(14)	C18	C13	C14	C15	-0.6(2)
N9	C8	C7	N24	127.57(13)	C18	C17	C16	C15	-0.4(2)
N9	C8	C7	C6	7.56(14)	C29	S20	N19	C14	-62.13(12)
N9	C8	C7	C10	-112.91(13)	C29	C34	C33	C32	0.2(2)
N19	S20	C29	C34	104.03(13)	C29	C30	C31	C32	0.1(2)
N19	S20	C29	C30	-74.80(13)	C9	N24	C7	C8	152.0(2)
N19	C14	C15	C16	177.26(14)	C9	N24	C7	C6	-94.7(3)

C1	N9	C8	O27	176.93(14)	C9	N24	C7	C10	34.0(3)
C1	N9	C8	C7	-5.72(16)	C17	C16	C15	C14	2.2(2)
C1	C6	C7	N24	-124.39(13)	C33	C34	C29	S20	-179.66(11)
C1	C6	C7	C8	-6.81(14)	C33	C34	C29	C30	-0.8(2)
C1	C6	C7	C10	109.10(13)	C33	C32	C31	C30	-0.7(2)
C1	C6	C5	C4	-1.6(2)	C28	N9	C1	C6	175.07(13)
C1	C2	C3	C4	-0.3(2)	C28	N9	C1	C2	-2.1(2)
C8	N9	C1	C6	1.25(17)	C28	N9	C8	O27	3.1(2)
C8	N9	C1	C2	-175.90(14)	C28	N9	C8	C7	-179.55(13)
C6	C1	C2	C3	-1.1(2)	C5	C6	C7	N24	54.7(2)
C6	C5	C4	C3	0.3(2)	C5	C6	C7	C8	172.27(15)
C13	C12	C11	C10	-176.97(13)	C5	C6	C7	C10	-71.8(2)
C13	C14	C15	C16	-1.7(2)	C31	C32	C33	C34	0.6(2)
C13	C18	C17	Cl23	178.72(11)	C35	C32	C33	C34	179.75(14)
C13	C18	C17	C16	-2.0(2)	C35	C32	C31	C30	-179.87(15)
C12	C13	C14	N19	-0.3(2)					

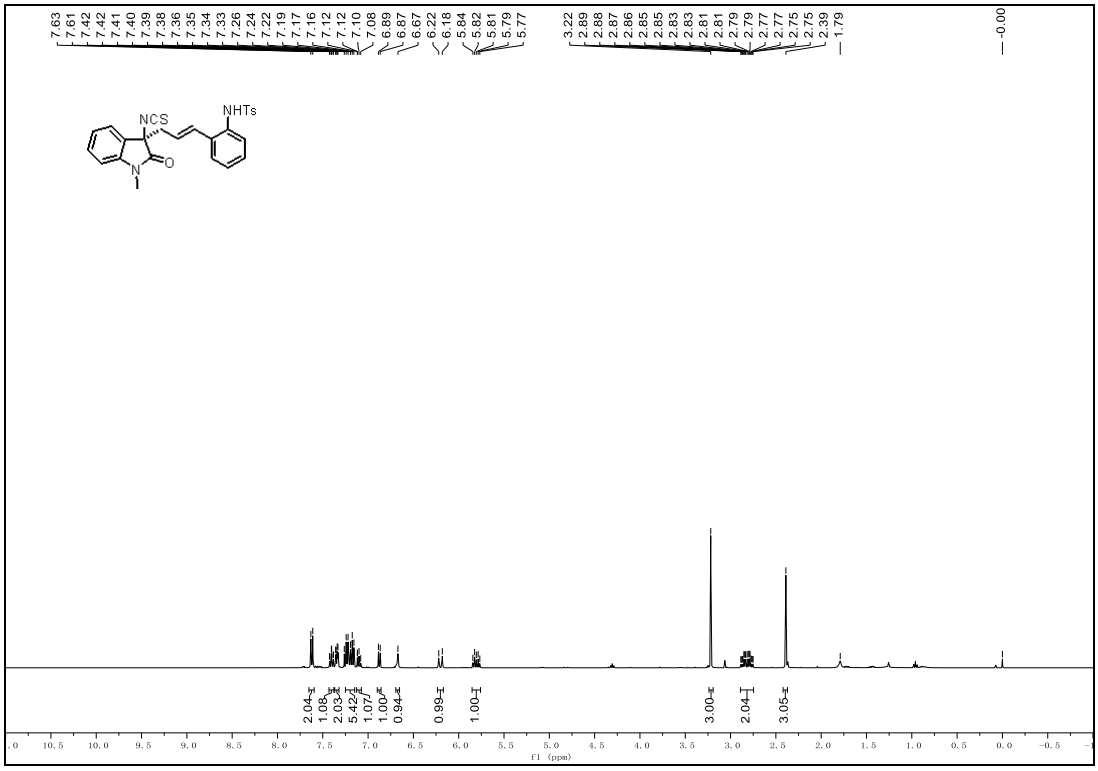
Table S28. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 20221214-ZYQ-2 (**3f**).

Atom	***x***	***y***	***z***	**U(eq)**
H19	2607	6201	1886	29
H12	3894	6013	4135	24
H10A	4627	5409	5965	24
H10B	4476	5697	7347	24
H2	7982	6322	10672	27
H34	-304	6950	4398	29
H11	4373	6661	6406	23

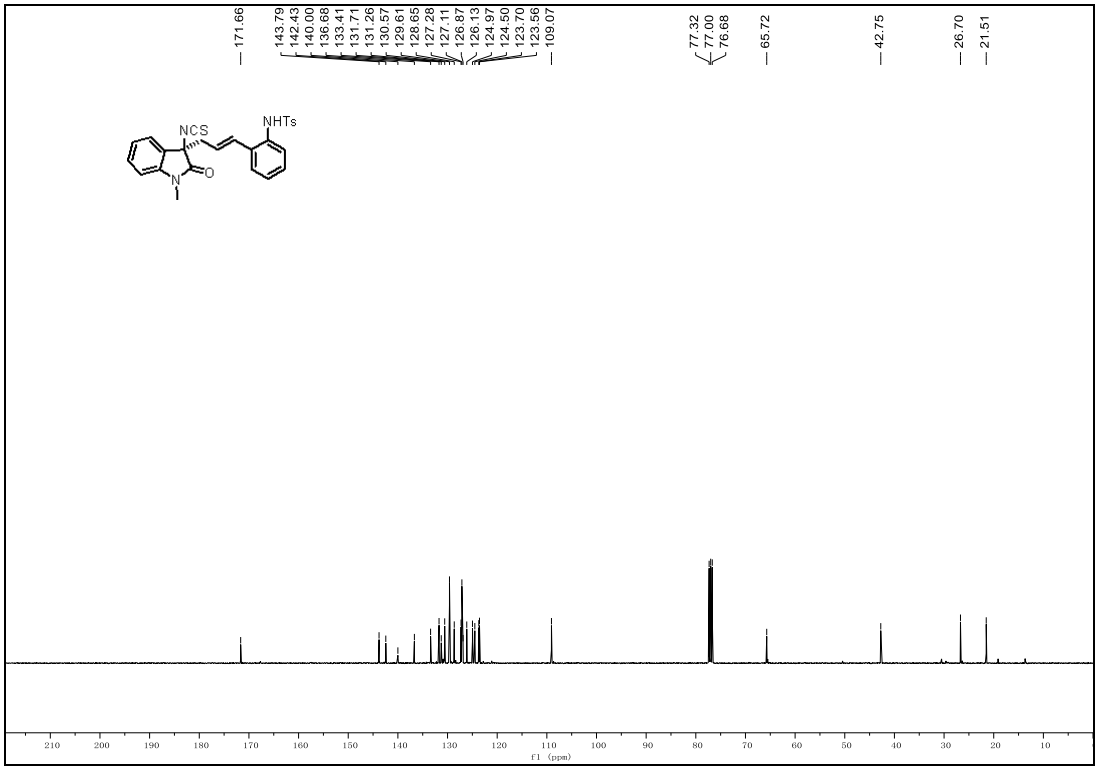
H18	4581	7462	5329	27
H33	-460	6799	6596	31
H28A	8444	5247	10340	40
H28B	7679	4688	9722	40
H28C	7039	5131	10663	40
H16	2406	8404	2655	35
H15	1711	7520	1657	33
H30	1390	5340	4210	34
H5	6580	7041	6514	30
H3	8067	7343	10193	34
H31	1232	5199	6402	35
H4	7396	7699	8146	37
H35A	1110	5868	8598	53
H35B	-168	5508	8262	53
H35C	-201	6213	8478	53

7. Copies of ^{1}H NMR and ^{13}C NMR Spectra

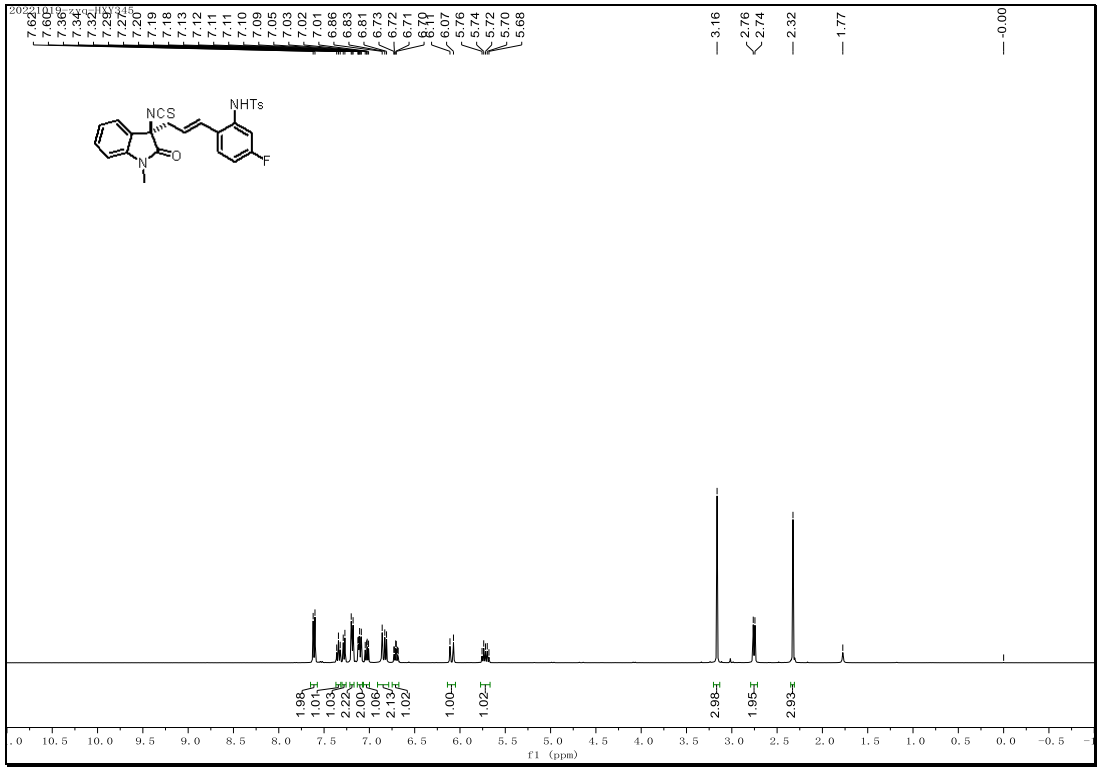
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3a



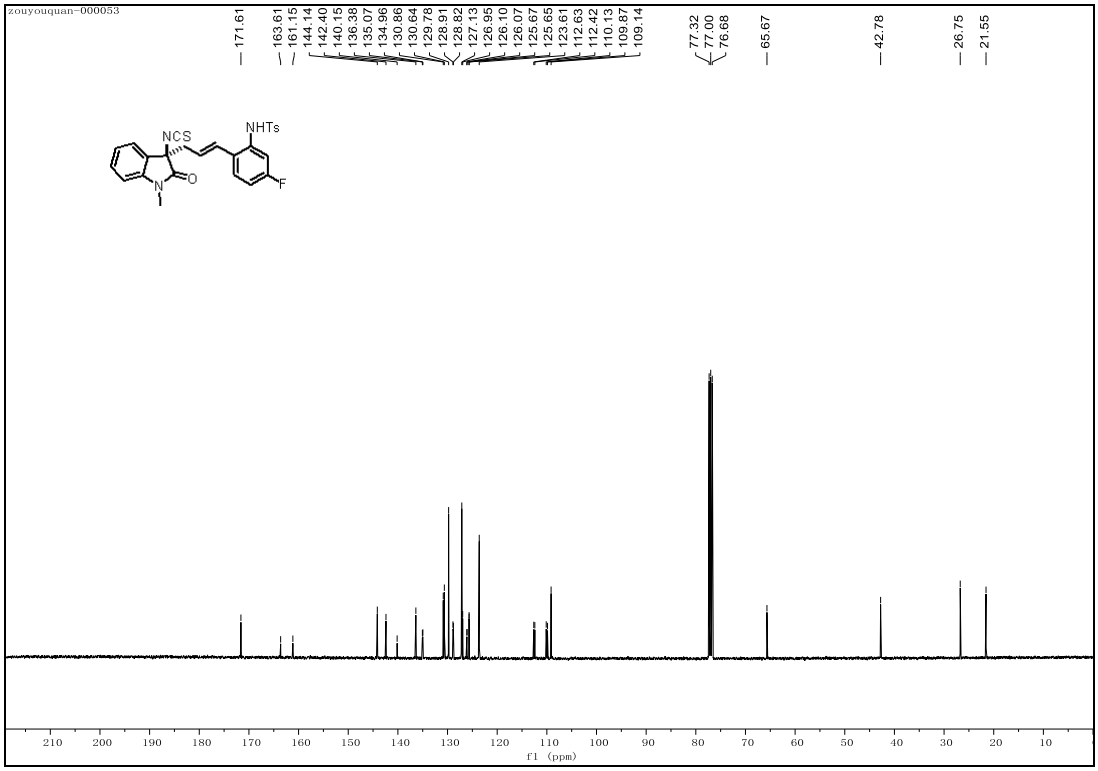
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3a



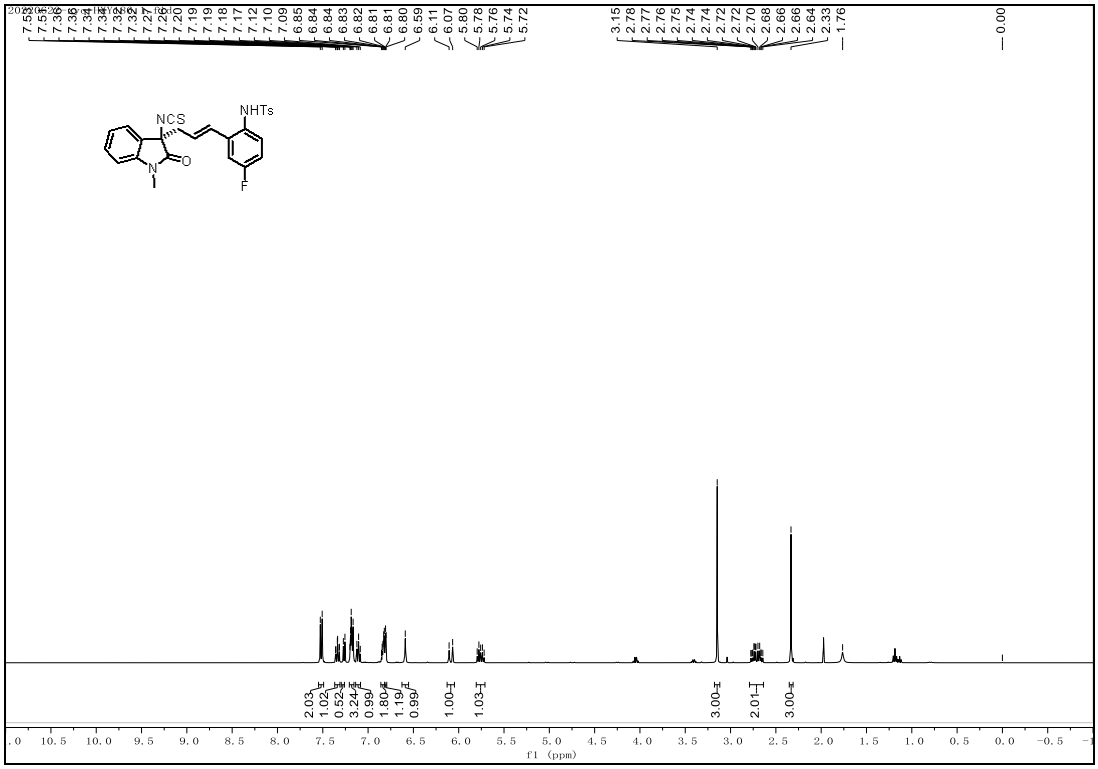
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3b



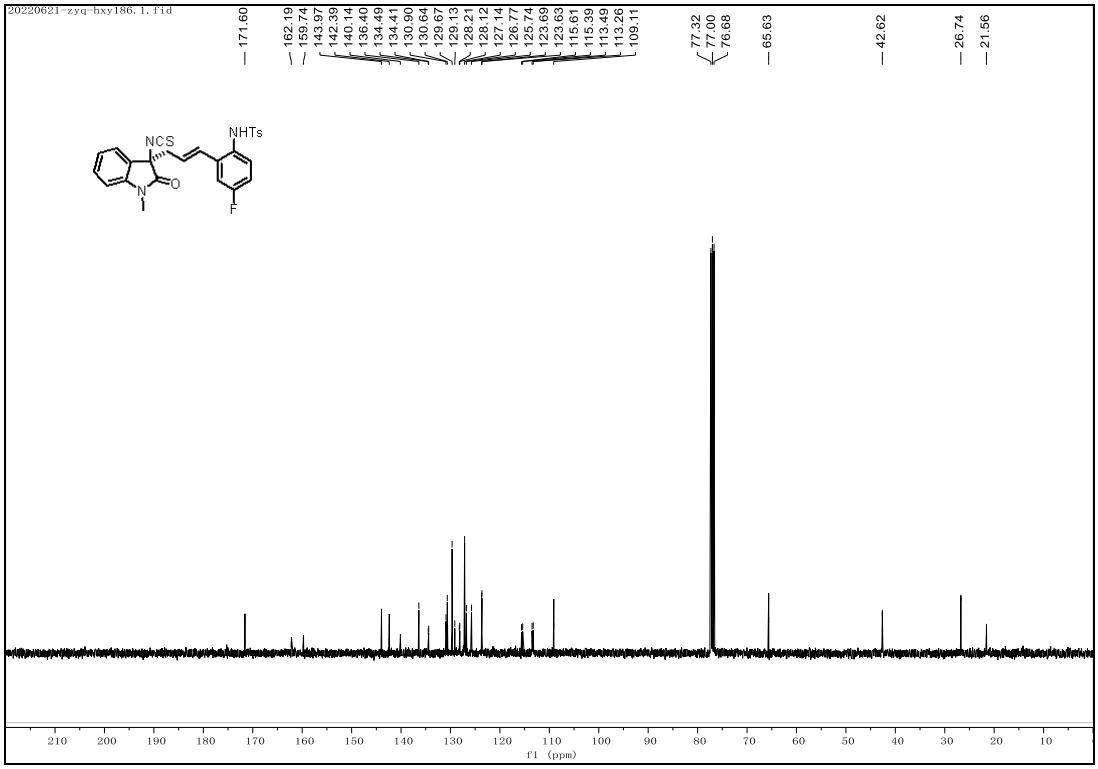
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3b



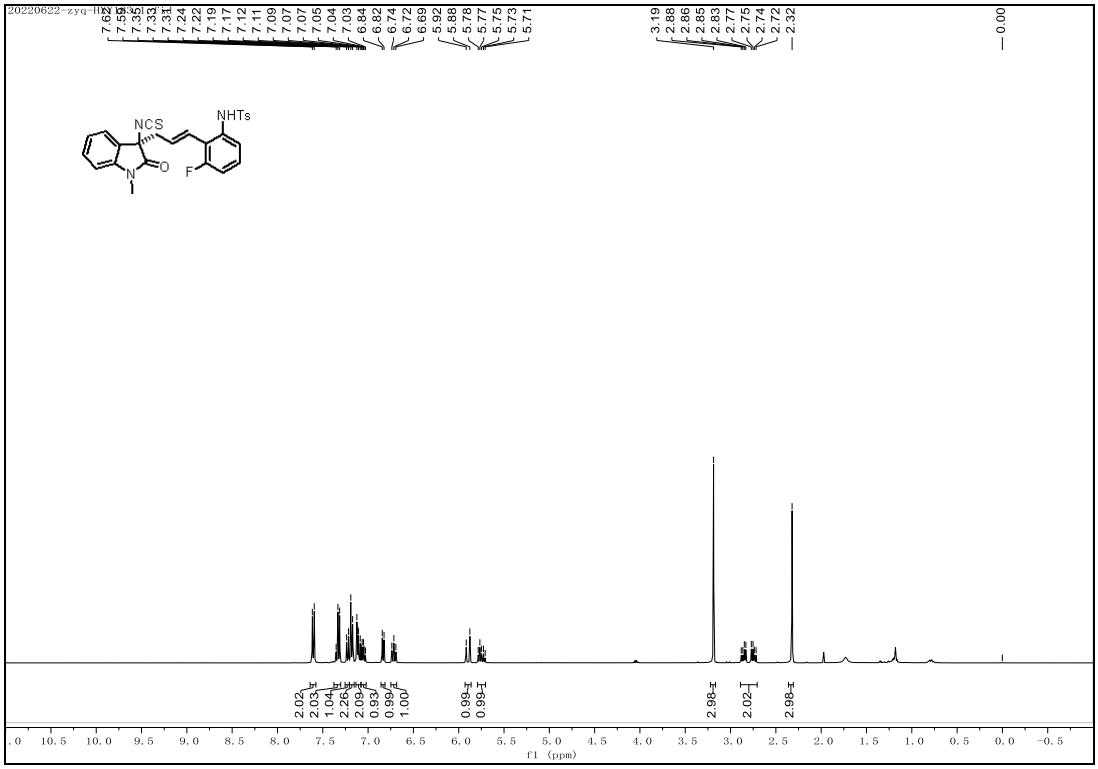
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3c



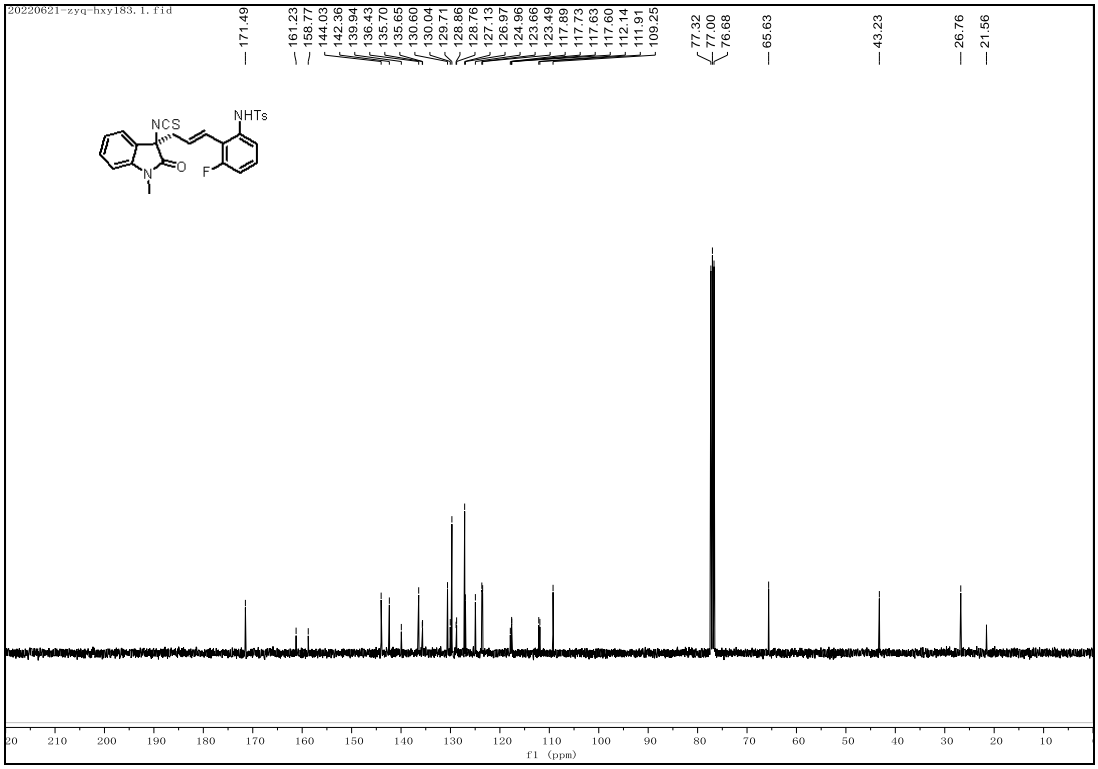
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3c



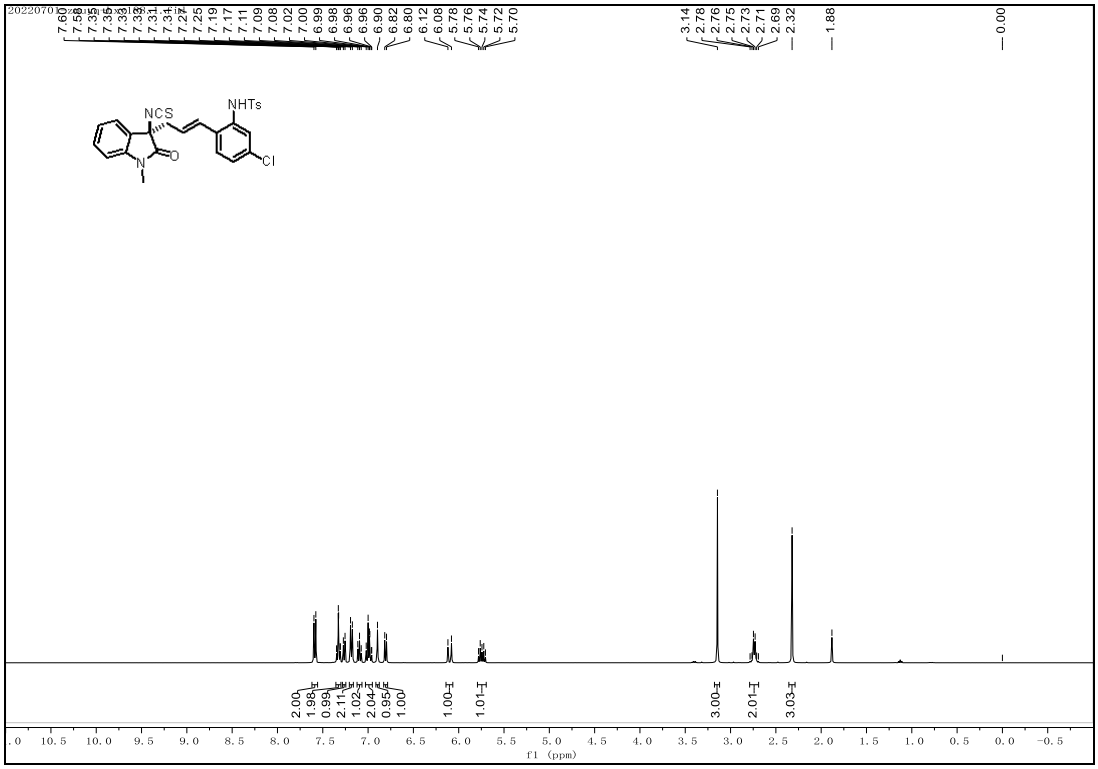
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3d



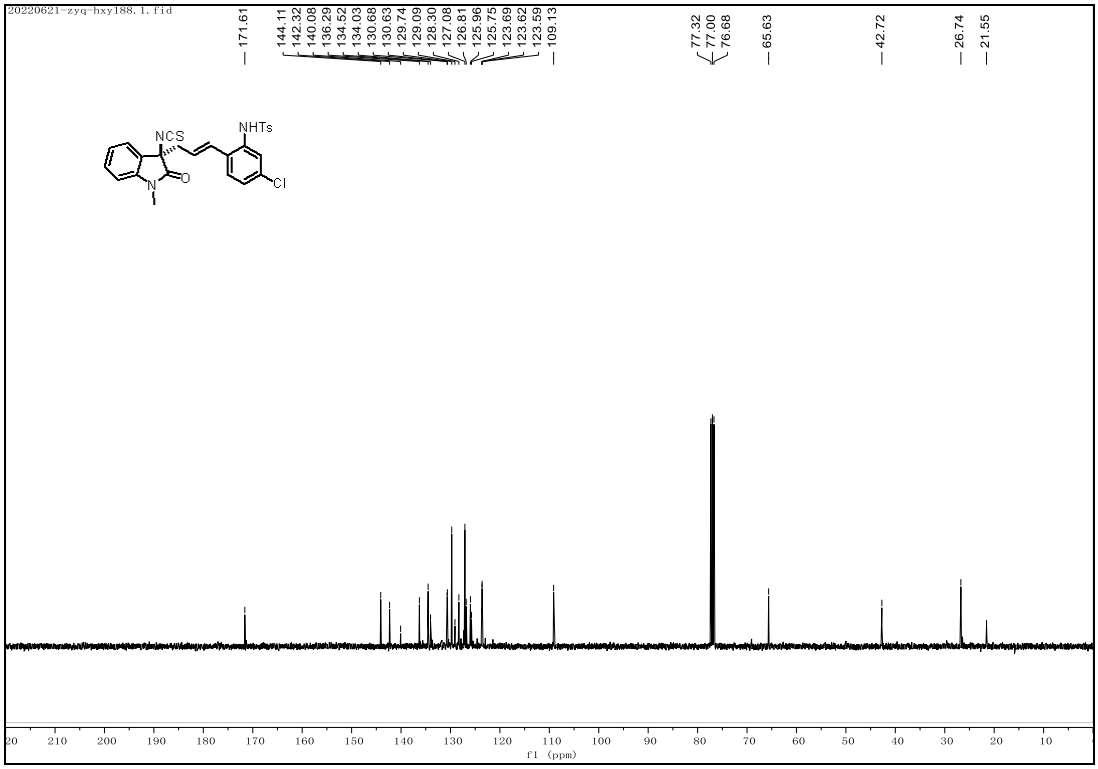
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3d



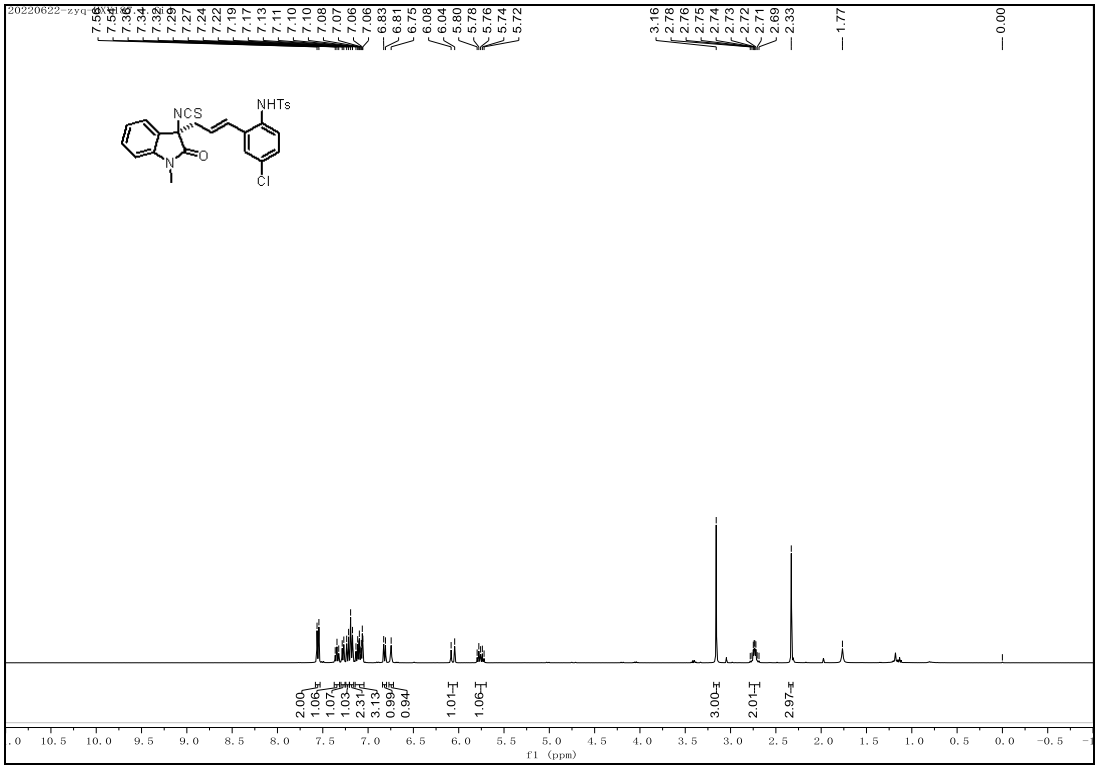
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3e



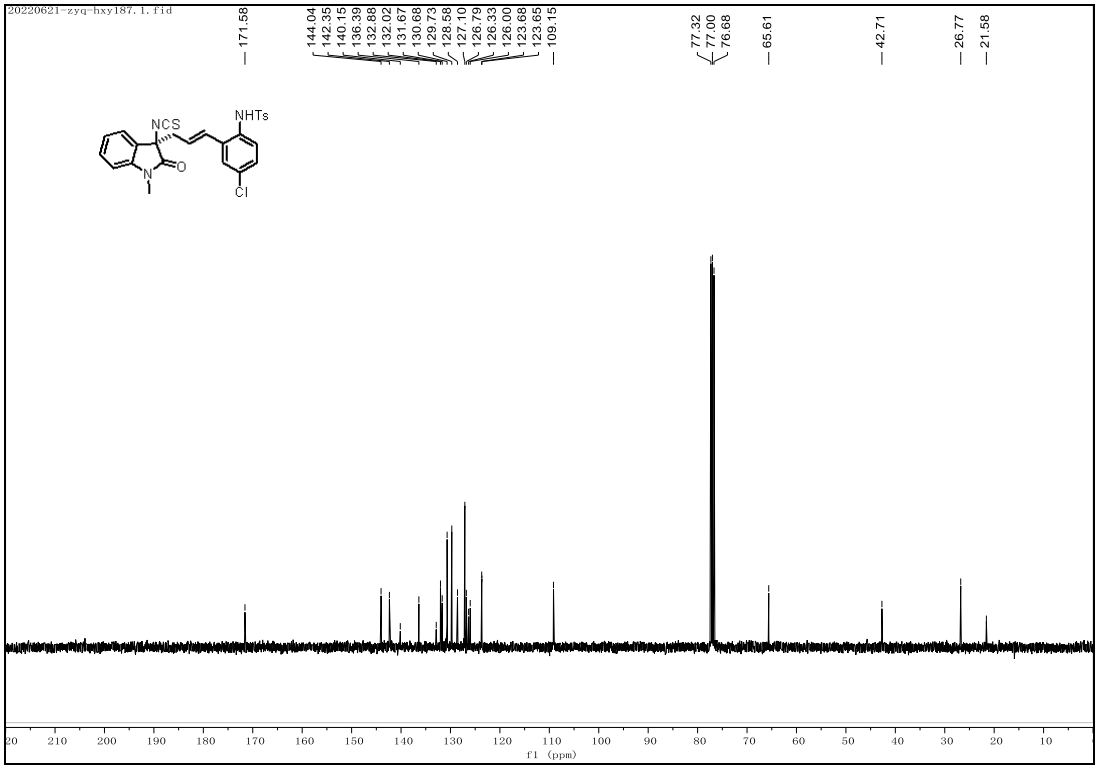
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3e



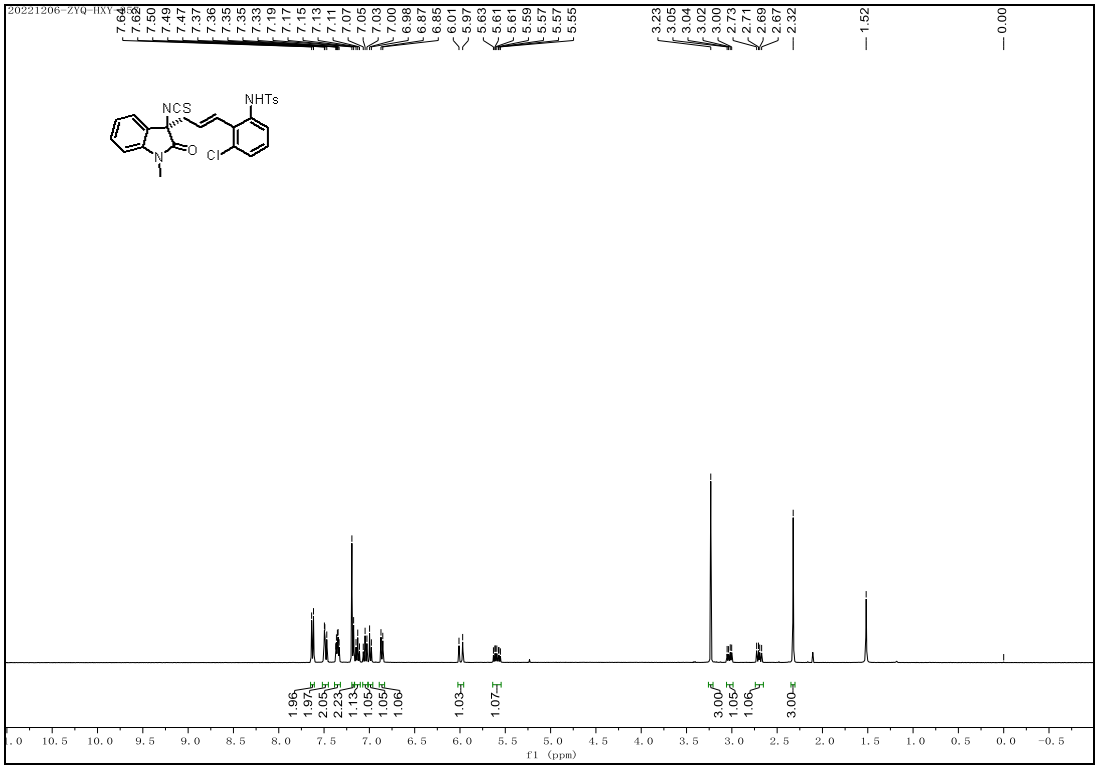
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3f



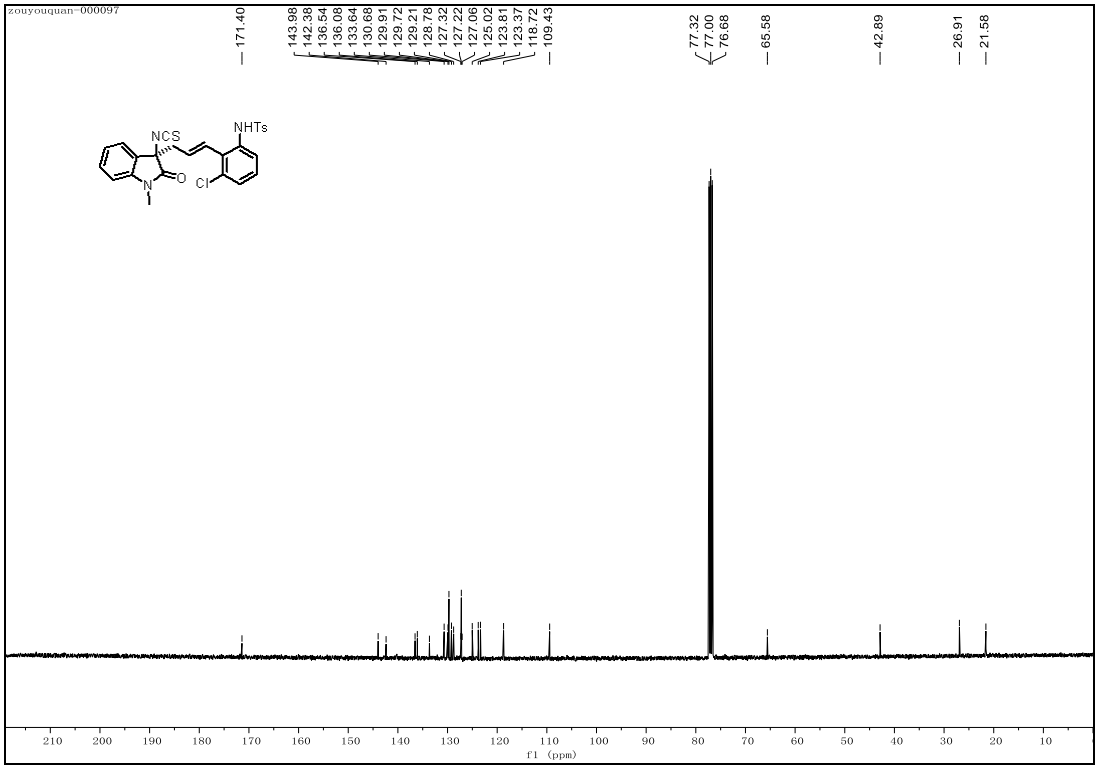
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3f



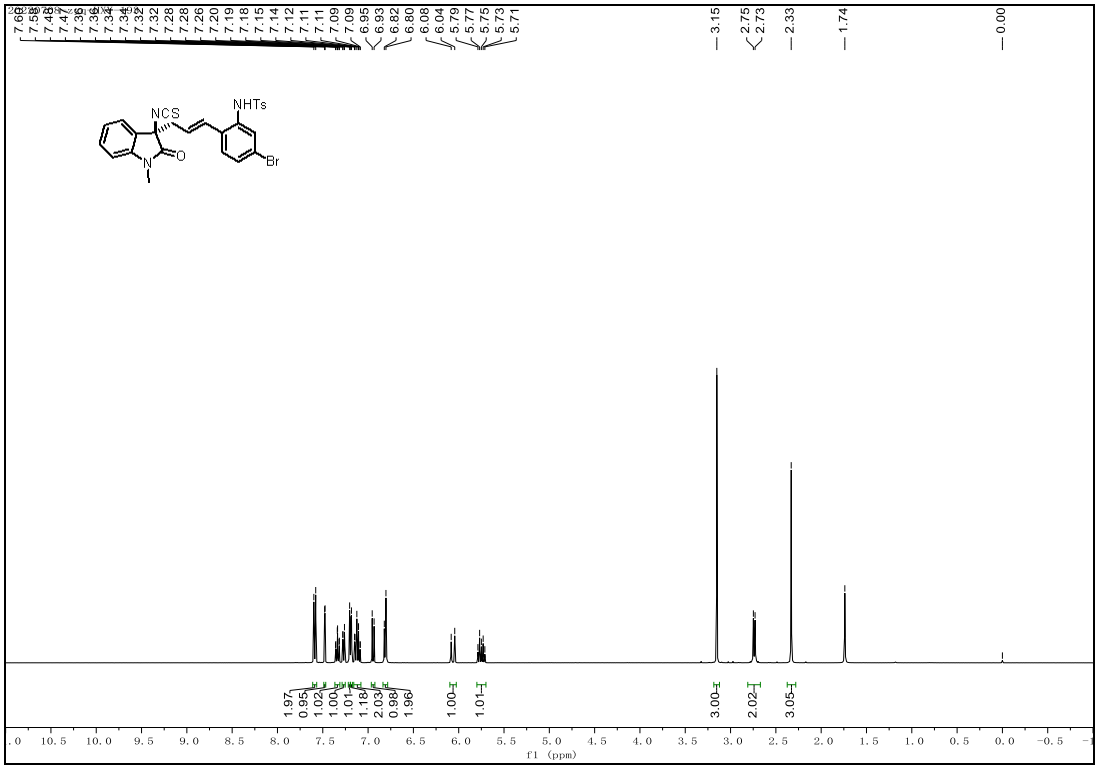
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3g



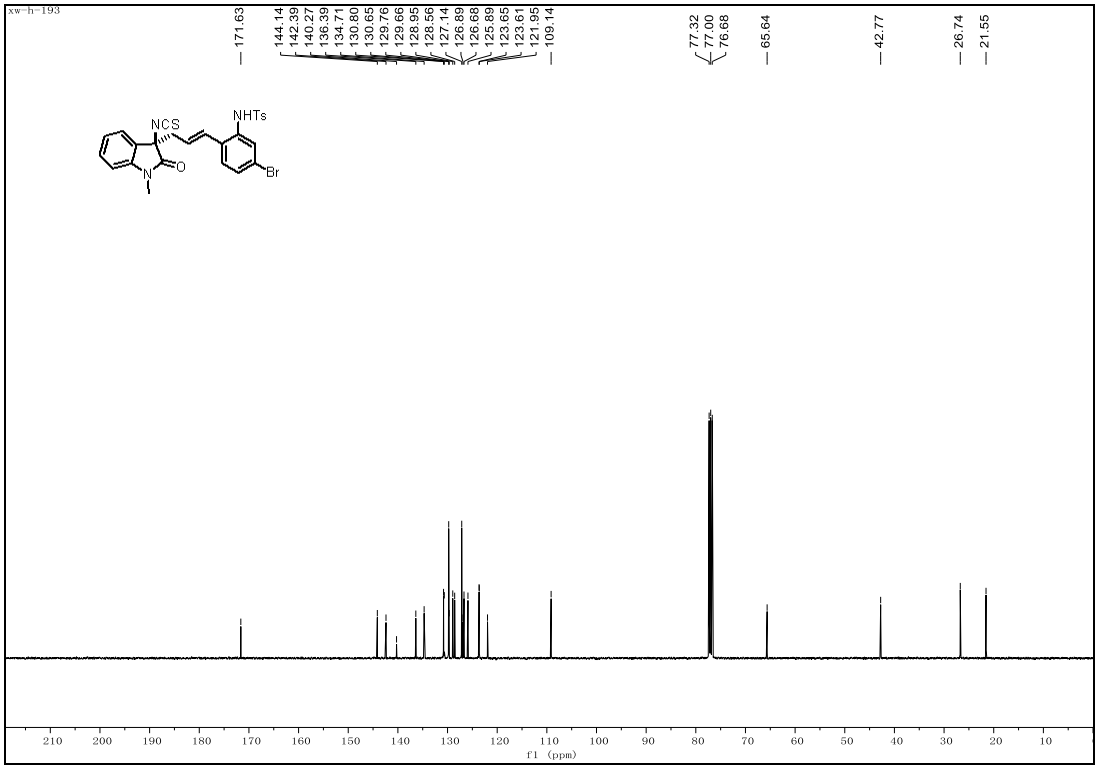
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3g



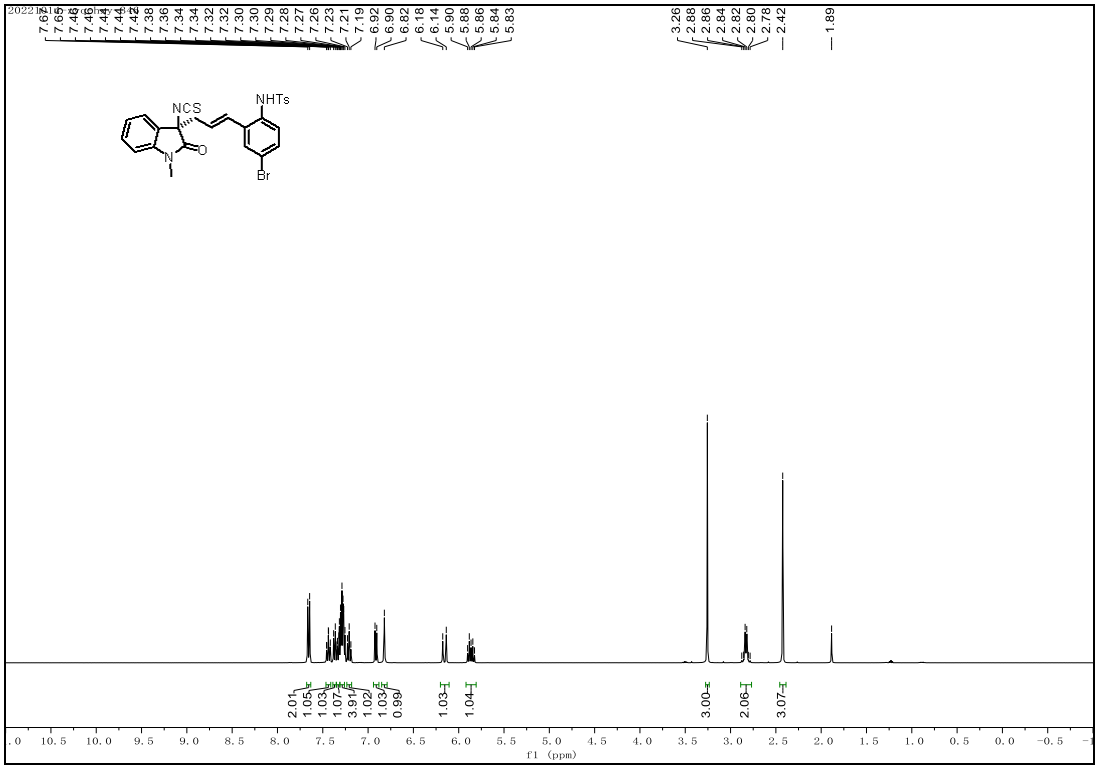
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3h



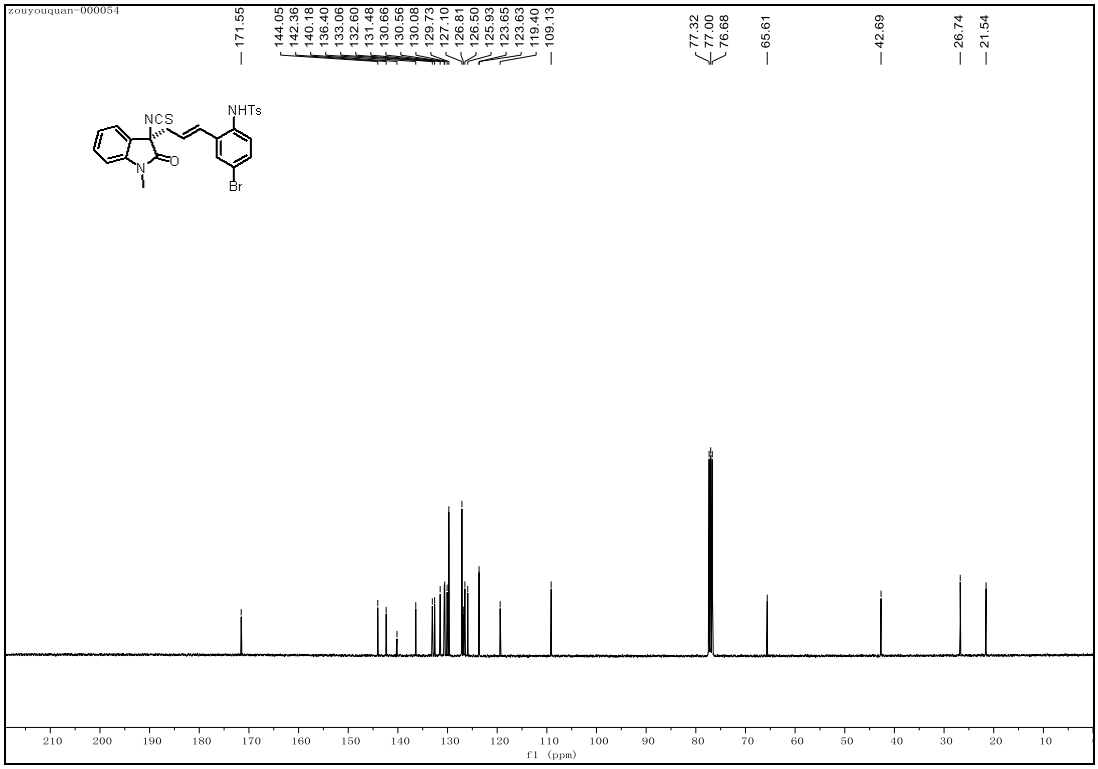
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3h



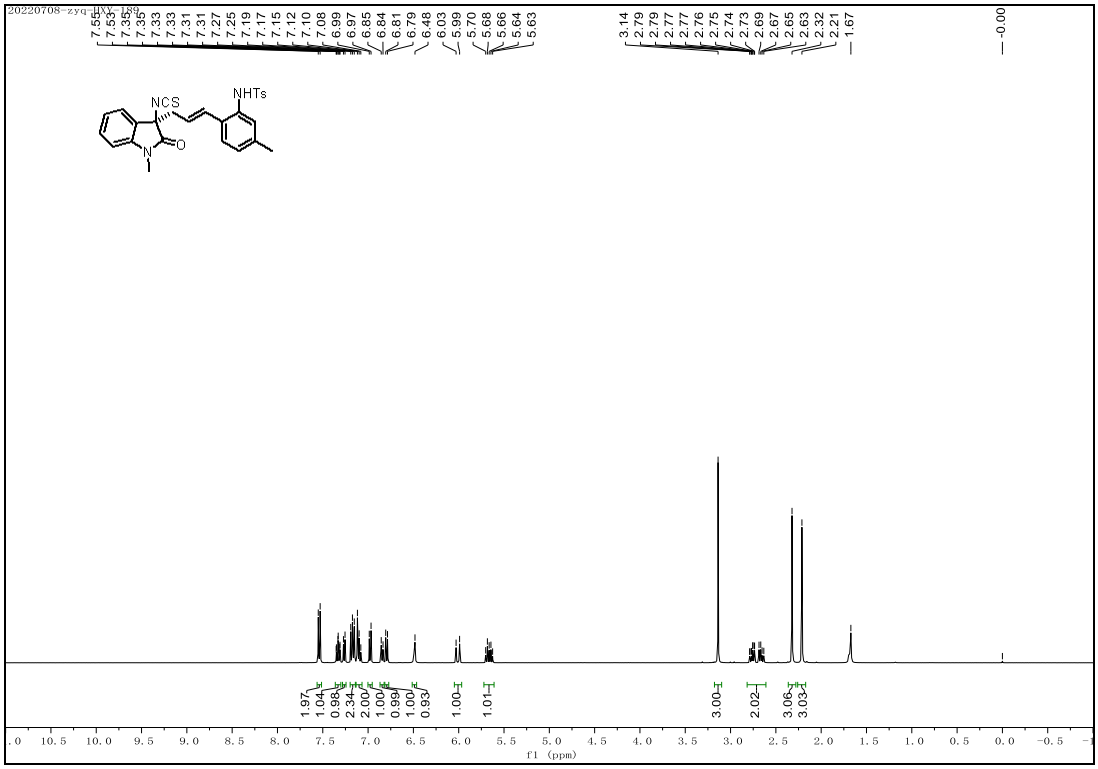
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3i



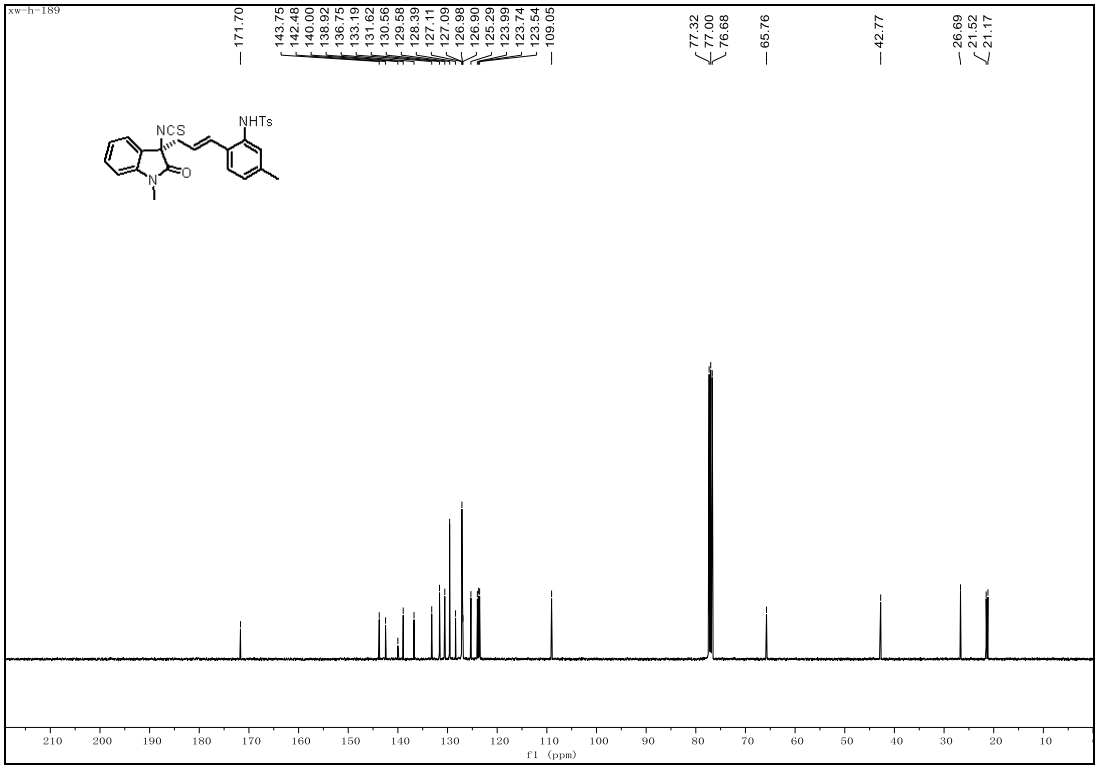
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3i



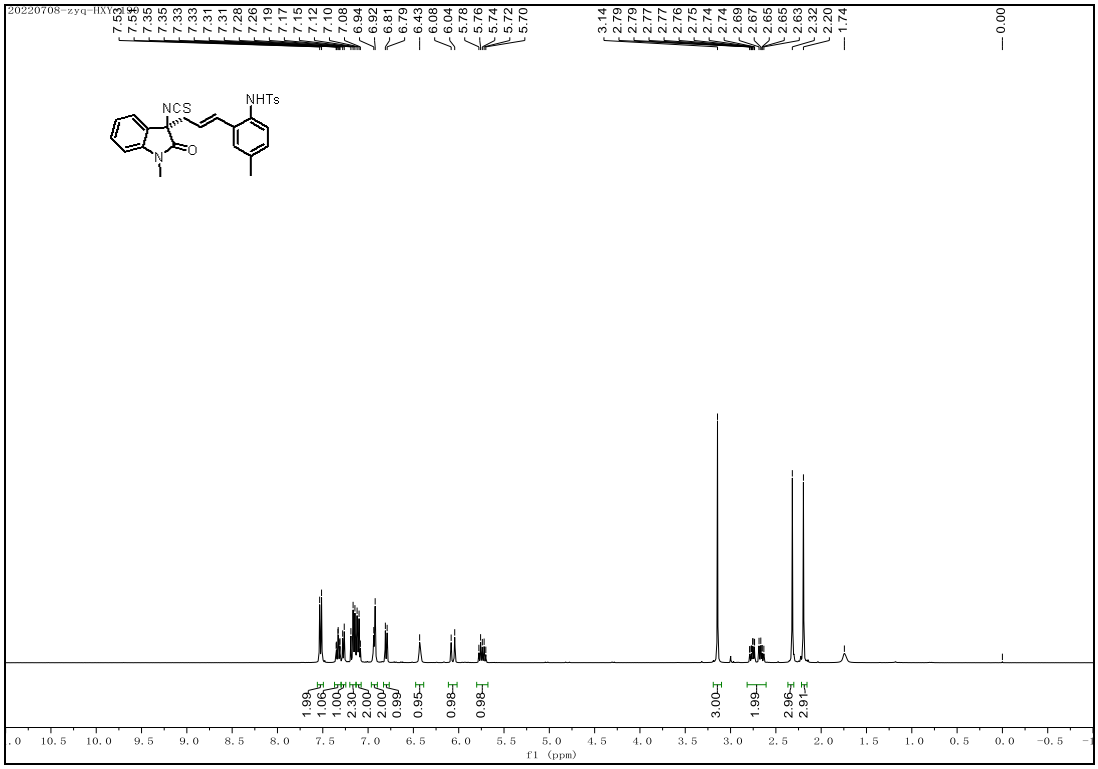
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3j



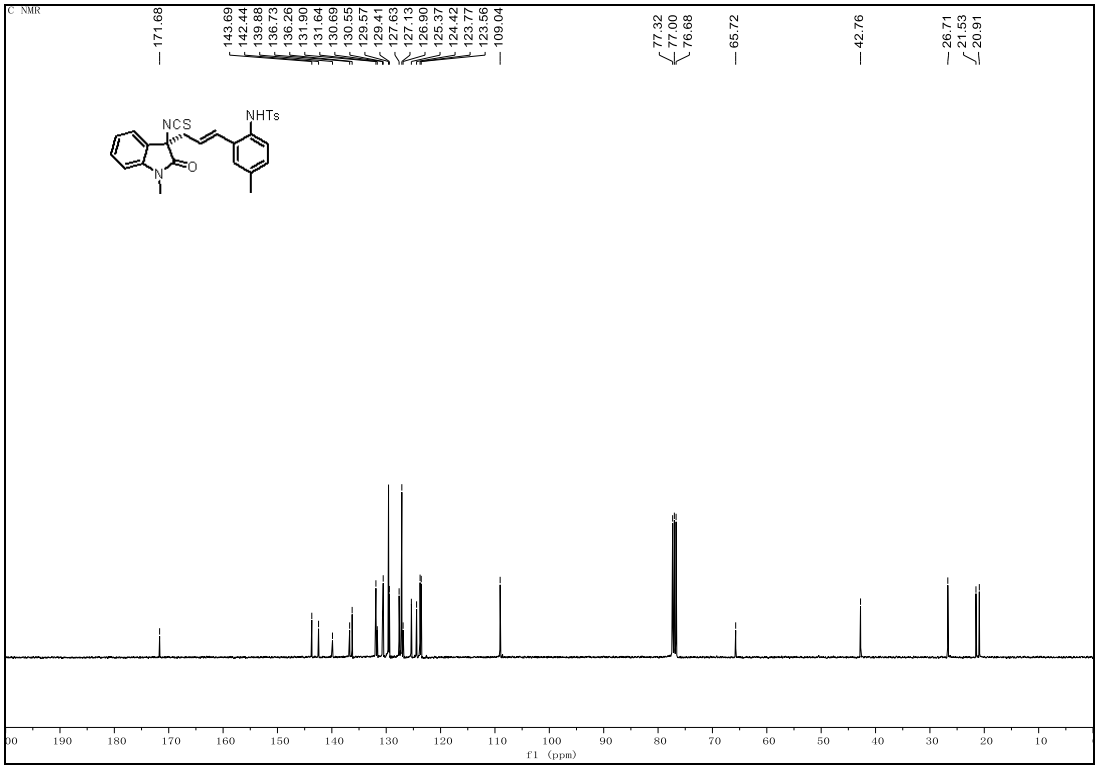
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3j



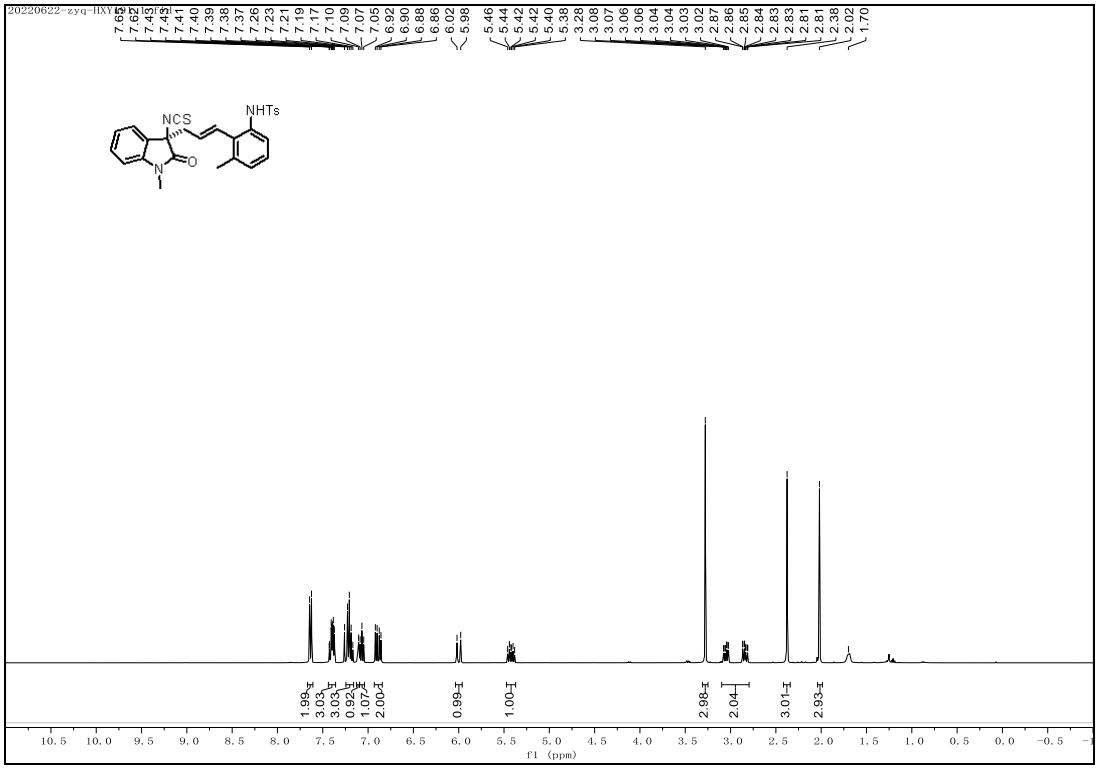
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3k



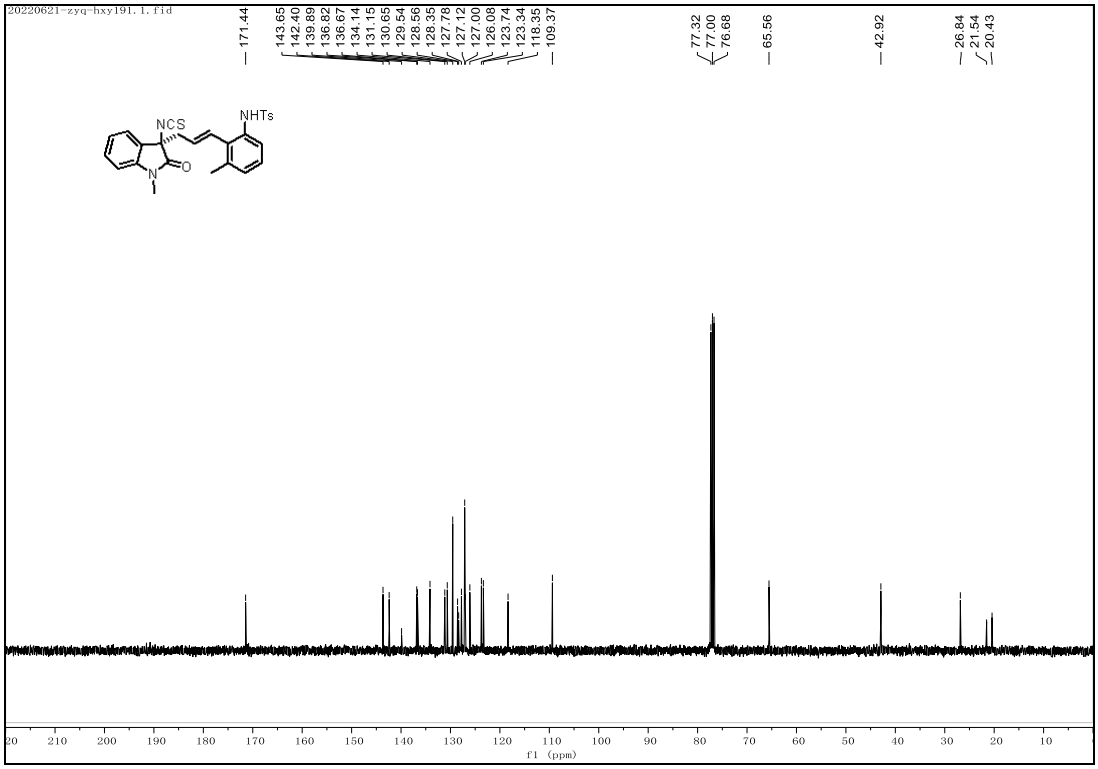
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3k



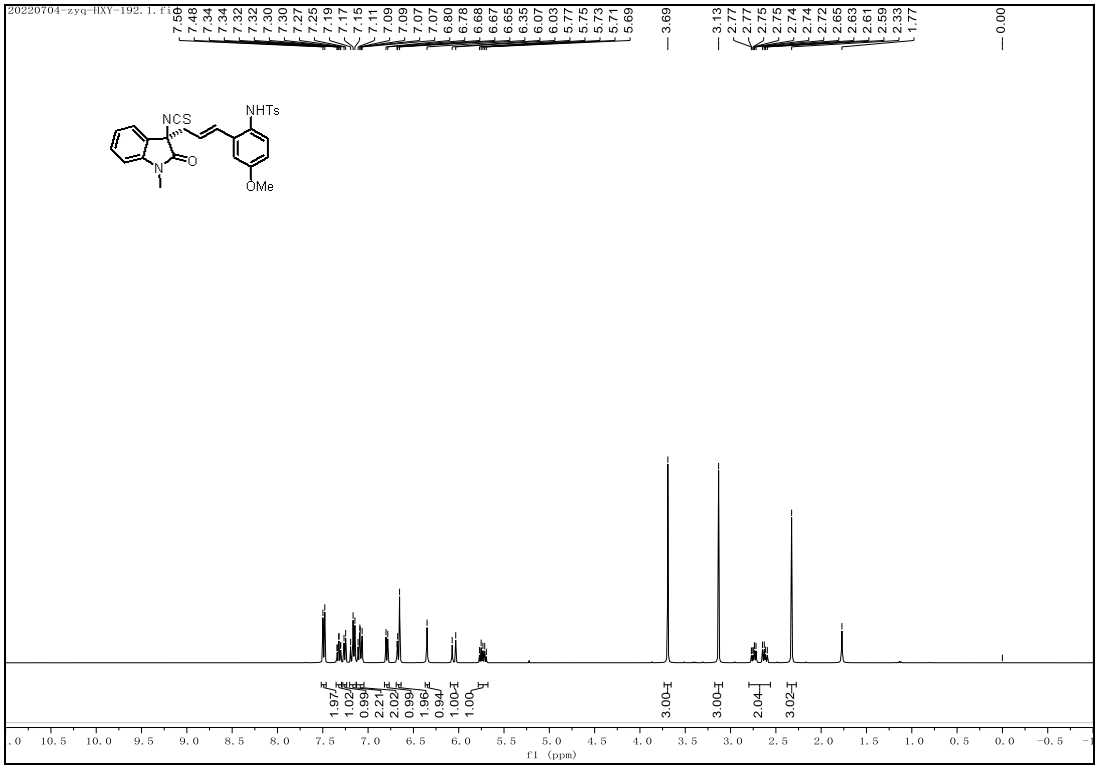
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3l



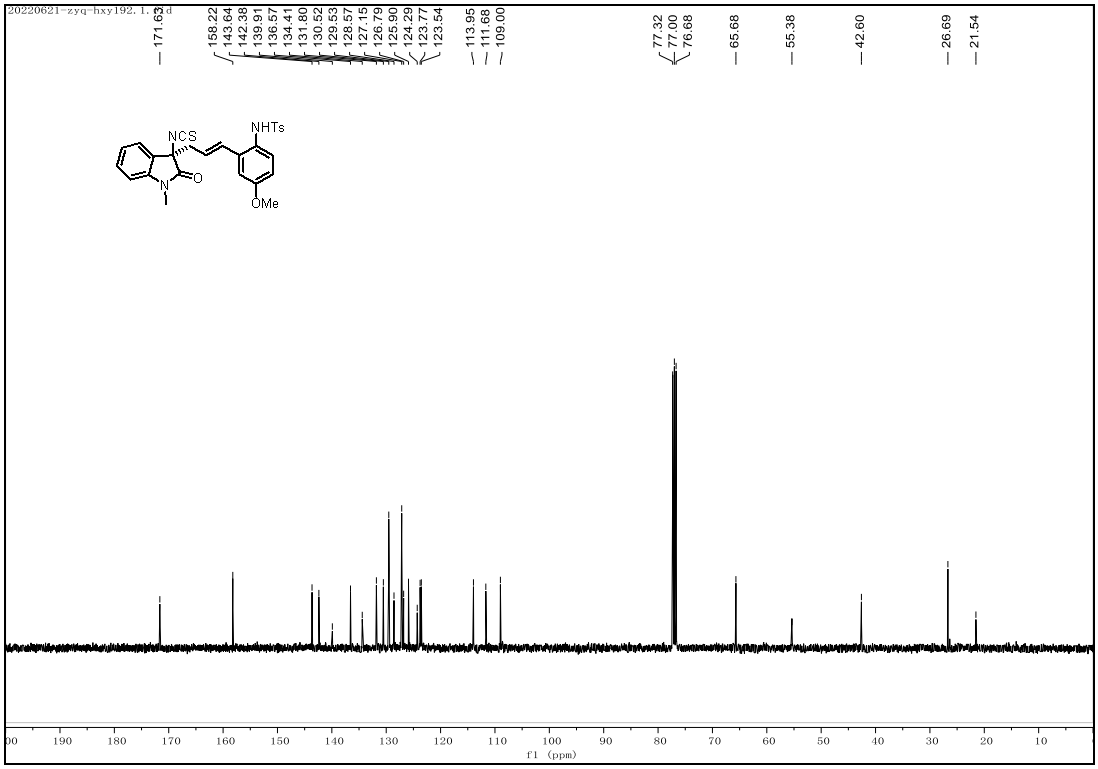
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3l



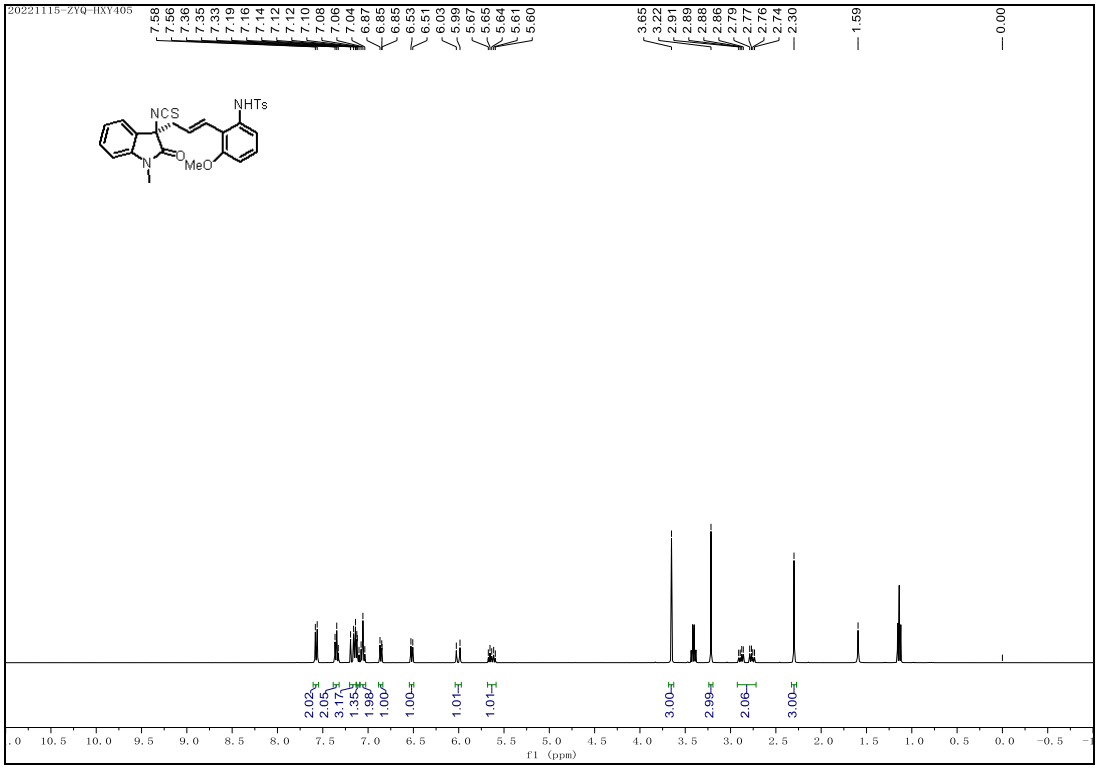
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3m



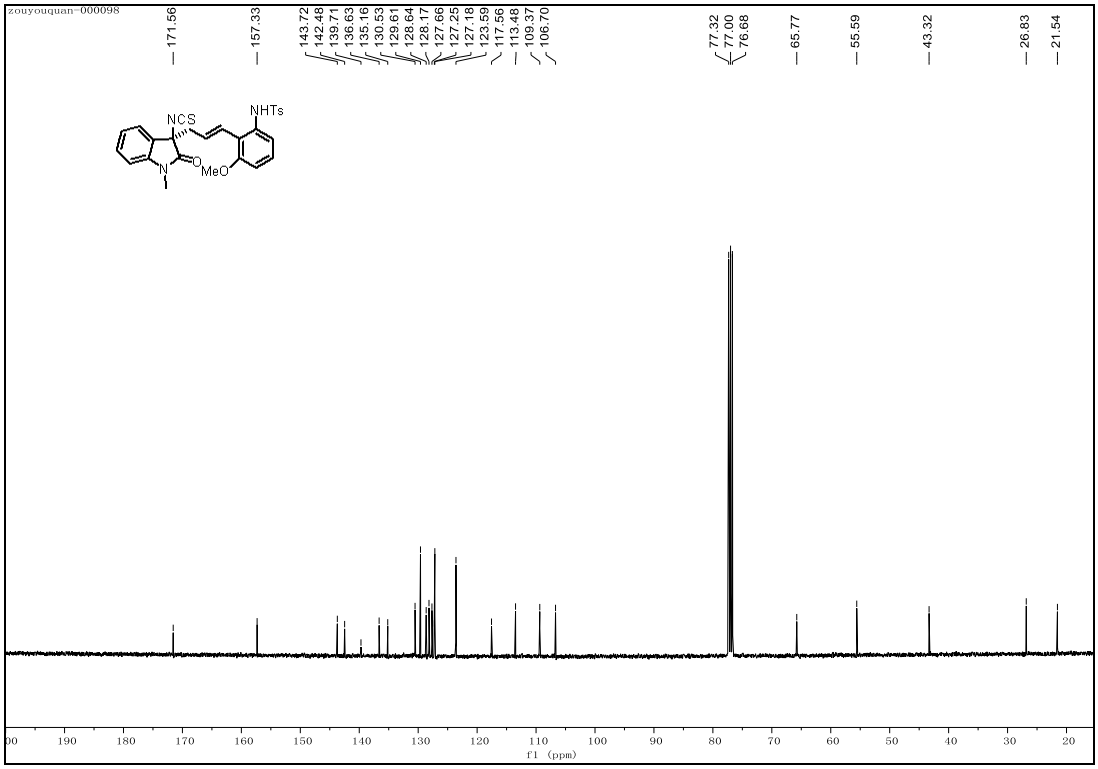
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3m



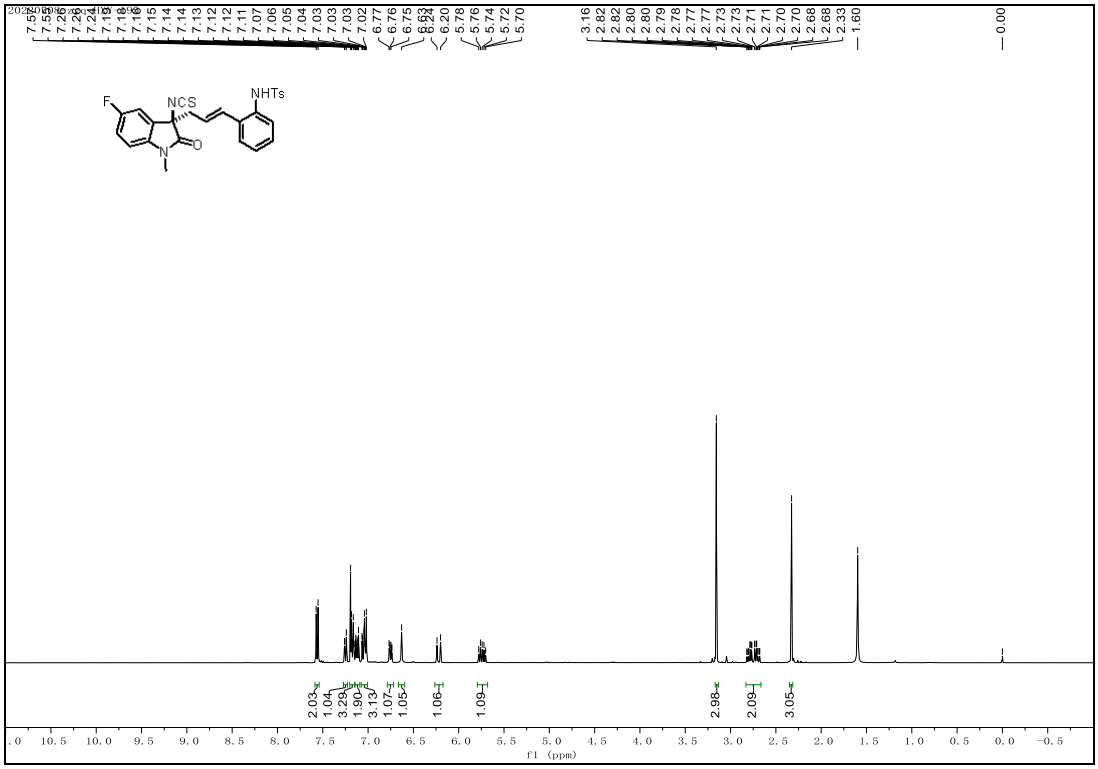
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3n



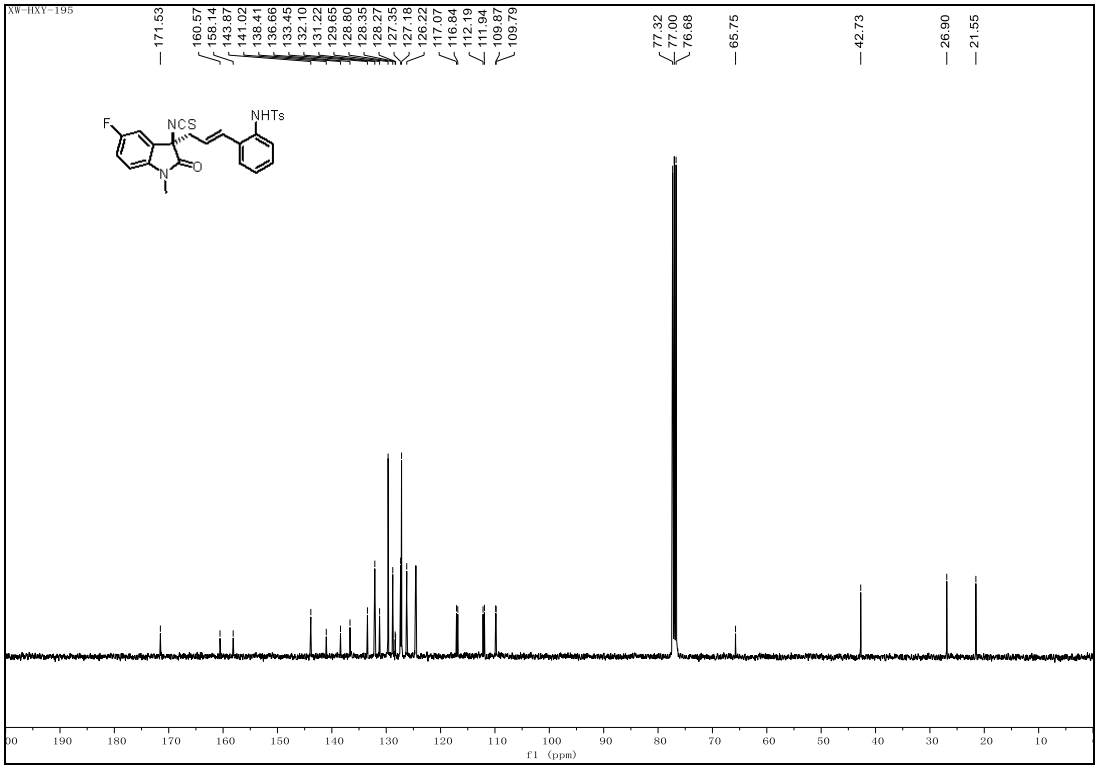
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3n



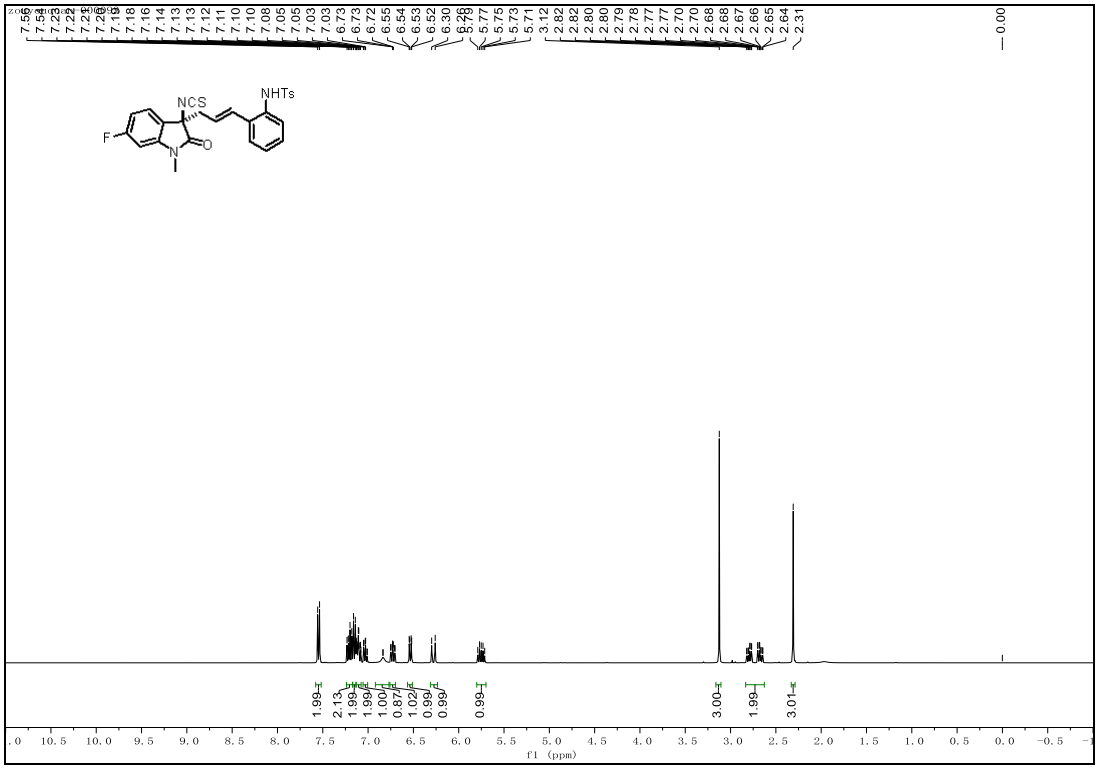
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3o



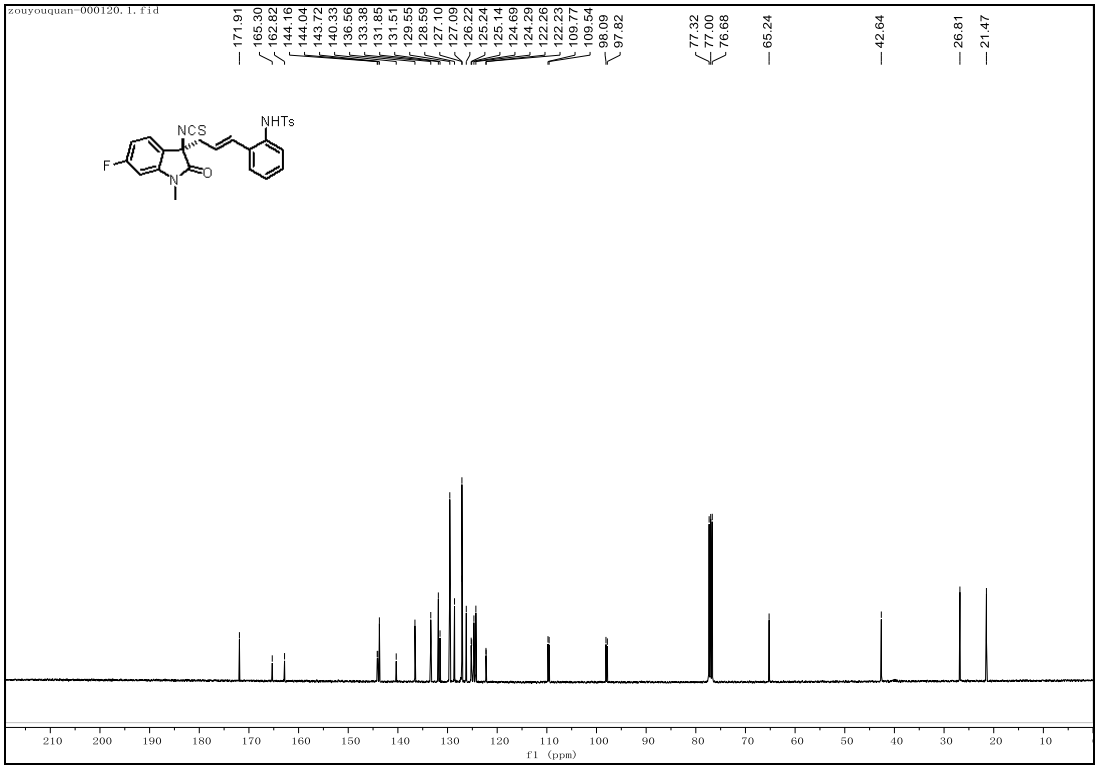
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3o



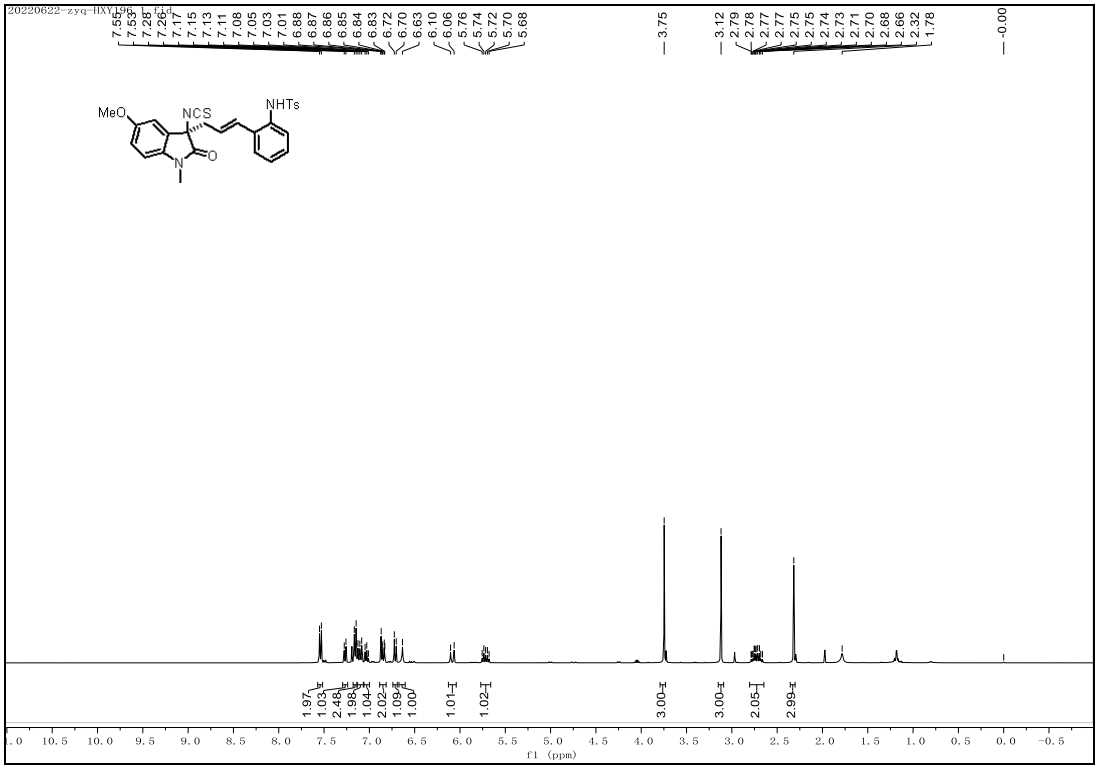
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3p



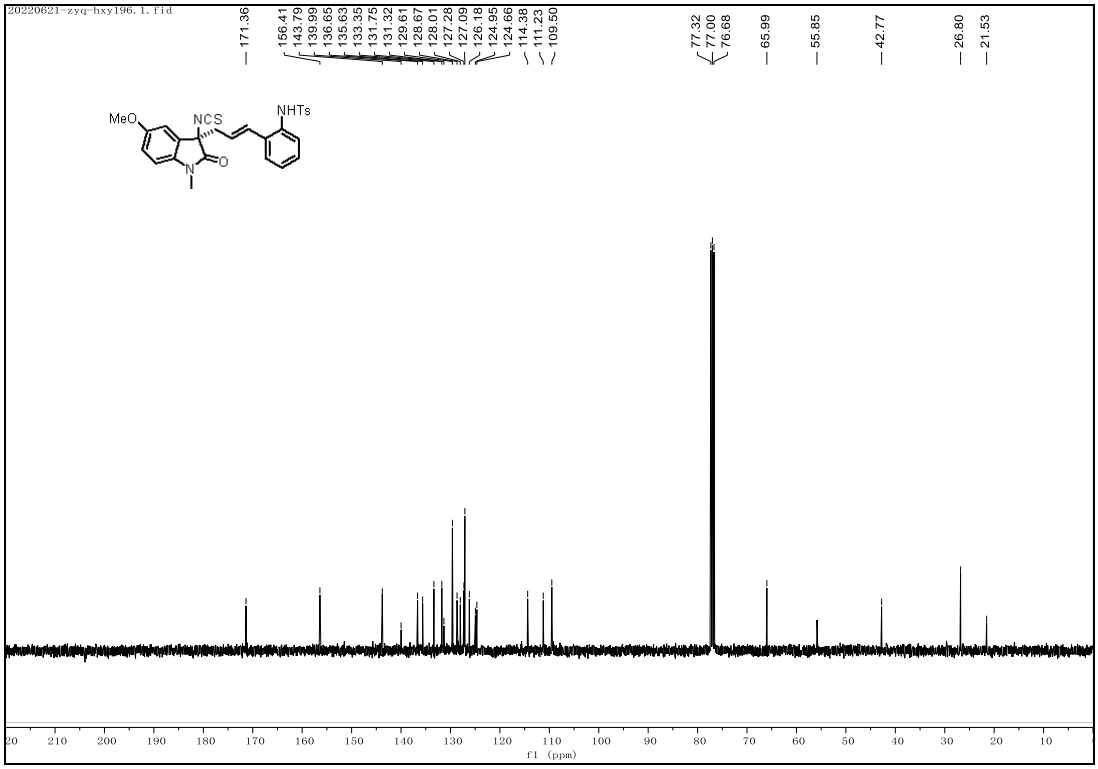
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3p



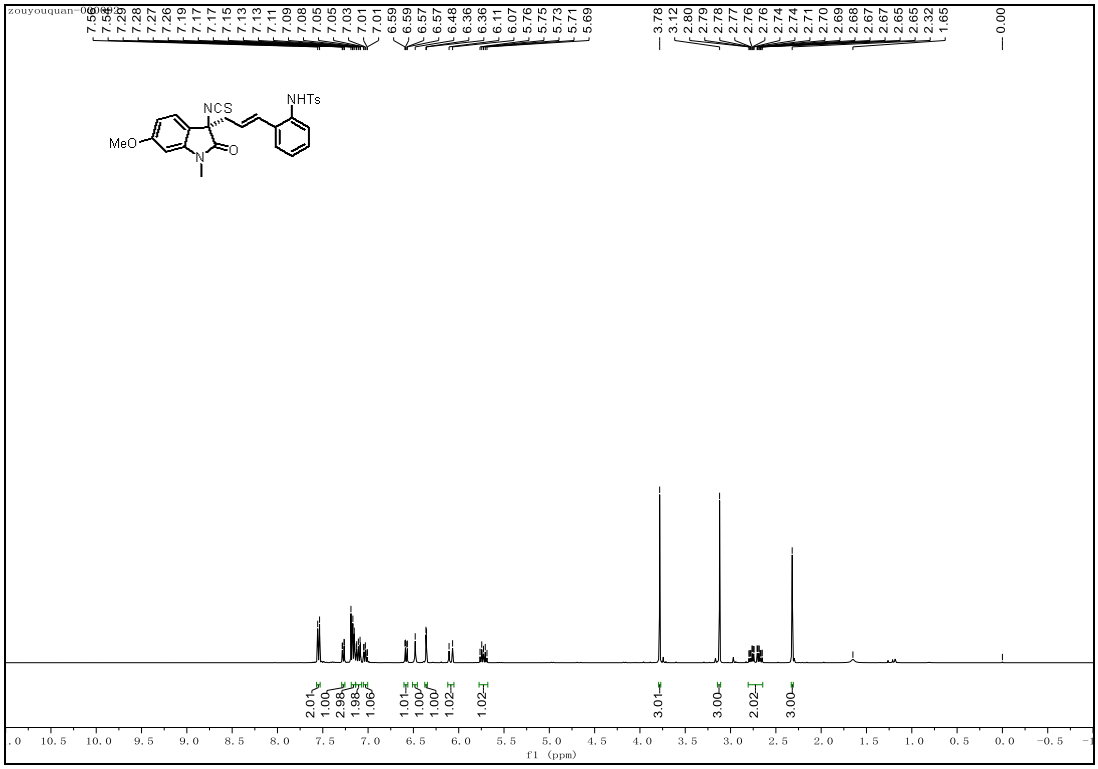
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3q



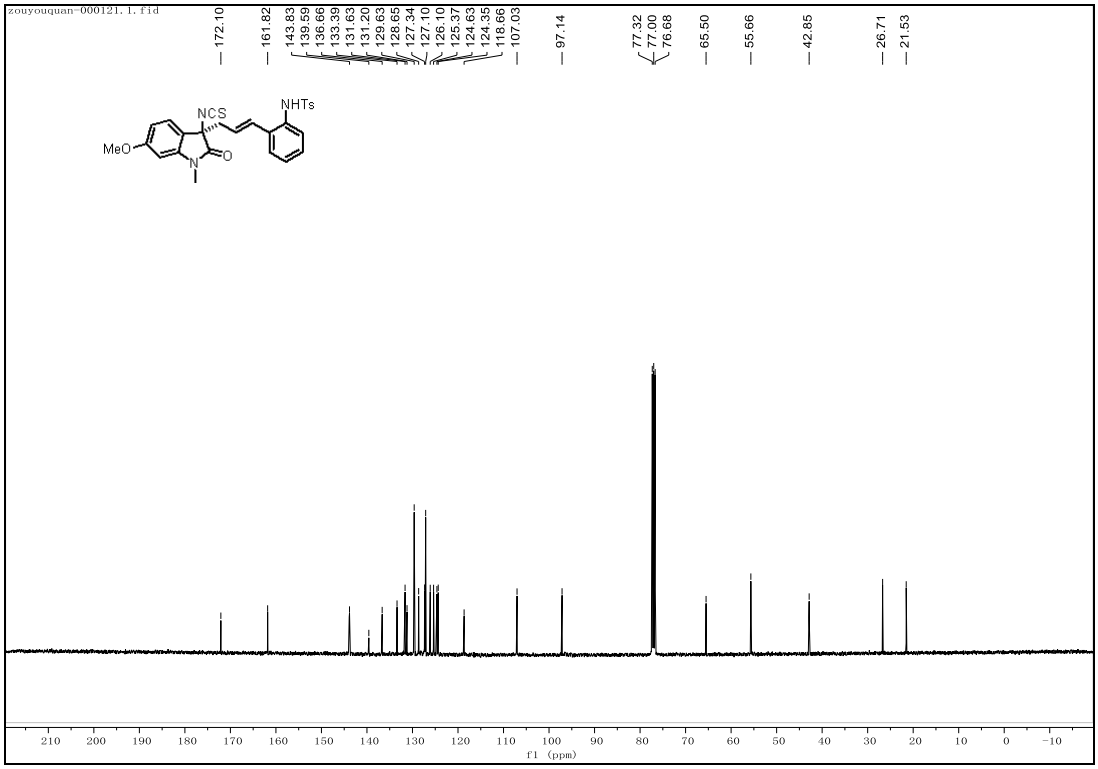
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3q



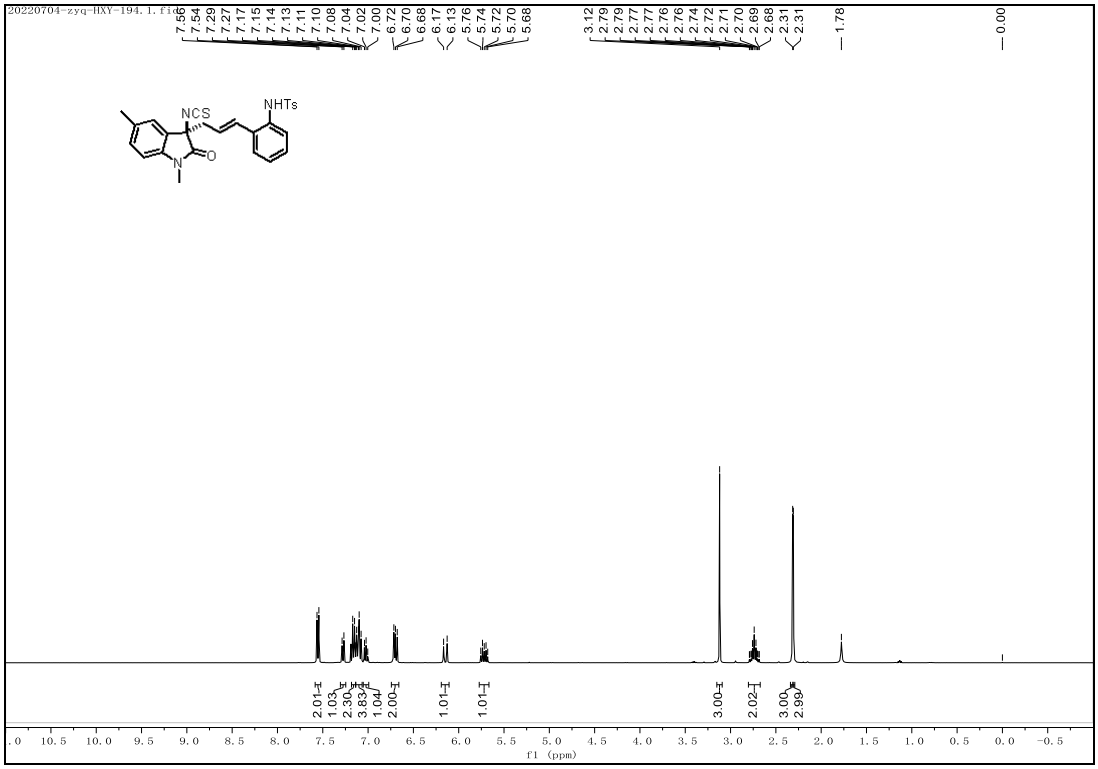
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3r



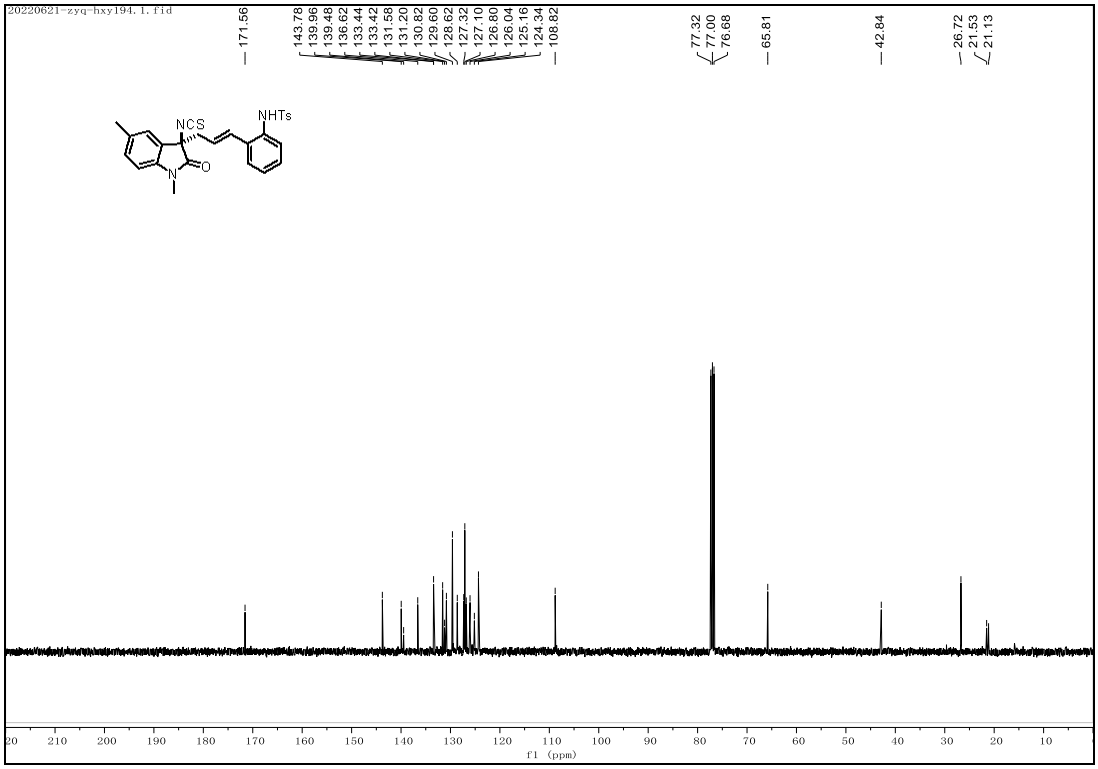
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3r



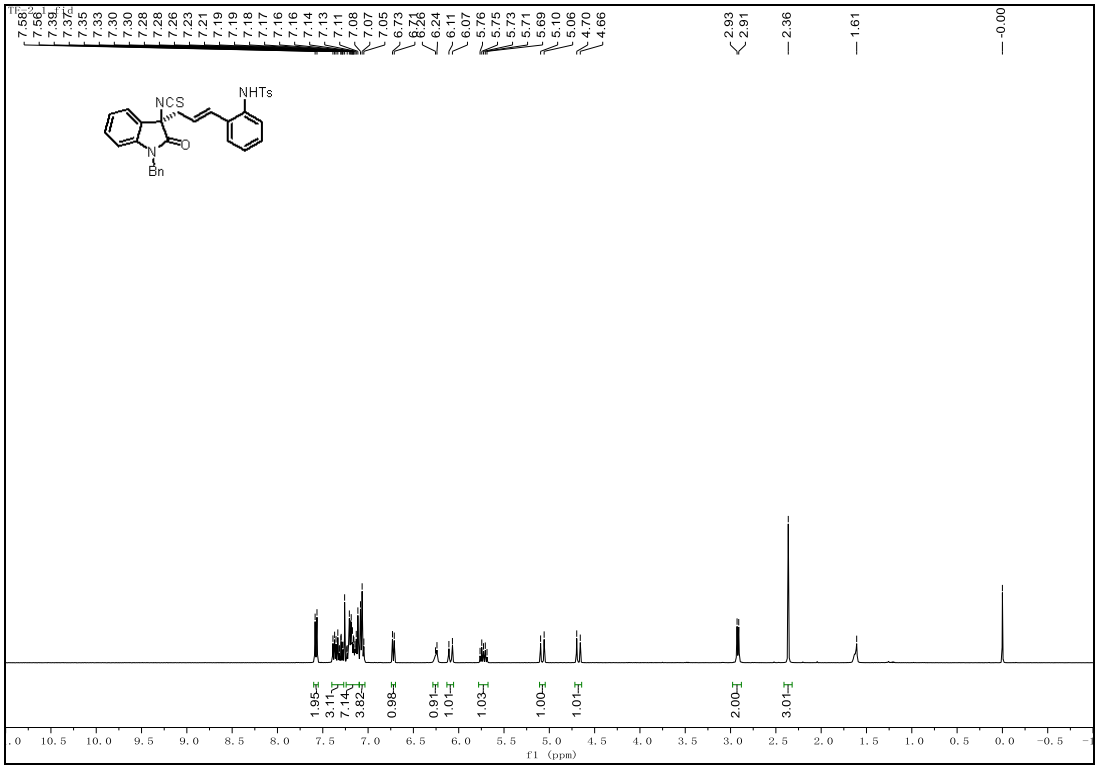
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3s



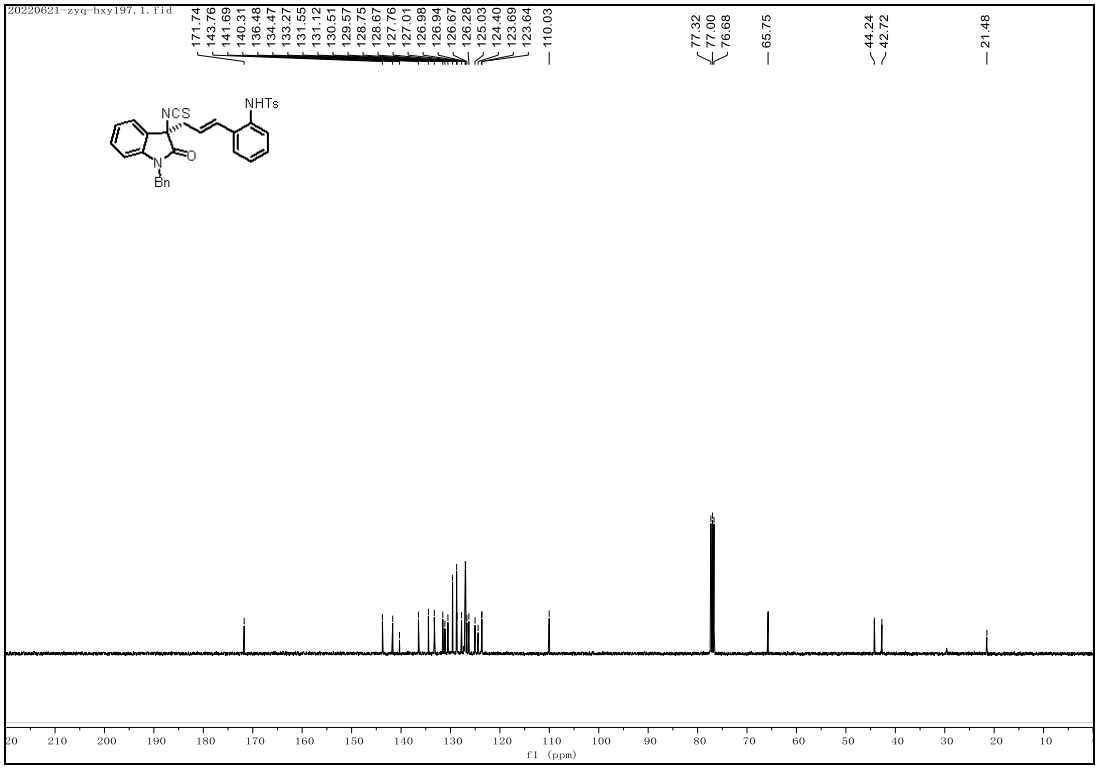
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3s



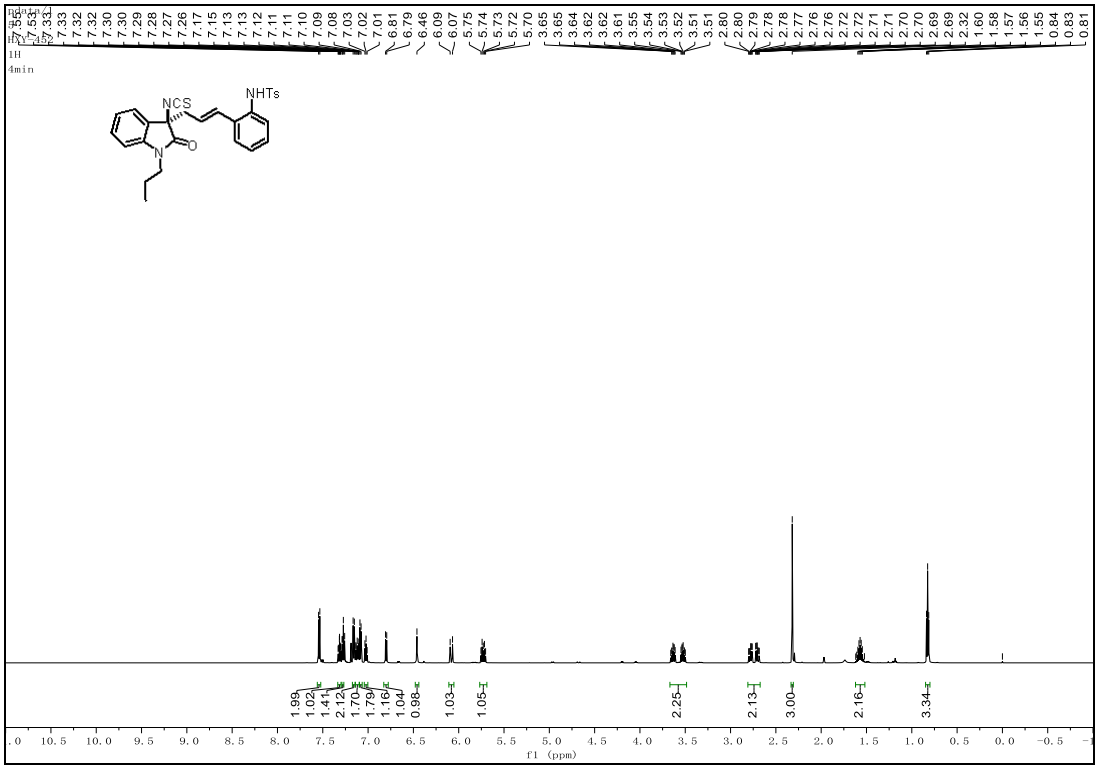
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for compound 3t



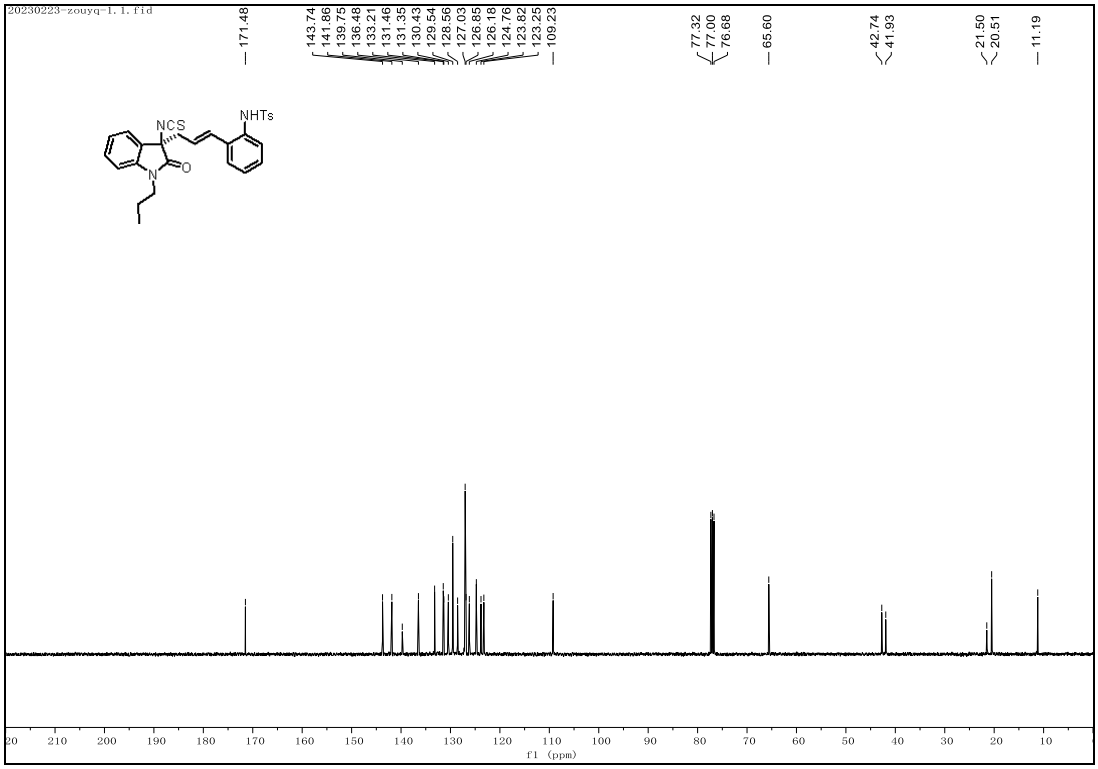
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3t



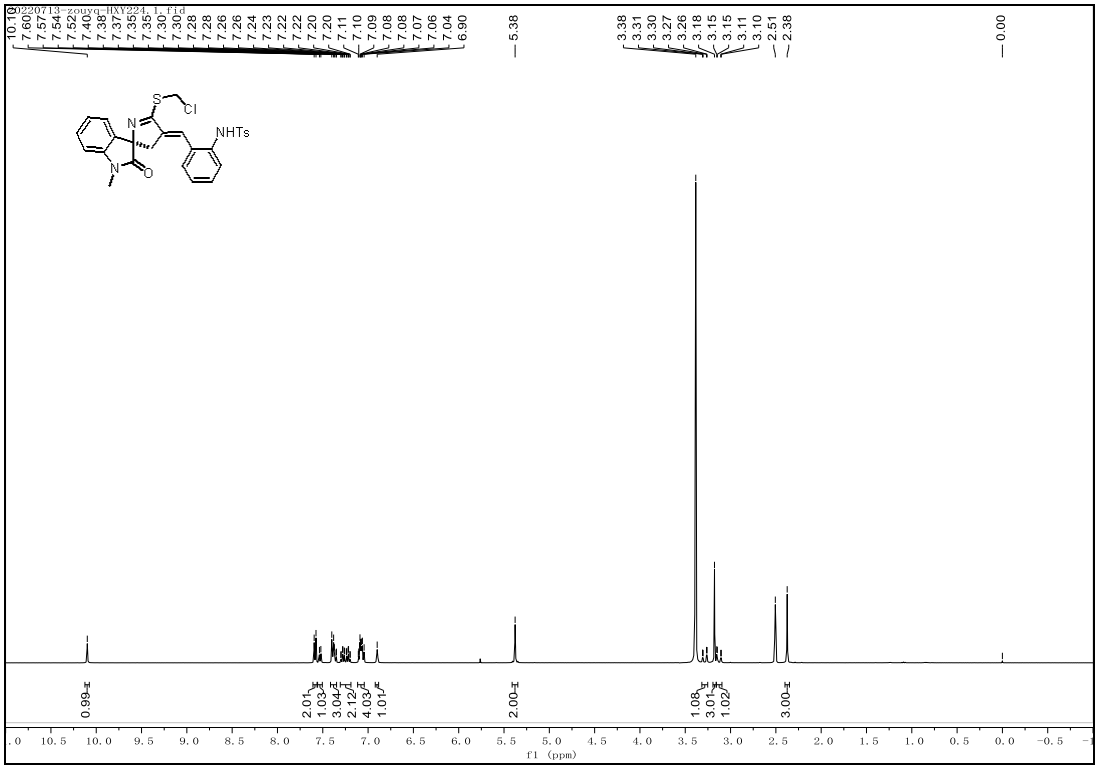
^{1}H NMR (600 MHz, $CDCl_3$) spectrum for compound 3u



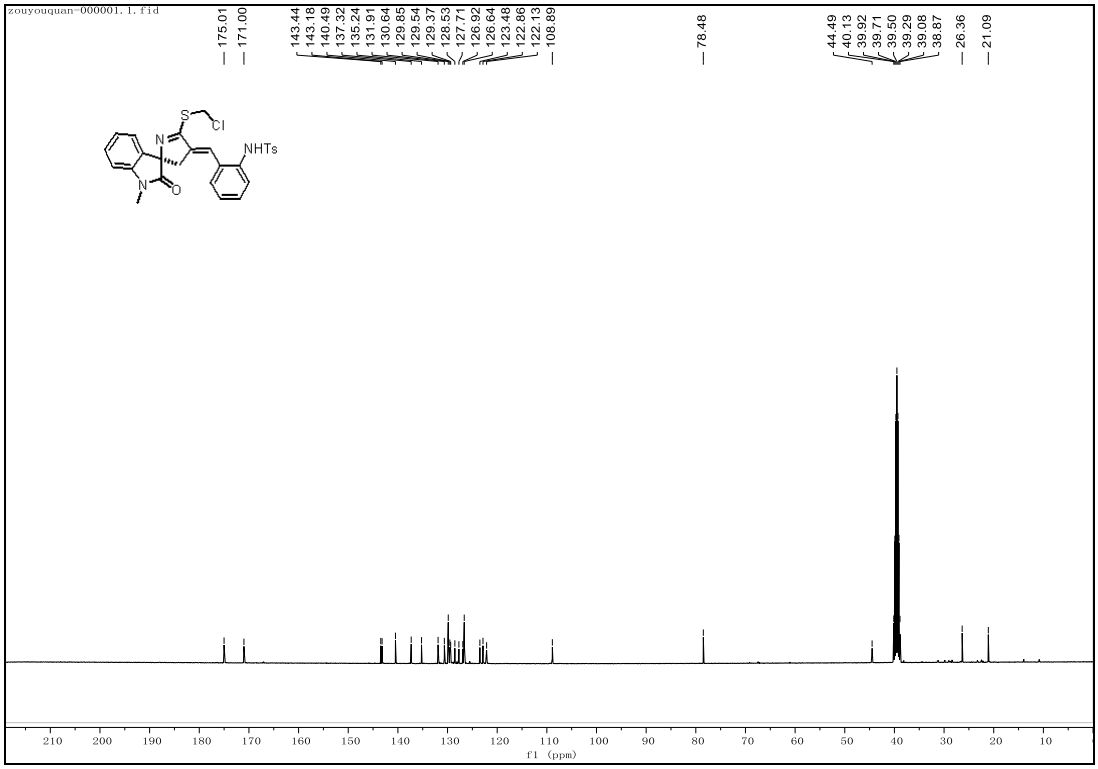
^{13}C NMR (100 MHz, $CDCl_3$) spectrum for compound 3u



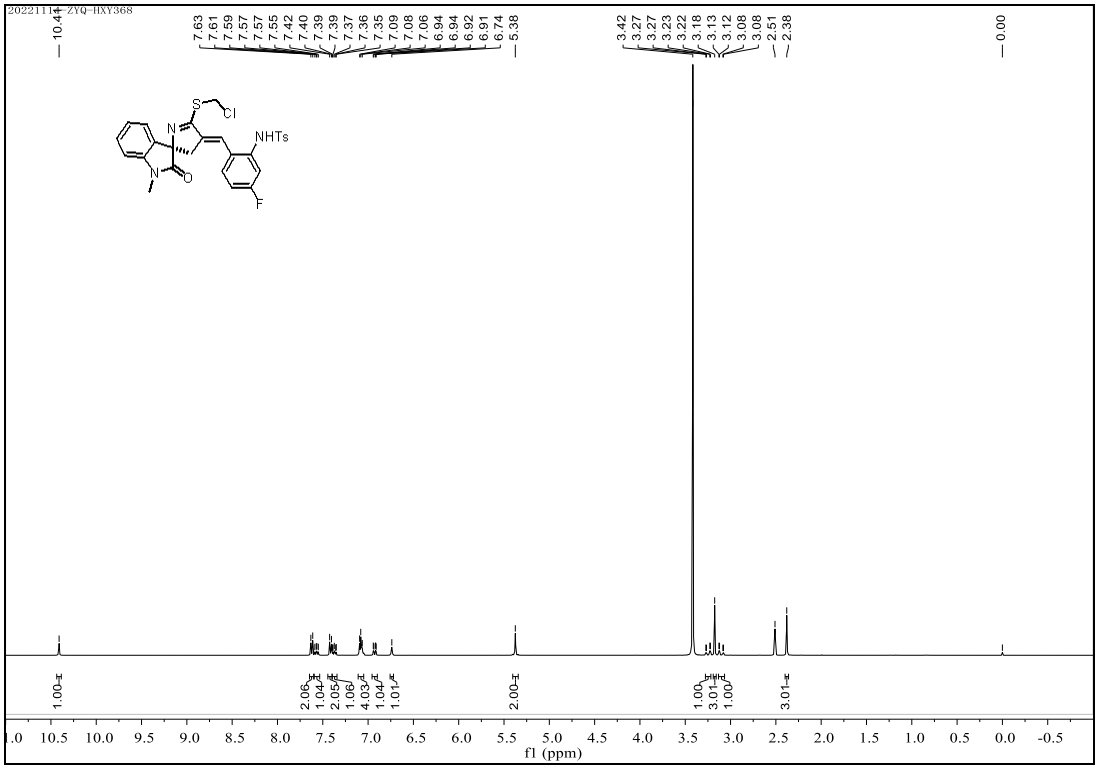
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4a



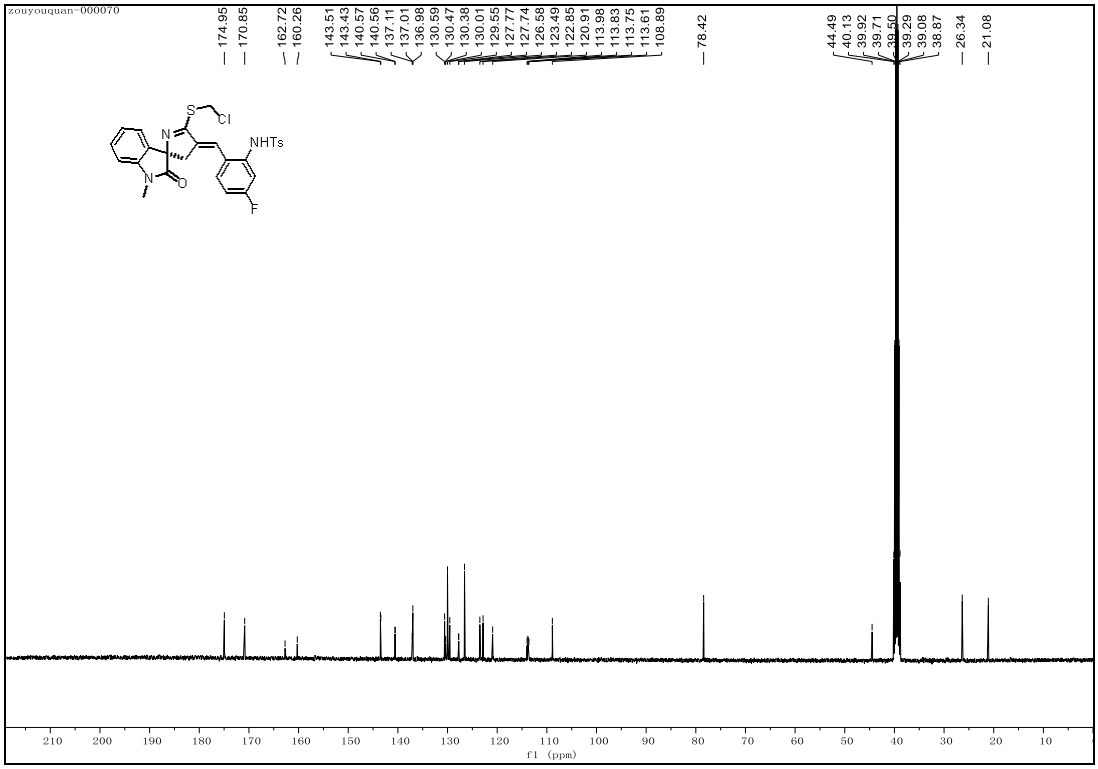
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4a



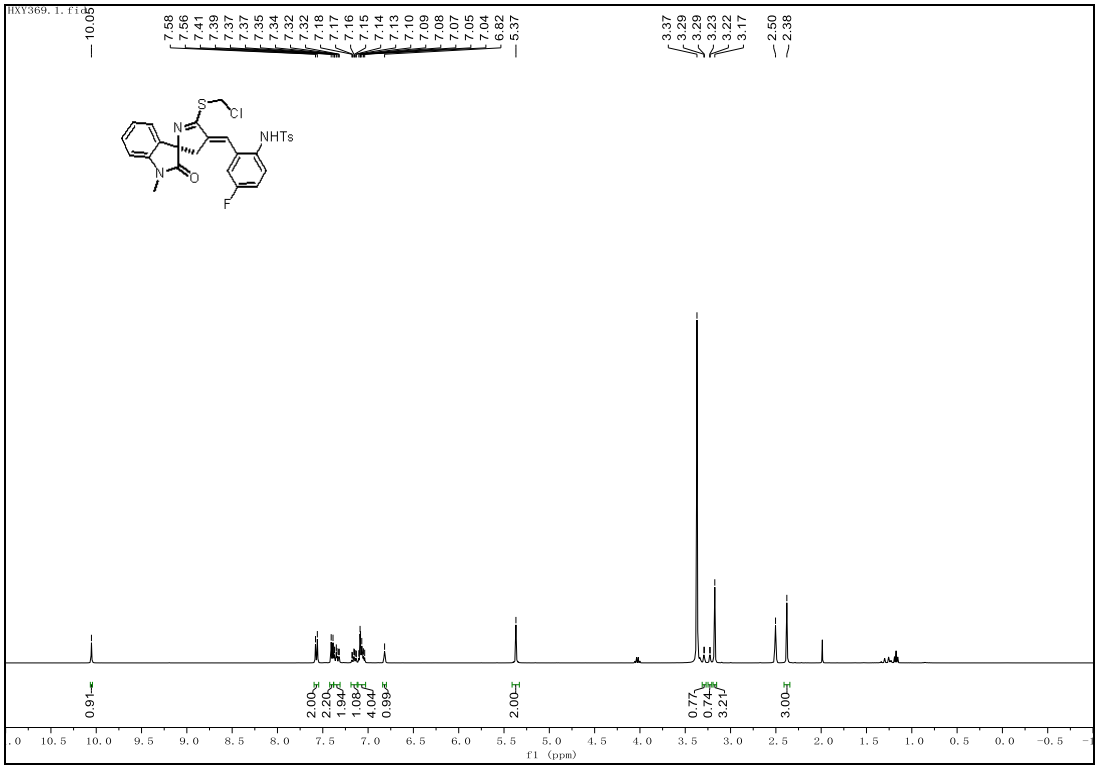
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4b



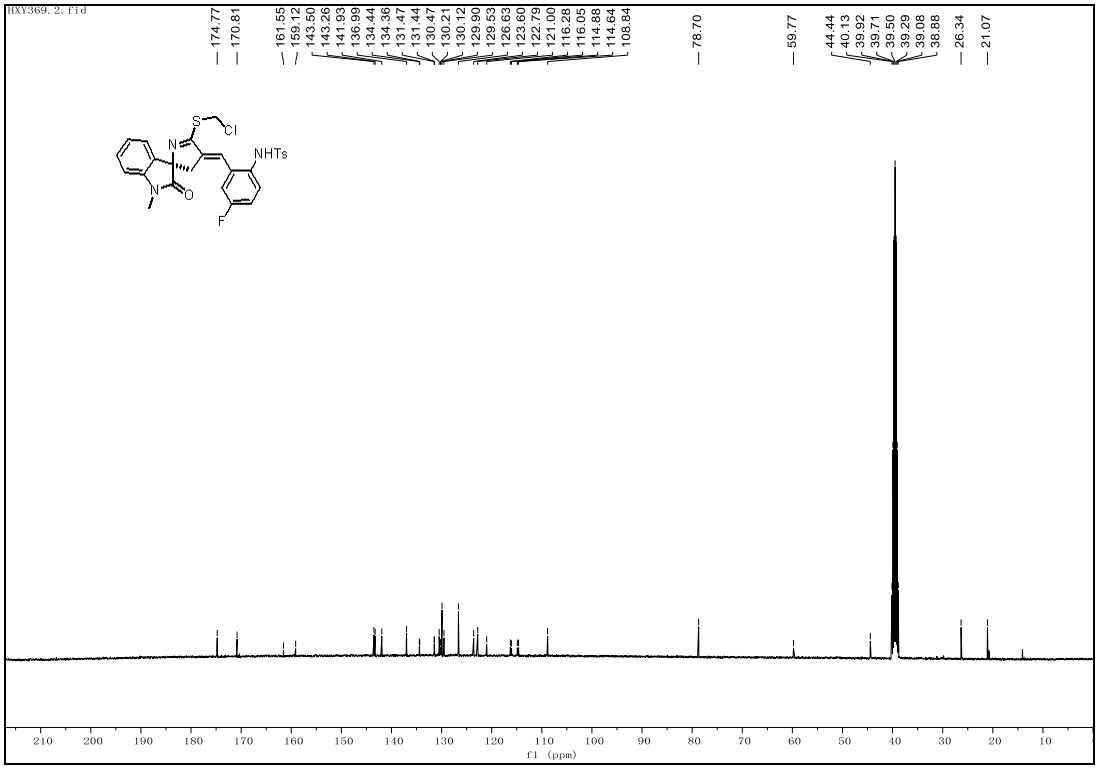
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4b



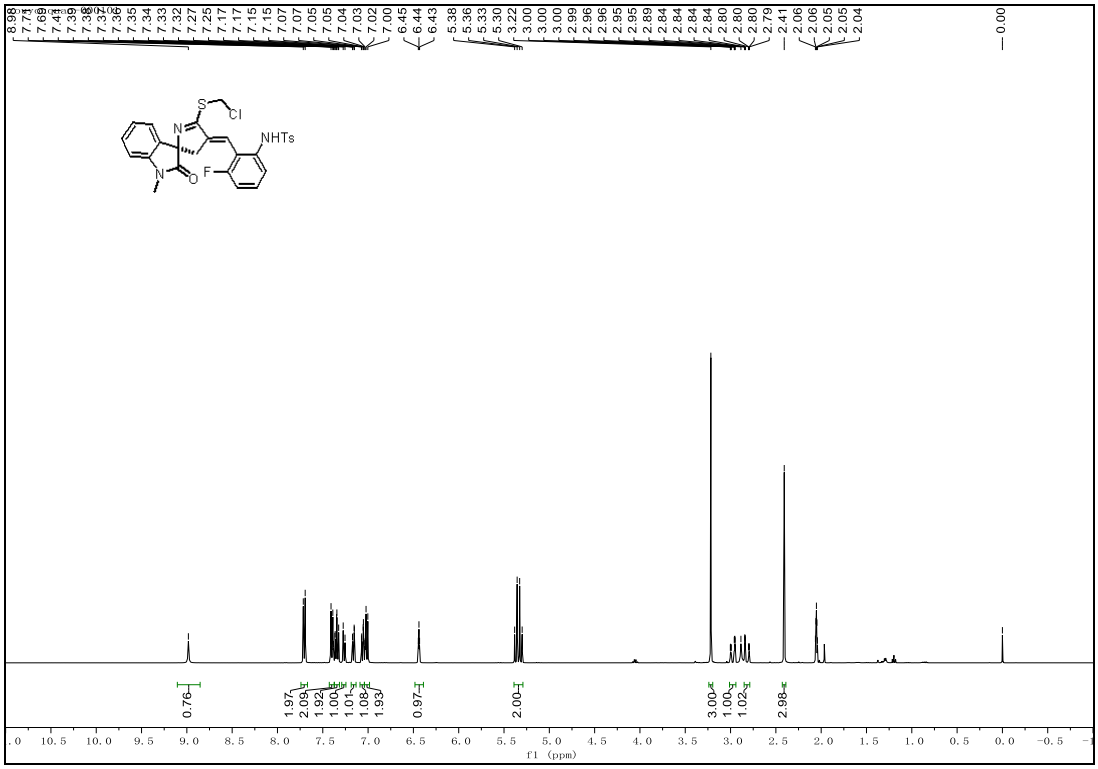
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4c



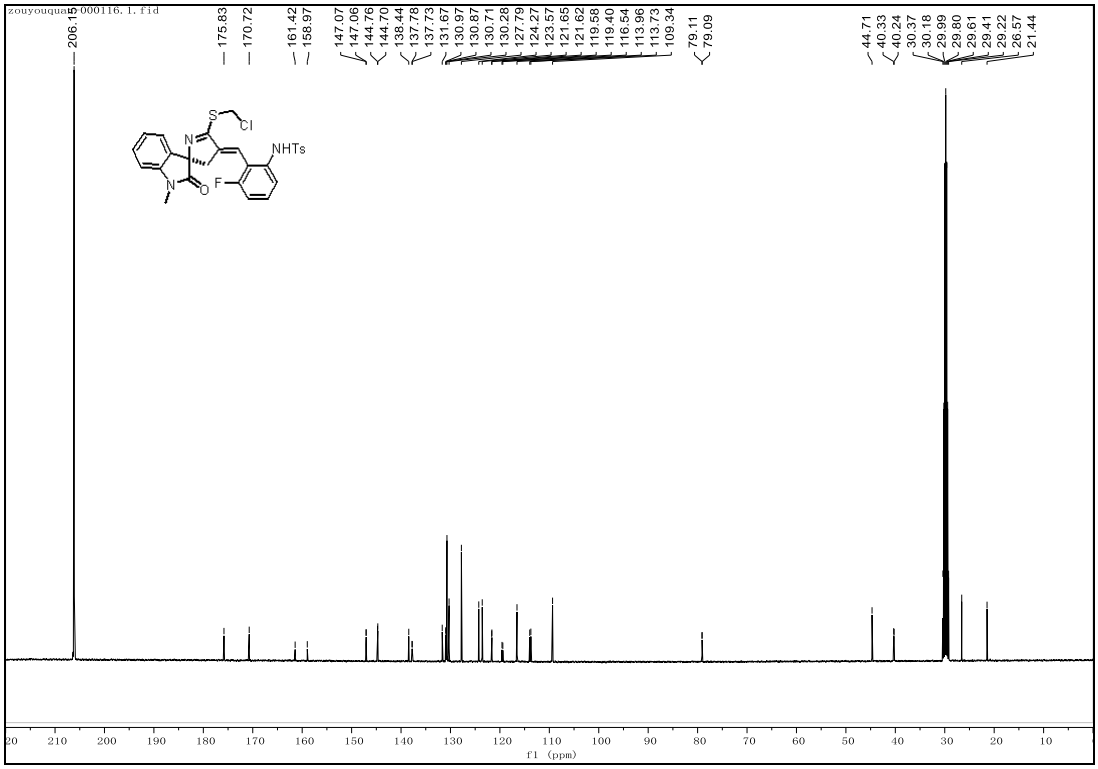
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4c



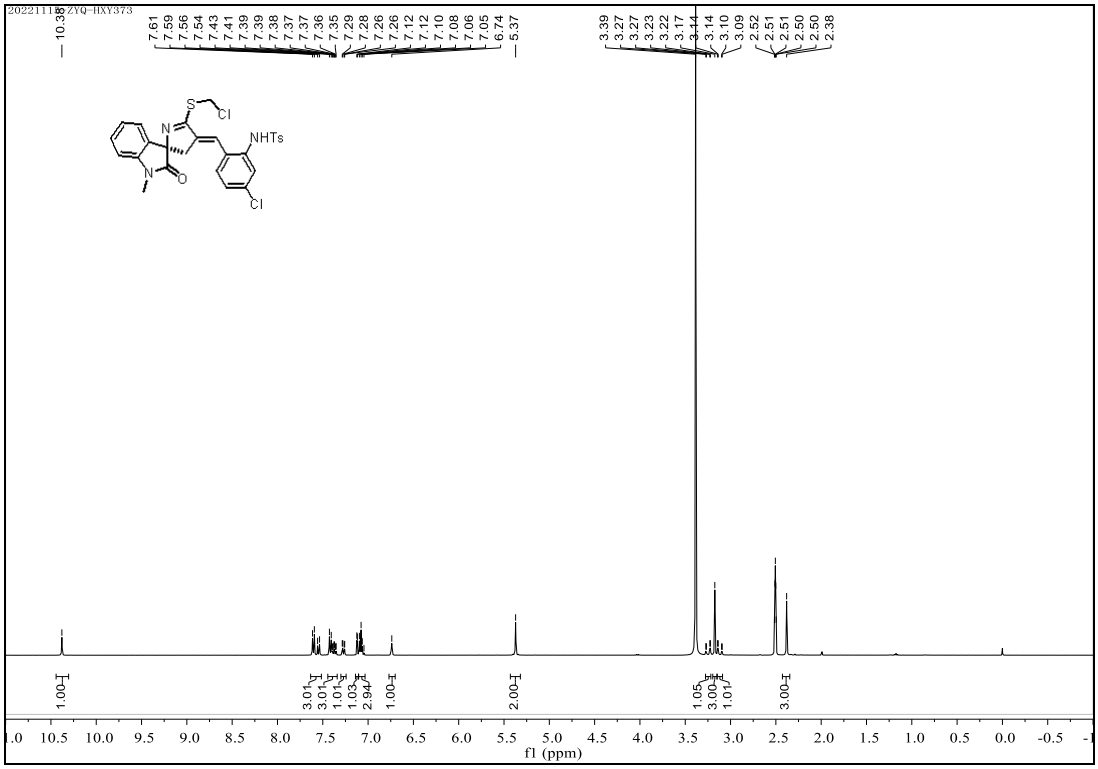
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4d



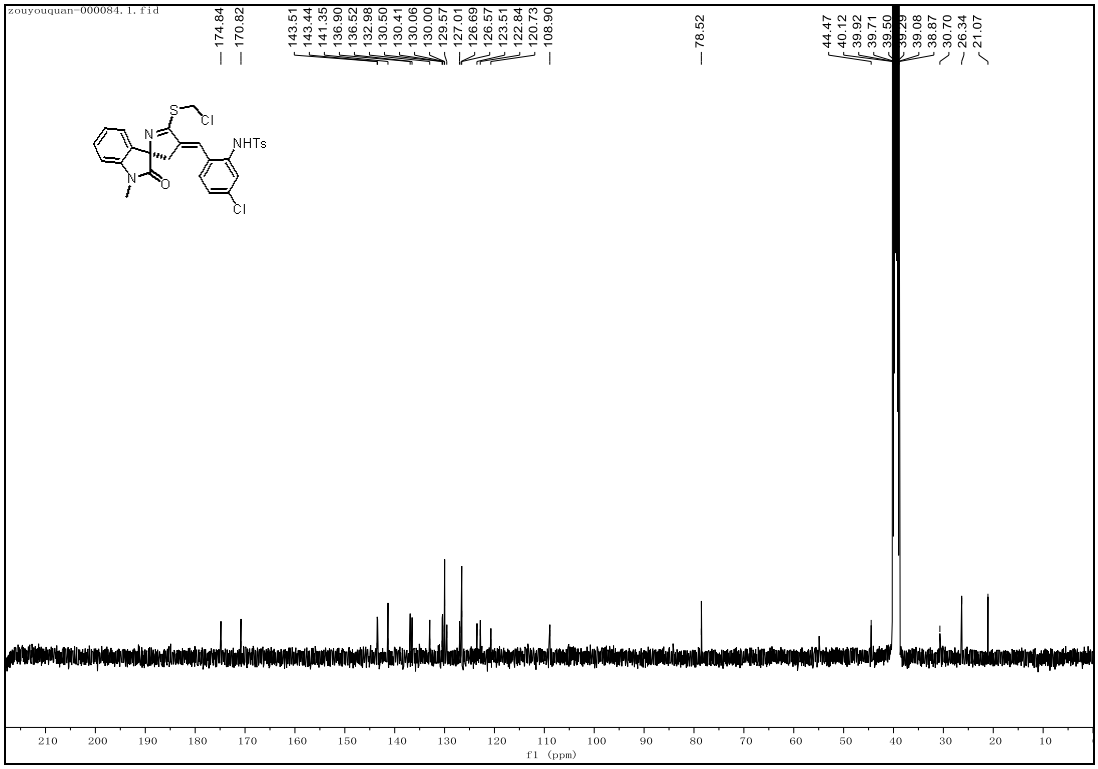
^{13}C NMR (100 MHz, acetone-d_6) spectrum for compound 4d



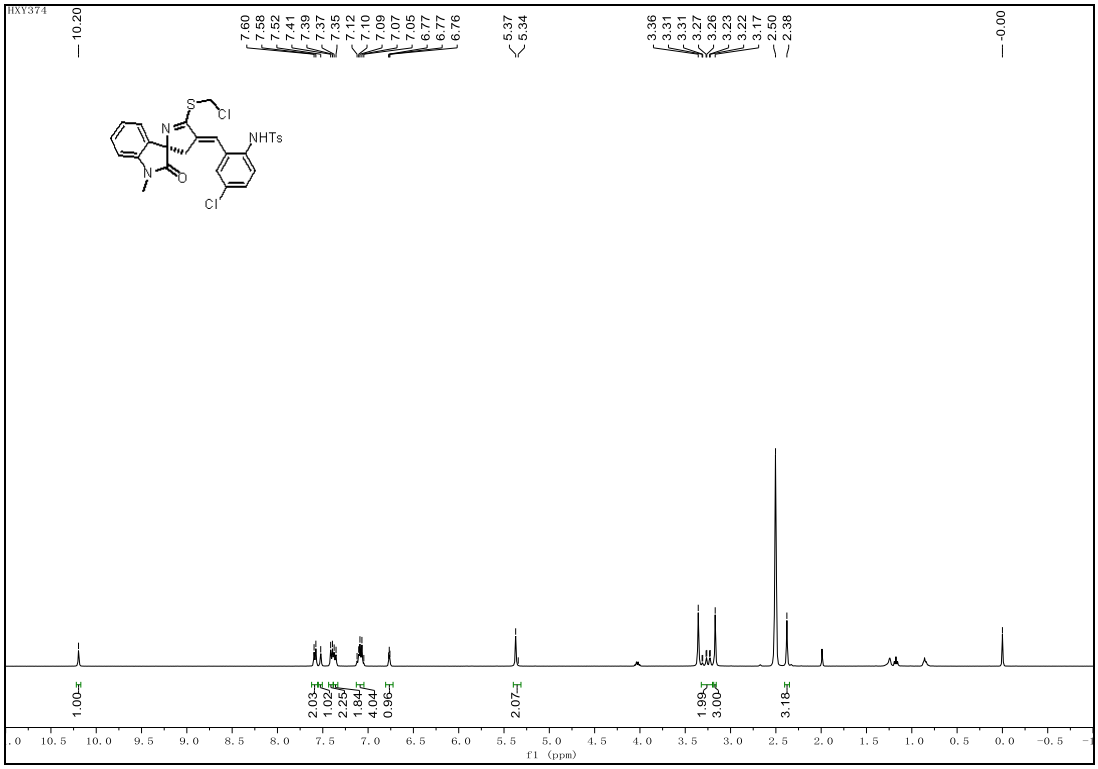
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4e



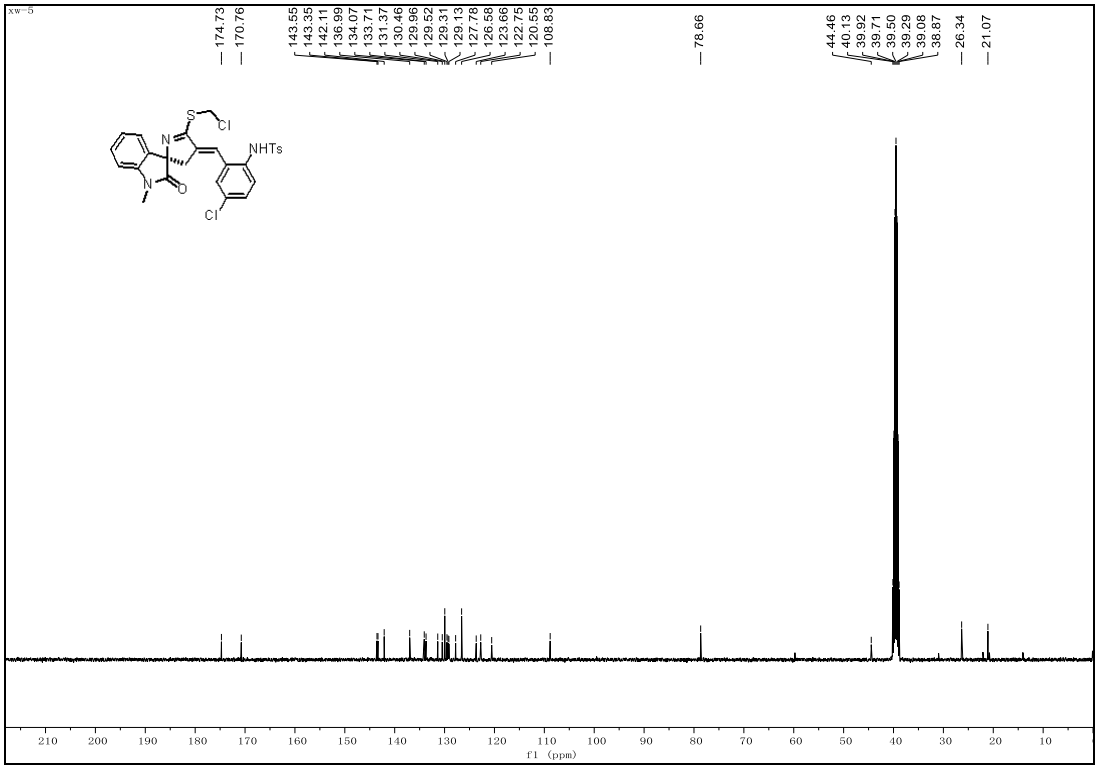
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4e



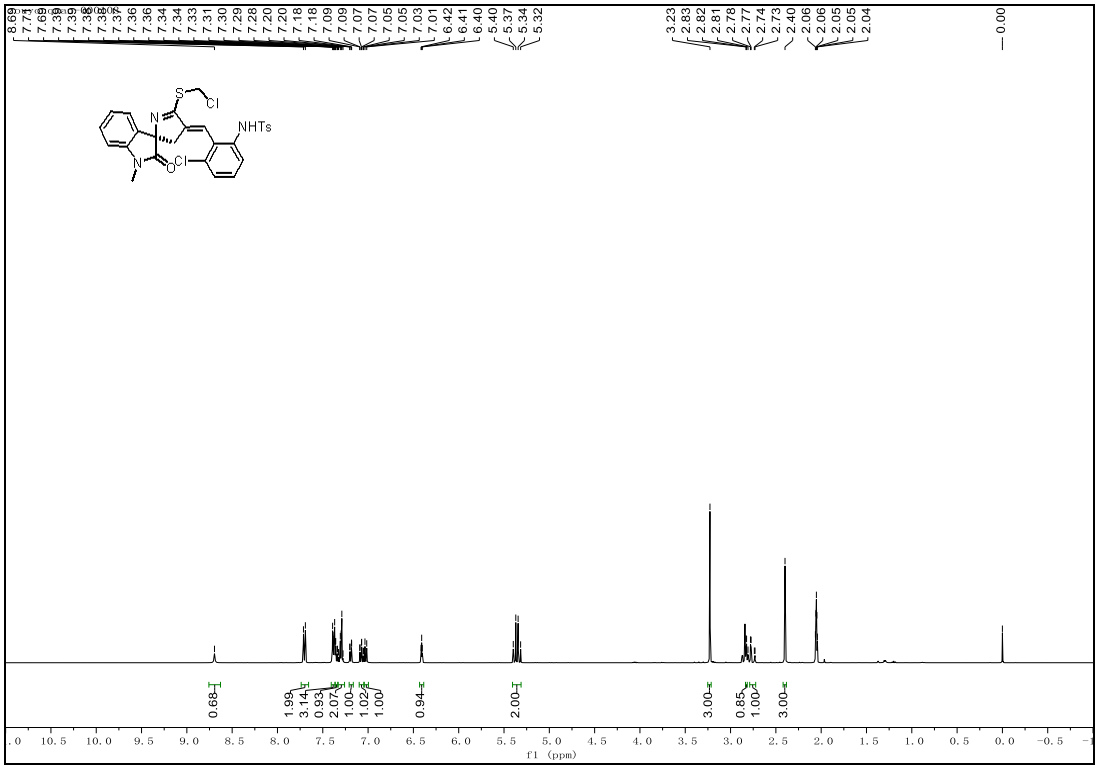
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4f



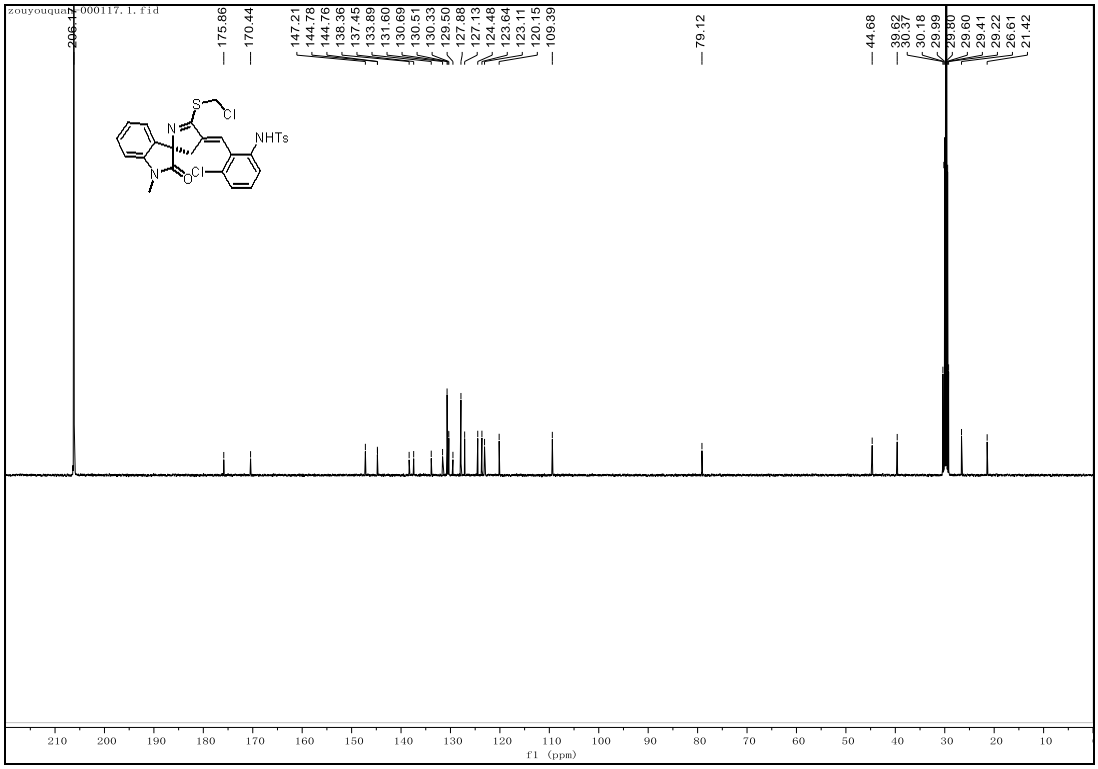
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4f



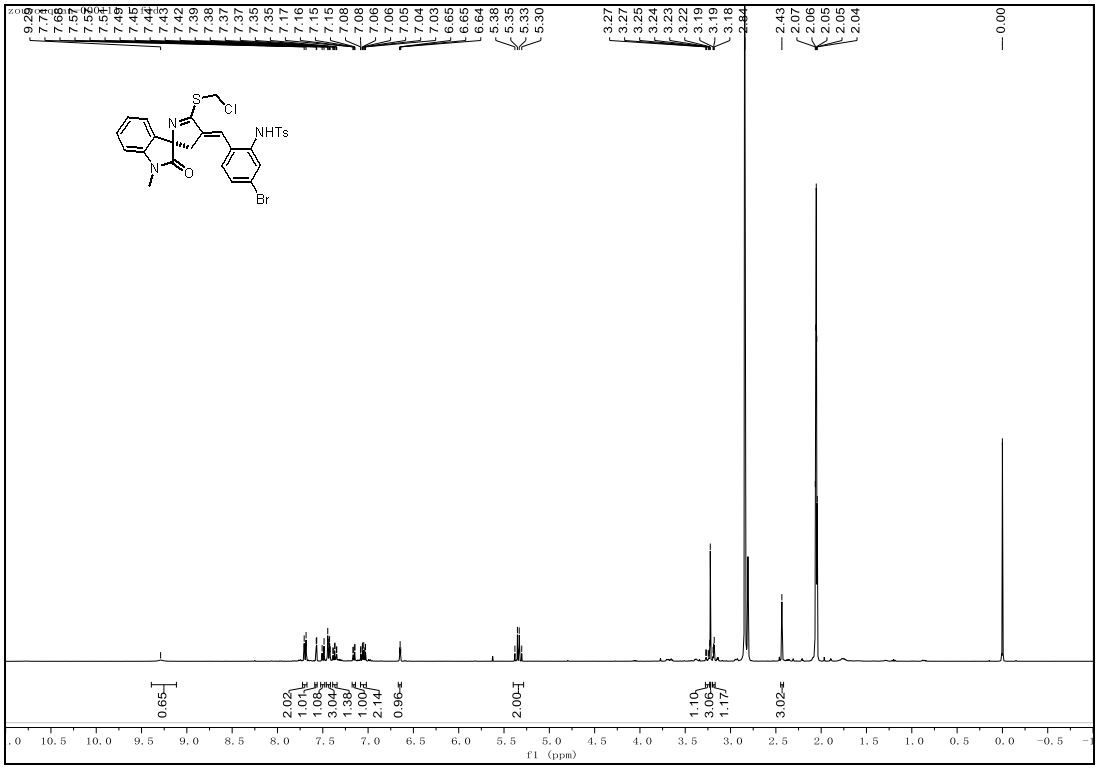
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4g



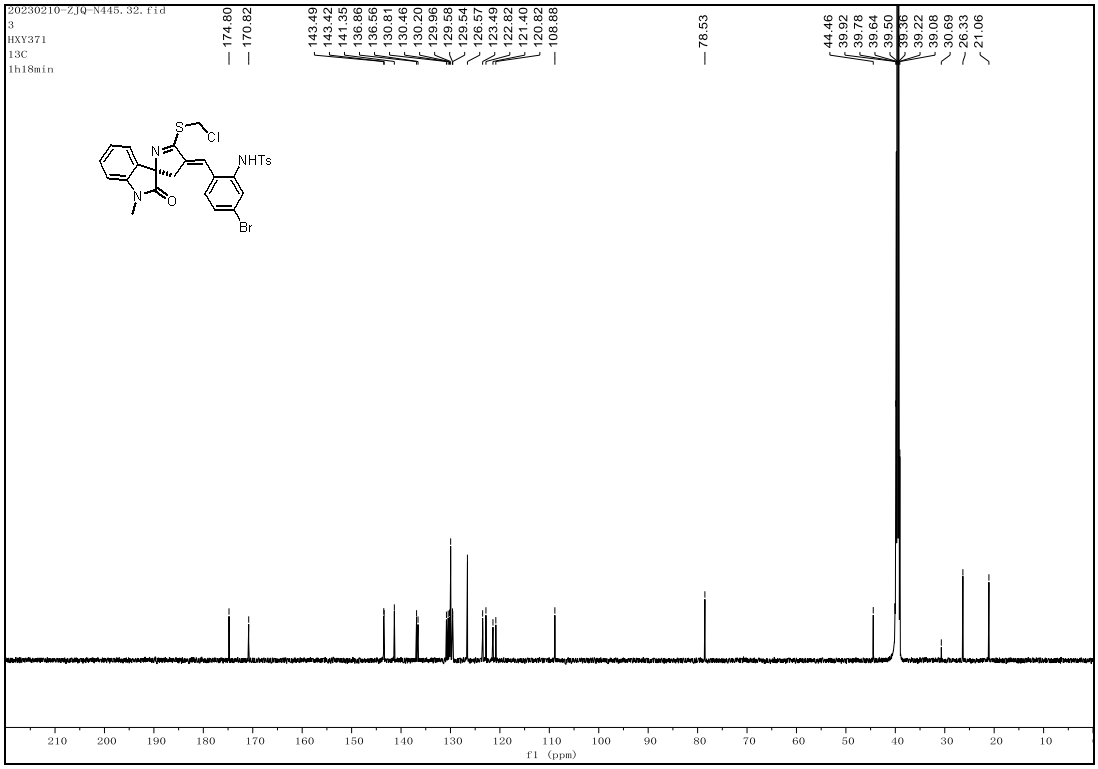
^{13}C NMR (100 MHz, acetone-d_6) spectrum for compound 4g



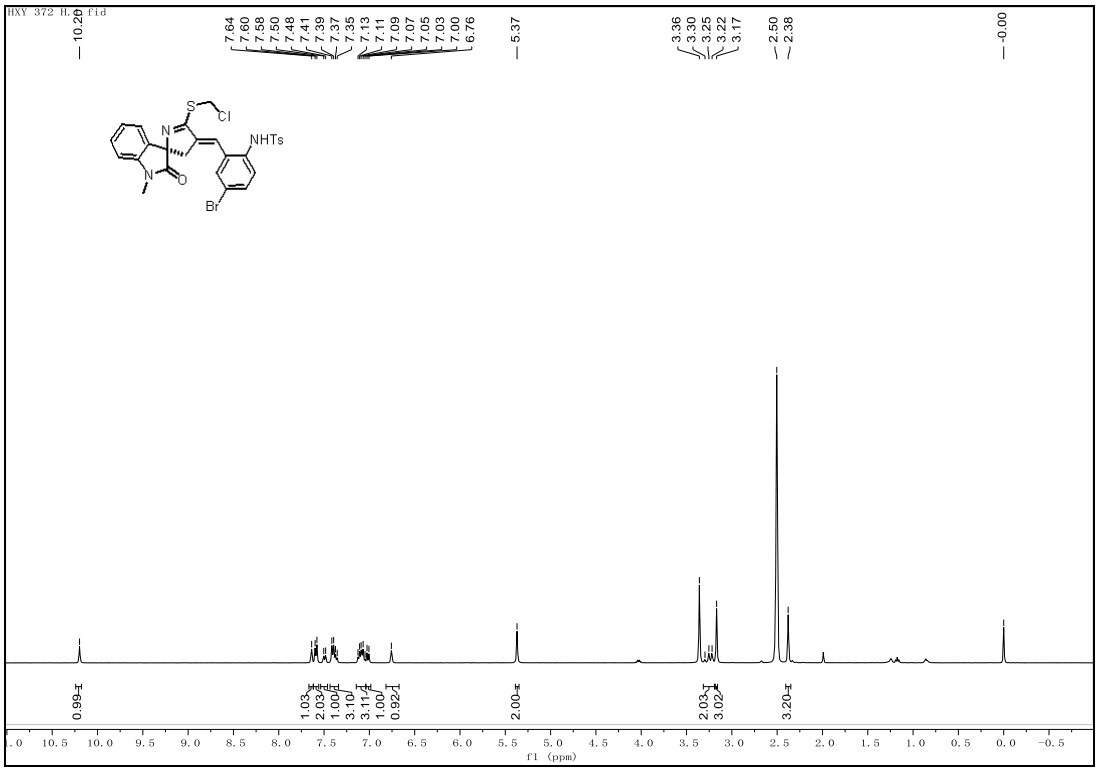
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4h



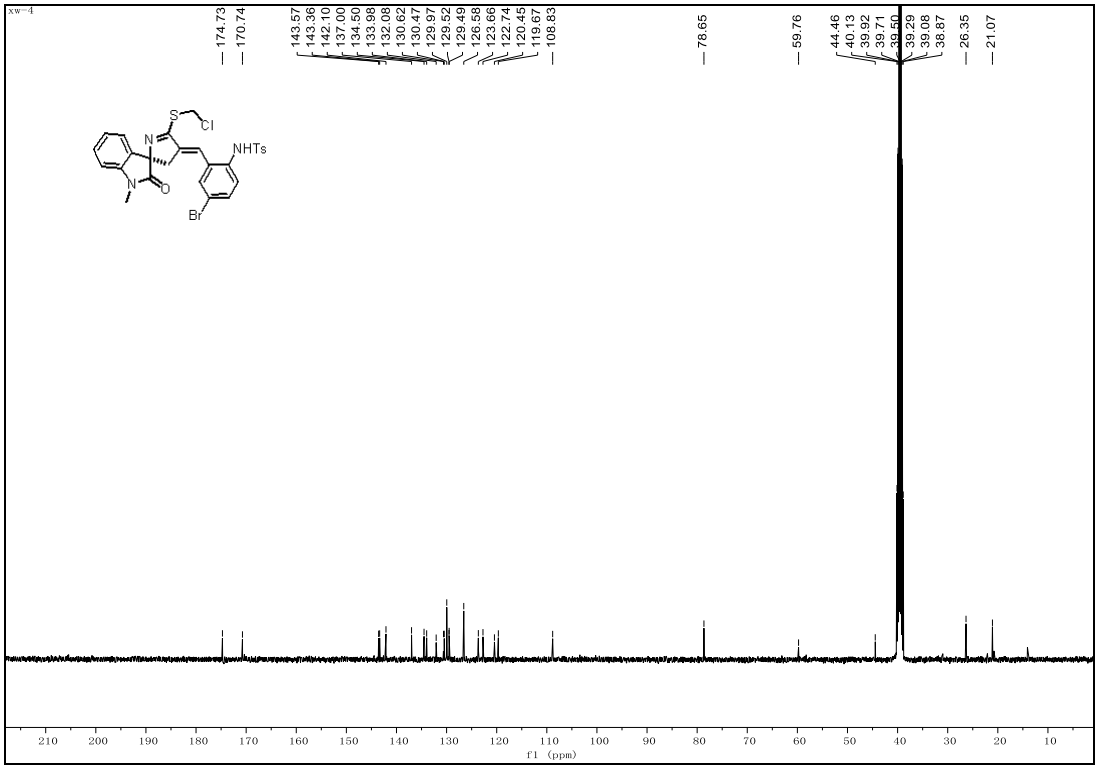
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4h



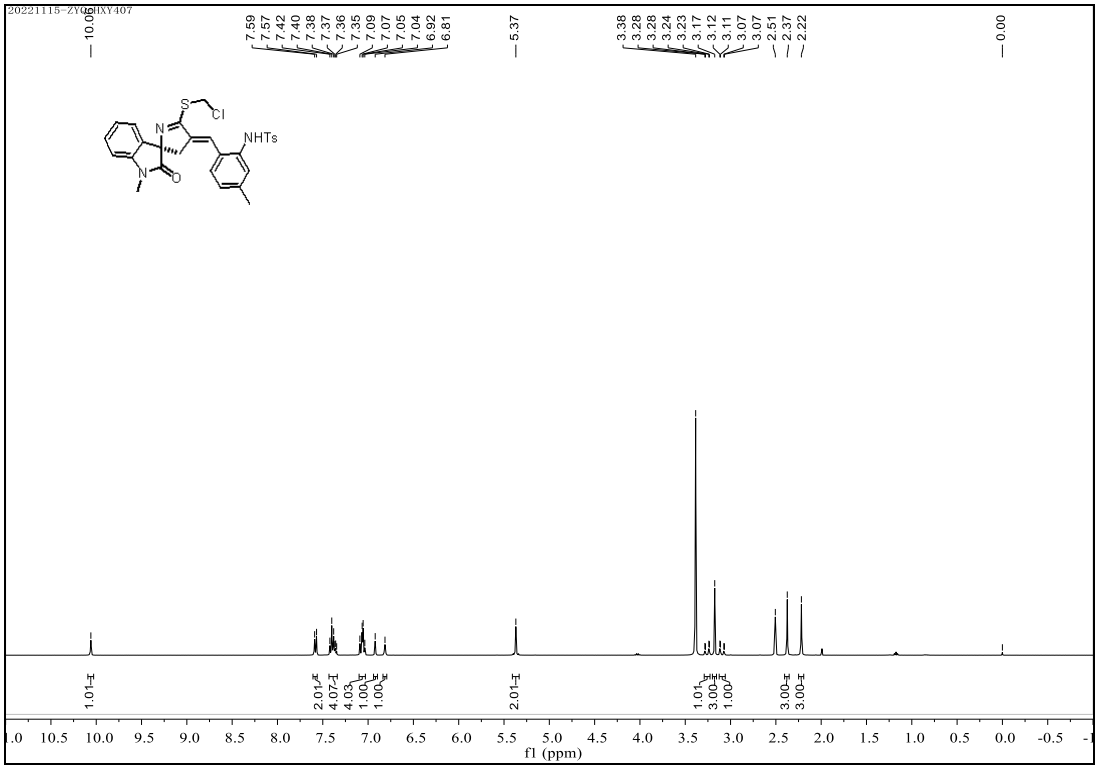
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4i



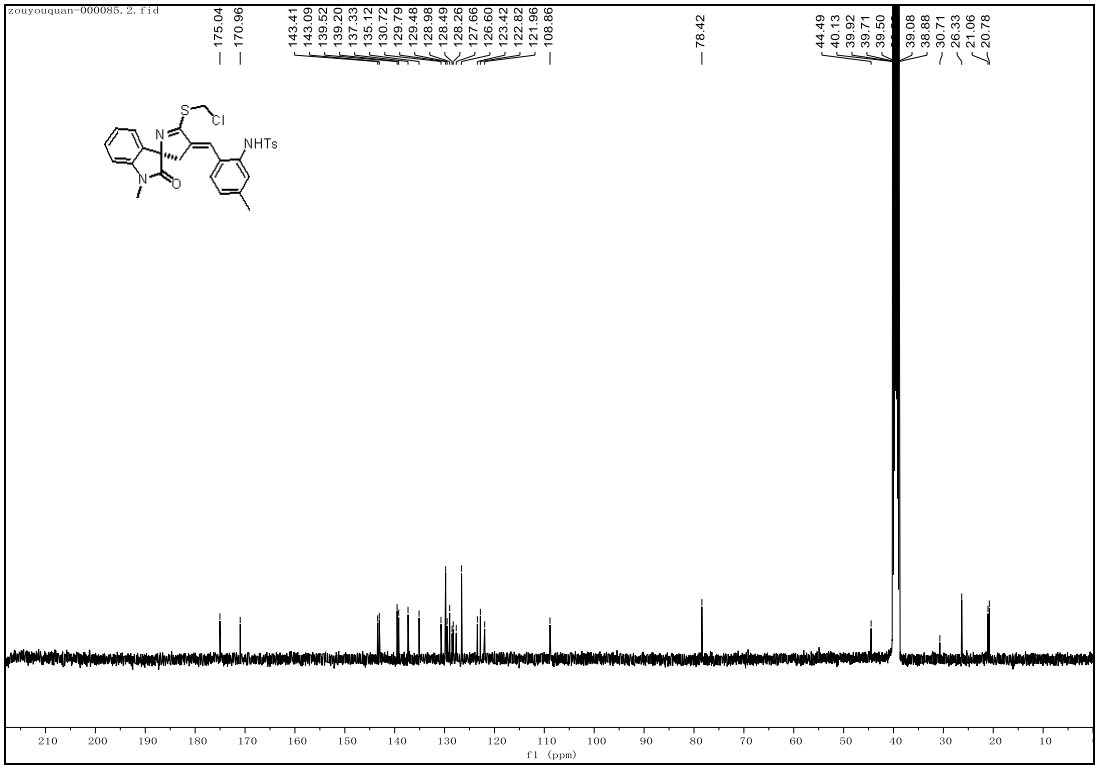
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4i



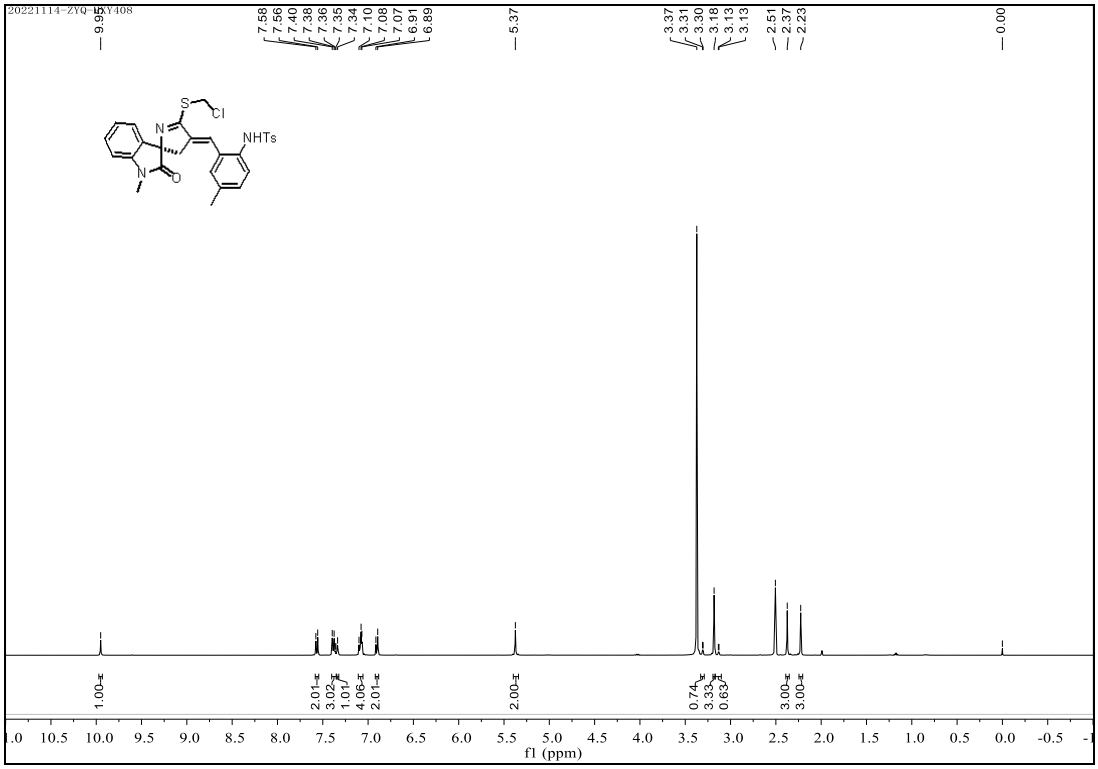
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4j



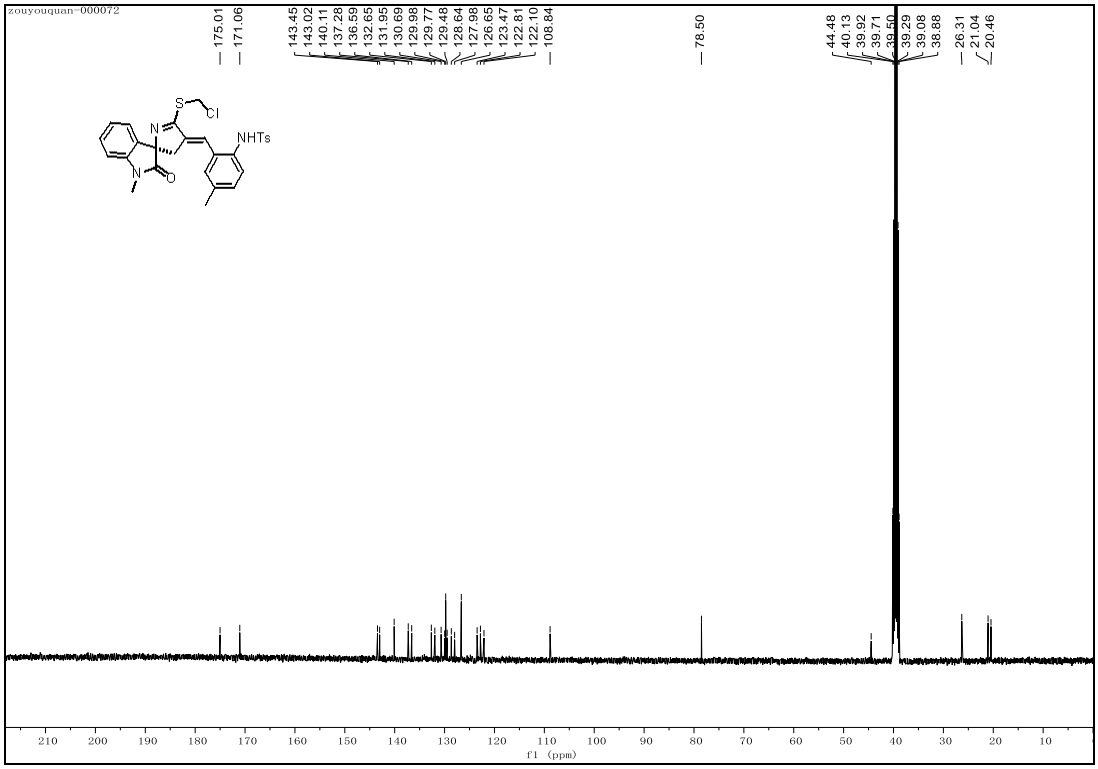
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4j



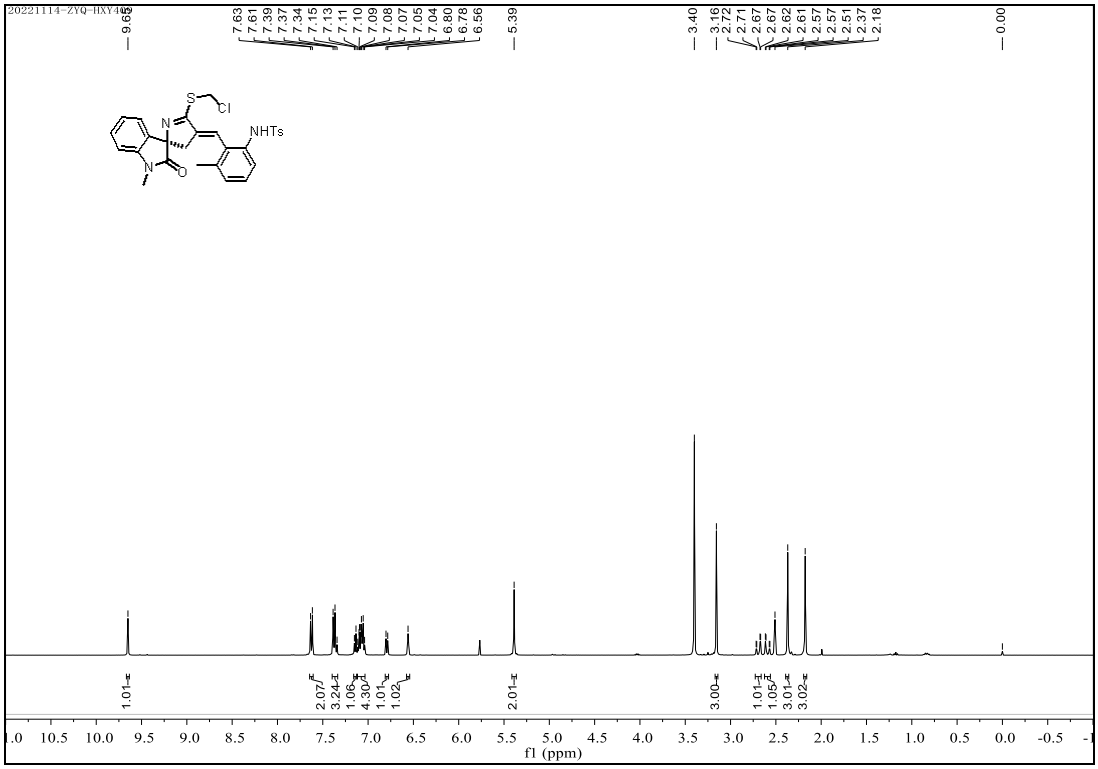
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4k



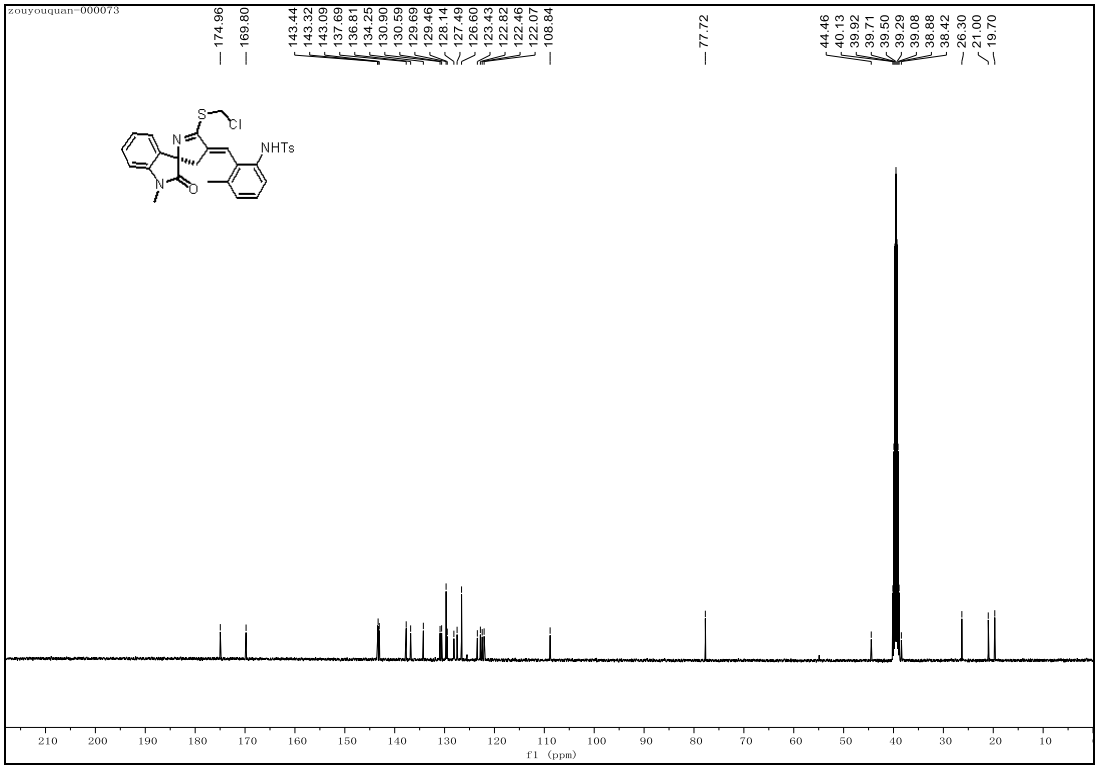
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4k



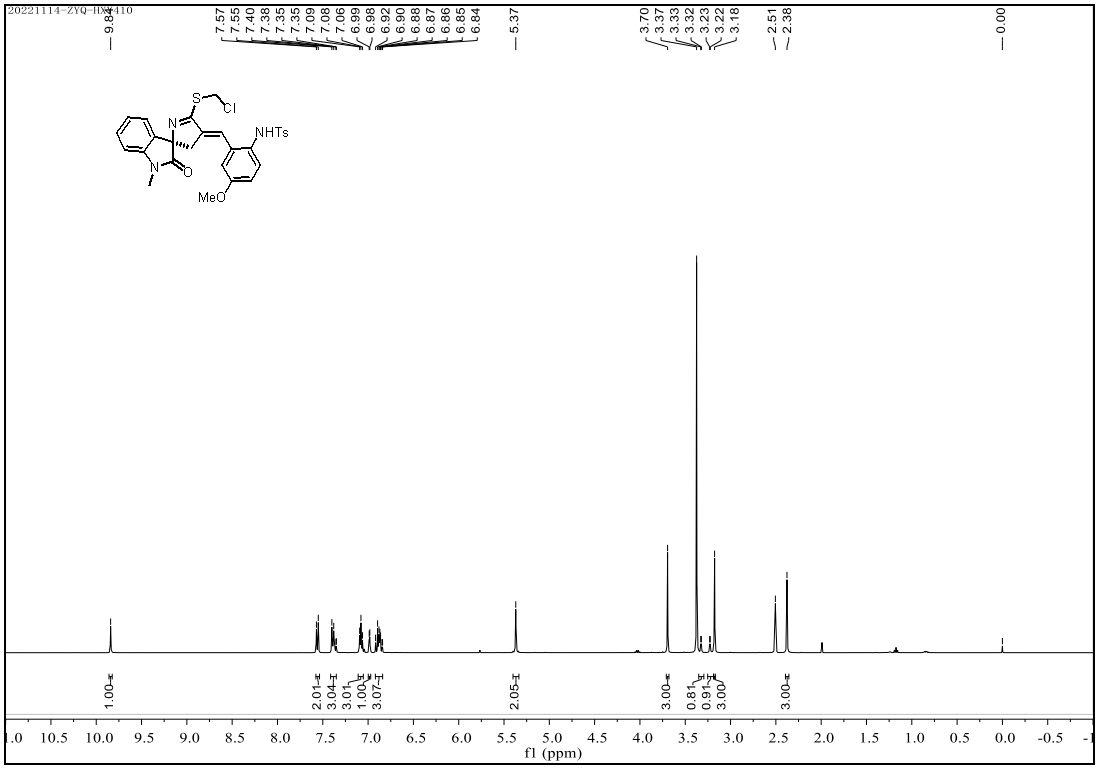
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4l



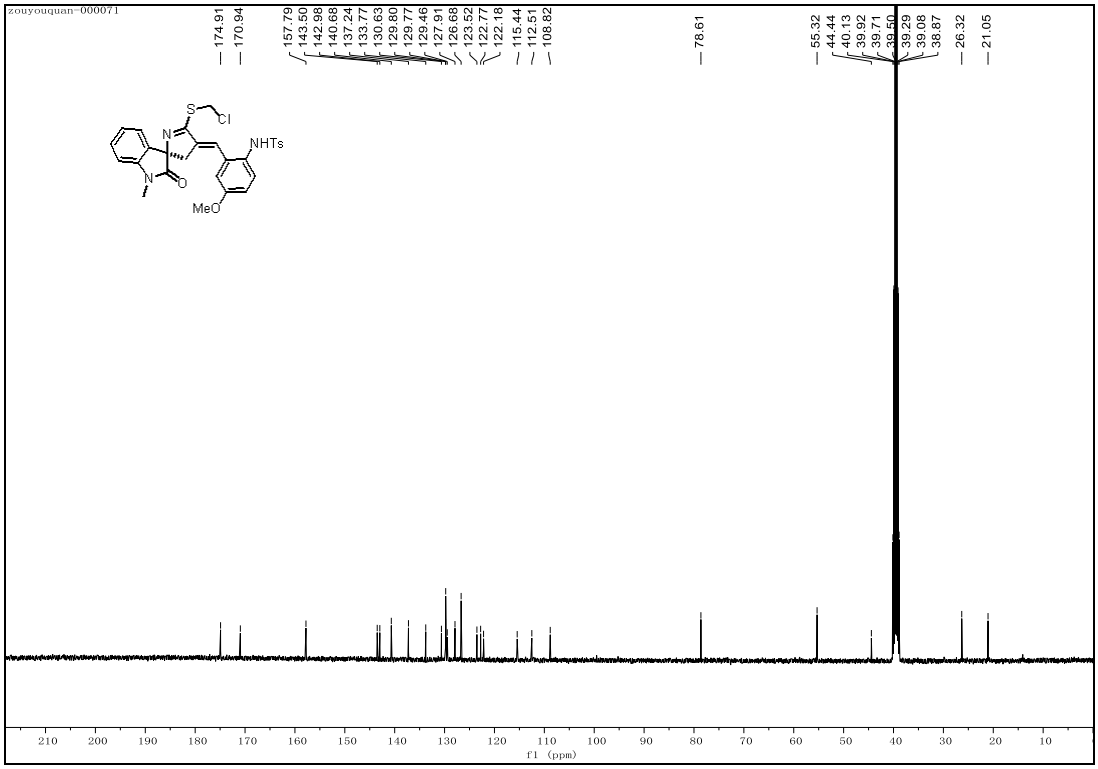
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4l



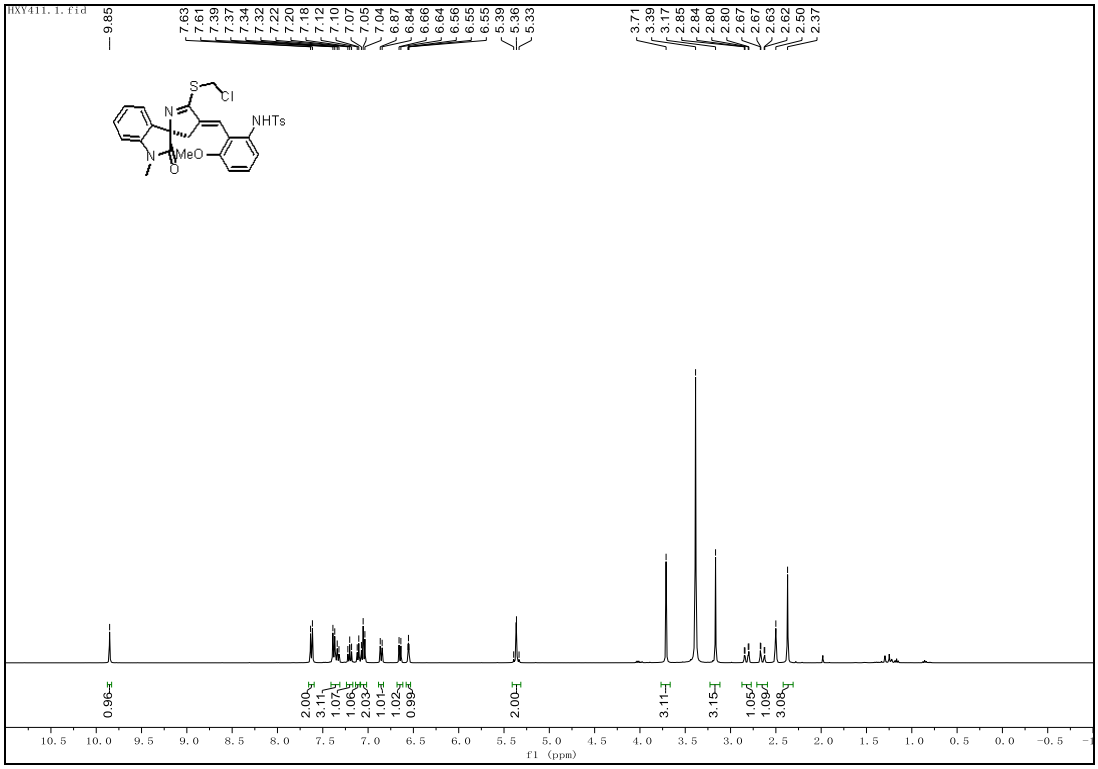
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4m



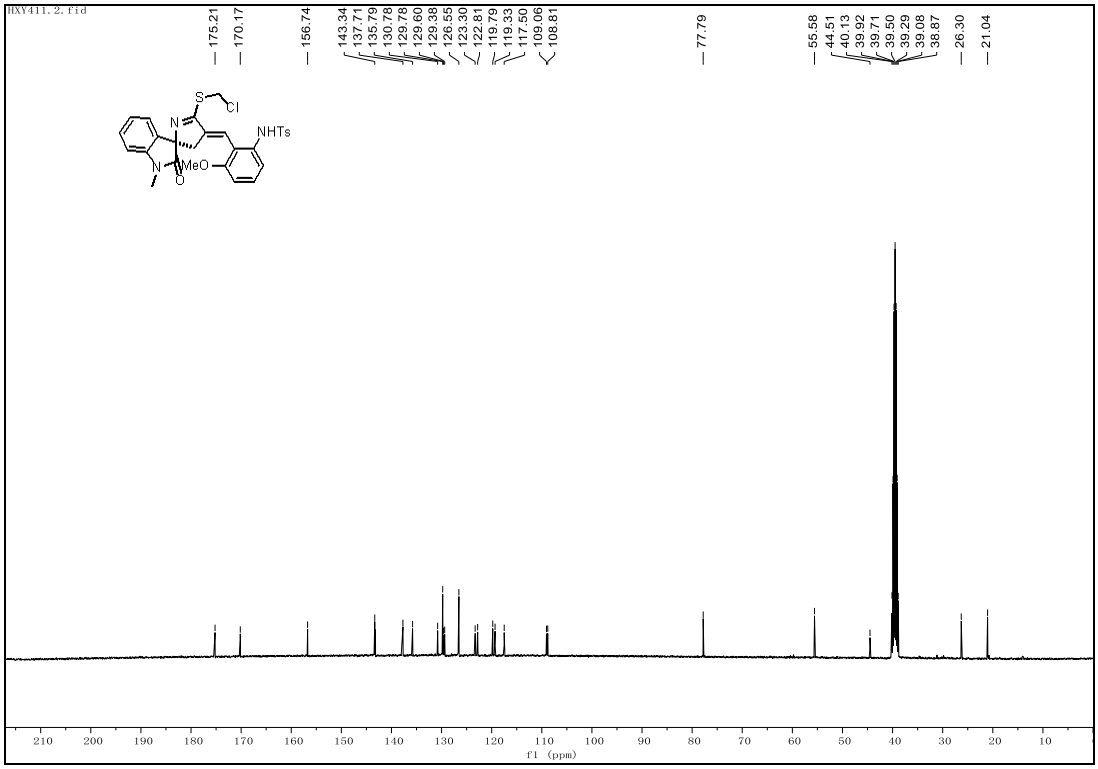
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4m



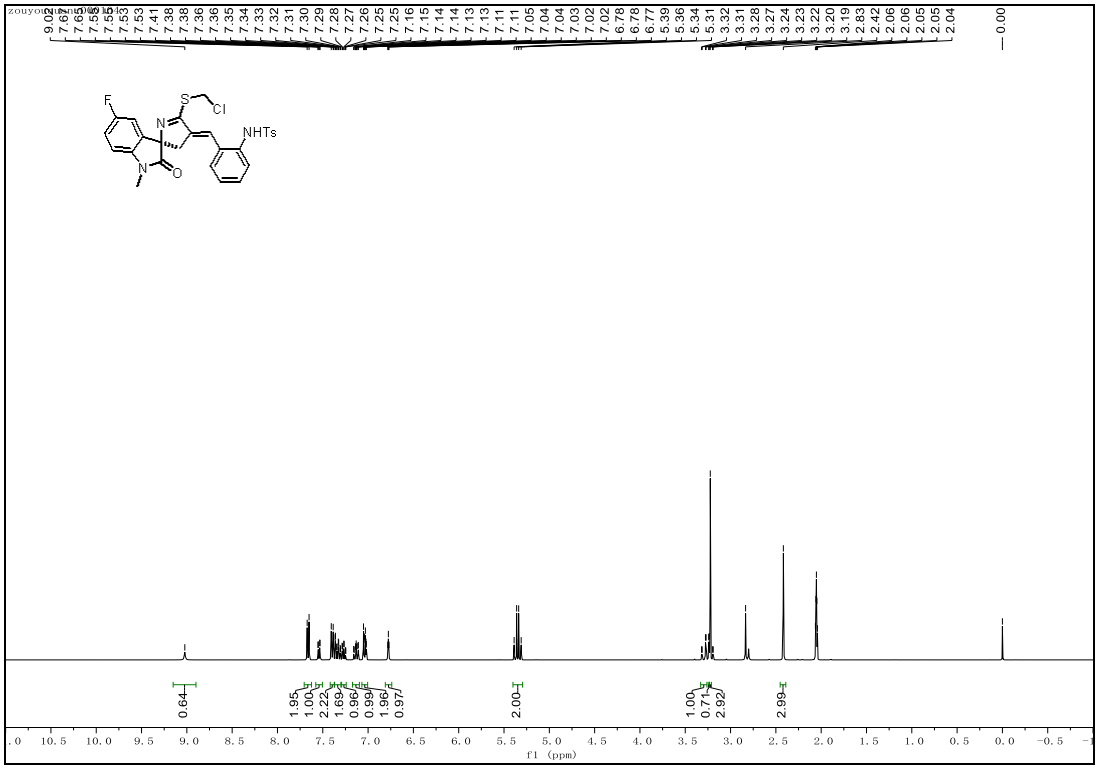
^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 4n



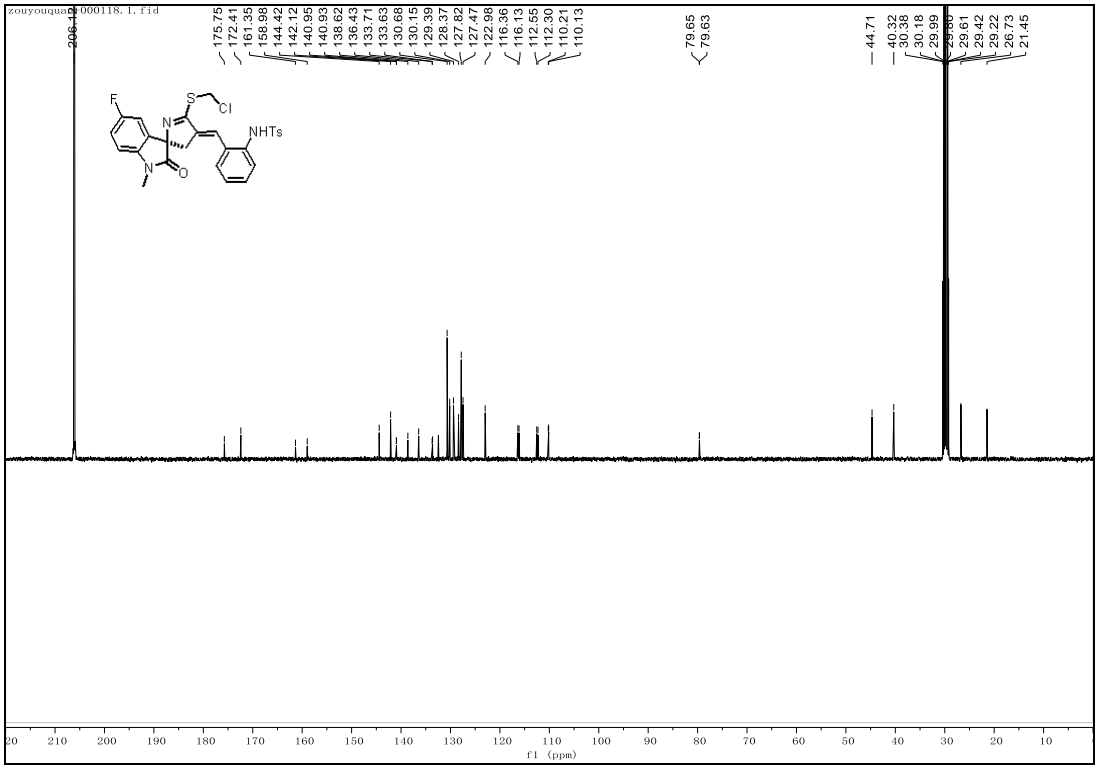
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4n



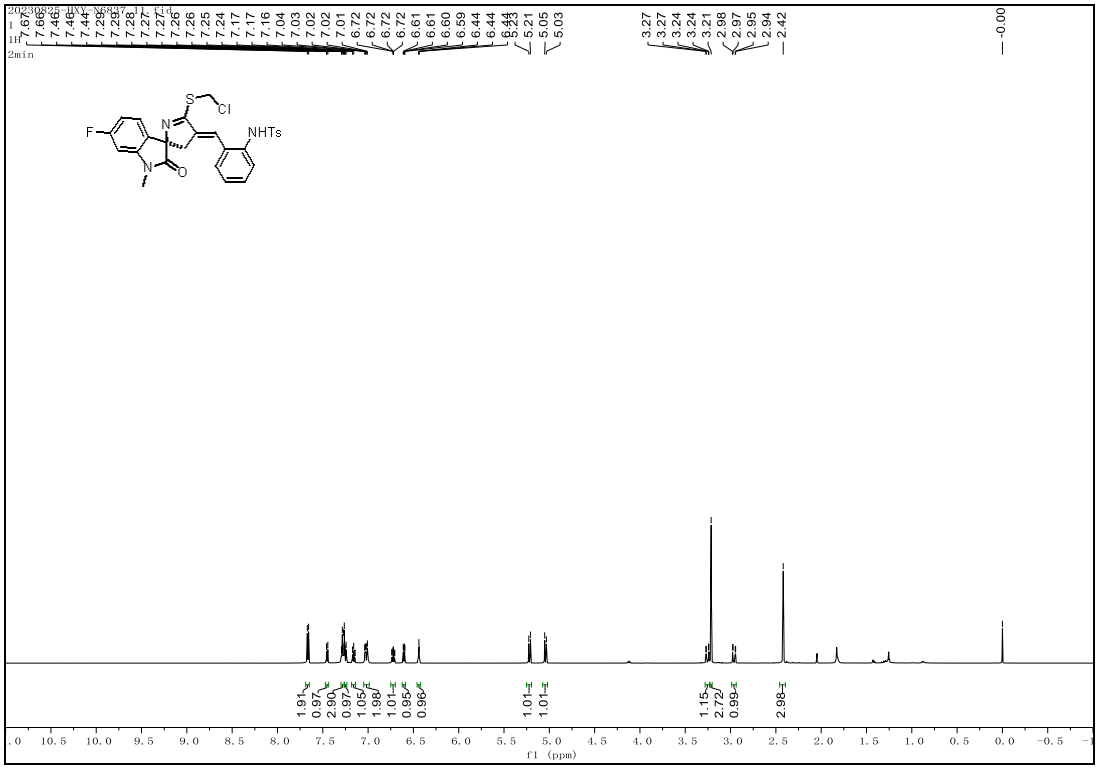
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4o



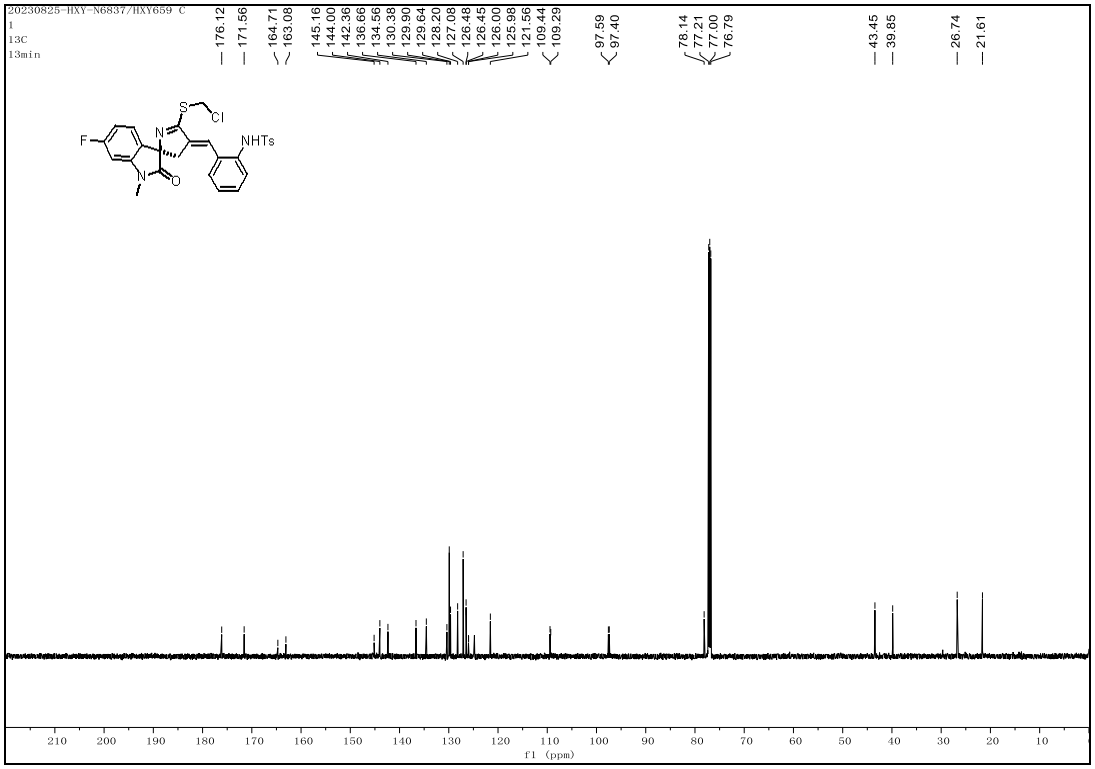
^{13}C NMR (100 MHz, acetone-d_6) spectrum for compound 4o



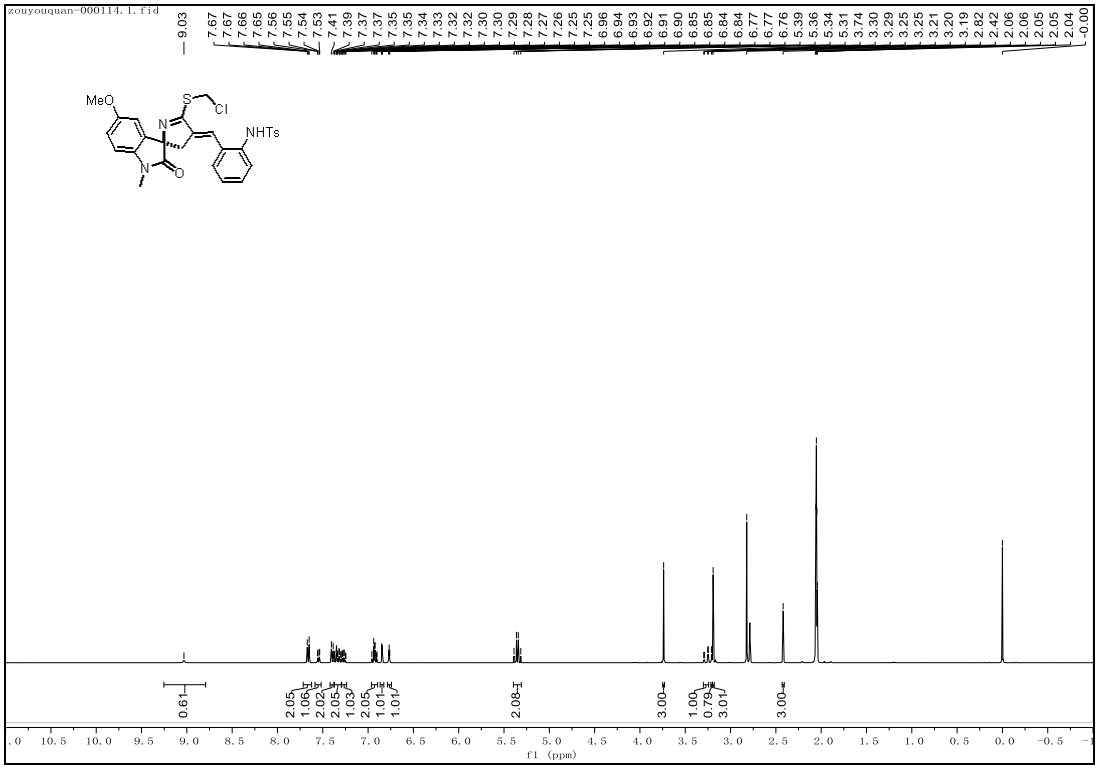
^{1}H NMR (600 MHz, $CDCl_3$) spectrum for compound 4p



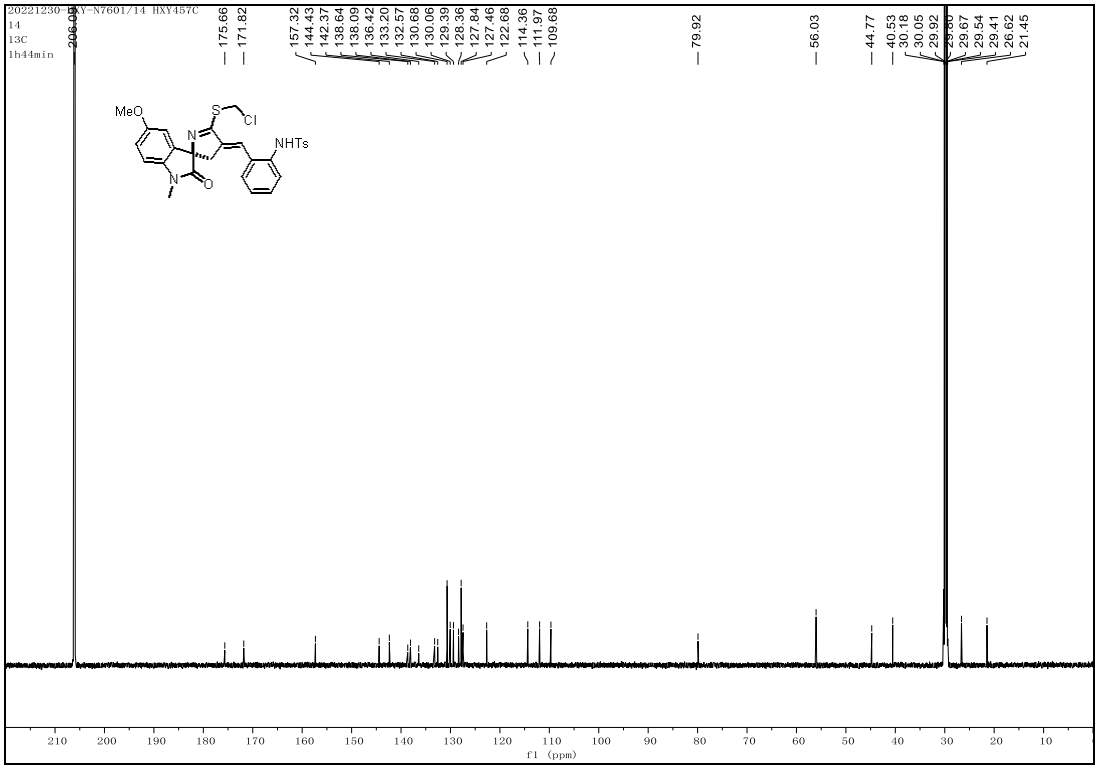
^{13}C NMR (150 MHz, $CDCl_3$) spectrum for compound 4p



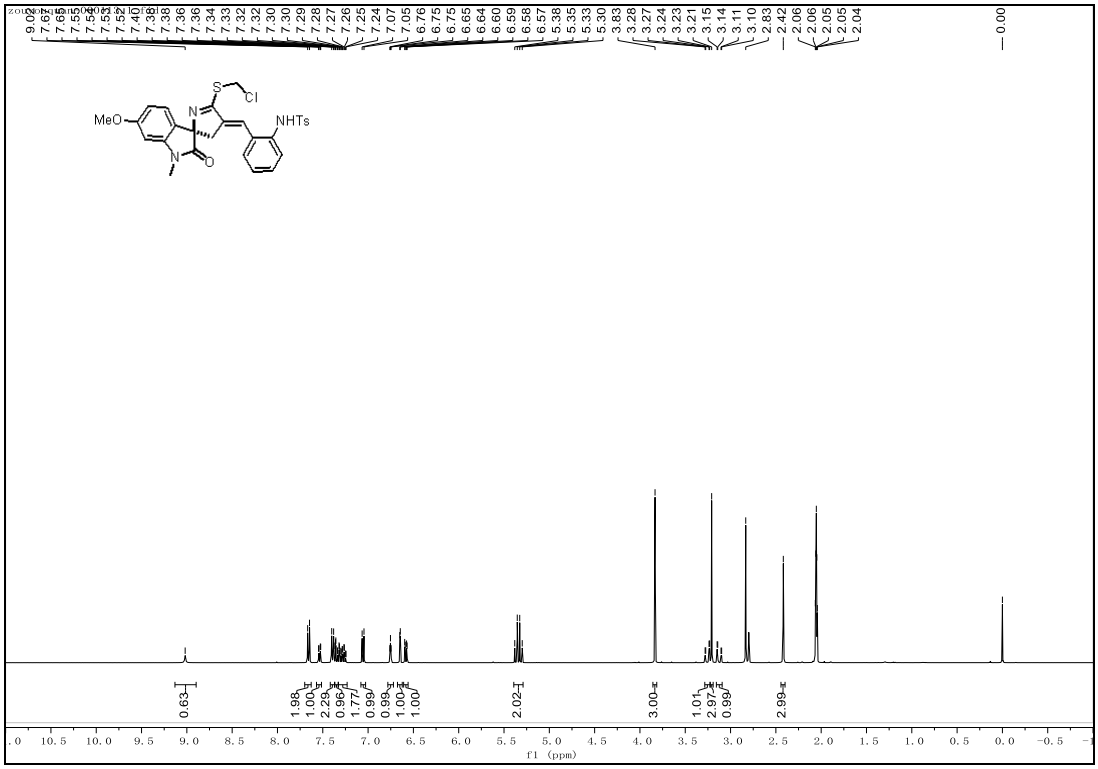
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4q



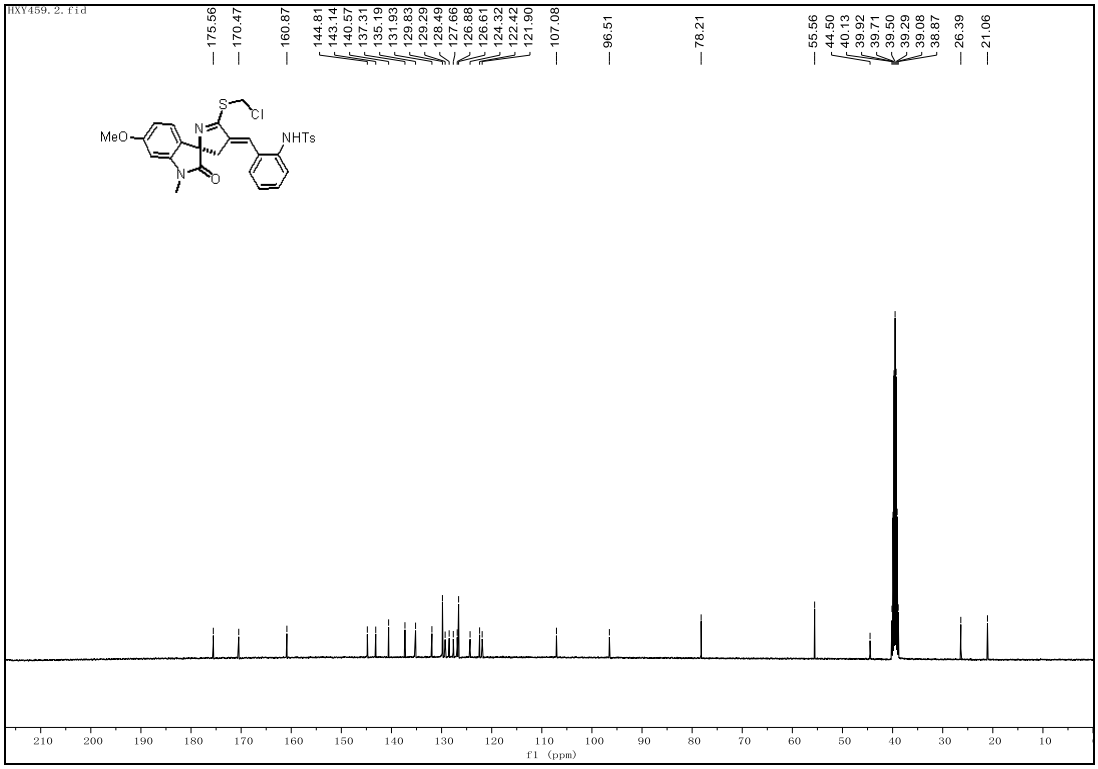
^{13}C NMR (150 MHz, acetone-d_6) spectrum for compound 4q



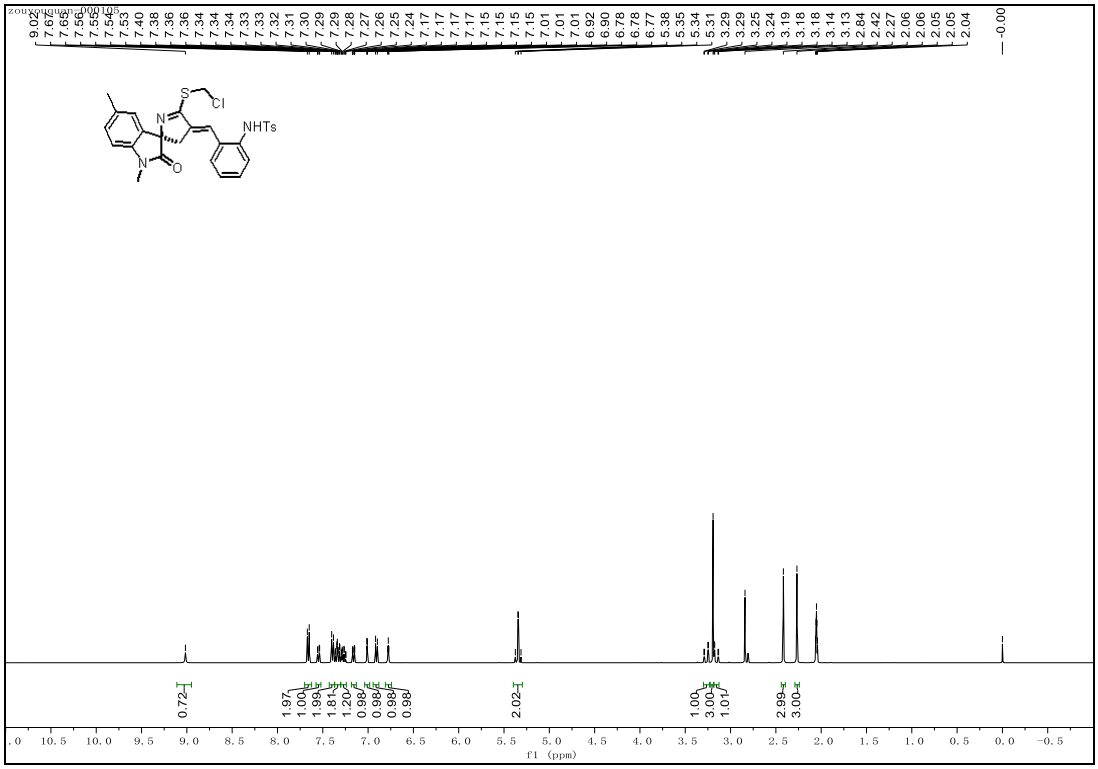
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4r



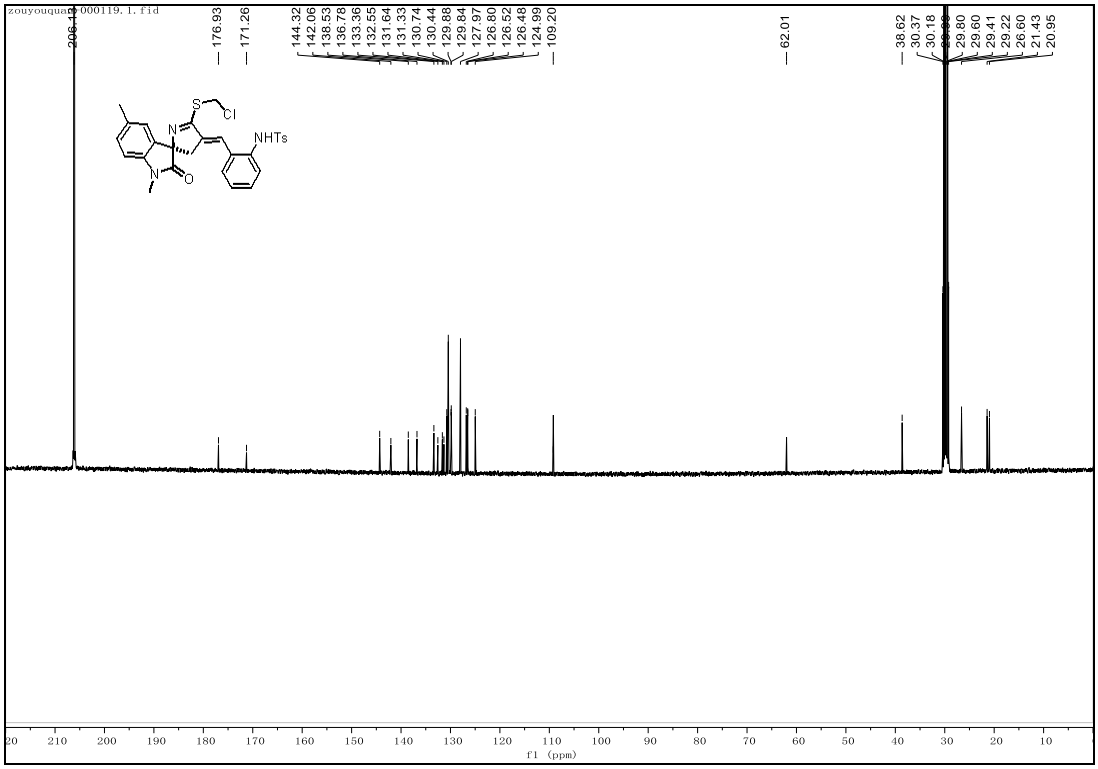
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4r



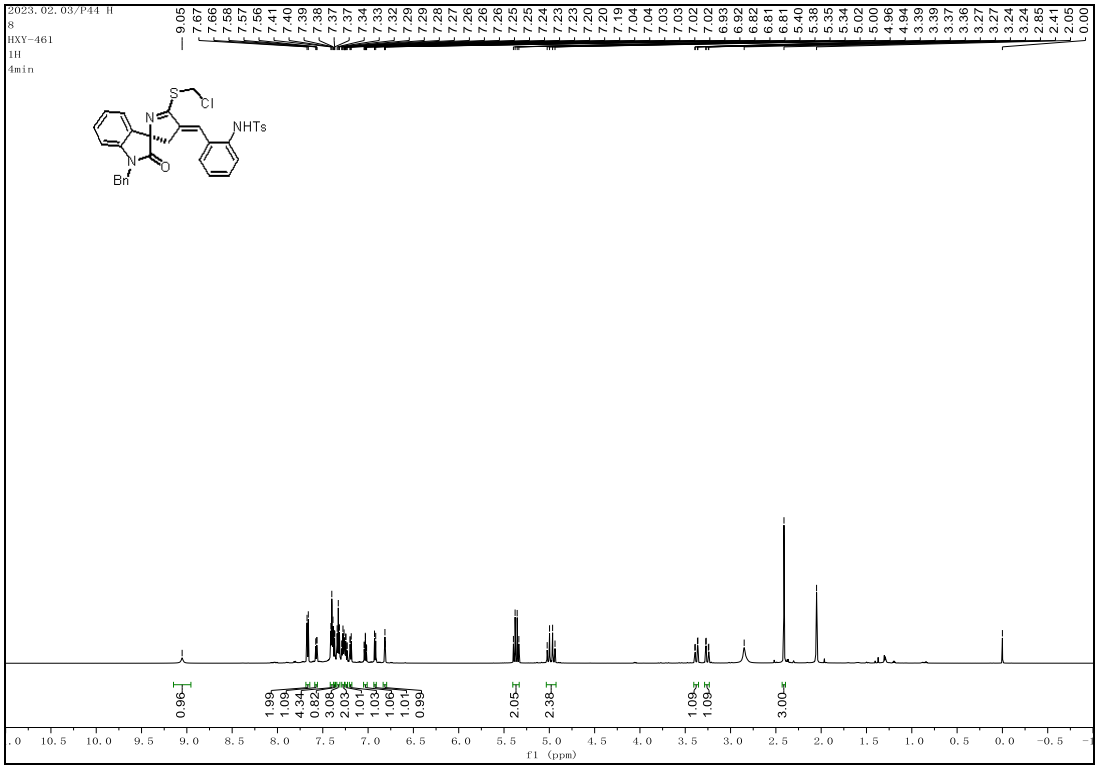
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4s



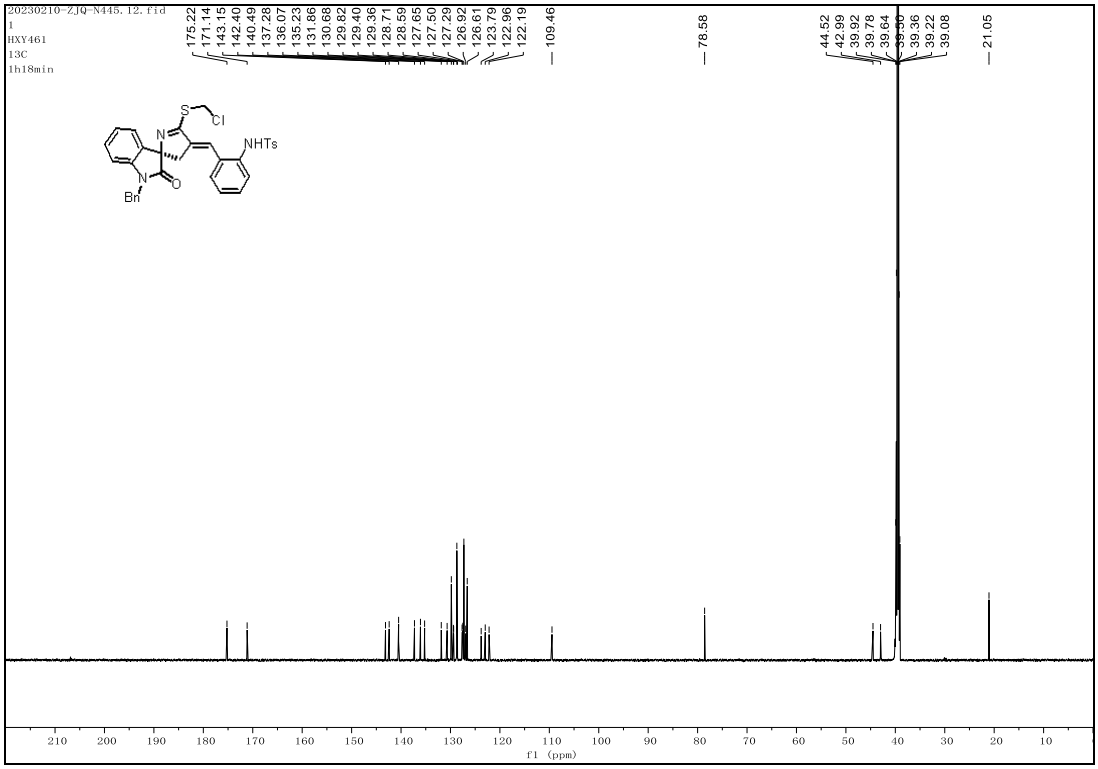
^{13}C NMR (100 MHz, acetone-d_6) spectrum for compound 4s



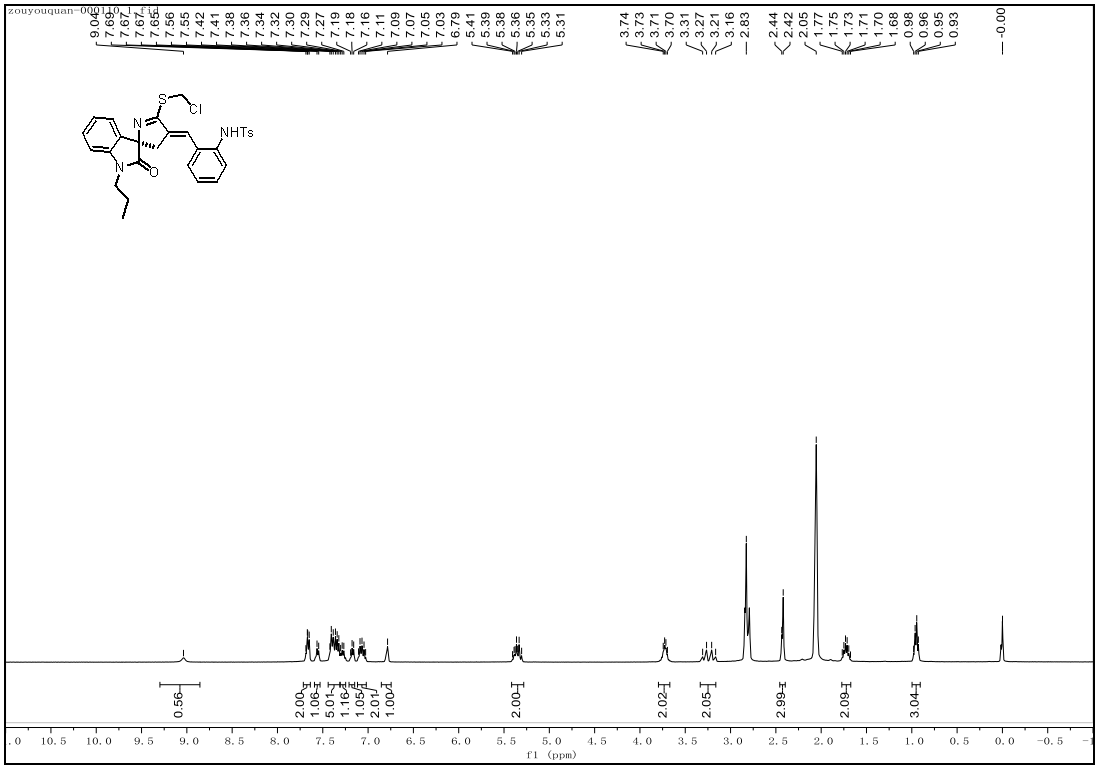
^{1}H NMR (600 MHz, acetone-d_6) spectrum for compound 4t



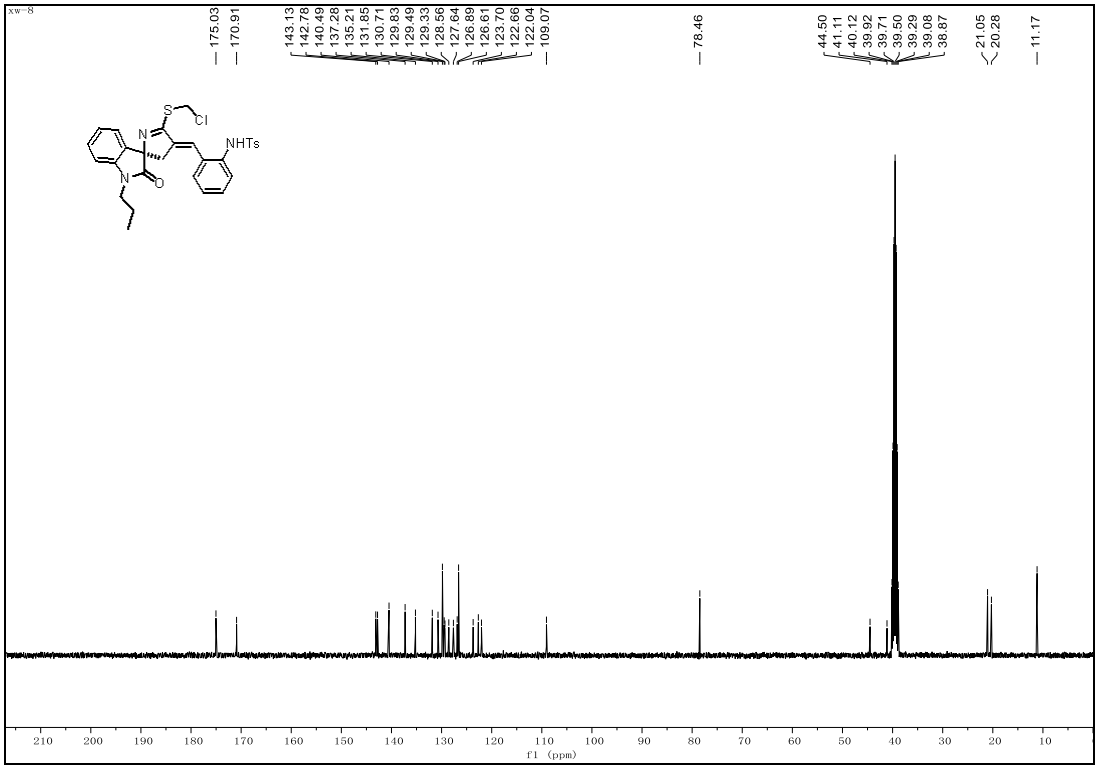
^{13}C NMR (150 MHz, DMSO-d_6) spectrum for compound 4t



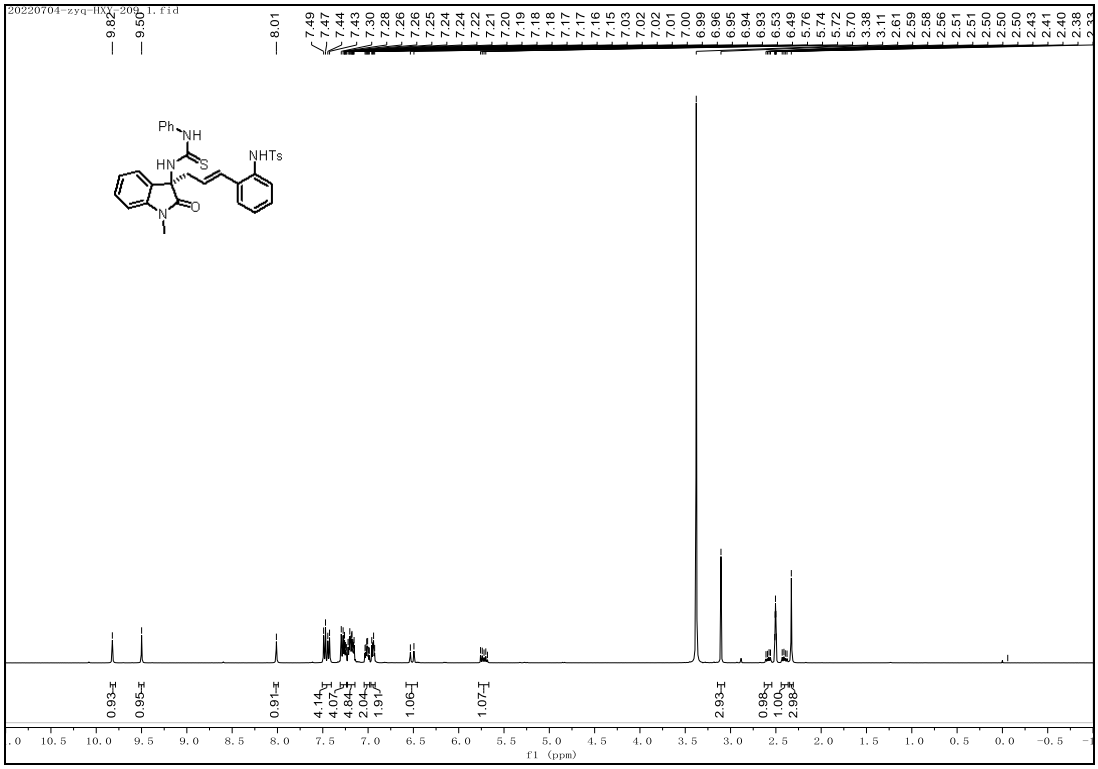
^{1}H NMR (400 MHz, acetone-d_6) spectrum for compound 4u



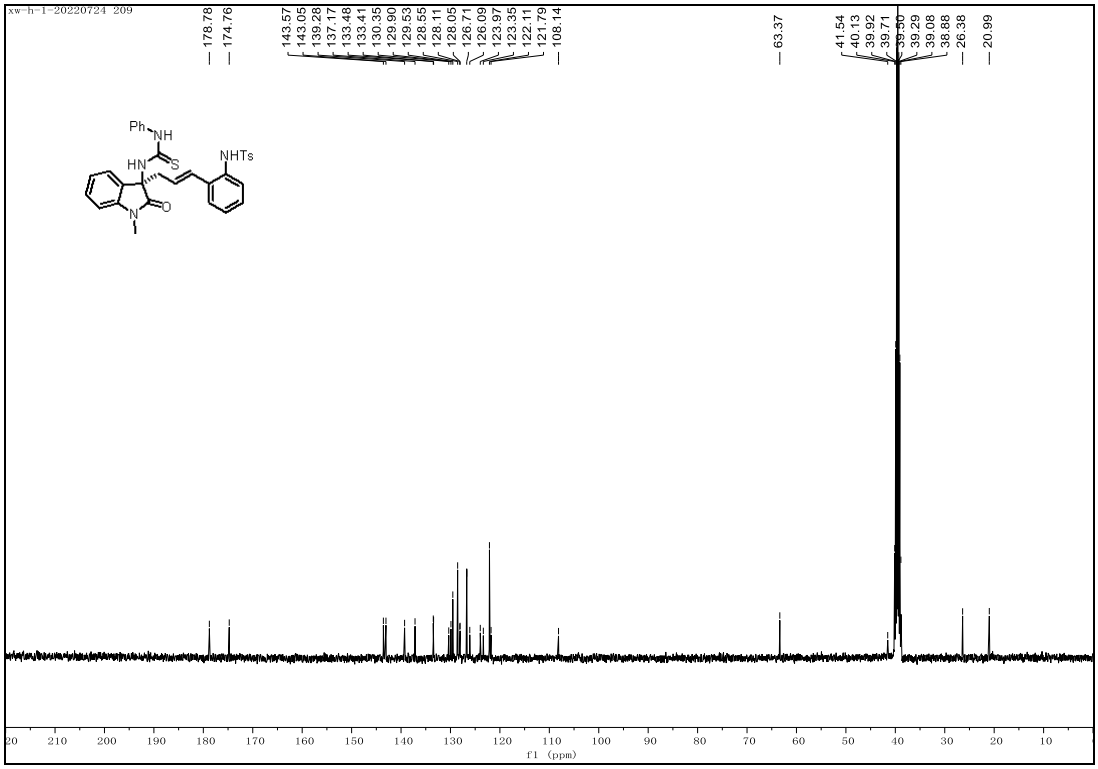
^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 4u



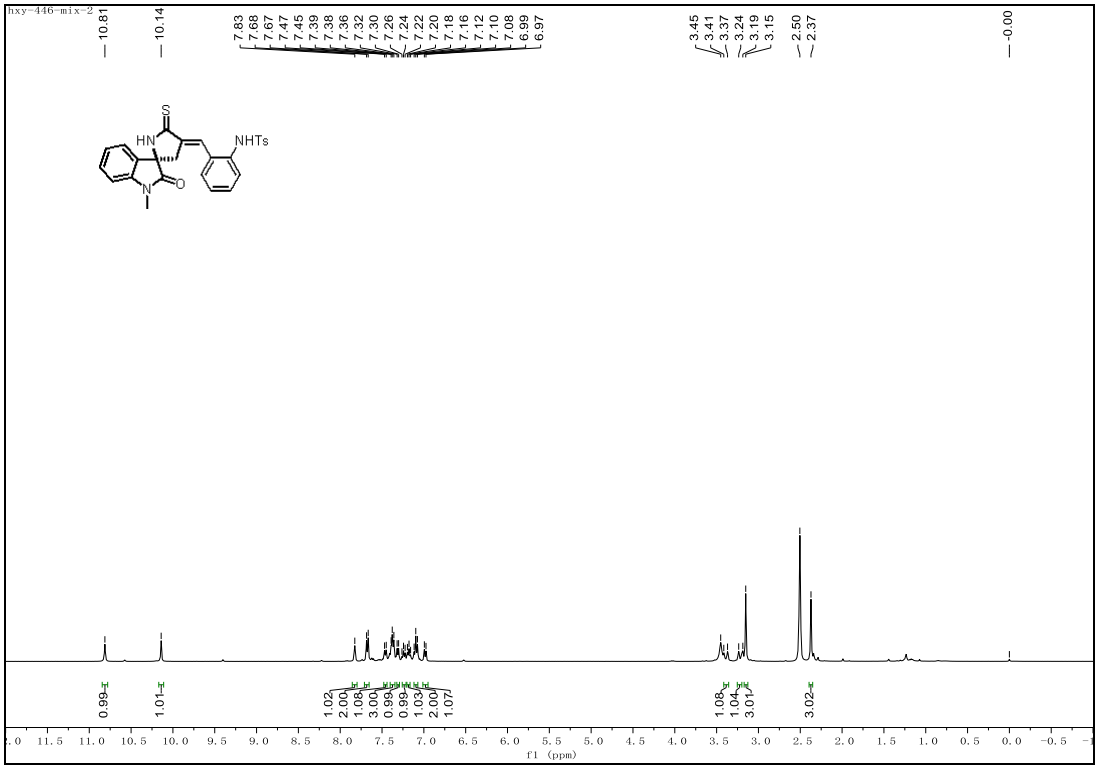
^{1}H NMR (400 MHz, DMSO- d_6) spectrum for compound 5



^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 5



^{1}H NMR (400 MHz, DMSO-d_6) spectrum for compound 6



^{13}C NMR (100 MHz, DMSO-d_6) spectrum for compound 6