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Supporting Information

for

COS-triggered Oxygen/Sulfur Atom Exchange of Isatins: Chemoselective Synthesis of Functionalized Isoindigos and Spirothiopyrans via Self-condensation and Thio-Diels-Alder Reaction

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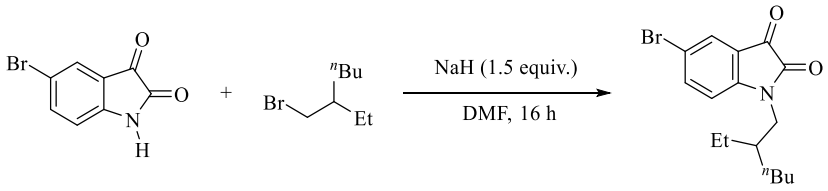
1. General Procedure

Unless otherwise stated, all manipulations of oxygen- and/or moisture-sensitive materials were performed in a glove box or using standard Schlenk techniques under a dry nitrogen or argon atmosphere. THPE-Bn-^{13}COS adducts and BIG were prepared according to previous procedures [1-2]. Solvents were dried by standard methods and distilled under argon. CH_3CN was distilled with P_2O_5. THF and toluene were distilled from sodium/benzophenone. DMSO and CH_2Cl_2 were distilled with CaH_2. All of the solvents were stored over 4A molecular sieves before used. NMR spectra were recorded on Varian Inova 400 and 500 MHz, Bruker 500 and 600 MHz spectrometers in $CDCl_3$ or DMSO and chemical shifts are expressed in parts per million (δ, ppm). Proton chemical shifts are referenced to 7.26 ppm ($CHCl_3$) or 2.50 ppm (DMSO) and carbon chemicalshifts are referenced to 77.16 ppm ($CHCl_3$) or 39.5 ppm (DMSO). High resolution mass spectra (HRMS) were recorded on a Q-TOF mass spectrometry equipped with Z-spray ionization source. Infrared spectra (IR) were measured using a Nicolet NEXUS FT-IR spectrophotometer. COS (99.9%), and other commercially available chemicals were used without further purification.

2. Synthetic procedure and characterization data for reaction substrate

Representative experimental procedure: Most of the functionalized isatins were synthesized following the synthetic procedure reported by Mironova. E, V [3]. Conjugated diene were prepared according to the literature procedure [4].

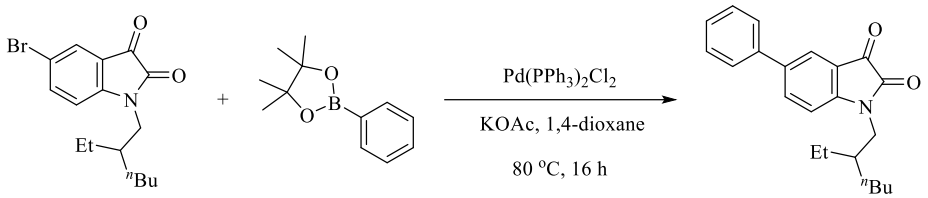
Procedure for preparation of *N*-(2-ethylhexyl)-5-bromoisatin: In a glove box, 5-bromoisatin (1.12 g, 5 mmol), NaH (0.18 g, 7.5 mmol), and DMF (10 mL) were introduced into a 50 mL Schlenk flask. The reaction was stirred at 0 °C for 0.5 h, then 2-ethylhexyl bromide (1.15 g, 6 mmol) was added to the reaction mixture and stirred continuously at 25°C for 16 h. The reaction was quenched with saturated salt water and the organic phase was extracted with dichloromethane. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the residue was purified by using silica gel column chromatography (petroleum ether/EtOAc 5/1) to give the desired product as red oil liquid (1.52 g, 4.5 mmol) in 90% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 (dd, J = 7.0, 2.0 Hz, 2H), 6.83 – 6.72 (m, 1H), 3.65 – 3.53 (m, 2H), 1.77 (dt, J = 12.4, 6.0 Hz, 1H), 1.40 – 1.23 (m, 8H), 0.97 – 0.83 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 182.5, 157.8, 150.2, 140.6, 128.1, 118.8, 116.4, 112.2, 44.6, 37.4, 30.6, 28.6, 24.0, 23.0, 14.1, 10.6; **IR** (neat cm^{-1}): 2959, 1740, 1606, 1470, 1438, 1331, 1259, 1184, 1119, 817, 708; **HRMS**(ESI): calcd. for $C_{16}H_{21}BrNO_2$ $[M+H]^+$ m/z 338.0756, found: 338.0751.



Yield: 90%

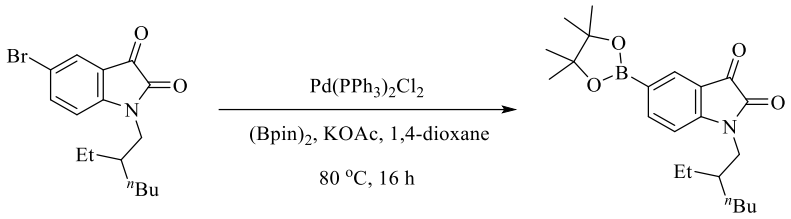
Procedure for preparation of 1i: In a glove box, the *N*-(2-ethylhexyl)-5-bromoisatin (0.41 g 1.16 mmol), (4,4,5,5,-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (0.36 g, 1.74 mmol), potassium acetate (0.34 g, 3.48 mmol) and $Pd(PPh_3)_2Cl_2$ (0.084 g, 0.12 mmol) were suspended in dry 1,4-dioxane (10 mL) and the reaction mixture was stirred at 80 °C for 16 h. The reaction mixture was filtered and the filtrate was dried in vacuum. Then the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) to give the desired product (0.35 g, 1.05 mmol) as red oil liquid in 90% yield. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.84 – 7.78 (m, 2H), 7.53 (d, J = 7.4 Hz, 2H), 7.46 (t, J = 7.4 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 6.95 (d, J = 8.1 Hz, 1H), 3.70 – 3.58 (m, 2H), 1.89 – 1.80 (m, 1H), 1.41 – 1.26 (m, 8H), 0.93 (dt, J = 12.0, 6.7 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 183.7, 158.6, 150.5, 139.0, 137.1, 136.8, 129.1, 127.9, 126.5, 123.8, 118.1, 110.8,

44.5, 37.5, 30.7, 28.6, 24.0, 23.1, 14.1, 10.6; **IR** (neat cm^{-1}): 2959, 1739, 1619, 1594, 1476, 1462, 1333, 1179, 1120, 827, 761; **HRMS**(ESI): calcd. for $C_{22}H_{26}NO_2$ $[M+H]^+$ m/z 336.1964, found: 336.1967.



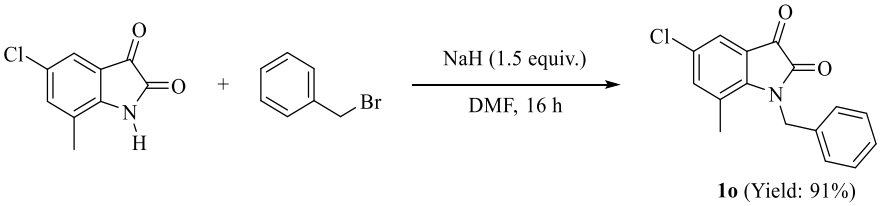
1i (Yield: 90%)

Procedure for preparation of 1j: In a glove box, the *N*-(2-ethylhexyl)-5-bromoisatin (0.49 g, 1.47 mmol), bis(pinacolato)diboron $(Bpin)_2$ (0.56 g, 2.21mmol), potassium acetate (0.43 g, 4.41 mmol) and $Pd(PPh_3)_2Cl_2$ (0.1 g, 0.147 mmol) were suspended in dry 1,4-dioxane (10 mL) and the reaction mixture was stirred at 80 °C for 16 h. The reaction mixture was filtered and the filtrate was dried in vacuum. Then the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) to give the desired product as red oil liquid (0.5 g, 1.34 mmol) in 91% yield. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.48 (dd, J = 16.2, 2.0 Hz, 2H), 7.35 (t, J = 6.1 Hz, 4H), 7.29 (dt, J = 8.5, 4.1 Hz, 1H), 5.14 (d, J = 15.3 Hz, 2H), 2.15 (s, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 182.3, 159.3, 146.9, 139.9, 137.1, 128.7, 127.4, 127.2, 125.7, 123.9, 121.8, 120.2, 44.5, 17.4; **IR** (neat cm^{-1}): 2920, 1728, 1593, 1452, 1466, 1402, 1331, 1239, 1157, 1085, 891, 751; **HRMS**(ESI): calcd. for $C_{16}H_{13}ClNO_2$ $[M+H]^+$ m/z 386.0635, found: 386.0630



1j (Yield: 91%)

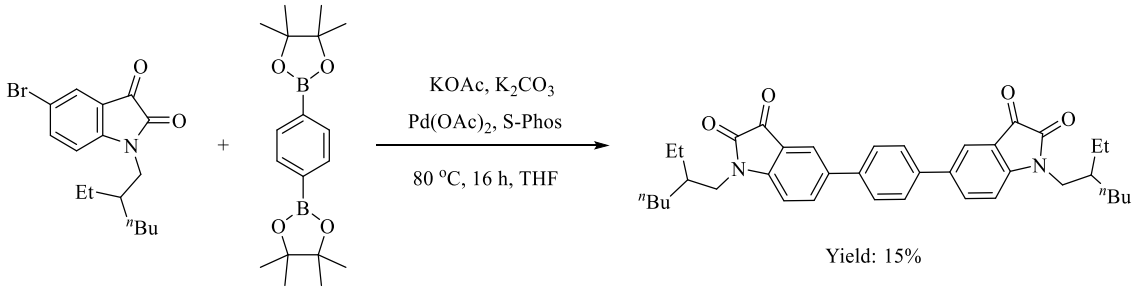
Procedure for preparation of 1o: In a glove box, 5-chloro-7-methylisatin (0.30g, 1.54 mmol), NaH (0.055g, 2.31 mmol) and DMF (10 mL) were introduced into a 50 mL Schlenk flask. The reaction was stirred at 0 °C for 0.5 h, then benzyl bromide (0.32 g, 1.85 mmol.) was added to the reaction mixture and stirred continuously at 25 °C for 16 h. The reaction was quenched with water and the organic phase was extracted with dichloromethane. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the residue was purified by using silica gel column chromatography (dichloromethane) to give the desired product as red solid (0.40 g, 1.4 mmol) in 91% yield. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.48 (dd, J = 16.2, 2.0 Hz, 2H), 7.35 (t, J = 6.1 Hz, 4H), 7.29 (dt, J = 8.5, 4.1 Hz, 1H), 5.14 (d, J = 15.3 Hz, 2H), 2.15 (s, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 182.3, 159.3, 146.9, 139.9, 137.1, 128.7, 127.4, 127.2, 125.7, 123.9, 121.8, 120.2, 44.5, 17.4; **IR** (neat cm^{-1}): 2920, 1728, 1593, 1452, 1466, 1402, 1331, 1239, 1157, 1085, 891, 751; **HRMS**(ESI): calcd. for $C_{16}H_{13}ClNO_2$ $[M+H]^+$ m/z 286.0635, found: 286.0630



1o (Yield: 91%)

Procedure for preparation of isatin-based monomer: Under argon atmosphere, *N*-(2-ethylhexyl)-5-bromoisatin (0.77 g, 2.3 mmol), 2,2'-benzene-1,4-diylbis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (0.53 g, 1.6 mmol), $Pd(OAc)_2$ (0.051 mg, 0.23 mmol), S-Phos (0.16 g, 0.46 mmol), K_2CO_3 (1.5 g, 11.5 mmol) and KOAc (0.56 g, 5.75 mmol) were mixed and dissolved in

degassed THF (40 mL) in a Schlenk tube. The reaction was stirred at 65 °C for 16 h. After removal of the solvent, the residue was purified by recrystallization in hexane and DCM to give the desired product as red solid (200 mg, 0.34 mmol) in 15% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91 – 7.82 (m, 4H), 7.63 (s, 4H), 6.98 (d, J = 8.2 Hz, 2H), 3.71 – 3.60 (m, 4H), 1.90 – 1.81 (m, 2H), 1.45 – 1.30 (m, 16H), 0.93 (dt, J = 13.9, 7.3 Hz, 12H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 183.8, 158.7, 150.9, 138.6, 136.7, 136.3, 127.3, 123.8, 118.3, 111.0, 44.7, 37.6, 30.8, 28.8, 24.1, 23.2, 14.2, 10.7; **IR** (neat cm^{-1}): 2958, 2851, 1736, 1619, 1592, 1476, 1381, 1338, 813, 722; **HRMS**(ESI): calcd. for $C_{38}H_{45}N_2O_4$ $[M+H]^+$ m/z 593.3379, found: 593.3369



3. COS-triggered Oxygen/Sulfur Atom Exchange of Isatins: Solvent-controlled Chemoselective Synthesis of Functionalized Isoindigos and Spirothiopyrans via Self-condensation and Thio-Diels-Alder Reaction

Representative experimental procedure of functionalized isoindigos: In a glove box, a 10 mL oven-dried autoclave containing a stir bar was charged with isatin (0.5 mmol), DBU (0.05 mmol, 10 mmol%) and CH_3CN (2 mL). After purging the autoclave with COS three times. The sealed autoclave was pressurized to 0.8 MPa with COS. The reaction mixture was stirred at 25 °C for 24 h, then the remaining COS in the autoclave was vented slowly. The crude reaction mixture was purified by washing in dichloromethane and methanol or column chromatography on silica gel (petroleum ether/EtOAc: 10/1-5/1) to give desired products.

Representative experimental procedure of spirothiopyrans (4aa-4pf'): In a glove box, a 10 mL oven-dried autoclave containing a stir bar was charged with isatin (0.5 mmol), conjugated diene (1.0 mmol), DBU (0.05 mmol, 10 mmol%) and DMSO (2.0 mL). After purging the autoclave with COS three times. The sealed autoclave was pressurized to 0.8 MPa with COS. The reaction mixture was stirred at 25 °C for 24 h, then the remaining COS in the autoclave was vented slowly. The crude reaction mixture was purified by column chromatography on silica gel (petroleum ether/EtOAc: 10/1-3/2) to give the desired product.

4. Crystallography

Single crystals of isoindigo **3v**, **3z**, and **elemental sulfur** suitable for X-ray structural analysis were obtained from chloroform or dichloromethane solution at room temperature. Diffraction data were collected at 273 K on a Bruker SMART-CCD diffractometer using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods and refined by full-matrix least squares on F2 [5]. All nonhydrogen atoms were refined anisotropically, and the hydrogen atoms were included in idealized positions. All calculations were performed using the SHELXTL crystallographic software packages [6]. CCDC: 1992590(**3v**), CCDC: 1992591(**3z**), CCDC: 1992592 (**elemental sulfur**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

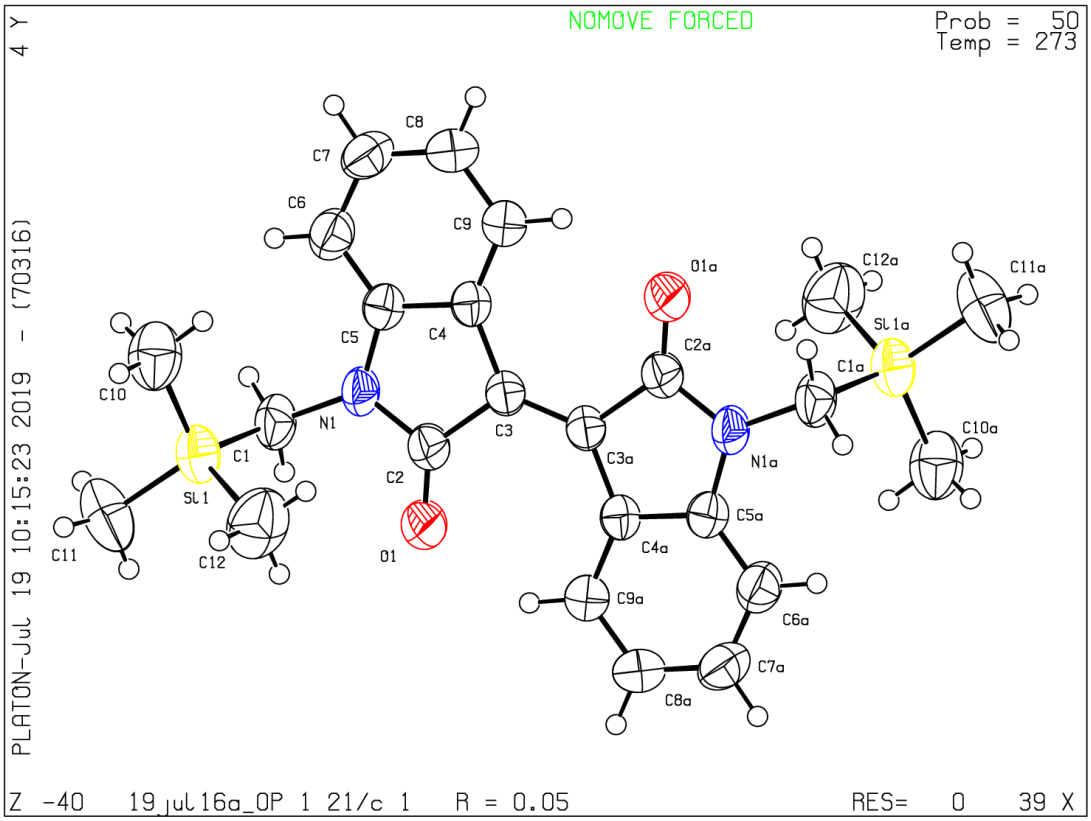


Figure S1. ORTEP Single Crystal X-Ray Diffraction of **3v**

Table S1. Crystal data and structure refinement for **3v**

Bond precision:	C-C = 0.0036 A	Wavelength=0.71073	
Cell:	a=12.0825(8)	b=6.2924(4)	c=15.8782(10)
	alpha=90	beta=90.701(4)	gamma=90
Temperature:	273 K		
	Calculated		Reported
Volume	1207.10(13)		1207.10(13)
Space group	P 21/c		P 1 21/c 1
Hall group	-P 2ybc		-P 2ybc
Moiety formula	C24 H30 N2 O2 Si2		C24 H30 N2 O2 Si2
Sum formula	C24 H30 N2 O2 Si2		C24 H30 N2 O2 Si2
Mr	434.68		434.68
Dx,g cm-3	1.196		1.196
Z	2		2
Mu (mm-1)	0.169		0.169
F000	464.0		464.0
F000'	464.48		
h,k,lmax	15,8,20		15,7,20
Nref	2765		2703
Tmin,Tmax			0.613,0.746
Tmin'			

Correction method= # Reported T Limits: Tmin=0.613 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.978 Theta(max)= 27.461

R(reflections)= 0.0537(1314) wR2(reflections)= 0.1466(2703)

S = 0.970 Npar= 139

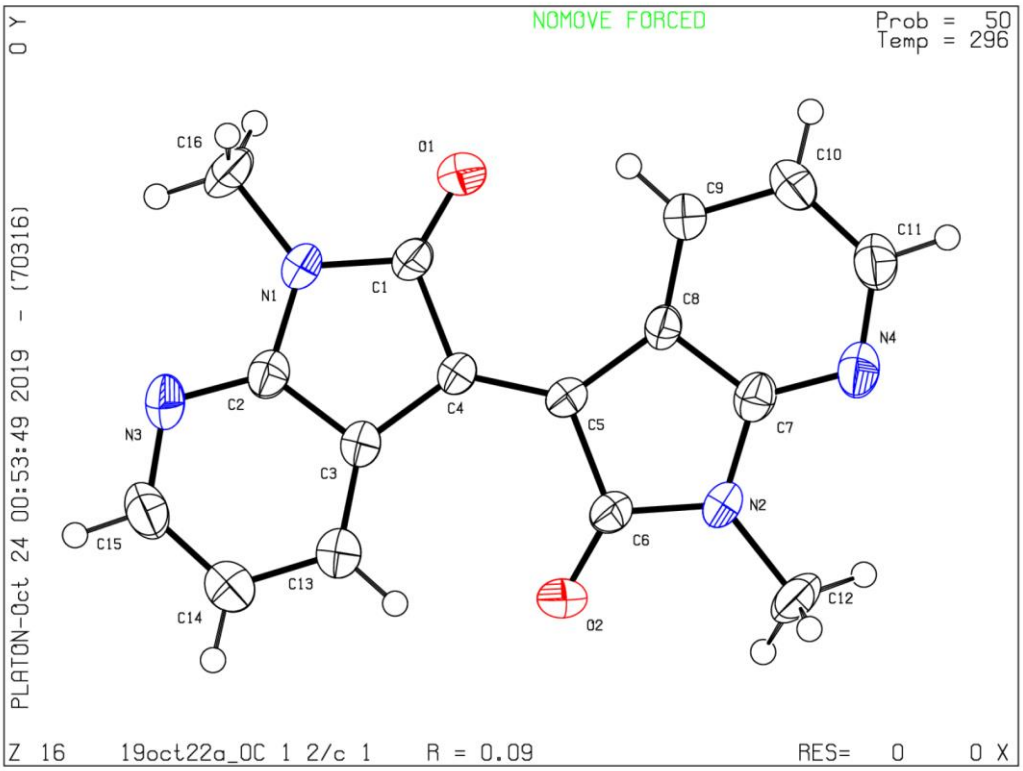


Figure S2. ORTEP Single Crystal X-Ray Diffraction of **3z**

Table S2. Crystal data and structure refinement for **3z**

Bond precision: C-C = 0.0052 A		Wavelength=0.71073	
Cell:	a=22.659(3)	b=8.6862(14)	c=15.721(3)
	alpha=90	beta=121.417(9)	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	2640.6(8)	2640.6(8)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C16 H12 N4 O2	C16 H12 N4 O2
Sum formula	C16 H12 N4 O2	C16 H12 N4 O2
Mr	292.30	292.30
Dx,g cm-3	1.470	1.470
Z	8	8
Mu (mm-1)	0.101	0.101
F000	1216.0	1216.0
F000'	1216.50	
h,k,lmax	30,11,21	30,11,21
Nref	3408	3348
Tmin,Tmax		0.475,0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.475 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 28.653

R(reflections)= 0.0945(2140) wR2(reflections)= 0.2786(3348)

S = 1.074 Npar= 203

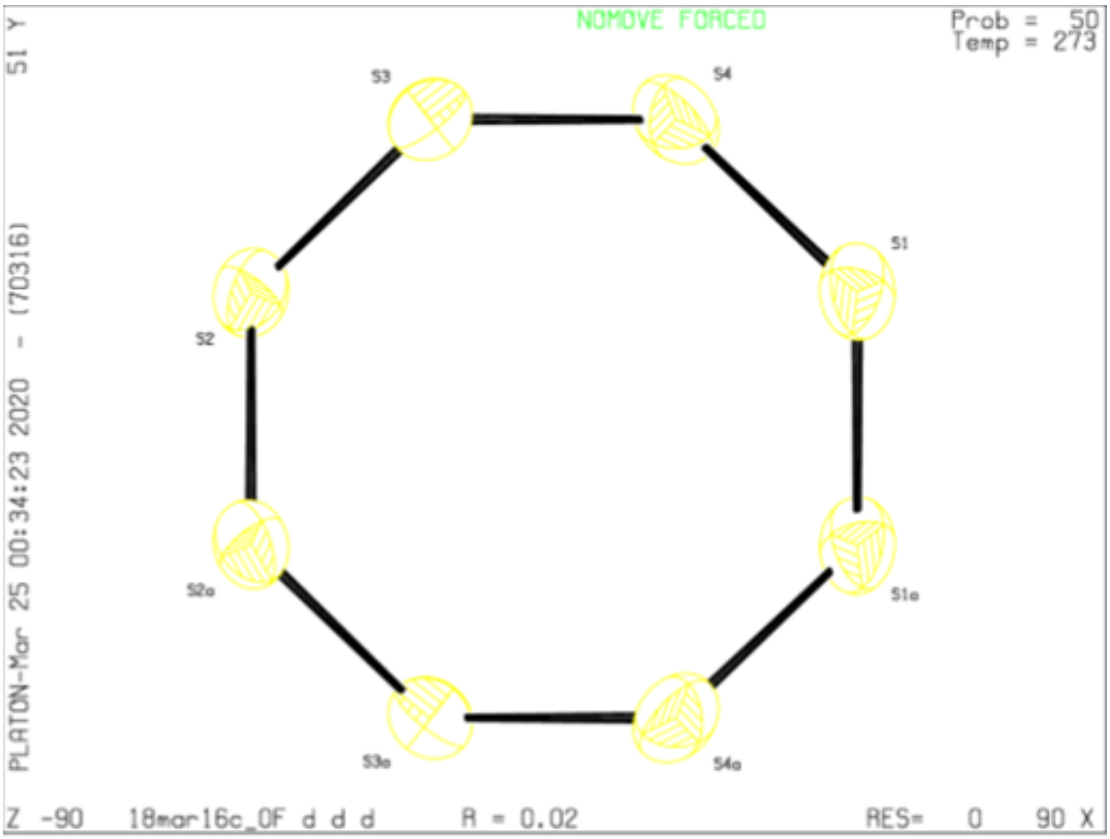


Figure S3. ORTEP Single Crystal X-Ray Diffraction of **elemental sulfur**

Table S3. Crystal data and structure refinement for **elemental sulfur**

Bond precision:	S- S = 0.0006 A	Wavelength=0.71073	
Cell:	a=10.4753(14)	b=12.8737(18)	c=24.510(3)
	alpha=90	beta=90	gamma=90
Temperature:	273 K		
	Calculated	Reported	
Volume	3305.3(8)	3305.3(8)	
Space group	F d d d	F d d d	
Hall group	-F 2uv 2vw	-F 2uv 2vw	
Moiety formula	S8	S8	
Sum formula	S8	S8	
Mr	256.48	256.48	
Dx,g cm-3	2.062	2.062	
Z	16	16	
Mu (mm-1)	2.060	2.060	
F000	2048.0	2048.0	
F000'	2063.99		
h,k,lmax	15,18,35	15,18,34	
Nref	1336	1276	
Tmin,Tmax	0.814,0.814	0.451,0.746	
Tmin'	0.814		

Correction method= # Reported T Limits: Tmin=0.451 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.955 Theta(max)= 31.132

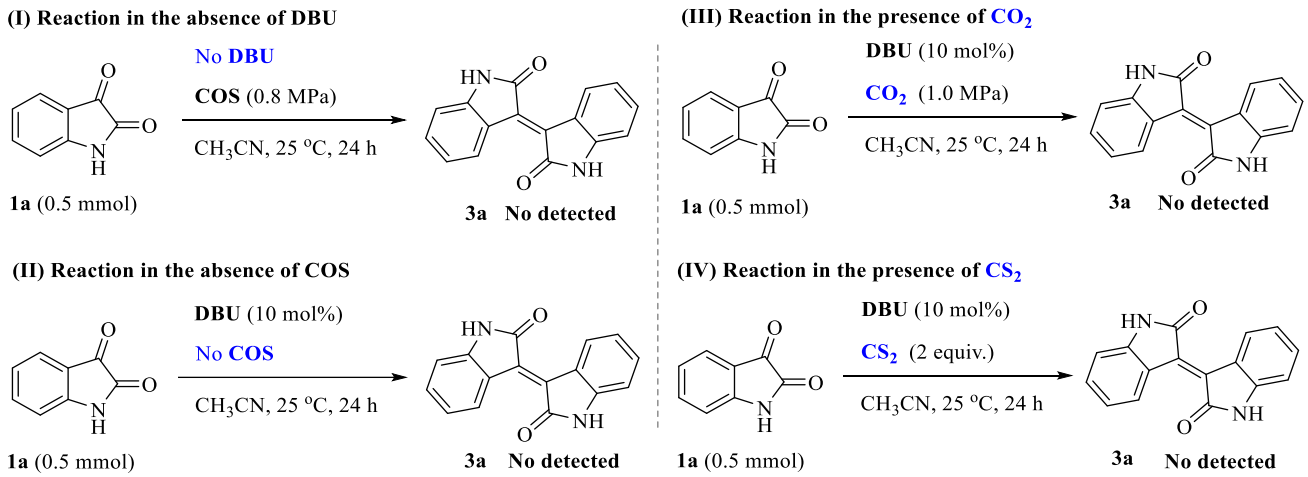
R(reflections)= 0.0200(1153) wR2(reflections)= 0.0499(1276)

S = 1.062 Npar= 38

5. Mechanistic studies

5.1 Control Experiments

In order to clarify the detailed reaction mechanism, several control experiments were designed and performed. As summarized in Scheme S1, in the absence of DBU or COS, and no desired product **3a** was observed (Scheme S1. **I** and **II**). Moreover, when changing COS to CO_2 or CS_2 under standard conditions, **3a** still was not observed and only the starting materials **1a** were retained, which indicates that CO_2 or CS_2 could not trigger this process (Scheme S1. **III** and **IV**).



Scheme S1. Control experiments

5.2 Detecting the interaction between DBU and COS

5.2.1 The interaction were detected by means of In-situ FTIR

To disclose the interaction between DBU and COS, the following experiments were designed and conducted: In a glove box, a 25 mL flask, equipped with a magnetic stir bar, was charged with DBU (0.5 mmol) and CH_3CN (2.0 mL), then In-situ FTIR probe was equipped to check the IR signals. As shown in Figure S4, the absorption peak at 1617 cm^{-1} is attributable to the C=N band of DBU. When introducing free COS (1.0 atm), the carbonyl peak of DBU-COS adduct at 1650 cm^{-1} gradually increased.

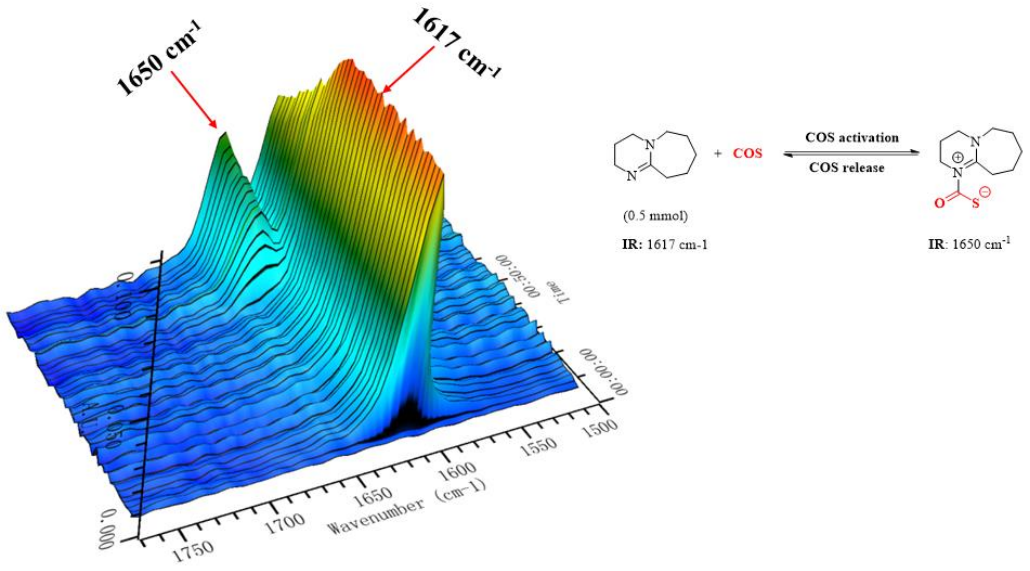


Figure S4. FTIR spectra of DBU with COS in CH_3CN

5.2.2 The interaction were detected by means of NMR control experiments

In a glove box, a dried NMR tube was charged with DBU (0.2 mmol) and CD_3CN (0.5 mL), which was characterized by ^{13}C-NMR spectroscopy (Figure S5. **I**). In the presence of COS atmosphere, a dried NMR tube was charged with DBU (0.2 mmol) and CD_3CN (0.5 mL), which was characterized by ^{13}C-NMR spectroscopy (Figure S5. **II**). Compared with the NMR data, it is obvious that when introducing COS atmosphere, a new signal at 210.1 ppm were observed from ^{13}C-NMR spectrum (Figure S5), which is attributable to in-situ generated DBU-COS adduct.

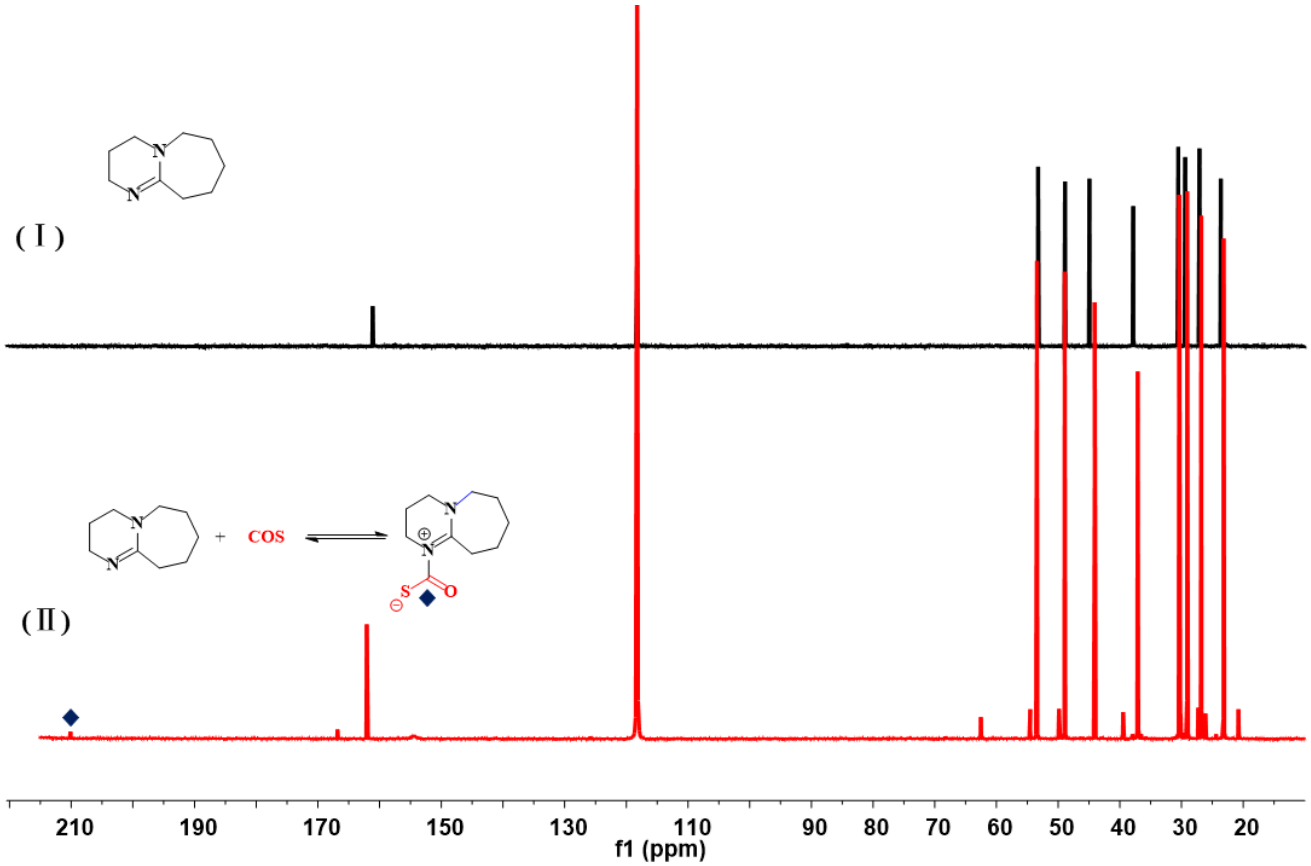


Figure S5. ^{13}C NMR comparison spectra to determine the interaction between DBU and COS

5.3 Detecting by-products experiments

5.3.1 Carbon dioxide tracking experiments by ^{13}C-NMR

The ^{13}C-NMR spectra of **1p**, CO_2 and **3p** in CD_3CN were characterized, respectively, as shown in Figure S6. The resonance of free CO_2 appears at 125.8 ppm (Figure S6, **II**). Due to the poor solubility of **3p** in CD_3CN, the resulting signals are very weak (Figure S6, **III**).

In the glove box, a dried NMR tube was charged with **1p** (0.25 mmol), THPE-Bn-^{13}COS (0.25 mmol) and CD_3CN (0.5 mL). After being sealed by NMR cap, the NMR tube was left for 24 h at room temperature. During this process, the insoluble red solid was gradually generated, which was later proved to be isoindigo **3p**. The reaction mixture in NMR tube was further characterized by ^{13}C-NMR spectroscopy (Figure S6. **IV**), and a strong ^{13}C-NMR signal at around 125.8 ppm was appeared. Through vacuum pumping and N_2 backfilling process, the reaction mixture was once again characterized by ^{13}C-NMR spectroscopy, and the ^{13}C-NMR signal at around 125.8 ppm was disappeared completely (Figure S6. **V**), which indicated that CO_2 as by-product occurred during this process.

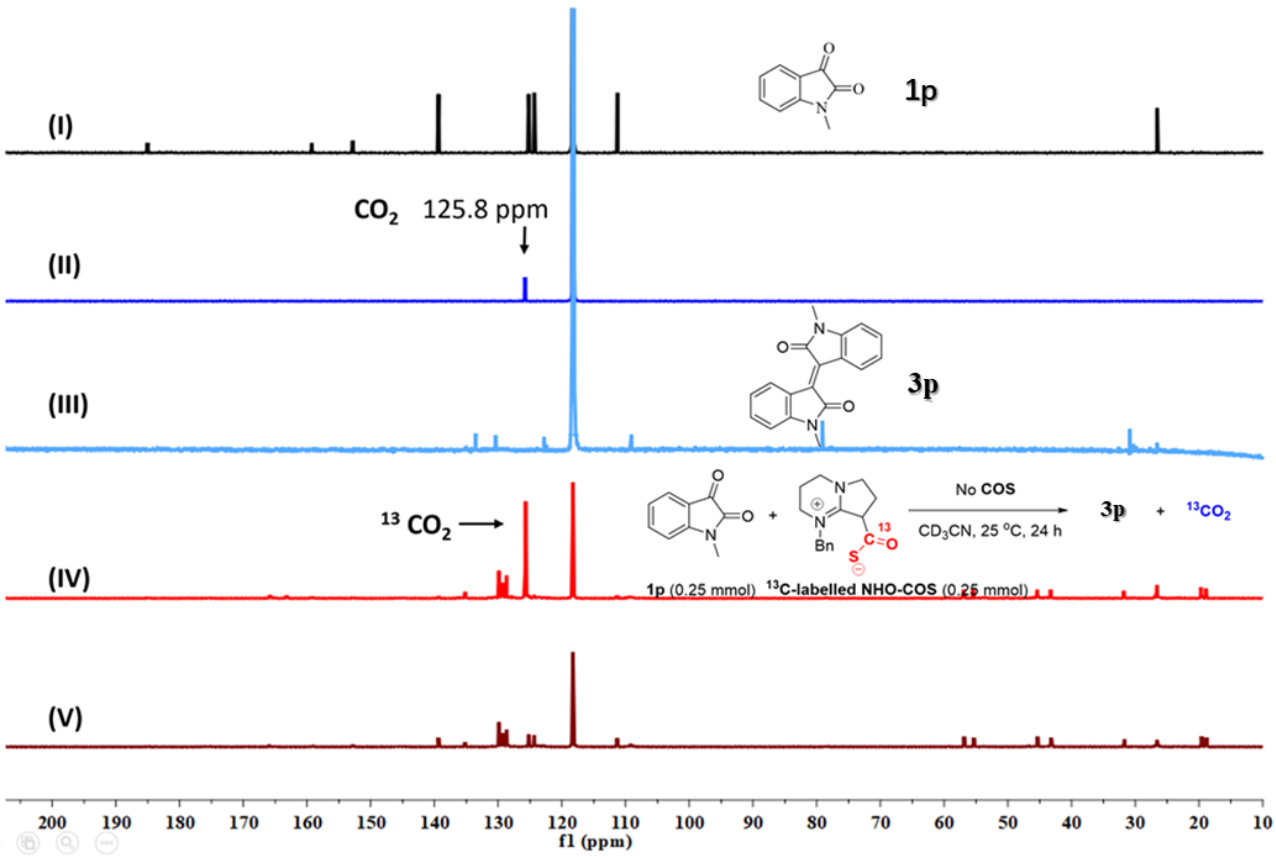


Figure S6. ^{13}C NMR comparison spectra to determine the presence of CO_2

5.3.2 Detecting Elemental sulfur experiments

In the glove box, a 10 mL oven-dried autoclave containing a stir bar was charged with isatin **1a** (1.5 mmol), DBU (0.15 mmol, 10 mmol%) and CH_3CN (2.0 mL). After purging the autoclave with COS three times. The sealed autoclave was pressurized to 0.8 MPa with COS. The reaction mixture was stirred at 25 °C for 24 h, then the remaining COS in the autoclave was vented slowly. The crude reaction mixture was purified by column chromatography on silica gel (dichormethane) to give isoindigo (0.73 mmol, 191 mg) in 98% yield and elemental sulfur (1.42 mmol, 45.6 mg) in 95% yield.

5.4 Trapping intermediate experiments

In the glove box, a 10 mL oven-dried autoclave containing a stir bar was charged with **1p** (1.0 mmol), DBU (0.1 mmol, 10 mmol%), 2,3-dimethyl-1,3-butadiene (2.0 mmol) and CH_3CN (2.0 mL). After purging the autoclave with COS three times. The sealed autoclave was pressurized to 0.8 MPa with COS. The reaction mixture was stirred at 25 °C for 24 h, then the remaining COS in the autoclave was vented slowly. The crude reaction mixture was purified by column chromatography on silica gel (petroleum ether/EtOAc: 5/1 and hexane) to give the corresponding cyclized product **4pa** (26 mg, 6% yield) [7], the 1,2-dithia-4,5-dimethyl-4-cyclohexene **6** (10.2 mg, 7% yield) and 1,2,3,4-tetrathia-6,7-dimethyl-6-cyclooctene **7** (10.5 mg, 5% yield) [8-9].

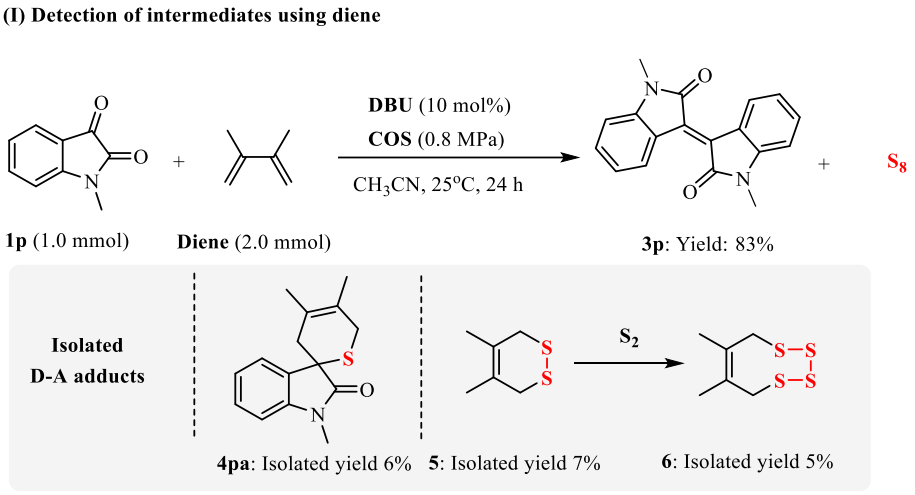


Figure S7. The capture of intermediate

1,2-dithia-4,5-dimethyl-4-cyclohexene (6). Colorless oil liquid, 10.2 mg, yield: 7%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.21 (s, 4H), 1.76 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ125.1, 34.1, 20.8. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [8].

1,2,3,4-tetrathia-6,7-dimethyl-6-cyclooctene (7). White solid, 10.5 mg, yield: 5%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 3.65 (s, 4H), 1.80 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 130.6, 43.0, 18.3. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [8].

5.5 The synthesis of 3-thioisatin in-situ

N-Chlorosulfenylsuccinimide (SuccNSCl) was firstly prepared according to previous literature [10].

Under N_2 atmosphere, oxindole (**8**) (133 mg, 1.0 mmol) and triethylamine (0.13 mL, 1.0 mmol) were dissolved in dry CH_2Cl_2 (3.0 mL) at room temperature. Then SuccNSCl (176 mg, 1.1 mmol in 3.0 mL CH_2Cl_2) was added dropwise over 15 min at -78 °C. Pyridine (1.7 mL, 3 mmol) was added slowly into the reaction mixture at room temperature for 10 minutes to obtain the CH_2Cl_2 solution of 3-thioisatin **5**, which was not purified and used directly for the subsequent transformation.

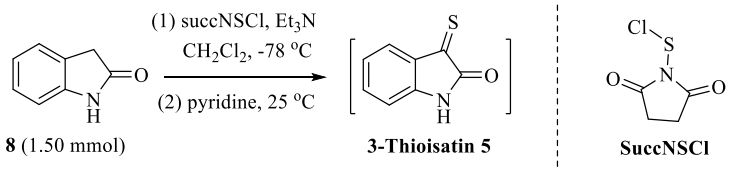
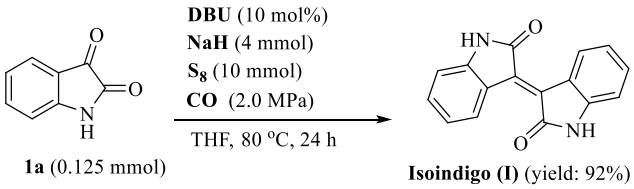


Figure S8. The synthesis of 3-thioisatin **5** in-situ

6. Self-condensation of isatin employing COS generated in-situ

In the glove box, a 10 mL oven-dried autoclave containing a stir bar was charged with elemental sulfur (320 mg, 10 mmol), NaH (96 mg, 4.0 mmol), THF (2.0 mL) and a 2 mL tube containing a stir bar was charged with **1a** (18.4 mg, 0.125 mmol), DBU (3.8 mg, 0.025 mmol) and THF (0.5 mL). Then the tube was transfered into autoclave, as shown in Figure S9. After purging the autoclave with CO three times, the sealed autoclave was pressurized to 2.0 MPa with CO. The reaction mixture was stirred at 80 °C for 24 h, then the remaining CO was vented slowly. The crude reaction mixture was purified by column chromatography on silica gel (dichloromethane) to give desired product **3a** (0.06 mmol, 18 mg) in 92% yield.



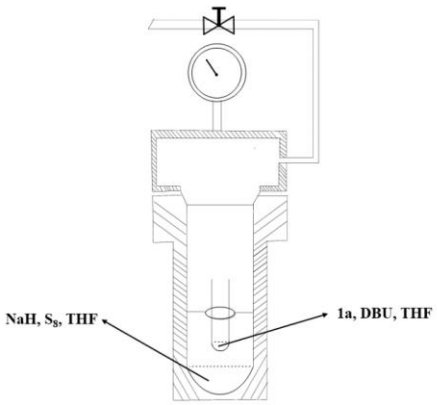
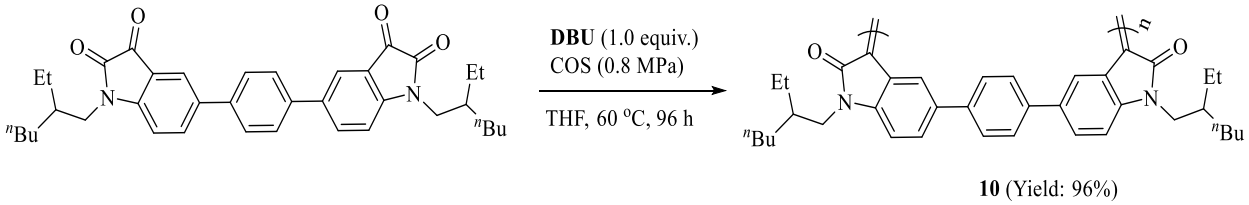


Figure S9. Experimental set-up for the formation of COS.

7. Synthesis of isoindigo based polymers

7.1 Synthesis of isoindigo based polymer 9

In the glove box, a 10 mL oven-dried autoclave containing a stir bar was charged with isatin-based monomer (120 mg, 0.2 mmol), DBU (30.6 mg, 0.2 mmol) and THF (1.0 mL). After purging the autoclave with COS three times, the sealed autoclave was pressurized to 0.8 MPa with COS. The reaction mixture was stirred at 60 °C for 96 h, then the remaining COS in the autoclave was vented slowly. The crude polymer was purified using Soxhlet extraction with methanol as washing and extracting solvent to give desired product as dark purple solid in 96% yield. GPC (DMF): M_n 9.70×10^4 g/mol, PDI 2.20.



10 (Yield: 96%)

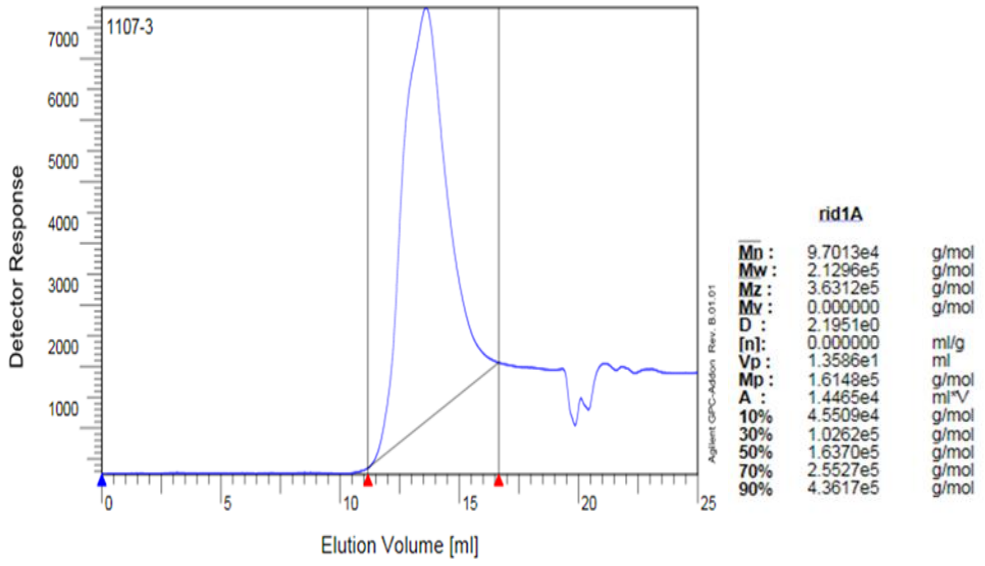
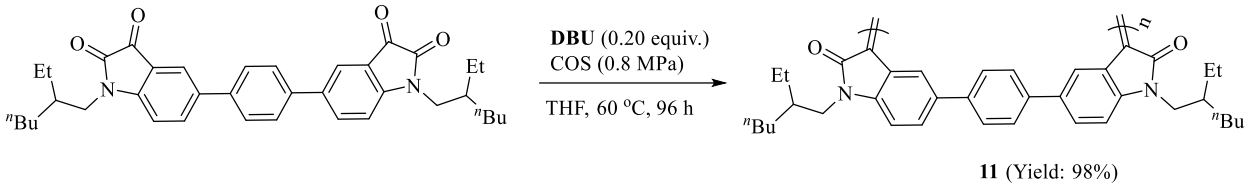


Figure S10. Gel-Permeation Chromatogram Analysis of **10**

7.2 Synthesis of isoindigo based polymer 10

In a glove box, a 10 mL oven-dried autoclave containing a stir bar was charged with isatin-based monomer (120 mg, 0.2 mmol), DBU (6.12 mg, 0.04 mmol) and THF (1.0 mL). After purging the autoclave with COS three times, the sealed autoclave was pressurized to 0.8 MPa with COS. The reaction mixture was stirred at 60 °C for 96 h, then the remaining COS in the autoclave was vented slowly. The crude polymer purified by Soxhlet extraction with methanol as washing and extracting solvent to give desired product as dark purple solid in 98% yield. GPC (THF): M_n 6.11×10^3 g/mol, PDI 1.62.



11 (Yield: 98%)

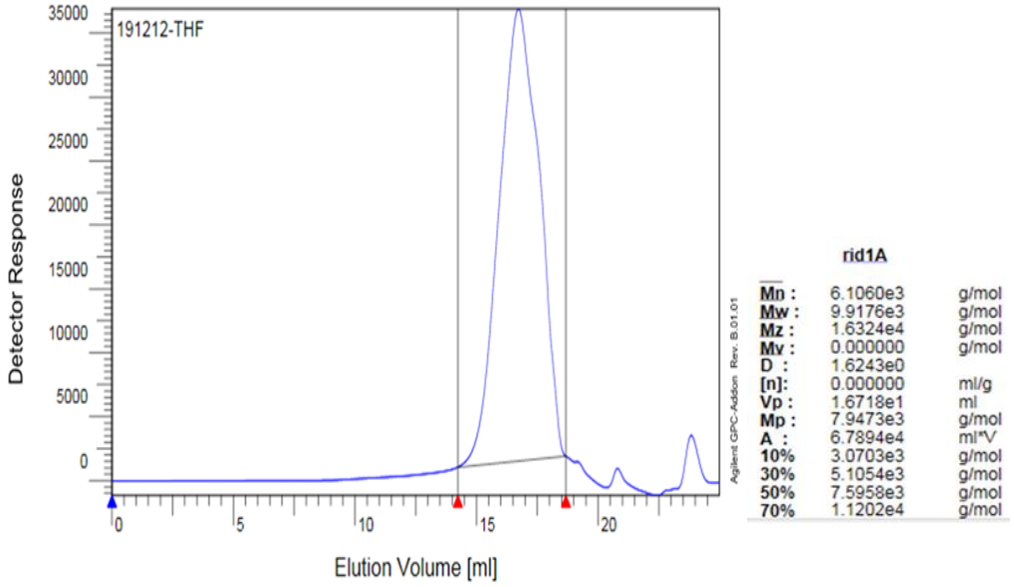


Figure S11. Gel-Permeation Chromatogram Analysis of **11**

8. Computational investigation of the reaction mechanism

Control experiments showed that 3-thioisatin is a key intermediate for this process. Both DBU and DBU-COS adducts have a certain catalytic activity and might promote the reaction. In terms of this fact, three possible pathways were proposed for the O/S exchange process (Figure S12). In **Pathway 1-1** (Figure S12), DBU acts as nucleophile reagent to activate isatin and further react with free COS to generate thiocarbonate intermediate **A**. Then, the intramolecular nucleophilic cyclization might take place to generate a four-membered cyclic thiocarbonate intermediate **B**. Finally, the selective ring-opening of intermediate **B** via DBU-involved aminolysis process and subsequent rearrangement process allow the production of 3-thioisatin. Alternatively, the four-membered cyclic thiocarbonate intermediate **B** could be generated in **Pathway 1-2** (Figure S12) employing DBU-COS adduct as nucleophile reagent. Meanwhile, a six-membered cyclic intermediate **D** could be selectively formed via the cyclization of intermediate **C** from the thiocarbonate anion to the C=O bond **(Pathway 1-3,** Figure S12**)**. Then, 3-thioisatin could be generated by subsequent rearrangement process.

In order to illustrate the process of O/S exchange, DFT calculation was performed with Gaussian 16 [11]. All geometries of the reactants, products, intermediates (**INT**), and transition states (**TS**) involved in this mechanistic study were fully optimized in CH_3CN solvent (experimentally used) with the continuum solvation model (SMD) at the M06-2X/6-31(d,p) level of theory. To improve the accuracy of the energy, the single-point energy of each optimized structure and transition state was calculated at the M06-2X (SMD, CH_3CN)/ 6-311++g(d,p) level.

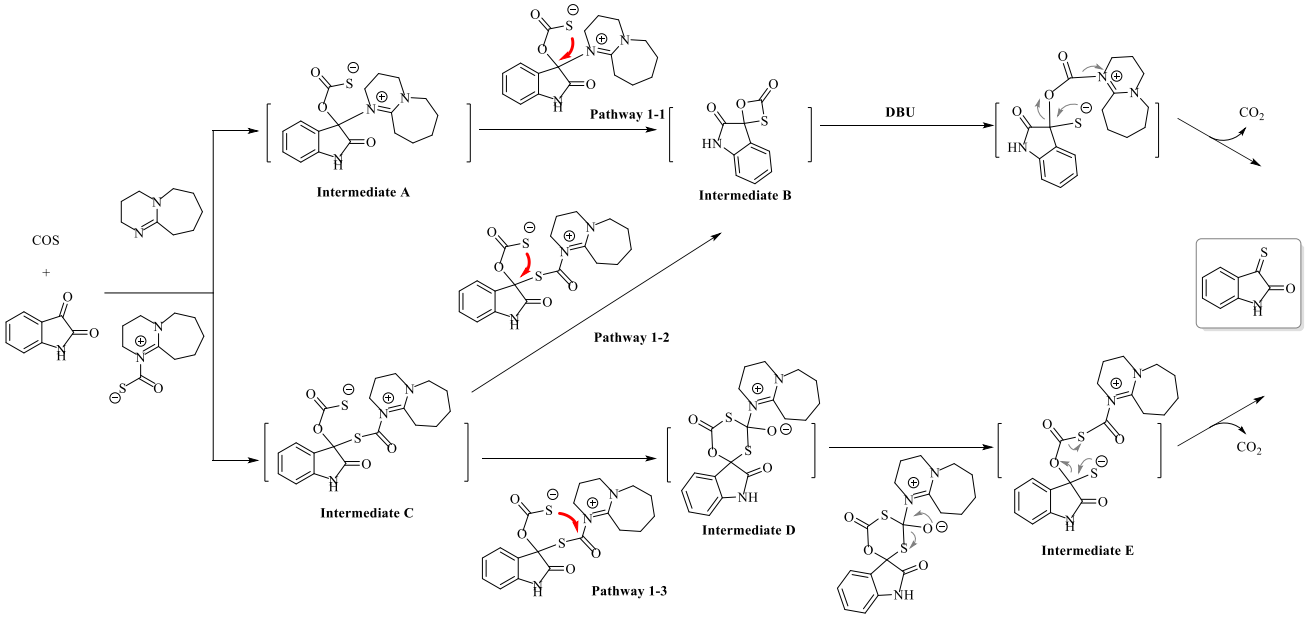


Figure S12. Proposed mechanism for the O/S exchange process.

Pathway 1-1: The computed potential energy surface of **Pathway 1-1** is presented in Figure S13. Firstly, DBU and free COS could synergistically activate isatin in the transition state **TS1-2** (4.6 kcal/mol), leading to the formation of intermediate **INT2** (-11.1 kcal/mol). Furthermore, the intramolecular nucleophilic cyclization of **INT2** via **TS2-3** produces a four-membered cyclic thiocarbonate **INT3** and releases DBU. Subsequently, the aminolysis process of resultant **INT3** by DBU takes place at **TS3-4** (11.0 kcal/mol), and the intermediate **INT4** (-12.1 kcal/mol) is formed. Finally, the zwitterionic intermediate **INT4** undergoes a rearrangement reaction (**TS4-S-isatin**) to generate 3-thioisatin and release the unstable DBU-CO_2 adduct. The overall process of O/S exchange is exothermic, and **TS2-3** is the highest stationary point with an energy barrier of 31.5 kcal/mol.

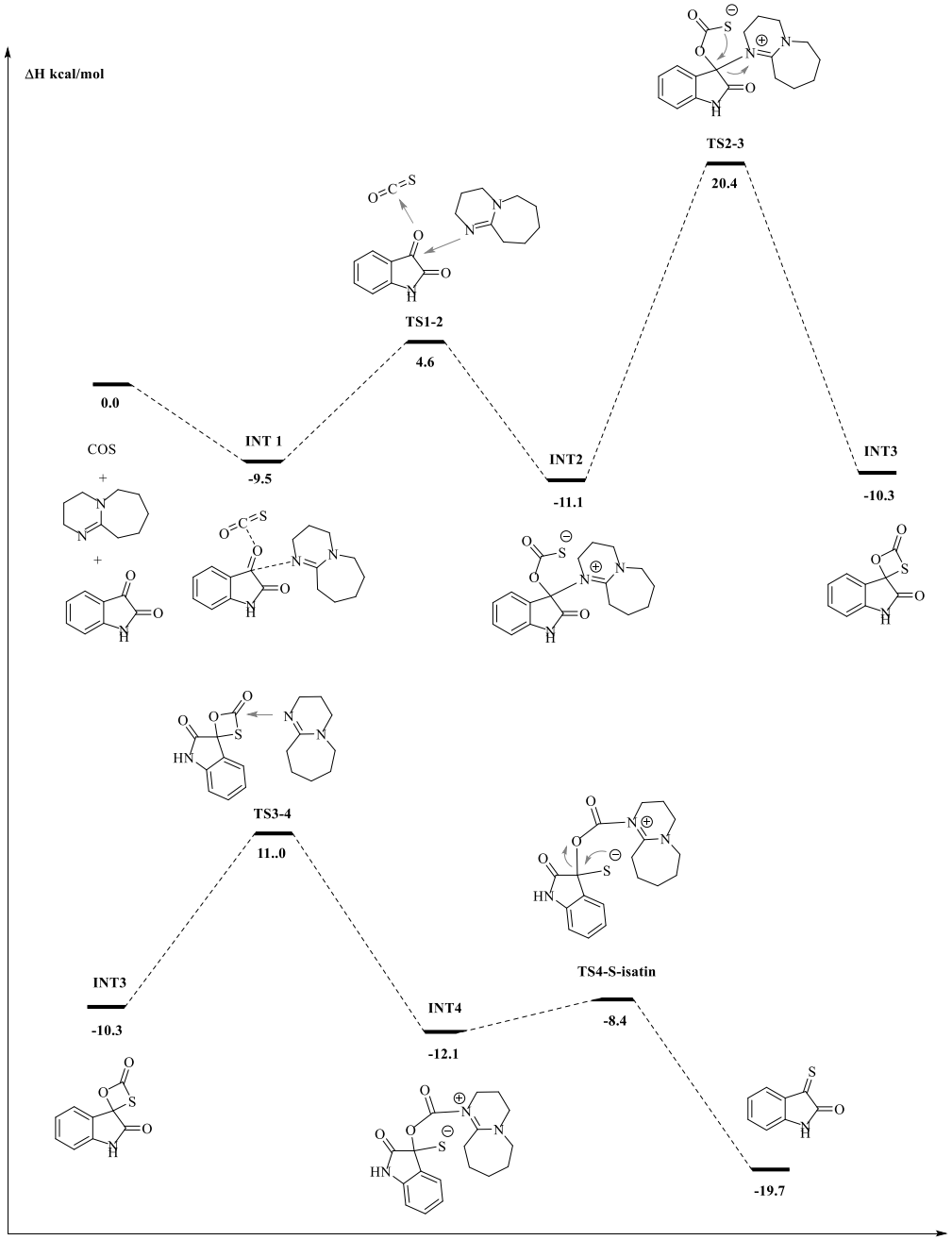


Figure S13. DBU-involved O/S exchange process (**Pathway 1-1**)

Pathway 1-2: On the other hand, the computed potential energy surface of **Pathway 1-2** is presented in Figure S14. Firstly, DBU-COS adduct and another free COS could synergistically activate isatin in the transition state **TS5-6** (4.9 kcal/mol), leading to the formation of intermediate **INT6**. Then, **INT6** can be ready to undergo an intramolecular nucleophilic cyclization from thiocarbonate anion to C-3 position of isatin with the associated energy of 7.9 kcal/mol (**TS6-3**), thus giving a four-membered cyclic thiocarbonate intermediate **INT3** and releasing the DBU-COS adduct. The subsequent reactions are the same as **Pathway 1-1**. Noting that the overall process of O/S exchange is exothermic by 19.7 kcal/mol and the nucleophilic ring opening of intermediate **INT3** is the rate determining step with an energy barrier of 28.5 kcal/mol.

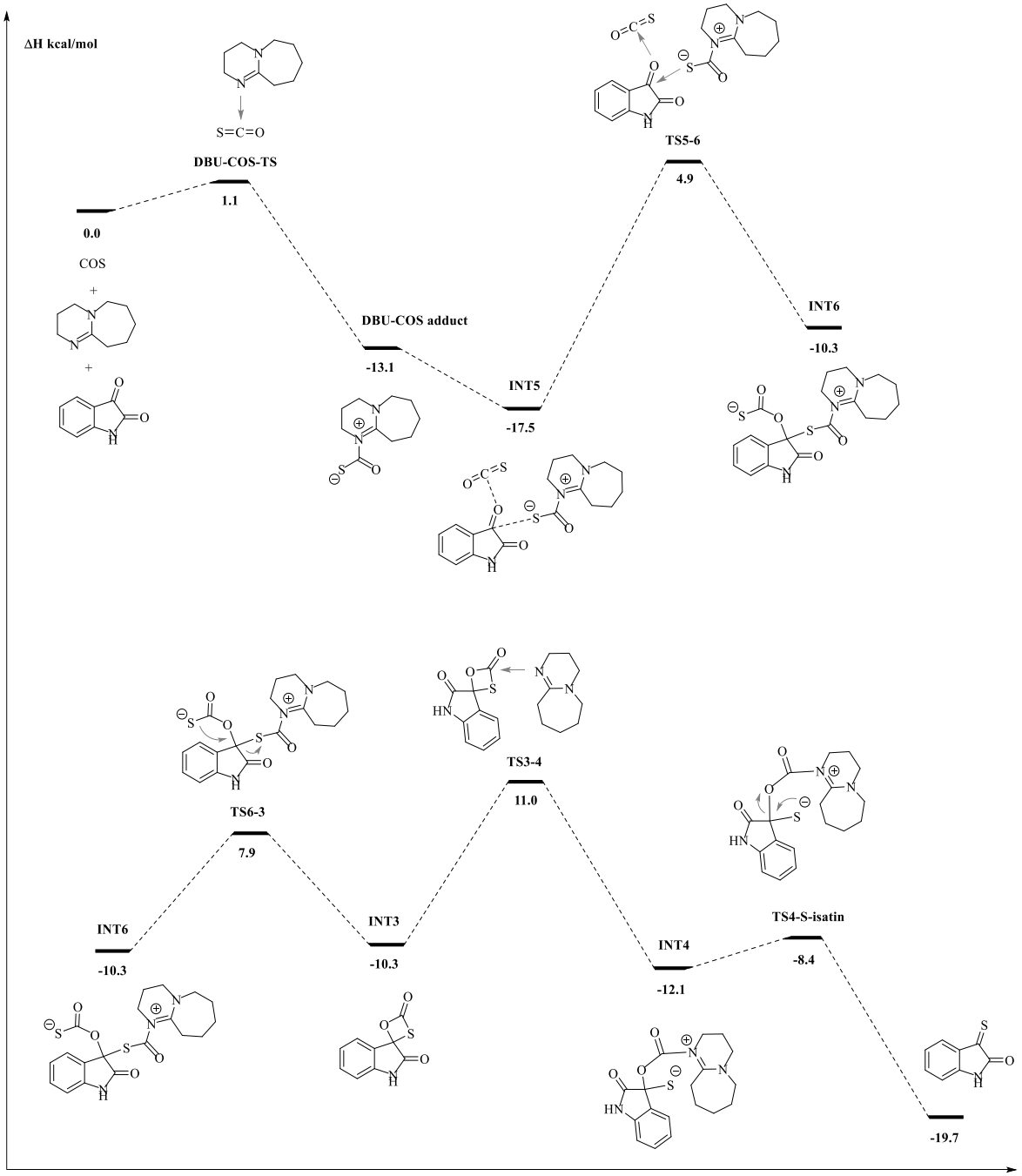


Figure S14. DBU-COS adduct-involved O/S exchange process (**Pathway 1-2**)

Pathway 1-3: In addition, another intramolecular cyclization process of thiocarbonate **INT 8** were computationally examined (Figure S15). The intramolecular nucleophilic addition from the thiocarboxylate anion to C=O bond takes place via **TS8-9** (8.9 kcal/mol) to give a tetrahedral intermediate **INT 9**. The tetrahedral intermediate **INT 9** also could experience a C-S bond cleavage **TS 9-10** (8.4 kcal/mol) to selectively form zwitterionic **INT10**, which further undergoes a rearrangement reaction (**TS10-S-isatin**: 1.5 kcal/mol) to form 3-thioisatin and release DBU-COS adduct, and free CO_2 (Figure S15). Through the detailed mechanistic studies, we observed that this is the lowest energy pathway for O/S exchange process in Figure S15, and the nucleophilic attack on C=O bond of **INT8** bond is the rate determining step with an energy barrier of 25.8 kcal/mol.

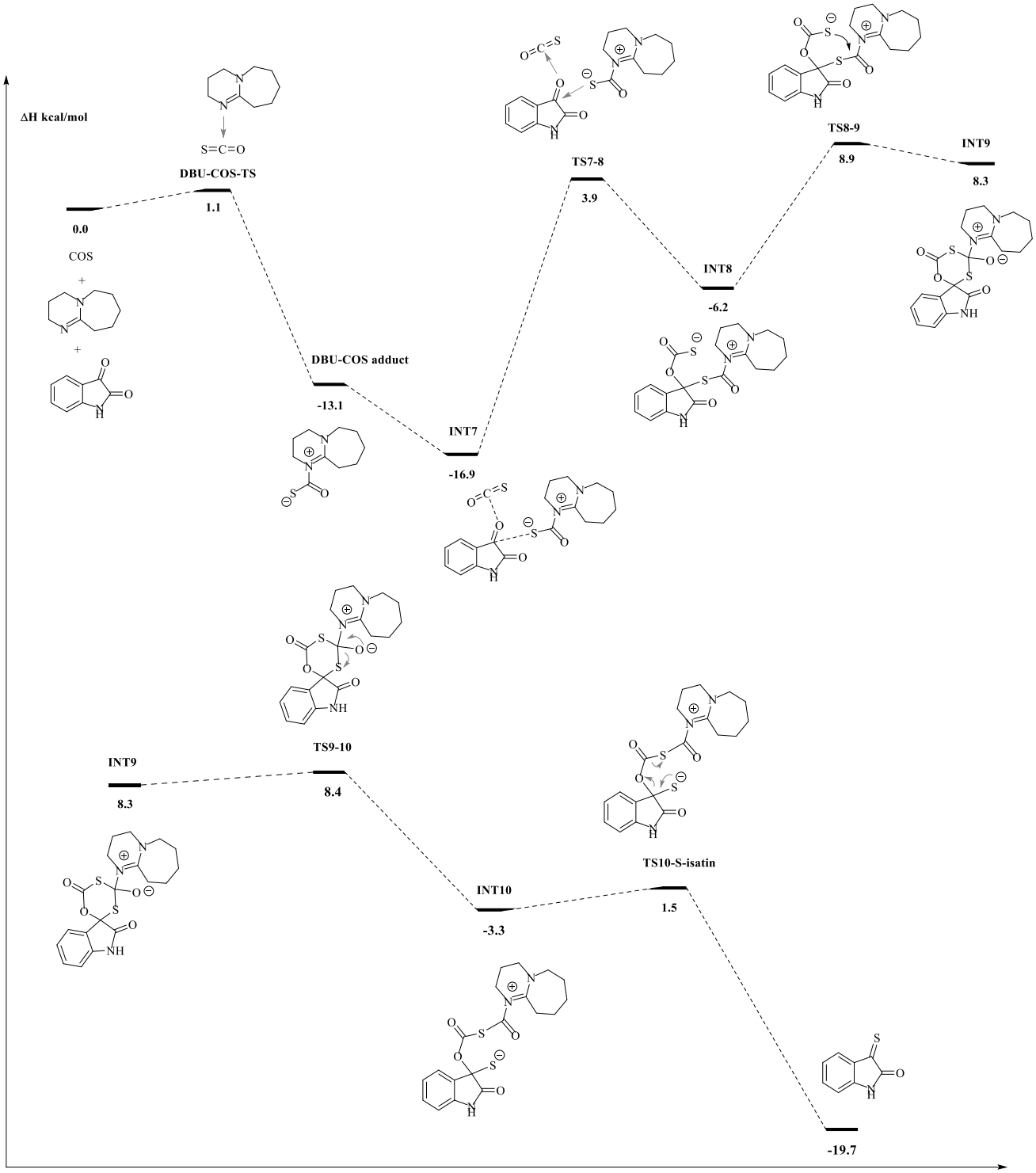


Figure S15. DBU-COS adduct-involved O/S exchange process **(Pathway 1-3)**

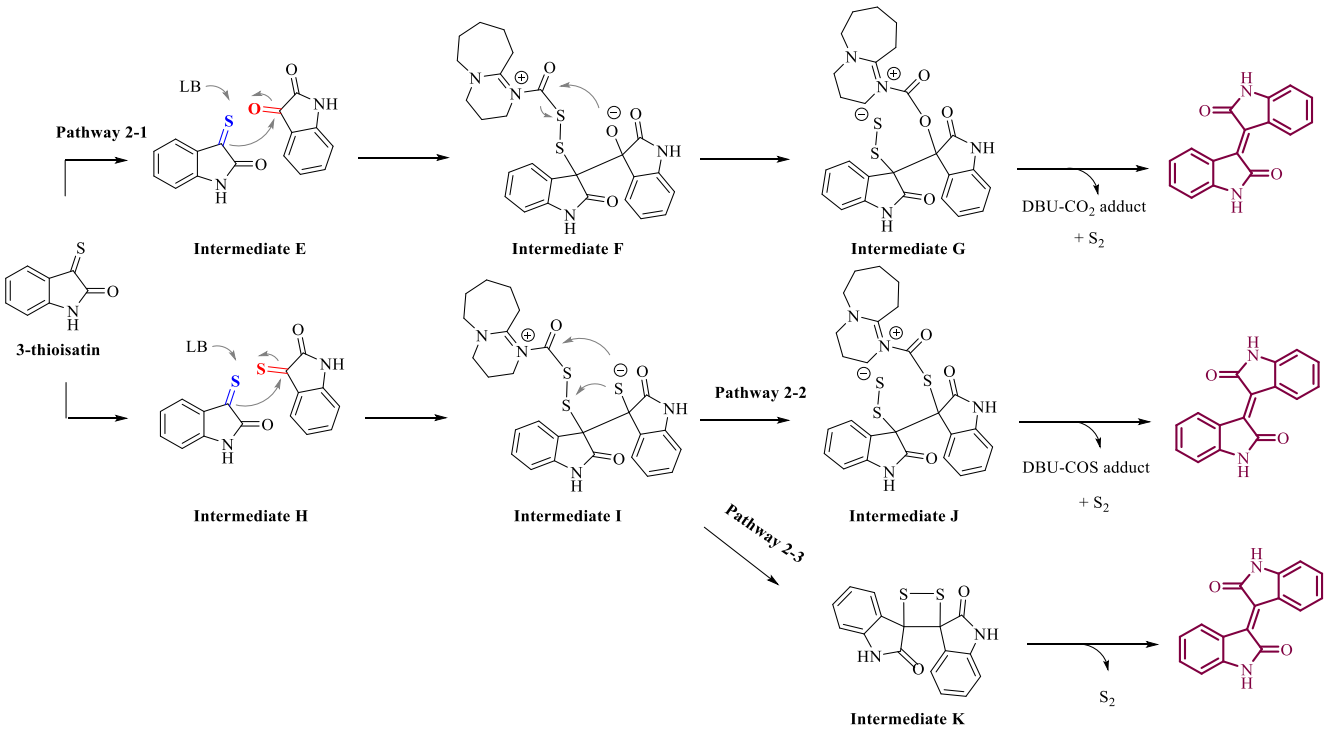
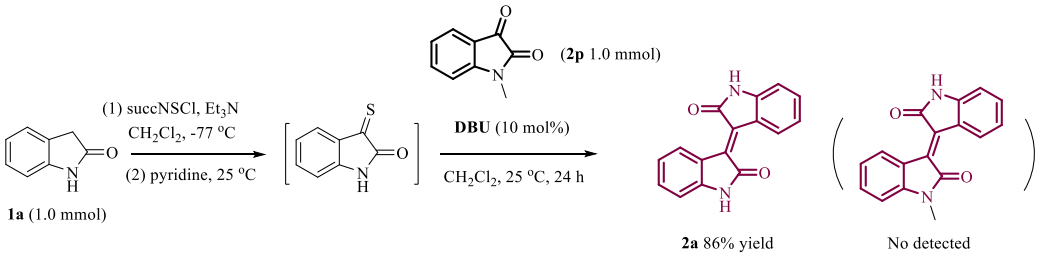


Figure S16. Proposed mechanism for the synthesis of isoindigo from 3-thioisatin

As shown in Figure S16, three proposed mechanisms for the formation of isoinidigo from 3-thioisatin were proposed. As seen from **Pathway 2-1** in Figure S16, thiophilic addition to a thiocarbonyl group of 3-thioisatin by DBU-COS adduct could take place firstly to form a carbanion, which further goes through a nucleophilic attack on the carbonyl carbon atom of isatin to generate intermediate **F**. Then intermediate **F** undergoes intramolecular transesterification to generate intermediate **G**. Finally, DBU-CO_2 adduct and diatomic sulfur (S_2) are eliminated respectively to afford isoindigo.

In addition, the carboanion generated from thiophilic addition of DBU-COS adduct with 3-thioisatin, also could attack the carbon atom of thiocarbonyl group of another 3-thioisatin to form intermediate **I**. There are two possible pathways for the formation of isoindigo from intermediate **I**. In pathway **2-2** (Figure S17), intermediate **I** goes through intramolecular transesterification and elimination process to generate isoindigo (similar to **Pathway 2-1**).

In **Pathway 2-3**, an intramolecular ring-closing reaction could proceed from intermediante **I** to afford 1,2-dithietane intermediate **K**. According to reported literatures, 1,2-dithietane derivatives could spontaneously extrudes the S_2 fragment under high temperature condition or photochemical conditions, to construct carbon-carbon double bond, thus forming corresponding isoindigo [9].



When isatin **1p** was added into the CH_2Cl_2 solution of 3-thioisatin in the presence of DBU (10 mol%) [10]. only **2a** was obtained in 86% yield. Unsymmetrical **Meisoindigo** was not detected. Based on the results, **Pathway 2-1** could be completely ruled out. Furthermore, **Pathway 2-2** and **2-3** were investigated by DFT calculations.

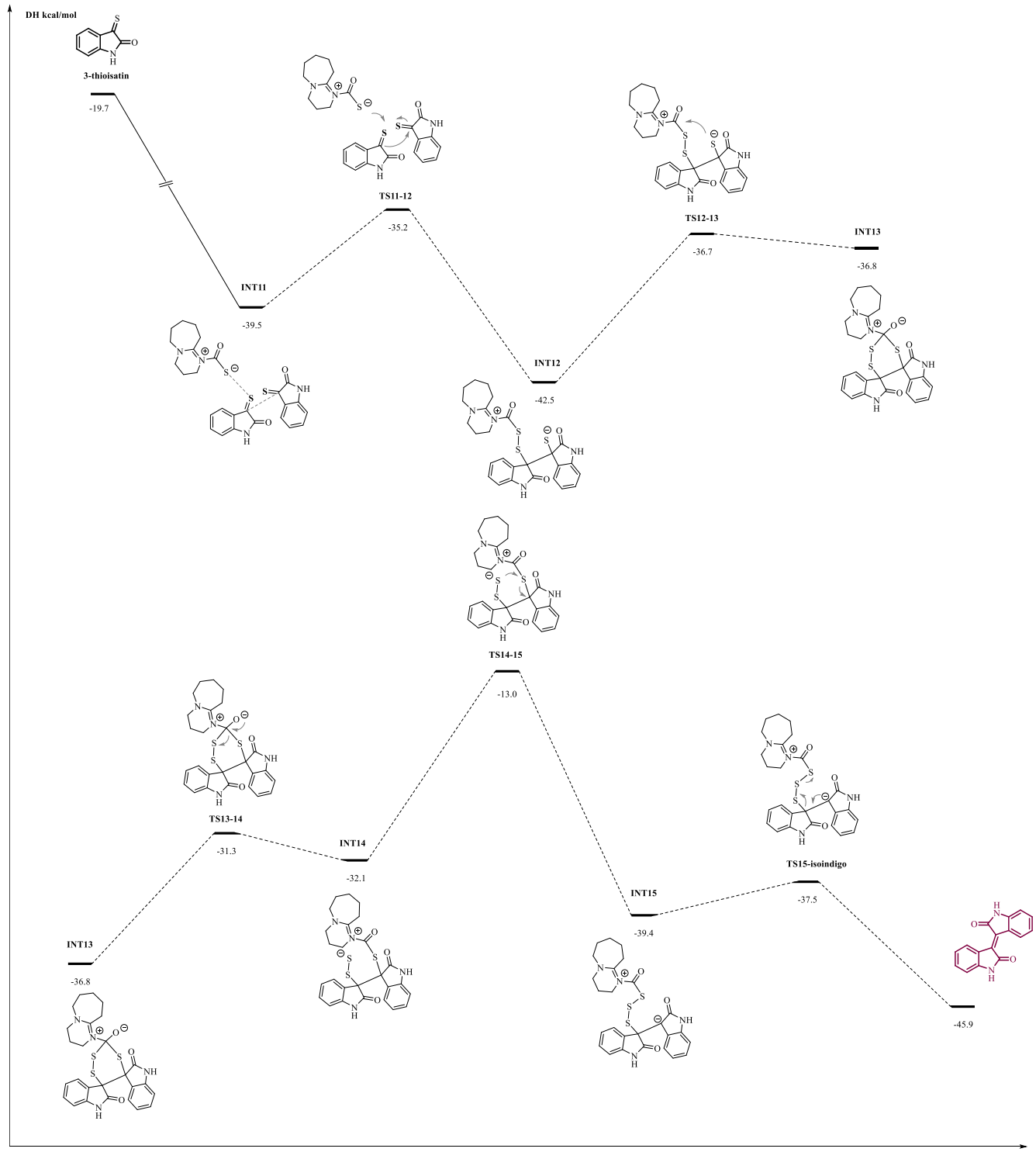


Figure S17. DBU-COS adduct-involved self-condensation of thioisatin **(Pathway 2-2)**

After the formation of 3-thioisatin, DBU-COS adduct further complex with two 3-thioisatins to form **INT 11**, as shown in Figure S17. Then **INT11** can traverse **TS11-12** (-35.2 kcal/mol) with an energy barrier of 4.3 kcal/mol to generate **INT 12**. The intramolecular nucleophilic cyclization of **INT 12** could take place vis **TS12-13** (-36.7 kcal/mol) to generate a cyclic tetrahedral **INT 13**. Furthermore, **INT 13** could break down via transition state **TS13-14** (-31.3 kcal/mol) to generate **INT 14**, which further undergoes a rearrangement (**TS14-15**, -13.0 kcal/mol) with an energy barrier of 29.5 kcal/mol to form **INT 15**. Finally, the S_2 fragment was ejected from **INT 15** vis **TS 15-isoindigo** (-37.5 kcal/mol), to generate isoindigo and release DBU-COS adduct for the next catalytic cycle.

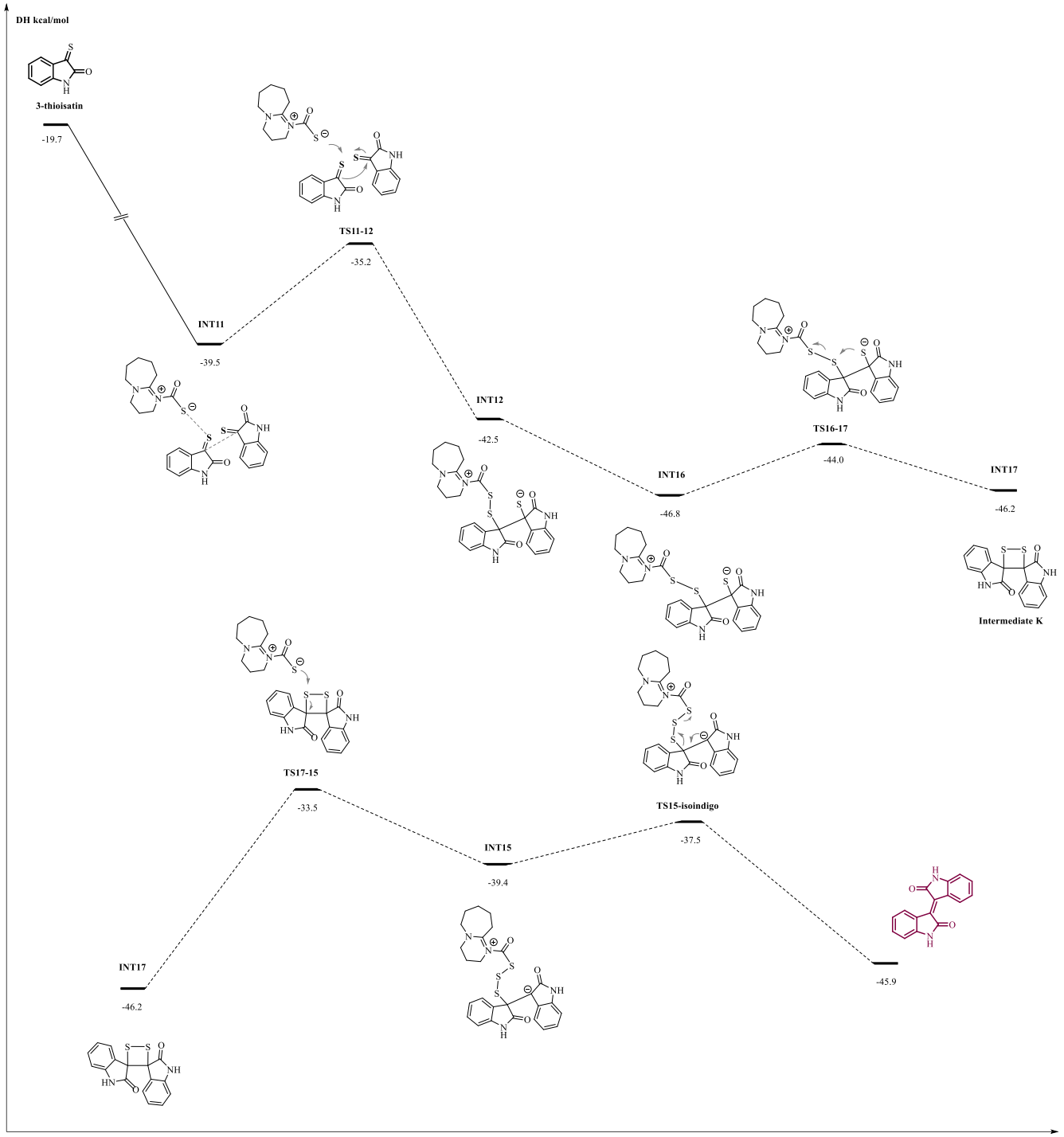
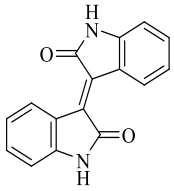


Figure S18. DBU-COS adduct-involved self-condensation of thioisatin **(Pathway 2-3)**

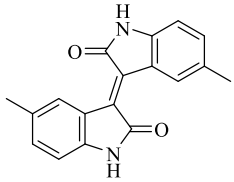
On the other hand, **INT 16** could form 1,2-dithietane **INT 17** via **TS 16-17** with an energy barrier of only 2.8 kcal/mol, as shown in Figure S18. Subsequently, thiophilic ring opening process of **INT 17** will take place via **TS17-15** (-33.5 kcal/mol) to form **INT 15**. Because the energy barrier for the rate determining step (**TS17-15**) is only 13.3 kcal/mol in **Pathway 2-3**, the self-condensation of 3-thioisatin perfers to proceed via **Pathway 2-3** than **Pathway 2-2**.

9. Characterization date of products



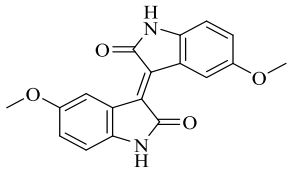
3a

(E)-[3,3'-biindolinylidene]-2-one. Red solid, 60.8 mg, yield: 98%. **^{1}H NMR (**400 MHz, DMSO-d_6) δ 10.90 (s, 2H), 9.05 (d, J = 7.1 Hz, 2H), 7.38 – 7.30 (m, 2H), 6.96 (t, J = 7.5 Hz, 2H), 6.84 (d, J = 6.6 Hz, 2H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 169.0, 144.2, 133.4, 132.7, 129.4, 121.8, 121.2, 109.6; **IR** (KBr cm^{-1}): 3075, 1703, 1650, 1618, 1575, 1463, 870, 778; **HRMS**(ESI): calcd. for $C_{16}H_{11}N_2O_2$: $[M+H]^+$ m/z 263.0821, found: 263.0824.



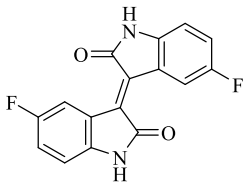
3b

(E)-5,5'-dimethyl-[3,3'-biindolinylidene]-2,2'-dione. Dark red solid, 63.8 mg, yield: 88%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.73 (s, 2H), 8.89 (s, 2H), 7.15 (d, J = 7.9 Hz, 2H), 6.73 (d, J = 7.9 Hz, 2H), 2.26 (s, 6H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 169.6, 142.4, 133.9, 133.2, 130.1, 122.6, 109.6, 21.3; **IR** (KBr cm^{-1}): 3182, 1704, 1621, 1484, 1327, 1258, 1221, 1139, 809, 771; **HRMS**(EI): calcd. for $C_{18}H_{14}N_2O_2$: [M] m/z 290.1055, found: 290.1059.



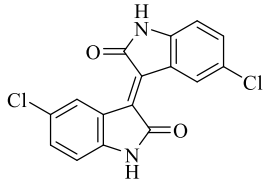
3c

(E)-5,5'-dimethoxy-[3,3'-biindolinylidene]-2,2'-dione. Blue-green solid, 63.8 mg, yield: 73%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.69 (s, 2H), 8.85 (d, J = 2.2 Hz, 2H), 6.97 (dd, J = 8.4, 2.4 Hz, 2H), 6.75 (d, J = 8.5 Hz, 2H), 3.73 (s, 6H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 168.7, 153.9, 137.8, 133.6, 122.1, 118.4, 115.4, 109.2, 55.4; **IR** (KBr cm^{-1}): 3157, 1684, 1651, 1623, 1593, 1478, 1447, 1317, 1223, 1150, 818, 774. **HRMS**(EI): calcd. for $C_{18}H_{14}N_2O_4$: [M] m/z 322.0954, found: 322.0952.



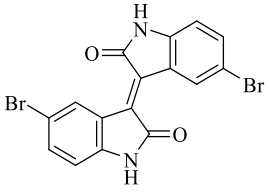
3d

(E)-5,5'-difluoro-[3,3'-biindolinylidene]-2,2'-dione. Dark red solid. 73 mg, yield: 98%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.99 (s, 2H), 8.99 (dd, J = 11.3, 2.4 Hz, 2H), 7.24 (td, J = 8.6, 2.4 Hz, 2H), 6.84 (dd, J = 8.5, 4.9 Hz, 2H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 169.1, 157.1 (d, J = 233.2 Hz), 140.9, 134.0 (d, J = 2.5 Hz), 122.2 (d, J = 10.2 Hz), 119.6 (d, J = 24.2 Hz), 116.3 (d, J = 28.2 Hz), 110.3 (d, J = 8.3 Hz). All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [12].



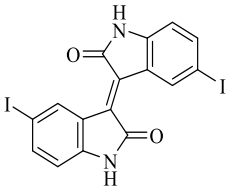
3e

(E)-5,5'-dichloro-[3,3'-biindolinylidene]-2,2'-dione. Dark red solid, 80 mg, yield: 98%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.12 (s, 2H), 9.19 (d, J = 1.7 Hz, 2H), 7.43 (dd, J = 8.3, 2.0 Hz, 2H), 6.88 (d, J = 8.3 Hz, 2H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.7, 143.1, 133.4, 132.4, 128.9, 125.1, 122.7, 111.0. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [13].



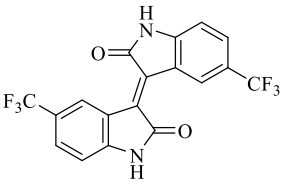
3f

(E)-5,5'-dibromo-[3,3'-biindolinylidene]-2,2'-dione. Purple-red solid, 102.4 mg, yield: 98%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.06 (s, 2H), 9.31 (s, 2H), 7.54 (d, J = 6.5 Hz, 2H), 6.83 (d, J = 5.7 Hz, 2H); **IR** (KBr cm^{-1}): 3112, 1701, 1614, 1448, 1319, 1181, 862, 813, 730; **HRMS**(EI): calcd. for $C_{16}H_8Br_2N_2O_2$: [M]$^+$ m/z 417.8953, found: 417.8938.



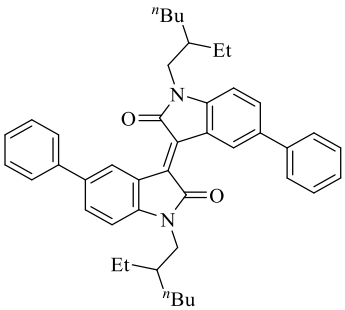
3g

(E)-5,5'-diiodo-[3,3'-biindolinylidene]-2,2'-dione. Dark red solid, 125.9 mg, yield: 98%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.02 (s, 2H), 9.46 (s, 2H), 7.69 (d, J = 7.5 Hz, 2H), 6.72 (d, J = 8.1 Hz, 2H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 183.3, 165.6, 158.9, 150.1, 146.1, 132.6, 120.1, 114.9; **IR** (KBr cm^{-1}): 3184, 1692, 1673, 1610, 1444, 1317, 1183, 1120, 881, 814, 771; **HRMS**(EI) calcd. for $C_{16}H_8I_2N_2O_2$ [M]$^+$ m/z 513.8675. found：513.8669.



3h

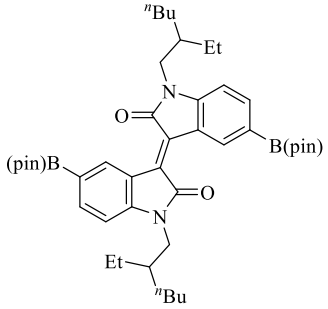
(E)-5,5'-bis(trifluoromethyl)-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 97.5 mg, yield: 98%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.32 (s, 2H), 9.54 (s, 2H), 7.71 (d, J = 8.1 Hz, 2H), 7.03 (d, J = 8.2 Hz, 2H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 168.8, 147.2, 133.2, 129.6 (dd, J = 7.5, 3.8 Hz), 126.4 (q, J = 4.1 Hz), 124.5 (q, J = 272.7 Hz), 122.3 (s), 121.83 (d, J = 31.8 Hz), 110.0; **IR** (KBr cm^{-1}): 3125, 1699, 1624, 1412, 1330, 1162, 1126, 855, 834; **HRMS**(ESI): calcd. for $C_{18}H_7F_6O_2N_2$: 397.0412 [M-H]$^-$, found: 397.0422.



3i

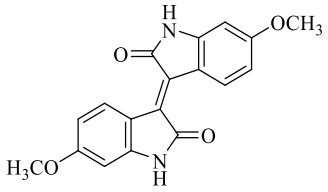
(E)-1,1'-bis(2-ethylhexyl)-5,5'-diphenyl-[3,3'-biindolinylidene]-2,2'-dione. Red oil liquid. 156.4 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.49 (s, 2H), 7.67 (d, J = 7.9 Hz, 4H), 7.59 (d, J = 8.1 Hz, 2H), 7.47 (t, J = 7.6 Hz, 4H), 7.35 (t, J = 7.0 Hz, 2H), 6.83 (d, J = 8.1 Hz, 2H), 3.76 – 3.63 (m, 4H), 1.93 – 1.84 (m, 2H), 1.43 – 1.28 (m, 16H), 0.99 – 0.89 (m, 12H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.4, 144.6, 141.2, 135.4, 134.0, 131.2, 128.9, 128.7, 127.0, 122.3, 108.5, 44.3, 37.7, 30.8, 28.8, 24.2, 23.2, 14.2, 10.9; **IR** (neat cm^{-1}): 2959, 1689, 1608, 1598, 1478, 1456, 1347, 1220, 1175, 1113, 810, 757; **HRMS**(ESI): calcd. for $C_{44}H_{51}N_2O_2$ $[M+H]^+$ m/z 639.3951, found：639.3938.



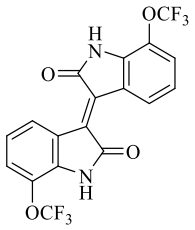
3j

(E)-1,1'-bis(2-ethylhexyl)-5,5'-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[3,3'-biindolinylidene]-2,2'-dione. Red oil liquid, 180.9 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.39 (s, 2H), 7.80 (d, J = 7.3 Hz, 2H), 6.77 (d, J = 7.7 Hz, 2H), 3.69 (m, 4H), 1.86 (m, 2H), 1.38 – 1.28 (m, 40H), 0.94 – 0.87 (m, 12H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 168.5, 147.8, 139.5, 135.8, 133.5, 130.0, 121.5, 107.9, 83.9, 44.3, 37.7, 30.8, 28.9, 25.0, 24.3, 23.3, 14.2, 10.9; **IR** (neat cm^{-1}):2951, 1739, 1612, 1470, 1352, 1191, 1126, 1073, 974, 756; **HRMS**(ESI): calcd. for $C_{44}H_{64}B_2N_2O_6$ $[M+H]^+$ m/z 739.5029, found: 739.5029.



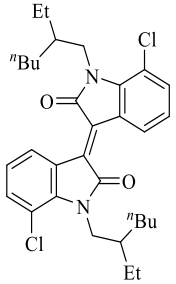
3k

(E)-6,6'-dimethoxy-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 40.3 mg, yield: 50%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.79 (s, 2H), 9.00 (s, 2H), 6.45 (d, J = 58.2 Hz, 4H), 3.81 (s, 6H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 170.0, 162.4, 145.7, 130.8, 129.7, 115.1, 106.64, 95.4, 55.4; **IR** (KBr cm^{-1}): 3161, 1685, 1630, 1508, 1453, 1334, 1199, 1125, 836, 617; **HRMS**(ESI): calcd. for $C_{18}H_{15}N_2O_4$ $[M+H]^+$ m/z 323.1032, found: 323.1026.



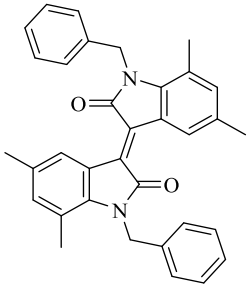
3l

(E)-7,7'-bis(trifluoromethoxy)-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 84.9 mg, yield: 79%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.70 (s, 2H), 7.64 (d, J = 8.3 Hz, 2H), 7.55 (d, J = 7.4 Hz, 2H), 7.15 (t, J = 7.9 Hz, 2H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 168.6, 137.3, 133.6, 131.1, 128.5, 125.6, 123.9, 121.6, 120.3 (d, J = 257.4 Hz); **IR** (KBr cm^{-1}): 3197, 1697, 1636, 1579, 1491, 1452, 1325, 1160, 865, 740; **HRMS**(EI) calcd. for $C_{18}H_8F_6N_2O_4$ $[M]^+$ m/z 430.0388, found: 430.0381.



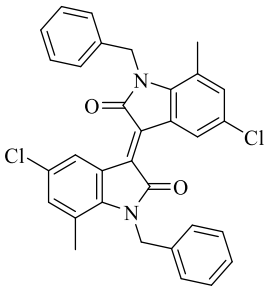
3m

(E)-7,7'-dichloro-1,1'-bis(2-ethylhexyl)-[3,3'-biindolinylidene]-2,2'-dione. Dark red solid, 135.7 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.97 (d, J = 7.9 Hz, 2H), 7.27 (d, J = 8.2 Hz, 2H), 6.94 (t, J = 8.0 Hz, 2H), 4.07 (d, J = 7.5 Hz, 4H), 2.10 – 1.80 (m, 2H), 1.42 – 1.16 (m, 16H), 1.00 – 0.74 (m, 12H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.3, 140.8, 135.3, 133.5, 128.1, 124.7, 123.0, 115.1, 46.0, 39.2, 30.2, 28.5, 23.4, 23.2, 14.2, 10.7; **IR** (neat cm^{-1}): 2958, 1697, 1591, 1466, 1451, 1217, 786, 729; **HRMS**(ESI): calcd. for $C_{32}H_{41}Cl_2N_2O_2$ $[M+H]^+$ m/z 555.2545, found: 555.2539.



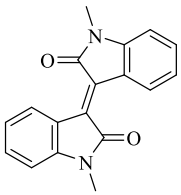
3n

(E)-1,1'-dibenzyl-5,5',7,7'-tetramethyl-[3,3'-biindolinylidene]-2,2'-dione. Purple-red solid, 122.1 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.85 (s, 2H), 7.34 (t, J = 7.3 Hz, 4H), 7.24 (t, J = 8.6 Hz, 6H), 6.87 (s, 2H), 5.32 (d, J = 5.1 Hz, 4H), 2.30 (s, 6H), 2.26 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.1, 140.4, 137.7, 137.6, 133.7, 131.6, 129.0, 128.0, 127.3, 125.8, 123.0, 119.0, 45.4, 21.1, 19.0. **IR** (neat cm^{-1}):2920, 1736, 1687, 1593, 1446, 1340, 1350, 869, 742; **HRMS**(ESI): calcd. for $C_{34}H_{31}N_2O_2$ $[M+H]^+$ m/z 499.2386, found: 499.2378.



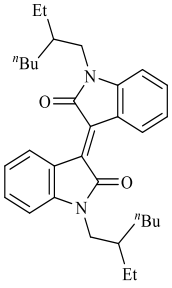
3o

(E)-1,1'-dibenzyl-5,5'-dichloro-7,7'-dimethyl-[3,3'-biindolinylidene]-2,2'-dione. Dark red solid, 131.8 mg, yield:98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.12 (s, 2H), 7.33 (t, J = 7.5 Hz, 4H), 7.27 (d, J = 6.6 Hz, 2H), 7.17 (d, J = 7.5 Hz, 4H), 7.05 (s, 2H), 5.30 (s, 4H), 2.26 (s, 6H); **^{13}C NMR** (101MHz, $CDCl_3$) δ 168.6, 141.4, 137.1, 136.4, 133.5, 129.2, 127.6, 127.6, 127.6, 125.7, 123.7, 120.8, 45.5, 19.00; **IR** (neat cm^{-1}): 2920, 1692, 1631, 1535, 1446, 1382, 1219, 1073, 912, 772; **HRMS**(ESI): calcd. for $C_{32}H_{25}Cl_2N_2O_2$ $[M+H]^+$ m/z 539.1293, found: 539.1265.



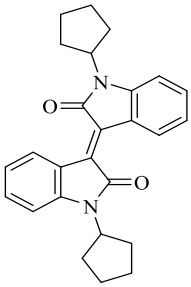
3p

(E)-1,1'-dimethyl-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 65.9 mg, yield: 91%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.22 (d, J = 7.4 Hz, 1H), 7.38 (td, J = 7.7, 1.1 Hz, 1H), 7.07 (td, J = 7.9, 1.0 Hz, 1H), 6.79 (d, J = 7.7 Hz, 1H), 3.29 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.1, 145.3, 133.5, 132.5, 130.0, 122.5, 121.7, 107.8, 26.2. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [14].



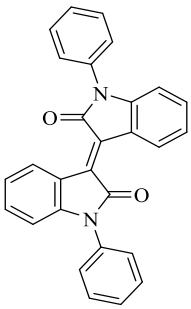
3q

(E)-1,1'-bis(2-ethylhexyl)-[3,3'-biindolinylidene]-2,2'-dione. Red oil liquid, 114.3 mg, yield: 94%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.16 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 7.7 Hz, 2H), 7.04 (t, J = 7.8 Hz, 2H), 6.77 (d, J = 7.8 Hz, 2H), 3.74 – 3.60 (m, 4H), 1.91 – 1.81 (m, 2H), 1.41 – 1.26 (m, 16H), 0.91 (dt, J = 13.7, 7.2 Hz, 12H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.4, 145.3, 133.7, 132.4, 129.9, 122.3, 121.9, 108.3, 44.4, 37.7, 30.9, 28.9, 24.2, 23.2, 14.2, 10.9; **IR** (neat cm^{-1}): 2953, 2921, 2851, 1691, 1607, 1463, 1349, 1194, 1100, 747, 593; **HRMS**(ESI) calcd. for $C_{32}H_{43}N_2O_2$ $[M+H]^+$ m/z 487.3325, found： 487.3315.



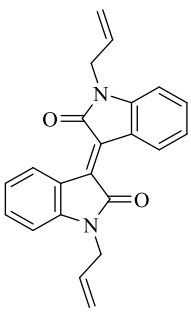
3r

(E)-1,1'-dicyclopentyl-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 97.5 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.13 (d, J = 7.9 Hz, 2H), 7.32 (t, J = 7.7 Hz, 2H), 7.03 (t, J = 7.8 Hz, 2H), 6.87 (d, J = 7.9 Hz, 2H), 4.90 – 4.81 (m, 2H), 2.23 – 2.08 (m, 4H), 2.02 – 1.89 (m, 8H), 1.79 – 1.68 (m, 8H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.9, 144.0, 133.8, 132.1, 130.0, 122.1, 121.9, 109.2, 52.4, 27.6, 25.3; **IR** (neat cm^{-1}): 3129, 2972, 2912, 1691, 1600, 1462, 1363, 1104, 741, 600, 458; **HRMS**(ESI) calcd. for $C_{26}H_{27}N_2O_2$ $[M+H]^+$ m/z 399.2073. found: 399.2069.



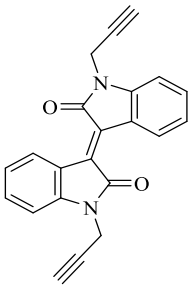
3s

(E)-1,1'-dibenzyl-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 108.3 mg, yield: 98%. **^{1}H NM**R (400 MHz, $CDCl_3$) δ 9.22 (d, J = 7.4 Hz, 2H), 7.36 – 7.26 (m, 12H), 7.09 – 7.01 (m, 2H), 6.72 (d, J = 7.8 Hz, 2H), 5.02 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.2, 144.6, 135.9, 132.6, 130.1, 129.0, 127.8, 127.4, 122.6, 121.9, 108.8, 43.8. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [12].



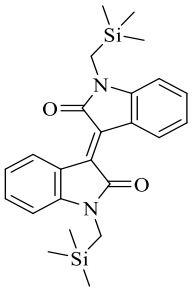
3t

(E)-1,1'-dibenzyl-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 83.8 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.06 (t, J = 7.6 Hz, 2H), 6.79 (d, J = 7.8 Hz, 2H), 5.88 (ddd, J = 22.3, 10.3, 5.1 Hz, 2H), 5.25 (t, J = 13.0 Hz, 4H), 4.44 (d, J = 5.1 Hz, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.8, 144.6, 133.5, 132.5, 131.3, 130.1, 122.5, 121.7, 117.7, 108.6, 42.4. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [12].



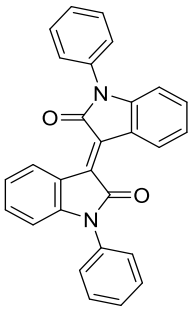
3u

(E)-1,1'-di(prop-2-yn-1-yl)-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 82.8 mg, yield: 98%.. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.10 (d, J = 8.0 Hz, 2H), 7.51 (t, J = 7.7 Hz, 2H), 7.17 – 7.09 (m, 4H), 4.66 (d, J = 2.1 Hz, 4H), 3.30 (s, 2H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 166.4, 143.3,133.1, 132.6, 129.3, 122.4, 120.9, 109.3, 77.9, 74.5, 29.0; **IR** (neat cm^{-1}): 3283, 2970, 1692, 1609, 1471, 1357, 1188, 1107, 1078, 774, 653, 464; **HRMS**(ESI) calcd. for $C_{22}H_{15}N_2O_2$ $[M+H]^+$ m/z 339.1143, found: 339.1133.



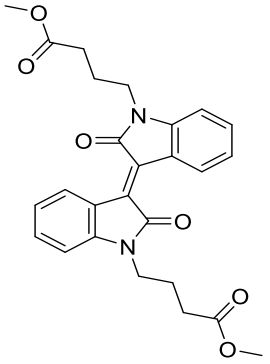
3v

(E)-1,1'-bis((trimethylsilyl)methyl)-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 106.4 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.17 (d, J = 8.0 Hz, 2H), 7.32 (t, J = 7.7 Hz, 2H), 7.02 (t, J = 7.8 Hz, 2H), 6.70 (d, J = 7.8 Hz, 2H), 3.30 (s, 4H), 0.14 (s, 18H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.6, 145.6, 133.5, 132.2, 129.6, 122.3, 122.1, 108.2, 31.5, -1.2; **IR** (neat cm^{-1}): 3130, 2953, 2851, 1687, 1605, 1467, 1353, 1176, 1101, 857, 844, 744; **HRMS**(ESI) calcd. for $C_{24}H_{31}N_2O_2Si_2$ $[M+H]^+$ m/z 435.1924, found: 435.1916.



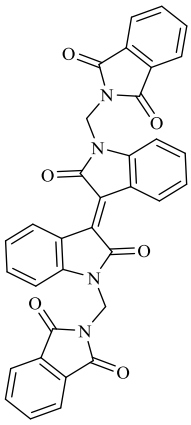
3w

(E)-1,1'-diphenyl-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 101.4 mg, yield: 98%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.23 (d, J = 8.0 Hz, 2H), 7.58 (dd, J = 9.9, 5.6 Hz, 4H), 7.50 – 7.43 (m, 6H), 7.31 – 7.26 (m, 2H), 7.09 – 7.02 (m, 2H), 6.75 (d, J = 7.8 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.6, 145.5, 132.7, 130.4, 129.9, 128.5, 127.3, 123.0, 121.7, 109.2. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [12].



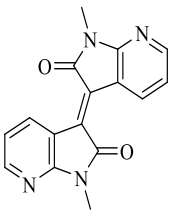
3x

Dimethyl 4,4'-(2,2'-dioxo-[3,3'-biindolinylidene]-1,1'-diyl)(E)-dibutyrate. Red solid, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.16 (d, J = 7.9 Hz, 2H), 7.37 (t, J = 7.7 Hz, 2H), 7.05 (t, J = 7.8 Hz, 2H), 6.88 (d, J = 7.8 Hz, 2H), 3.85 (t, J = 7.2 Hz, 4H), 3.67 (s, 6H), 2.44 (t, J = 7.1 Hz, 4H), 2.05 (p, J = 7.2 Hz, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.4, 168.1, 144.6, 133.6, 132.7, 130.1, 122.5, 121.8, 108.1, 51.9, 39.2, 31.1, 22.7; **IR** (neat cm^{-1}): 2919, 2852, 1733, 1687, 1603, 1464, 1355, 1161, 1077, 773, 750; **HRMS**(ESI) calcd. for $C_{26}H_{27}N_2O_6$ $[M+H]^+$ m/z 463.1869, found: 463.1857.



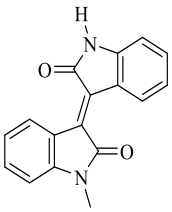
3y

(E)-2,2'-((2,2'-dioxo-[3,3'-biindolinylidene]-1,1-diyl)bis(methylene))bis(isoindoline-1,3-dione). Red solid, 142.1 mg, yield: 98%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.10 (d, J = 8.0 Hz, 2H), 7.88 – 7.84 (m, 8H), 7.45 (t, J = 7.7 Hz, 2H), 7.26 (d, J = 7.9 Hz, 2H), 7.10 (t, J = 7.8 Hz, 2H), 5.69 (s, 4H); **IR** (KBr cm^{-1}): 3429, 1776, 1726, 1611, 1470, 1405, 1326, 1301, 1101, 1022, 925, 779, 749, 724, 709; **HRMS**(ESI) calcd. for $C_{34}H_{21}N_4O_6$ $[M+H]^+$ m/z 581.1461, found：581.1454.



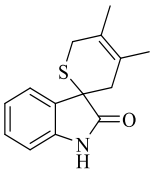
3z

(E)-1,1'-dimethyl-[3,3'-bipyrrolo[2,3-b]pyridinylidene]-2,2'(1H,1'H)-dione. Red solid, 66.4 mg, yield: 91%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.46 (d, J = 7.7 Hz, 2H), 8.24 (d, J = 4.5 Hz, 2H), 7.02 (dd, J = 7.6, 5.3 Hz, 2H), 3.38 (s, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.8, 157.8, 150.4, 137.6, 132.3, 118.8, 116.2, 25.5; **IR** (neat cm^{-1}): 2921, 1705, 1598, 1463, 1339, 1260, 1194, 1020, 803, 759; **HRMS**(ESI) calcd. for $C_{16}H_{13}N_4O_2$ $[M+H]^+$ m/z 293.1039, found: 293.1034 $[M+H]^+$.



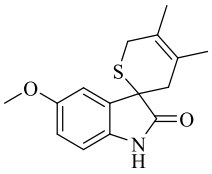
9

(E)-1-methyl-[3,3'-biindolinylidene]-2,2'-dione. Red solid, 20 mg, yield: 29%. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.89 (s, 1H), 9.07 (d, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.06 – 6.92 (m, 3H), 6.83 (d, *J* = 7.6 Hz, 1H), 3.21 (s, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 168.9, 167.2, 145.0, 144.2, 133.8, 132.9, 132.6, 132.3, 129.5, 129.0, 121.8, 121.7, 121.2, 120.8, 109.6, 108.5, 26.1. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values [13].



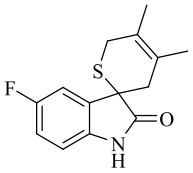
4aa

4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 111.5 mg, yield: 91%. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.88 (s, 1H), 7.27 – 7.20 (m, 2H), 7.05 (dd, *J* = 15.5, 7.9 Hz, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 3.80 (d, *J* = 16.7 Hz, 1H), 3.07 (d, *J* = 16.8 Hz, 1H), 2.64 – 2.47 (m, 2H), 1.91 (s, 3H), 1.78 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 178.6, 139.8, 132.2, 128.9, 124.8, 123.9, 123.8, 122.9, 110.0, 47.1, 37.8, 30.2, 20.5, 19.7; **IR** (neat cm^{-1}): 2920, 1710, 1601, 1471, 1372, 1279, 1180, 1225, 1141, 1108, 1017, 724; **HRMS**(APCI): calcd. for $C_{14}H_{16}NOS$: [M+H]$^+$ m/z 246.0953, found: 246.0947.



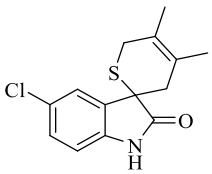
4ca

5-methoxy-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 119.7 mg, yield: 87%. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 8.76 (s, 1H), 6.82 (dd, *J* = 12.4, 5.4 Hz, 2H), 6.76 (dd, *J* = 8.4, 2.6 Hz, 1H), 3.75 (d, *J* = 17.6 Hz, 4H), 3.08 (d, *J* = 16.7 Hz, 1H), 2.61 – 2.45 (m, 2H), 1.88 (s, 3H), 1.76 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 179.3, 156.0, 133.7, 133.4, 124.9, 123.9, 113.4, 110.9, 110.6, 55.9, 47.8, 37.9, 30.2, 20.5, 19.7; **IR** (neat cm^{-1}): 1720, 1609, 1595, 1499, 1480, 1370, 1180, 1075, 753; **HRMS**(ESI): calcd. for $C_{15}H_{16}NO_2S$: [M-H]$^-$ m/z 274.0902, found: 274.0906.



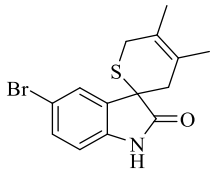
4da

5-fluoro-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 117.1 mg, yield: 89%. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 9.13 (s, 1H), 7.02 – 6.61 (m, 3H), 3.68 (d, *J* = 16.8 Hz, 1H), 3.12 (d, *J* = 16.8 Hz, 1H), 2.52 (dd, *J* = 57.7, 17.3 Hz, 2H), 1.89 (s, 3H), 1.76 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 179.4, 160.0, 158.4, 135.9 (d, *J* = 3.0 Hz), 134.1 (d, *J* = 9.1 Hz), 124.8, 124.0, 113.4 (dd, *J* = 90.6 Hz), 110.9 (d, *J* = 3.0 Hz), 48.1, 37.7, 30.1, 20.6, 19.7; **IR** (neat cm^{-1}): 1711, 1629, 1487, 1180, 1142, 815; **HRMS**(ESI): calcd. for $C_{14}H_{13}FNOS$: [M-H]$^-$ m/z 262.0702, found: 262.0713.



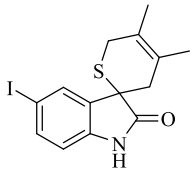
4ea

5-chloro-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 128.4 mg, yield: 92%. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 8.28 (s, 1H), 7.21 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.16 (s, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 3.72 (d, *J* = 16.8 Hz, 1H), 3.07 (d, *J* = 16.8 Hz, 1H), 2.59 – 2.44 (m, 2H), 1.89 (s, 3H), 1.76 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 178.9, 137.4, 132.4, 132.2, 129.3, 124.7, 124.6, 123.8, 109.7, 47.1, 37.8, 30.2, 20.5, 19.8; **IR** (neat cm^{-1}): 3223, 1712, 1617, 1478, 1439, 1307, 1180, 1142, 1075, 811; **HRMS**(ESI): calcd. for $C_{14}H_{13}ClNOS$: [M-H]$^-$ m/z 278.0406, found: 278.0412.



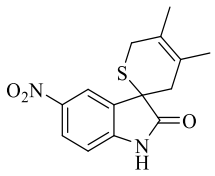
4fa

5-bromo-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 148.6 mg, yield: 92%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.36 (d, J = 8.2 Hz, 1H), 7.29 (s, 1H), 6.80 (d, J = 8.2 Hz, 1H), 3.73 (d, J = 16.8 Hz, 1H), 3.07 (d, J = 16.7 Hz, 1H), 2.57 – 2.45 (m, 2H), 1.89 (s, 3H), 1.76 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 178.5, 138.9, 134.4, 131.8, 127.1, 124.6, 124.0, 115.4, 111.6, 47.5, 37.6, 30.1, 20.5, 19.7； **IR** (neat cm^{-1}): 1711, 1616, 1474, 1306, 1180, 1142, 1076, 810; **HRMS**(ESI): calcd. for $C_{14}H_{13}BrNOS^-$ [M-H]$^-$ m/z 323.9881, found: 323.9884.



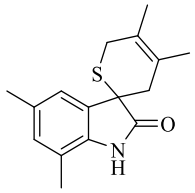
4ga

5-iodo-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 165.1 mg, yield: 89%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.55 (dd, J = 8.2, 1.6 Hz, 1H), 7.48 (d, J = 1.3 Hz, 1H), 6.68 (d, J = 8.2 Hz, 1H), 3.76 (d, J = 16.8 Hz, 1H), 3.03 (d, J = 16.7 Hz, 1H), 2.57 – 2.43 (m, 2H), 1.88 (s, 3H), 1.76 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 177.9, 139.5, 137.7, 134.6, 132.8, 124.5, 123.9, 112.0, 47.0, 37.6, 30.1, 20.5, 19.7； **IR** (neat cm^{-1}): 1713, 1610, 1473, 1229, 1180, 1132, 1076; **HRMS**(ESI): calcd. for $C_{14}H_{13}INOS^-$ [M-H]$^-$ m/z 369.9763, found: 369.9763.



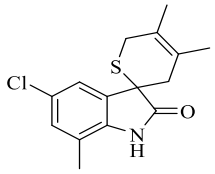
4a*a

4',5'-dimethyl-5-nitro-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 130.5 mg, yield: 90%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.23 (dd, J = 8.6, 2.3 Hz, 1H), 8.09 (d, J = 2.2 Hz, 1H), 7.05 (d, J = 8.6 Hz, 1H), 3.73 (d, J = 16.7 Hz, 1H), 3.13 (d, J = 16.8 Hz, 1H), 2.58 (s, 2H), 1.93 (s, 3H), 1.79 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.3, 145.7, 143.8, 133.3, 126.0, 124.4, 124.2, 119.9, 110.1, 47.4, 37.4, 30.1, 20.6, 19.7; **IR** (neat cm^{-1}): 1721, 1624, 1604, 1523, 1337, 1180, 734; **HRMS**(ESI): calcd. for $C_{14}H_{13}N_2O_3S^-$ [M-H]$^-$ m/z 289.0647, found: 289.0654.



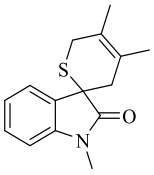
4b*a

4',5,5',7-tetramethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Yellow solid, 127.0 mg, yield: 93%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 6.86 (d, J = 6.7 Hz, 2H), 3.80 (d, J = 16.7 Hz, 1H), 3.04 (d, J = 16.7 Hz, 1H), 2.53 (q, J = 17.6 Hz, 2H), 2.29 (s, 3H), 2.25 (s, 3H), 1.87 (s, 3H), 1.76 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.9, 136.4, 132.2, 131.8, 130.8, 124.6, 123.6, 121.7, 119.3, 47.5, 37.9, 30.2, 21.3, 20.5, 19.6, 16.4； **IR** (neat cm^{-1}): 1699, 1622, 1473, 1180, 1142, 1075; **HRMS**(ESI): calcd. for $C_{16}H_{18}NOS^-$ [M-H]$^-$ m/z 272.1109, found: 272.1123.



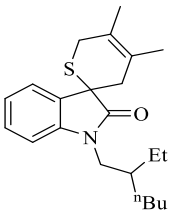
4c*a

5-chloro-4',5',7-trimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. White solid, 133.3 mg, yield: 91%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.04 (d, J = 27.6 Hz, 2H), 3.74 (d, J = 16.6 Hz, 1H), 3.06 (d, J = 16.7 Hz, 1H), 2.51 (s, 2H), 2.24 (s, 3H), 1.87 (s, 3H), 1.76 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.0, 137.3, 133.4, 130.1, 127.9, 124.5, 123.8, 121.6, 121.0, 47.7, 31.0, 30.2, 20.5, 19.6, 16.4; **IR** (neat cm^{-1}): 1709, 1624, 1463, 1307, 1198, 1180, 1142, 1075; **HRMS**(ESI): calcd. for $C_{15}H_{16}ClNOS$: $[M-H]^-$ m/z 292.0563, found: 292.0565.



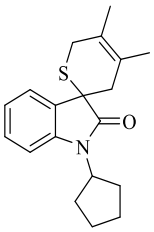
4pa

1,4',5'-trimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. White solid, 107.5 mg, yield: 83%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 (t, J = 7.7 Hz, 1H), 7.22 (d, J = 7.4 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 6.85 (d, J = 7.8 Hz, 1H), 3.78 (d, J = 16.4 Hz, 1H), 3.22 (s, 3H), 3.06 (d, J = 16.8 Hz, 1H), 2.58 – 2.43 (m, 2H), 1.88 (s, 3H), 1.75 (s, 3H); **^{13}C NMR** (126 MHz, CDCl3) δ 176.9, 142.8, 131.8, 129.0, 124.7, 123.7, 123.5, 122.9, 108.4, 46.7, 38.0, 30.3, 26.5, 20.6, 19.7; **IR**(neat cm^{-1}): 2922, 1715, 1610, 1492, 1469, 1372, 1342, 1260, 1086, 752; **HRMS**(ESI): calcd for $C_{15}H_{17}NOS$ $[M+H]+$ m/z 260.1109, found: 260.1106 $[M+H]+$.



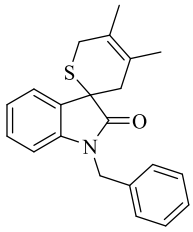
4qa

1-(2-ethylhexyl)-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Colorless oil liquid, 151.8 mg, yield: 85%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 – 7.21 (m, 1H), 7.05 (t, J = 7.5 Hz, 1H), 6.86 (d, J = 7.8 Hz, 1H), 3.80 (d, J = 16.8 Hz, 1H), 3.67 (ddd, J = 13.9, 7.9, 5.9 Hz, 1H), 3.59 – 3.47 (m, 1H), 3.05 (d, J = 16.8 Hz, 1H), 2.53 (q, J = 17.5 Hz, 1H), 1.89 (s, 2H), 1.77 (s, 1H), 1.37 (dtt, J = 12.5, 9.9, 3.8 Hz, 4H), 0.93 (ddd, J = 19.3, 10.8, 5.9 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.1, 142.6, 131.8, 128.8, 124.66 (d, J = 3.03 Hz), 123.67 (d, J = 2.02 Hz), 123.5, 122.5, 108.8, 46.5, 44.0, 37.96 (d, J = 9.09 Hz), 37.45 (d, J = 11.11 Hz), 30.68 (d, J = 10.1 Hz), 30.20 (d, J = 5.05 Hz), 28.69 (d, J = 36.36 Hz), 24.08 (d, J = 9.09 Hz), 23.13 (d, J = 3.03 Hz), 20.5, 19.7, 14.1, 10.73 (d, J = 36.36 Hz); **IR** (neat cm^{-1}): 2958, 1715, 1610, 1487, 1466, 1348, 1178, 751; **HRMS**(ESI): calcd. for $C_{22}H_{31}NOS$: $[M+H]^+$ m/z 358.2205, found: 358.2205.



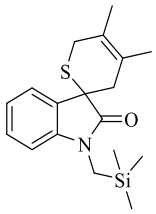
4ra

1-cyclopentyl-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. White solid, 134.6 mg, yield: 86%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.27 – 7.20 (m, 2H), 7.02 (t, J = 7.5 Hz, 1H), 6.93 (d, J = 7.9 Hz, 1H), 3.77 (d, J = 16.7 Hz, 1H), 3.03 (d, J = 16.8 Hz, 1H), 2.58 – 2.44 (m, 2H), 2.12 – 2.02 (m, 2H), 1.93 (dt, J = 14.7, 7.5 Hz, 4H), 1.87 (s, 3H), 1.75 (s, 3H), 1.69 (dd, J = 7.2, 4.2 Hz, 2H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 176.6, 141.2, 132.0, 128.4, 124.6, 123.6, 123.5, 122.2, 109.7, 52.4, 46.4, 38.0, 30.1, 27.7, 27.6, 25.3, 20.4, 19.5; **IR** (neat cm^{-1}): 2958, 1708, 1607, 1483, 1465, 1358, 752; **HRMS**(ESI): calcd. for $C_{19}H_{24}NOS$: $[M+H]^+$ m/z 314.1579, found: 314.1574.



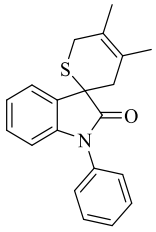
4sa

1-benzyl-4',5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 142.4 mg, yield: 85%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 4H), 7.22 – 7.19 (m, 2H), 7.13 (td, *J* = 7.8, 1.0 Hz, 1H), 6.98 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 4.94 (d, *J* = 15.8 Hz, 1H), 4.80 (d, *J* = 15.8 Hz, 1H), 3.81 (d, *J* = 16.7 Hz, 1H), 3.02 (d, *J* = 16.8 Hz, 1H), 2.58 (d, *J* = 17.5 Hz, 1H), 2.50 (d, *J* = 17.5 Hz, 1H), 1.85 (s, 3H), 1.74 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 176.9, 141.9, 135.9, 131.6, 128.9, 128.9, 127.7, 127.3, 124.7, 124.5, 123.8, 123.6, 123.6, 123.2, 122.9, 109.4, 46.7, 43.7, 37.9, 30.3, 20.6, 19.7; **IR** (neat cm^{-1}): 1721, 1611, 1466, 1348, 1258, 1142, 1076, 801, 751; **HRMS**(ESI): calcd. for $C_{21}H_{22}NOS$: $[M+H]^+$ m/z 336.1422, found: 336.1416.



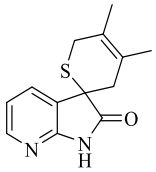
4va

4',5'-dimethyl-1-((trimethylsilyl)methyl)-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. White solid, 142.4 mg, yield: 86%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.16 (ddd, *J* = 7.7, 6.6, 1.0 Hz, 7H), 7.09 (d, *J* = 7.3 Hz, 6H), 6.90 (t, *J* = 7.5 Hz, 6H), 6.67 (d, *J* = 7.8 Hz, 6H), 3.65 (d, *J* = 16.8 Hz, 6H), 3.18 (d, *J* = 15.4 Hz, 6H), 3.01 (d, *J* = 15.4 Hz, 6H), 2.94 (d, *J* = 16.8 Hz, 6H), 2.06 (s, 1H), 1.76 (s, 18H), 1.63 (s, 18H), -0.00 (s, 52H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 176.2, 143.1, 132.1, 128.7, 124.8, 123.7, 123.3, 122.3, 108.7, 46.5, 37.9, 31.3, 30.2, 20.5, 19.7, -1.3; **IR** (neat cm^{-1}): 1704, 1609, 1196, 1180, 1142, 1075, 848; **HRMS**(ESI): calcd. for $C_{18}H_{26}NOSSi$: $[M+H]^+$ m/z 332.1504, found: 332.1500.



4wa

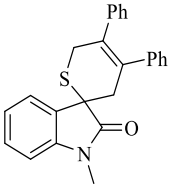
4',5'-dimethyl-1-phenyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 134.9 mg, yield: 84%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 10.7, 4.6 Hz, 2H), 7.44 (t, *J* = 4.3 Hz, 2H), 7.41 – 7.35 (m, 1H), 7.30 (dd, *J* = 7.4, 0.7 Hz, 1H), 7.23 (td, *J* = 8.2, 1.6 Hz, 1H), 7.10 (dd, *J* = 10.9, 4.1 Hz, 1H), 6.86 (d, *J* = 7.9 Hz, 1H), 3.85 (d, *J* = 16.8 Hz, 1H), 3.04 (d, *J* = 16.8 Hz, 1H), 2.71 (d, *J* = 17.5 Hz, 1H), 2.58 (d, *J* = 17.5 Hz, 1H), 1.87 (s, 3H), 1.78 (s, 3H)； **^{13}C NMR** (151 MHz, $CDCl_3$) δ 175.9, 142.7, 134.4, 131.3, 129.6, 128.9, 128.1, 126.6, 124.4, 123.8, 123.8, 123.3, 109.7, 46.6, 38.1, 30.4, 20.5, 19.6； **IR** (neat cm^{-1}): 1721, 1670, 1594, 1499, 1465 ,1369, 1323, 1164, 752; **HRMS**(ESI): calcd. for $C_{20}H_{19}BNOS$: $[M+H]^+$ m/z 322.1266, found: 322.1270..



4d*a

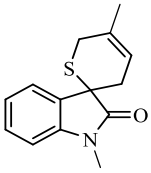
4',5'-dimethyl-3',6'-dihydrospiro[pyrrolo[2,3-b]pyridine-3,2'-thiopyran]-2(1H)-one. Pale yellow solid, 110.7 mg, yield: 90%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.22 – 8.17 (m, 2H), 7.44 (dd, *J* = 7.4, 1.4 Hz, 2H), 6.97 (td, *J* = 7.6, 3.7 Hz, 2H), 3.71

(d, *J* = 16.8 Hz, 2H), 3.09 (t, *J* = 16.5 Hz, 2H), 2.62 (d, *J* = 17.3 Hz, 2H), 2.49 (d, *J* = 17.3 Hz, 2H), 1.92 – 1.85 (m, 7H), 1.76 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 177.4, 155.5, 146.9, 131.6, 127.2, 124.7, 123.9, 118.4, 47.2, 37.4, 30.2, 20.5, 19.7; **IR** (neat cm^{-1}): 1731, 1606, 1519, 1471, 1435 ,1216, 1110, 778; **HRMS**(ESI): calcd. for $C_{13}H_{13}N_2OS$: $[M+H]^+$ m/z 245.0749, found: 245.0756.



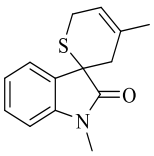
4pb

1-methyl-4',5'-diphenyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 160.9 mg, yield: 84%. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.41 – 7.29 (m, 2H), 7.09 (dtd, *J* = 21.5, 14.7, 7.7 Hz, 11H), 6.90 (d, *J* = 7.8 Hz, 1H), 4.24 (d, *J* = 17.0 Hz, 1H), 3.59 (d, *J* = 17.0 Hz, 1H), 3.28 (s, 3H), 3.12 – 2.93 (m, 2H); **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 176.8, 142.9, 142.7, 142.1, 134.0, 133.7, 131.4, 129.3, 129.3, 129.2, 128.1, 127.9, 126.7, 126.5, 123.8, 123.0, 108.5, 47.2, 39.1, 31.1, 26.6; **IR** (neat cm^{-1}): 1712, 1611, 1491, 1470, 1442, 1418, 1371, 1344, 1180, 752; **HRMS**(ESI): calcd. for $C_{25}H_{22}NOS$: $[M+H]^+$ m/z 384.1422, found: 384.1413.



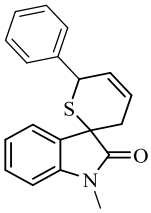
4pc

1,5'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.43 – 7.12 (m, 2H), 7.06 (tdd, *J* = 7.6, 2.1, 1.0 Hz, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 5.66 (ddd, *J* = 4.7, 3.1, 1.6 Hz, 1H), 3.82 – 3.71 (m, 1H), 3.22 (s, 3H), 3.02 (d, *J* = 16.8 Hz, 1H),2.62 (m, 3H),1.90 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 176.7, 142.9, 131.3, 131.0, 129.1, 123.5, 122.8, 119.5, 108.4, 44.9, 32.2, 28.8, 26.4, 24.5; **HRMS**(ESI): calcd. for $C_{14}H_{15}NOS$: $[M+H]^+$ m/z 246.0953, found: 246.0952.



4pc′

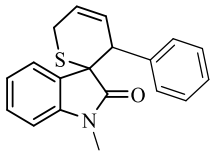
1,4'-dimethyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.43 – 7.12 (m, 2H), 7.06 (tdd, *J* = 7.6, 2.1, 1.0 Hz, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 5.86 (ddd, *J* = 4.9, 3.2, 1.6 Hz, 1H), 3.76 (d, *J* = 1.0 Hz, 1H), 3.22 (s, *J* = 1.2 Hz, 3H), 3.16 (m, 1H), 3.00 (s, 1H), 2.45 (t, *J* = 14.8 Hz, 2H), 1.81 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 176.5, 142.7, 132.5, 131.4, 128.9, 123.4, 122.8, 117.8, 108.2, 46.1, 35.8, 26.3, 25.2, 24.8; **HRMS**(ESI): calcd. for $C_{14}H_{15}NOS$: $[M+H]^+$ m/z 246.0953, found: 246.0952.



4pd

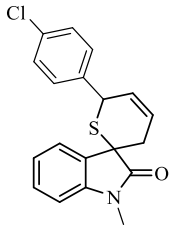
1-methyl-6'-phenyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 84.5 mg, yield: 55%. **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.47 (d, *J* = 7.3 Hz, 1H), 7.26 (dd, *J* = 14.2, 6.6 Hz, 1H), 7.19 – 6.99 (m, 4H), 6.91 (d, *J* = 6.9 Hz, 2H), 6.56 (d, *J* = 7.7 Hz, 1H), 6.34 – 6.17 (m, 1H), 5.99 (d, *J* = 10.9 Hz, 1H), 4.29 (t, *J* = 15.3 Hz, 1H), 4.24 (s, 1H), 3.21 – 3.05 (m, 1H), 2.86 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) *δ* 174.8, 143.3, 138.3, 129.4, 129.2, 129.2, 127.7, 127.1, 124.8, 123.8,

122.5, 107.9, 49.0, 48.2, 25.8, 25.1; **IR** (neat cm^{-1}): 3446, 1708, 1611, 1493, 1470, 1373, 1180, 1142, 753; **HRMS**(ESI): calcd. for $C_{19}H_{17}NNaOS$: $[M+Na]^+$ m/z 330.0929, found: 330.0929.



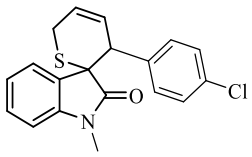
4pd′

1-methyl-3'-phenyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 53.7 mg, yield: 35%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.16 (tt, J = 7.4, 3.7 Hz, 1H), 7.14 – 7.09 (m, 3H), 7.07 – 7.02 (m, 2H), 6.88 – 6.83 (m, 1H), 6.72 (d, J = 7.4 Hz, 1H), 6.65 (d, J = 7.8 Hz, 1H), 6.32 – 6.21 (m, 1H), 6.10 – 6.04 (m, 1H), 4.22 – 4.07 (m, 1H), 3.66 (tt, J = 36.1, 18.0 Hz, 1H), 3.56 (dd, J = 17.9, 1.2 Hz, 1H), 3.10 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 175.5, 142.5, 139.0, 130.5, 130.1, 129.7, 127.7, 127.3, 125.2, 124.4, 122.2, 108.2, 50.9, 45.9, 26.5, 25.1; **IR** (neat cm^{-1}): 3441, 1710, 1609, 1491, 1470, 1372, 1180, 1141, 753; **HRMS**(ESI): calcd. for $C_{19}H_{17}NNaOS$: $[M+Na]^+$ m/z 330.0929, found: 330.0930.



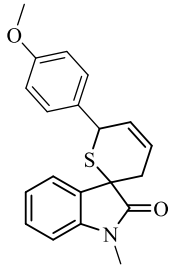
4pe

6'-(4-chlorophenyl)-1-methyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 104.0 mg, yield: 61%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.41 (d, J = 7.3 Hz, 1H), 7.23 (t, J = 7.7 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 6.99 (d, J = 8.4 Hz, 1H), 6.82 (d, J = 8.4 Hz, 1H), 6.57 (d, J = 7.7 Hz, 1H), 6.28 – 6.17 (m, 1H), 5.88 (d, J = 10.9 Hz, 1H), 4.25 (d, J = 17.4 Hz, 1H), 4.18 (s, 1H), 3.14 – 3.01 (m, 1H), 2.87 (s, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.5, 143.1, 136.9, 132.9, 130.7, 129.3, 128.8, 128.5, 127.8, 125.1, 123.6, 122.5, 48.7, 47.3, 25.8, 25.0; **IR** (neat cm^{-1}): 3446, 1712, 1605, 1490, 1470, 1409, 1372, 1193, 1180, 1142, 1076, 753; **HRMS**(ESI): calcd. for $C_{19}H_{17}ClNOS$: $[M+H]^+$ m/z 342.0719, found: 342.0715.



4pe′

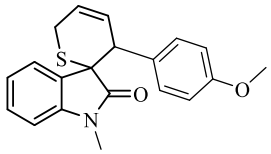
3'-(4-chlorophenyl)-1-methyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 52.9 mg, yield: 31%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.18 (td, J = 7.7, 1.1 Hz, 1H), 7.07 (d, J = 8.5 Hz, 2H), 6.97 (d, J = 8.4 Hz, 2H), 6.89 (td, J = 7.6, 0.8 Hz, 1H), 6.80 (d, J = 7.2 Hz, 1H), 6.68 (d, J = 7.7 Hz, 1H), 6.32 – 6.24 (m, 1H), 6.02 (dd, J = 10.8, 2.9 Hz, 1H), 4.19 (d, J = 23.6 Hz, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 175.17, 142.46, 137.57, 133.15, 131.36, 130.07, 129.44, 128.75, 127.91, 125.01, 124.84, 122.36, 108.44, 50.79, 45.36, 26.53, 25.11; **IR** (neat cm^{-1}): 3444, 1709, 1609, 1490, 1470, 1409, 1372, 1180, 1142, 1076, 753; **HRMS**(ESI): calcd. for $C_{19}H_{17}ClNOS$: $[M+H]^+$ m/z 342.0719, found: 342.0712.



4pf

6'-(4-methoxyphenyl)-1-methyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 97.4 mg, yield: 76%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.3 Hz, 1H), 7.26 (d, J = 6.6 Hz, 1H), 7.12 (t, J = 7.5 Hz, 1H), 6.82 (d, J =

8.7 Hz, 2H), 6.58 (d, J = 8.6 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.0, 158.6, 143.4, 130.5, 130.5, 129.6, 129.4, 129.2, 124.7, 123.8, 122.5, 113.1, 108.0, 55.2, 49.0, 47.3, 25.9, 25.1; **IR** (neat cm^{-1}): 3445, 1635, 1609, 1510, 1257, 1180, 1142; **HRMS**(ESI): calcd. for $C_{20}H_{19}NnaO_2S$: $[M+Na]^+$ m/z 360.1034, found: 360.1026.



4pf′

3'-(4-methoxyphenyl)-1-methyl-3',6'-dihydrospiro[indoline-3,2'-thiopyran]-2-one. Pale yellow solid, 16.7 mg, yield: 13%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 – 7.11 (m, 1H), 6.96 (d, J = 8.6 Hz, 2H), 6.87 (t, J = 7.6 Hz, 1H), 6.75 (d, J = 7.5 Hz, 1H), 6.65 (t, J = 9.2 Hz, 3H), 6.25 (ddd, J = 10.6, 6.5, 3.8 Hz, 1H), 6.05 (dd, J = 10.9, 2.9 Hz, 1H), 4.11 (dd, J = 7.4, 4.8 Hz, 1H), 3.72 (s, 3H), 3.66 (ddd, J = 8.5, 4.4, 2.1 Hz, 1H), 3.58 – 3.48 (m, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6, 158.8, 142.6, 131.2, 131.2, 130.8, 129.9, 128.5, 125.3, 124.2, 122.2, 113.1, 108.2, 55.3, 51.0, 45.1, 26.5, 25.2; **IR** (neat cm^{-1}): 3445, 1709, 1609, 1491, 1470, 1372, 1180, 1142, 753; **HRMS**(ESI): calcd. for $C_{20}H_{19}NnaO_2S$: $[M+Na]^+$ m/z 360.1034, found: 360.1028.

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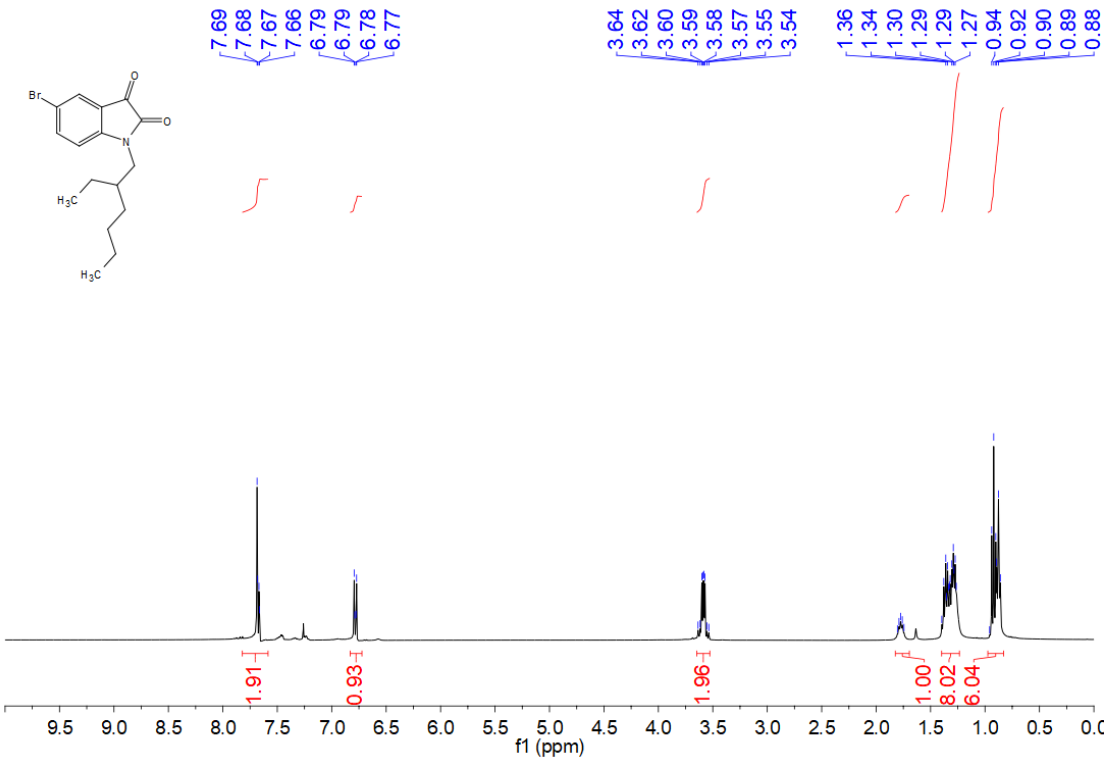
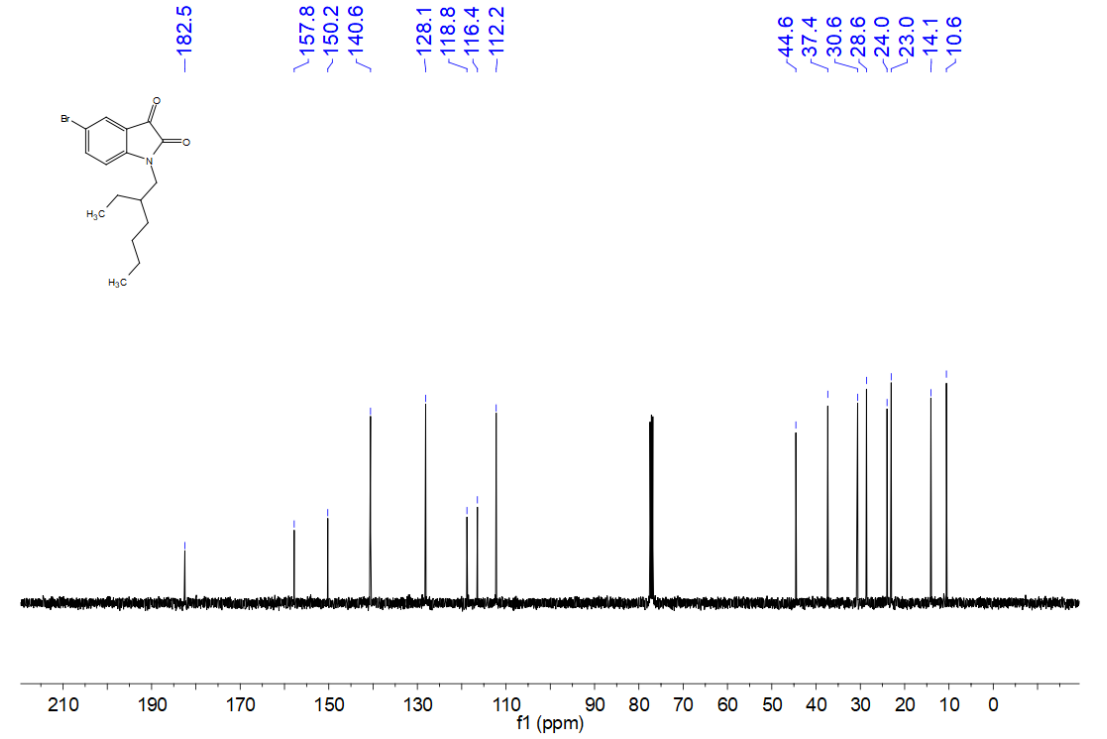
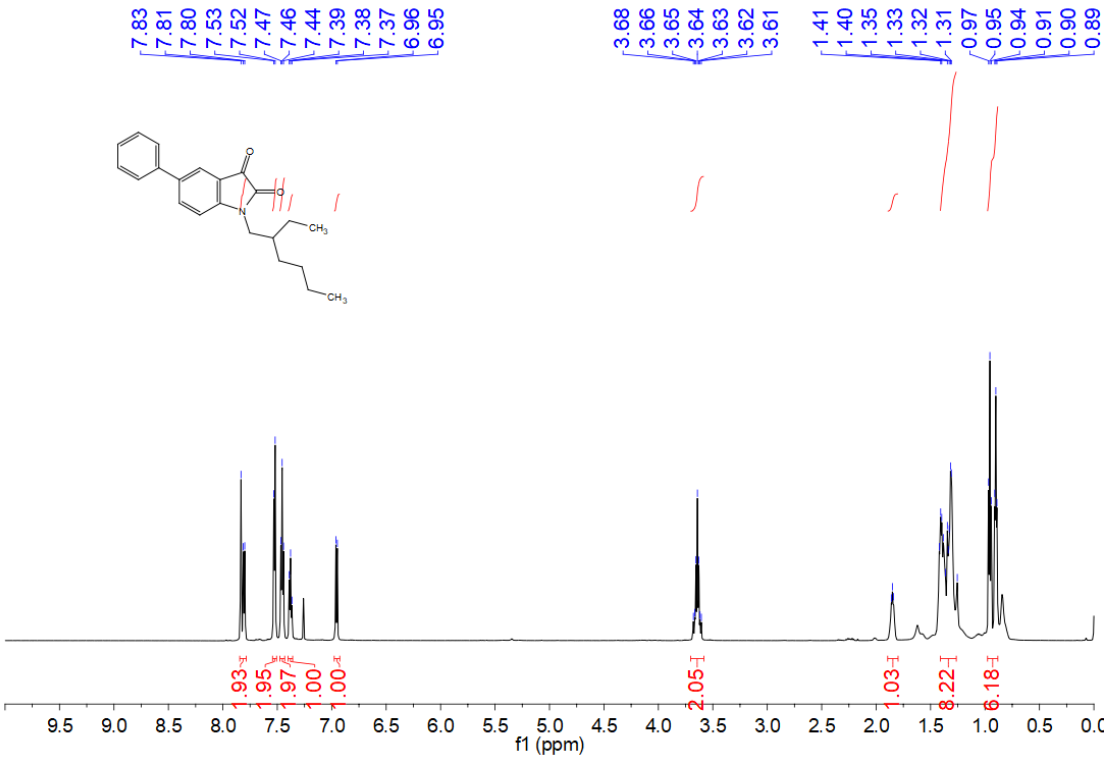
11. NMR spectra



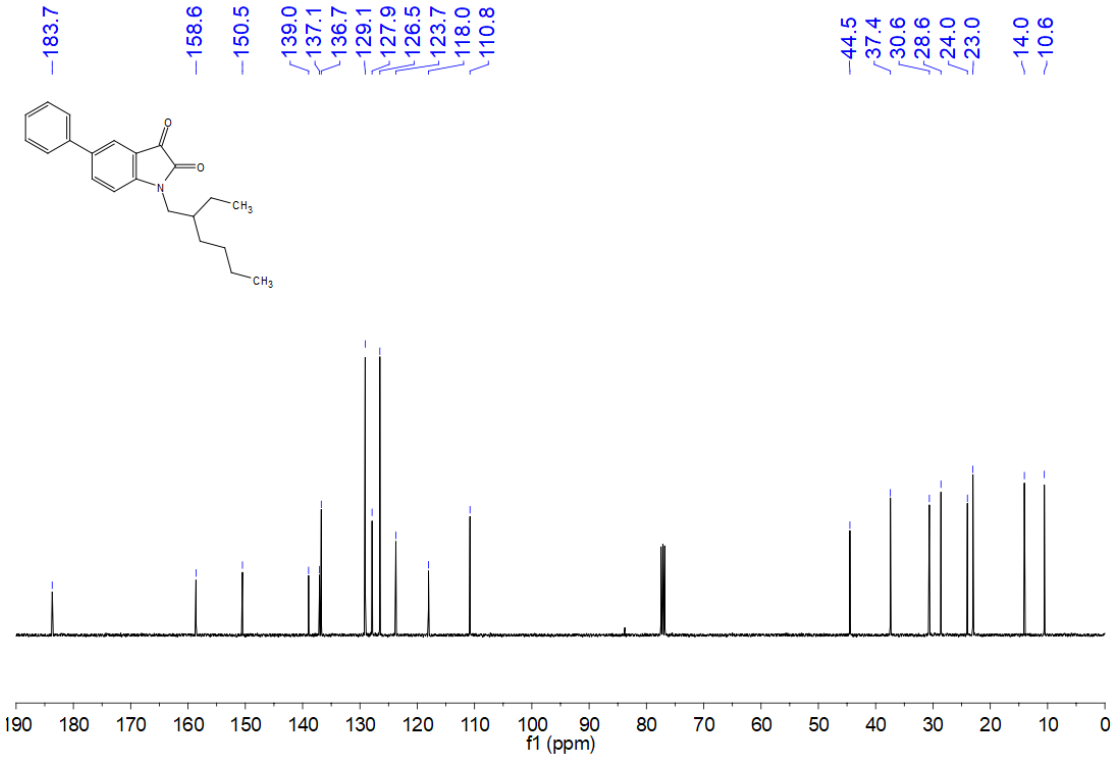
^{1}H NMR spectrum of *N*-(2-ethylhexyl)-5-bromoisatin (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of *N*-(2-ethylhexyl)-5-bromoisatin (101 MHz, $CDCl_3$)



^{1}H NMR spectrum of 1i (600 MHz, $CDCl_3$)



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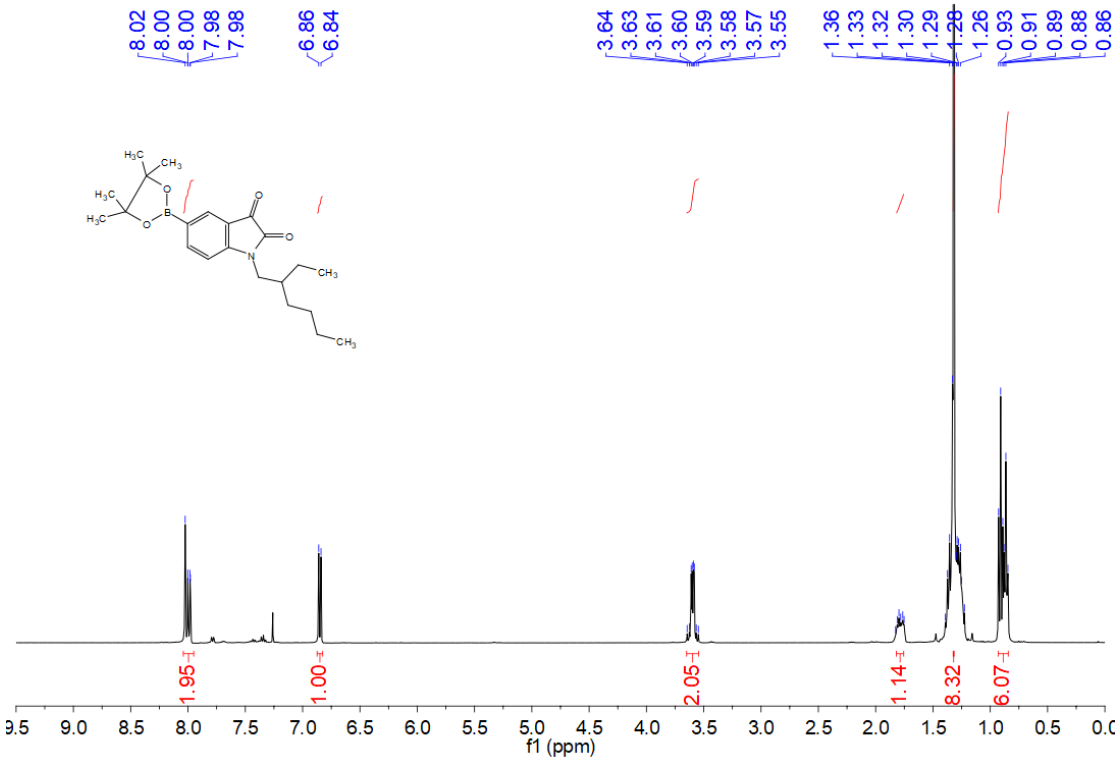

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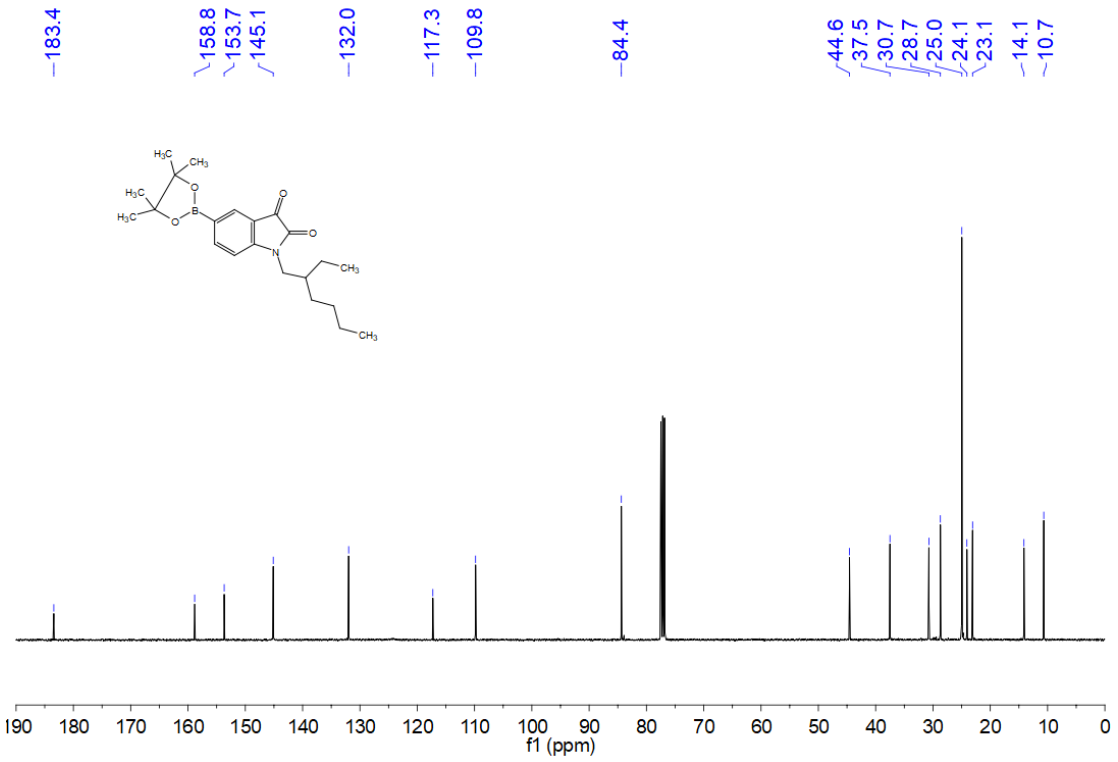

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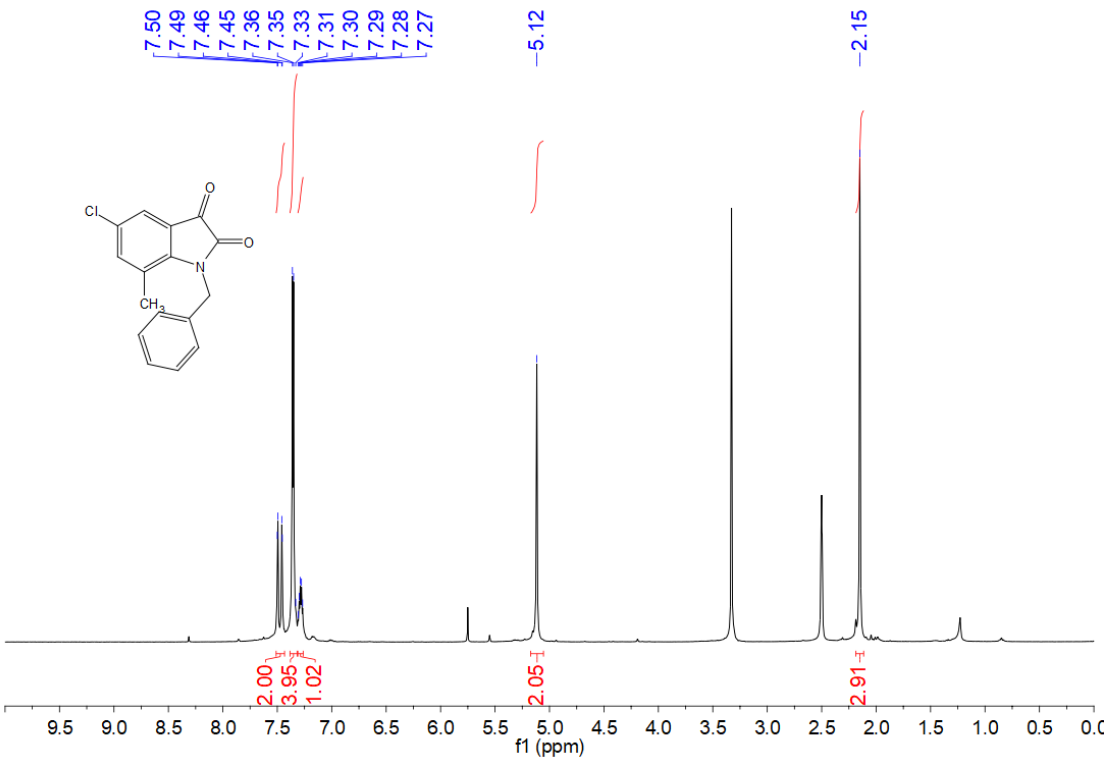
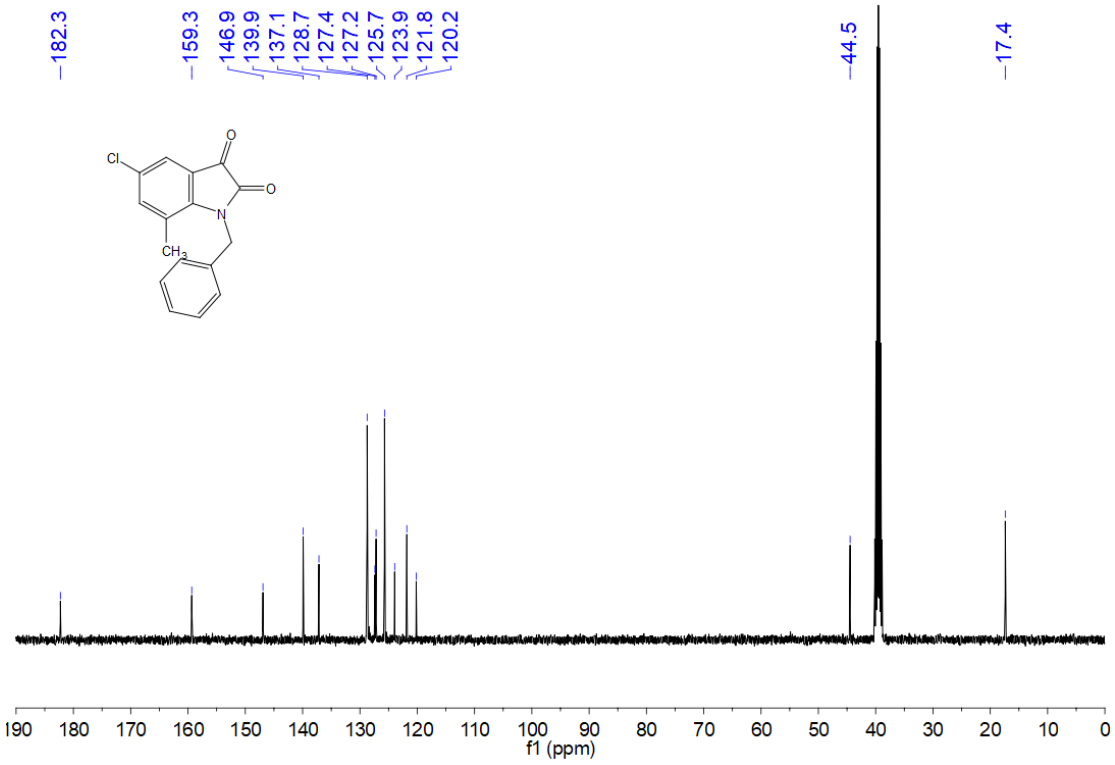
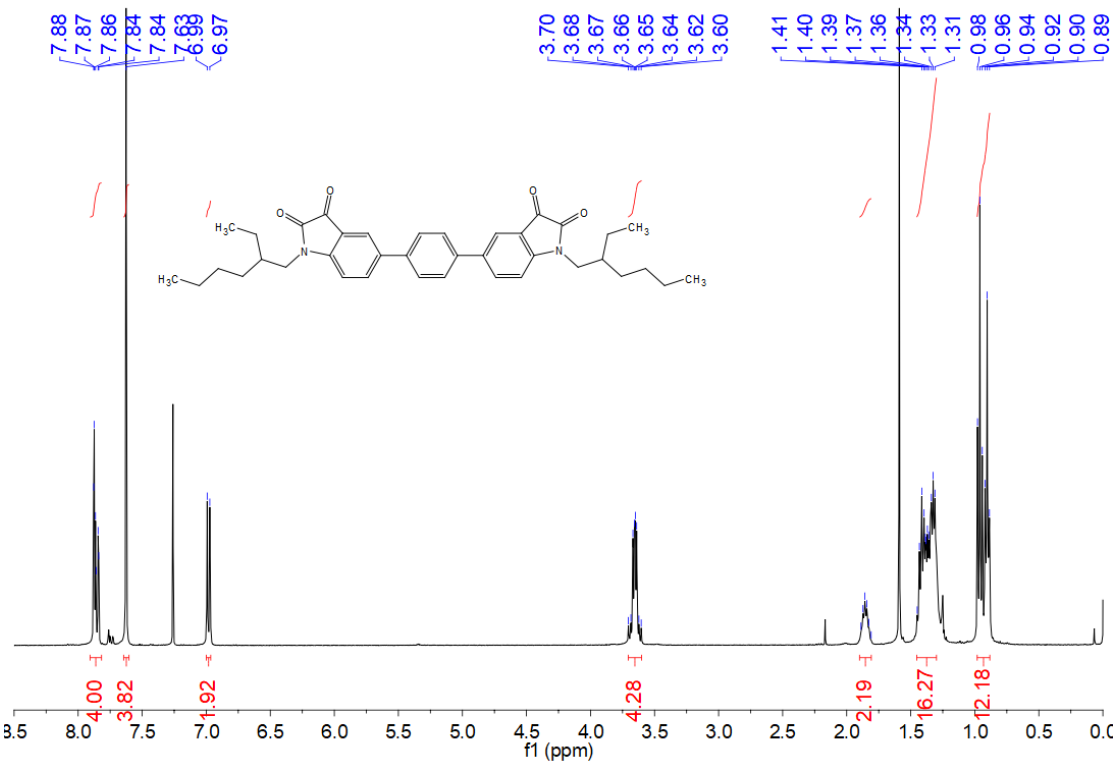


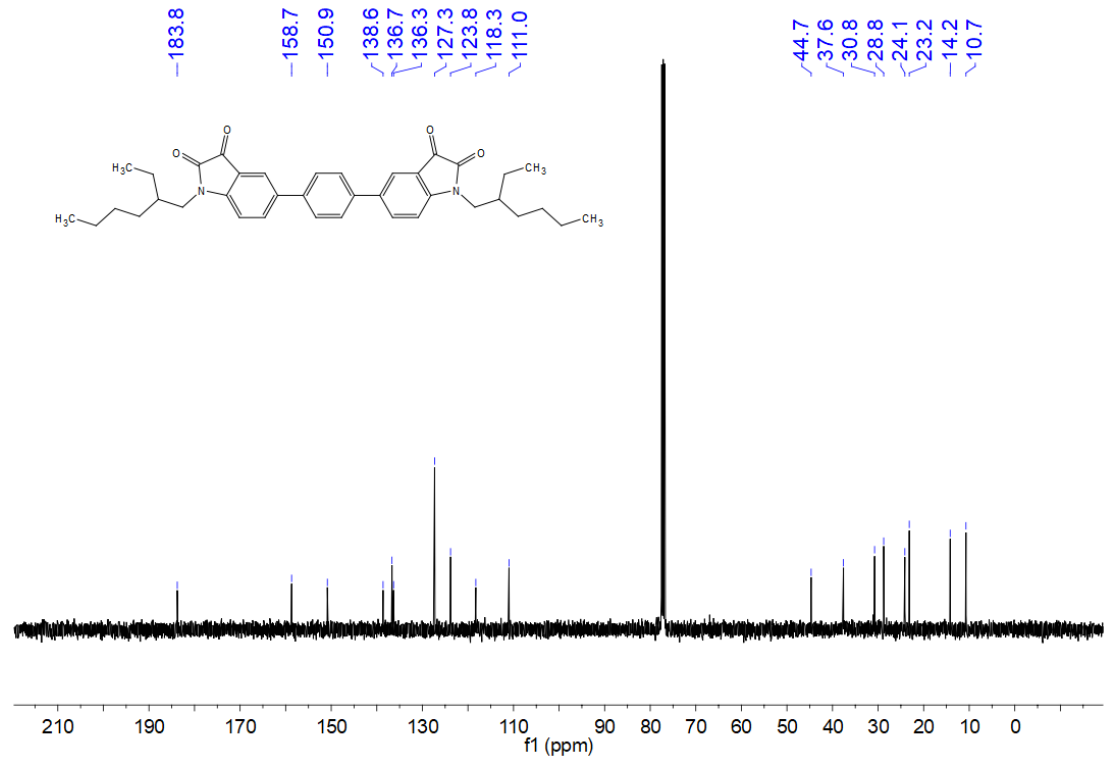
^{1}H NMR spectrum of 1o (400 MHz, $CDCl_3$)



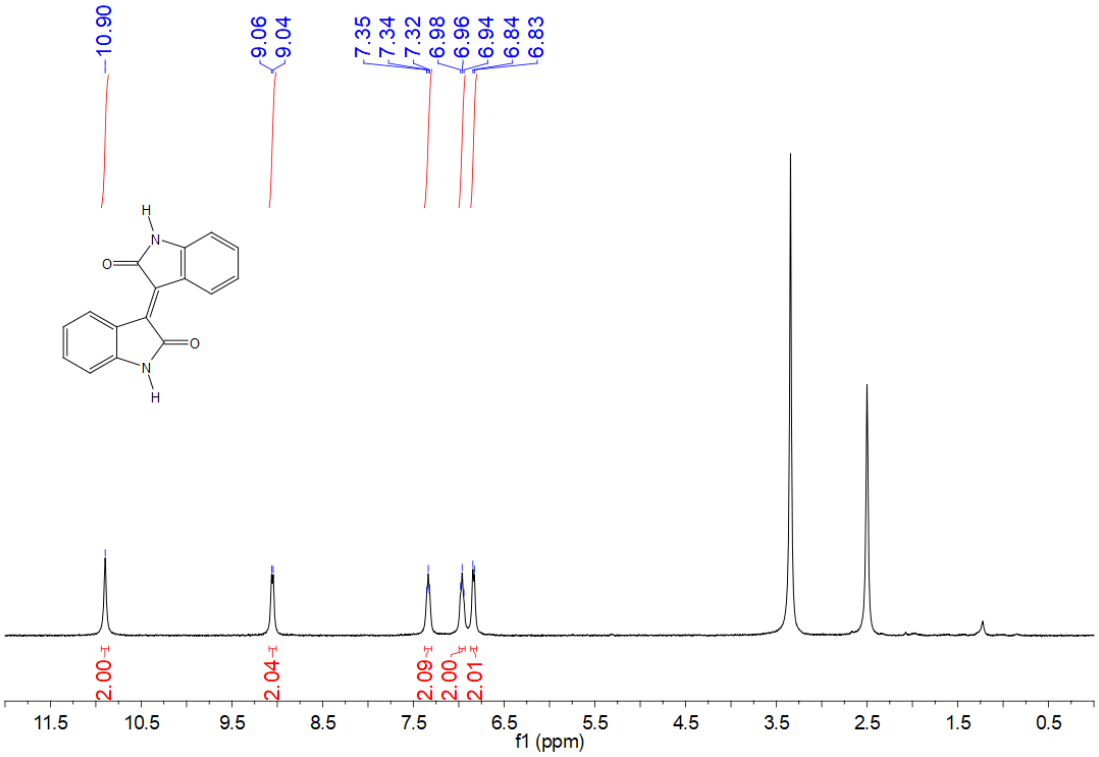
^{13}C NMR spectrum of 1o (101 MHz, $CDCl_3$)



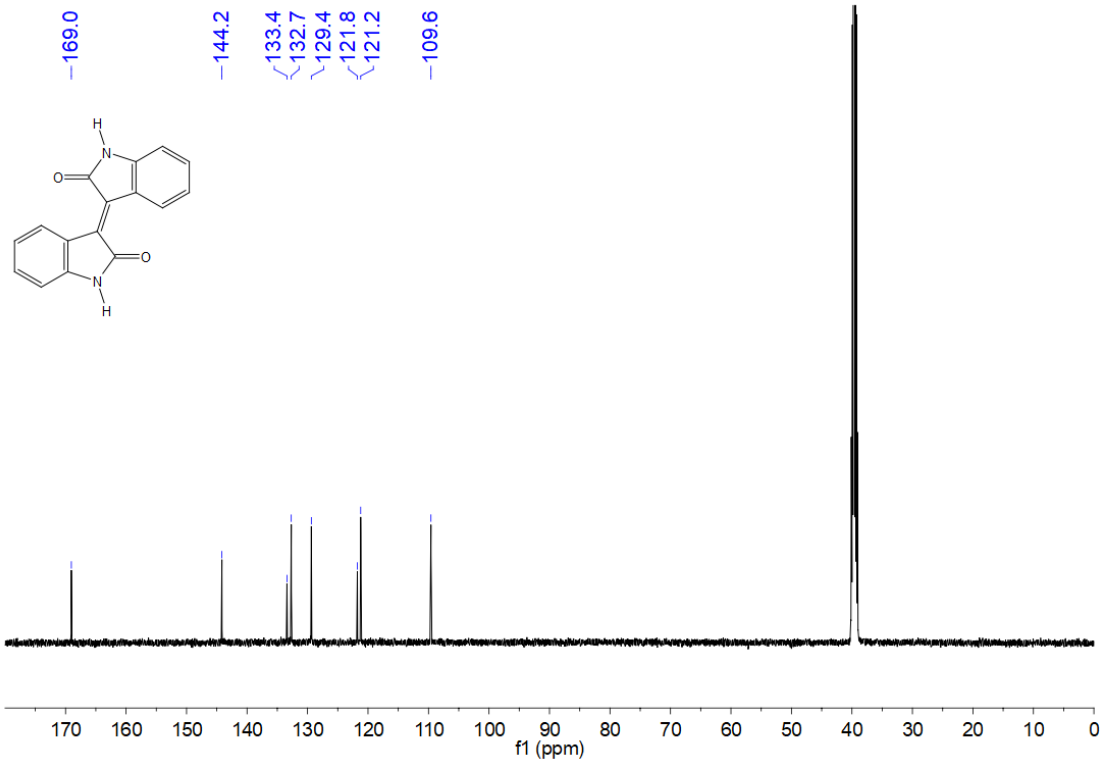
^{1}H NMR spectrum of isatin-based monomer (400 MHz, $CDCl_3$)



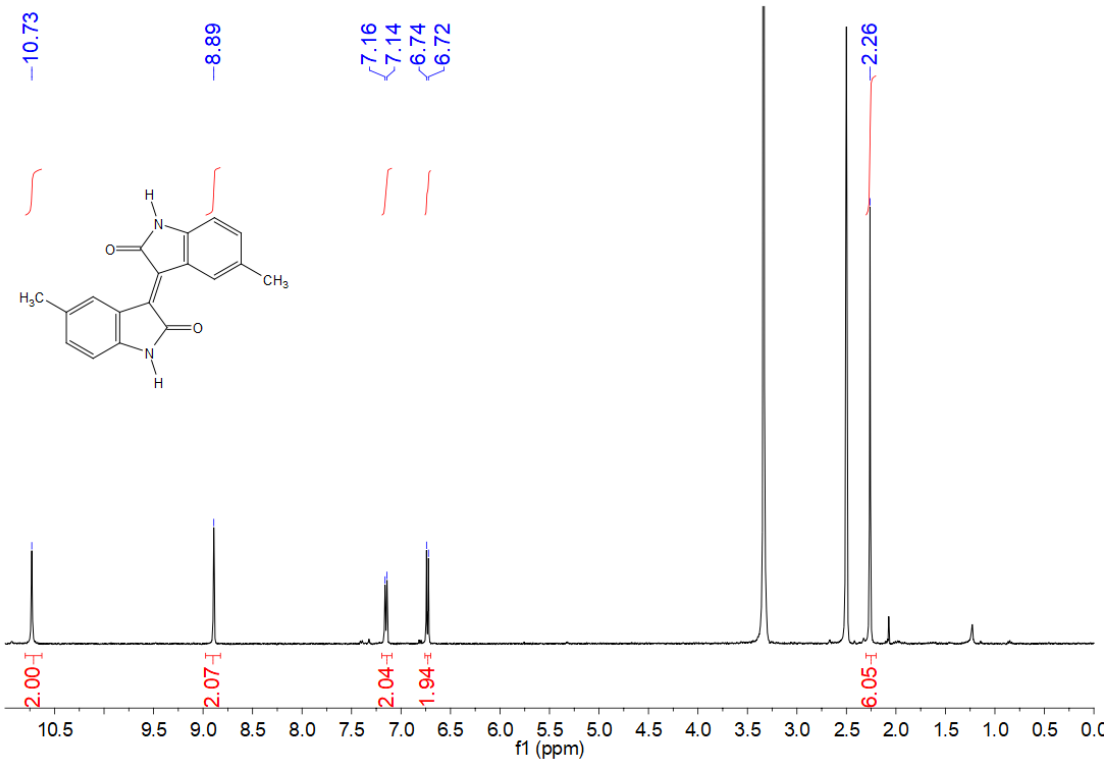
^{13}C NMR spectrum of isatin-based monomer (101 MHz, $CDCl_3$)



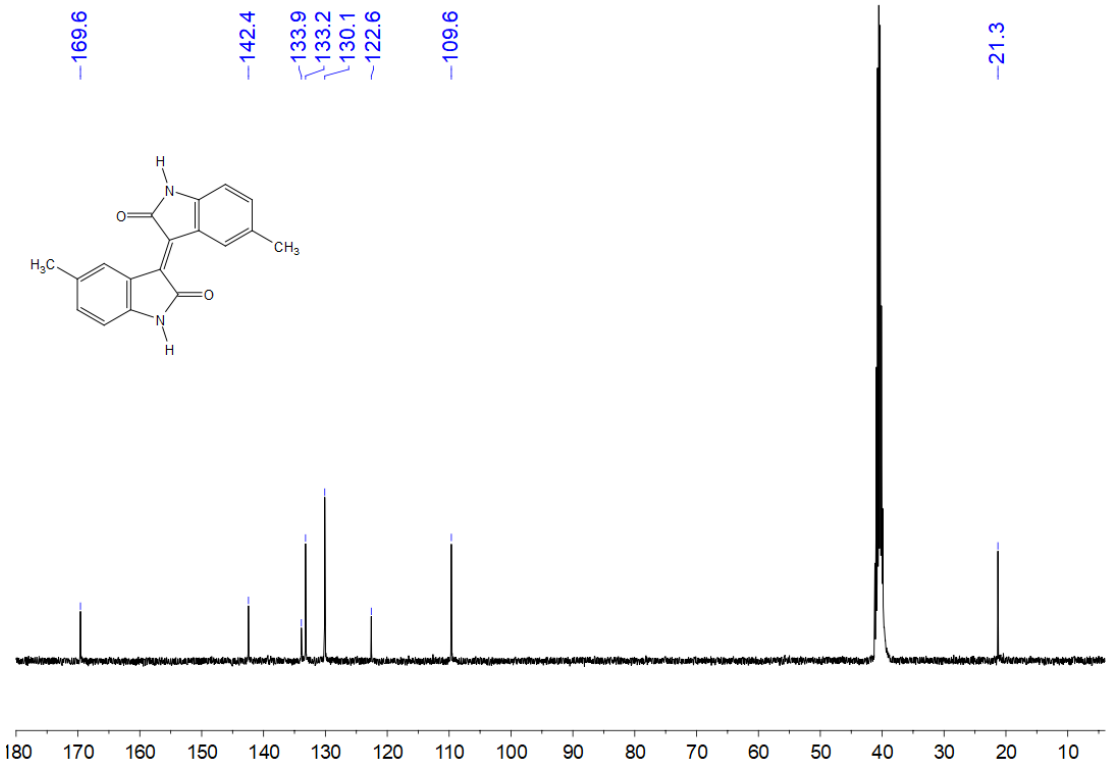
^{1}H NMR spectrum of 3a (400 MHz, DMSO-d_6)



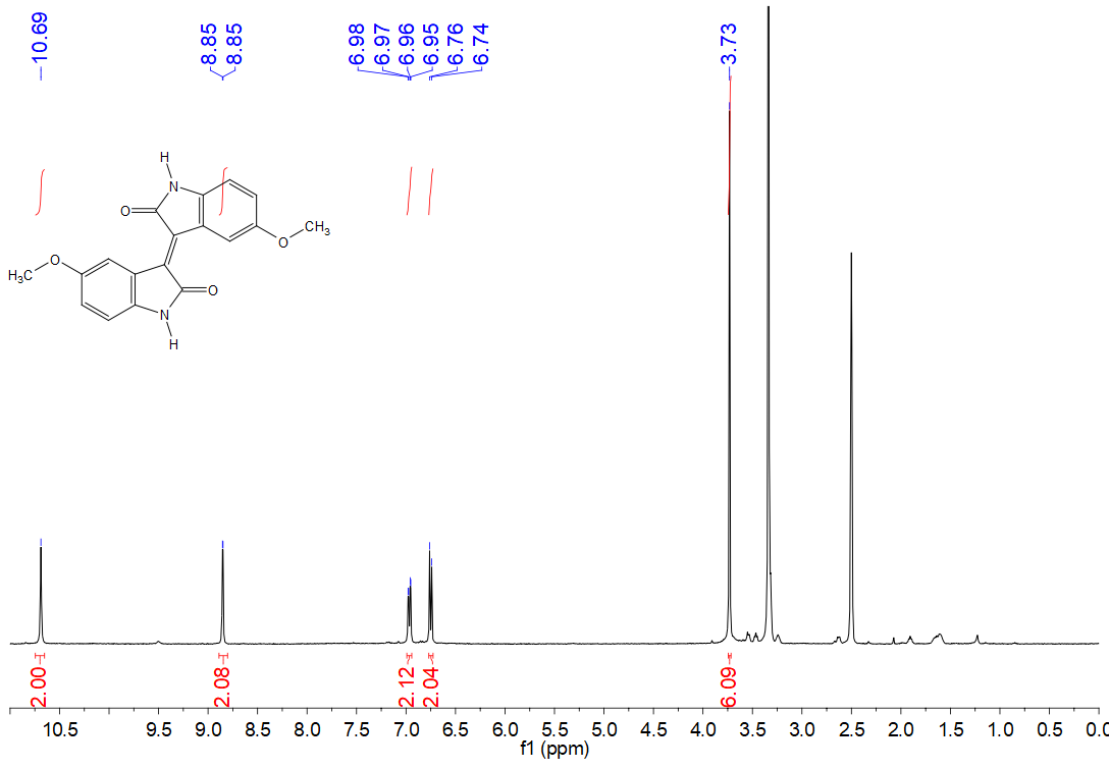
^{13}C NMR spectrum of 3a (126 MHz, DMSO-d_6)



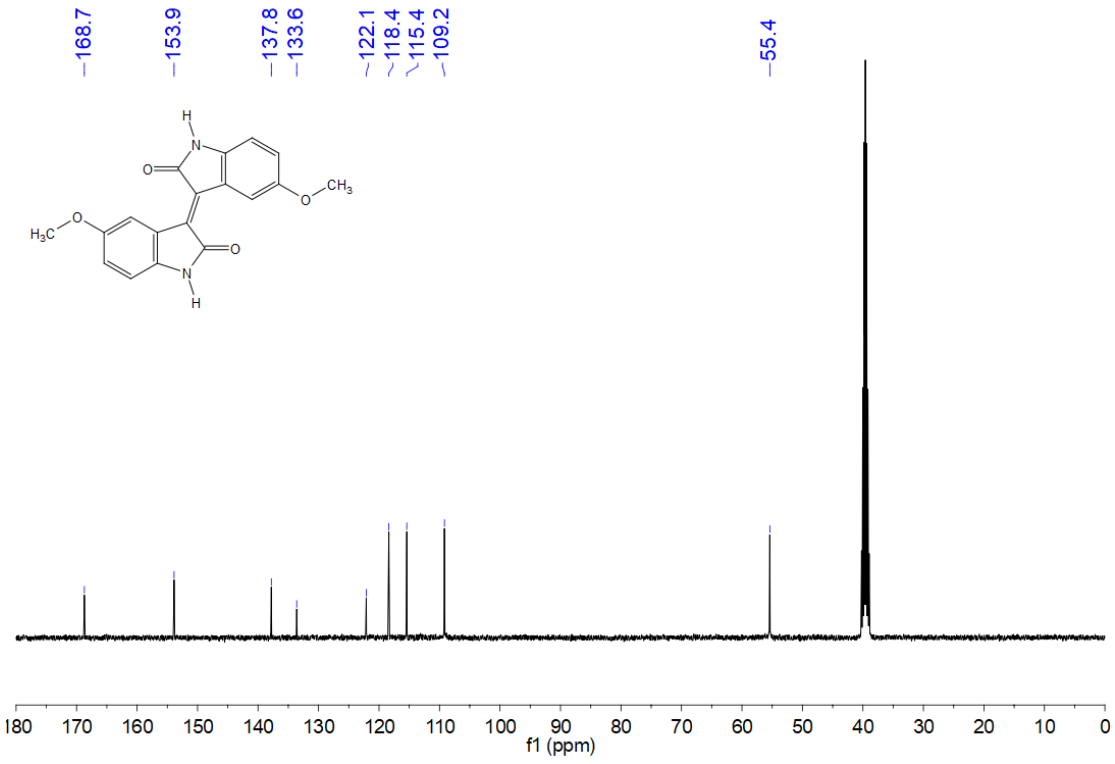
^{1}H NMR spectrum of 3b (400 MHz, DMSO-d_6)



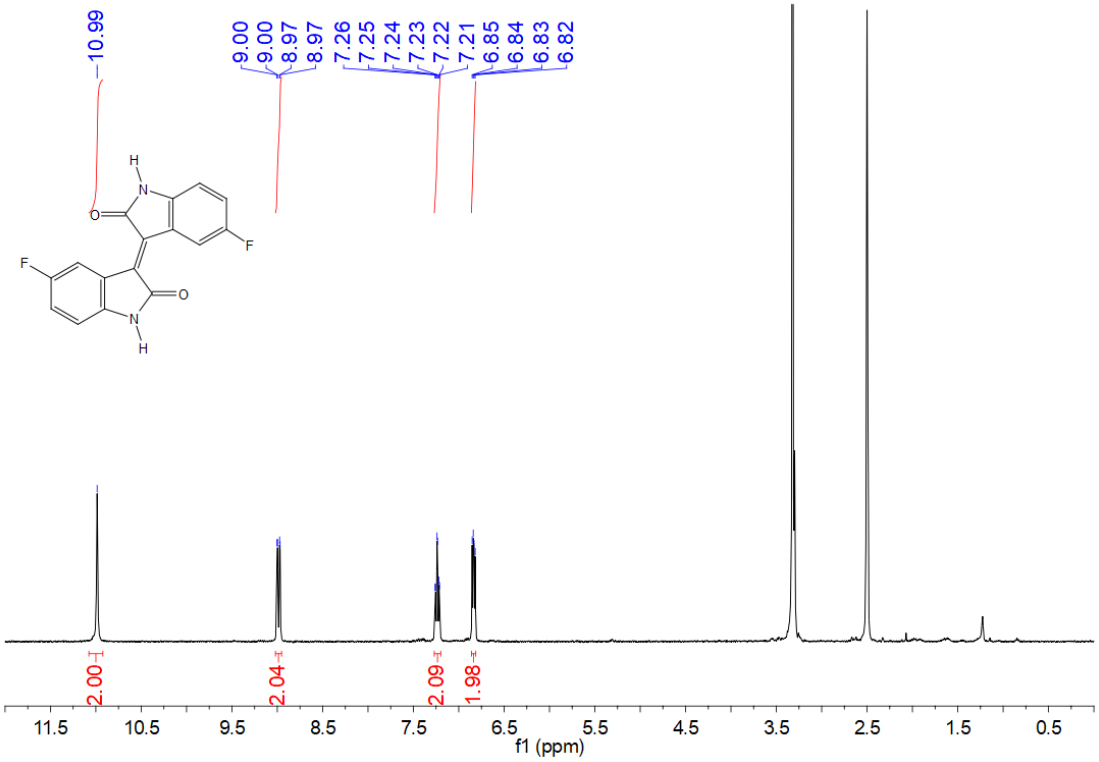
^{13}C NMR spectrum of 3b (101 MHz, DMSO-d_6)



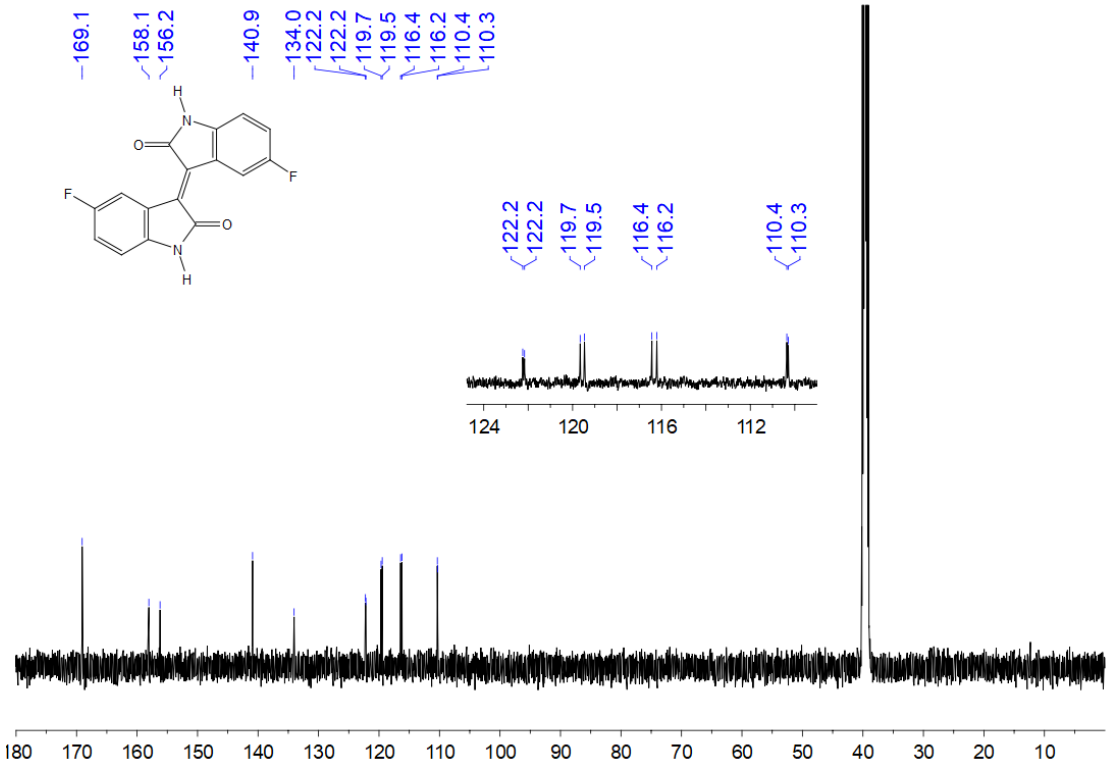
^{1}H NMR spectrum of 3c (400 MHz, DMSO-d_6)



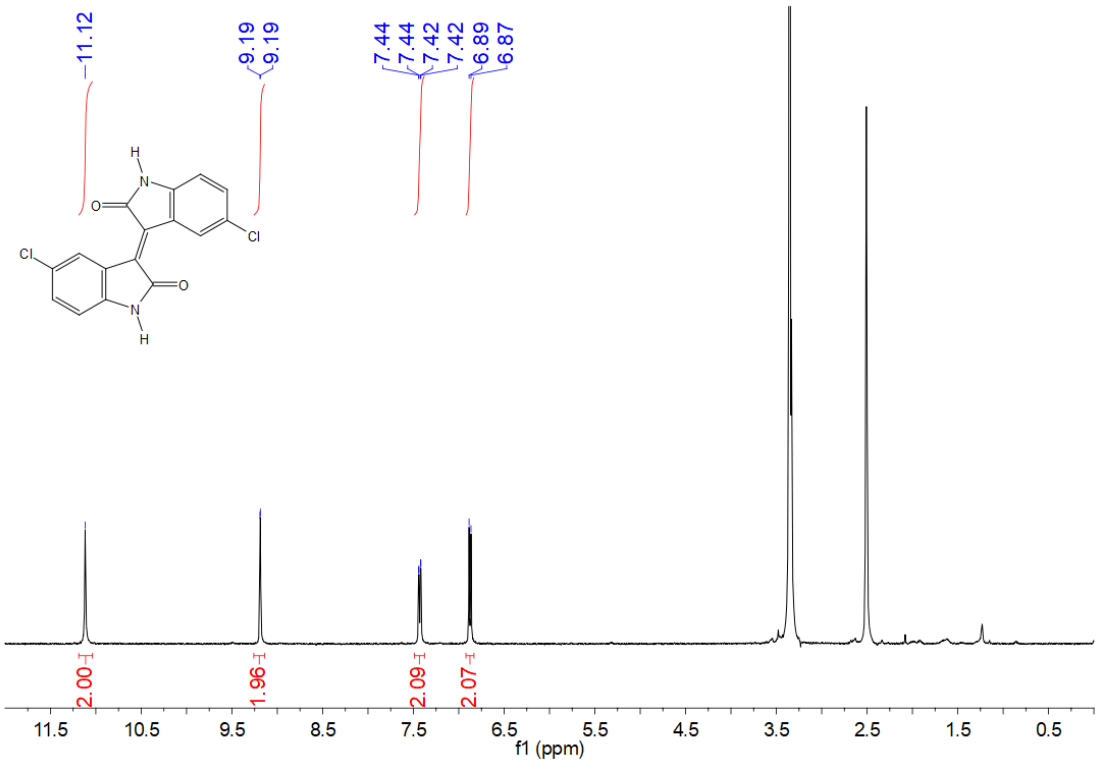
^{13}C NMR spectrum of 3c (101 MHz, DMSO-d_6)



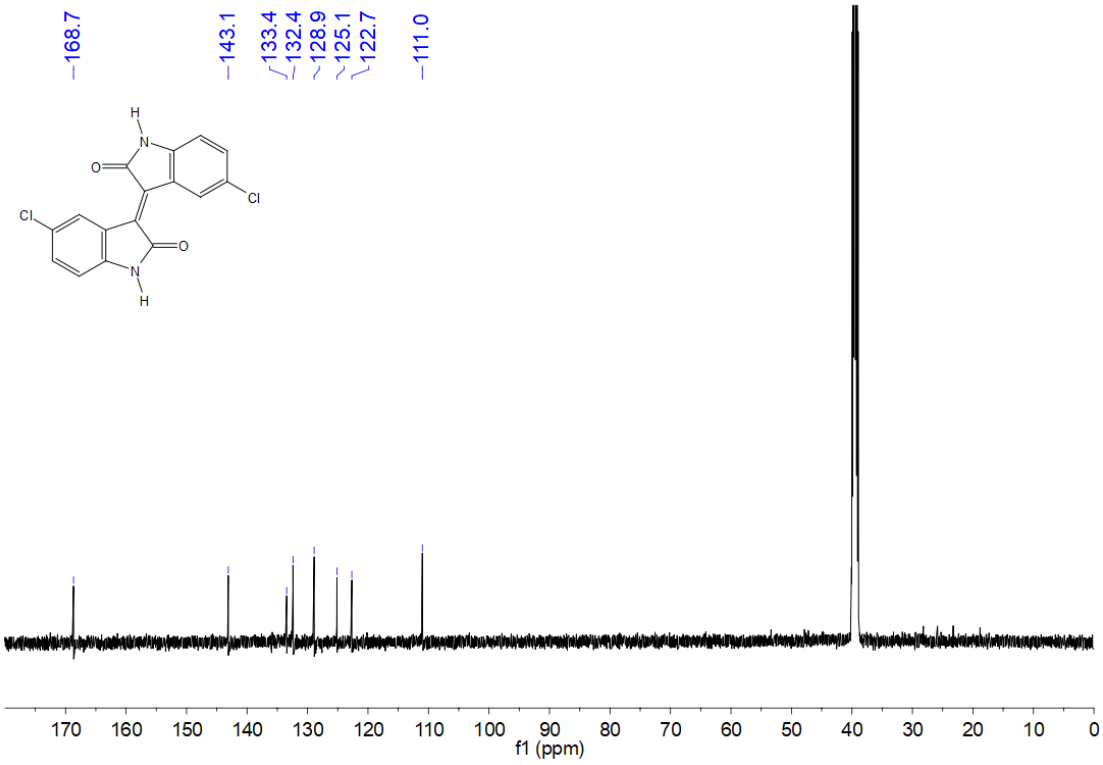
^{1}H NMR spectrum of 3d (400 MHz, DMSO-d_6)



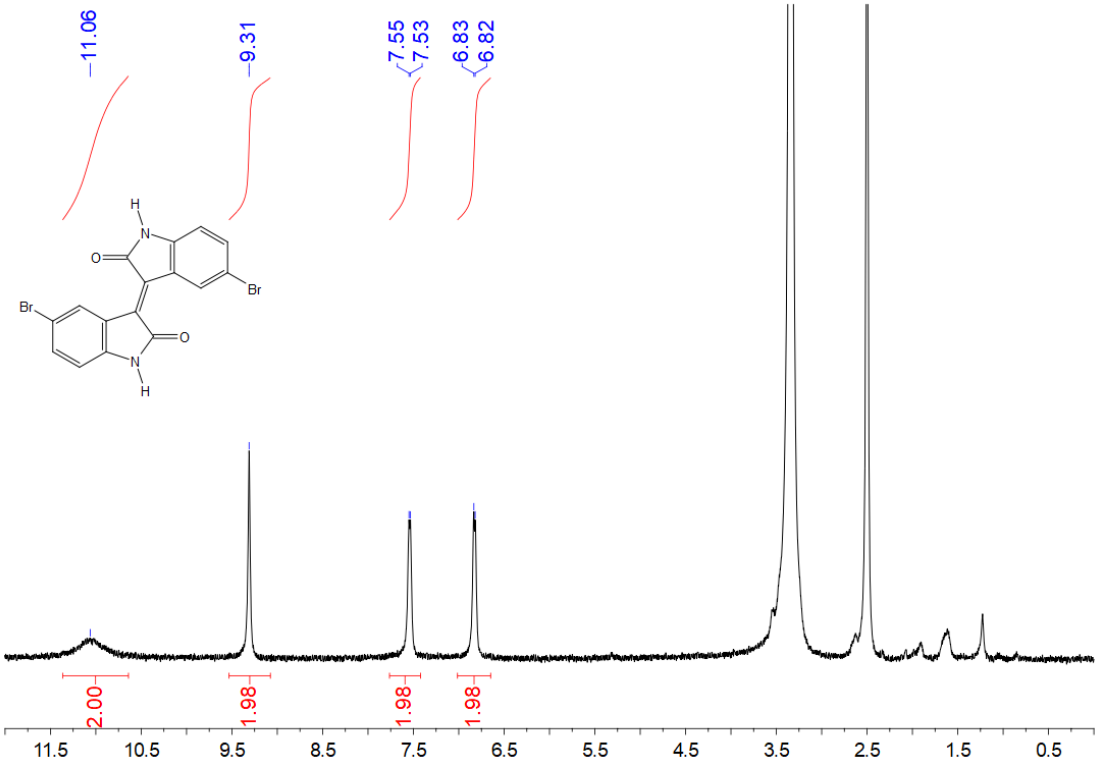
^{13}C NMR spectrum of 3d (126 MHz, DMSO-d_6)



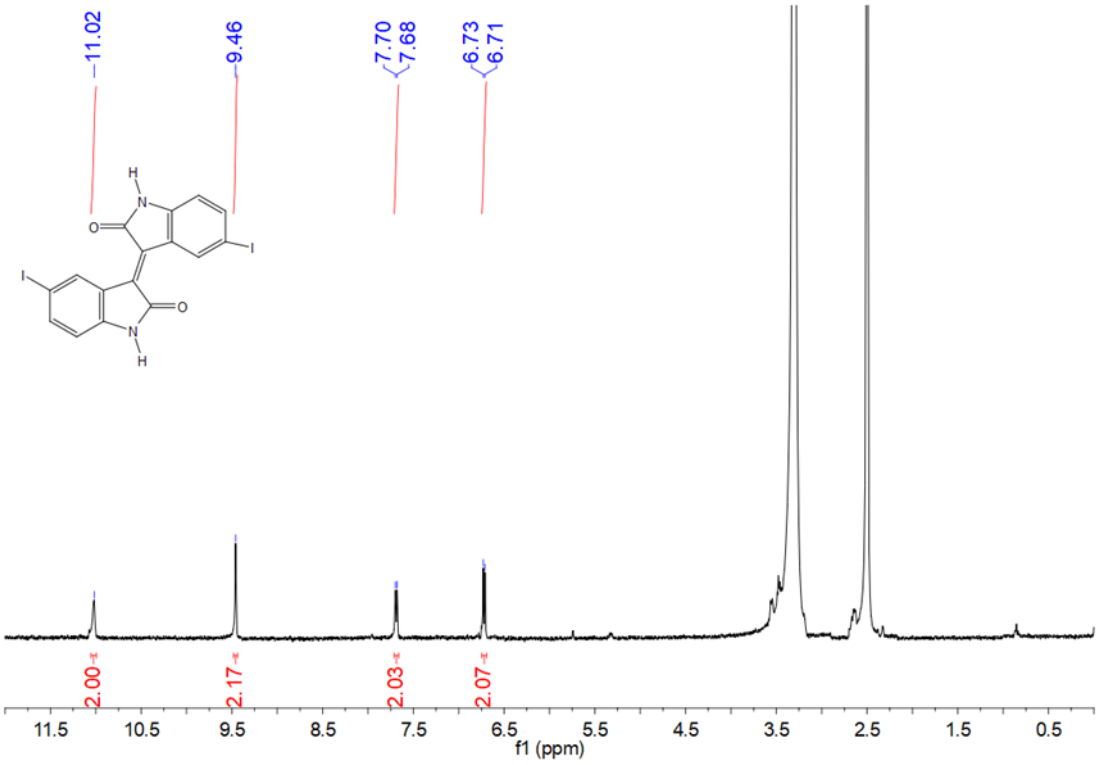
^{1}H NMR spectrum of 3e (400 MHz, DMSO-d_6)



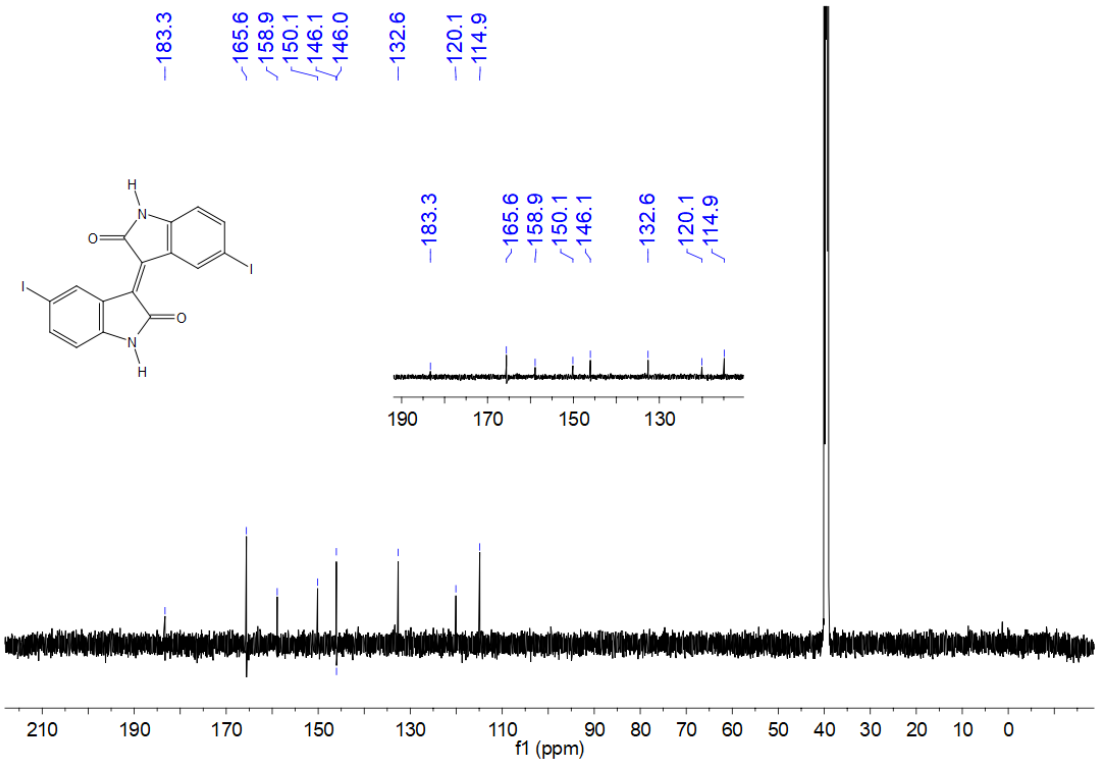
^{13}C NMR spectrum of 3e (126 MHz, DMSO-d_6)



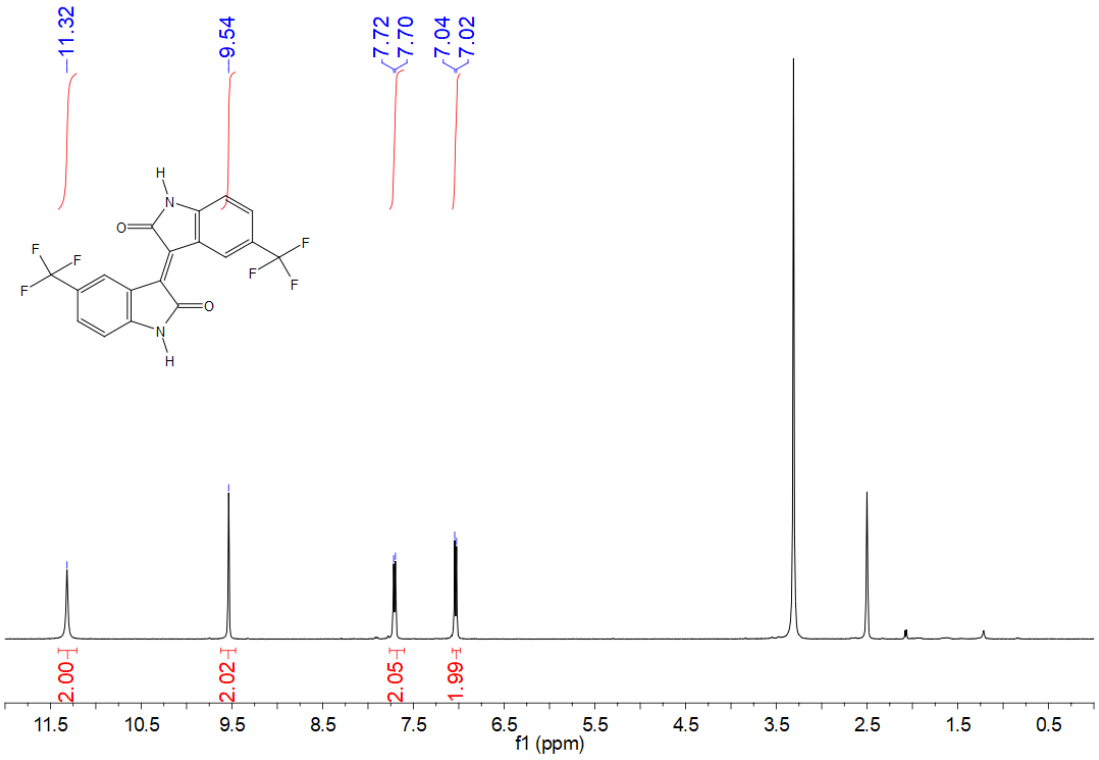
^{1}H NMR spectrum of 3f (400 MHz, DMSO-d_6)



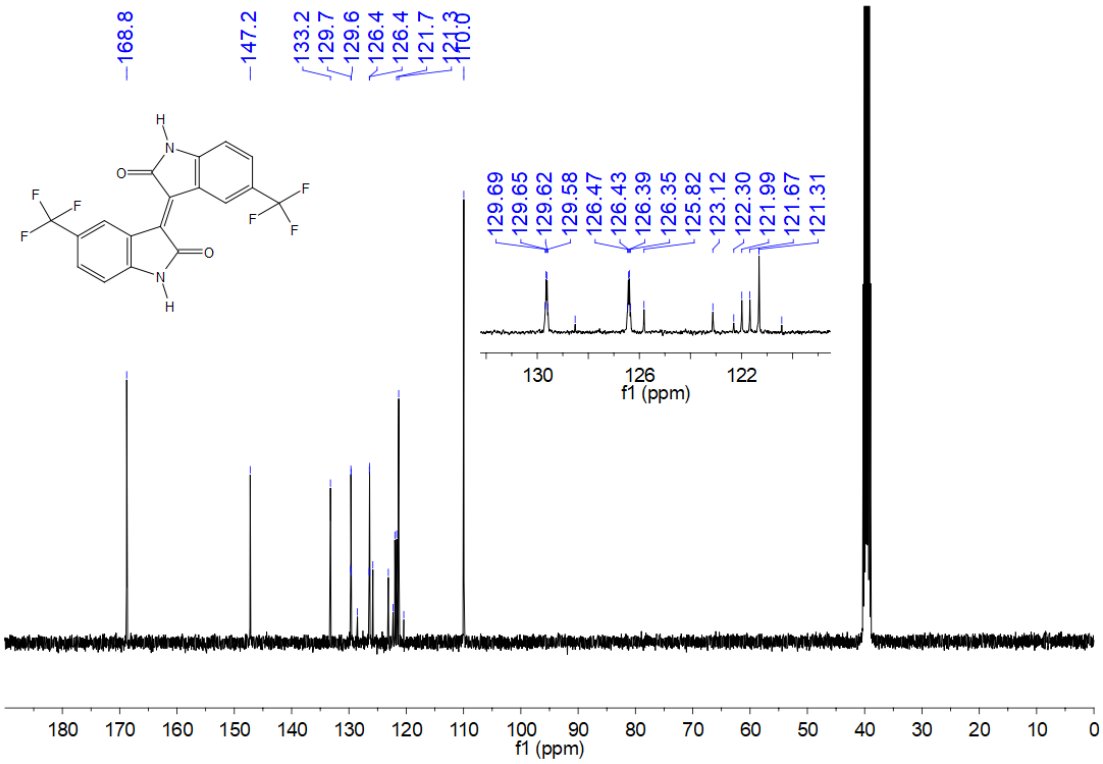
^{1}H NMR spectrum of 3g (400 MHz, DMSO-d_6)



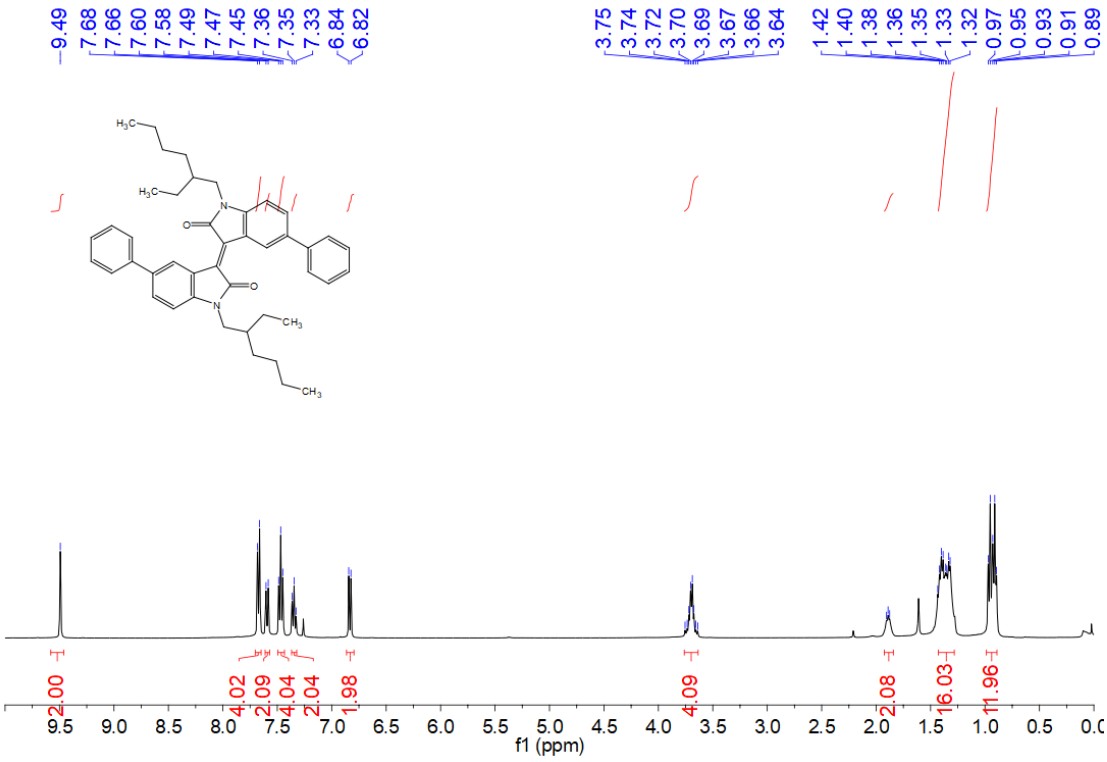
^{13}C NMR spectrum of 3g (151 MHz, DMSO-d_6)



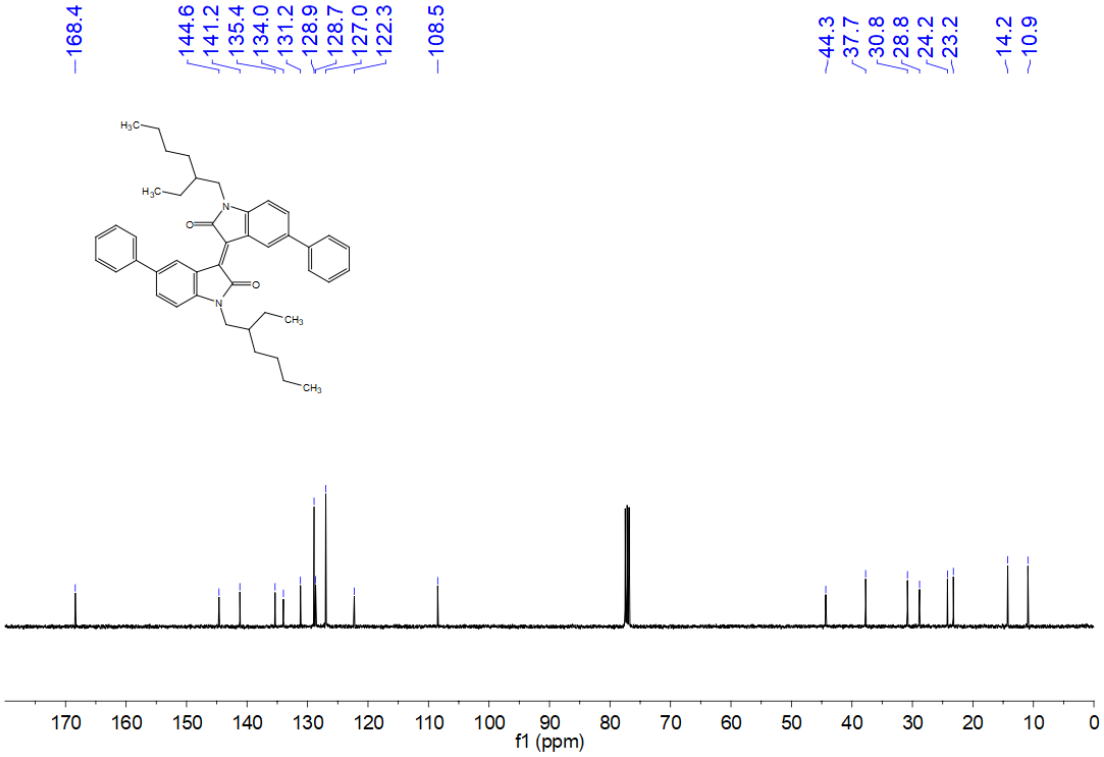
^{1}H NMR spectrum of 3h (400 MHz, DMSO-d_6)



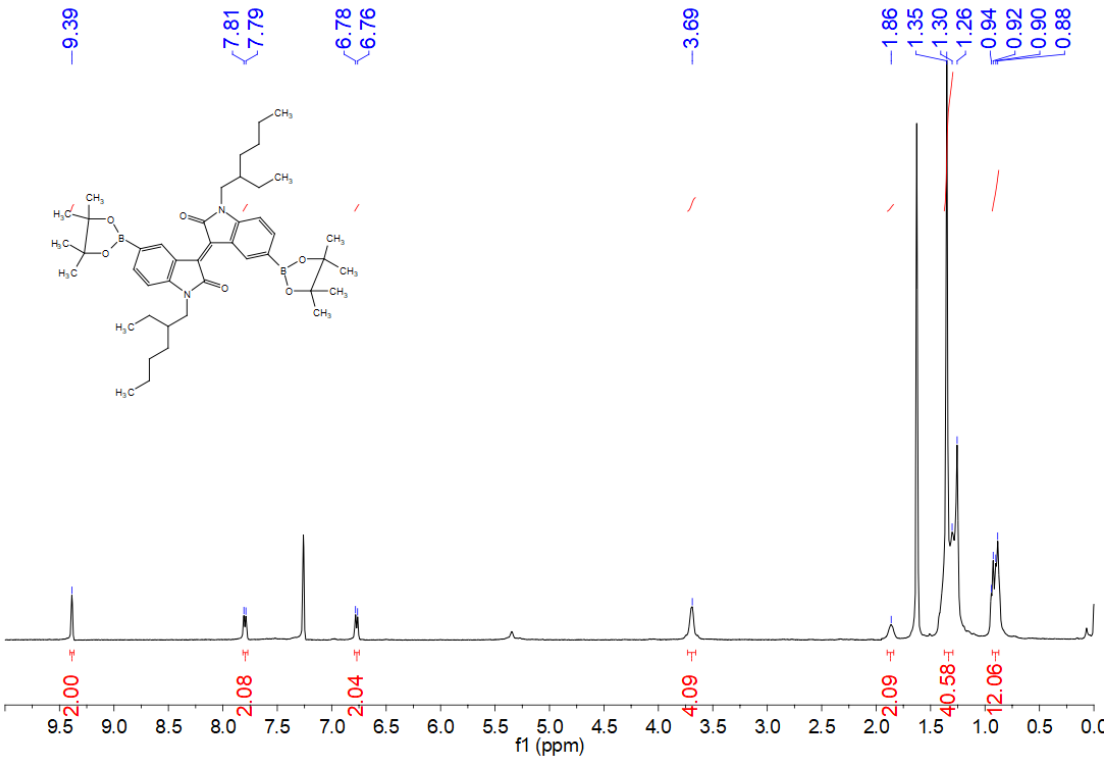
^{13}C NMR spectrum of 3h (101 MHz, DMSO-d_6)



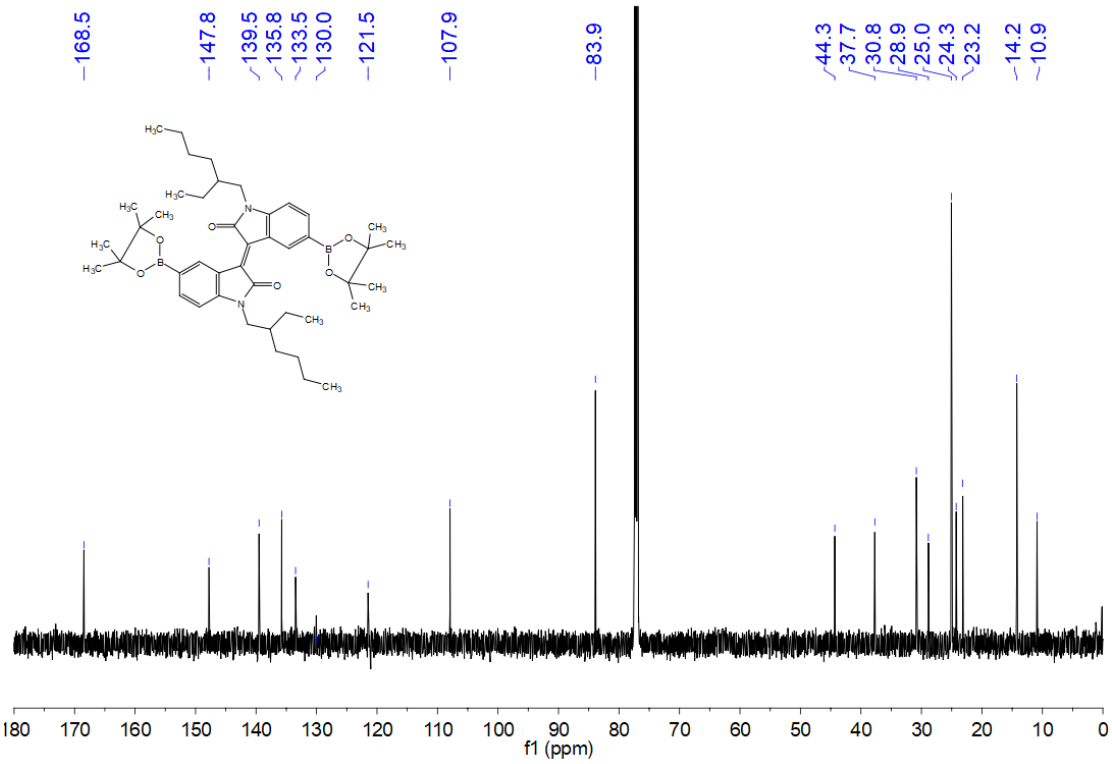
^{1}H NMR spectrum of 3i (400 MHz, $CDCl_3$)



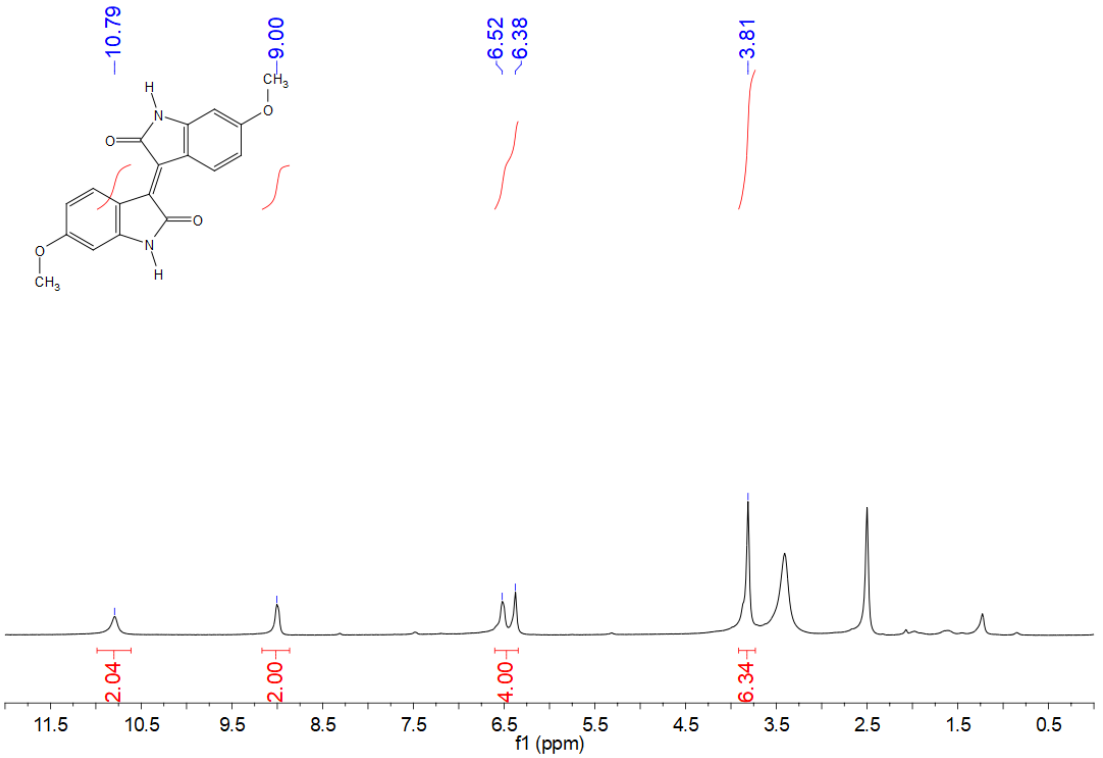
^{13}C NMR spectrum of 3i (101 MHz, $CDCl_3$)



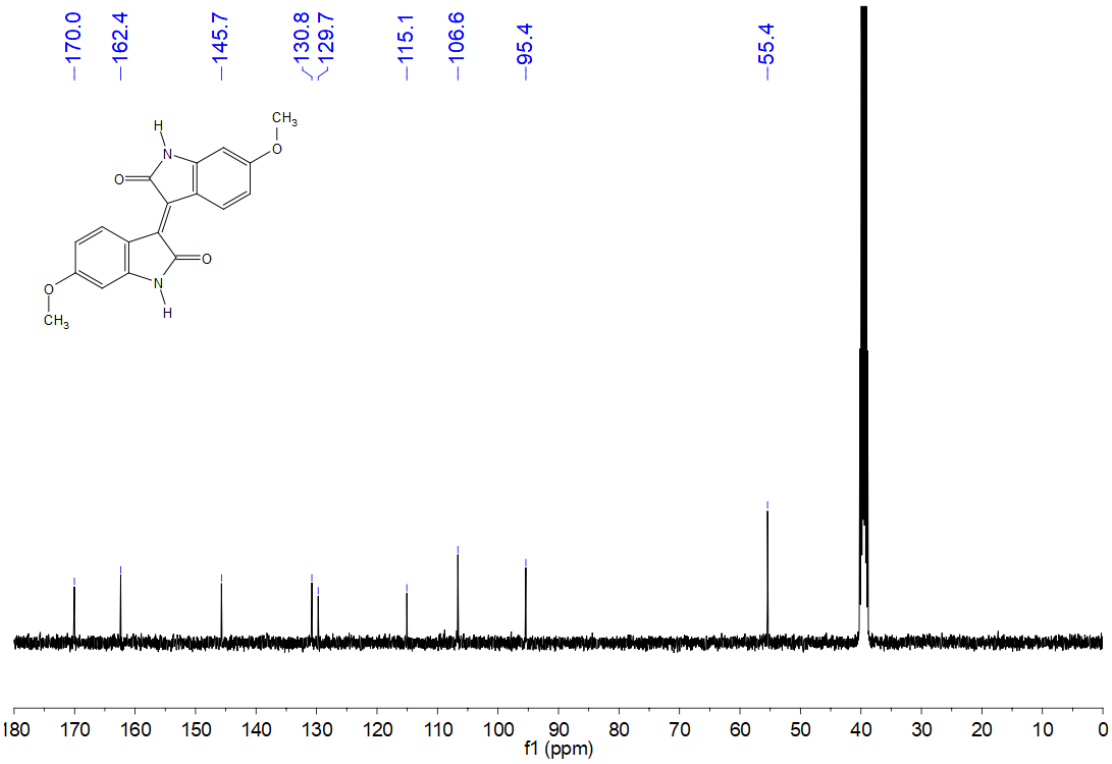
^{1}H NMR spectrum of 3j (400 MHz, $CDCl_3$)



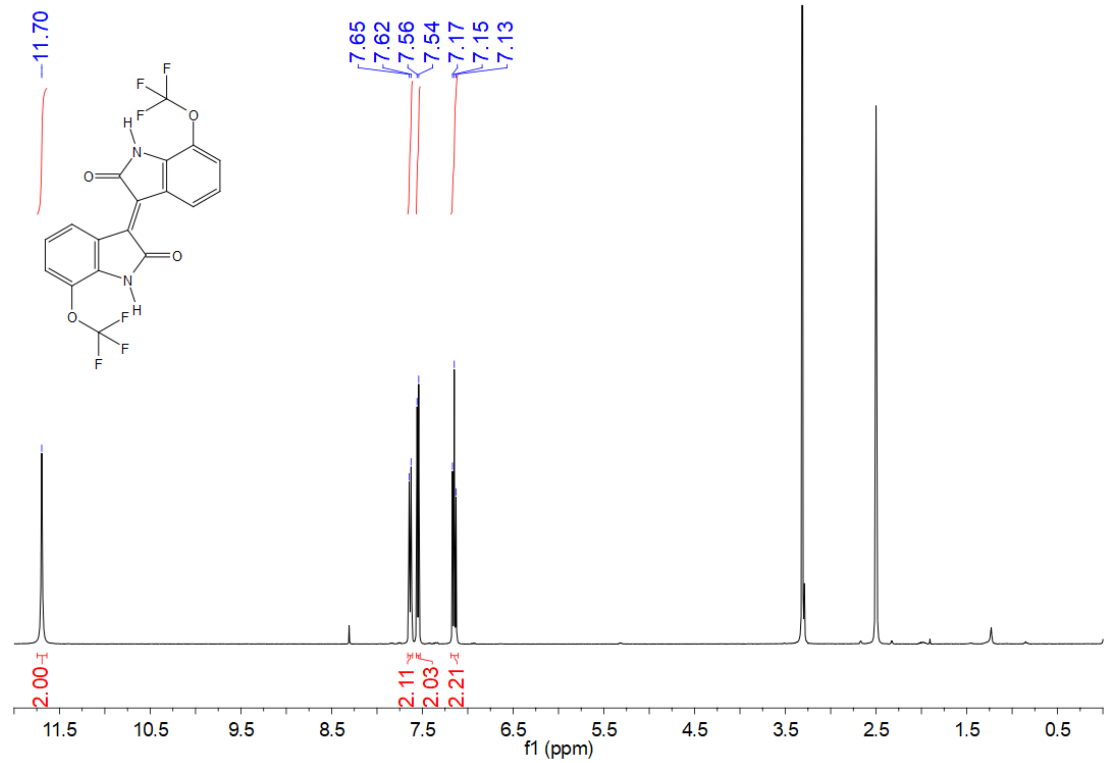
^{13}C NMR spectrum of 3j (151 MHz, $CDCl_3$)



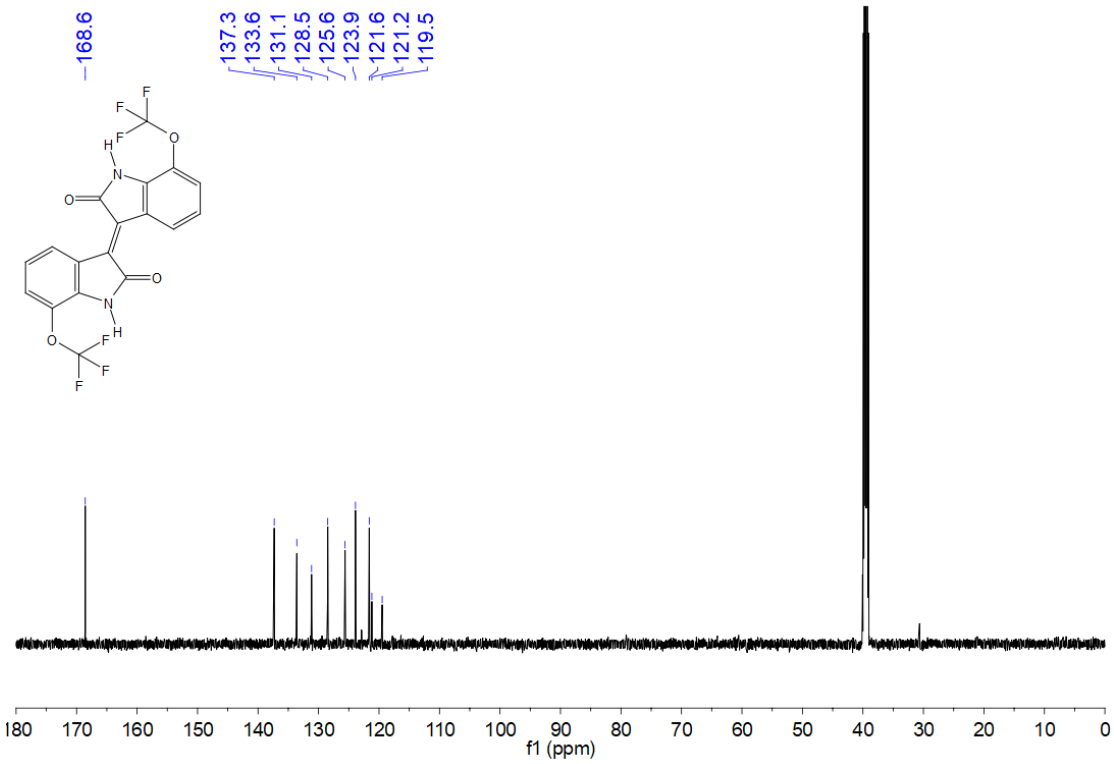
^{1}H NMR spectrum of 3k (400 MHz, DMSO-d_6)



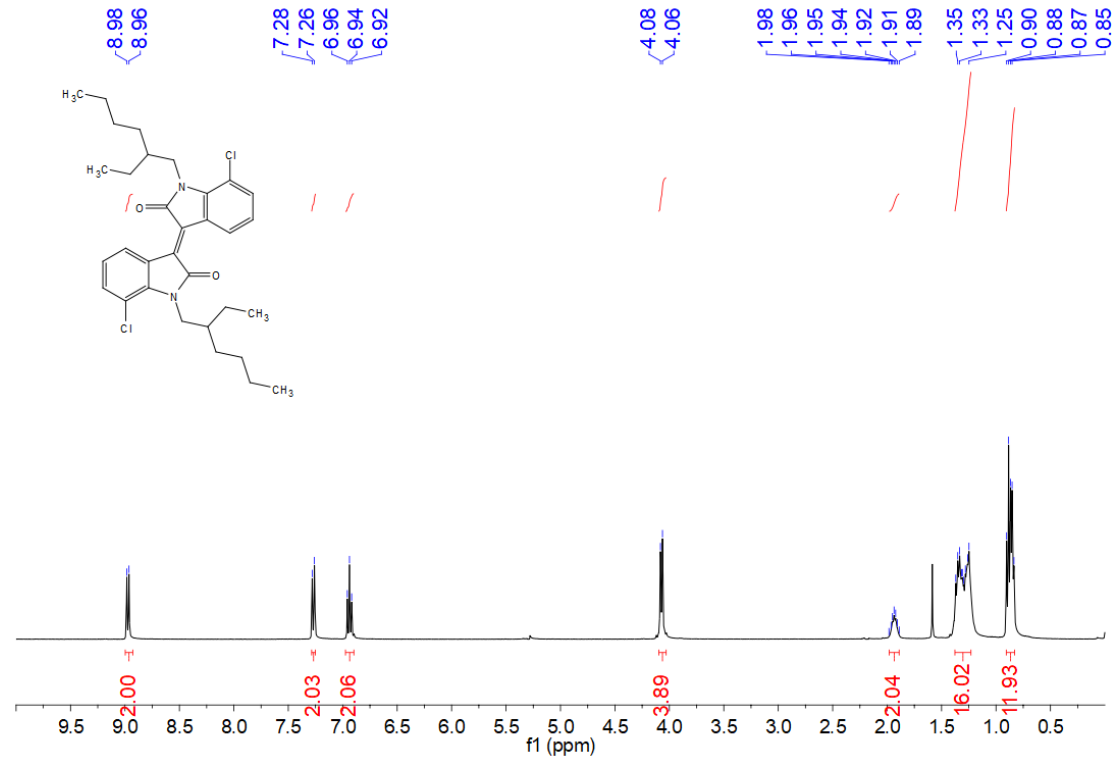
^{13}C NMR spectrum of 3k (101 MHz, DMSO-d_6)



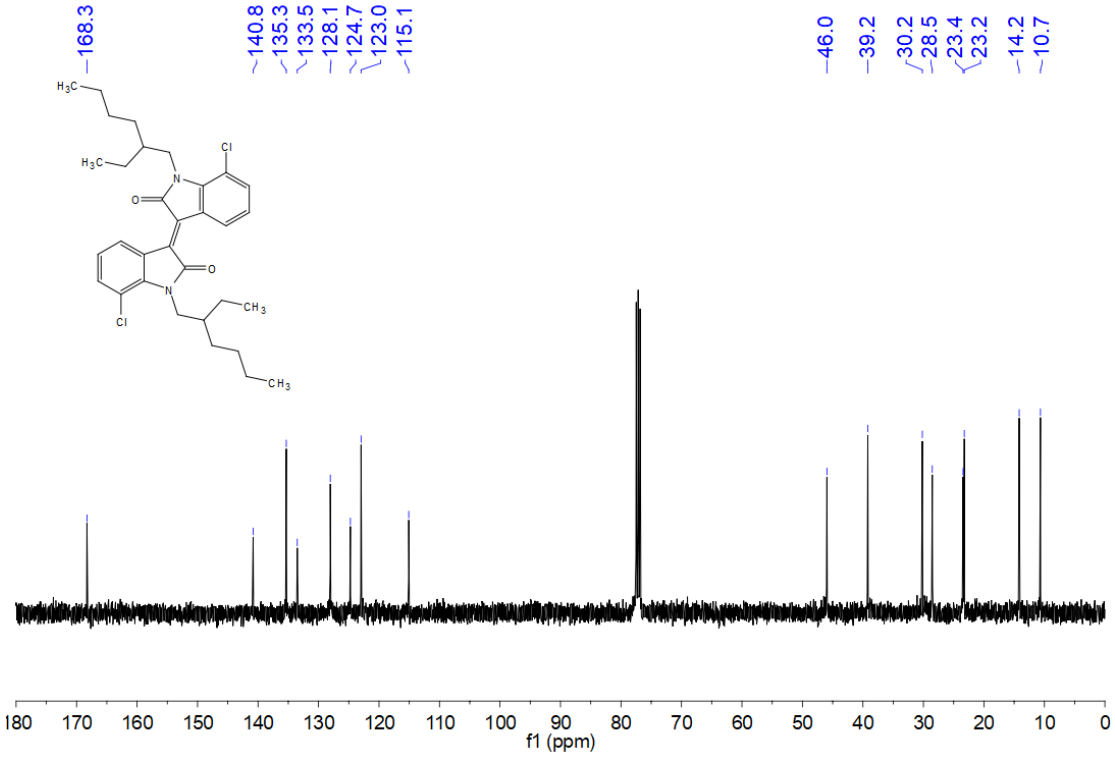
^{1}H NMR spectrum of 3l (400 MHz, DMSO-d_6)



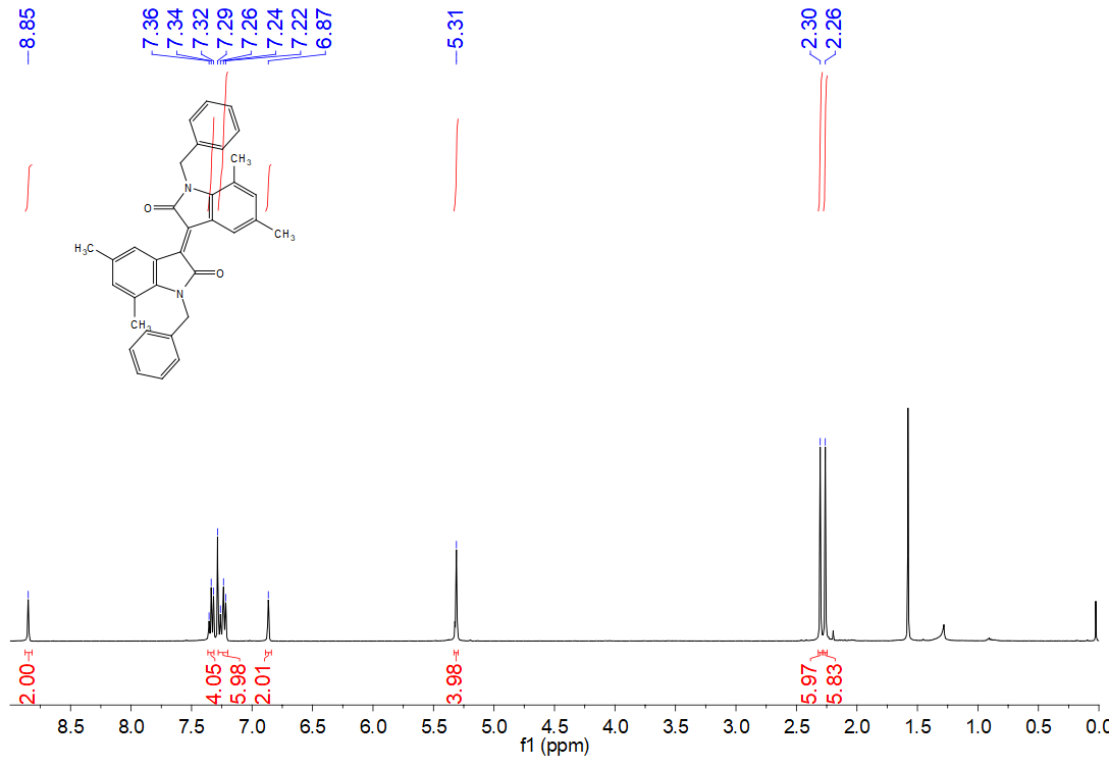
^{13}C NMR spectrum of 3l (151 MHz, DMSO-d_6)



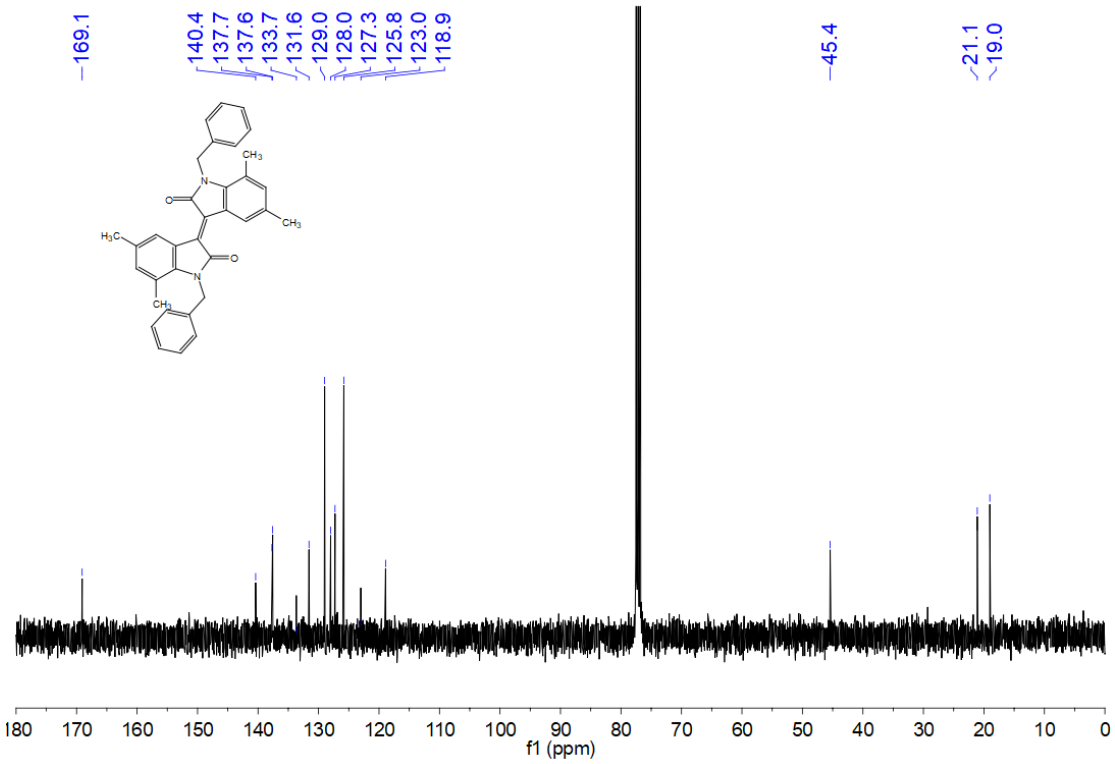
^{1}H NMR spectrum of 3m (400 MHz, $CDCl_3$)



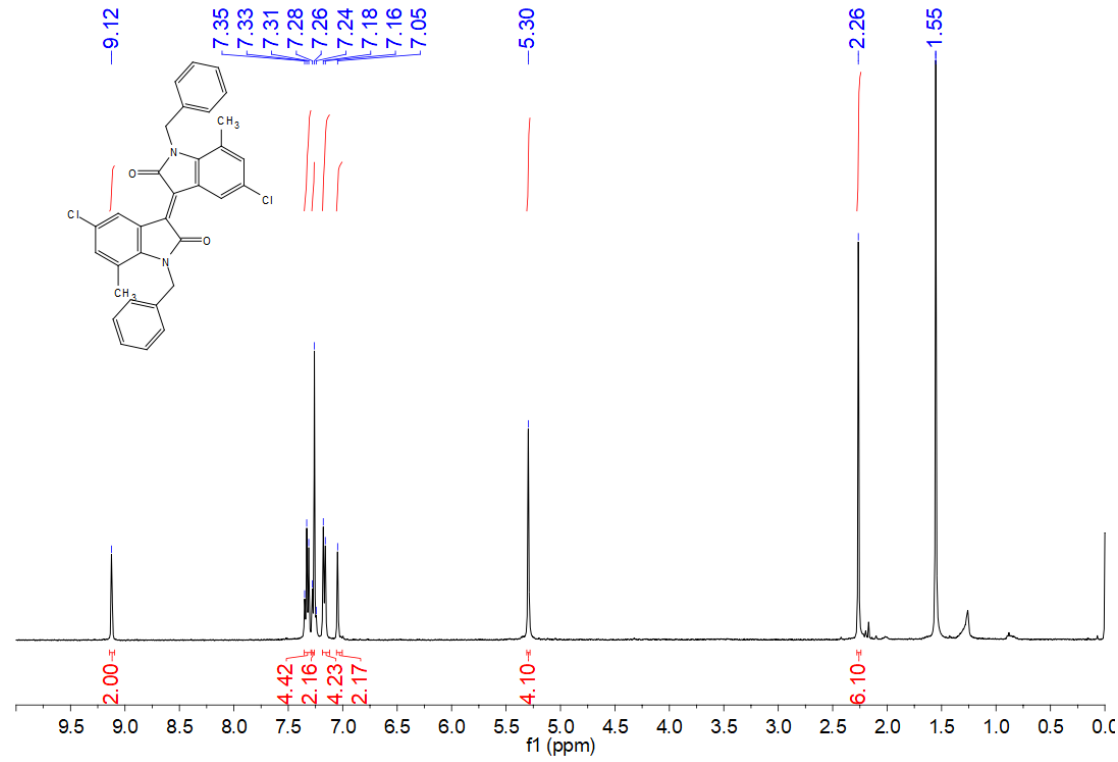
^{13}C NMR spectrum of 3m (101 MHz, $CDCl_3$)



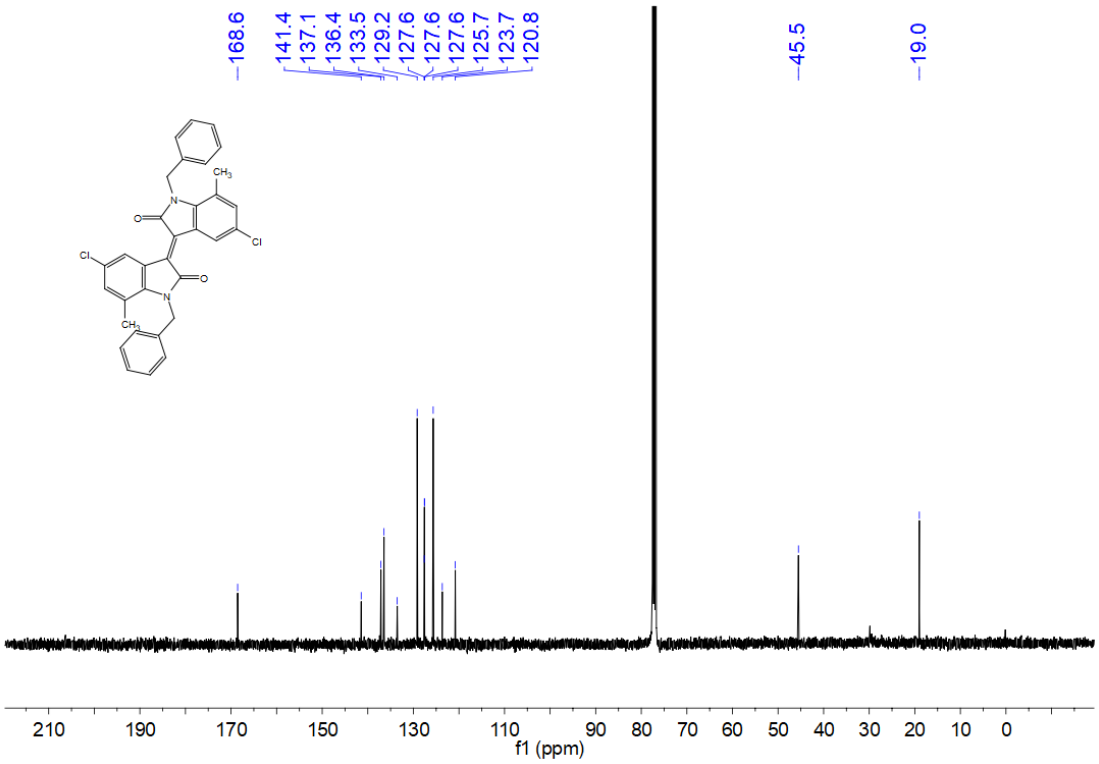
^{1}H NMR spectrum of 3n (400 MHz, $CDCl_3$)



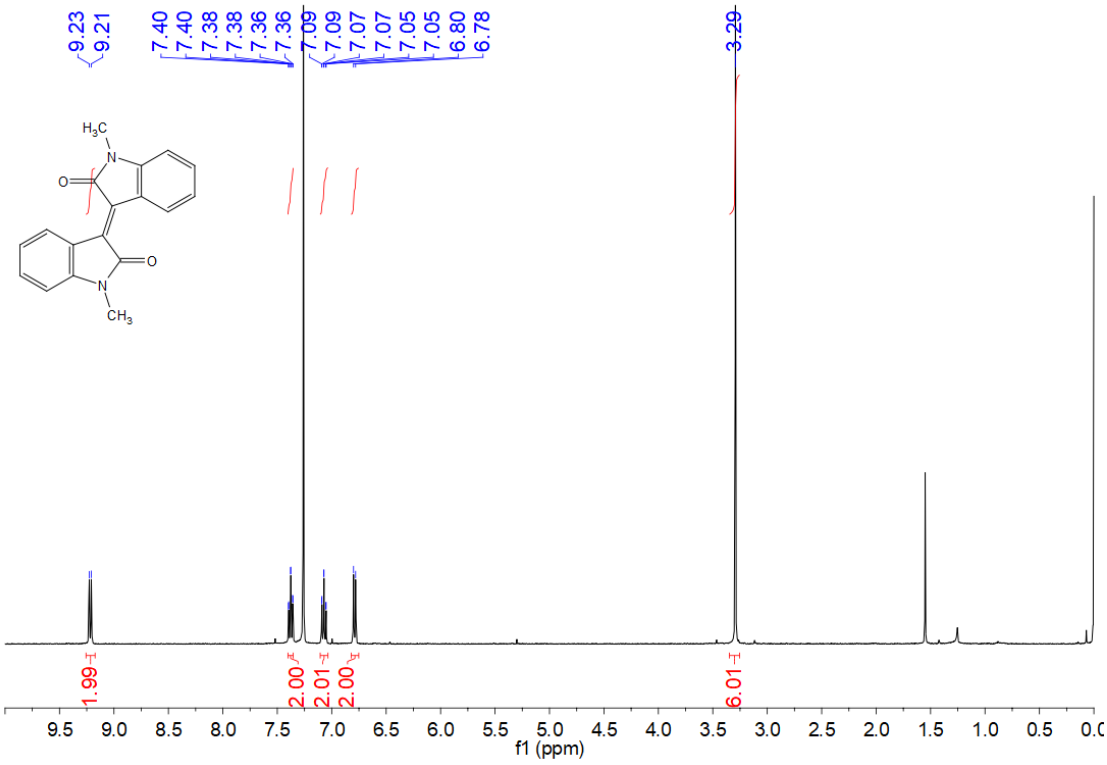
^{13}C NMR spectrum of 3n (101 MHz, $CDCl_3$)



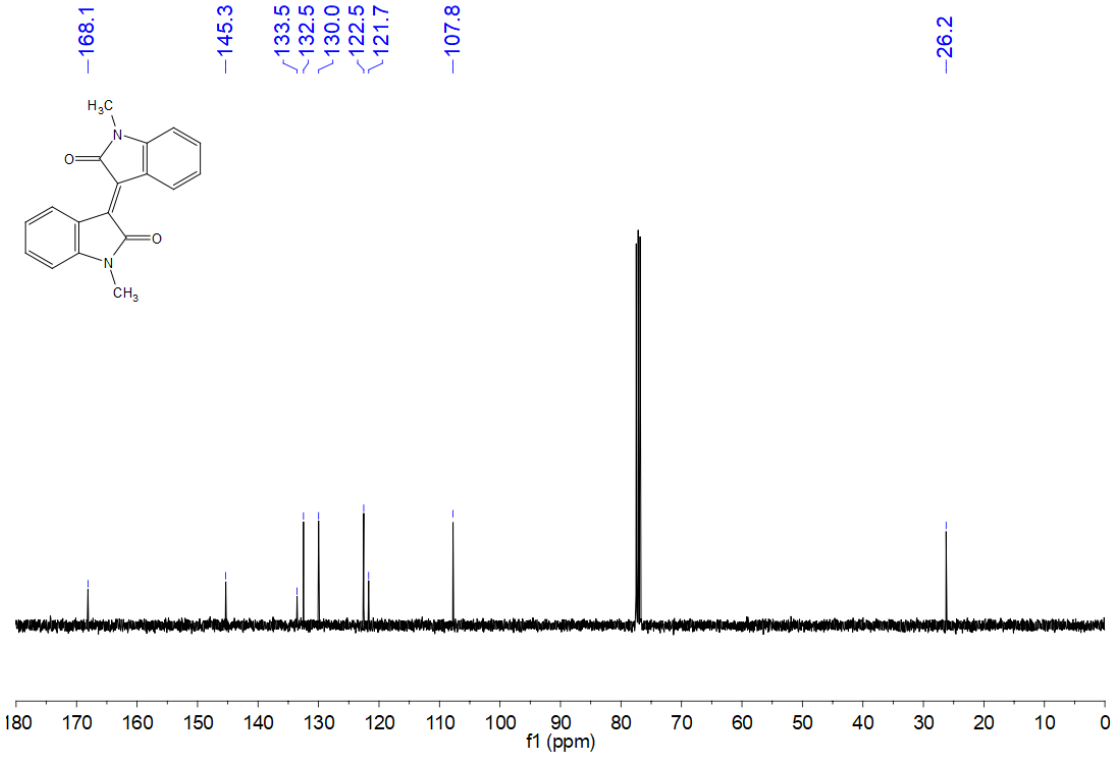
^{1}H NMR spectrum of 3o (400 MHz, $CDCl_3$)



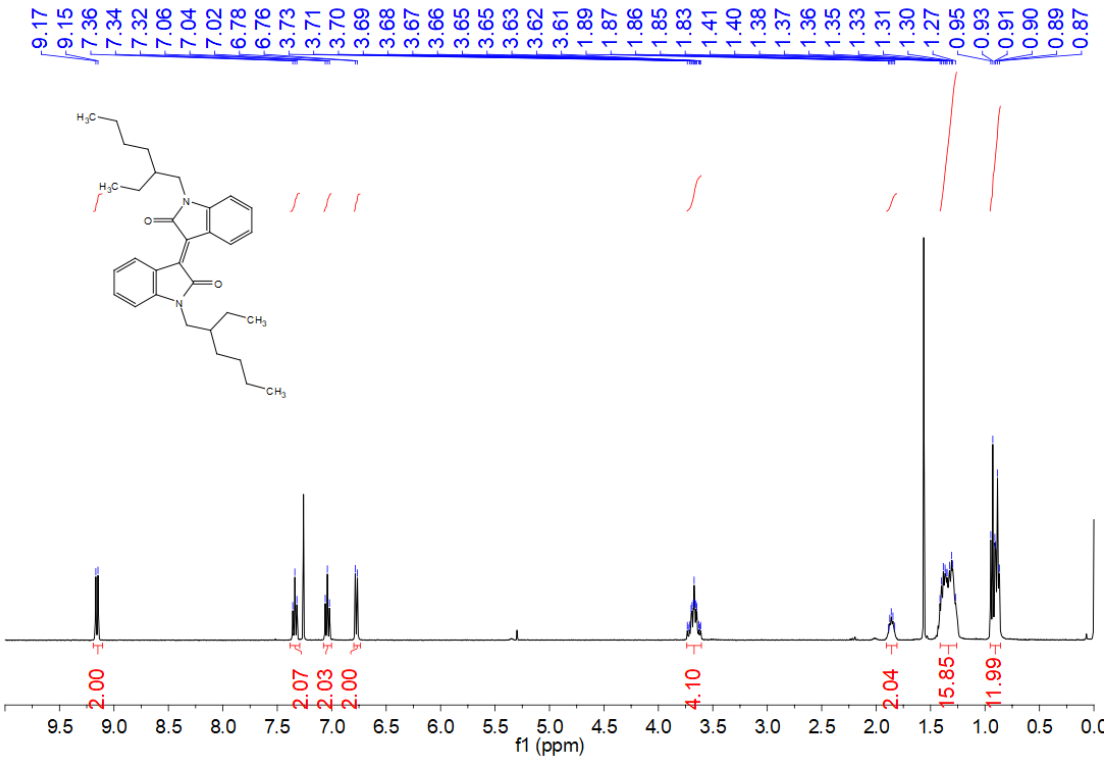
^{13}C NMR spectrum of 3o (101 MHz, $CDCl_3$)



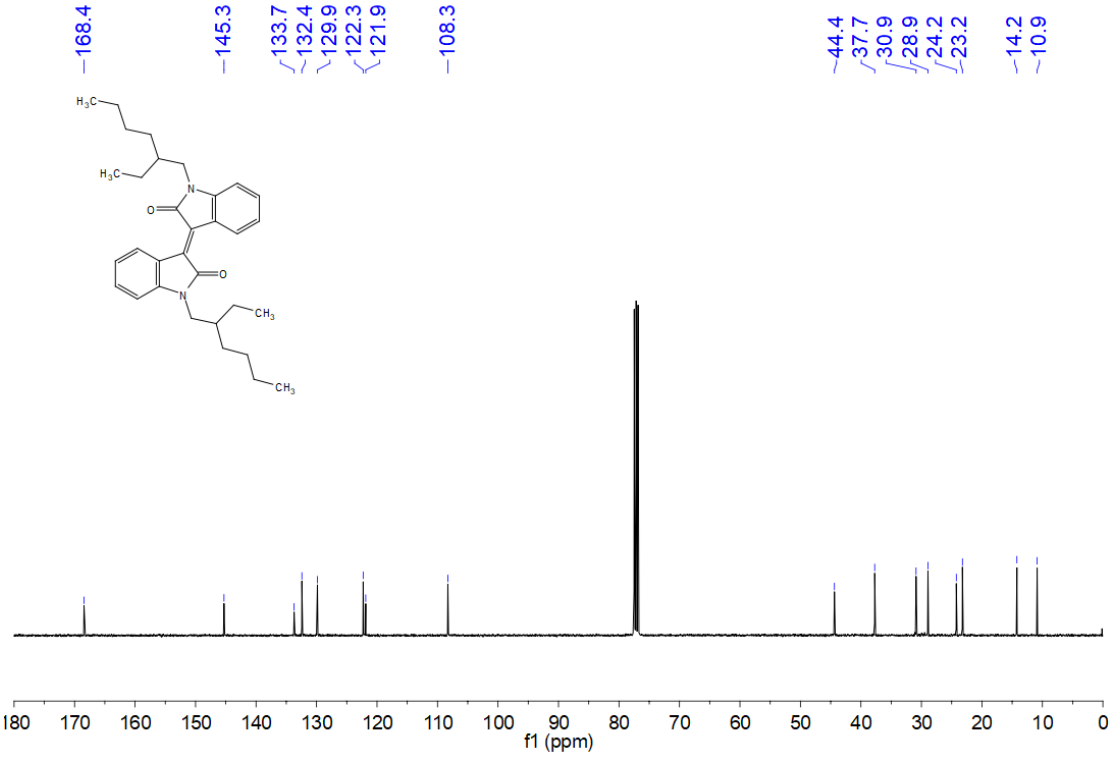
^{1}H NMR spectrum of 3p (400 MHz, $CDCl_3$)



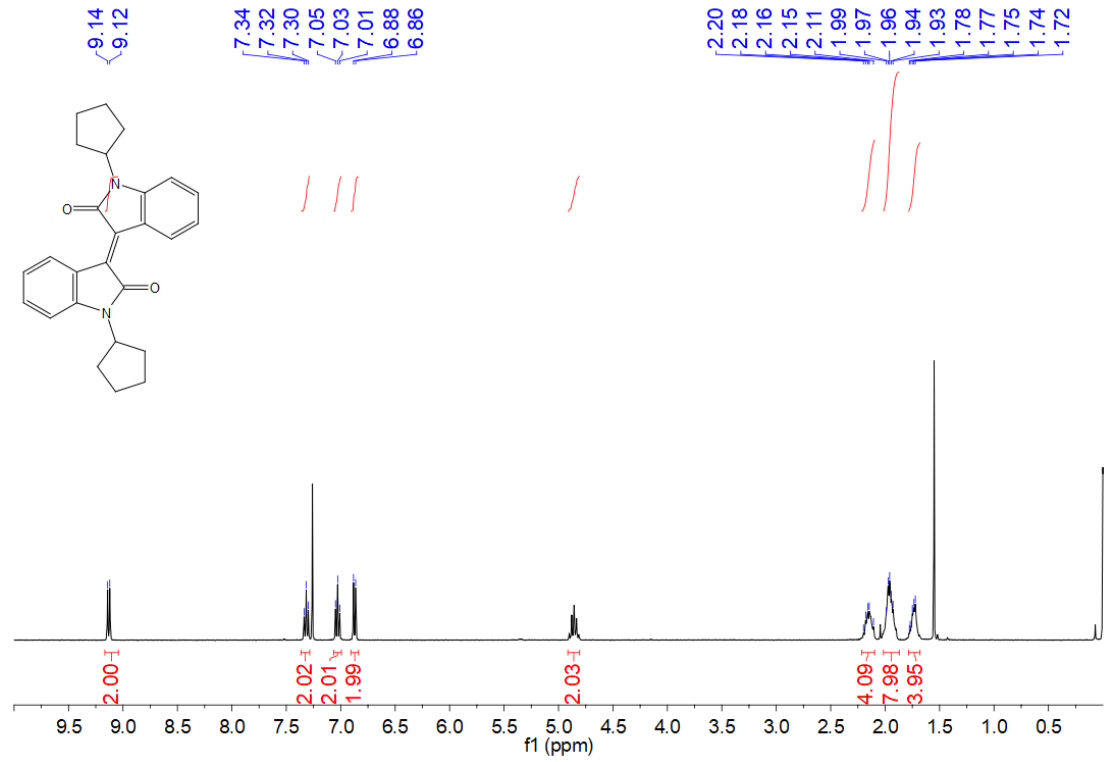
^{13}C NMR spectrum of 3p (101 MHz, $CDCl_3$)



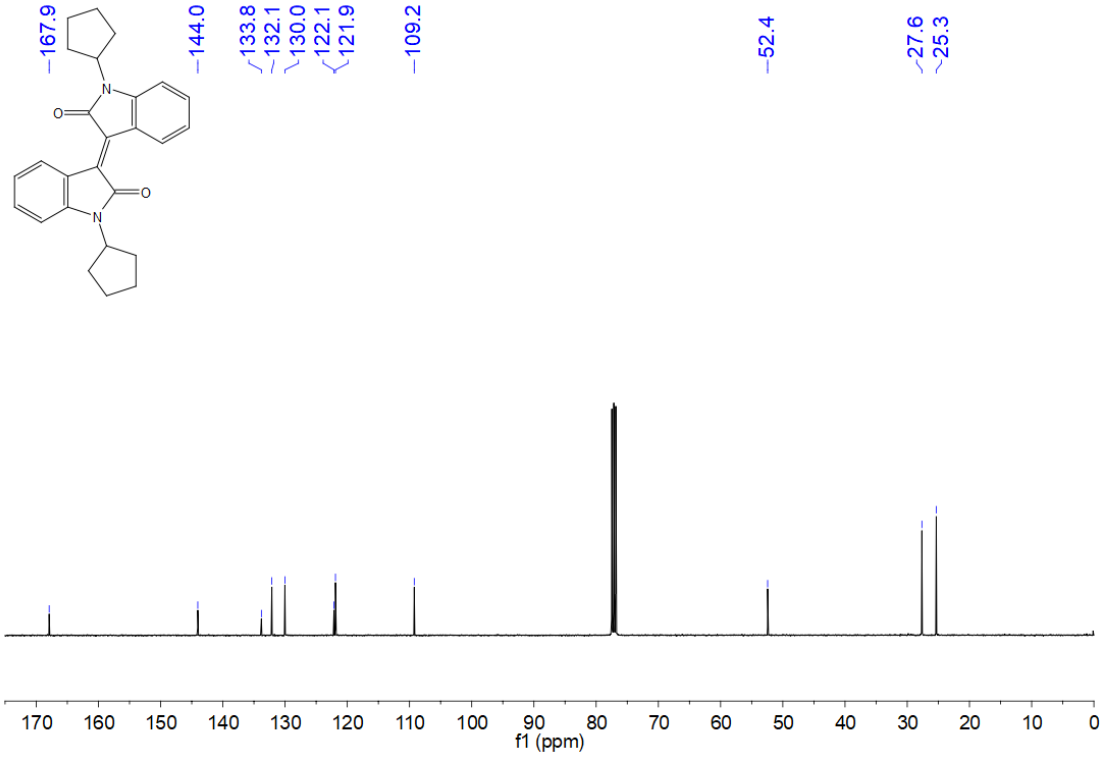
^{1}H NMR spectrum of 3q (400 MHz, $CDCl_3$)



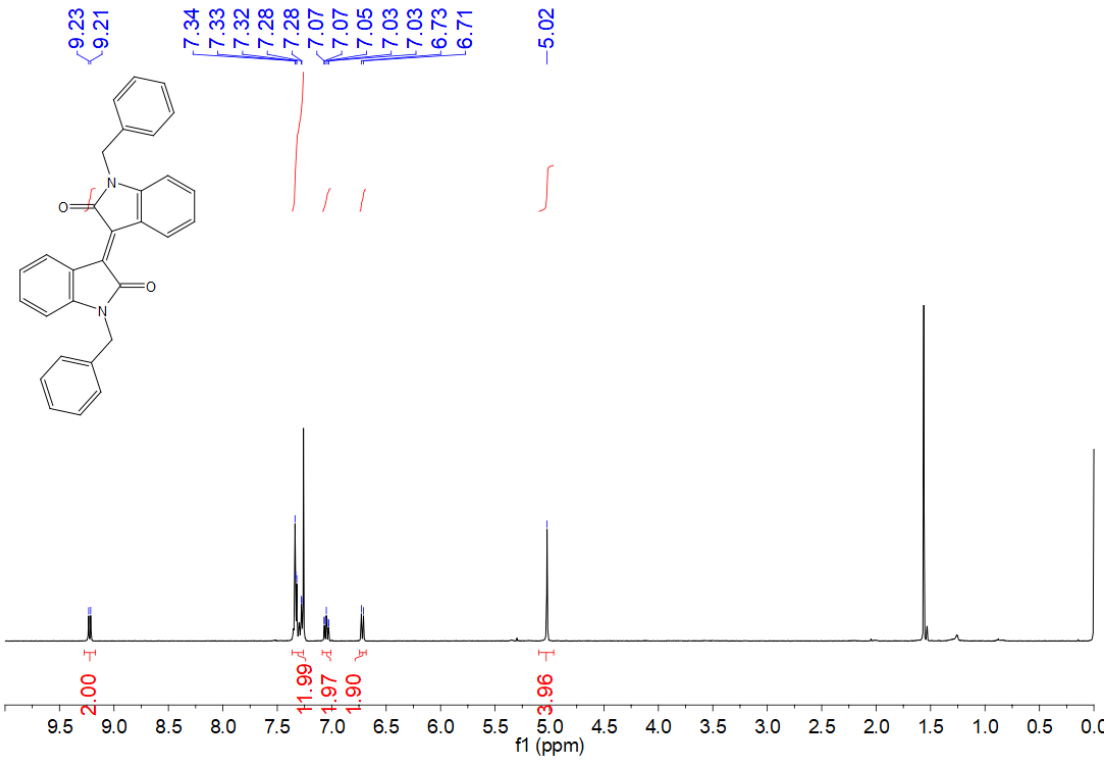
^{13}C NMR spectrum of 3q (101 MHz, $CDCl_3$)



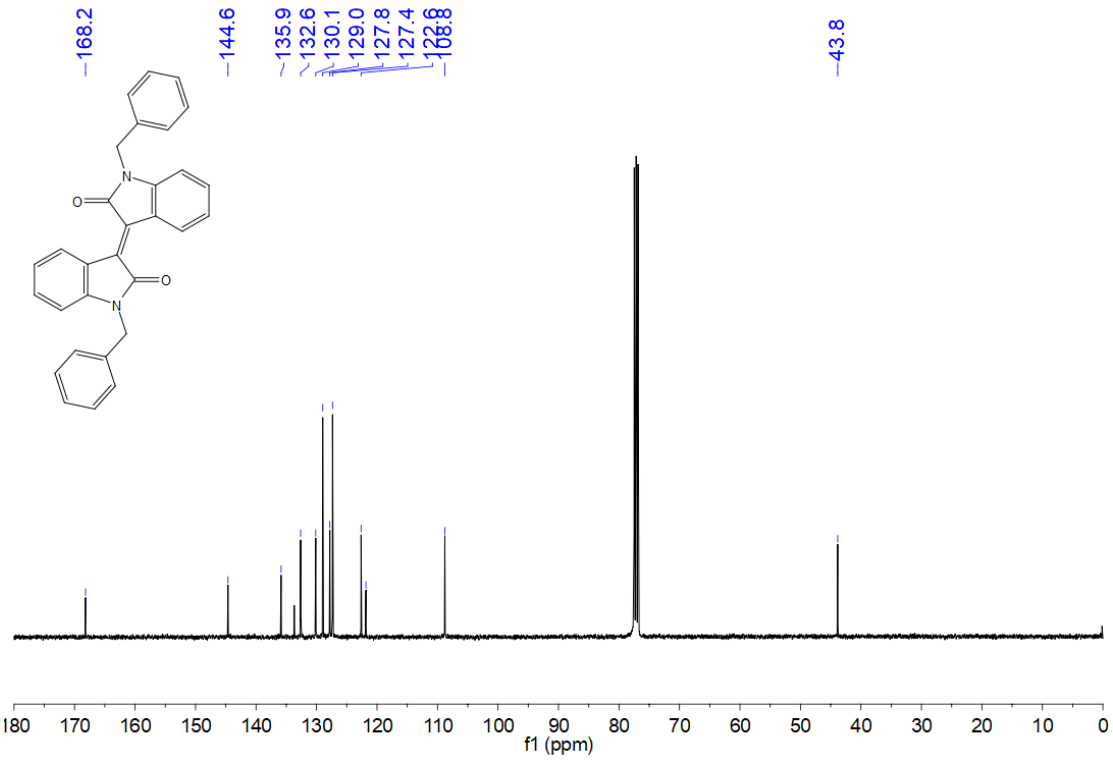
^{1}H NMR spectrum of 3r (400 MHz, $CDCl_3$)



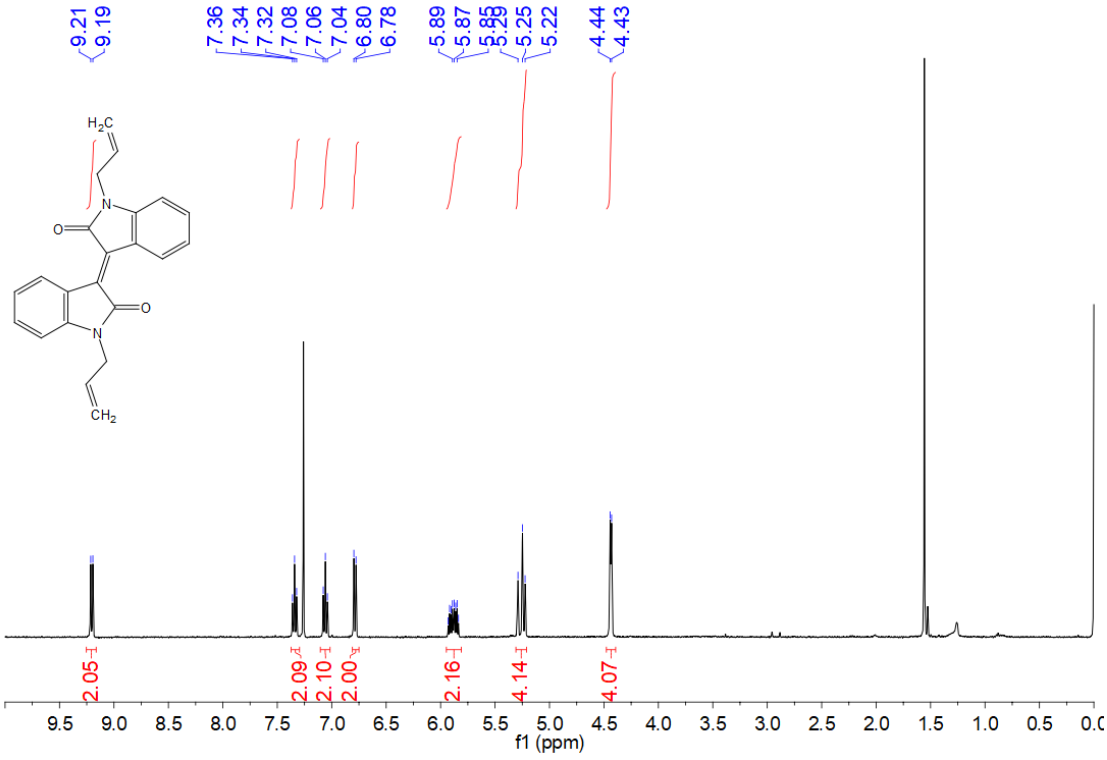
^{13}C NMR spectrum of 3r (101 MHz, $CDCl_3$)



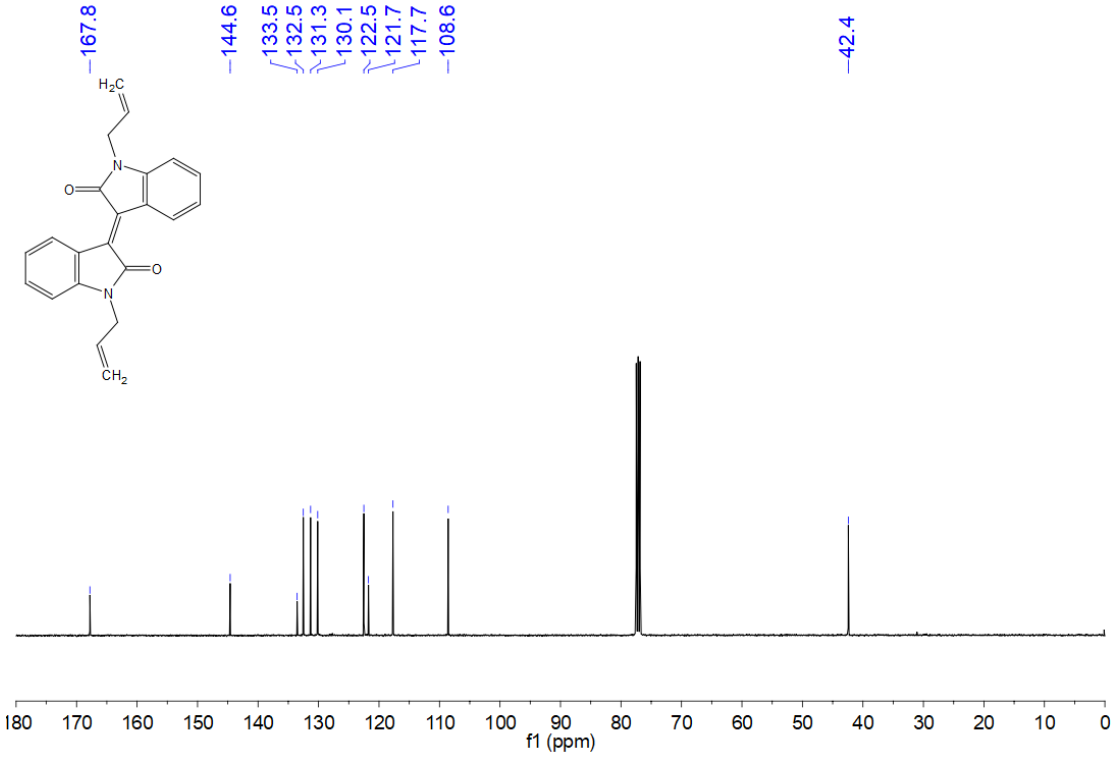
^{1}H NMR spectrum of 3s (400 MHz, $CDCl_3$)



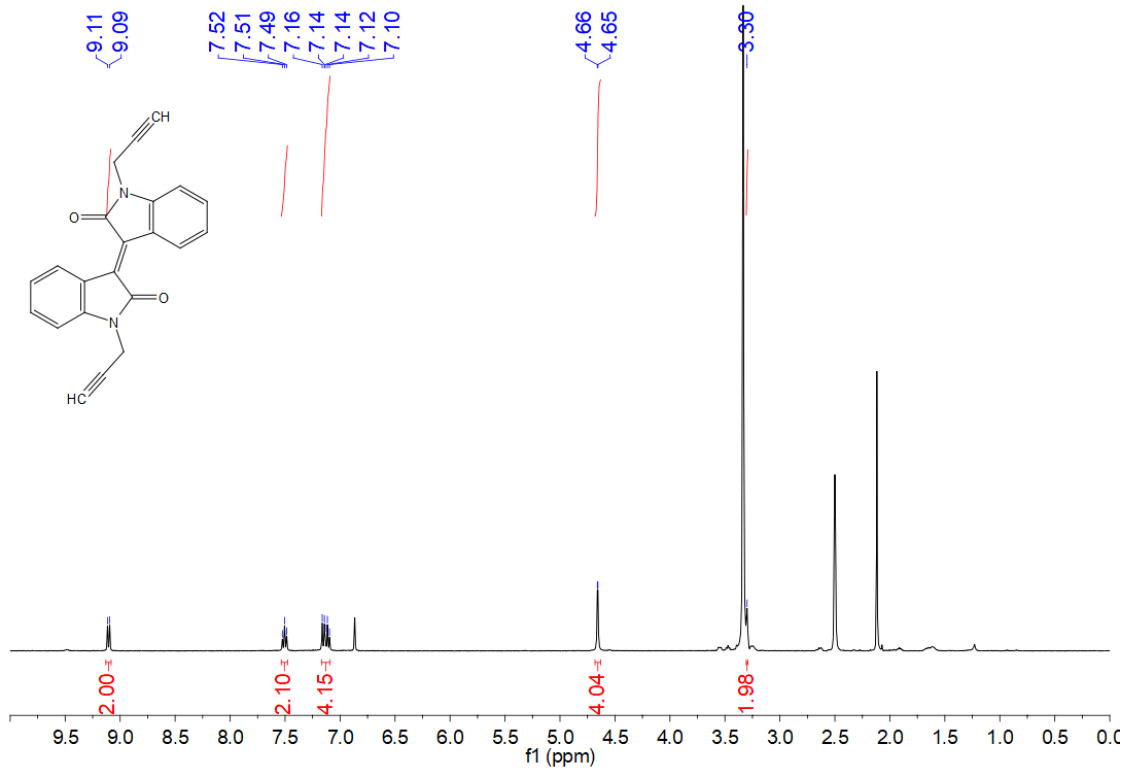
^{13}C NMR spectrum of 3s (101 MHz, $CDCl_3$)



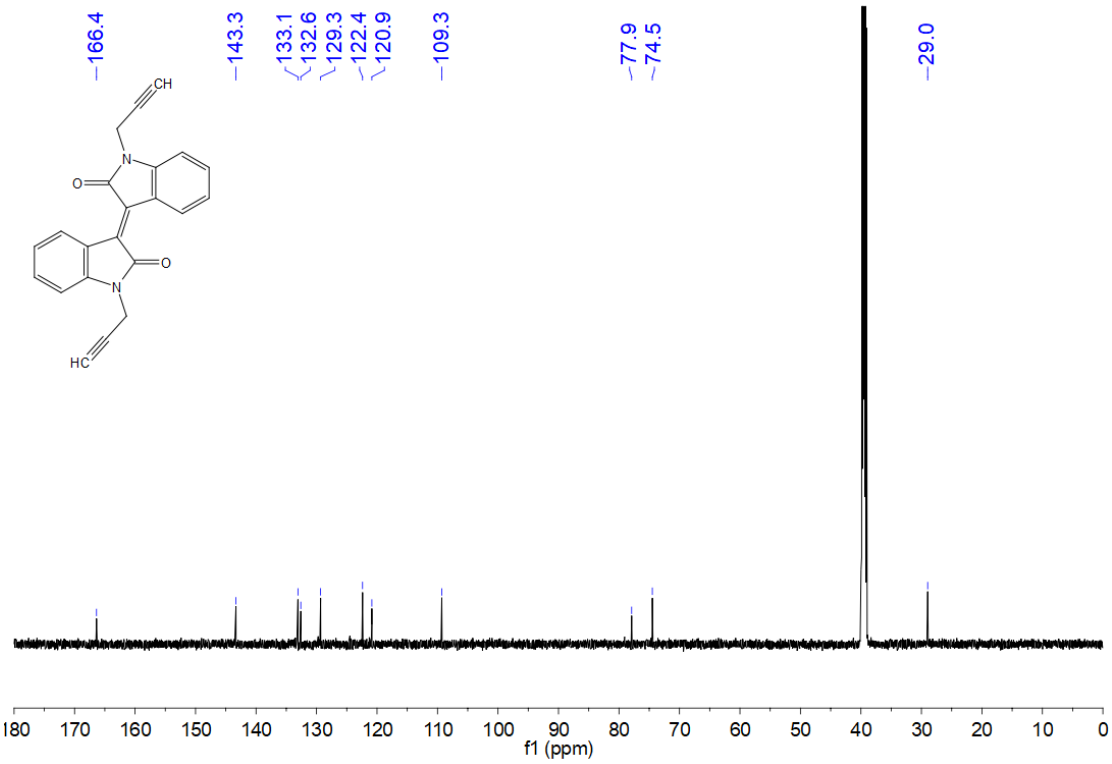
^{1}H NMR spectrum of 3t (400 MHz, $CDCl_3$)



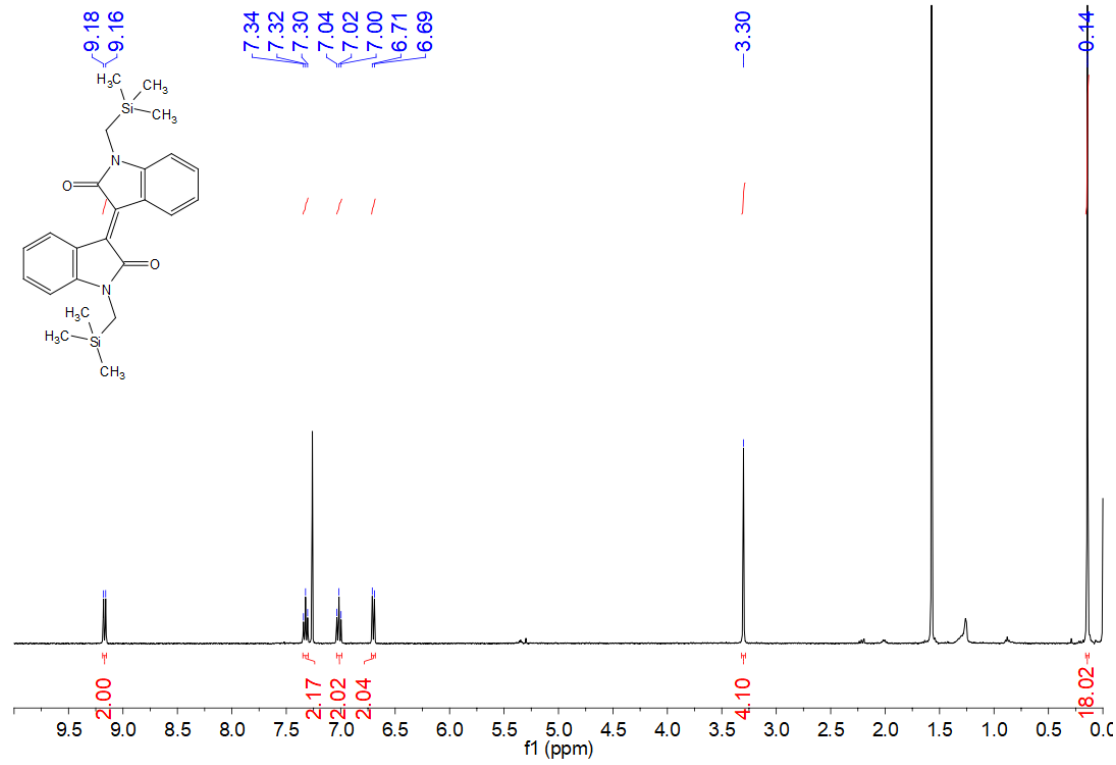
^{13}C NMR spectrum of 3t (101 MHz, $CDCl_3$)



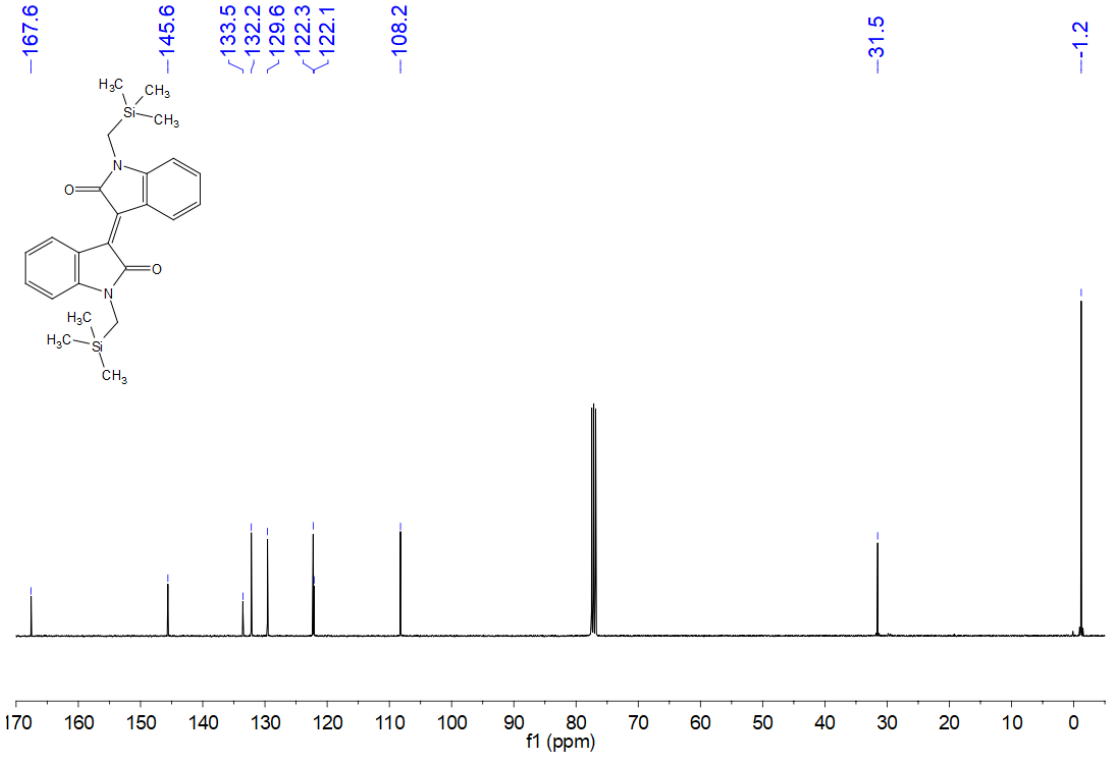
^{1}H NMR spectrum of 3u (400 MHz, DMSO-d_6)



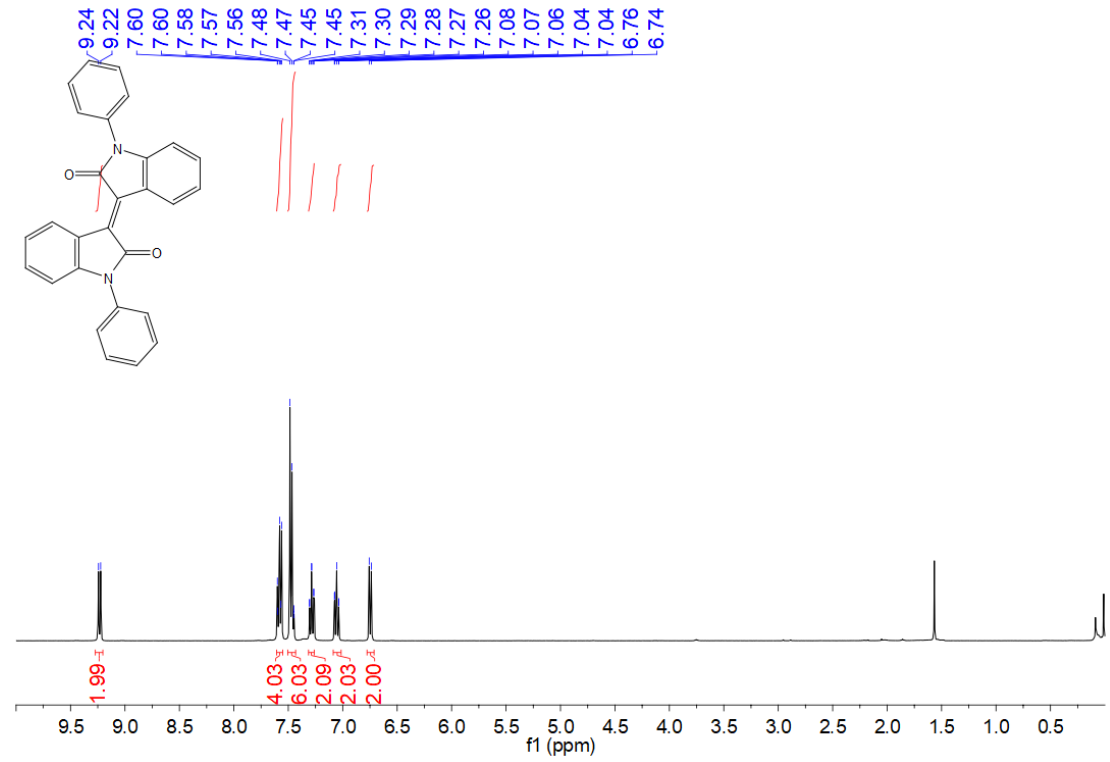
^{13}C NMR spectrum of 3u (151 MHz, DMSO-d_6)



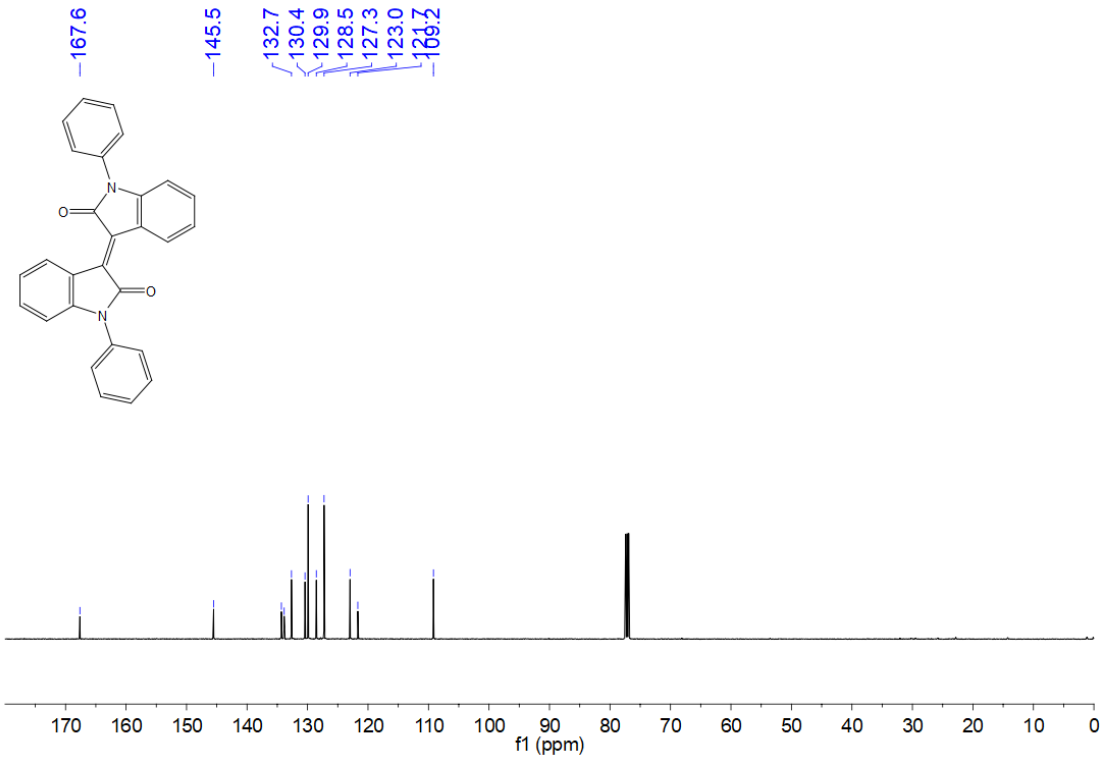
^{1}H NMR spectrum of 3v (400 MHz, $CDCl_3$)



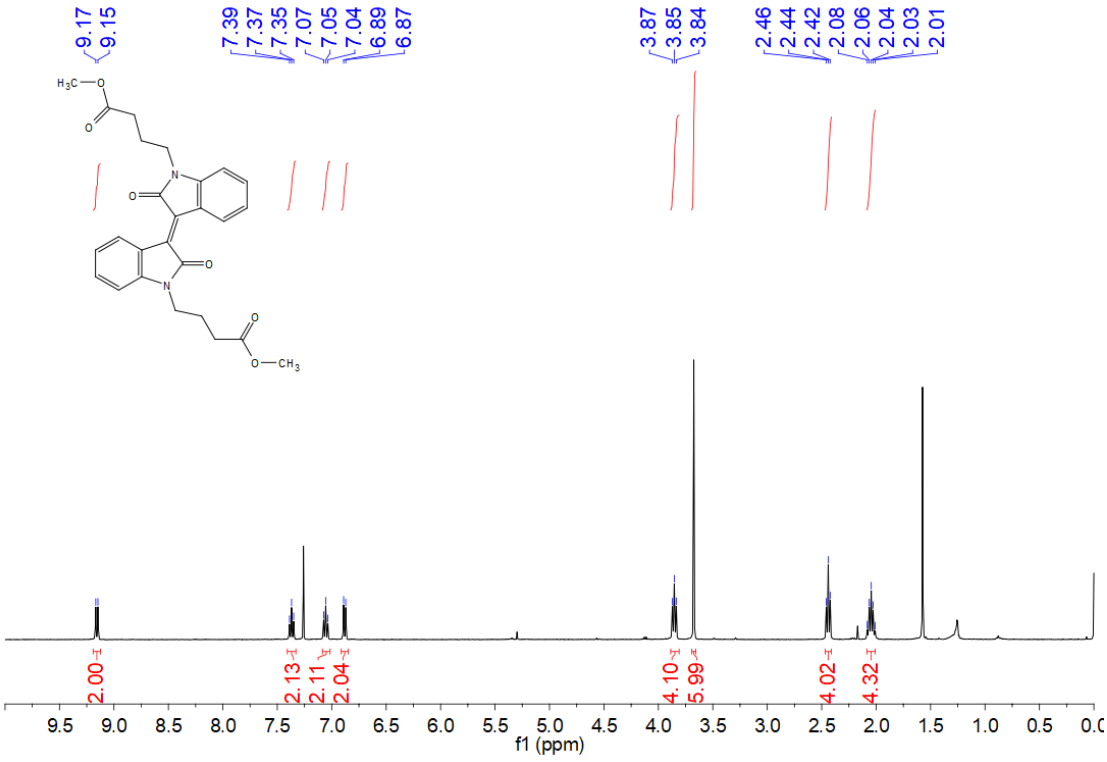
^{13}C NMR spectrum of 3v (101 MHz, $CDCl_3$)



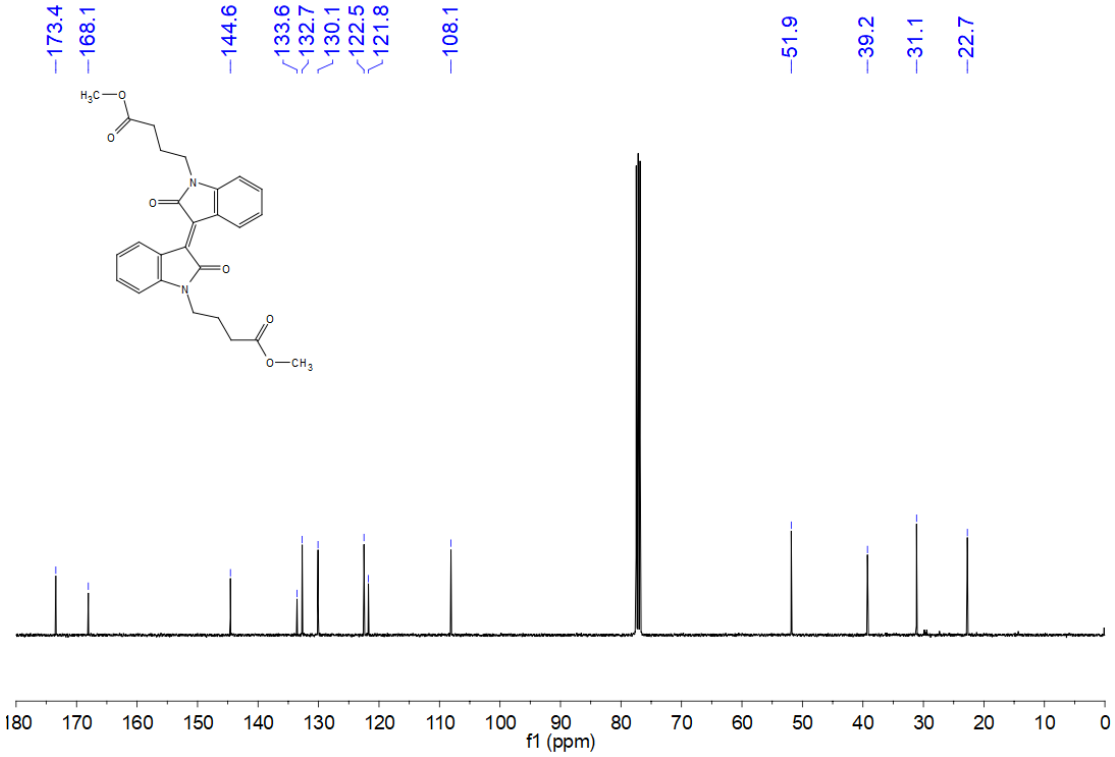
^{1}H NMR spectrum of 3w (400 MHz, $CDCl_3$)



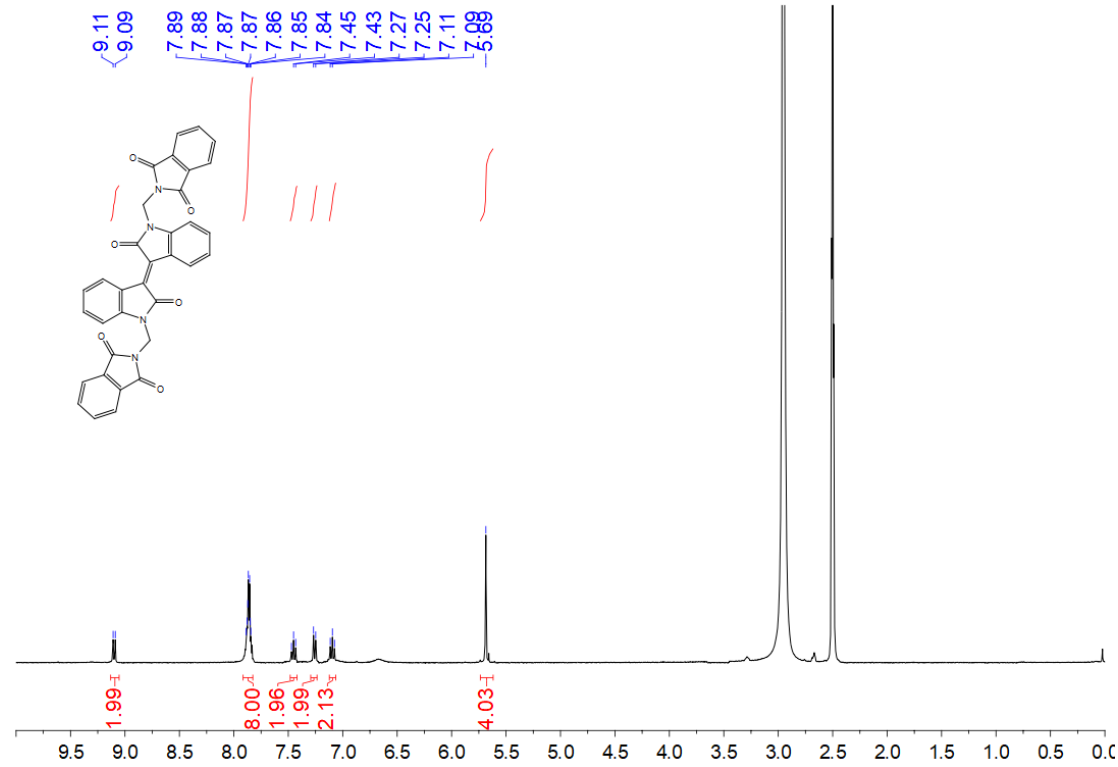
^{13}C NMR spectrum of 3w (126 MHz, $CDCl_3$)



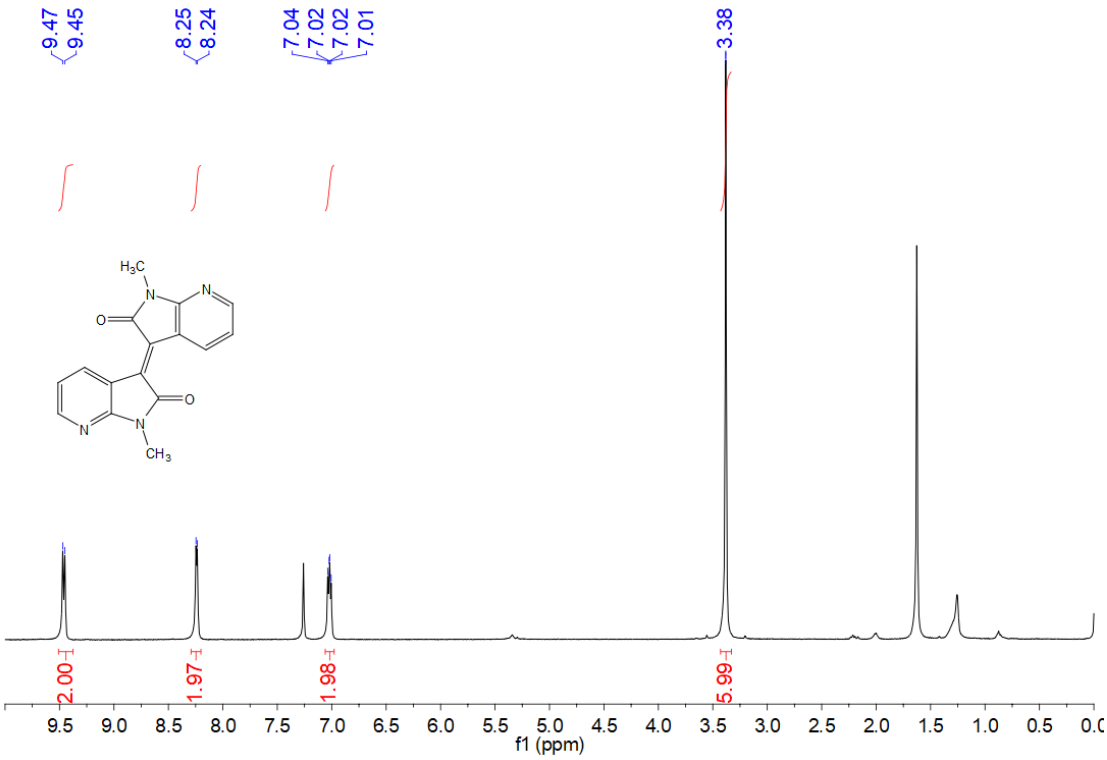
^{1}H NMR spectrum of 3x (400 MHz, $CDCl_3$)



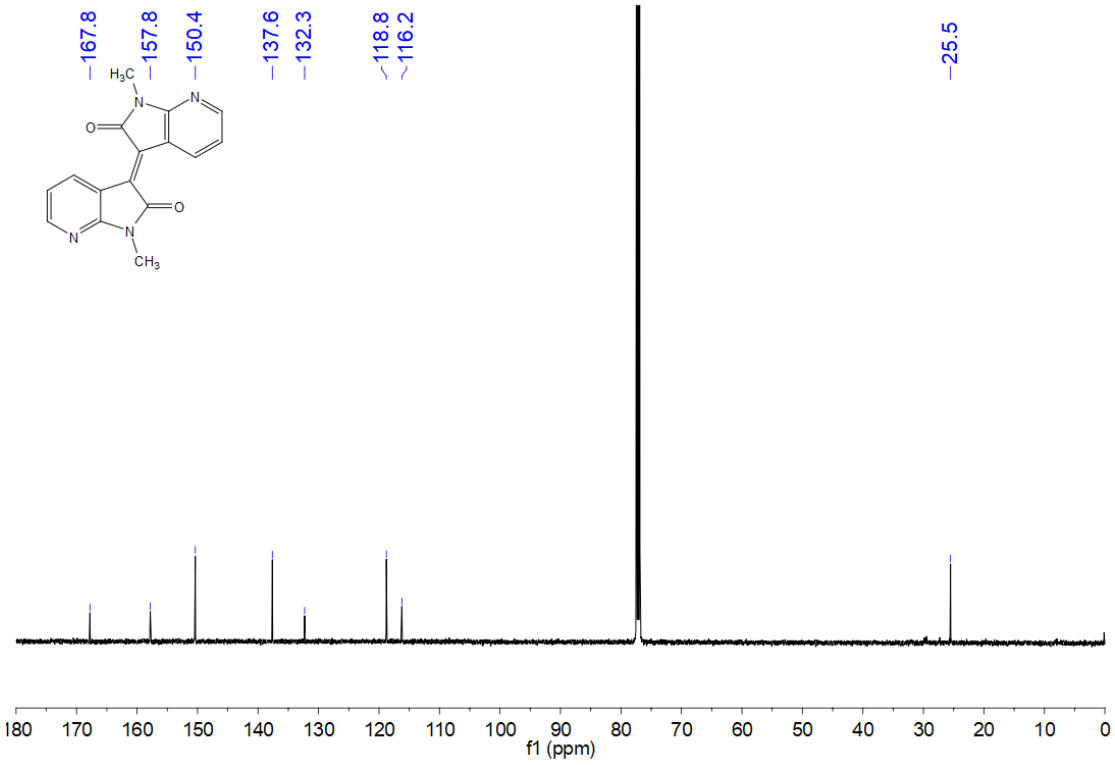
^{13}C NMR spectrum of 3x (101 MHz, $CDCl_3$)



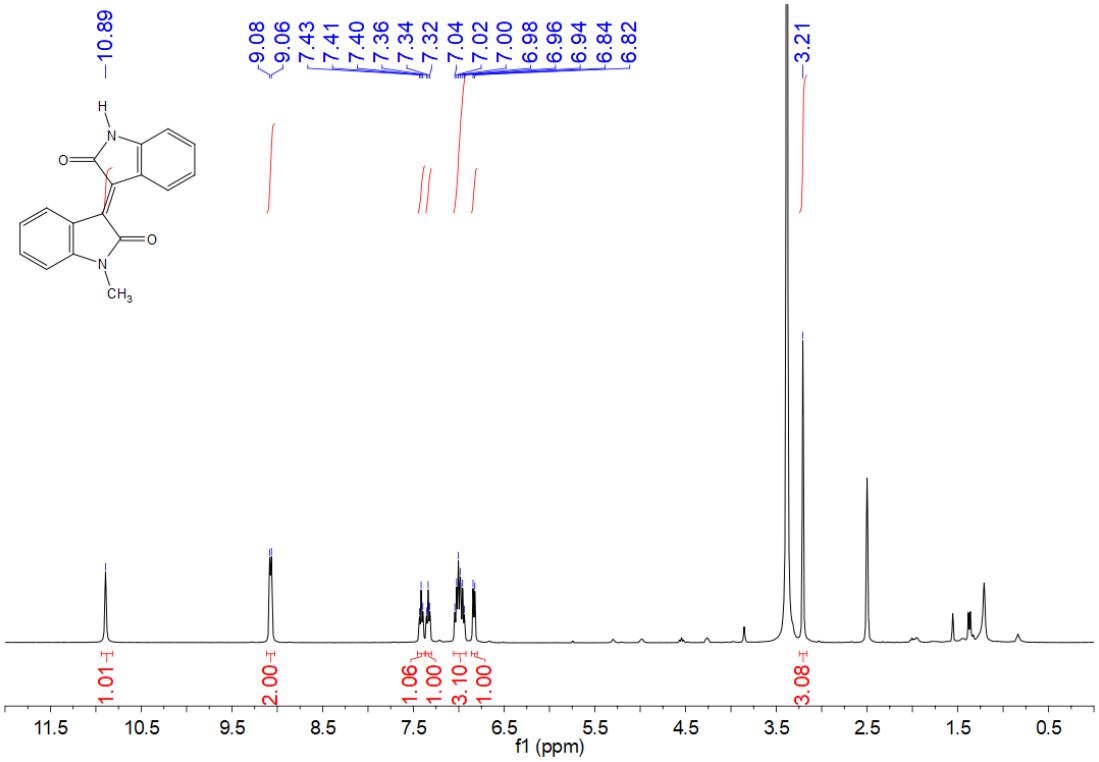
^{1}H NMR spectrum of 3y (400 MHz, DMSO-d_6)



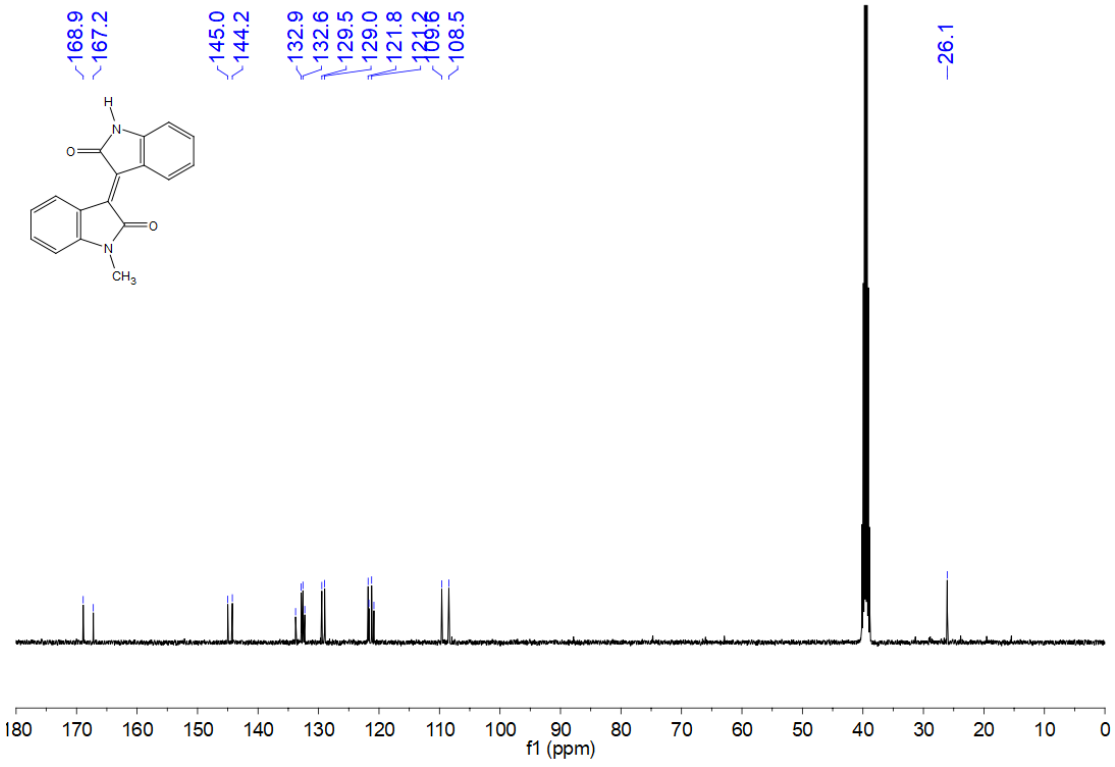
^{1}H NMR spectrum of 3z (400 MHz, CDCl3)



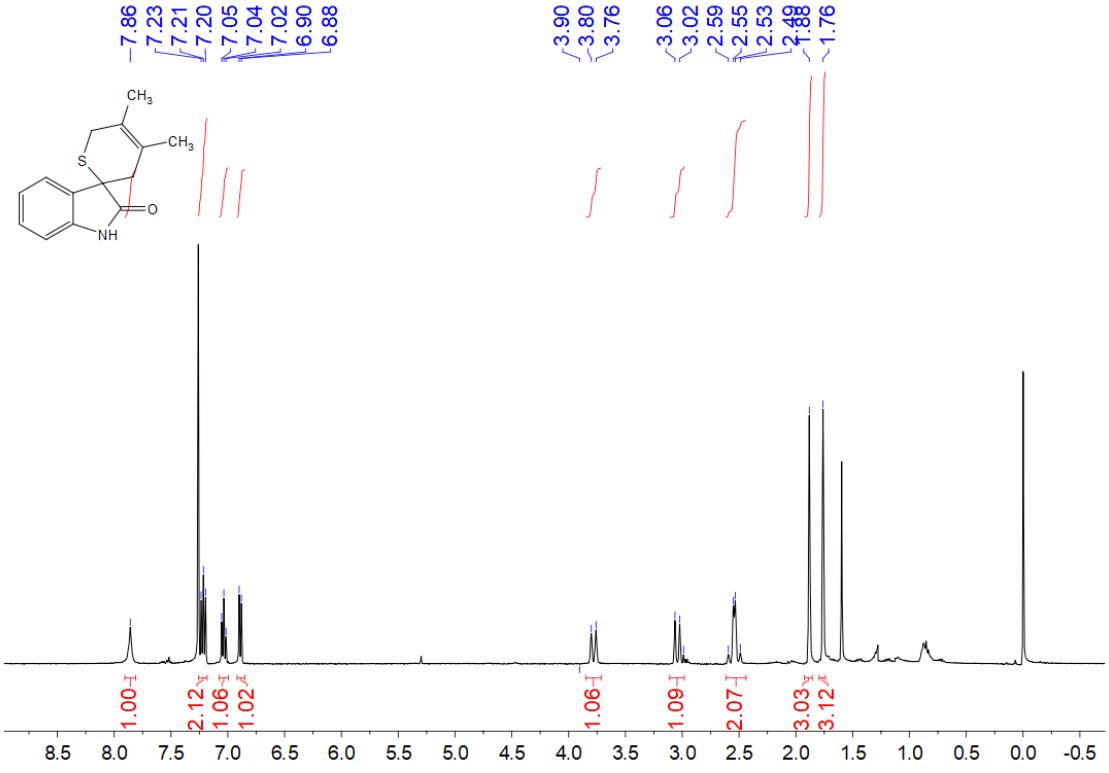
^{13}C NMR spectrum of 3z (126 MHz, CDCl3)



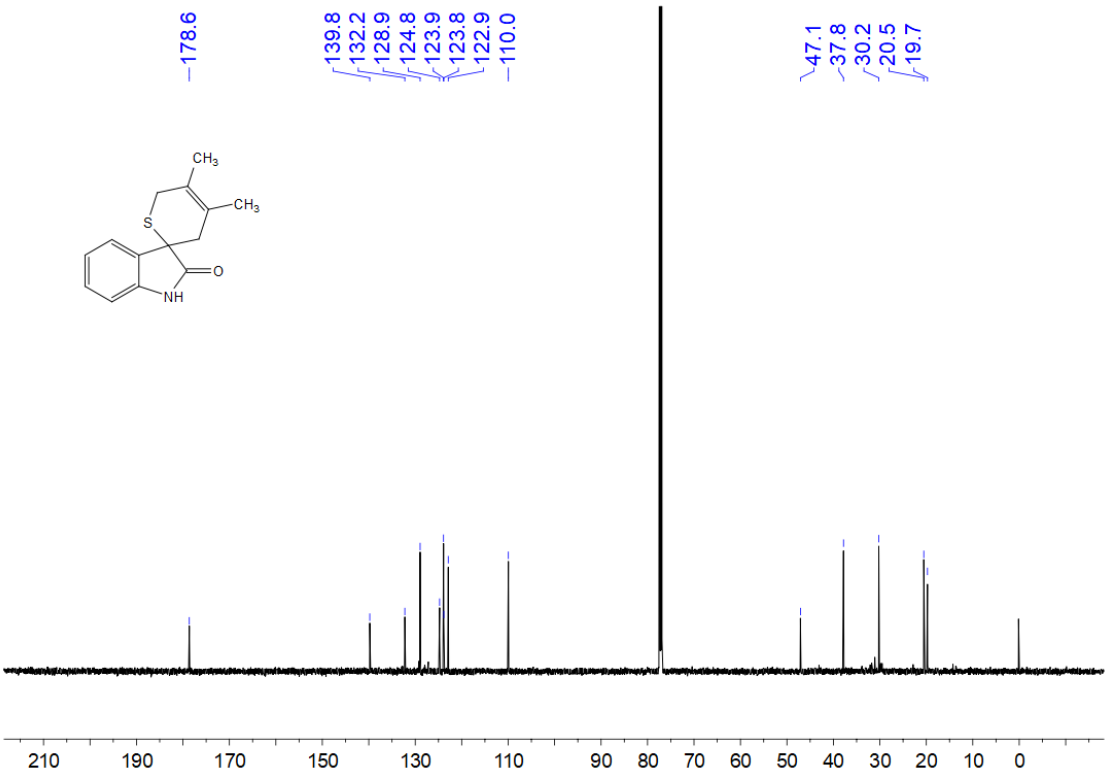
^{1}H NMR spectrum of Meisoindigo (400 MHz, DMSO-d_6)



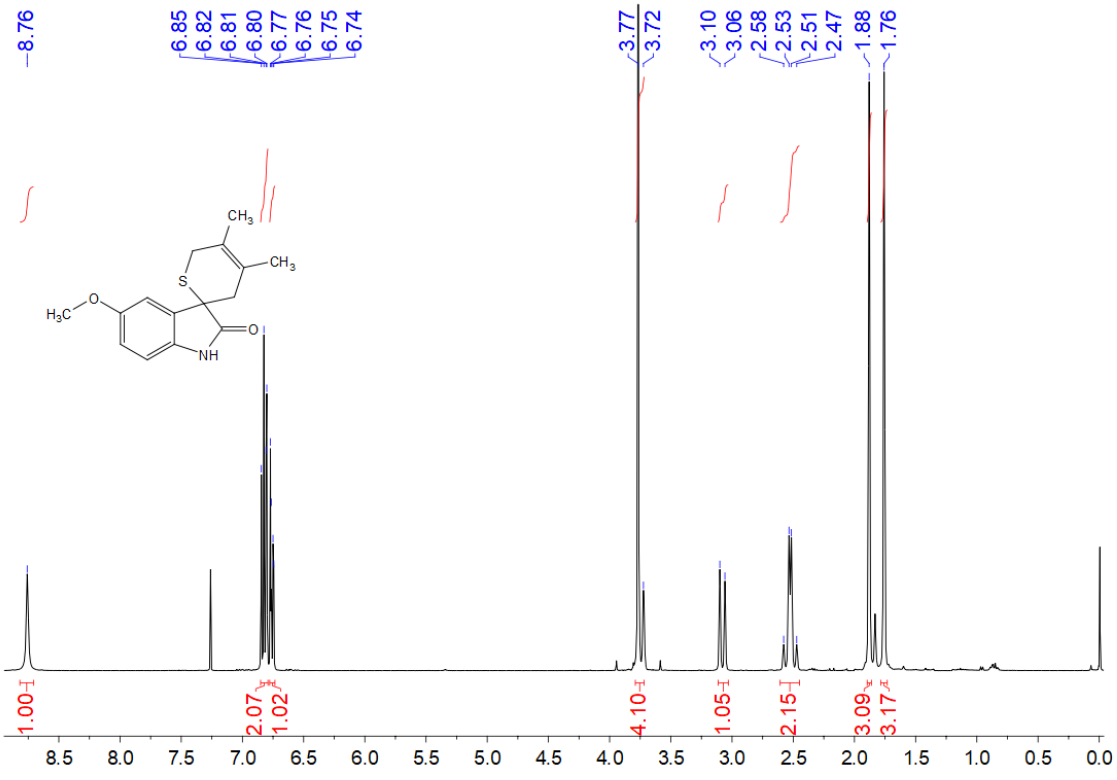
^{13}C NMR spectrum of Meisoindigo (101 MHz, DMSO-d_6)



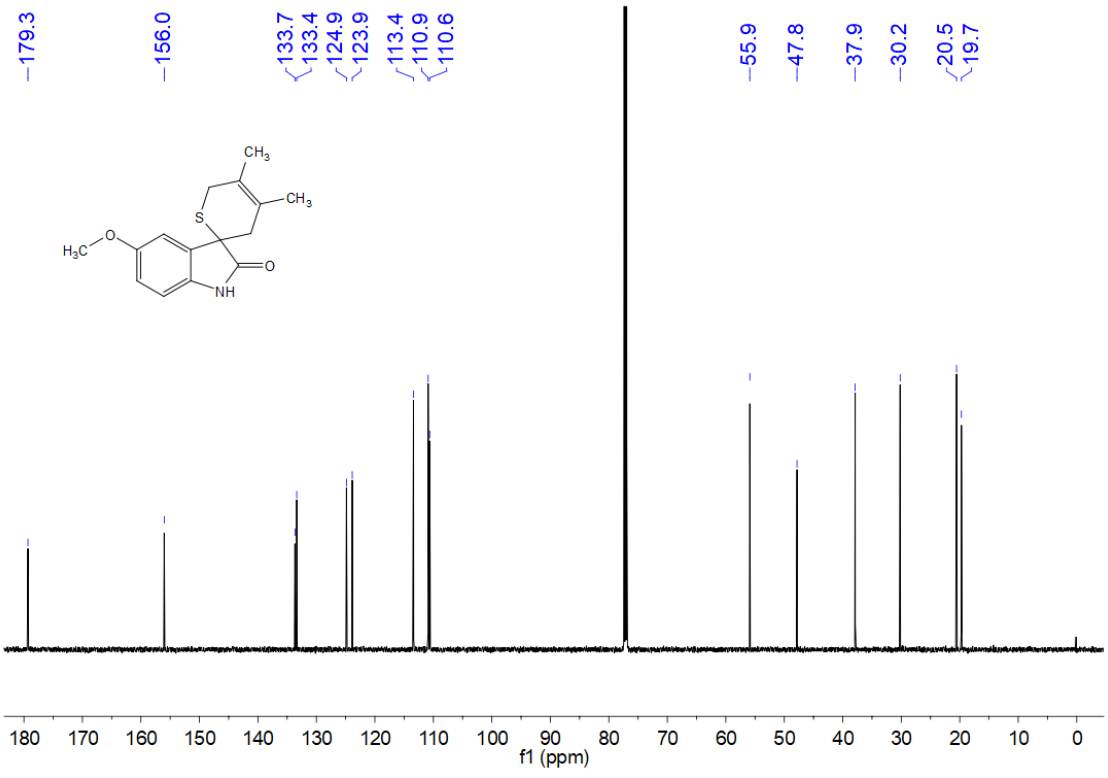
^{1}H NMR spectrum of 4aa (400 MHz, $CDCl_3$)



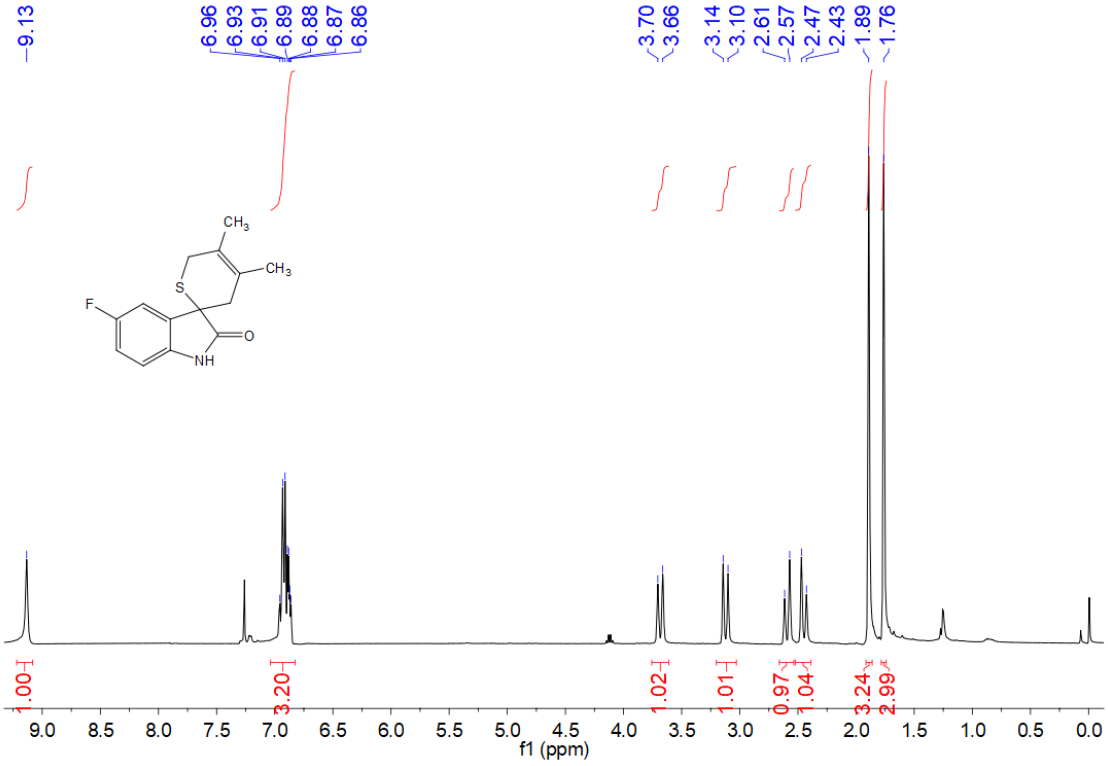
^{13}C NMR spectrum of 4aa (151 MHz, $CDCl_3$)



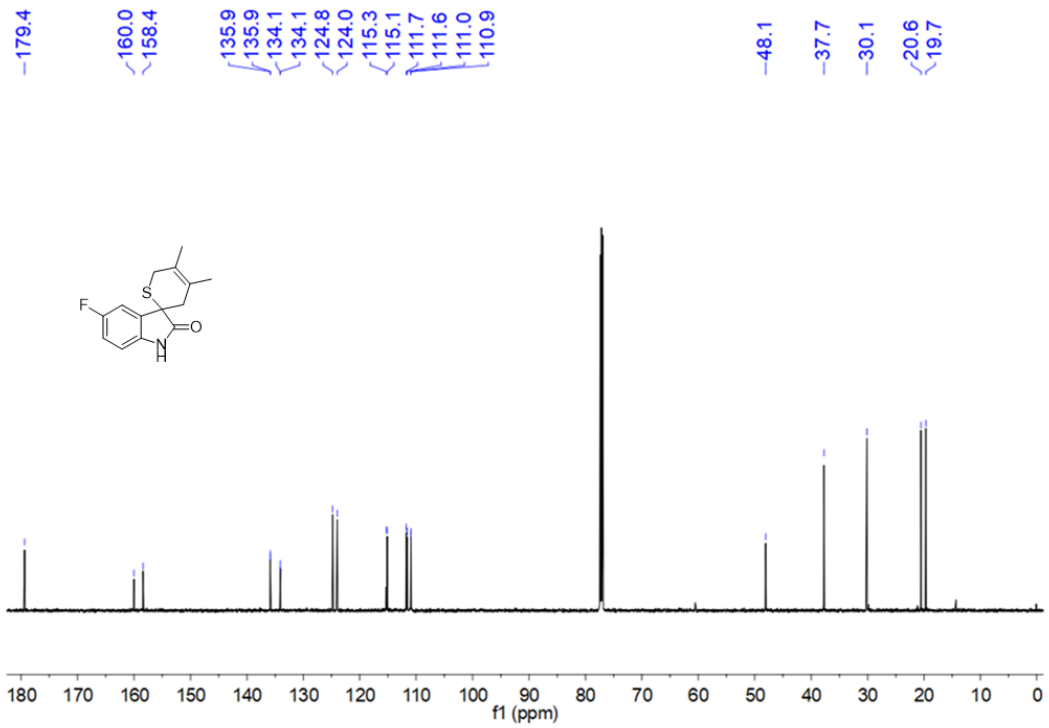
^{1}H NMR spectrum of 4ca (400 MHz, $CDCl_3$)



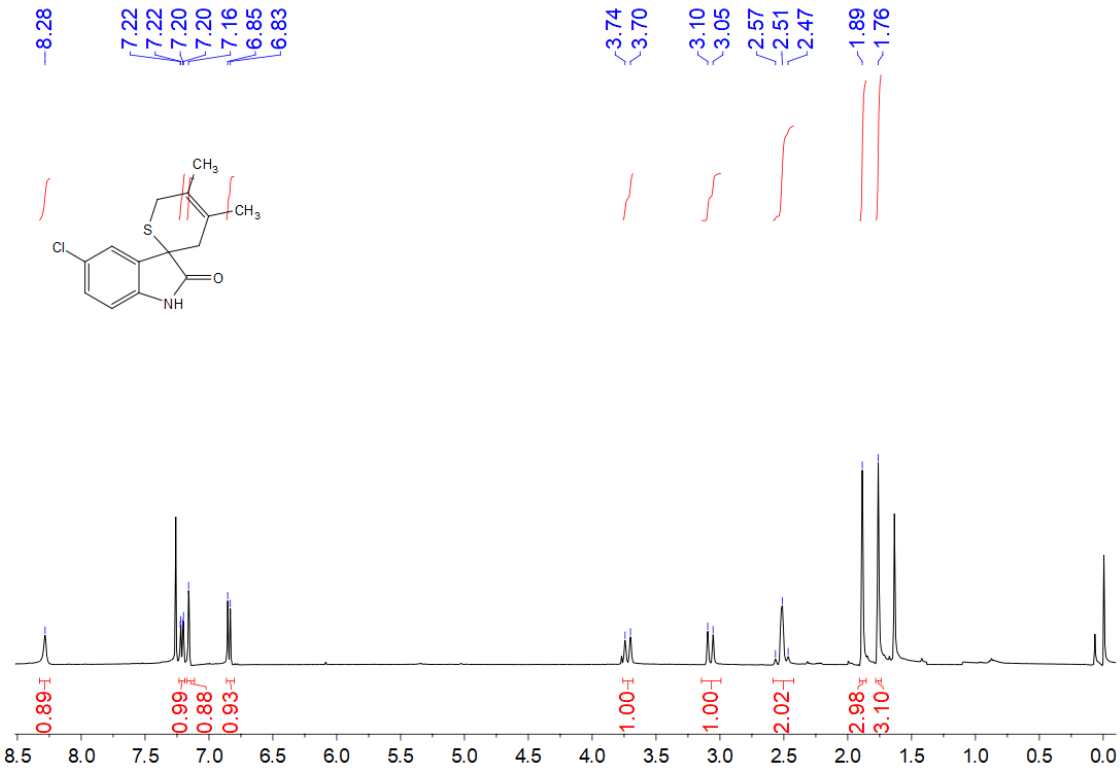
^{13}C NMR spectrum of 4ca (151 MHz, $CDCl_3$)



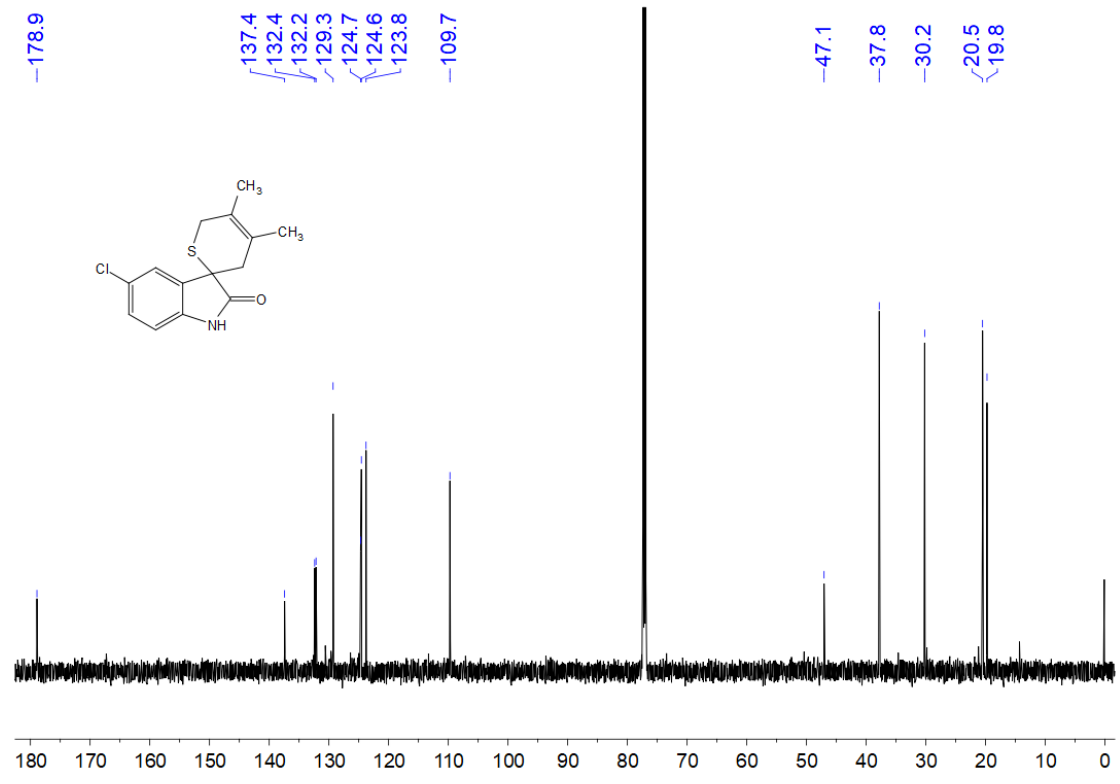
^{1}H NMR spectrum of 4da (400 MHz, $CDCl_3$)



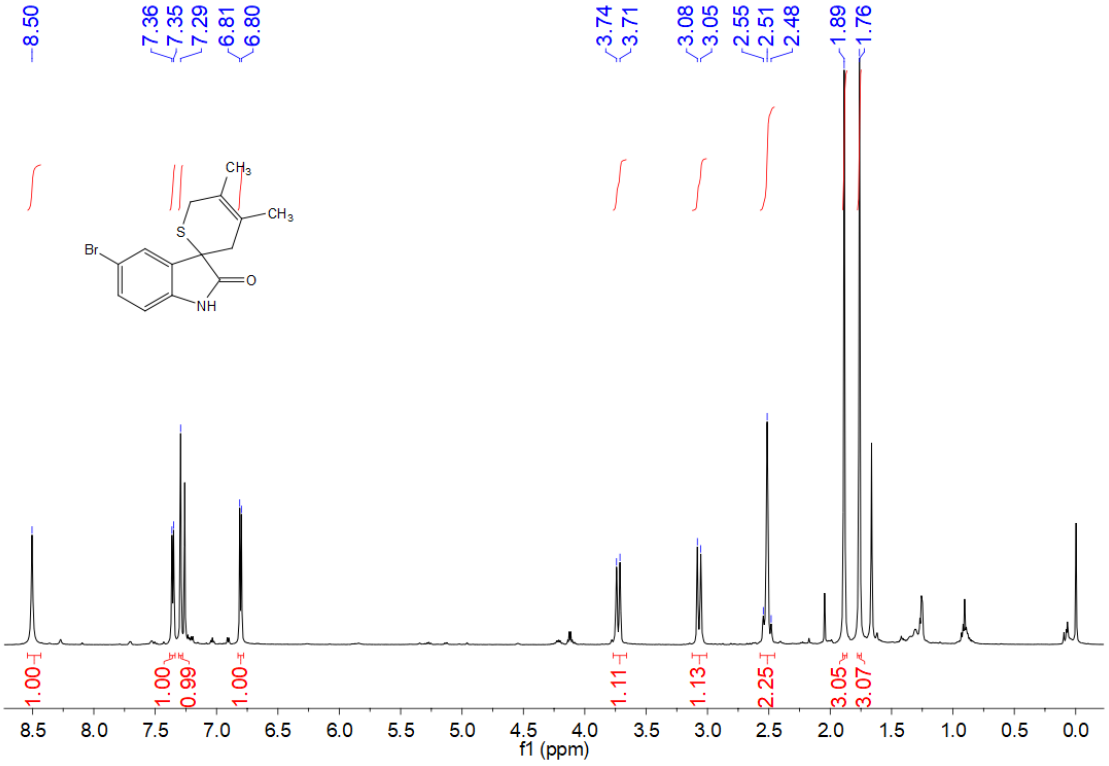
^{13}C NMR spectrum of 4da (151 MHz, $CDCl_3$)



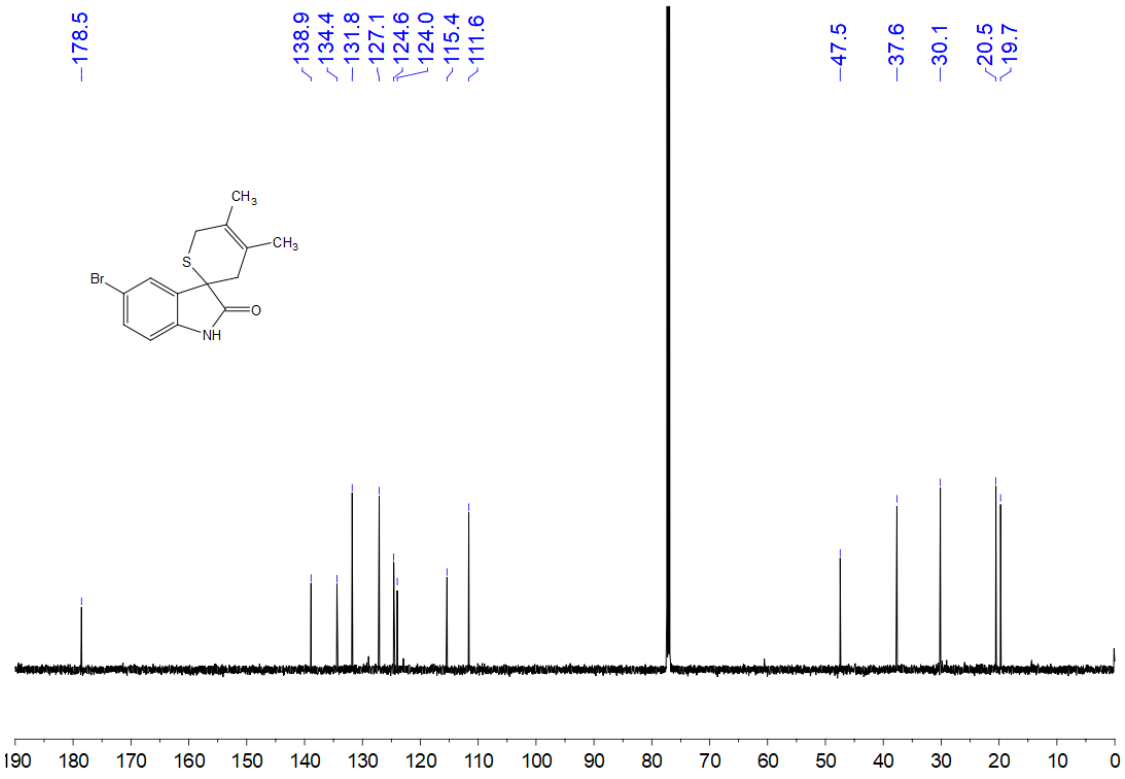
^{1}H NMR spectrum of 4ea (400 MHz, $CDCl_3$)



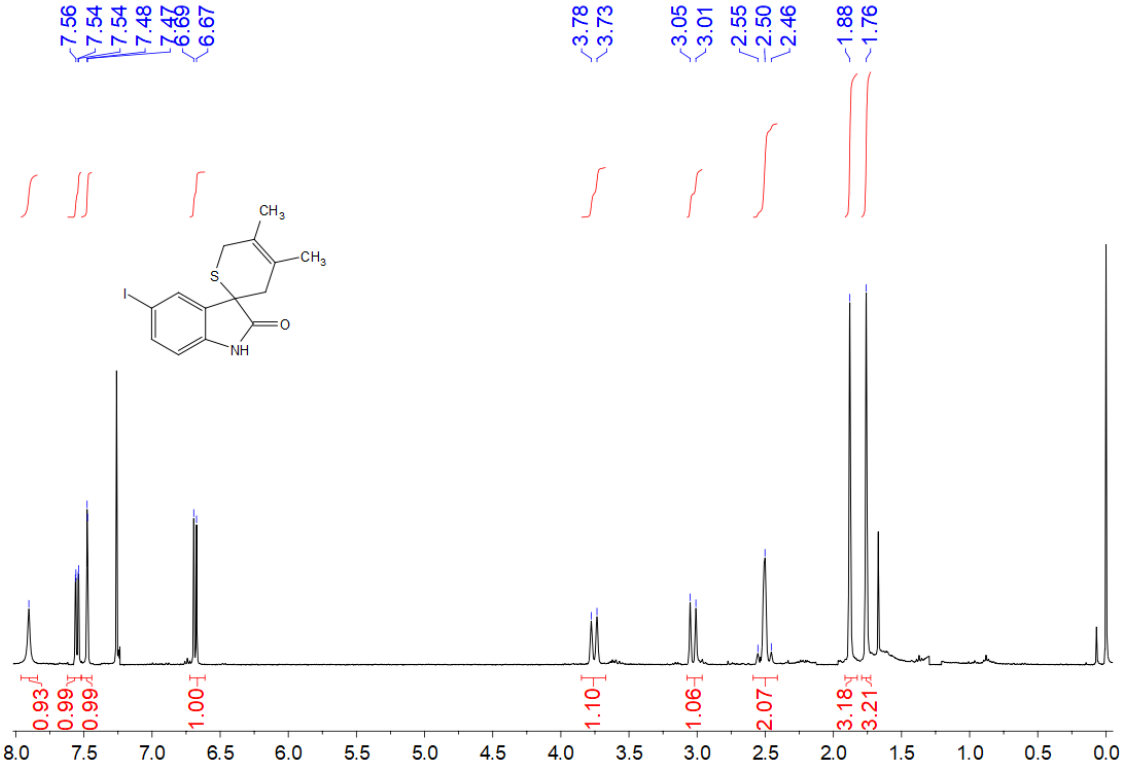
^{13}C NMR spectrum of 4ea (151 MHz, $CDCl_3$)



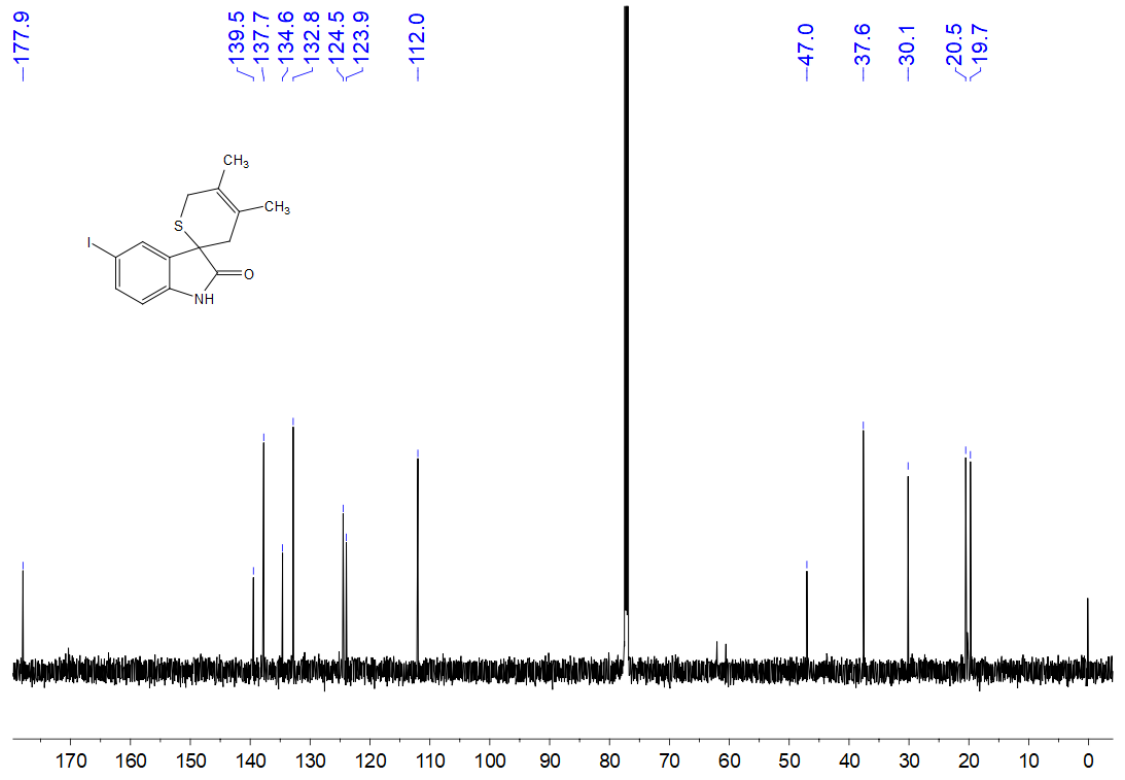
[1]H NMR spectrum of 4fa (600 MHz, $CDCl_3$)



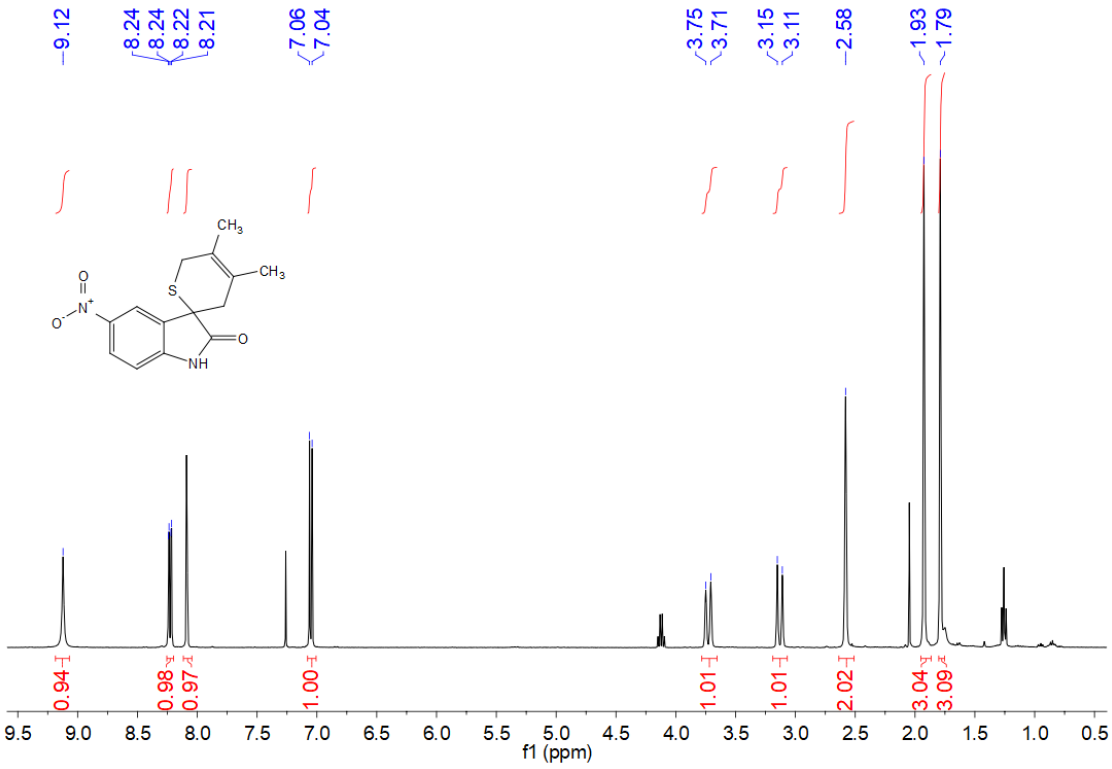
[13]C NMR spectrum of 4fa (151 MHz, $CDCl_3$)



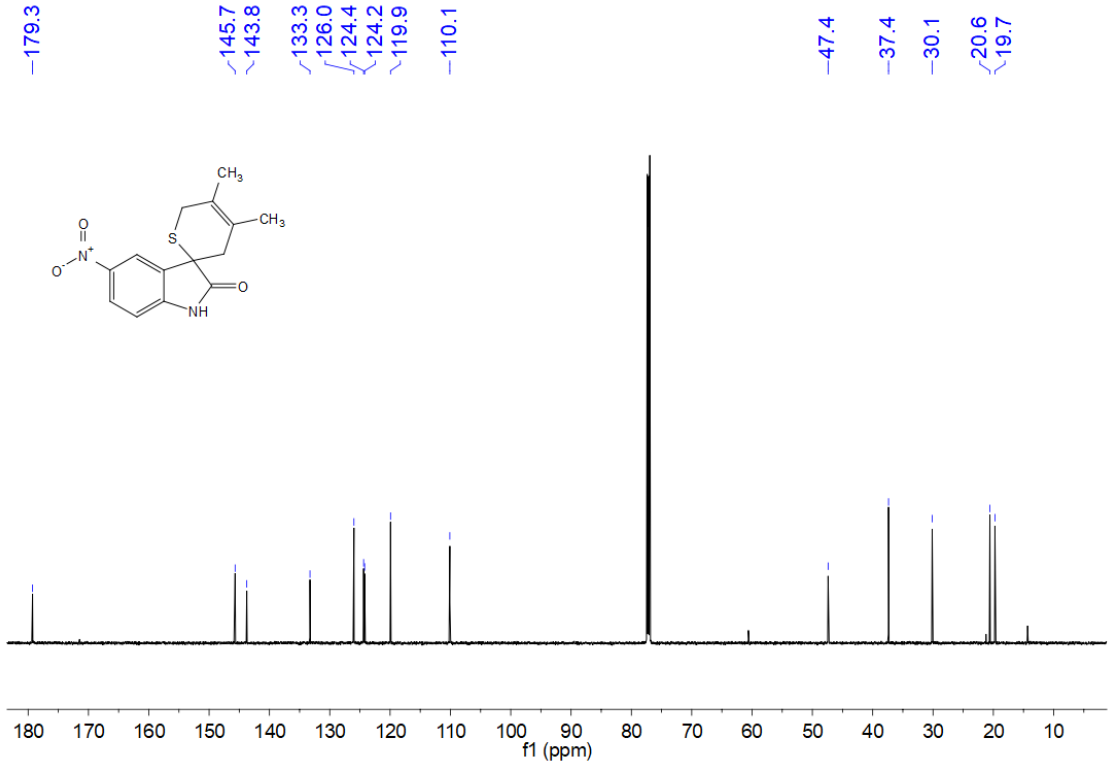
^{1}H NMR spectrum of 4ga (400 MHz, $CDCl_3$)



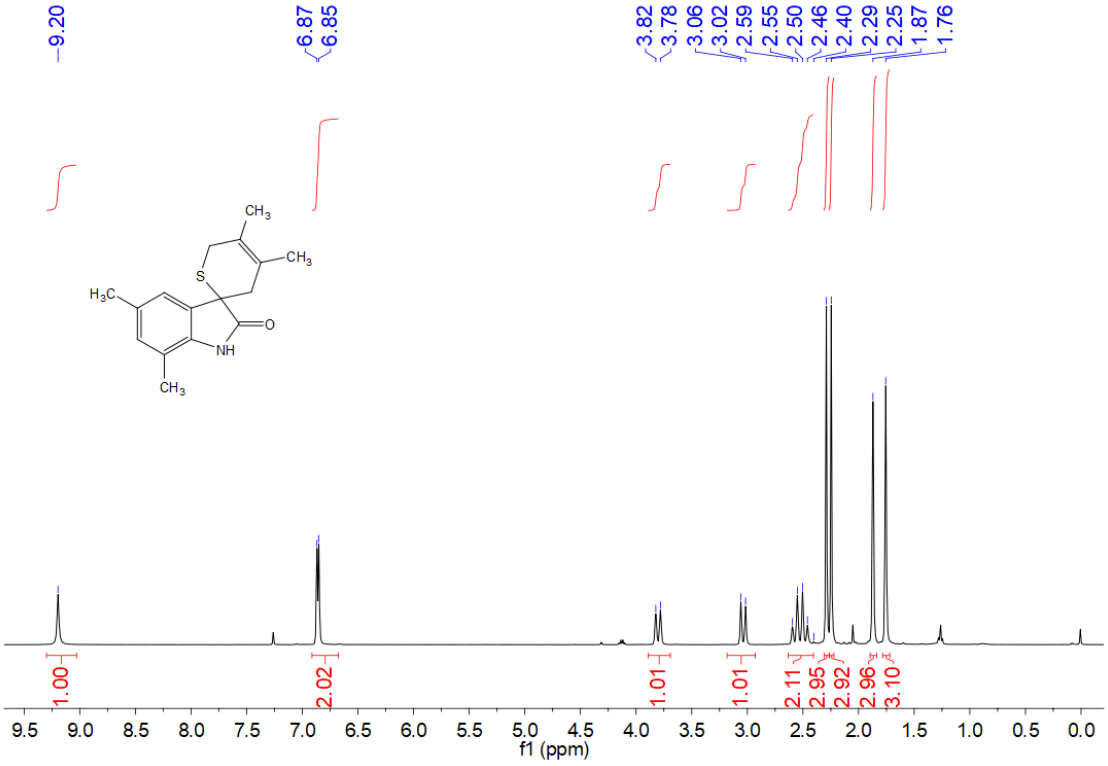
^{13}C NMR spectrum of 4ga (151 MHz, $CDCl_3$)



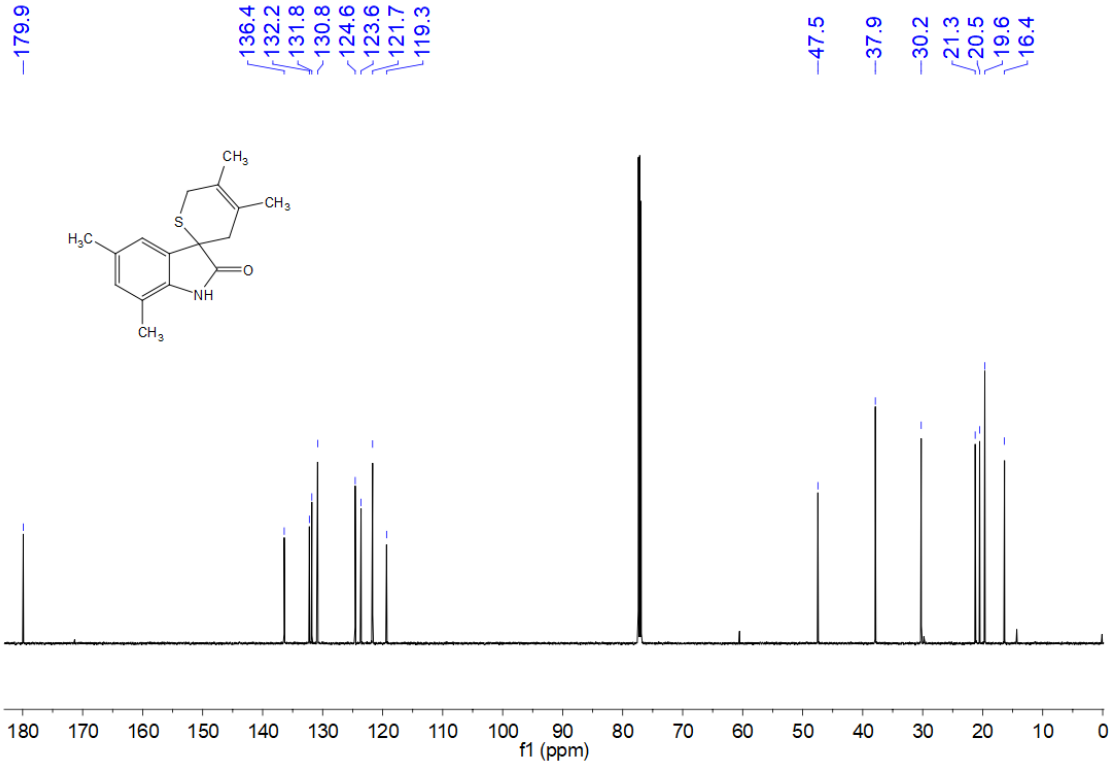
^{1}H NMR spectrum of 4a*a (400 MHz, $CDCl_3$)



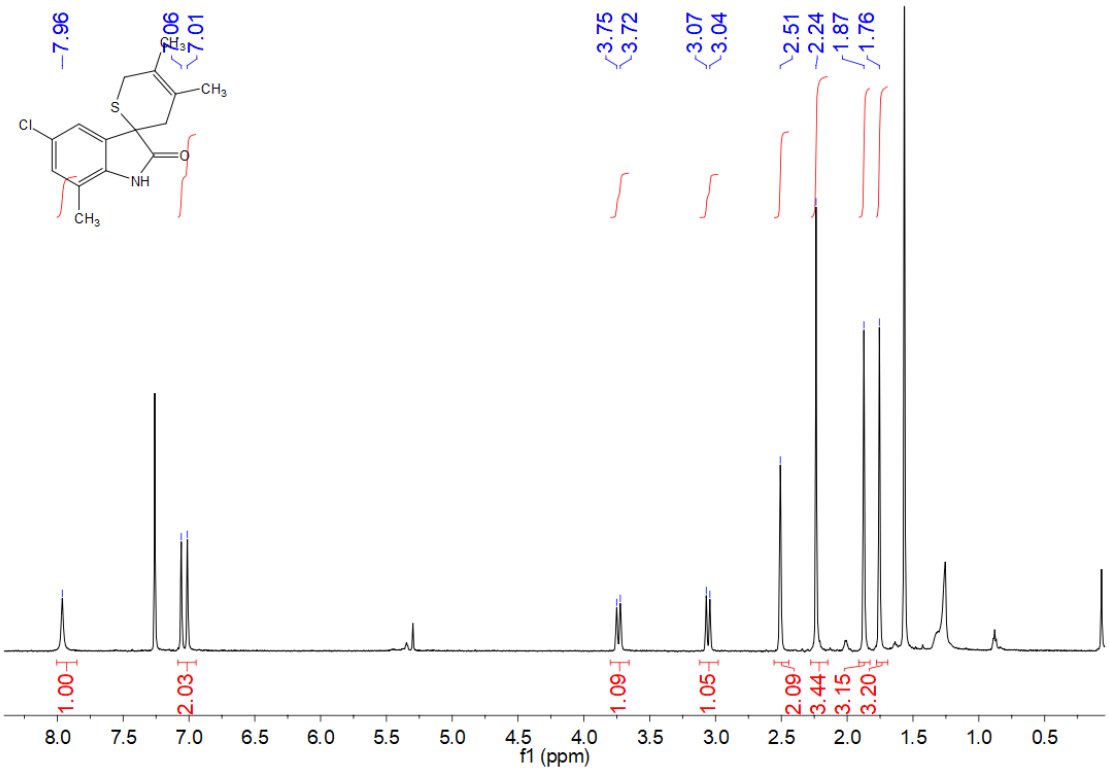
^{13}C NMR spectrum of 4a*a (151 MHz, $CDCl_3$)



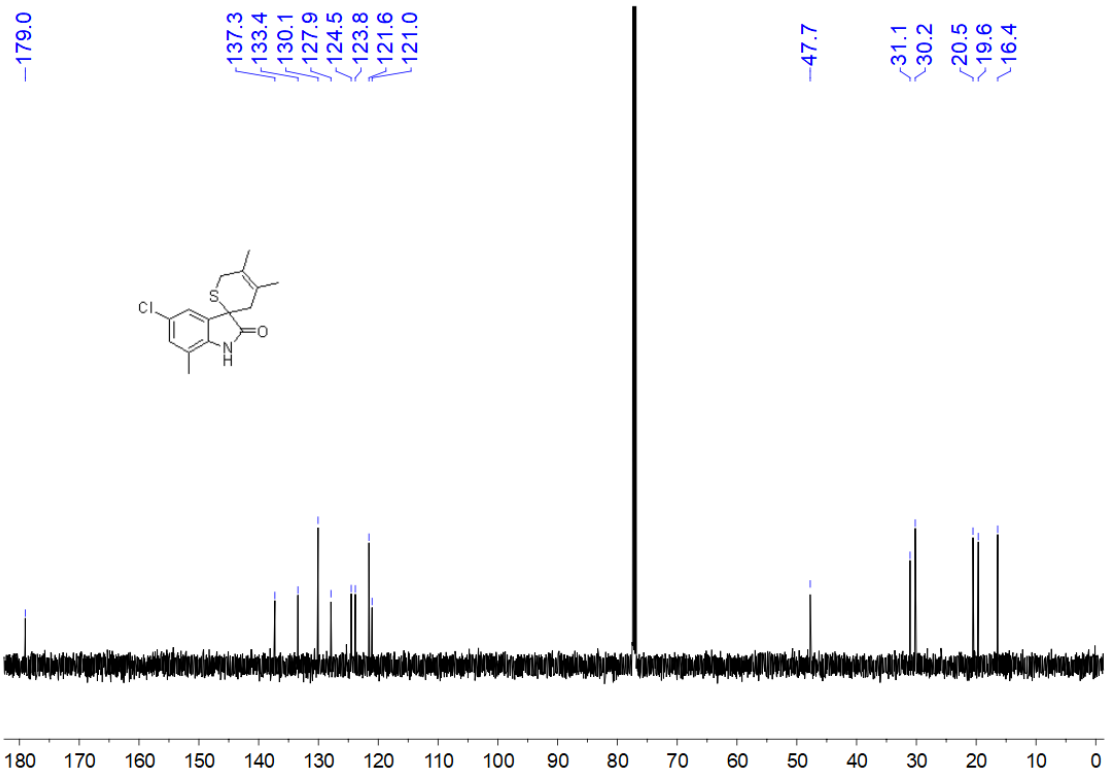
^{1}H NMR spectrum of 4b*a (400 MHz, $CDCl_3$)



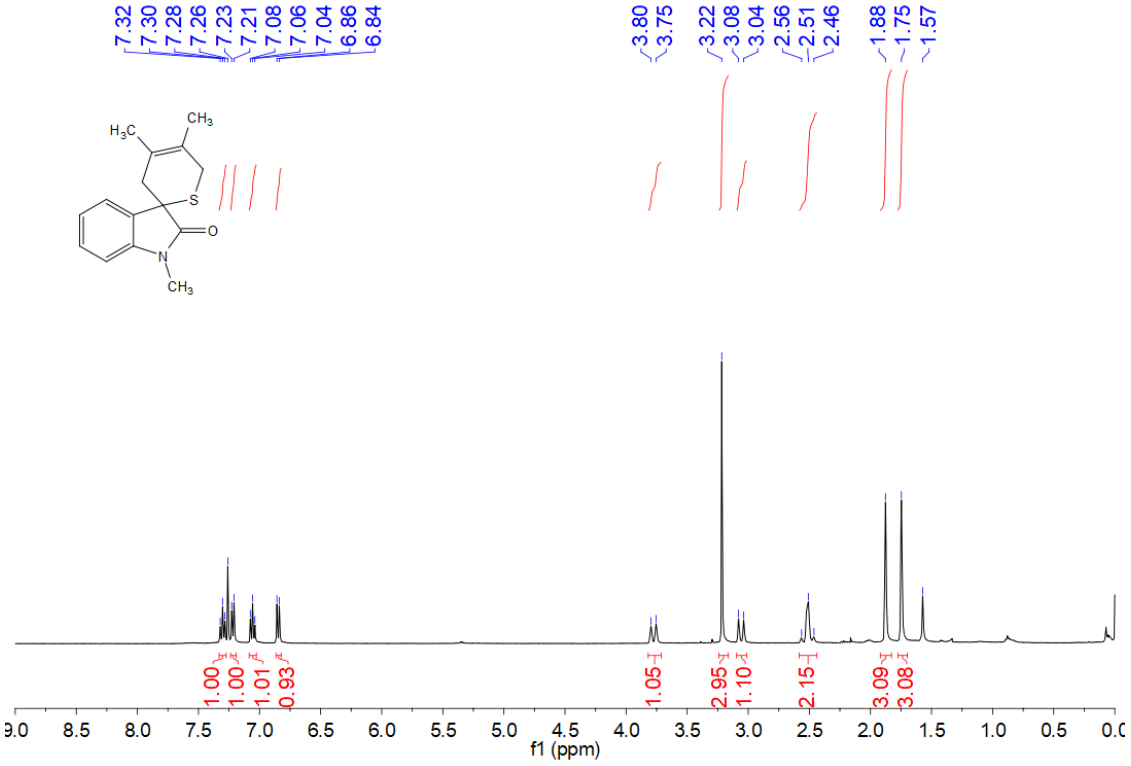
^{13}C NMR spectrum of 4b*a (151 MHz, $CDCl_3$)



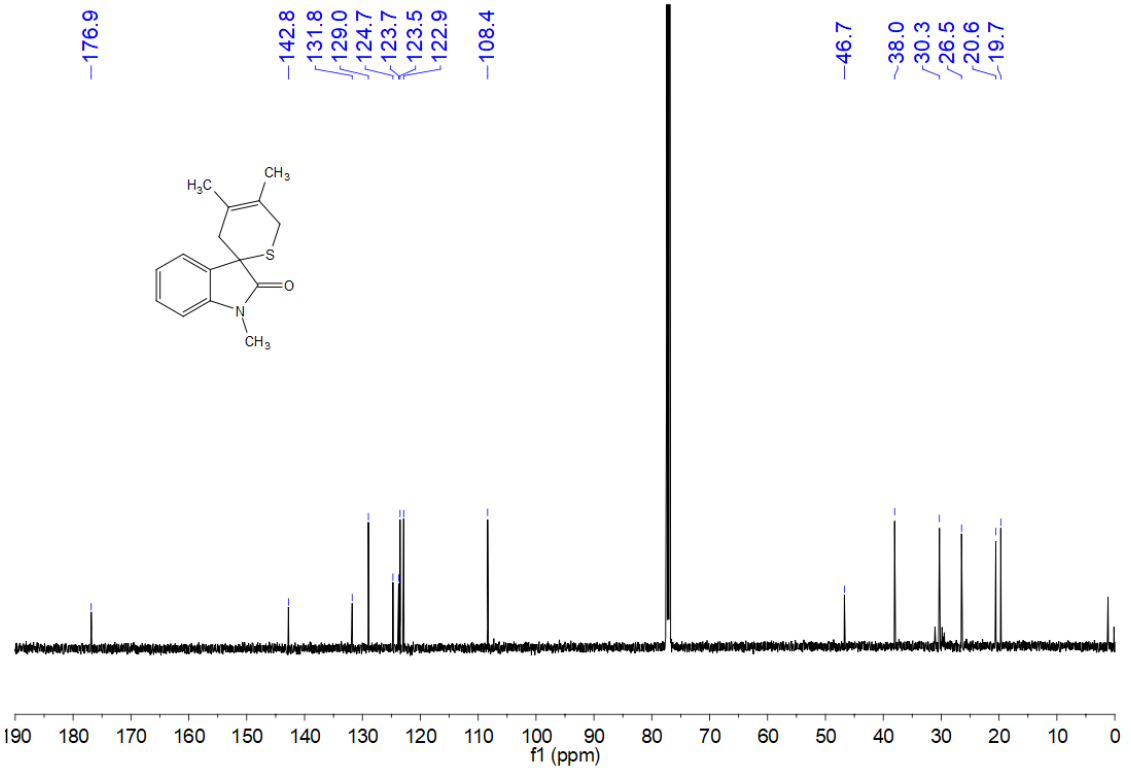
^{1}H NMR spectrum of 4c*a (600 MHz, $CDCl_3$)



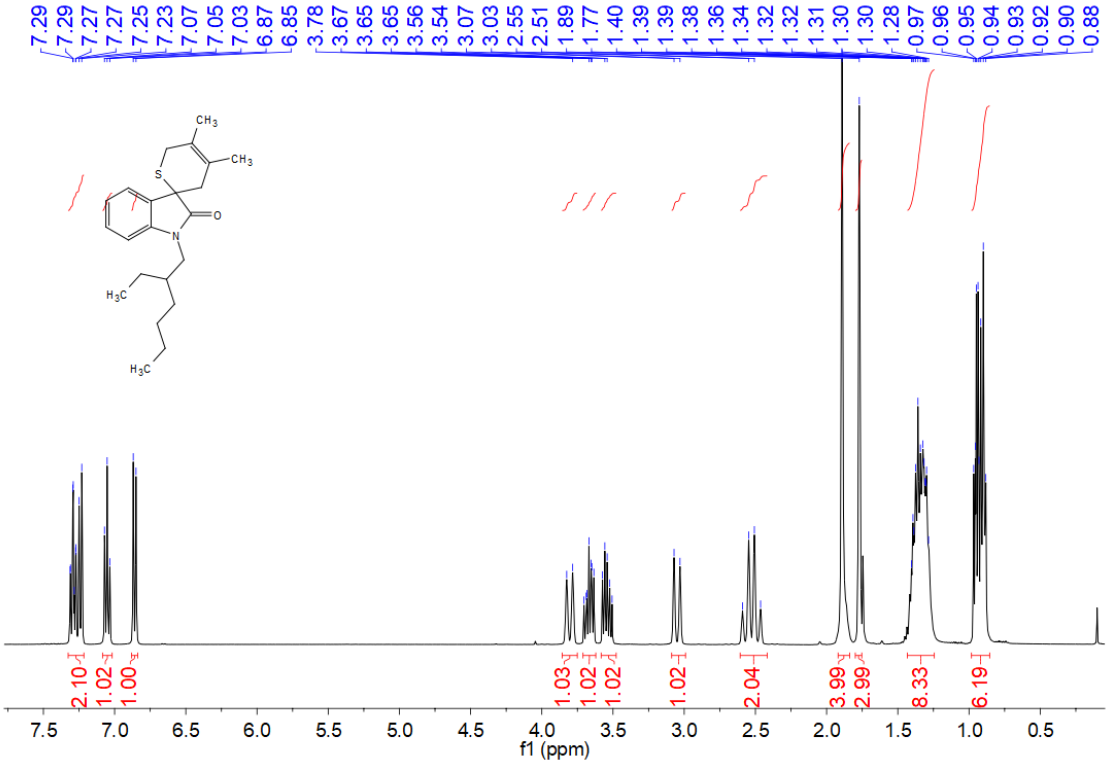
^{13}C NMR spectrum of 4c*a (151 MHz, $CDCl_3$)



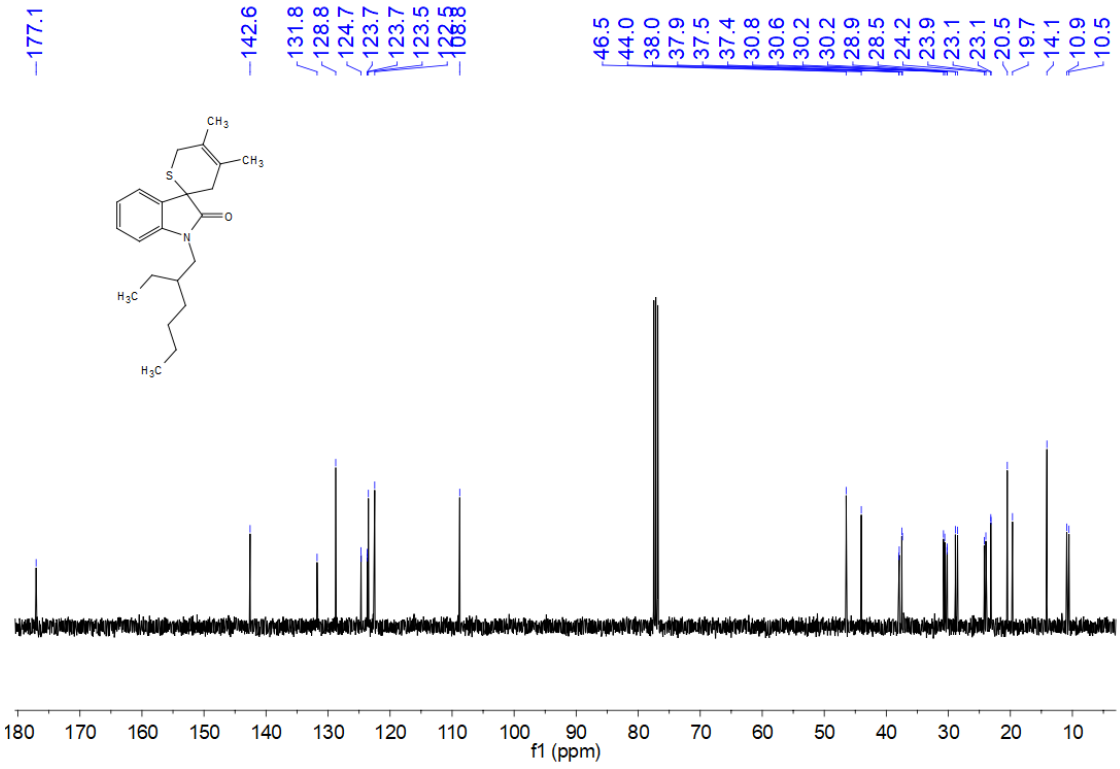
^{1}H NMR spectrum of 4pa (400 MHz, $CDCl_3$)



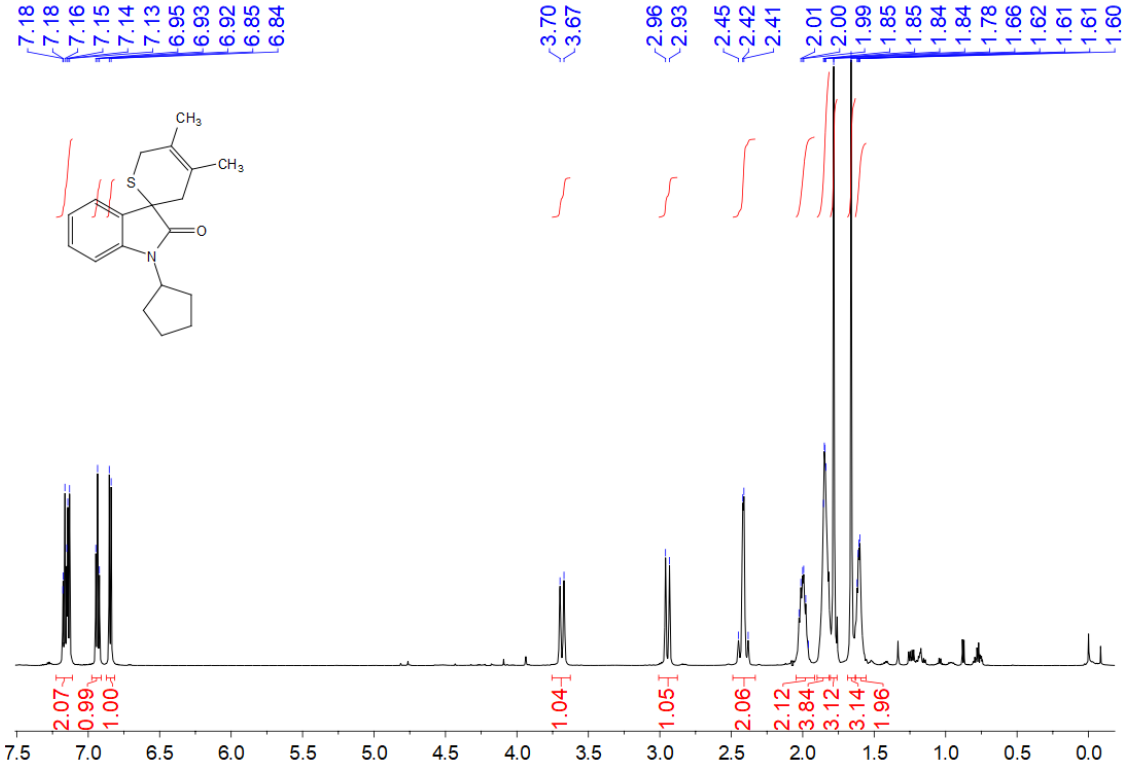
^{13}C NMR spectrum of 4pa (126 MHz, $CDCl_3$)



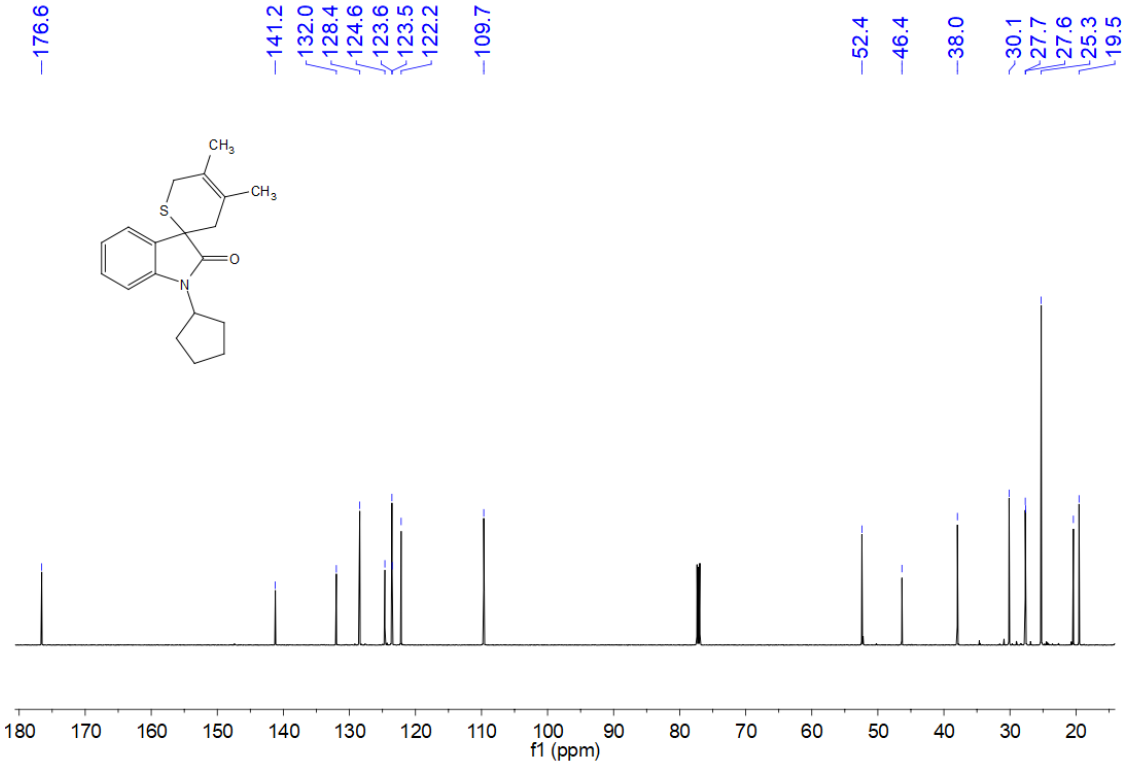
^{1}H NMR spectrum of 4qa (400 MHz, $CDCl_3$)



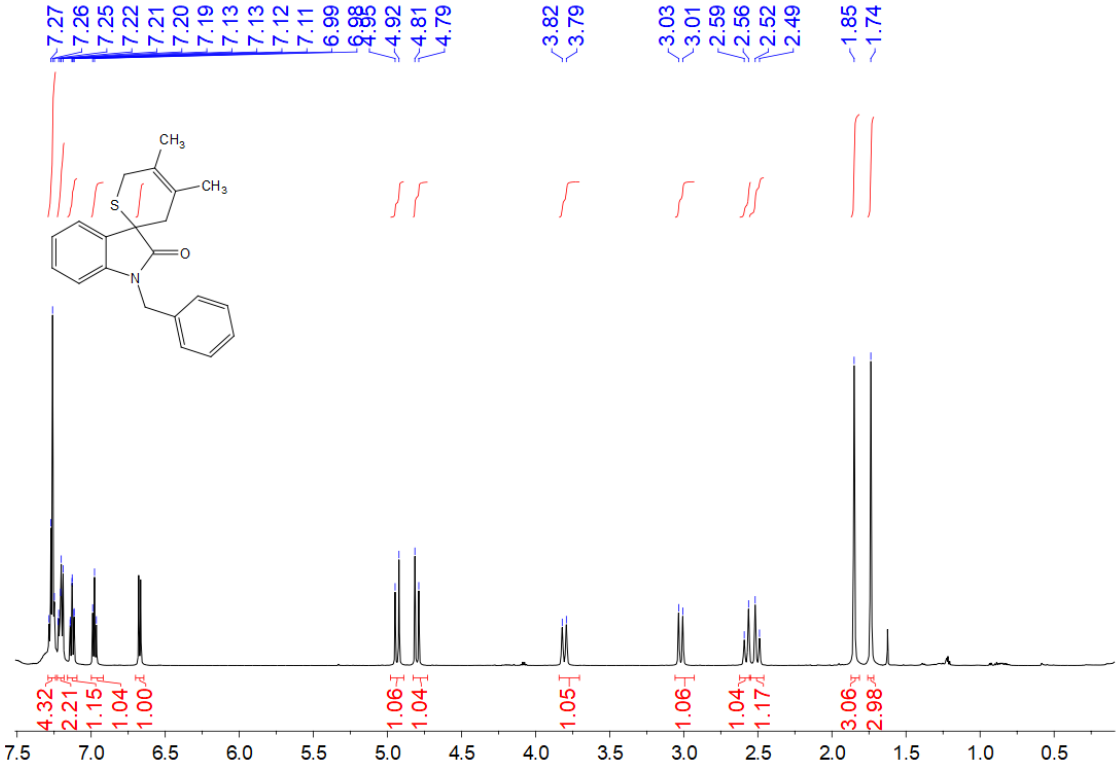
^{13}C NMR spectrum of 4qa (101 MHz, $CDCl_3$)



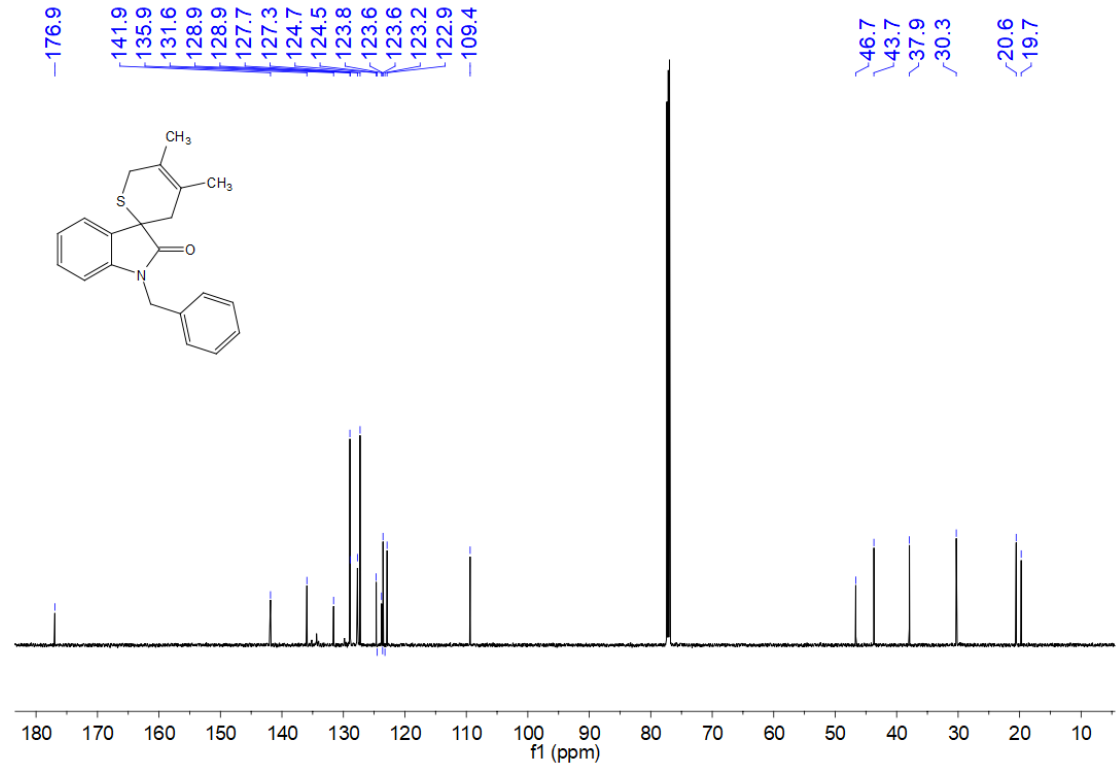
^{1}H NMR spectrum of 4ra (600 MHz, $CDCl_3$)



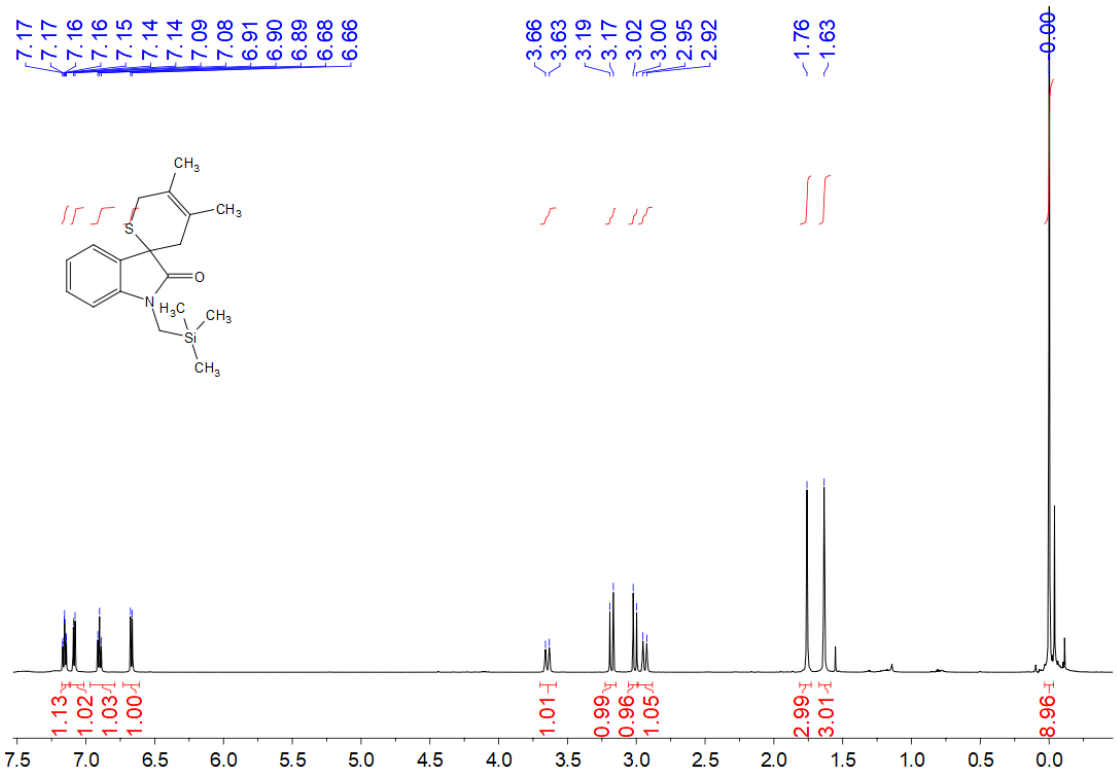
^{13}C NMR spectrum of 4ra (151 MHz, $CDCl_3$)



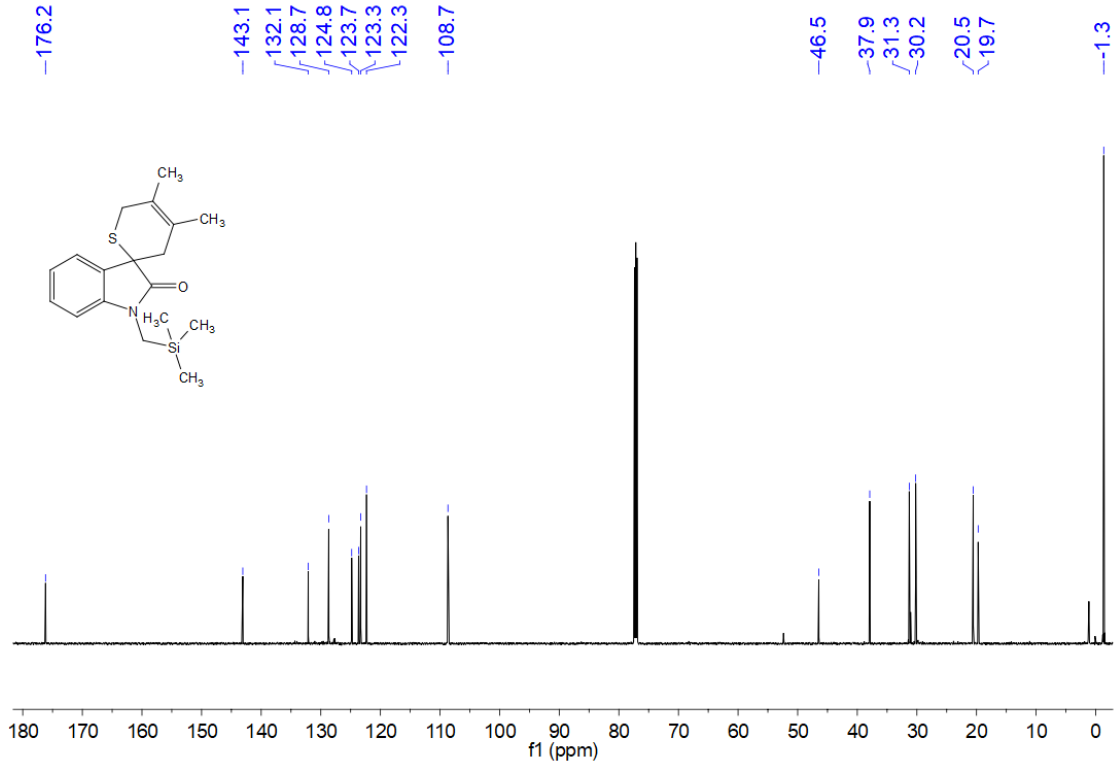
^{1}H NMR spectrum of 4sa (600 MHz, $CDCl_3$)



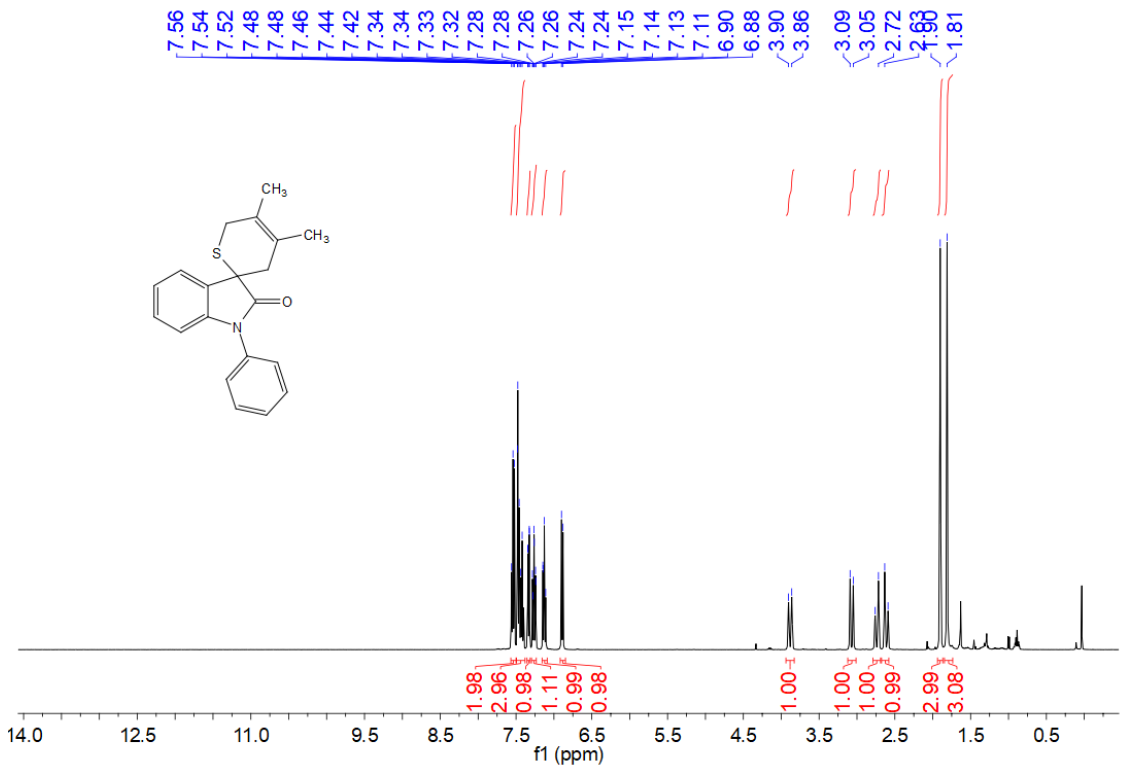
^{13}C NMR spectrum of 4sa (151MHz, $CDCl_3$)



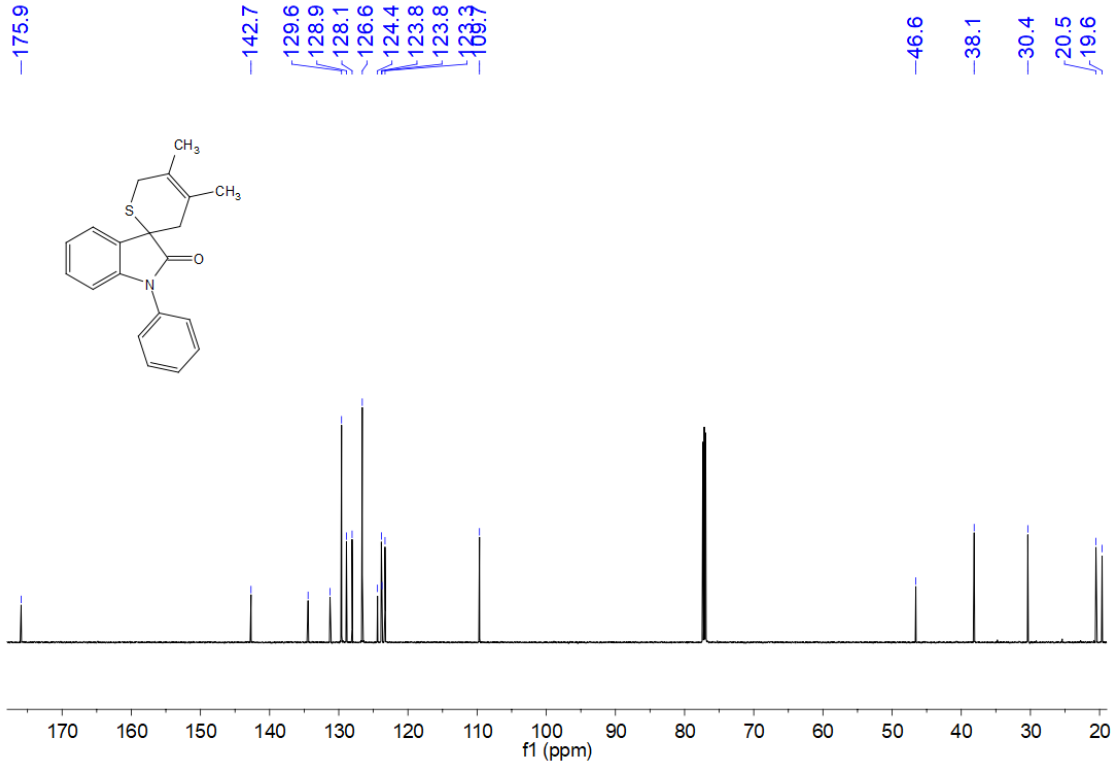
^{1}H NMR spectrum of 4va (600 MHz, $CDCl_3$)



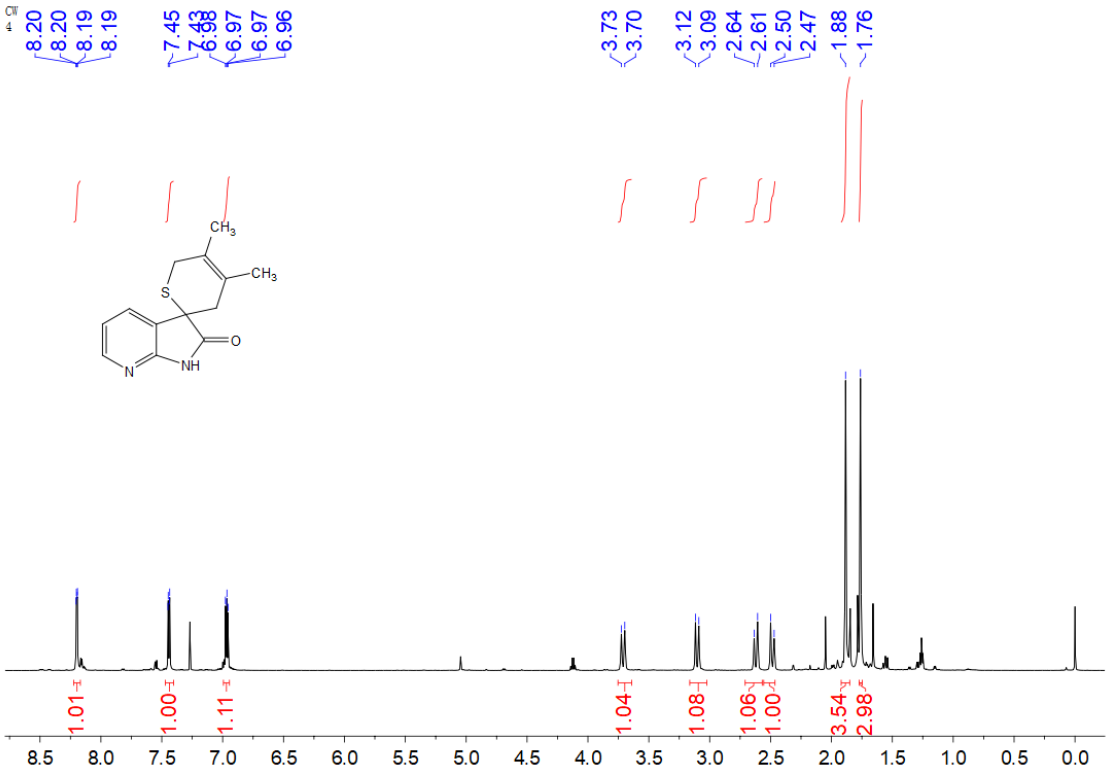
^{13}C NMR spectrum of 4va (151 MHz, $CDCl_3$)



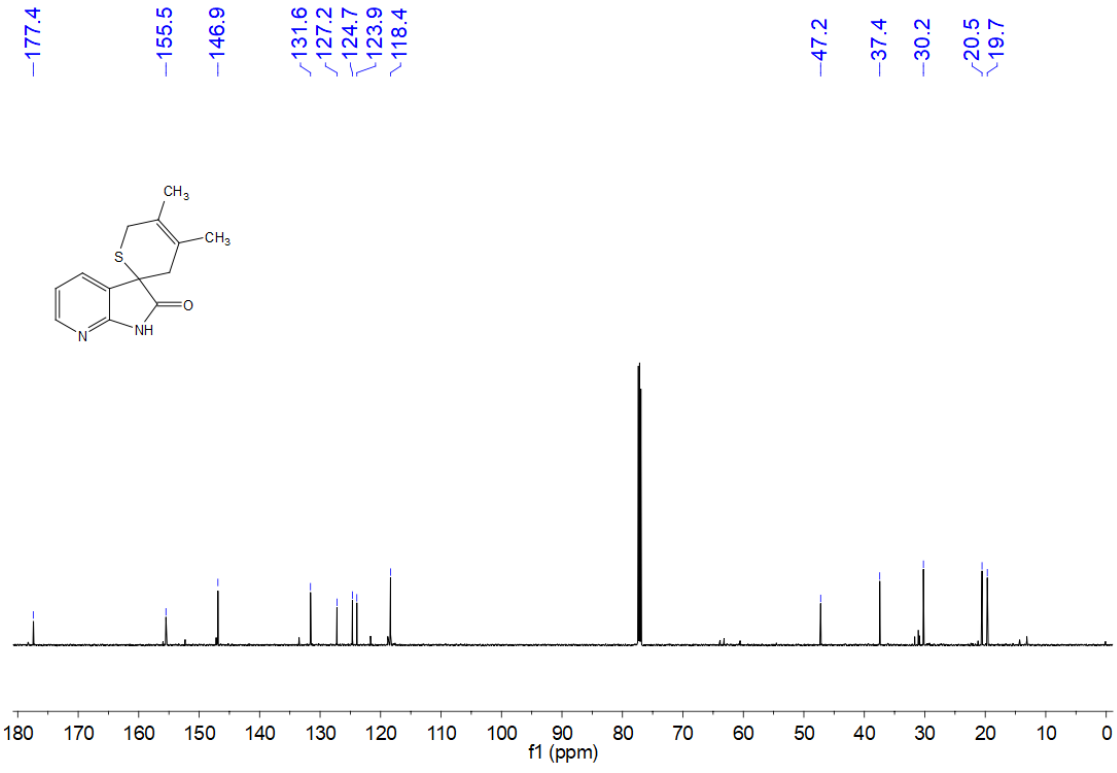
^{1}H NMR spectrum of 4wa (400 MHz, $CDCl_3$)



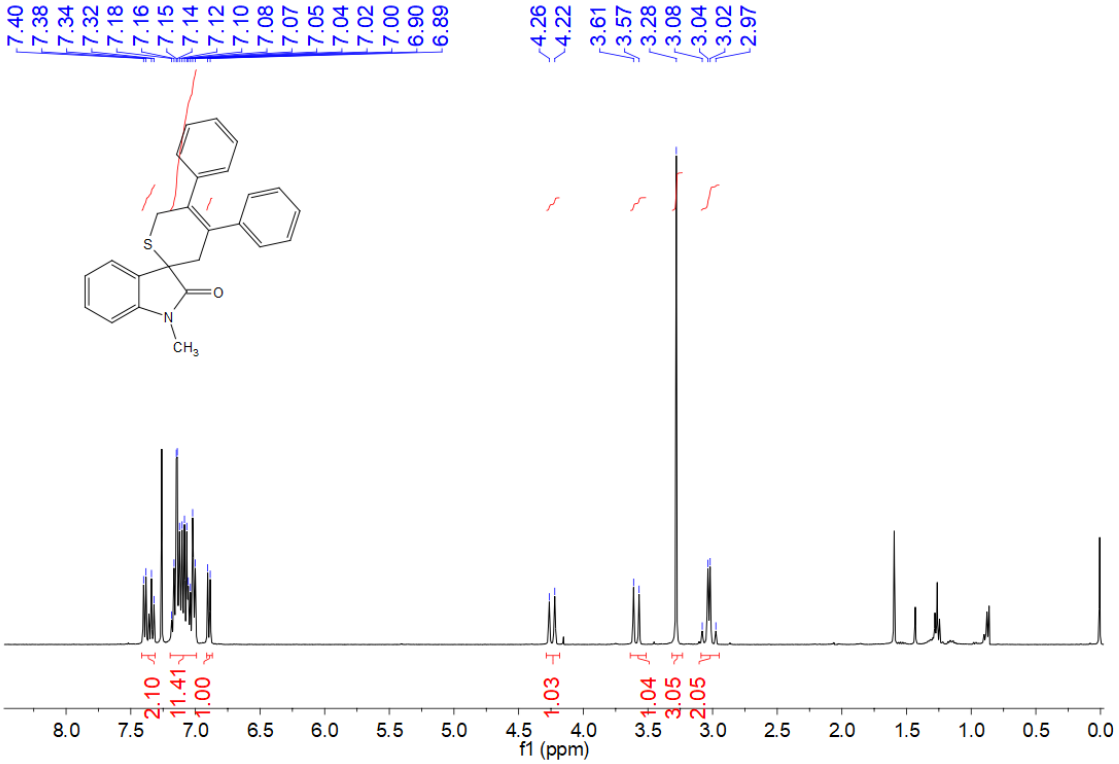
^{13}C NMR spectrum of 4wa (151 MHz, $CDCl_3$)



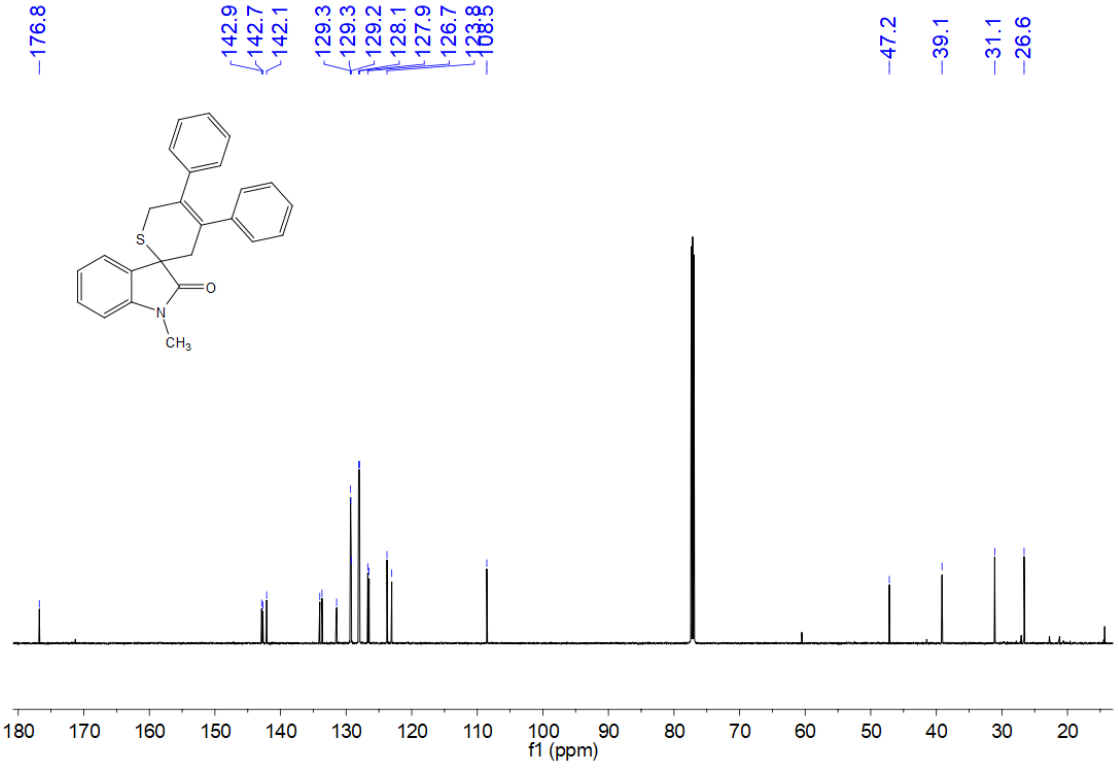
^{1}H NMR spectrum of 4d*a (600 MHz, $CDCl_3$)



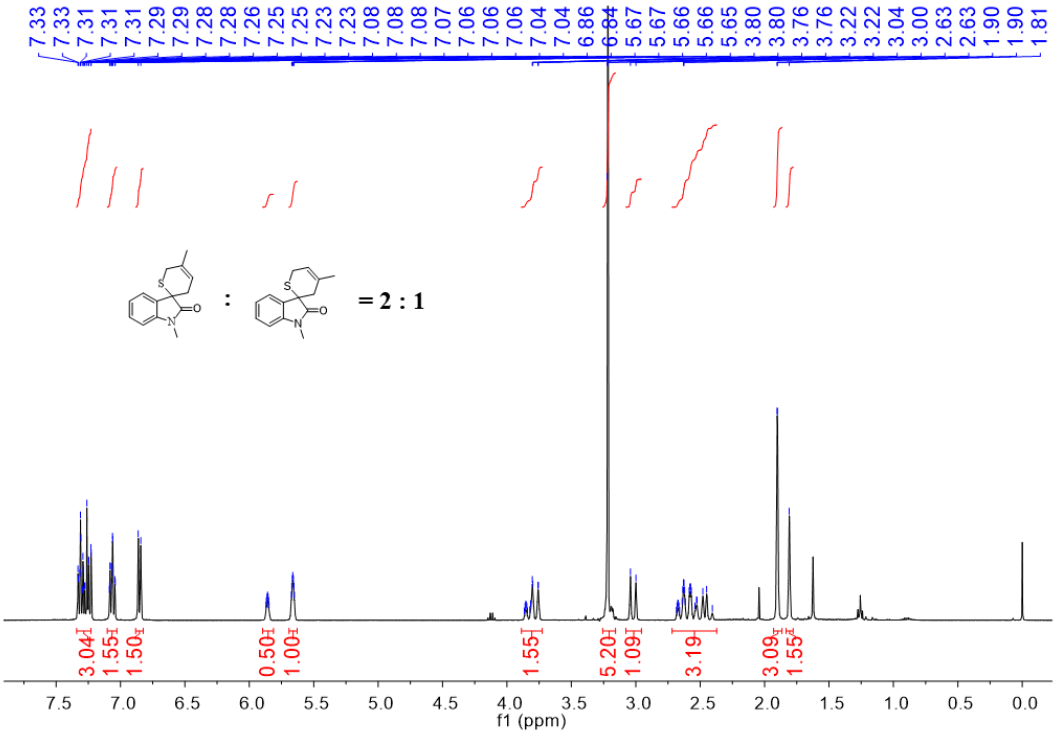
^{13}C NMR spectrum of 4d'a (151 MHz, $CDCl_3$)



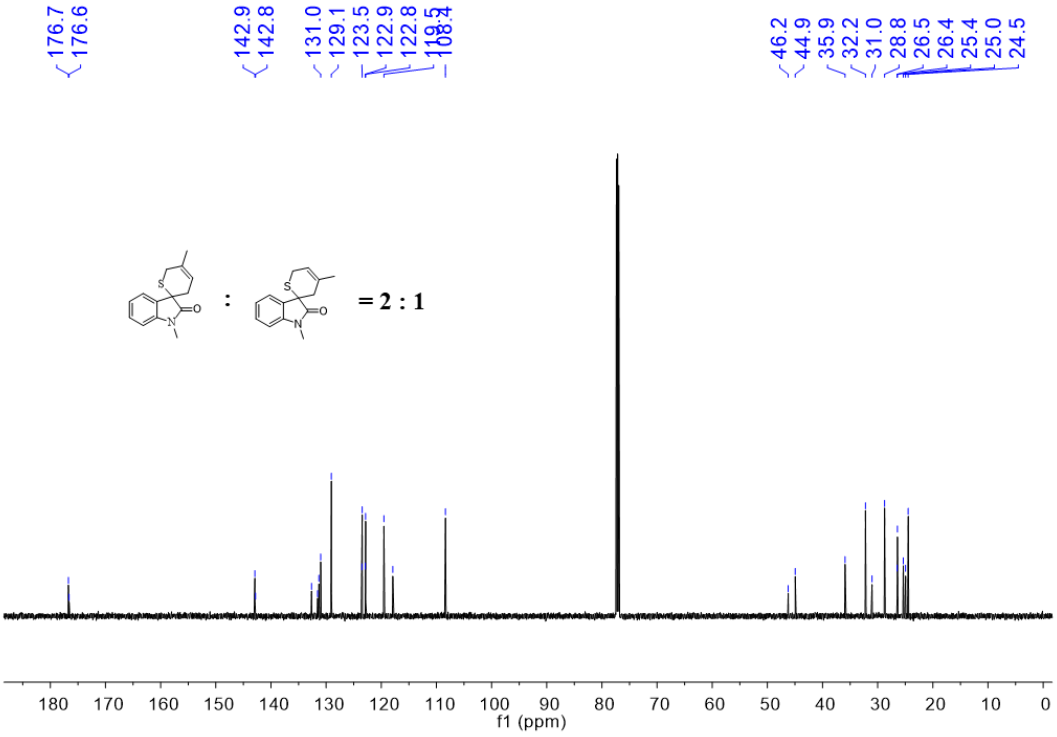
^{1}H NMR spectrum of 4pb (400 MHz, $CDCl_3$)



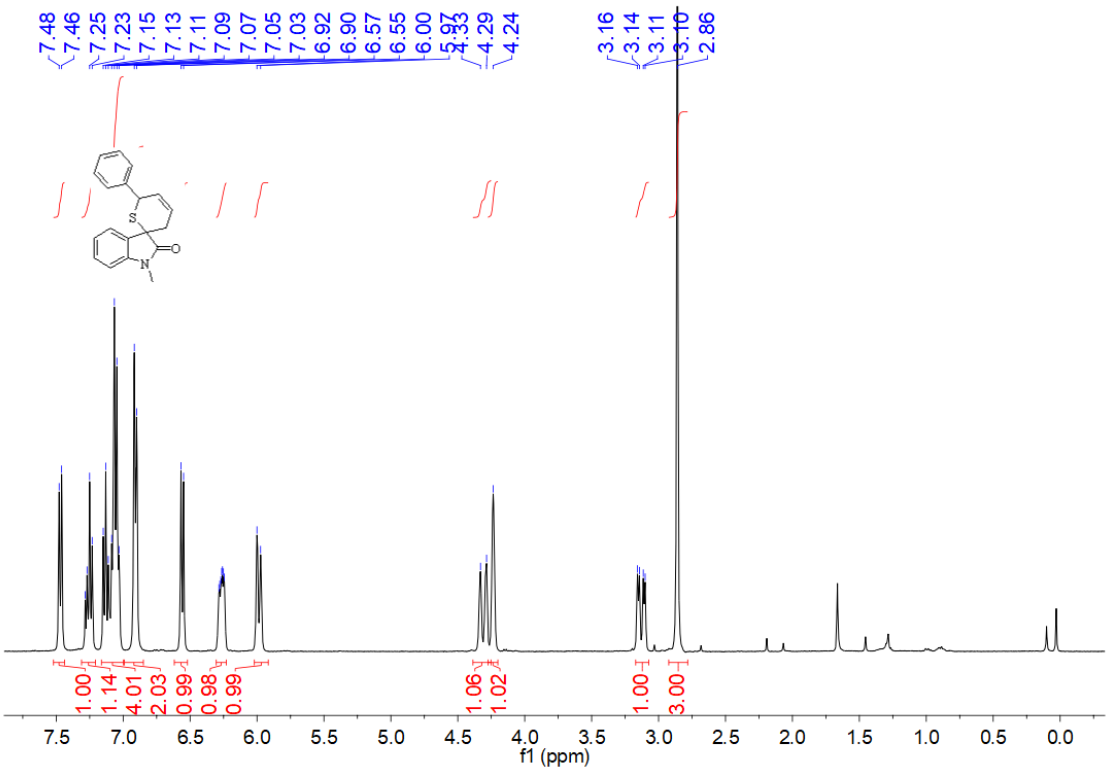
^{13}C NMR spectrum of 4pb (151 MHz, $CDCl_3$)



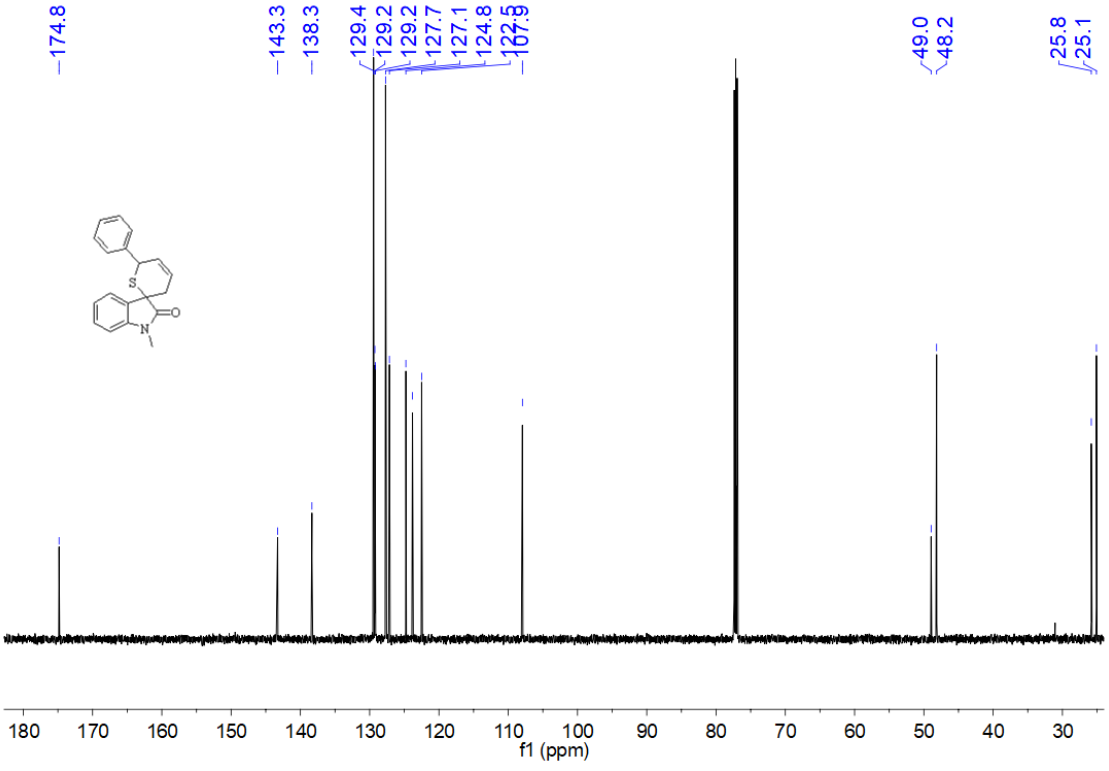
^{1}H NMR spectrum of 4pc and 4pc' (400 MHz, $CDCl_3$)



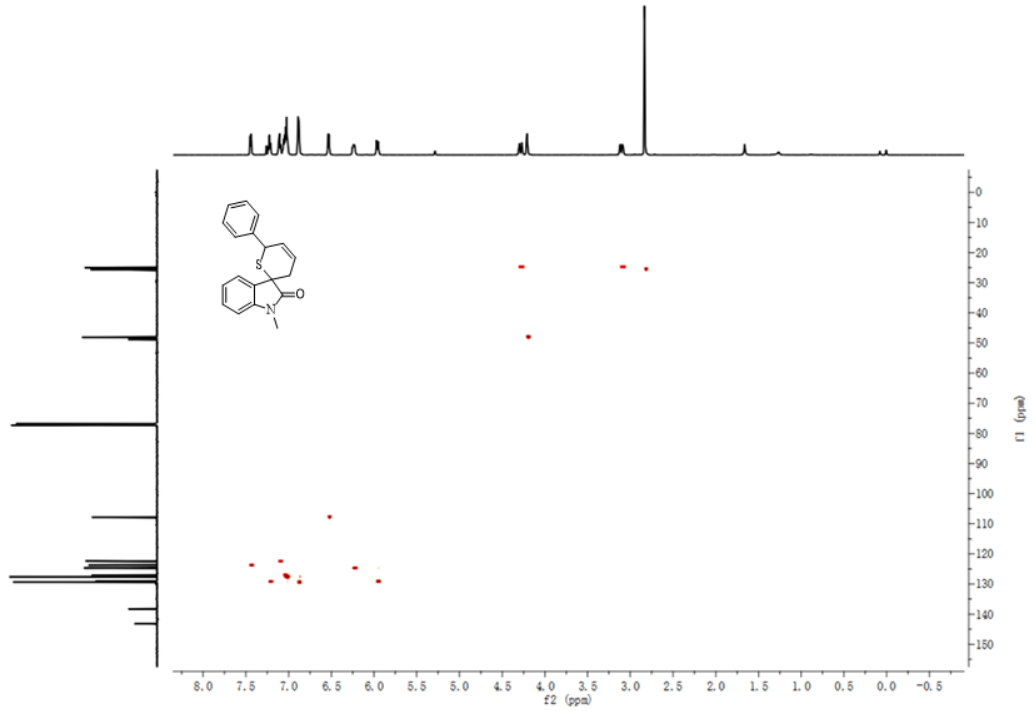
^{13}C NMR spectrum of 4pc and 4pc' (151 MHz, $CDCl_3$)



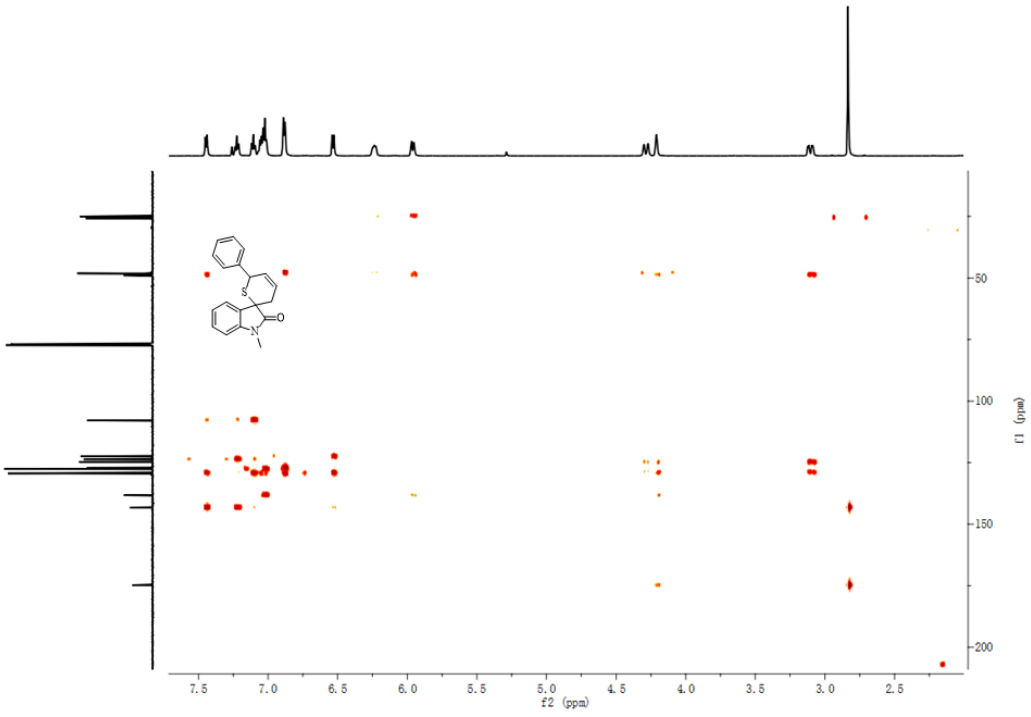
^{1}H NMR spectrum of 4pd (400 MHz, $CDCl_3$)



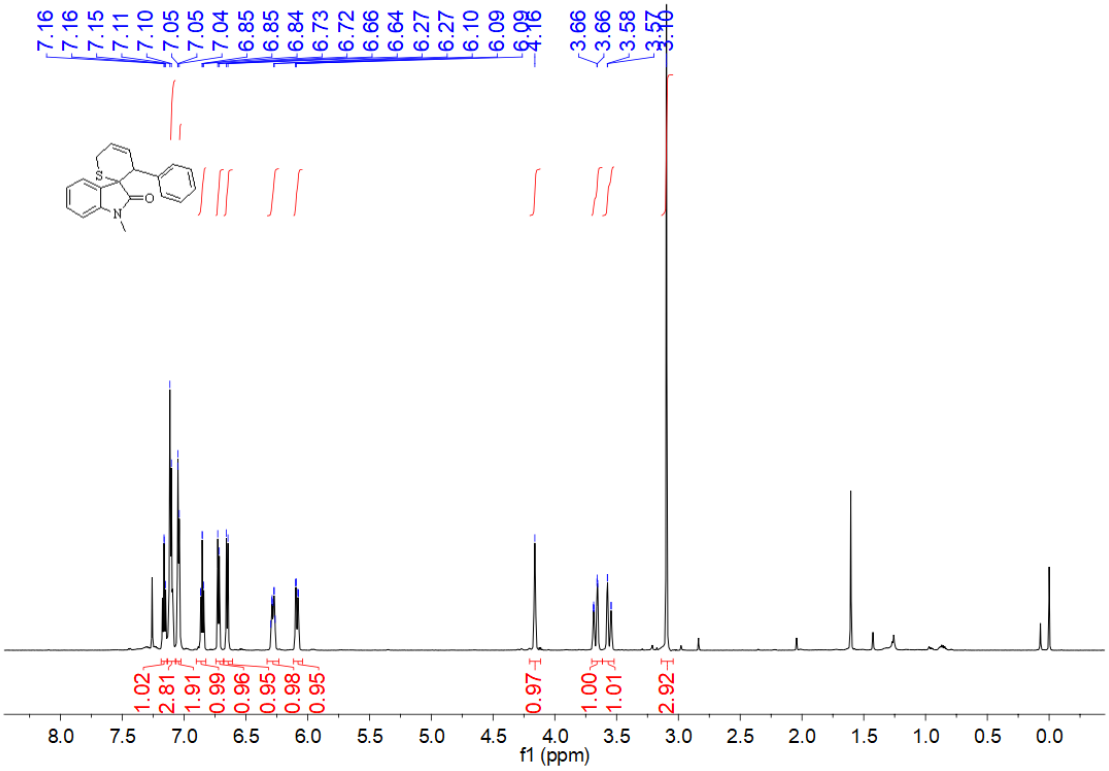
^{13}C NMR spectrum of 4pd (151 MHz, $CDCl_3$)



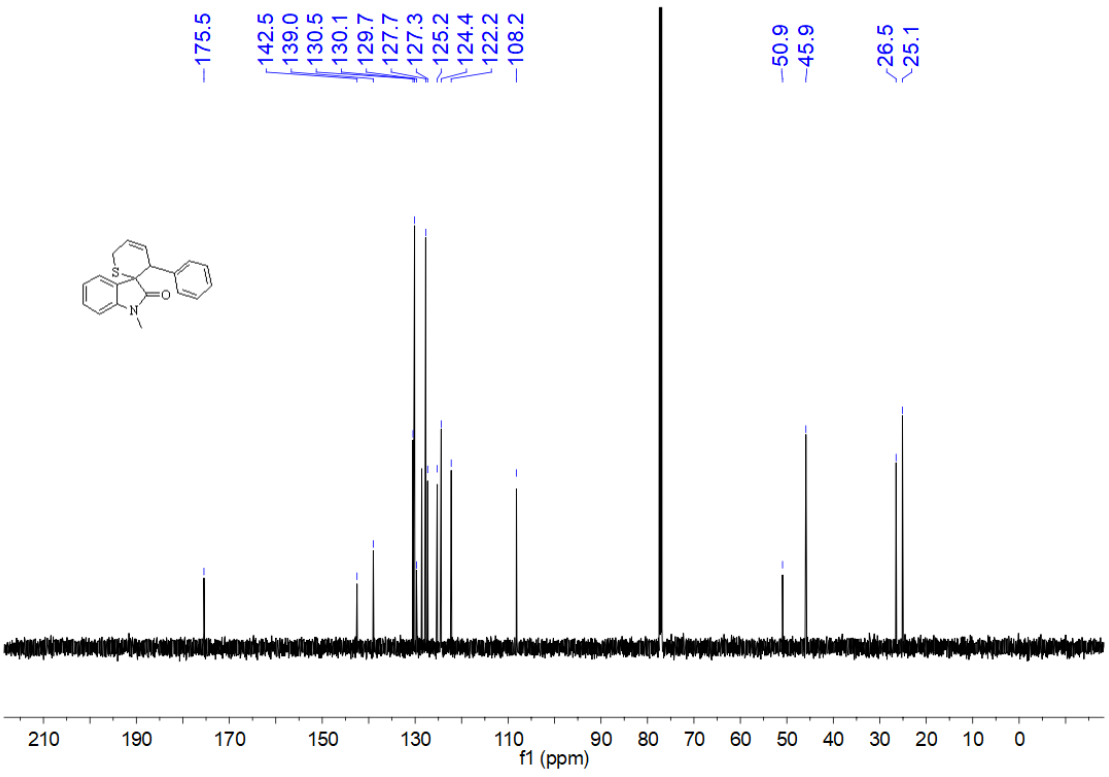
^{1}H-^{13}C HSQC NMR spectrum of 4pd



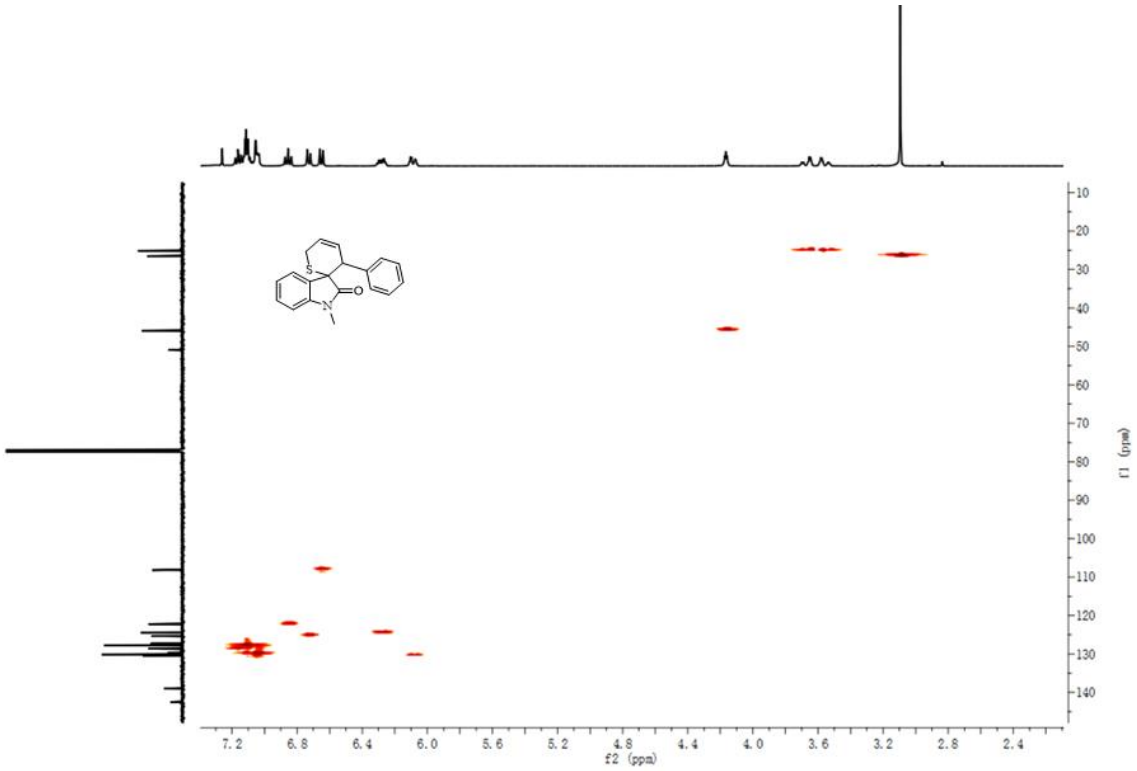
^{1}H-^{13}C HMBC NMR spectrum of 4pd



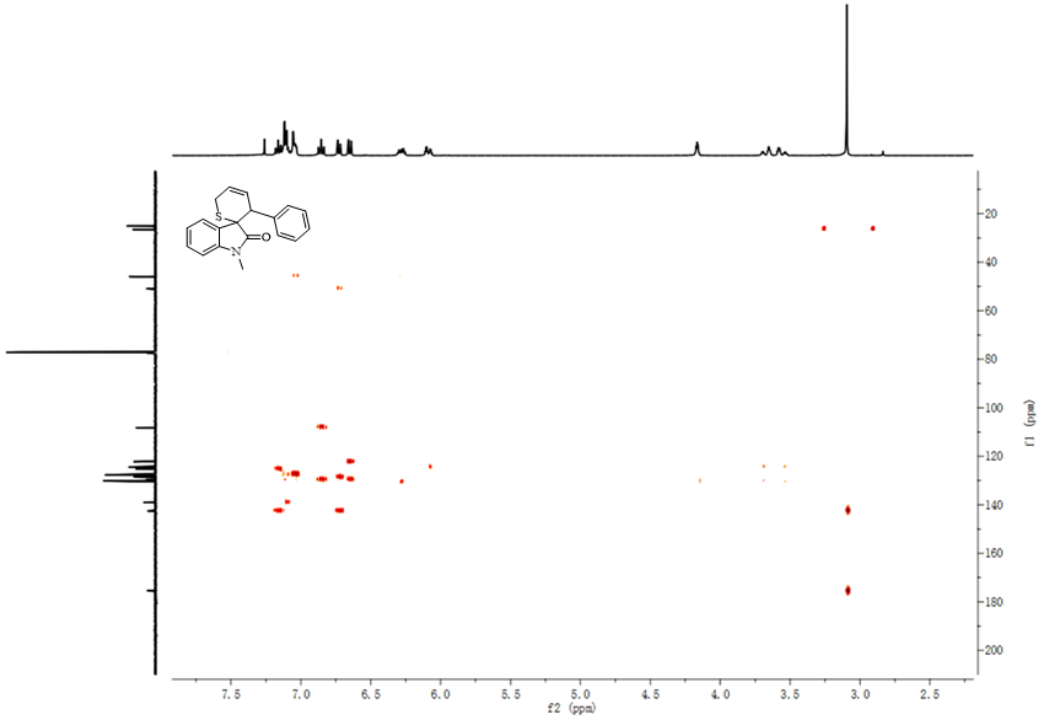
^{1}H NMR spectrum of 4pd' (600 MHz, $CDCl_3$)



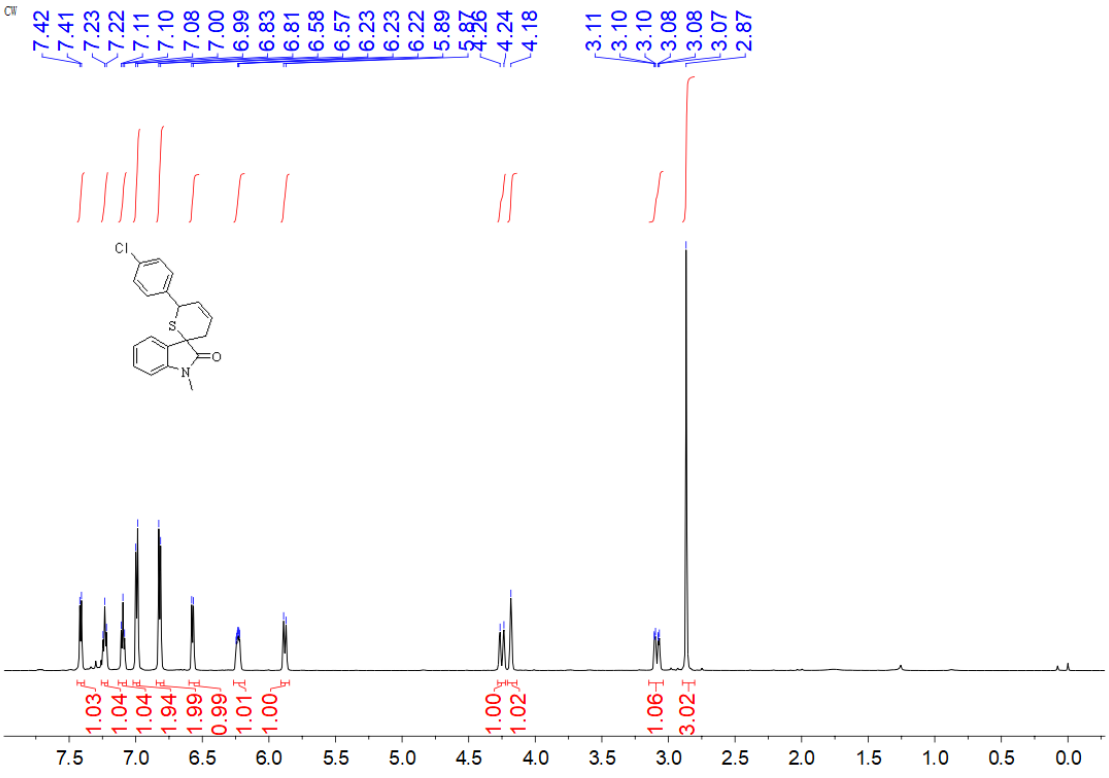
^{13}C NMR spectrum of 4pd' (151 MHz, $CDCl_3$)



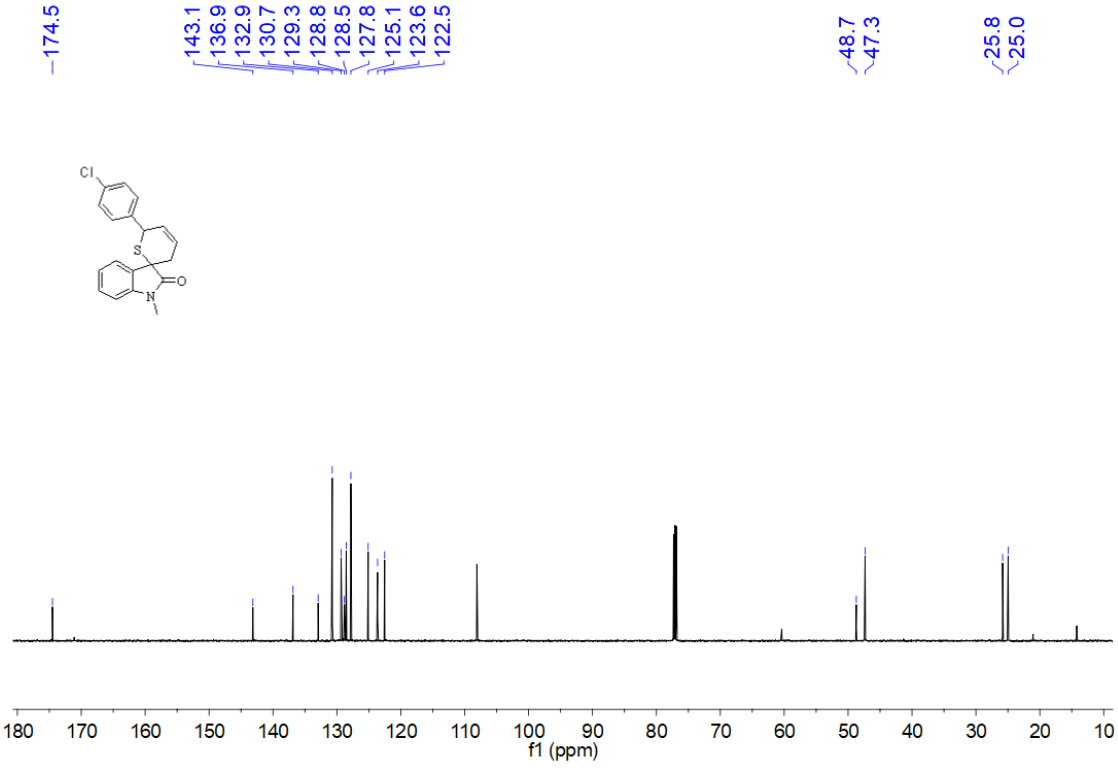
^{1}H-^{13}C HSQC NMR spectrum of 4pd′



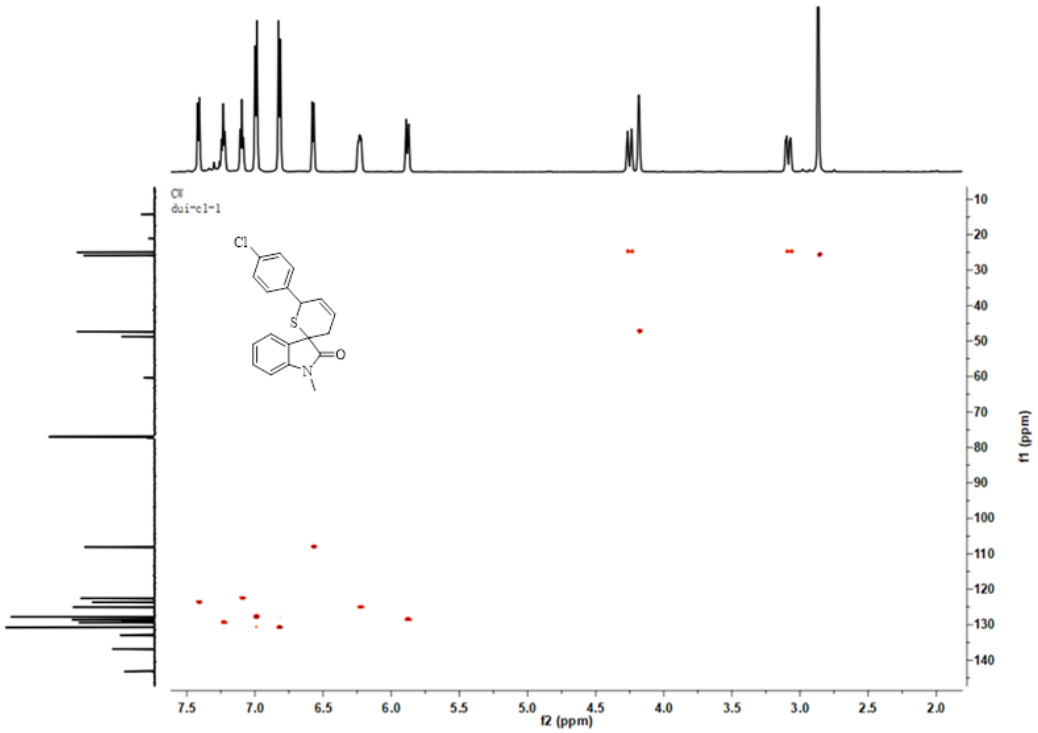
^{1}H-^{13}C HMBC NMR spectrum of 4pd′



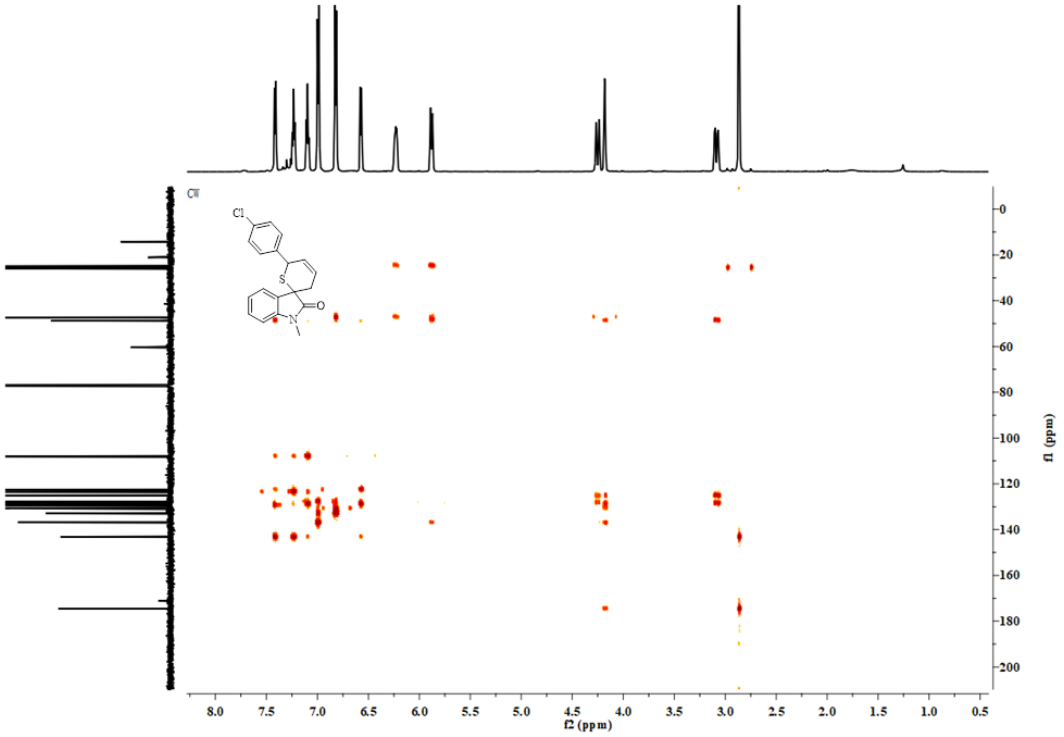
^{1}H NMR spectrum of 4pe (600 MHz, $CDCl_3$)



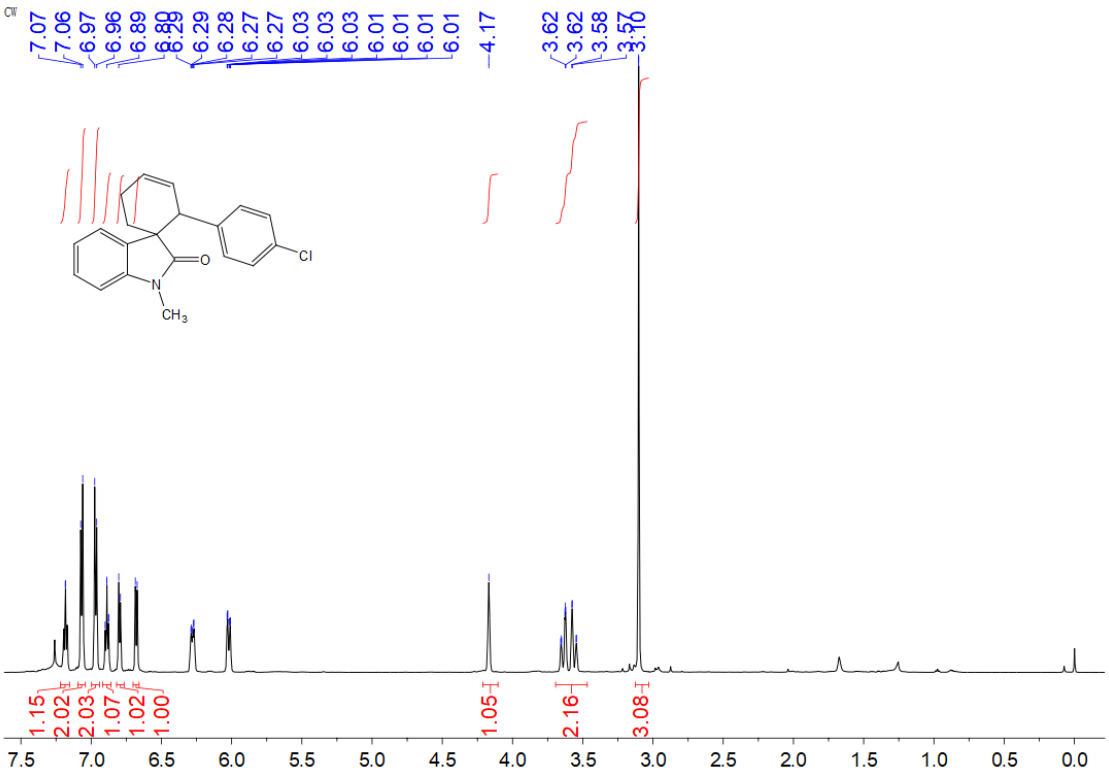
^{13}C NMR spectrum of 4pe (151 MHz, $CDCl_3$)



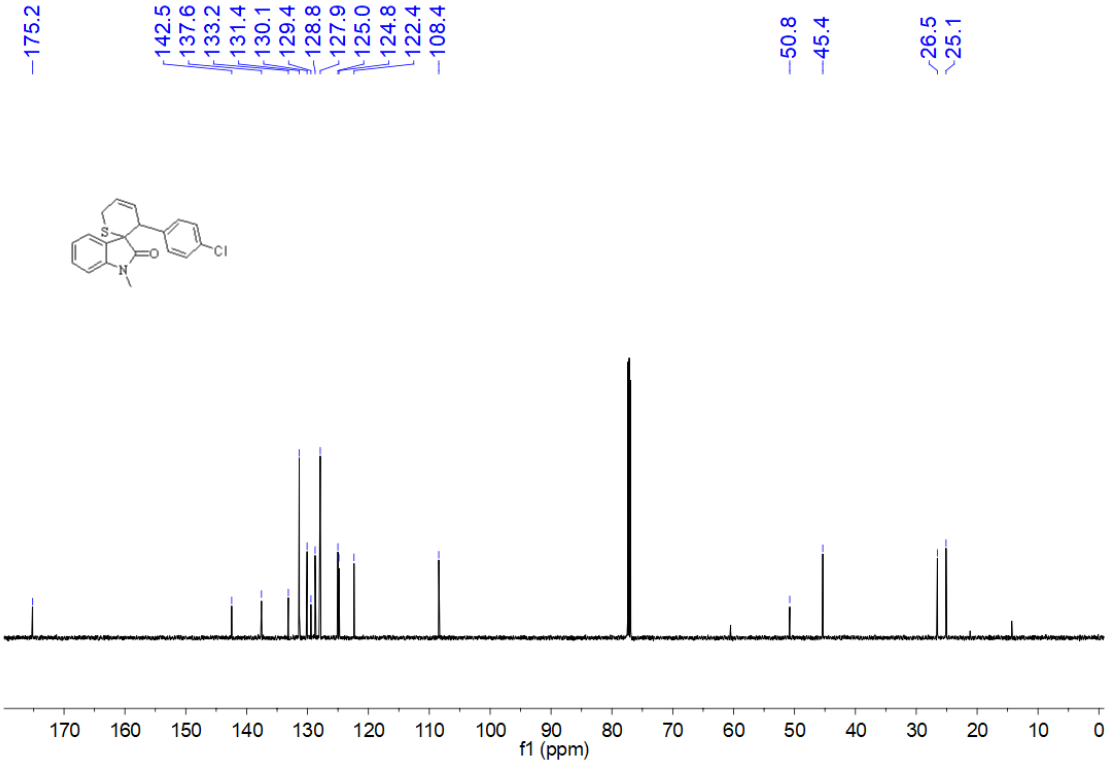
^{1}H-^{13}C HSQC NMR spectrum of 4pe



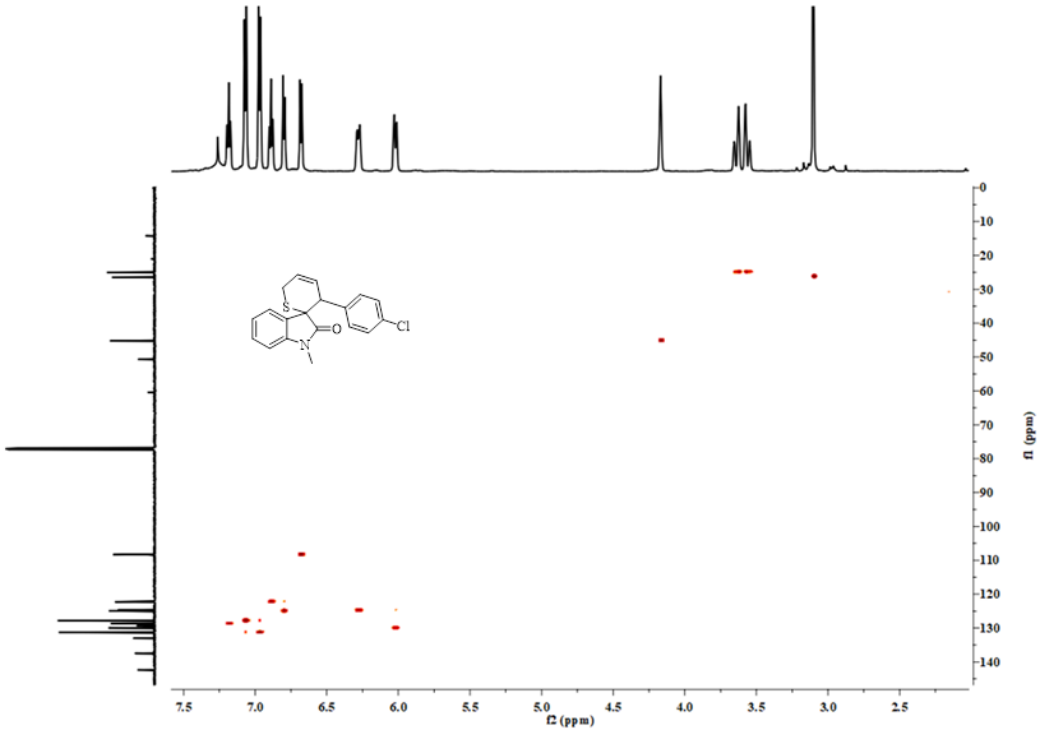
^{1}H-^{13}C HMBC NMR spectrum of 4pe



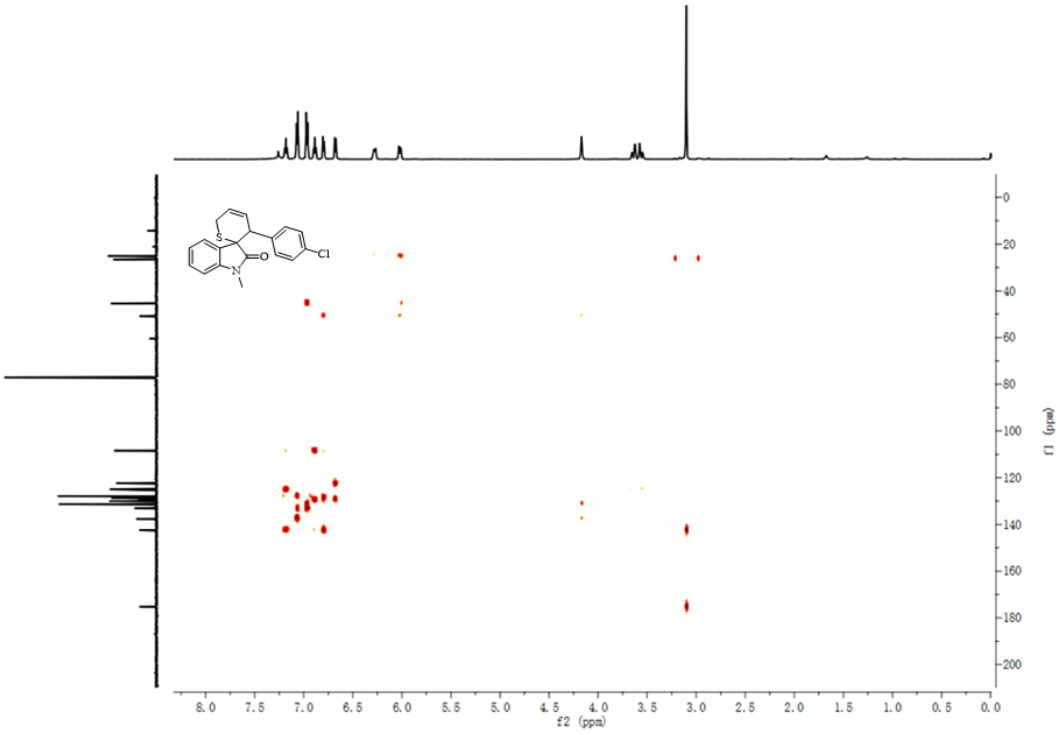
^{1}H NMR spectrum of 4pe′(600 MHz, $CDCl_3$)



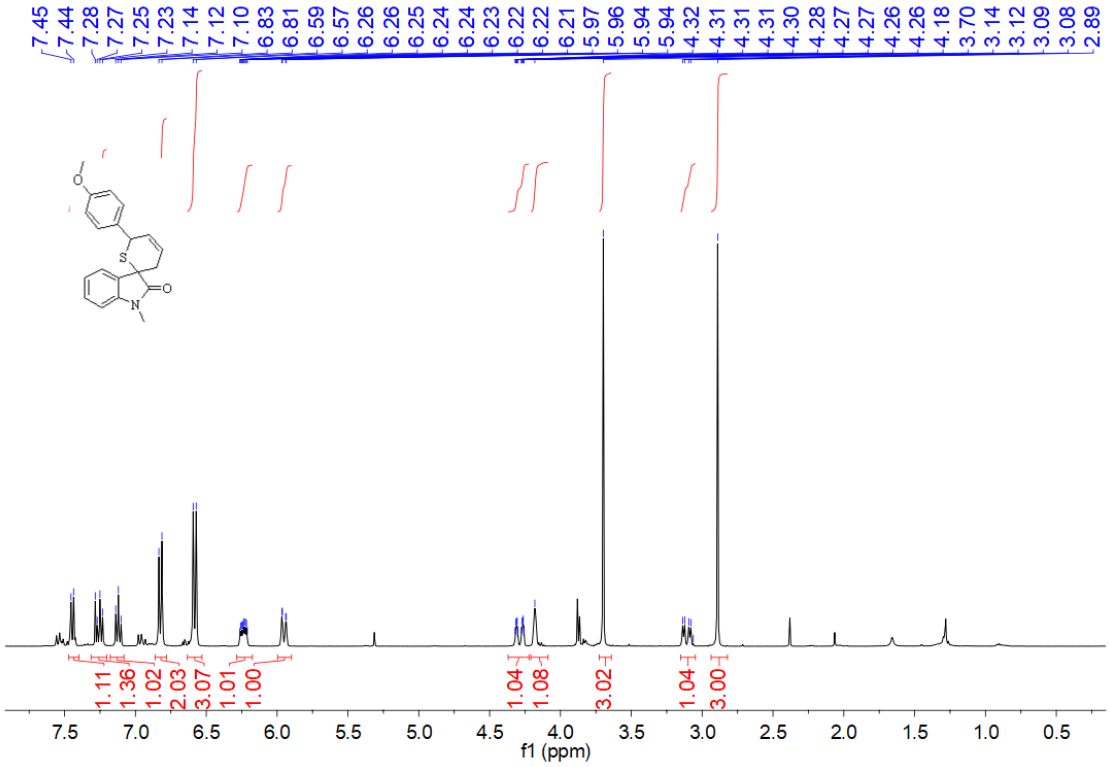
^{13}C NMR spectrum of 4pe′ (151 MHz, $CDCl_3$)



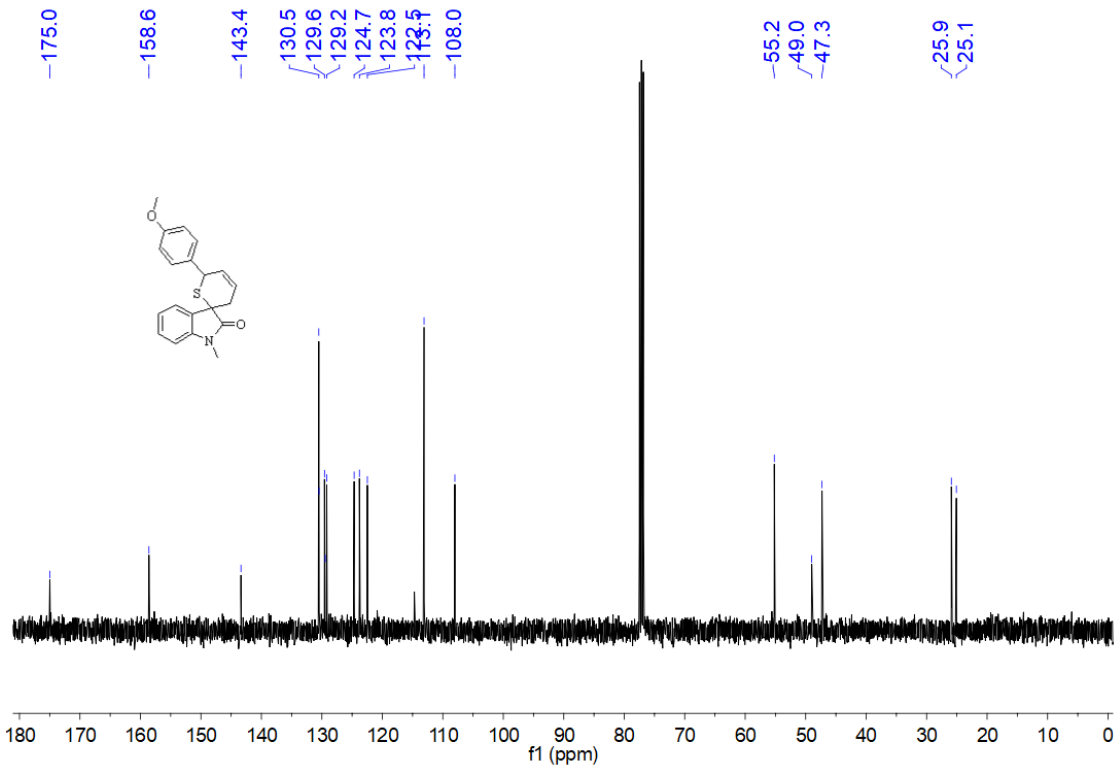
^{1}H-^{13}C HSQC NMR spectrum of 4pe′



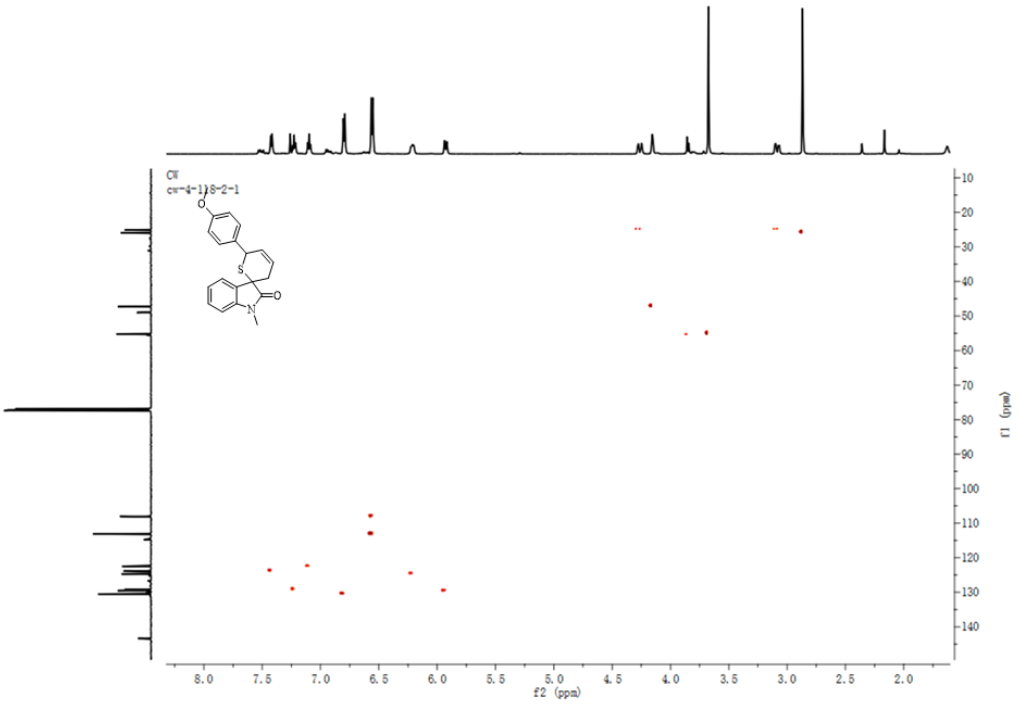
^{1}H-^{13}C HMBC NMR spectrum of 4pe′



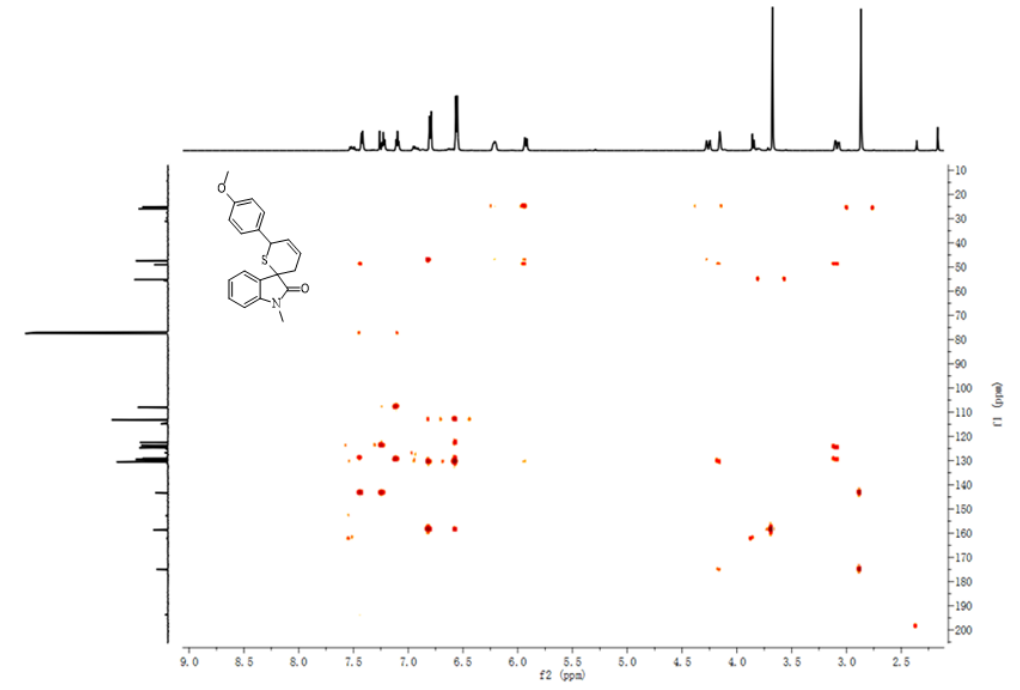
^{1}H NMR spectrum of 4pf (400 MHz, $CDCl_3$)



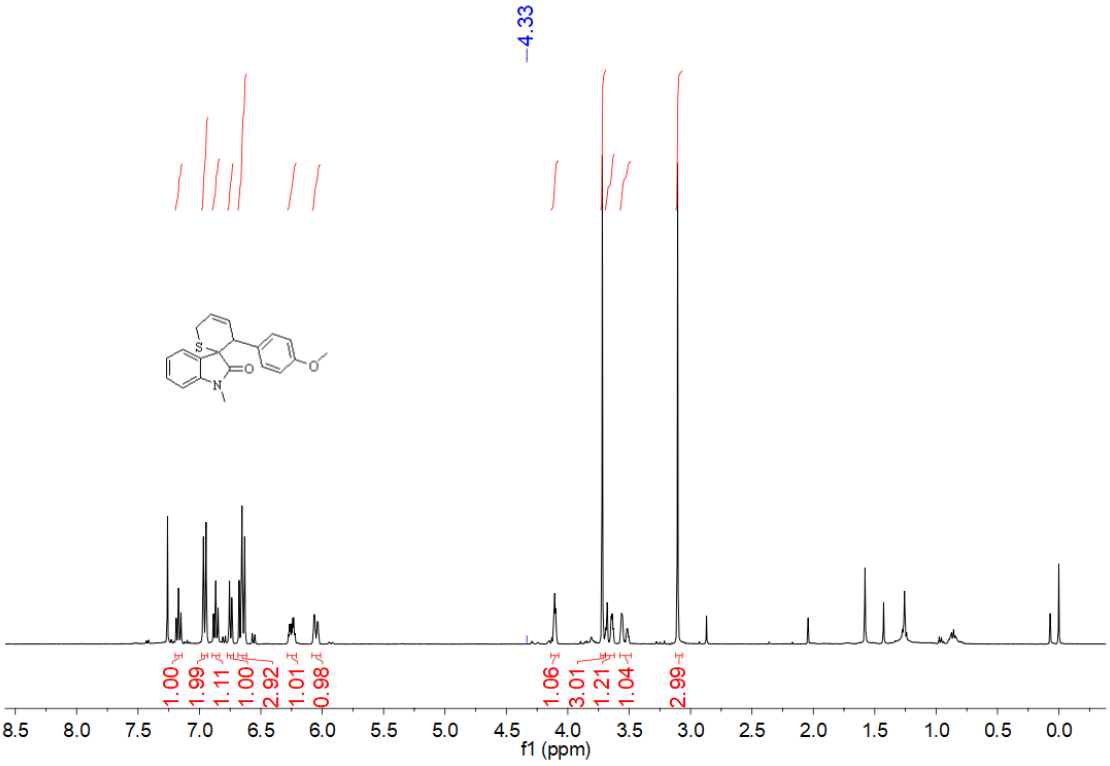
^{13}C NMR spectrum of 4pf (101 MHz, $CDCl_3$)



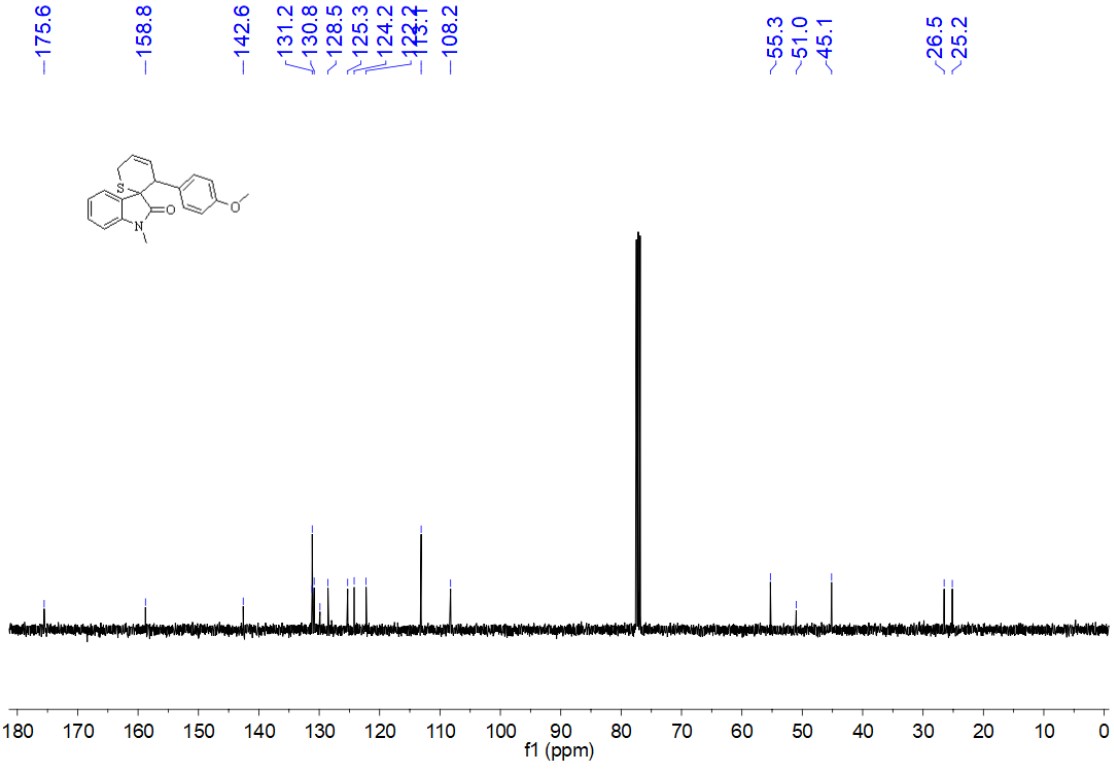
^{1}H-^{13}C HSQC NMR spectrum of 4pf



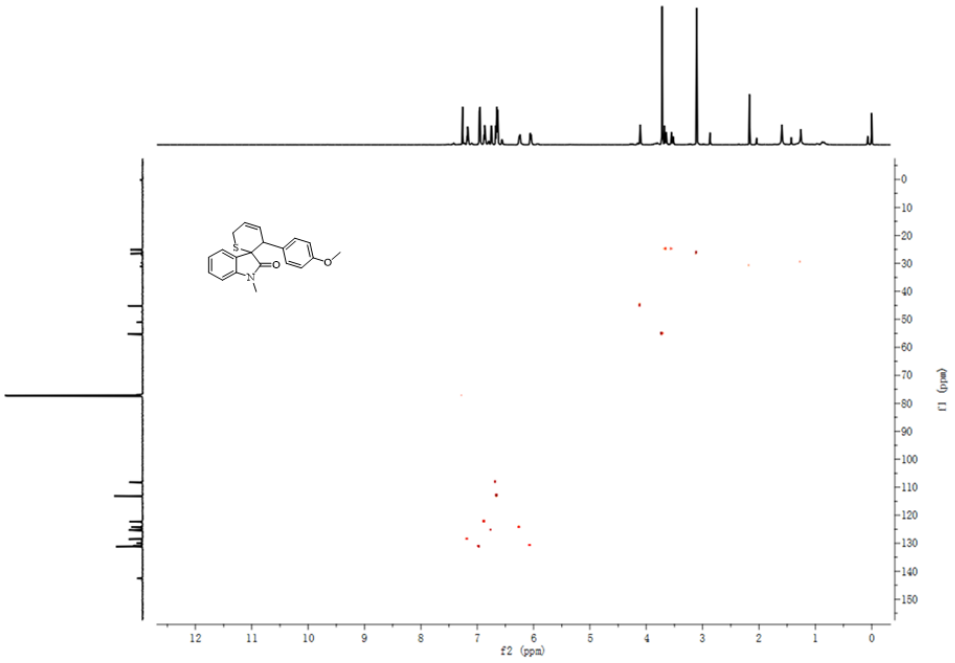
^{1}H-^{13}C HMBC NMR spectrum of 4pf



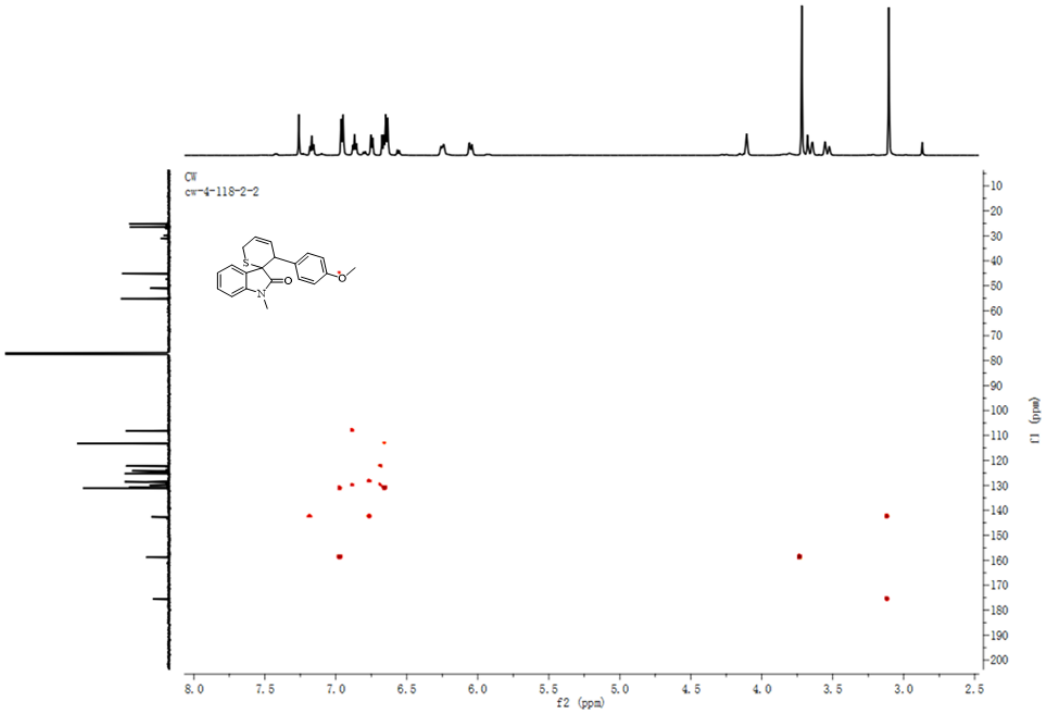
^{1}H NMR spectrum of 4pf′ (400 MHz, $CDCl_3$)



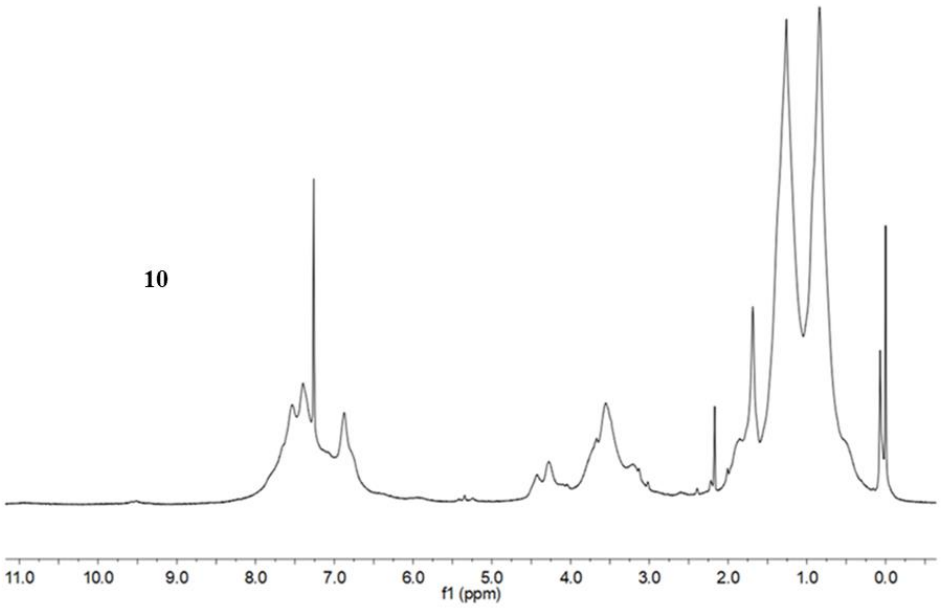
^{13}C NMR spectrum of 4pf′ (101 MHz, $CDCl_3$)



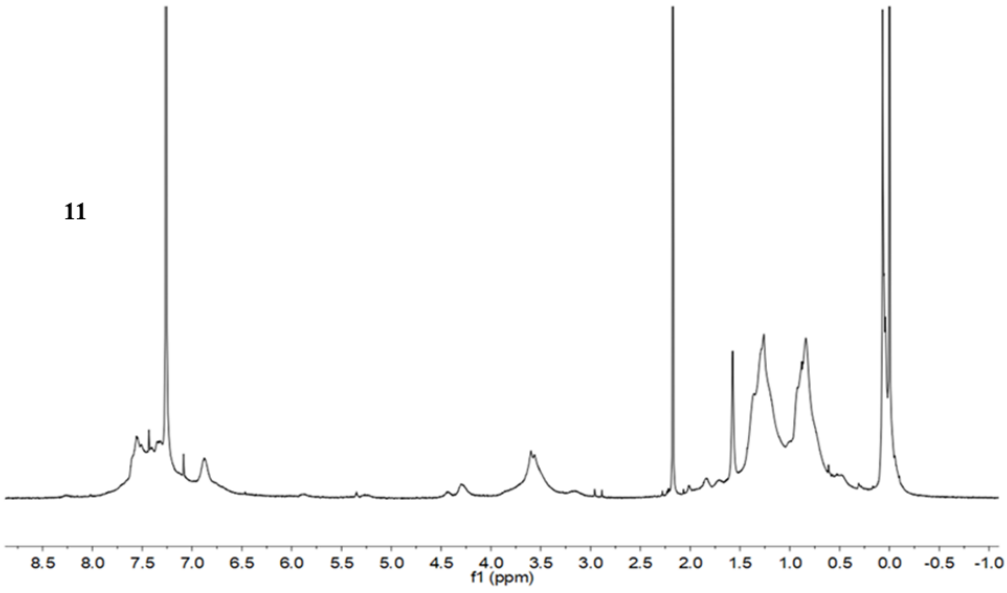
^{1}H-^{13}C HSQC NMR spectrum of 4pf′



^{1}H-^{13}C HMBC NMR spectrum of 4pf′



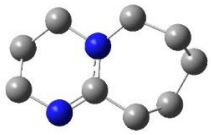
^{1}H NMR spectrum of polymer 9 (600 MHz, $CDCl_3$)



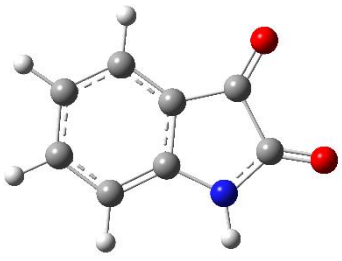
^{1}H NMR spectrum of polymer 10 (600 MHz, $CDCl_3$)

12. Cartesian coordinates of intermediates

C	-0.32862	0.05495	0.41235
O	-1.04497	0.17393	1.31134
S	0.64572	-0.10757	-0.8103



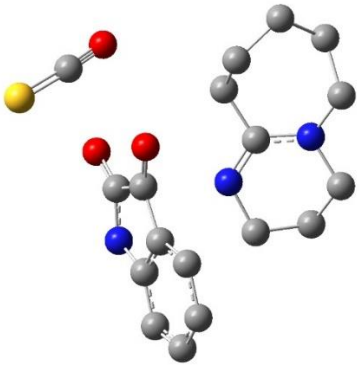
C	2.29726	0.66638	0.75783
C	2.58187	-0.71547	0.17789
N	1.35805	-1.48641	-0.00943
C	0.3206	-0.82172	-0.39274
N	0.2847	0.52955	-0.64405
C	1.36655	1.40736	-0.18838
C	-0.97471	-1.57669	-0.61141
C	-2.14141	-1.16887	0.33316
C	-1.93003	0.12886	1.12129
C	-1.87923	1.38537	0.24864
C	-0.97334	1.19009	-0.97343
H	3.21632	1.24085	0.90006
H	1.81691	0.54799	1.73582
H	3.10403	-0.60115	-0.78452
H	3.2522	-1.27944	0.83439
H	0.91967	2.27335	0.31316
H	1.92307	1.78241	-1.05714
H	-0.73189	-2.63121	-0.47434
H	-1.27572	-1.4557	-1.65694
H	-3.06514	-1.08736	-0.25097
H	-2.30025	-1.97773	1.05231
H	-2.73228	0.23281	1.85914
H	-0.99708	0.04814	1.69303
H	-1.52507	2.23133	0.84885
H	-2.88355	1.64364	-0.10728
H	-0.73018	2.15242	-1.43361
H	-1.49569	0.60589	-1.73473



Isatin

H	-1.26654	2.48351	-0.00017
H	-1.72417	-2.50598	0.00019
H	-3.73321	-1.04428	0.00002
H	-3.53296	1.41355	-0.0001
O	3.08451	-0.69356	-0.00023

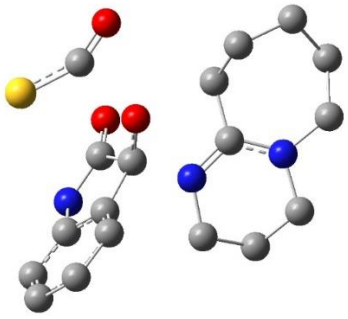
O	1.76695	1.9426	0.00025
C	1.178	0.88924	0.00002
C	1.89075	-0.502	-0.00009
C	-1.37947	1.4037	-0.00013
C	-0.25838	0.58312	-0.00002
C	-0.3816	-0.81568	0.00004
C	-1.62555	-1.42603	0.00007
C	-2.7467	-0.59104	0. 0000
C	-2.63692	0.80309	-0.00009
N	0.88177	-1.42548	0.0001
H	1.03205	-2.42723	0.0004



INT1

C	-2.298	-2.77491	1.25324
C	-0.87946	-2.299	0.98093
N	-0.78946	-0.84796	0.87806
C	-1.82386	-0.16595	0.51135
N	-3.06783	-0.69193	0.22089
C	-3.21405	-2.14848	0.21854
C	-1.6337	1.33819	0.46697
C	-1.99681	1.98625	-0.87533
C	-3.45806	2.43797	-0.9253
C	-4.40052	1.42323	-0.27135
C	-4.07811	-0.02956	-0.61645
C	1.94045	-3.31409	-1.97971
C	2.43096	-3.92848	-0.82315
C	2.59311	-3.22966	0.37641
C	2.24376	-1.88785	0.38226
C	1.75563	-1.26003	-0.77408
C	1.59924	-1.96156	-1.96092
C	1.82373	0.24915	1.09525
C	1.46791	0.1377	-0.41671
O	1.75527	1.24703	1.77906
C	1.78982	3.59818	0.1285
O	0.67668	3.72635	0.40615
H	-2.36809	-3.86493	1.20467
H	-2.61058	-2.45938	2.25492
H	-0.19896	-2.62486	1.7771
H	-0.50663	-2.75564	0.05168
H	-4.26154	-2.37884	0.43701
H	-2.9901	-2.55301	-0.7805

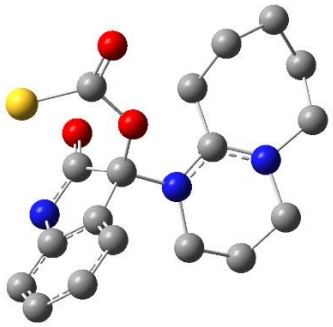
H	-2.21899	1.79857	1.273
H	-0.5826	1.50925	0.698
H	-1.33315	2.8379	-1.0506
H	-1.7938	1.27363	-1.68361
H	-3.75684	2.59863	-1.96748
H	-3.56482	3.40172	-0.41402
H	-4.39497	1.52864	0.81869
H	-5.42704	1.62319	-0.59452
H	-4.98729	-0.6221	-0.48316
H	-3.80572	-0.11211	-1.68076
H	1.82837	-3.89207	-2.89039
H	2.69353	-4.98153	-0.85337
H	2.96858	-3.71757	1.26948
H	1.21426	-1.46239	-2.8451
N	2.28798	-0.98768	1.45372
H	2.58025	-1.2299	2.39223
O	1.10422	1.06854	-1.09735
S	3.31498	3.52587	-0.25796



TS1-2

C	-1.27444	-3.17953	0.72247
C	-0.11352	-2.34253	0.23078
N	-0.48457	-0.92363	0.18445
C	-1.73934	-0.51184	0.19838
N	-2.77001	-1.38168	0.0559
C	-2.49699	-2.81199	-0.09112
C	-2.07647	0.93816	0.44338
C	-2.7916	1.58298	-0.75378
C	-4.31324	1.54314	-0.58919
C	-4.79593	0.23953	0.05763
C	-4.1054	-1.01579	-0.47229
C	3.56346	-1.63818	-1.89823
C	4.42645	-1.79001	-0.81445
C	4.07574	-1.35109	0.46522
C	2.82594	-0.77223	0.62193
C	1.9423	-0.6429	-0.4506
C	2.31165	-1.04251	-1.71934
C	1.082	0.45172	1.49913
C	0.70497	0.12158	-0.00318
O	0.43691	1.10802	2.28096
C	0.89058	2.91019	-0.38266
O	-0.10319	3.50365	-0.55338

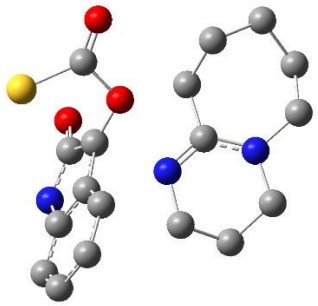
H	-1.04514	-4.24137	0.6107
H	-1.4672	-2.98071	1.78129
H	0.74549	-2.43137	0.90115
H	0.21369	-2.66642	-0.76196
H	-3.37891	-3.35327	0.26082
H	-2.3503	-3.06418	-1.15131
H	-2.71423	0.94473	1.33291
H	-1.18082	1.48346	0.70087
H	-2.42783	2.60637	-0.85972
H	-2.48431	1.06993	-1.67135
H	-4.7953	1.66767	-1.56491
H	-4.64446	2.38233	0.03143
H	-4.69583	0.26717	1.14655
H	-5.86497	0.11015	-0.14032
H	-4.73675	-1.8749	-0.23313
H	-4.03955	-0.96664	-1.56918
H	3.87425	-1.96658	-2.88402
H	5.40058	-2.24393	-0.96596
H	4.76405	-1.44562	1.29857
H	1.63622	-0.87224	-2.55275
N	2.24567	-0.2381	1.78409
H	2.76528	-0.0295	2.62494
O	0.31119	1.09251	-0.78744
S	2.47702	2.8527	-0.02569



INT2

C	-1.21445	-3.2005	0.36582
C	-0.02188	-2.30636	0.12808
N	-0.42676	-0.8814	0.13018
C	-1.71755	-0.48816	0.15379
N	-2.68098	-1.34657	-0.15987
C	-2.32982	-2.72474	-0.53806
C	-2.09671	0.9157	0.56147
C	-2.93438	1.6359	-0.50702
C	-4.43172	1.50415	-0.21933
C	-4.78414	0.11695	0.32095
C	-4.11484	-1.03529	-0.41791
C	3.68883	-1.4089	-1.77517
C	4.52532	-1.55795	-0.66871
C	4.11741	-1.18116	0.61485
C	2.8402	-0.65965	0.74814
C	1.99139	-0.52186	-0.35039

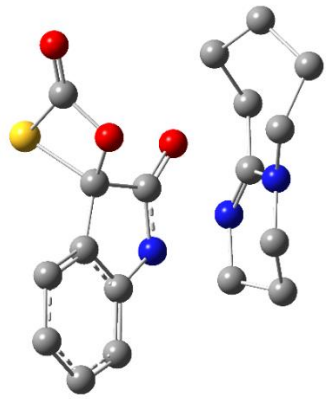
C	2.40372	-0.8787	-1.61998
C	1.02685	0.45824	1.61328
C	0.69446	0.10986	0.10682
O	0.30582	1.02102	2.40662
C	0.80499	2.42976	-0.78087
O	0.15565	3.17327	-1.48523
H	-0.94161	-4.23058	0.13041
H	-1.5431	-3.15678	1.40814
H	0.72763	-2.43767	0.91324
H	0.43819	-2.54089	-0.83347
H	-3.22397	-3.33656	-0.42607
H	-2.02309	-2.74412	-1.59043
H	-2.66103	0.8105	1.4931
H	-1.21419	1.4778	0.82527
H	-2.6345	2.68541	-0.54504
H	-2.69992	1.21918	-1.49245
H	-5.00045	1.7001	-1.13431
H	-4.73805	2.25608	0.51569
H	-4.57376	0.03406	1.39093
H	-5.85992	-0.05314	0.21332
H	-4.6429	-1.953	-0.15689
H	-4.21488	-0.89909	-1.50229
H	4.03775	-1.70232	-2.75934
H	5.52103	-1.96874	-0.80366
H	4.77626	-1.28084	1.47075
H	1.74124	-0.74867	-2.47109
N	2.20534	-0.18054	1.89819
H	2.6638	-0.07126	2.79476
O	0.25499	1.12668	-0.738
S	2.24778	2.74929	0.0999



TS2-3

C	-1.11211	-3.26549	0.35674
C	-0.00835	-2.25047	0.1136
N	-0.4632	-0.89553	0.40157
C	-1.72734	-0.58615	0.31345
N	-2.70427	-1.46303	-0.06394
C	-2.33288	-2.83317	-0.42763
C	-2.1472	0.80681	0.73138
C	-2.88818	1.58527	-0.36614
C	-4.40592	1.42804	-0.24618
C	-4.80828	-0.00027	0.13382

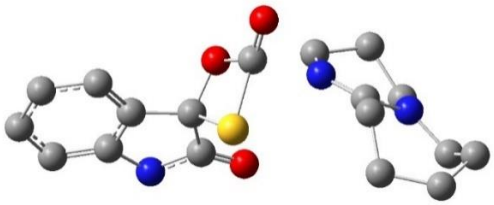
C	-4.02421	-1.08209	-0.60496
C	3.45066	-1.61515	-1.855
C	4.10464	-2.12807	-0.72638
C	3.77528	-1.72685	0.56891
C	2.75888	-0.79139	0.70434
C	2.10222	-0.26911	-0.42418
C	2.43832	-0.67196	-1.71225
C	1.21516	0.66288	1.60398
C	1.12071	0.66139	0.07577
O	0.2614	1.39388	-0.68028
O	0.57089	1.29702	2.40639
C	0.7384	2.70759	-0.76807
O	0.06882	3.53242	-1.32061
S	2.29983	2.77552	-0.01446
H	-0.79278	-4.26094	0.03908
H	-1.35493	-3.30764	1.42372
H	0.8528	-2.46617	0.75407
H	0.33729	-2.319	-0.92539
H	-3.18791	-3.47695	-0.20413
H	-2.14022	-2.89753	-1.50783
H	-2.78503	0.70542	1.61663
H	-1.25843	1.33331	1.0598
H	-2.60923	2.64127	-0.31218
H	-2.54804	1.2357	-1.34754
H	-4.87906	1.70331	-1.19524
H	-4.79147	2.1182	0.51261
H	-4.70978	-0.1676	1.2110
H	-5.86594	-0.15224	-0.10317
H	-4.61039	-2.00332	-0.57692
H	-3.91551	-0.80948	-1.6652
H	3.73954	-1.95562	-2.84305
H	4.89313	-2.86192	-0.86065
H	4.28512	-2.13216	1.43587
H	1.91971	-0.25737	-2.57118
N	2.22165	-0.24187	1.86469
H	2.53702	-0.45199	2.80362



INT3

C	-1.34975	-3.3635	0.27739
C	-0.18383	-2.40282	0.45106

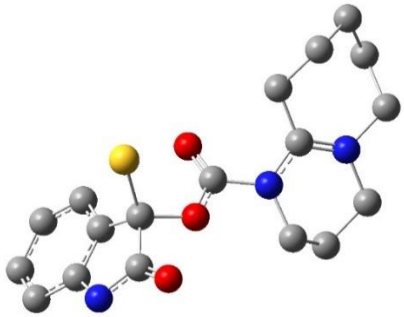
N	-0.60362	-1.05622	0.82209
C	-1.79596	-0.65694	0.52893
N	-2.76032	-1.40861	-0.12188
C	-2.36368	-2.71548	-0.64617
C	-2.16185	0.73329	1.01613
C	-2.71097	1.6753	-0.06415
C	-4.23537	1.60707	-0.17335
C	-4.7556	0.1706	-0.06844
C	-3.91303	-0.84526	-0.83811
C	3.11351	-1.83637	-1.91258
C	3.5394	-2.57629	-0.80753
C	3.32854	-2.13199	0.50075
C	2.66783	-0.92464	0.66315
C	2.24955	-0.17011	-0.43923
C	2.46814	-0.6099	-1.73299
C	1.54386	0.82929	1.61604
C	1.61878	1.06681	0.08572
O	0.36753	1.47288	-0.48102
O	0.99309	1.55173	2.41382
C	0.69442	2.74019	-0.83009
O	-0.00714	3.55816	-1.32774
S	2.4077	2.69799	-0.32237
H	-1.01815	-4.31932	-0.13755
H	-1.81938	-3.56039	1.24776
H	0.50322	-2.7671	1.22447
H	0.40275	-2.35759	-0.47893
H	-3.26486	-3.33104	-0.72747
H	-1.94344	-2.61259	-1.6588
H	-2.88865	0.64558	1.83392
H	-1.24301	1.13319	1.44271
H	-2.39862	2.701	0.15563
H	-2.25007	1.42461	-1.02642
H	-4.55427	2.04553	-1.12588
H	-4.69141	2.21002	0.6204
H	-4.81145	-0.15036	0.97719
H	-5.77695	0.12595	-0.45962
H	-4.54625	-1.70481	-1.07415
H	-3.59672	-0.41808	-1.80325
H	3.29028	-2.21226	-2.91433
H	4.04659	-3.52311	-0.96426
H	3.65097	-2.71484	1.35681
H	2.1399	-0.01676	-2.58187
N	2.29495	-0.28659	1.85385
H	2.37744	-0.70319	2.77341



TS3-4

C	2.44994	2.66867	1.24904
C	1.13224	1.91436	1.19002
N	1.3375	0.49435	0.9391
C	2.44242	0.03494	0.44893
N	3.48697	0.8239	0.03174
C	3.2794	2.2735	0.04169
C	2.6057	-1.47034	0.40486
C	2.89512	-2.03228	-0.99417
C	4.39808	-2.13718	-1.26792
C	5.1777	-0.94076	-0.71354
C	4.50096	0.40713	-0.95241
C	-5.45626	-0.96124	0.67964
C	-6.00198	-0.2339	-0.37895
C	-5.20008	0.5171	-1.24393
C	-3.83449	0.51045	-1.00729
C	-3.27609	-0.2225	0.04351
C	-4.07516	-0.96201	0.89658
C	-1.58653	0.97723	-1.15171
C	-1.79202	-0.02819	0.01719
O	-1.23912	0.41674	1.25775
O	-0.53838	1.46413	-1.51404
C	-0.31409	-0.59894	1.4941
O	-0.03629	-1.03498	2.57303
S	-0.73423	-1.5215	-0.07905
H	2.27798	3.74802	1.25132
H	2.99633	2.40946	2.16234
H	0.58653	2.00239	2.13633
H	0.4866	2.32139	0.40645
H	4.26323	2.74934	0.06996
H	2.77954	2.59163	-0.88566
H	3.41433	-1.74238	1.0926
H	1.70293	-1.90403	0.83031
H	2.42922	-3.01706	-1.09424
H	2.41846	-1.39091	-1.74461
H	4.5658	-2.21689	-2.34759
H	4.79178	-3.05507	-0.81721
H	5.36248	-1.05286	0.35985
H	6.16179	-0.90281	-1.19095
H	5.26682	1.18557	-0.90985
H	4.07405	0.44069	-1.9667
H	-6.10674	-1.53067	1.33456
H	-7.07566	-0.24697	-0.53798
H	-5.62671	1.086	-2.06287

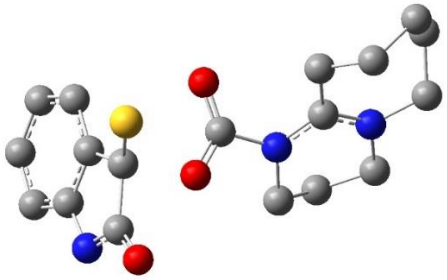
H	-3.63255	-1.52707	1.71234
N	-2.82061	1.18574	-1.70134
H	-2.97436	1.80499	-2.48797



INT 4

C	-2.01486	2.86901	-0.63616
C	-1.16526	2.14235	0.38264
N	-1.30677	0.69573	0.12682
C	-2.54227	0.15079	-0.05644
N	-3.56589	0.94002	-0.29791
C	-3.44573	2.40735	-0.48628
C	-2.68045	-1.34858	0.13678
C	-3.93967	-1.80804	0.88238
C	-5.13139	-2.00064	-0.0504
C	-5.24969	-0.83104	-1.02532
C	-4.9911	0.51203	-0.35342
C	3.75751	-0.90816	-2.64004
C	4.90487	-0.14989	-2.41053
C	5.09976	0.50765	-1.19364
C	4.10406	0.38992	-0.23449
C	2.93702	-0.35852	-0.44921
C	2.77241	-1.02704	-1.65349
C	2.91795	0.66119	1.712
C	2.1187	-0.33629	0.82835
O	0.84453	0.40075	0.67891
O	2.58215	1.12052	2.78237
C	-0.13178	-0.09754	-0.05096
O	-0.09909	-1.04713	-0.78985
S	1.95257	-1.91569	1.66244
H	-1.96997	3.94764	-0.47471
H	-1.64095	2.65273	-1.64058
H	-0.11412	2.39916	0.29131
H	-1.4951	2.35142	1.40453
H	-4.02867	2.65256	-1.37549
H	-3.92764	2.87281	0.37933
H	-2.60808	-1.83425	-0.84146
H	-1.80573	-1.66703	0.70045
H	-3.69705	-2.74951	1.38177
H	-4.18009	-1.09423	1.67708
H	-6.0479	-2.08582	0.54256
H	-5.01885	-2.9342	-0.61134
H	-4.55587	-0.94413	-1.86512

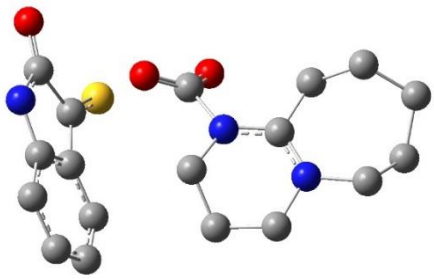
H	-6.25413	-0.7957	-1.4557
H	-5.48875	1.29952	-0.91766
H	-5.39124	0.53988	0.66544
H	3.62949	-1.41789	-3.58953
H	5.66371	-0.07135	-3.18304
H	5.99475	1.08989	-0.99979
H	1.88807	-1.63034	-1.8187
N	4.0837	0.9443	1.0472
H	4.78864	1.56924	1.4167



TS4-S-isatin

C	1.97141	2.89054	-0.68295
C	0.98697	1.82782	-1.11711
N	1.24454	0.61268	-0.32674
C	2.49037	0.20891	-0.02339
N	3.52741	0.99896	-0.26574
C	3.37448	2.35179	-0.84735
C	2.64683	-1.19663	0.53136
C	3.85326	-1.98846	0.0113
C	5.11747	-1.73001	0.82643
C	5.2938	-0.23662	1.09761
C	4.95635	0.62007	-0.11784
C	-3.68632	0.8879	2.59675
C	-4.43655	1.80436	1.85377
C	-4.50142	1.73366	0.45745
C	-3.78154	0.72204	-0.16237
C	-3.01713	-0.19932	0.56908
C	-2.97046	-0.12713	1.95268
C	-2.94165	-0.69155	-1.76769
C	-2.40314	-1.1554	-0.3894
O	-0.80739	-0.22074	-0.78439
O	-2.74271	-1.20014	-2.85154
C	0.05592	-0.10767	0.15029
O	0.0079	-0.46653	1.31233
S	-2.13653	-2.78525	-0.08034
H	1.85747	3.78862	-1.29508
H	1.78612	3.15902	0.36242
H	-0.04244	2.13178	-0.93027
H	1.09385	1.59308	-2.18161
H	4.09318	2.99719	-0.3395
H	3.65615	2.29031	-1.90491
H	2.66082	-1.14141	1.62587
H	1.74079	-1.73989	0.26628

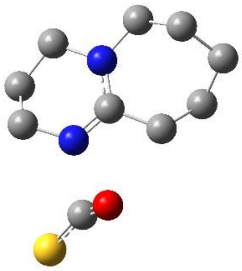
H	3.59234	-3.05039	0.05323
H	4.0205	-1.75643	-1.04703
H	5.98747	-2.11546	0.28206
H	5.06403	-2.27157	1.77817
H	4.67496	0.08748	1.94261
H	6.33148	-0.02366	1.37397
H	5.48419	1.57044	-0.04112
H	5.28533	0.14256	-1.04856
H	-3.65965	0.96578	3.67953
H	-4.9886	2.58647	2.3678
H	-5.09472	2.43741	-0.11876
H	-2.37818	-0.84514	2.51149
N	-3.70014	0.42383	-1.52704
H	-4.19784	0.92303	-2.25742



3-thioisatin

C	-1.01092	-2.33584	0.14435
C	-0.46666	-1.30589	-0.82131
N	-1.05424	-0.00307	-0.49588
C	-2.35697	0.09574	-0.22452
N	-3.09664	-0.99981	-0.02835
C	-2.51616	-2.35936	0.00826
C	-2.9794	1.48195	-0.21359
C	-4.3488	1.60348	-0.89455
C	-5.50574	1.31493	0.05799
C	-5.22057	0.06919	0.89483
C	-4.57509	-1.04323	0.07557
C	2.27696	-2.65396	1.2154
C	2.76157	-3.08812	-0.02354
C	3.2869	-2.19886	-0.96588
C	3.31024	-0.85357	-0.62896
C	2.82306	-0.40116	0.61444
C	2.30275	-1.29894	1.541
C	3.56889	1.4171	-0.72157
C	2.95753	1.04458	0.64153
O	0.87344	1.03194	-1.21752
O	3.86458	2.51821	-1.12199
C	-0.06661	1.17277	-0.42815
O	-0.34309	2.03465	0.40498
S	2.60668	2.11283	1.80519
H	-0.6095	-3.32845	-0.07321
H	-0.72077	-2.06554	1.16454
H	0.61356	-1.20122	-0.75481

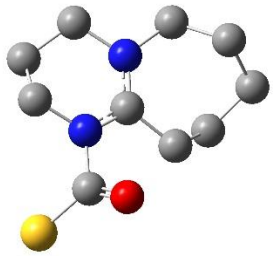
H	-0.72301	-1.57117	-1.85392
H	-2.97257	-2.8767	0.85497
H	-2.8203	-2.87757	-0.90821
H	-3.02786	1.83417	0.82209
H	-2.2728	2.13706	-0.71267
H	-4.43544	2.62018	-1.28758
H	-4.39112	0.93773	-1.76361
H	-6.42716	1.17438	-0.51729
H	-5.6659	2.17261	0.72013
H	-4.56871	0.30387	1.74302
H	-6.15031	-0.32289	1.31682
H	-4.78968	-2.00042	0.55053
H	-4.99946	-1.08673	-0.93435
H	1.8756	-3.3751	1.91917
H	2.73143	-4.14664	-0.26364
H	3.65874	-2.54547	-1.92397
H	1.92384	-0.93913	2.49345
N	3.77201	0.22339	-1.37564
H	4.1115	0.16492	-2.32683



DBU-COS-TS

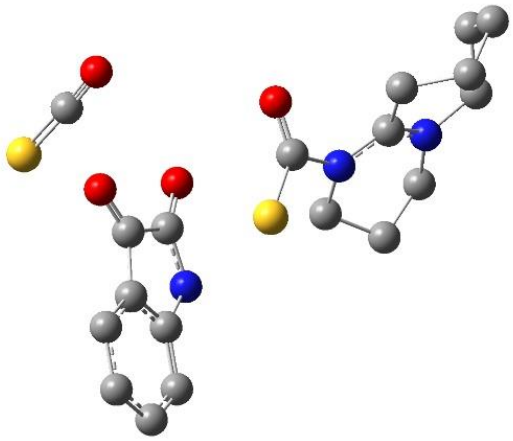
C	-0.36145	2.71325	-0.42595
C	-1.2933	1.79676	0.35363
N	-0.93498	0.40729	0.14067
C	0.31517	0.0839	0.01371
N	1.33677	0.98725	0.05151
C	1.06002	2.42831	0.01893
C	0.59333	-1.39226	-0.23699
C	1.82478	-1.70777	-1.08816
C	3.10092	-1.77895	-0.25039
C	3.16873	-0.62944	0.75437
C	2.777	0.71229	0.14829
C	-2.5895	-1.05043	0.44386
O	-2.09722	-1.76591	1.21979
S	-3.76119	-0.49286	-0.50965
H	-0.59627	3.76667	-0.25442
H	-0.46911	2.50968	-1.49671
H	-1.24439	2.04244	1.42468
H	-2.33345	1.92876	0.03751
H	1.77973	2.88744	-0.66817
H	1.24348	2.85022	1.0161
H	-0.30435	-1.76843	-0.7308
H	0.65316	-1.91453	0.72553
H	1.66613	-2.65962	-1.60349

H	1.92901	-0.94642	-1.87021
H	3.13865	-2.73293	0.28754
H	3.97605	-1.74715	-0.90897
H	4.18733	-0.53606	1.14297
H	2.52398	-0.82733	1.61792
H	3.24367	0.83447	-0.84016
H	3.17652	1.51007	0.78375



DBU-COS adduct

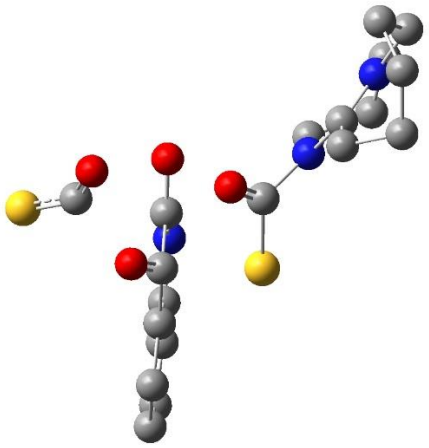
C	-0.76071	2.5741	-0.46591
C	-1.57434	1.65469	0.42018
N	-1.06055	0.28767	0.28256
C	0.22961	0.03446	0.07618
N	1.11062	1.02937	-0.00982
C	0.69343	2.4428	-0.07282
C	0.6193	-1.41694	-0.1424
C	1.85809	-1.65365	-1.00658
C	3.15479	-1.55806	-0.20763
C	3.14146	-0.3306	0.70082
C	2.58573	0.9046	0.00644
C	-2.0448	-0.83272	0.47615
O	-1.79035	-1.58876	1.39181
S	-3.34683	-0.84812	-0.63558
H	-1.08081	3.60986	-0.33876
H	-0.90241	2.2924	-1.51397
H	-1.50459	1.95842	1.47073
H	-2.62306	1.62826	0.12647
H	1.34497	2.92798	-0.80451
H	0.88043	2.89947	0.90539
H	-0.24088	-1.88174	-0.62882
H	0.71318	-1.90476	0.83296
H	1.76828	-2.64587	-1.45691
H	1.86589	-0.93836	-1.8366
H	3.28679	-2.46048	0.39875
H	4.00466	-1.50322	-0.89612
H	4.15677	-0.09439	1.03167
H	2.55586	-0.51963	1.60748
H	2.95822	0.9854	-1.02181
H	2.92293	1.79526	0.5429



INT5

C	-4.94359	-2.89597	1.00265
C	-4.47858	-3.50688	-0.16534
C	-3.56892	-2.87806	-1.0214
C	-3.13611	-1.61107	-0.66551
C	-3.5927	-0.98958	0.50727
C	-4.49933	-1.61993	1.34799
C	-2.02988	0.39827	-0.68593
C	-2.95255	0.33338	0.57281
O	-1.31604	1.32256	-1.01009
C	-2.70619	3.73748	-0.09295
O	-1.81996	3.92811	0.61999
H	-5.65012	-3.41752	1.63874
H	-4.83319	-4.50068	-0.42084
H	-3.21697	-3.36087	-1.92654
H	-4.84479	-1.12454	2.25026
N	-2.2429	-0.77656	-1.35218
H	-1.77327	-1.03045	-2.21281
O	-3.10558	1.24835	1.34535
S	-3.93215	3.5676	-1.06902
C	2.17219	-1.66521	-2.08916
C	1.21643	-0.81475	-1.28187
N	1.87332	-0.39254	-0.03807
C	3.19519	-0.22088	0.04932
N	3.97176	-0.37183	-1.01993
C	3.44729	-0.88242	-2.29987
C	3.77243	0.04604	1.42961
C	5.19038	-0.47767	1.66499
C	6.25708	0.50838	1.19696
C	5.90926	1.05978	-0.1836
C	5.40607	-0.01826	-1.13197
C	0.98065	-0.02635	1.11035
O	1.18422	1.06633	1.59753
S	-0.1665	-1.22209	1.56181
H	1.73076	-1.91524	-3.05572
H	2.38382	-2.59608	-1.55364
H	0.90191	0.07419	-1.8396
H	0.32926	-1.37457	-0.98608

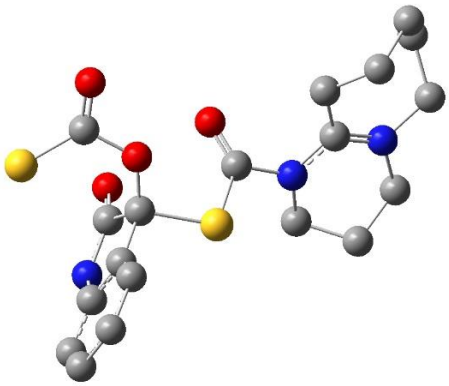
H	4.23018	-1.51302	-2.72861
H	3.28643	-0.0321	-2.97181
H	3.09516	-0.44142	2.13253
H	3.70354	1.11706	1.64112
H	5.30321	-0.67242	2.73488
H	5.31359	-1.44288	1.1614
H	6.34107	1.33451	1.91098
H	7.23039	0.00747	1.1642
H	6.79127	1.51504	-0.64296
H	5.15383	1.85011	-0.11312
H	6.00046	-0.93573	-1.04399
H	5.5108	0.33716	-2.16005



TS5-6

C	-5.21	-1.53358	1.8304
C	-5.44714	-2.32381	0.70449
C	-4.65618	-2.22073	-0.44409
C	-3.61782	-1.30231	-0.42174
C	-3.36398	-0.51315	0.7081
C	-4.15767	-0.61336	1.83708
C	-1.86143	0.02406	-1.0858
C	-2.20917	0.38127	0.3882
O	-0.99818	0.53949	-1.76793
C	-1.95442	2.95327	-0.43816
O	-0.94468	3.49194	-0.20277
H	-5.84686	-1.63416	2.70274
H	-6.26863	-3.03342	0.71373
H	-4.851	-2.82761	-1.32199
H	-3.95836	0.0097	2.70398
N	-2.70744	-0.99	-1.44075
H	-2.70104	-1.42138	-2.35699
O	-2.10485	1.57338	0.81422
S	-3.3607	2.95537	-1.29771
C	2.4141	-2.46785	-1.53687
C	1.35191	-1.42706	-1.26823
N	1.77245	-0.6039	-0.11729
C	3.07509	-0.32547	0.11637
N	4.00801	-0.78599	-0.6968
C	3.7198	-1.75012	-1.77972

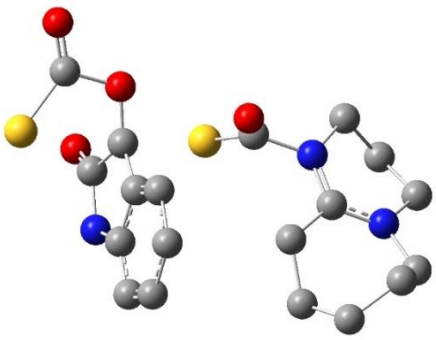
C	3.41333	0.42607	1.39259
C	4.77123	0.09441	2.01526
C	5.90158	0.92165	1.41
C	5.78769	0.94801	-0.11201
C	5.44659	-0.41551	-0.69262
C	0.73015	0.09401	0.62679
O	0.83965	1.27188	0.84006
S	-0.60088	-0.91491	1.19022
H	2.15025	-3.0525	-2.41984
H	2.50109	-3.14609	-0.6827
H	1.20823	-0.77234	-2.13243
H	0.39419	-1.87744	-1.01147
H	4.56007	-2.44818	-1.79945
H	3.70544	-1.2006	-2.72645
H	2.62946	0.17039	2.10642
H	3.31461	1.49976	1.20748
H	4.69926	0.28414	3.08934
H	4.97532	-0.97611	1.90421
H	5.86511	1.94485	1.79816
H	6.86606	0.49565	1.70528
H	6.73415	1.26421	-0.55933
H	5.03334	1.6717	-0.43959
H	6.00482	-1.21751	-0.19641
H	5.72107	-0.43342	-1.74978



INT6

C	-4.4981	-1.15783	2.50745
C	-5.1519	-2.02153	1.62875
C	-4.77447	-2.12726	0.28581
C	-3.72097	-1.33586	-0.14481
C	-3.06217	-0.46499	0.73067
C	-3.43164	-0.37048	2.05954
C	-2.21208	-0.24507	-1.50135
C	-1.94717	0.20621	-0.0288
O	-1.60849	0.09902	-2.49037
C	-2.56987	2.56657	-0.20736
O	-2.16287	3.67248	0.07295
H	-4.81714	-1.0972	3.54234
H	-5.97601	-2.62816	1.99115
H	-5.28868	-2.79677	-0.39543
H	-2.91253	0.30875	2.72986

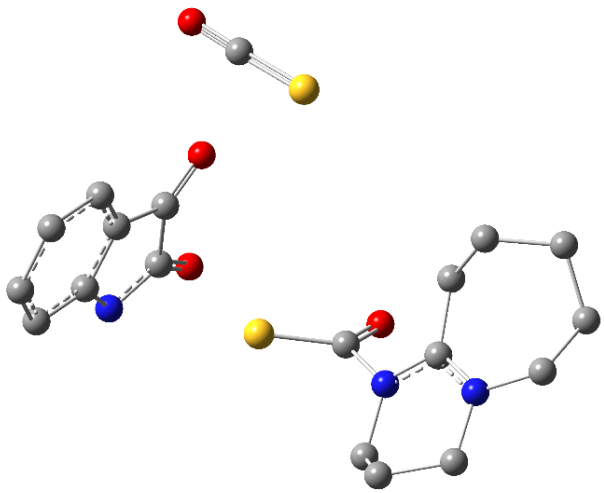
N	-3.1625	-1.23593	-1.41916
H	-3.54376	-1.6821	-2.24425
O	-1.6868	1.54292	0.21177
S	-4.03372	2.11721	-1.00095
C	3.10036	-2.96469	-0.36312
C	2.04364	-2.10993	-1.02506
N	2.06654	-0.77841	-0.38365
C	3.22251	-0.19357	0.01452
N	4.35832	-0.847	-0.09342
C	4.43221	-2.26616	-0.50996
C	3.10819	1.17896	0.64812
C	4.15799	1.50996	1.71109
C	5.45271	2.04352	1.10493
C	5.87928	1.20003	-0.09429
C	5.71654	-0.293	0.14863
C	0.85627	0.00873	-0.47683
O	0.80354	1.02687	-1.09738
S	-0.42969	-0.72849	0.50771
H	3.15019	-3.94138	-0.84702
H	2.85313	-3.10932	0.69248
H	2.24301	-1.98502	-2.09411
H	1.04422	-2.52572	-0.90132
H	5.19251	-2.72974	0.12245
H	4.78425	-2.28736	-1.54583
H	2.12125	1.21928	1.11315
H	3.10137	1.92897	-0.1505
H	3.72372	2.25248	2.38513
H	4.35442	0.61958	2.3179
H	5.31645	3.08298	0.78926
H	6.2398	2.03526	1.86586
H	6.93305	1.37762	-0.32594
H	5.31515	1.47589	-0.99208
H	6.0237	-0.57794	1.16085
H	6.34874	-0.8421	-0.55189



TS6-3

C	-0.71847	2.80706	-1.09788
C	-0.65784	3.41808	0.15598
C	-1.15672	2.78951	1.30141
C	-1.72013	1.52945	1.1534
C	-1.75674	0.89713	-0.10467
C	-1.27463	1.53294	-1.23738

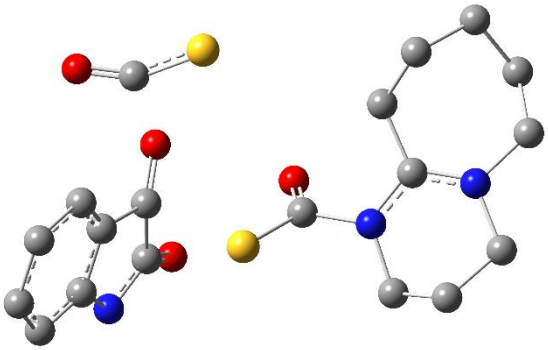
C	-2.82533	-0.46539	1.56259
C	-2.37333	-0.42375	0.10127
O	-3.32826	-1.3735	2.17228
C	-4.19481	-0.897	-1.21192
O	-4.71711	-1.5435	-2.06632
H	-0.34973	3.33338	-1.97202
H	-0.23354	4.41387	0.24638
H	-1.13335	3.28336	2.26721
H	-1.34227	1.04013	-2.20003
N	-2.32112	0.71964	2.10314
H	-2.50929	0.9787	3.05865
O	-2.84625	-1.2349	-0.87043
S	-4.73358	0.44719	-0.26246
C	3.44778	-2.92261	0.82025
C	2.37771	-2.86929	-0.25422
N	1.91316	-1.48525	-0.36569
C	2.69694	-0.43822	-0.16872
N	3.99244	-0.61111	0.12151
C	4.54005	-1.93742	0.45222
C	2.02995	0.92253	-0.21843
C	2.74733	2.05905	0.50429
C	3.88495	2.66122	-0.31525
C	4.76163	1.56747	-0.92567
C	5.04155	0.42635	0.04629
C	0.45447	-1.27412	-0.68777
O	0.20625	-0.85813	-1.78501
S	-0.54841	-1.64567	0.65598
H	3.87037	-3.92601	0.89947
H	3.0011	-2.66104	1.7842
H	2.76287	-3.20013	-1.22513
H	1.51028	-3.47954	0.00362
H	5.23524	-1.79571	1.28556
H	5.11796	-2.2994	-0.40725
H	1.04537	0.7885	0.24629
H	1.81629	1.17128	-1.2642
H	1.99753	2.82137	0.72975
H	3.11613	1.69741	1.47139
H	3.47643	3.28772	-1.11474
H	4.49148	3.31344	0.32163
H	5.72138	1.98483	-1.24276
H	4.29732	1.14979	-1.82633
H	5.2509	0.80537	1.05466
H	5.9348	-0.11212	-0.28433



INT 7

C	4.1224	-0.51549	-2.67354
C	4.36832	-1.87398	-2.45279
C	4.26451	-2.4504	-1.18391
C	3.90163	-1.61873	-0.13554
C	3.64613	-0.2537	-0.34615
C	3.75663	0.30898	-1.61059
C	3.33819	-0.87462	1.95932
C	3.28014	0.32134	0.95727
O	3.03009	1.45773	1.2817
O	3.11845	-0.82817	3.14707
C	2.48143	3.75465	-0.35524
O	3.61588	3.94888	-0.25514
S	0.93334	3.53357	-0.52107
H	4.21661	-0.10647	-3.67331
H	4.65083	-2.50411	-3.29055
H	4.4603	-3.50507	-1.02367
H	3.56337	1.36667	-1.76161
N	3.74132	-1.95143	1.21439
H	3.82415	-2.89071	1.58263
C	-3.28551	-2.856	-1.17959
C	-2.48447	-2.73811	0.10004
N	-2.29202	-1.31675	0.40705
C	-3.20854	-0.39756	0.1146
N	-4.35213	-0.74305	-0.47315
C	-4.58402	-2.10294	-0.99549
C	-2.84601	1.04815	0.40302
C	-3.50983	2.09371	-0.49334
C	-4.90355	2.4808	-0.00662
C	-5.71175	1.23951	0.3653
C	-5.54937	0.11111	-0.64335
C	-1.0363	-0.94373	1.14364
O	-1.20653	-0.44563	2.23705
S	0.41628	-1.27696	0.29802
H	-3.49998	-3.90296	-1.40158
H	-2.7115	-2.4345	-2.01066

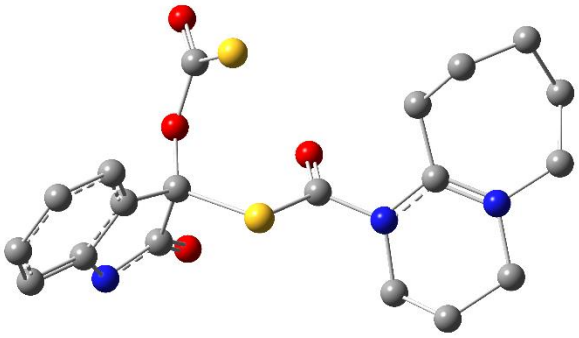
H	-3.00603	-3.21689	0.93622
H	-1.49233	-3.17775	0.00167
H	-5.10913	-1.98711	-1.9473
H	-5.24934	-2.62768	-0.301
H	-1.76369	1.11021	0.27152
H	-3.03346	1.2519	1.46215
H	-2.86338	2.9756	-0.51689
H	-3.55419	1.71637	-1.52105
H	-4.82518	3.14029	0.86421
H	-5.42174	3.04125	-0.79191
H	-6.77645	1.48407	0.41773
H	-5.42941	0.86999	1.35745
H	-5.56815	0.49073	-1.67203
H	-6.38856	-0.58144	-0.53926



TS7-8

C	4.74876	0.20375	-2.20896
C	5.43183	-0.96294	-1.86066
C	5.10441	-1.68281	-0.71036
C	4.07862	-1.19078	0.08347
C	3.39138	-0.01015	-0.24557
C	3.71556	0.68569	-1.40317
C	2.57612	-0.9739	1.81164
C	2.36139	0.19435	0.81461
O	1.88722	1.27162	1.25189
O	2.03041	-1.13781	2.87742
C	2.01725	2.80394	0.23972
O	3.10577	3.20217	0.42727
S	0.56436	3.03462	-0.4782
H	5.01842	0.7379	-3.11349
H	6.23275	-1.32424	-2.49813
H	5.62924	-2.59341	-0.44169
H	3.17292	1.57953	-1.69276
N	3.57643	-1.73918	1.26439
H	3.94458	-2.5698	1.71087
C	-3.05424	-2.94771	-1.18341
C	-2.05405	-2.68587	-0.07869
N	-1.94861	-1.23244	0.1233
C	-2.99683	-0.41138	-0.03198
N	-4.17735	-0.8947	-0.38923
C	-4.36503	-2.30251	-0.79527

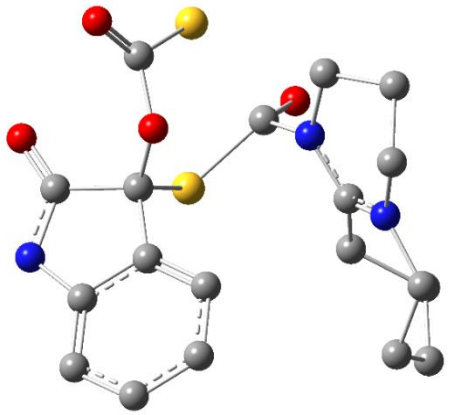
C	-2.73541	1.07354	0.1329
C	-3.61838	1.99837	-0.70594
C	-4.95294	2.30039	-0.02961
C	-5.56935	1.02673	0.54421
C	-5.46429	-0.15754	-0.4054
C	-0.67035	-0.71947	0.66016
O	-0.68829	-0.13491	1.71271
S	0.69274	-1.02982	-0.36897
H	-3.2023	-4.02105	-1.31427
H	-2.68326	-2.52963	-2.12403
H	-2.37147	-3.15183	0.86034
H	-1.0604	-3.0522	-0.33462
H	-5.06249	-2.29148	-1.63636
H	-4.8391	-2.83457	0.03618
H	-1.69242	1.23052	-0.15062
H	-2.79524	1.32357	1.19741
H	-3.06498	2.92649	-0.87506
H	-3.78008	1.55218	-1.69342
H	-4.80705	3.02875	0.775
H	-5.63715	2.75176	-0.75568
H	-6.63106	1.18253	0.75523
H	-5.10034	0.75837	1.49723
H	-5.68238	0.13522	-1.43908
H	-6.20276	-0.91004	-0.11820



INT8

C	4.74488	0.55692	-2.30271
C	5.6231	-0.45684	-1.92367
C	5.36326	-1.26456	-0.81384
C	4.20151	-1.01384	-0.1008
C	3.31077	0.00703	-0.46276
C	3.57392	0.79291	-1.57508
C	2.55669	-1.17234	1.49331
C	2.15733	-0.01166	0.52233
O	1.98786	1.08456	1.34638
O	1.92789	-1.53412	2.46066
C	1.46756	2.36311	1.03518
O	1.54161	3.1143	1.98234
S	0.82784	2.69413	-0.5334
H	4.96835	1.16747	-3.17101

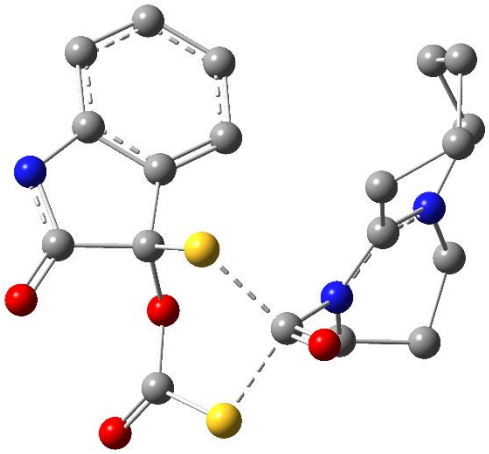
H	6.52671	-0.62869	-2.50017
H	6.04009	-2.05853	-0.51726
H	2.87805	1.57464	-1.8579
N	3.73162	-1.68808	1.03012
H	4.20993	-2.45795	1.48265
C	-2.76377	-3.08125	-0.81888
C	-1.8621	-2.60611	0.29979
N	-1.82839	-1.13259	0.25517
C	-2.91291	-0.39251	-0.05429
N	-4.03344	-0.98856	-0.40579
C	-4.12498	-2.44888	-0.63143
C	-2.73354	1.11076	-0.03079
C	-3.60493	1.89887	-1.00958
C	-4.99843	2.18234	-0.45539
C	-5.5893	0.93664	0.20179
C	-5.34969	-0.33024	-0.60664
C	-0.62994	-0.48363	0.75754
O	-0.62696	0.12149	1.7887
S	0.67703	-0.66195	-0.40786
H	-2.86488	-4.1673	-0.78792
H	-2.33438	-2.79747	-1.78409
H	-2.23903	-2.91958	1.27849
H	-0.8391	-2.96612	0.18624
H	-4.74568	-2.58279	-1.5204
H	-4.65115	-2.8823	0.22483
H	-1.68328	1.30745	-0.26745
H	-2.87947	1.45652	0.99929
H	-3.08819	2.83691	-1.23046
H	-3.67102	1.3525	-1.95681
H	-4.94937	2.99196	0.28014
H	-5.65051	2.5206	-1.26729
H	-6.67103	1.04846	0.31693
H	-5.18489	0.79386	1.2099
H	-5.48562	-0.15928	-1.68038
H	-6.07185	-1.09105	-0.30294



TS8-9

C	-0.31726	3.32296	1.18391
C	0.58595	4.32725	0.83637

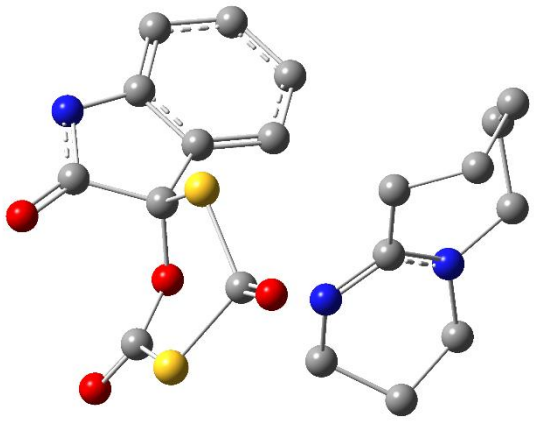
C	1.81176	4.02826	0.23478
C	2.09108	2.69328	-0.01172
C	1.18146	1.67859	0.30438
C	-0.0214	1.9819	0.91645
C	3.21909	0.77012	-0.54939
C	1.77677	0.36249	-0.11879
O	4.11235	-0.00002	-0.82006
C	2.48977	-1.73391	0.90742
O	3.37914	-1.93124	1.6911
H	-1.25435	3.58069	1.66667
H	0.34101	5.3638	1.04493
H	2.52421	4.80587	-0.01838
H	-0.7164	1.19563	1.19695
N	3.25748	2.13481	-0.55553
H	4.09759	2.65962	-0.7691
O	1.81823	-0.51091	0.97816
S	1.81702	-2.8921	-0.2044
C	0.0591	-1.83169	-1.1163
O	-0.33803	-2.56207	-2.00988
S	0.9692	-0.29074	-1.66588
C	-2.12956	-2.45572	1.95464
C	-0.81946	-2.45448	1.20304
N	-0.88315	-1.54602	0.0384
C	-1.91433	-0.69676	-0.14812
N	-2.69171	-0.35803	0.87465
C	-2.54354	-1.02172	2.17907
C	-2.19896	-0.15776	-1.53892
C	-3.69222	0.00096	-1.85944
C	-4.21101	1.38649	-1.48157
C	-3.67311	1.80244	-0.11588
C	-3.74836	0.68557	0.91264
H	-1.99597	-2.96843	2.90884
H	-2.9056	-2.9763	1.38515
H	-0.00509	-2.13713	1.85878
H	-0.59122	-3.44873	0.819
H	-3.50877	-0.95787	2.68319
H	-1.80137	-0.47707	2.77568
H	-1.75868	-0.85931	-2.24203
H	-1.67008	0.79193	-1.66646
H	-3.82934	-0.17523	-2.92938
H	-4.26568	-0.77637	-1.3425
H	-3.90083	2.11934	-2.23387
H	-5.306	1.37911	-1.46681
H	-4.25475	2.63876	0.28326
H	-2.63884	2.15442	-0.18877
H	-4.72121	0.18035	0.87681
H	-3.64481	1.12137	1.90973



INT9

C	-0.18382	3.27275	1.21615
C	0.74546	4.26773	0.91251
C	1.9682	3.9629	0.30773
C	2.22112	2.63111	0.01796
C	1.28988	1.62554	0.29921
C	0.08499	1.9356	0.9053
C	3.29381	0.70806	-0.62048
C	1.85486	0.31572	-0.17898
O	4.15811	-0.07688	-0.94105
C	2.43771	-1.84856	0.80902
O	3.35661	-2.21532	1.48657
H	-1.12083	3.53528	1.69636
H	0.52118	5.30181	1.15407
H	2.69657	4.73401	0.08137
H	-0.63564	1.15816	1.14396
N	3.37226	2.06872	-0.55445
H	4.21952	2.58386	-0.76251
O	1.95808	-0.57289	0.92921
S	1.52143	-2.95798	-0.21583
C	0.03543	-1.93451	-0.94577
O	-0.49623	-2.59840	-1.84311
S	0.99247	-0.35104	-1.6555
C	-2.05058	-2.17469	2.20341
C	-0.71012	-1.84219	1.58312
N	-0.90457	-1.4272	0.18239
C	-1.9763	-0.67307	-0.1213
N	-2.82844	-0.29509	0.83557
C	-2.87883	-0.91856	2.17074
C	-2.20423	-0.23553	-1.55564
C	-3.66436	-0.0119	-1.96099
C	-4.11826	1.41891	-1.68082
C	-3.64933	1.85654	-0.29586
C	-3.85699	0.77197	0.74902
H	-1.91477	-2.50348	3.2354
H	-2.53223	-2.97996	1.64096
H	-0.22162	-1.0319	2.13576

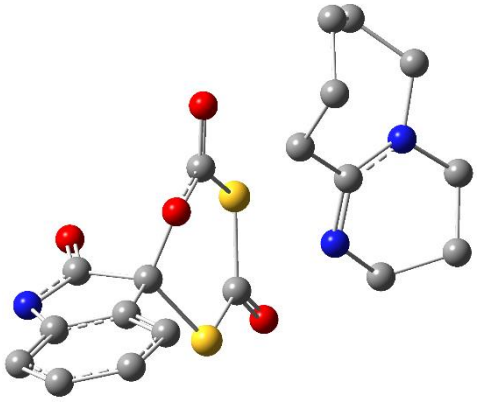
H	-0.06333	-2.71307	1.59884
H	-3.93292	-1.11878	2.38331
H	-2.51548	-0.18871	2.90248
H	-1.76764	-1.00889	-2.1808
H	-1.61072	0.66952	-1.72455
H	-3.75827	-0.23483	-3.0271
H	-4.30846	-0.72833	-1.43922
H	-3.70987	2.09587	-2.43874
H	-5.20988	1.4815	-1.74315
H	-4.20718	2.73702	0.03602
H	-2.59274	2.14649	-0.30746
H	-4.83722	0.29449	0.6309
H	-3.8401	1.23016	1.74189



TS9-10

C	0.01179	3.39985	-1.03571
C	-1.03173	4.30284	-0.8266
C	-2.27527	3.88705	-0.34245
C	-2.43266	2.53607	-0.07608
C	-1.38964	1.6255	-0.26896
C	-0.16056	2.04228	-0.75011
C	-3.37601	0.52004	0.47192
C	-1.87418	0.26812	0.1493
O	-4.17812	-0.35338	0.71645
C	-2.24358	-1.90759	-0.89059
O	-2.99273	-2.3365	-1.71901
H	0.96253	3.7531	-1.4207
H	-0.87974	5.35462	-1.04712
H	-3.0874	4.58882	-0.18732
H	0.64508	1.32932	-0.90793
N	-3.57576	1.86439	0.39054
H	-4.4824	2.29791	0.52166
O	-1.80618	-0.62	-0.94915
S	-1.49639	-2.98448	0.30389
C	-0.29341	-1.91341	1.22692
O	0.32729	-2.49999	2.08796
S	-1.03882	-0.29214	1.69766
C	2.19117	-2.18027	-2.17231
C	0.84394	-1.77714	-1.59599

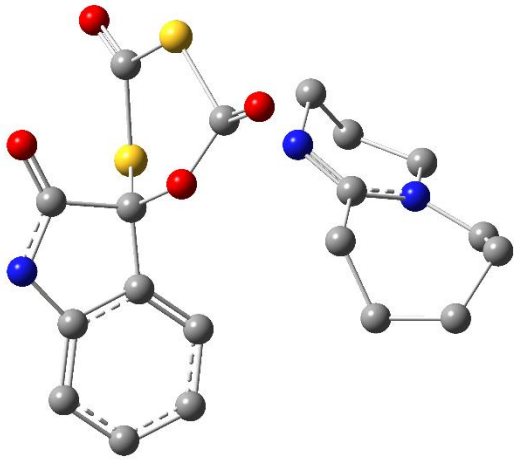
N	0.99766	-1.33307	-0.2145
C	2.04671	-0.59704	0.07112
N	2.96384	-0.24615	-0.8686
C	3.06776	-0.95022	-2.15467
C	2.22254	-0.12583	1.50525
C	3.66542	0.09375	1.96771
C	4.1524	1.50815	1.65667
C	3.75579	1.91304	0.23813
C	3.99885	0.79932	-0.77031
H	2.08687	-2.54778	-3.19565
H	2.62576	-2.9781	-1.56172
H	0.41003	-0.96918	-2.20111
H	0.15522	-2.62168	-1.62513
H	4.12218	-1.20914	-2.30229
H	2.7799	-0.25901	-2.95631
H	1.75052	-0.88199	2.12875
H	1.63781	0.7917	1.63925
H	3.71993	-0.09115	3.04428
H	4.32054	-0.64636	1.49405
H	3.72215	2.21601	2.37379
H	5.24124	1.55858	1.76687
H	4.33679	2.78312	-0.08179
H	2.70156	2.21081	0.19439
H	4.97358	0.32526	-0.58929
H	4.04291	1.23675	-1.77323



INT10

C	-3.10399	2.84097	1.6785
C	-4.38256	2.90303	1.12248
C	-4.81939	1.9797	0.1672
C	-3.924	0.9943	-0.21324
C	-2.6421	0.9272	0.33921
C	-2.2142	1.83522	1.2916
C	-2.96536	-0.77904	-1.3083
C	-1.93985	-0.25623	-0.25597
O	-2.74513	-1.66271	-2.10608
C	0.08702	-0.67912	-1.52876
O	0.81294	-0.27309	-2.39136
H	-2.80055	3.57481	2.41671

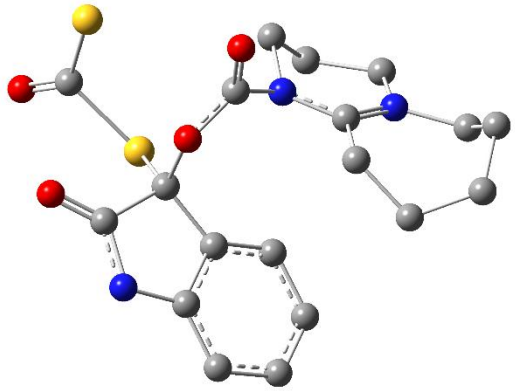
H	-5.06168	3.68865	1.43786
H	-5.81414	2.03247	-0.26084
H	-1.21628	1.75738	1.71441
N	-4.09402	-0.03762	-1.14926
H	-4.91706	-0.16037	-1.72861
O	-0.75893	0.15345	-0.9099
S	0.25987	-2.40887	-1.09804
C	-0.74428	-2.73648	0.34905
O	-0.65848	-3.82107	0.85427
S	-1.72912	-1.46692	1.09647
C	3.12279	-1.00459	2.63409
C	1.67804	-1.03404	2.15335
N	1.35432	0.16056	1.38659
C	2.27839	0.6464	0.61883
N	3.53488	0.11199	0.47676
C	4.01487	-0.91029	1.4113
C	1.90349	1.92274	-0.12306
C	3.04115	2.9224	-0.34362
C	3.8124	2.62445	-1.63042
C	4.06952	1.12587	-1.79248
C	4.55997	0.46347	-0.51147
H	3.37875	-1.89765	3.21014
H	3.27149	-0.13024	3.2773
H	1.53405	-1.94194	1.54583
H	0.98158	-1.1068	2.99524
H	5.03968	-0.6463	1.69922
H	4.06158	-1.87923	0.89466
H	1.10756	2.36569	0.47838
H	1.44872	1.66181	-1.08603
H	2.63159	3.93626	-0.38372
H	3.72073	2.89684	0.51674
H	3.24317	2.98714	-2.4941
H	4.7657	3.16513	-1.62555
H	4.82908	0.9638	-2.56363
H	3.16494	0.60859	-2.13129
H	5.33285	1.08771	-0.0367
H	5.04528	-0.48388	-0.77458



TS10-11

C	-0.53193	3.5149	1.29621
C	-1.68368	4.25903	1.03812
C	-2.80538	3.69071	0.42657
C	-2.72802	2.35165	0.07773
C	-1.5783	1.598	0.33162
C	-0.47386	2.16268	0.94547
C	-3.24744	0.28123	-0.77312
C	-1.80757	0.19922	-0.17495
O	-3.83151	-0.62688	-1.31982
C	-0.22519	-1.29083	-1.4114
O	0.39907	-1.40706	-2.4418
H	0.3207	3.98573	1.7734
H	-1.71523	5.3071	1.31847
H	-3.69892	4.27236	0.22816
H	0.41055	1.56445	1.14867
N	-3.69222	1.55167	-0.55015
H	-4.60461	1.87604	-0.84906
O	-0.92029	-0.10914	-1.21679
S	-1.19141	-2.83322	-0.98187
C	-2.07383	-2.51278	0.51982
O	-2.69588	-3.37852	1.0737
S	-1.87816	-0.89802	1.28846
C	1.9858	-1.77297	2.23932
C	1.2813	-2.26755	0.98813
N	1.11247	-1.16683	0.04754
C	2.13181	-0.35552	-0.12234
N	3.2713	-0.44947	0.60897
C	3.34962	-1.26989	1.82613
C	1.99422	0.74346	-1.163
C	2.71554	2.0554	-0.8414
C	4.1546	2.05484	-1.35411
C	4.83803	0.72651	-1.03426
C	4.54993	0.2498	0.38229
H	2.09313	-2.57289	2.97544
H	1.39372	-0.96846	2.68917
H	1.86475	-3.07433	0.52185

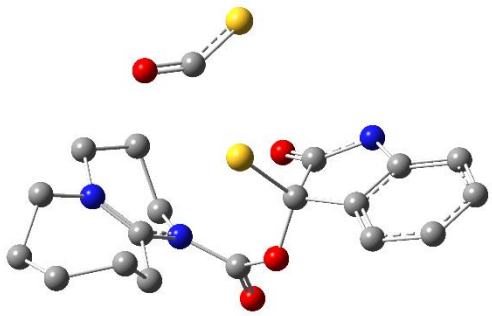
H	0.30872	-2.68231	1.24695
H	3.79869	-0.65102	2.61085
H	4.02975	-2.10922	1.63654
H	0.92946	0.93043	-1.2647
H	2.31841	0.34751	-2.13171
H	2.1571	2.88295	-1.28926
H	2.70066	2.22642	0.24202
H	4.16377	2.21969	-2.43723
H	4.71243	2.87969	-0.89725
H	5.92282	0.82907	-1.13299
H	4.53474	-0.05306	-1.74117
H	4.63082	1.08614	1.09064
H	5.31574	-0.47861	0.66776



INT11

C	1.30311	2.70881	1.61141
C	0.91819	3.96712	1.15062
C	-0.20889	4.1291	0.34245
C	-0.91373	2.98787	-0.0089
C	-0.50719	1.70832	0.39505
C	0.58257	1.56879	1.24217
C	-2.59995	1.63369	-0.7761
C	-1.5136	0.70708	-0.13367
O	-3.64976	1.27515	-1.25207
C	-0.23363	-1.02908	-1.40361
O	-0.12948	-1.66012	-2.41509
H	2.16228	2.61086	2.2664
H	1.48819	4.84329	1.44286
H	-0.5383	5.10974	0.01654
H	0.86242	0.59662	1.63591
N	-2.11101	2.90898	-0.72264
H	-2.63876	3.70998	-1.04868
O	-1.08469	-0.01375	-1.31418
S	-3.28501	-2.34043	-0.79066
C	-3.62803	-1.36666	0.56132
O	-4.58821	-1.3111	1.2886
S	-2.18894	-0.24557	1.24566
C	0.84626	-2.4401	1.85287
C	0.23108	-2.55408	0.47595
N	0.59381	-1.32192	-0.25467

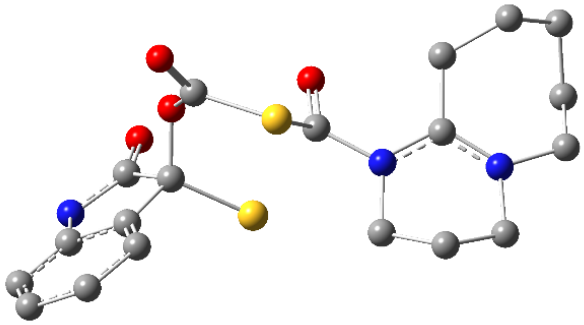
C	1.87658	-0.89387	-0.26736
N	2.73302	-1.36938	0.60949
C	2.34637	-2.29513	1.70186
C	2.22559	0.14547	-1.30954
C	3.34283	1.12658	-0.9495
C	4.73029	0.5575	-1.22928
C	4.84651	-0.87923	-0.72153
C	4.19212	-1.08614	0.63844
H	0.63429	-3.33596	2.4395
H	0.41351	-1.5787	2.36953
H	0.62424	-3.41737	-0.07267
H	-0.85706	-2.6092	0.50385
H	2.80209	-1.90035	2.61349
H	2.81367	-3.2579	1.47472
H	1.31074	0.71163	-1.49925
H	2.45591	-0.39142	-2.23889
H	3.18235	2.04187	-1.52532
H	3.24842	1.40692	0.10416
H	4.93501	0.58014	-2.30465
H	5.4821	1.187	-0.74243
H	5.89898	-1.1591	-0.62396
H	4.40403	-1.58494	-1.43323
H	4.36427	-0.23848	1.31063
H	4.62233	-1.97004	1.11212



TS 11-4

C	4.47386	2.40123	-0.83605
C	5.42531	1.39102	-0.69466
C	5.07155	0.11449	-0.24632
C	3.73729	-0.10544	0.05637
C	2.77178	0.89595	-0.09324
C	3.1285	2.15443	-0.54209
C	1.81487	-1.06525	0.8404
C	1.42559	0.30649	0.24052
O	1.08204	-1.78516	1.48939
C	-0.07559	0.61629	2.15805
O	0.09095	0.66727	3.34657
H	4.77882	3.38397	-1.17977
H	6.46417	1.59604	-0.93323
H	5.81059	-0.67104	-0.12971
H	2.3777	2.93043	-0.66108
N	3.13143	-1.27083	0.551

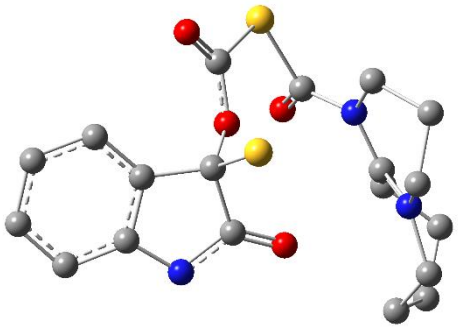
H	3.63678	-2.09024	0.86622
O	0.84229	1.11307	1.30746
S	0.57161	-3.20435	-1.588
C	-0.45697	-1.97708	-1.88504
O	-1.46286	-1.60652	-2.37195
S	0.40267	0.14228	-1.2402
C	-2.04904	-2.18668	1.24941
C	-1.73457	-1.16504	2.32004
N	-1.258	0.04529	1.62326
C	-2.01159	0.56819	0.61414
N	-2.96724	-0.16933	0.09537
C	-3.13589	-1.6174	0.36608
C	-1.84342	2.03892	0.30973
C	-2.22464	2.51603	-1.09256
C	-3.71593	2.80816	-1.2315
C	-4.55407	1.69998	-0.59444
C	-3.99996	0.30566	-0.86225
H	-2.40376	-3.1192	1.69355
H	-1.13243	-2.38825	0.69059
H	-2.61933	-0.9109	2.91281
H	-0.93716	-1.49661	2.97891
H	-3.16997	-2.11207	-0.60792
H	-4.11638	-1.72384	0.8398
H	-0.80367	2.28575	0.50361
H	-2.43508	2.56283	1.07371
H	-1.64281	3.41595	-1.31031
H	-1.90595	1.76362	-1.81917
H	-3.95927	3.7647	-0.75689
H	-3.96806	2.90162	-2.29297
H	-5.57522	1.72885	-0.98451
H	-4.63329	1.8405	0.48914
H	-3.59241	0.20778	-1.87388
H	-4.80687	-0.42174	-0.76644



TS9-12

C	4.65263	2.19522	0.65213
C	5.77898	1.74273	-0.03404
C	5.746	0.56603	-0.78703
C	4.55334	-0.14076	-0.8148
C	3.41384	0.29819	-0.13066
C	3.45417	1.47589	0.59774

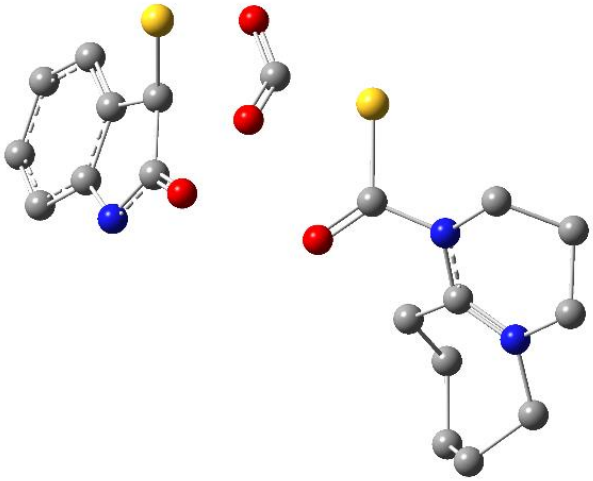
C	2.99198	-1.76564	-1.26653
C	2.29178	-0.68524	-0.38732
O	2.49963	-2.79813	-1.65897
C	1.56873	-0.81053	1.93293
O	2.10303	-1.02836	2.98643
H	4.70201	3.11509	1.22487
H	6.70017	2.3152	0.01008
H	6.61773	0.2142	-1.32847
H	2.56832	1.84125	1.10928
N	4.27058	-1.33307	-1.48904
H	4.94353	-1.86355	-2.02857
O	1.96708	-1.43603	0.80974
S	0.17291	0.29162	1.84858
C	-2.40948	2.87473	-0.09512
C	-1.33034	1.88713	-0.4717
N	-1.74185	0.53149	-0.0606
C	-3.04924	0.18101	-0.05093
N	-3.95869	1.02454	-0.52006
C	-3.67281	2.44573	-0.79653
C	-3.46092	-1.12553	0.6095
C	-4.88841	-1.18154	1.1549
C	-5.90611	-1.56659	0.08618
C	-5.66183	-0.75776	-1.18452
C	-5.36221	0.70174	-0.88337
C	-0.68258	-0.43427	0.31022
O	-0.88139	-1.628	0.28676
S	0.88505	0.02851	-1.28751
H	-2.1268	3.87701	-0.42125
H	-2.55251	2.88767	0.99002
H	-1.16016	1.89739	-1.5529
H	-0.38527	2.10725	0.02125
H	-4.54249	3.00688	-0.4451
H	-3.59128	2.57902	-1.88034
H	-2.76501	-1.26126	1.43583
H	-3.2626	-1.95447	-0.07542
H	-4.89969	-1.91447	1.96614
H	-5.14966	-0.21866	1.60734
H	-5.83028	-2.63615	-0.1359
H	-6.91923	-1.38225	0.45864
H	-6.54239	-0.78414	-1.83244
H	-4.8348	-1.17853	-1.76691
H	-6.02077	1.094	-0.10004
H	-5.53854	1.29664	-1.78330



INT 12

C	-5.48342	0.41309	0.51515
C	-5.45199	1.75334	0.8994
C	-4.27238	2.49844	0.82251
C	-3.13658	1.84914	0.36303
C	-3.14715	0.50156	-0.02167
C	-4.3296	-0.21899	0.03969
C	-0.96326	1.43789	-0.23846
C	-1.77196	0.15027	-0.54579
O	0.24031	1.58036	-0.34705
C	-1.40571	-2.08573	0.37514
O	-2.41815	-2.617	0.01956
H	-6.41254	-0.14373	0.57959
H	-6.35708	2.23148	1.26085
H	-4.24105	3.544	1.11076
H	-4.34743	-1.25631	-0.27411
N	-1.85159	2.37985	0.19416
H	-1.57724	3.31973	0.45224
O	-1.06076	-0.81463	0.33341
S	-0.08823	-3.07149	1.14556
C	2.3089	-1.48189	-2.27073
C	1.47238	-2.03185	-1.14231
N	1.82368	-1.35227	0.13631
C	2.64014	-0.22219	0.16262
N	2.77777	0.4778	-0.92597
C	2.21419	0.02332	-2.20965
C	3.41799	0.07292	1.42793
C	4.74767	0.80161	1.21681
C	4.56623	2.31488	1.1448
C	3.38701	2.66462	0.24199
C	3.36217	1.84214	-1.03458
C	1.17459	-1.74304	1.31221
O	1.36822	-1.28433	2.40449
S	-1.6889	-0.25157	-2.28885
H	1.89931	-1.84555	-3.21508
H	3.35296	-1.80087	-2.19705
H	0.42091	-1.83756	-1.36928
H	1.64115	-3.0991	-1.00151
H	2.80129	0.50168	-2.99427
H	1.17152	0.36354	-2.25565

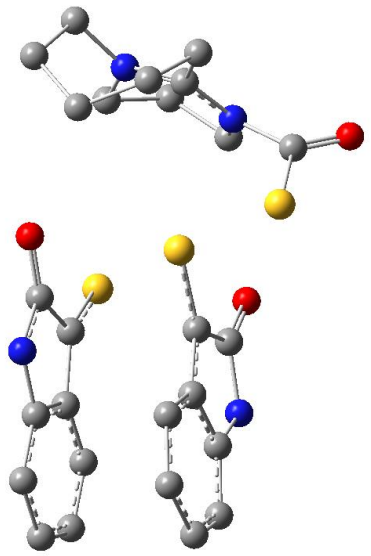
H	3.60358	-0.89846	1.88627
H	2.77868	0.61649	2.13003
H	5.40384	0.53762	2.05023
H	5.23431	0.42794	0.30919
H	4.39221	2.71842	2.14771
H	5.48214	2.77676	0.76203
H	3.43404	3.7153	-0.05839
H	2.42867	2.53123	0.75469
H	4.35454	1.74598	-1.48846
H	2.70876	2.33034	-1.76046



TS12-S-isatiin

C	4.70743	2.10952	-1.63931
C	4.3678	3.15769	-0.78235
C	3.78092	2.92027	0.46397
C	3.53851	1.59981	0.81291
C	3.8681	0.53702	-0.04055
C	4.46005	0.78498	-1.26779
C	2.96194	-0.27158	2.01892
C	3.50816	-0.73925	0.64213
O	2.57759	-0.96146	2.93519
S	4.44178	-2.15055	0.54599
H	5.16639	2.3254	-2.59839
H	4.56789	4.18159	-1.08304
H	3.52852	3.734	1.13563
H	4.71193	-0.04514	-1.9189
N	2.99369	1.10116	1.99843
H	2.70486	1.66955	2.78439
C	1.65175	-1.1834	-1.17997
O	2.40205	-1.27791	-2.11616
O	1.81146	-0.97825	0.05848
S	-0.16924	-1.50875	-1.62576
C	-4.17237	-2.64644	-0.18754
C	-2.69413	-2.37984	-0.03932
N	-2.43184	-0.94213	-0.2893
C	-3.38145	0.02055	-0.09834
N	-4.54795	-0.29536	0.41333

C	-4.92745	-1.6943	0.70712
C	-3.06492	1.41349	-0.61252
C	-4.26524	2.183	-1.17247
C	-5.01849	2.94305	-0.08427
C	-5.21509	2.06248	1.14681
C	-5.63688	0.64562	0.79287
C	-1.05954	-0.54032	-0.43049
O	-0.61388	0.40148	0.16446
H	-4.38754	-3.67531	0.10506
H	-4.47963	-2.50876	-1.22844
H	-2.34428	-2.62736	0.96741
H	-2.12141	-2.95732	-0.76263
H	-6.003	-1.76264	0.53658
H	-4.72855	-1.88417	1.76665
H	-2.32917	1.28232	-1.40666
H	-2.56589	1.98171	0.17763
H	-3.89097	2.87768	-1.92859
H	-4.9354	1.49056	-1.69344
H	-4.462	3.8433	0.19611
H	-5.99013	3.26773	-0.47044
H	-5.9961	2.477	1.79025
H	-4.30485	2.02096	1.75432
H	-6.38391	0.63119	-0.00869
H	-6.08695	0.17592	1.66975

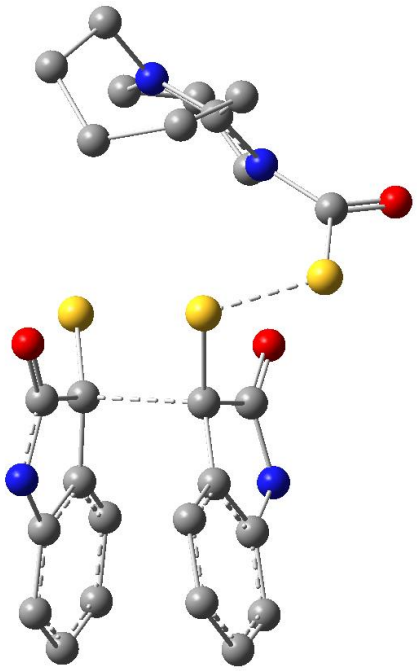


INT13

C	3.74428	0.18808	0.0525
C	3.14763	-1.9845	0.92326
H	2.09344	-2.03045	0.62227
H	3.58265	-2.9812	0.85652
N	3.86483	-1.12251	-0.02706
N	3.12546	0.7511	1.10434
C	3.30306	-1.39446	2.31437
H	4.3623	-1.38102	2.58703
H	2.76642	-2.00465	3.04412

C	2.71752	0.00229	2.32386
H	3.07604	0.58201	3.17646
H	1.62267	-0.01509	2.32835
C	4.66977	-1.7391	-1.09652
H	5.6084	-1.1892	-1.17983
H	4.91704	-2.74612	-0.76032
C	3.93635	-1.77033	-2.44248
H	3.28881	-2.65168	-2.48649
H	4.69459	-1.88183	-3.22472
C	3.08152	-0.52601	-2.68051
H	2.19532	-0.59699	-2.04183
H	2.71449	-0.53747	-3.71159
C	3.78273	0.81548	-2.43666
H	3.05553	1.61335	-2.61876
H	4.59342	0.95113	-3.15905
C	4.37998	1.02874	-1.02189
H	4.33661	2.08103	-0.74464
H	5.44108	0.76227	-1.01358
C	-3.16046	1.61062	0.5554
C	-2.20761	1.51486	-0.49324
C	-2.60953	1.78151	-1.80374
C	-3.93607	2.1404	-2.04801
C	-4.86166	2.22565	-1.00178
C	-4.4816	1.96429	0.31822
C	-0.9697	1.09003	0.1088
H	-1.89325	1.71145	-2.61835
H	-4.25551	2.35317	-3.06377
H	-5.88974	2.50274	-1.21388
H	-5.19557	2.02915	1.13395
H	-2.95192	1.31948	2.6616
S	0.53644	0.92376	-0.64655
C	-1.17476	1.01305	1.54286
O	-0.37857	0.76622	2.45518
N	-2.52165	1.31245	1.74715
C	2.7318	2.1356	1.14081
O	3.07221	2.83154	2.05986
S	1.66551	2.7384	-0.15182
C	-2.9982	-1.59524	-0.99693
C	-2.78539	-1.76162	0.38581
C	-3.86145	-1.72303	1.2719
C	-5.14053	-1.53053	0.7612
C	-5.33447	-1.37351	-0.61864
C	-4.26949	-1.4014	-1.51968
C	-1.36615	-1.9671	0.59693
H	-3.69029	-1.84527	2.33769
H	-5.99417	-1.50027	1.42969
H	-6.33991	-1.22269	-0.99994
H	-4.42496	-1.27351	-2.5856
H	-1.66768	-1.61989	-2.67432

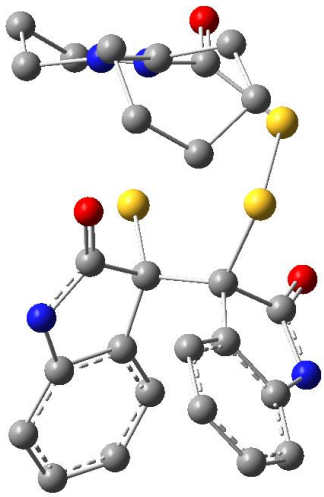
S	-0.53054	-2.26718	1.96057
C	-0.74531	-1.94027	-0.80504
O	0.41337	-2.14517	-1.10713
N	-1.78266	-1.68246	-1.67079



TS13-14

C	3.67723	0.32213	0.03097
C	3.84337	-1.29281	1.84414
H	2.87301	-1.79985	1.82079
H	4.61495	-2.00751	2.12626
N	4.15744	-0.81904	0.48789
N	2.92283	1.11492	0.81989
C	3.81674	-0.09594	2.77491
H	4.80687	0.36849	2.80277
H	3.5542	-0.41452	3.78564
C	2.76756	0.87517	2.28386
H	2.86146	1.84786	2.76654
H	1.75833	0.48842	2.42961
C	5.03478	-1.65441	-0.35653
H	5.79567	-1.01508	-0.80704
H	5.5496	-2.34162	0.31395
C	4.26087	-2.41891	-1.43381
H	3.81657	-3.31868	-0.99695
H	4.99112	-2.74529	-2.18178
C	3.15641	-1.5826	-2.08072
H	2.30524	-1.52053	-1.39417
H	2.78434	-2.10548	-2.96726
C	3.5812	-0.1699	-2.49553
H	2.72609	0.32269	-2.97015
H	4.36931	-0.22472	-3.25283
C	4.09622	0.745	-1.35357
H	3.81074	1.77802	-1.53414
H	5.18963	0.74214	-1.33079

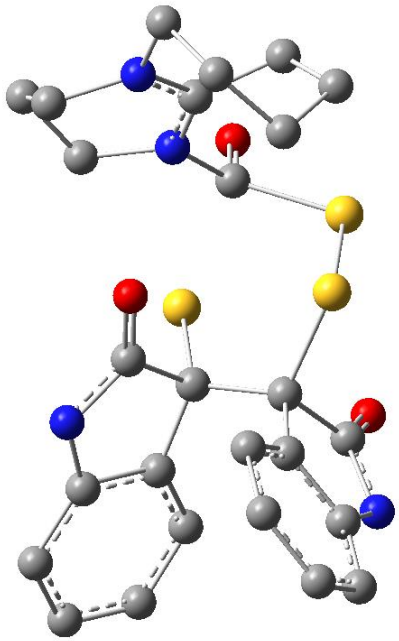
C	-3.07715	1.62095	0.01706
C	-2.31033	0.94388	-0.95703
C	-2.88177	0.64251	-2.18937
C	-4.21323	0.99548	-2.42268
C	-4.96525	1.63574	-1.43367
C	-4.40447	1.96264	-0.19562
C	-1.02657	0.61701	-0.33978
H	-2.30015	0.13043	-2.95149
H	-4.6699	0.76666	-3.38029
H	-6.00178	1.89215	-1.62974
H	-4.98122	2.46901	0.5719
H	-2.55433	2.36529	1.95433
S	0.47832	0.48589	-1.24526
C	-1.0027	1.34979	0.94545
O	-0.06126	1.51606	1.71144
N	-2.27936	1.84452	1.13212
C	2.33912	2.34729	0.37518
O	2.53826	3.36767	0.9741
S	1.27531	2.40525	-1.07633
C	-3.39435	-1.79074	-0.07182
C	-2.5953	-1.32708	0.98594
C	-3.18886	-0.88971	2.16029
C	-4.5835	-0.89052	2.25233
C	-5.36314	-1.33203	1.18043
C	-4.7796	-1.79699	-0.00198
C	-1.17962	-1.3963	0.56341
H	-2.57003	-0.54124	2.98258
H	-5.06532	-0.54532	3.16121
H	-6.44547	-1.32227	1.26621
H	-5.38255	-2.14996	-0.8323
H	-2.89732	-2.56985	-2.00314
S	0.11716	-1.69907	1.60374
C	-1.23873	-2.02509	-0.8302
O	-0.31444	-2.32467	-1.56497
N	-2.57034	-2.20643	-1.11686



INT 14

C	3.38943	-0.01531	-0.00242
C	3.53405	-0.60276	-2.37096
H	2.51669	-0.45075	-2.73979
H	4.2506	-0.32944	-3.14447
N	3.76018	0.29812	-1.23028
N	2.82562	-1.21491	0.25843
C	3.74081	-2.02495	-1.89377
H	4.77729	-2.15791	-1.56902
H	3.53987	-2.72713	-2.70532
C	2.77344	-2.29875	-0.76712
H	3.01994	-3.22431	-0.24853
H	1.73861	-2.3422	-1.10921
C	4.44186	1.57857	-1.50299
H	5.2016	1.74441	-0.73707
H	4.96294	1.46149	-2.45249
C	3.45904	2.74612	-1.54932
H	2.89537	2.72129	-2.4876
H	4.05023	3.66803	-1.54323
C	2.49698	2.70625	-0.36263
H	1.73005	1.94785	-0.55437
H	1.9778	3.66572	-0.27437
C	3.1942	2.39012	0.96474
H	2.48821	2.55433	1.78252
H	4.01892	3.09324	1.11989
C	3.76035	0.94684	1.10061
H	3.49047	0.524	2.06401
H	4.85548	0.96596	1.08987
C	-2.96173	1.75433	1.16003
C	-1.84605	1.4341	0.37469
C	-1.46849	2.2718	-0.66668
C	-2.23748	3.41161	-0.9255
C	-3.35666	3.70231	-0.14687
C	-3.73736	2.87732	0.91433
C	-1.2386	0.14159	0.89789
H	-0.58984	2.05305	-1.26639
H	-1.95681	4.07428	-1.73703
H	-3.94391	4.58949	-0.36221
H	-4.60152	3.10508	1.52909
H	-3.8153	0.83064	2.88812
S	0.40222	0.72801	1.51701
C	-2.13599	-0.16707	2.12198
O	-2.01596	-1.06751	2.92279
N	-3.11483	0.79767	2.15772
C	2.39998	-1.66155	1.55135
O	2.7791	-2.7161	1.98485
S	1.2857	-0.74317	2.62732
C	-2.7118	-0.91479	-2.04891
C	-2.67202	-1.18989	-0.67635
C	-3.82258	-1.61805	-0.03213

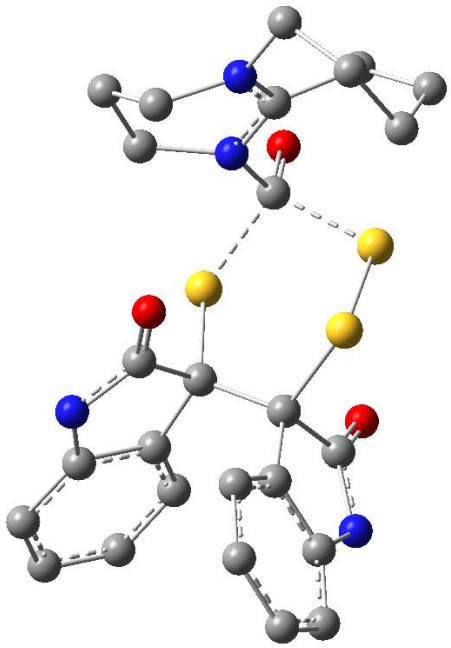
C	-5.00729	-1.74034	-0.76707
C	-5.02779	-1.45474	-2.13201
C	-3.87127	-1.04168	-2.79966
C	-1.2532	-0.99603	-0.17028
H	-3.79875	-1.87609	1.02294
H	-5.91506	-2.06936	-0.27172
H	-5.95289	-1.55967	-2.69024
H	-3.87674	-0.82654	-3.86324
H	-1.19237	-0.28318	-3.42326
S	-0.50024	-2.6002	0.2813
C	-0.53704	-0.49765	-1.44138
O	0.62132	-0.11975	-1.54577
N	-1.43933	-0.52428	-2.4715



TS14-15

C	3.40503	-0.28996	0.08421
C	3.59618	-1.22661	-2.15066
H	2.64629	-0.94223	-2.61628
H	4.38364	-1.22909	-2.904
N	3.95893	-0.24135	-1.12923
N	2.47987	-1.20507	0.3745
C	3.47079	-2.56587	-1.44974
H	4.42345	-2.81971	-0.97491
H	3.21568	-3.35479	-2.16011
C	2.35384	-2.44086	-0.43749
H	2.35499	-3.268	0.27635
H	1.39536	-2.42315	-0.9502
C	4.92892	0.80765	-1.48039
H	5.69143	0.87309	-0.70172
H	5.43229	0.4803	-2.39001
C	4.2589	2.16883	-1.69075
H	3.79729	2.20254	-2.68305
H	5.04784	2.92864	-1.67146
C	3.19895	2.46519	-0.62885

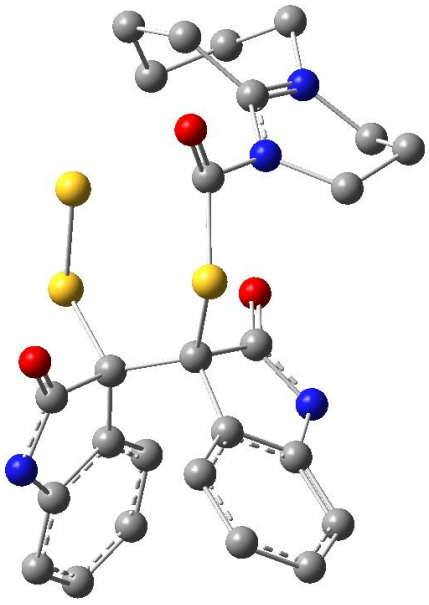
H	2.30234	1.87026	-0.84105
H	2.89772	3.51511	-0.69953
C	3.65777	2.17217	0.80348
H	2.88013	2.50709	1.49699
H	4.55481	2.75682	1.03271
C	3.96119	0.68173	1.09767
H	3.63115	0.40358	2.09294
H	5.04033	0.50419	1.08206
C	-3.17578	2.09585	0.42794
C	-2.02529	1.62202	-0.21772
C	-1.69197	2.10634	-1.47606
C	-2.54129	3.03514	-2.08698
C	-3.69407	3.47544	-1.43898
C	-4.029	3.01504	-0.1636
C	-1.32492	0.63999	0.70461
H	-0.78515	1.78098	-1.97581
H	-2.29522	3.41787	-3.0716
H	-4.34283	4.1958	-1.9273
H	-4.91723	3.36427	0.35178
H	-4.00364	1.70877	2.36201
S	0.28985	1.44705	1.10089
C	-2.23795	0.65355	1.95476
O	-2.09395	0.0314	2.98461
N	-3.27417	1.51301	1.6872
C	1.72386	-1.30731	1.68307
O	2.15577	-2.12873	2.49083
S	1.17996	0.28309	2.52888
C	-2.62916	-1.62208	-1.60069
C	-2.54531	-1.38075	-0.22386
C	-3.60303	-1.73102	0.60247
C	-4.74742	-2.29663	0.02964
C	-4.81693	-2.51809	-1.34506
C	-3.75127	-2.18784	-2.18644
C	-1.18712	-0.78014	0.08833
H	-3.53839	-1.58366	1.67613
H	-5.58416	-2.57117	0.66321
H	-5.71067	-2.96059	-1.77365
H	-3.79512	-2.36676	-3.2555
H	-1.24409	-1.29135	-3.2026
S	-0.2429	-2.0126	1.08053
C	-0.55016	-0.68588	-1.32133
O	0.5392	-0.22407	-1.61383
N	-1.4426	-1.21569	-2.21228



INT 15

C	3.53655	-0.49676	0.08235
C	3.49222	-1.08194	-2.24143
H	2.56792	-0.5574	-2.51154
H	4.18554	-1.05824	-3.08114
N	4.12069	-0.40567	-1.1076
N	2.39738	-1.1907	0.19918
C	3.17541	-2.49554	-1.77668
H	4.10167	-2.97527	-1.44783
H	2.74788	-3.08975	-2.58688
C	2.16165	-2.38792	-0.64977
H	2.20609	-3.25268	0.01976
H	1.16318	-2.31664	-1.06471
C	5.35138	0.37249	-1.29746
H	6.05996	0.11869	-0.50574
H	5.79397	0.05107	-2.24047
C	5.06975	1.87701	-1.30453
H	4.64028	2.16788	-2.26869
H	6.03261	2.39013	-1.20696
C	4.12815	2.2985	-0.17287
H	3.09667	2.03219	-0.43945
H	4.14695	3.38813	-0.0763
C	4.46641	1.66578	1.17914
H	3.83391	2.12435	1.94244
H	5.50603	1.89138	1.4393
C	4.26181	0.13106	1.25052
H	3.77467	-0.16855	2.17382
H	5.2328	-0.37757	1.25088
C	-3.17537	2.27211	0.23609
C	-2.15803	1.62817	-0.48248
C	-2.0082	1.88536	-1.83953
C	-2.90803	2.75462	-2.46534

C	-3.92828	3.3647	-1.73799
C	-4.07534	3.13691	-0.36813
C	-1.34988	0.77883	0.48379
H	-1.20349	1.43141	-2.40797
H	-2.80436	2.95779	-3.52577
H	-4.6182	4.03656	-2.23883
H	-4.85751	3.61951	0.2079
H	-3.71908	2.24151	2.30457
S	0.32491	1.56825	0.52638
C	-2.07771	1.02848	1.82822
O	-1.82283	0.54498	2.91005
N	-3.09943	1.90827	1.57625
C	1.61684	-1.16513	1.50295
O	2.07646	-1.85937	2.42536
S	1.30225	0.64675	2.07088
C	-3.0324	-1.77968	-1.15891
C	-2.7093	-1.33687	0.1298
C	-3.60754	-1.53059	1.16973
C	-4.83459	-2.14358	0.89444
C	-5.14357	-2.56452	-0.39813
C	-4.24085	-2.39302	-1.45056
C	-1.31828	-0.72637	0.1043
H	-3.35772	-1.22305	2.18007
H	-5.54806	-2.29737	1.69697
H	-6.09929	-3.04027	-0.59442
H	-4.47056	-2.72644	-2.45691
H	-1.94546	-1.74277	-3.00536
S	-0.25195	-1.82937	1.14344
C	-0.93045	-0.88508	-1.38753
O	0.09893	-0.52063	-1.92499
N	-1.97067	-1.50567	-2.02087

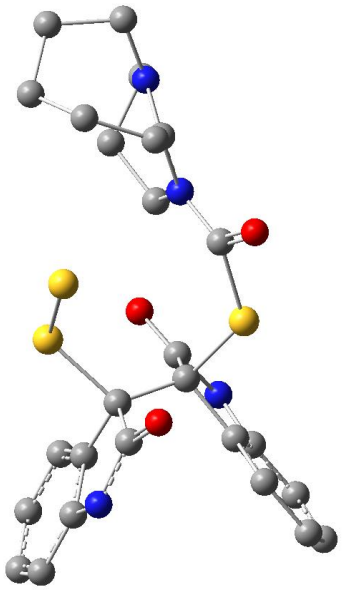


TS15-16

C	3.51455	0.43755	-0.19883
C	3.47744	1.67929	1.87134

H	2.56514	1.26827	2.31625
H	4.20014	1.89817	2.65582
N	4.07089	0.68175	0.97633
N	2.42025	1.13196	-0.56015
C	3.15973	2.89825	1.02407
H	4.07846	3.25819	0.55294
H	2.74453	3.70278	1.63385
C	2.13195	2.48895	-0.01288
H	2.13202	3.17913	-0.86118
H	1.13876	2.49424	0.42983
C	5.24973	-0.07189	1.42791
H	5.95816	-0.14729	0.60015
H	5.72687	0.51544	2.21262
C	4.85211	-1.46008	1.92615
H	4.35189	-1.37818	2.89671
H	5.77608	-2.02829	2.07891
C	3.94802	-2.17503	0.91755
H	2.91723	-1.80909	1.00502
H	3.91717	-3.24346	1.15147
C	4.41408	-1.98313	-0.52717
H	3.86606	-2.67917	-1.163
H	5.4787	-2.23153	-0.60069
C	4.19192	-0.55995	-1.10799
H	3.64909	-0.60755	-2.04585
H	5.15582	-0.08751	-1.3384
C	-3.63826	-1.84933	0.15008
C	-2.44815	-1.36623	0.71071
C	-2.2803	-1.37702	2.08856
C	-3.33256	-1.82799	2.89278
C	-4.51914	-2.28065	2.31805
C	-4.68924	-2.30614	0.93175
C	-1.50137	-0.98411	-0.41299
H	-1.34579	-1.05626	2.53811
H	-3.21789	-1.8334	3.97143
H	-5.32535	-2.63032	2.95533
H	-5.6038	-2.67332	0.47852
H	-4.27483	-2.09373	-1.87738
S	-0.13927	-2.22822	-0.29019
C	-2.35358	-1.27241	-1.66922
O	-2.05891	-1.07827	-2.82965
N	-3.55177	-1.79044	-1.23687
C	1.65832	0.82558	-1.77321
O	2.18178	0.92062	-2.86178
S	1.24952	-1.69816	-1.71094
C	-2.35169	2.11507	0.89048
C	-2.32995	1.40015	-0.31241
C	-3.32771	1.59538	-1.25625
C	-4.35824	2.4954	-0.9638
C	-4.37317	3.18697	0.24619

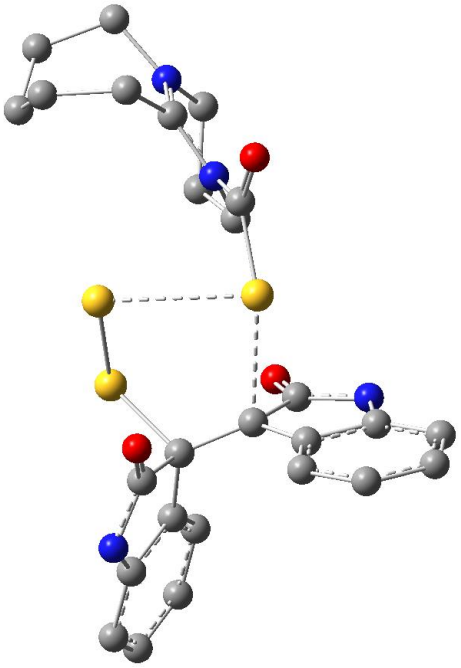
C	-3.36371	3.01098	1.1965
C	-1.09411	0.51362	-0.33153
H	-3.30673	1.07091	-2.20673
H	-5.14911	2.65709	-1.68818
H	-5.18069	3.88071	0.45744
H	-3.36658	3.55287	2.13599
H	-1.0348	2.12445	2.58011
S	-0.12227	1.25839	-1.73379
C	-0.45402	0.82404	1.04476
O	0.54259	0.32009	1.52141
N	-1.2362	1.76839	1.65302



INT 16

C	3.78668	0.74763	-0.23084
C	4.24149	1.13913	2.11715
H	5.04225	0.80735	2.77764
H	4.1173	2.22232	2.21892
N	4.66051	0.83638	0.74016
N	2.47856	1.05139	0.04259
C	2.9403	0.40307	2.37414
H	2.58708	0.58631	3.39021
H	3.1069	-0.67238	2.25305
C	1.90076	0.8985	1.39363
H	1.50678	1.86913	1.70369
H	1.08844	0.17986	1.31302
C	6.07334	0.48247	0.52257
H	6.36714	0.84637	-0.46303
H	6.65214	1.02964	1.26736
C	6.26786	-1.02705	0.63022
H	6.20747	-1.33966	1.6779
H	7.28022	-1.24965	0.27748
C	5.22686	-1.76851	-0.21132
H	4.27266	-1.82715	0.32442
H	5.55448	-2.80008	-0.36947
C	4.98757	-1.11165	-1.57341

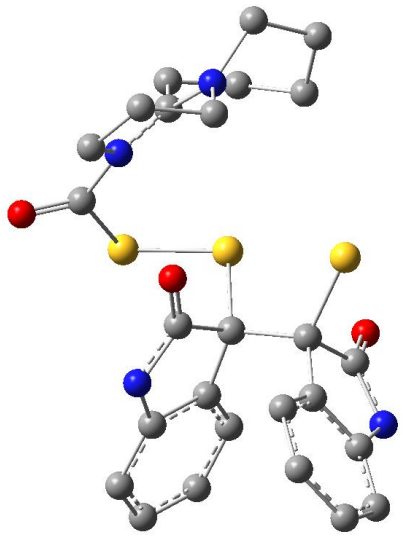
H	4.39703	-1.79891	-2.1839
H	5.94912	-0.97859	-2.08051
C	4.23302	0.25591	-1.5866
H	3.35376	0.15878	-2.2128
H	4.85612	1.04061	-2.02872
C	-3.4696	-2.07393	-0.47018
C	-2.66762	-1.44936	0.49735
C	-3.00333	-1.56162	1.84043
C	-4.16197	-2.26296	2.19246
C	-4.9573	-2.85696	1.21454
C	-4.61787	-2.77716	-0.13808
C	-1.47399	-0.81867	-0.20114
H	-2.37586	-1.12887	2.61217
H	-4.43679	-2.34907	3.23837
H	-5.85239	-3.39848	1.50423
H	-5.22336	-3.24901	-0.90464
H	-3.3166	-2.2013	-2.59857
S	-0.0544	-1.92174	0.30202
C	-1.78585	-1.09044	-1.68618
O	-1.17286	-0.69525	-2.65434
N	-2.91713	-1.87095	-1.72889
C	1.64038	1.45922	-0.99093
O	2.06122	1.90017	-2.03332
S	1.50324	-1.83231	-1.06484
C	-3.27241	2.02642	0.73504
C	-2.66611	1.41415	-0.36686
C	-3.23155	1.55185	-1.62859
C	-4.42354	2.27091	-1.75584
C	-5.02402	2.85462	-0.64107
C	-4.4526	2.74601	0.62806
C	-1.39294	0.704	0.09683
H	-2.75278	1.12277	-2.50218
H	-4.87908	2.38013	-2.73404
H	-5.94875	3.4106	-0.75842
H	-4.90678	3.20623	1.49883
H	-2.75428	2.08485	2.81121
S	-0.14901	1.77292	-0.81889
C	-1.42393	0.99523	1.63069
O	-0.67612	0.57506	2.49045
N	-2.51179	1.78344	1.87476



TS16-17

C	-3.98239	-0.58438	0.04666
C	-4.28275	0.19526	2.32466
H	-4.93712	0.94514	2.76889
H	-4.35527	-0.72932	2.90693
N	-4.77184	-0.06062	0.9626
N	-2.71738	-0.93361	0.36617
C	-2.84711	0.67581	2.23001
H	-2.43829	0.86661	3.22394
H	-2.81739	1.60957	1.6584
C	-2.01465	-0.38928	1.55043
H	-1.80197	-1.21922	2.23091
H	-1.07163	0.03249	1.20383
C	-6.08946	0.48428	0.5986
H	-6.56506	-0.19905	-0.10587
H	-6.69196	0.49095	1.50736
C	-5.94698	1.88158	-0.00503
H	-5.75622	2.61287	0.78744
H	-6.90614	2.13967	-0.46591
C	-4.82228	1.92866	-1.04197
H	-3.85035	1.98721	-0.53696
H	-4.91263	2.84419	-1.63371
C	-4.81412	0.72927	-1.99424
H	-4.06904	0.91962	-2.77068
H	-5.78505	0.65791	-2.49514
C	-4.49216	-0.66699	-1.37275
H	-3.75515	-1.16878	-1.98967
H	-5.38039	-1.30414	-1.36967
C	3.88294	2.23881	-0.68819
C	3.03495	1.72612	0.30704
C	3.17562	2.15332	1.61984
C	4.18719	3.07052	1.92431

C	5.0298	3.55854	0.92694
C	4.88755	3.15092	-0.40126
C	2.04198	0.80247	-0.36637
H	2.50951	1.78436	2.39097
H	4.31128	3.40759	2.94803
H	5.80875	4.27056	1.18086
H	5.53409	3.53111	-1.18506
H	4.00511	1.90469	-2.79796
S	0.44512	1.89019	-0.36428
C	2.51155	0.7939	-1.8271
O	2.04905	0.14064	-2.74008
N	3.54281	1.69342	-1.92255
C	-2.00118	-1.87364	-0.451
O	-2.6124	-2.76867	-0.99774
S	-0.93983	0.97781	-1.49333
C	2.47913	-2.57691	1.07363
C	2.53999	-1.75083	-0.07802
C	3.17606	-2.2516	-1.22476
C	3.75024	-3.51772	-1.18579
C	3.68554	-4.30394	-0.02971
C	3.0445	-3.84329	1.1183
C	1.84704	-0.51952	0.24507
H	3.21223	-1.6687	-2.13553
H	4.24774	-3.90386	-2.06905
H	4.1384	-5.29041	-0.02504
H	2.98878	-4.44413	2.01975
H	1.66145	-2.25999	3.02086
S	-0.24643	-1.78756	-0.52509
C	1.45121	-0.63829	1.69424
O	0.91027	0.18622	2.41539
N	1.82727	-1.90027	2.08998

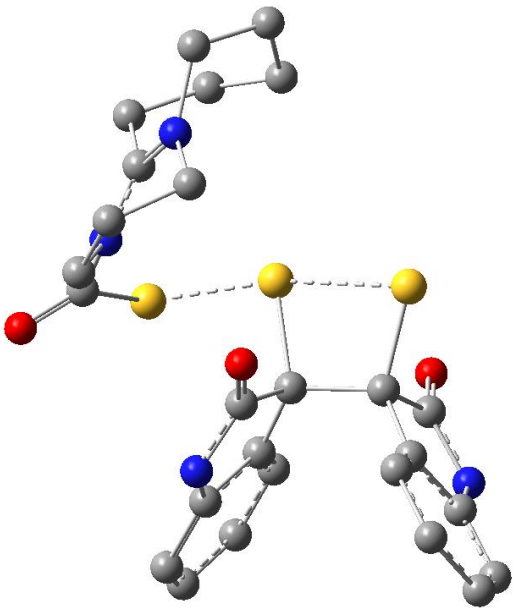


INT18

C	3.49297	0.27012	0.14162
C	3.06829	-1.30657	1.87332
H	1.98425	-1.28732	1.70264

H	3.38986	-2.3145	2.12976
N	3.72115	-0.92812	0.61254
N	2.8607	1.16192	0.96102
C	3.48915	-0.27444	2.91036
H	4.57637	-0.30404	3.01959
H	3.04073	-0.50203	3.87943
C	3.02029	1.10068	2.45152
H	3.72527	1.88525	2.73035
H	2.03863	1.33268	2.86004
C	4.71877	-1.81488	-0.01918
H	5.58649	-1.2033	-0.27522
H	5.03271	-2.52217	0.74827
C	4.18119	-2.53424	-1.25787
H	3.64505	-3.4387	-0.95358
H	5.0485	-2.85018	-1.84657
C	3.23678	-1.66193	-2.08317
H	2.2797	-1.6126	-1.55523
H	3.03524	-2.16031	-3.0366
C	3.73003	-0.24215	-2.38955
H	2.95365	0.26209	-2.97496
H	4.61763	-0.28669	-3.02786
C	4.08005	0.66642	-1.18159
H	3.82897	1.7047	-1.39448
H	5.16341	0.6588	-1.00523
C	-2.33672	2.05356	0.39078
C	-1.99557	1.23851	-0.69514
C	-2.61947	1.43137	-1.91978
C	-3.59623	2.42651	-2.02987
C	-3.93472	3.21474	-0.93068
C	-3.30341	3.04333	0.30344
C	-0.939	0.2508	-0.2443
H	-2.34514	0.82715	-2.77864
H	-4.0911	2.58771	-2.98171
H	-4.6953	3.98236	-1.03339
H	-3.55027	3.66147	1.15999
H	-1.55911	2.19131	2.38414
S	0.61303	0.32485	-1.23868
C	-0.65458	0.71994	1.20589
O	0.197	0.30213	1.96666
N	-1.54798	1.71162	1.49171
C	2.18003	2.31114	0.5364
O	2.19192	3.32386	1.18716
S	1.14688	2.3001	-0.95384
C	-3.75341	-1.79046	-0.11475
C	-2.64613	-1.4055	0.65281
C	-2.77518	-1.29949	2.02941
C	-4.01923	-1.55072	2.61858
C	-5.11194	-1.92171	1.8356
C	-4.99312	-2.05508	0.44969

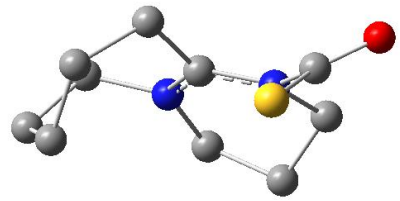
C	-1.44435	-1.23978	-0.26043
H	-1.91626	-1.04377	2.64331
H	-4.13128	-1.46437	3.6945
H	-6.07002	-2.11847	2.30671
H	-5.83549	-2.35477	-0.1652
H	-3.99035	-2.13127	-2.21701
S	-0.16021	-2.50929	0.04276
C	-2.06361	-1.52215	-1.64812
O	-1.51466	-1.44931	-2.73208
N	-3.37911	-1.8613	-1.4568

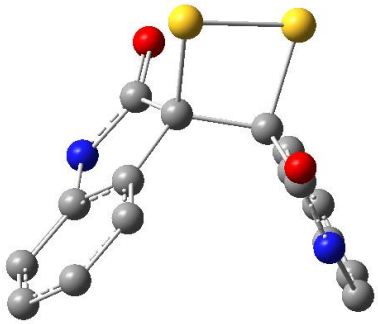


TS18-19

C	3.52686	0.21802	0.24331
C	3.13601	-1.46395	1.89568
H	2.07255	-1.58254	1.66041
H	3.56684	-2.42464	2.17136
N	3.81982	-0.98511	0.68867
N	2.76635	1.03154	1.01274
C	3.33037	-0.40656	2.97254
H	4.40069	-0.28387	3.15913
H	2.85227	-0.71431	3.90467
C	2.70289	0.89447	2.49866
H	3.20937	1.76373	2.91936
H	1.64638	0.93211	2.76588
C	4.90324	-1.77948	0.0773
H	5.76368	-1.12108	-0.05502
H	5.1849	-2.53136	0.81371
C	4.50952	-2.43724	-1.25387
H	4.10583	-3.4355	-1.06118
H	5.42684	-2.56536	-1.83767
C	3.47125	-1.64079	-2.04162
H	2.51732	-1.70885	-1.50822
H	3.3137	-2.12349	-3.01103
C	3.8099	-0.16653	-2.28818
H	2.95382	0.30336	-2.78436

H	4.65661	-0.09065	-2.97724
C	4.16127	0.67584	-1.04001
H	3.93061	1.72513	-1.21175
H	5.23978	0.62755	-0.85017
C	-1.93645	2.07129	0.80493
C	-1.7863	1.45255	-0.44247
C	-2.31151	2.06574	-1.57167
C	-3.00478	3.27179	-1.428
C	-3.1631	3.85673	-0.17266
C	-2.62279	3.26397	0.9706
C	-1.00991	0.1692	-0.2508
H	-2.17409	1.62301	-2.55163
H	-3.41816	3.75802	-2.30535
H	-3.70472	4.7927	-0.07851
H	-2.7233	3.71952	1.94995
H	-1.1954	1.58339	2.75687
S	0.5696	-0.05731	-1.20027
C	-0.65865	0.22084	1.26225
O	0.03562	-0.55453	1.89227
N	-1.27142	1.32377	1.78046
C	2.10568	2.21108	0.5367
O	2.09584	3.19035	1.24472
S	1.22511	2.16321	-0.99883
C	-4.09004	-1.49293	-0.21
C	-2.8271	-1.56015	0.39443
C	-2.72306	-2.00078	1.70585
C	-3.88783	-2.33586	2.40536
C	-5.13574	-2.24208	1.79132
C	-5.2564	-1.82277	0.46416
C	-1.7794	-1.14272	-0.61621
H	-1.75008	-2.08957	2.17681
H	-3.81642	-2.67848	3.43238
H	-6.03044	-2.50775	2.34582
H	-6.2217	-1.76378	-0.02757
H	-4.70497	-1.03815	-2.20953
S	-0.46282	-2.35329	-0.99645
C	-2.63693	-0.91317	-1.89182
O	-2.24815	-0.63476	-3.00742
N	-3.94913	-1.08712	-1.53751

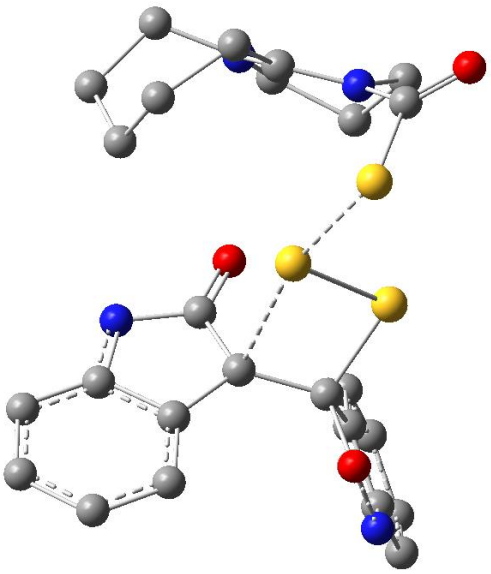




INT19

C	-4.57584	2.85205	1.19981
C	-4.80752	3.32944	-0.08918
C	-3.97481	2.97598	-1.15429
C	-2.91759	2.12464	-0.87792
C	-2.68373	1.61193	0.40587
C	-3.50607	1.98887	1.45813
C	-0.97883	0.92576	-1.11597
C	-1.48356	0.70766	0.33957
O	0.05882	0.51796	-1.60102
H	-5.22707	3.15529	2.01248
H	-5.64306	3.99764	-0.27238
H	-4.13772	3.35923	-2.15582
H	-3.31822	1.62155	2.46084
N	-1.92579	1.66972	-1.75407
H	-1.81803	1.98325	-2.7116
S	-0.09412	0.95864	1.53024
C	-2.42949	-2.85714	-2.57051
C	-3.6851	-3.32357	-2.18494
C	-4.23188	-2.98998	-0.94348
C	-3.47931	-2.17284	-0.11528
C	-2.22148	-1.67815	-0.49088
C	-1.68608	-2.03015	-1.72244
C	-2.77561	-1.01784	1.73649
C	-1.70257	-0.81641	0.62874
O	-2.72755	-0.62009	2.8803
H	-2.02156	-3.13967	-3.53503
H	-4.24919	-3.96464	-2.85506
H	-5.20237	-3.36015	-0.63105
H	-0.7091	-1.6686	-2.02329
N	-3.79258	-1.73567	1.17399
H	-4.60179	-2.03849	1.70299
S	-0.01304	-1.14599	1.31639
C	3.8302	0.04379	-0.32937

C	2.89816	-0.84638	-2.44452
H	2.1528	-0.30062	-3.02965
H	3.61947	-1.29993	-3.13257
N	3.62184	0.14882	-1.63734
N	3.53249	-1.08255	0.32101
C	2.23097	-1.88107	-1.56508
H	1.95596	-2.75171	-2.16497
H	1.33002	-1.45337	-1.11922
C	3.17961	-2.28507	-0.45254
H	4.09432	-2.73969	-0.84837
H	2.71554	-2.99008	0.23551
C	4.00183	1.37135	-2.36106
H	5.00956	1.66529	-2.06456
H	4.04561	1.10548	-3.41877
C	3.00682	2.5102	-2.11765
H	2.11832	2.36125	-2.74036
H	3.48554	3.43953	-2.44511
C	2.57294	2.60266	-0.65378
H	1.85764	1.79876	-0.44856
H	2.02801	3.54011	-0.49925
C	3.7127	2.51991	0.36518
H	3.28068	2.62791	1.36445
H	4.41223	3.34954	0.21858
C	4.52039	1.19827	0.35106
H	4.77828	0.90812	1.36557
H	5.46211	1.32901	-0.19049
C	3.62076	-1.29765	1.78936
O	4.15392	-2.34595	2.09753
S	2.85963	-0.14705	2.82051

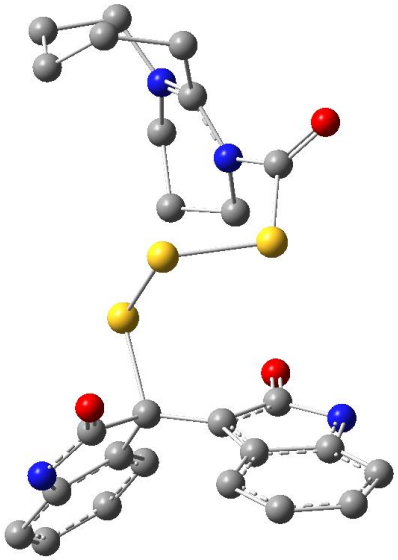


TS19-17

C	-3.3017	3.83373	1.13832
C	-2.76742	4.69027	0.17395
C	-1.88346	4.19848	-0.78804
C	-1.56319	2.84886	-0.74928

C	-2.077	1.95254	0.22903
C	-2.96314	2.47898	1.17847
C	-0.6768	0.79555	-1.24546
C	-1.45918	0.65514	-0.02485
O	-0.00891	-0.0334	-1.88364
H	-3.991	4.22577	1.88029
H	-3.03966	5.74103	0.16696
H	-1.46033	4.8431	-1.55274
H	-3.38397	1.85296	1.95481
N	-0.74148	2.13618	-1.60068
H	-0.22319	2.52043	-2.3789
S	0.50503	0.26861	1.41959
C	-3.29153	-2.75966	-2.55835
C	-4.56673	-2.98171	-2.04036
C	-4.93193	-2.49351	-0.78272
C	-3.97674	-1.78043	-0.07495
C	-2.69442	-1.53701	-0.58468
C	-2.34151	-2.03385	-1.83043
C	-2.92141	-0.63322	1.61168
C	-1.92756	-0.70815	0.42365
O	-2.70997	-0.16707	2.71208
H	-3.03148	-3.15472	-3.53496
H	-5.29155	-3.54683	-2.61812
H	-5.91978	-2.66884	-0.36989
H	-1.34859	-1.84192	-2.22206
N	-4.08909	-1.21344	1.19819
H	-4.88419	-1.33411	1.81393
S	-0.41751	-1.5969	1.03963
C	3.49413	-0.24913	-0.17394
C	2.85655	-1.11249	-2.40069
H	2.13801	-0.56195	-3.0128
H	3.66632	-1.48554	-3.03517
N	3.45949	-0.1264	-1.48259
N	3.14519	-1.42036	0.40251
C	2.16295	-2.23031	-1.64916
H	2.03869	-3.08806	-2.3139
H	1.18129	-1.88569	-1.31425
C	2.99825	-2.62266	-0.446
H	3.99412	-2.97473	-0.73315
H	2.5109	-3.38983	0.15494
C	4.02246	1.07087	-2.1359
H	4.99854	1.27576	-1.69324
H	4.19125	0.79678	-3.17813
C	3.10473	2.29259	-2.02873
H	2.3397	2.24613	-2.81136
H	3.71896	3.17728	-2.22625
C	2.41088	2.38992	-0.67168
H	1.6401	1.61632	-0.63531
H	1.89125	3.35067	-0.59647

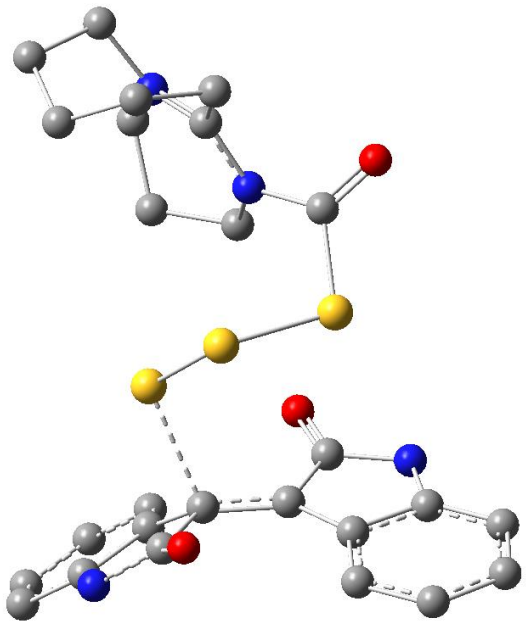
C	3.31907	2.22351	0.54811
H	2.70056	2.32099	1.44689
H	4.0605	3.02742	0.58589
C	4.07884	0.87704	0.63663
H	4.17904	0.56652	1.67445
H	5.10145	0.99088	0.26206
C	3.06614	-1.64252	1.81126
O	3.63503	-2.58669	2.29541
S	2.00331	-0.61492	2.80819



INT 17

C	4.02314	0.66575	0.31652
C	4.20727	-1.32195	1.74385
H	4.61405	-2.29935	1.47811
H	4.60142	-1.03375	2.72303
N	4.71642	-0.36476	0.7437
N	2.79174	0.9212	0.80993
C	2.69264	-1.33628	1.72718
H	2.31972	-1.93966	2.55699
H	2.33527	-1.77884	0.79263
C	2.17054	0.07734	1.86438
H	2.44675	0.50413	2.83479
H	1.08213	0.12513	1.75351
C	5.99927	-0.71042	0.10594
H	6.56162	0.20734	-0.06807
H	6.5585	-1.30581	0.82868
C	5.7648	-1.46971	-1.20053
H	5.49891	-2.50959	-0.98587
H	6.71308	-1.47974	-1.74754
C	4.66688	-0.81659	-2.04373
H	3.68285	-1.08009	-1.63503
H	4.69447	-1.22974	-3.05579
C	4.78515	0.70778	-2.13549
H	4.04373	1.06538	-2.85353
H	5.7699	0.97212	-2.53269
C	4.5744	1.5028	-0.80951

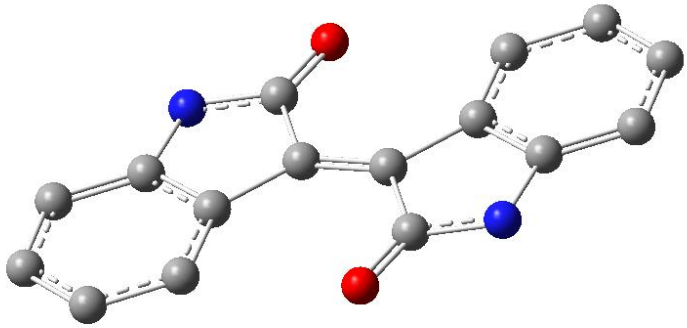
H	3.90492	2.33828	-0.99994
H	5.51436	1.93722	-0.4588
C	-2.86057	-3.06316	-0.67069
C	-2.25453	-2.21338	0.26475
C	-2.01331	-2.65898	1.55619
C	-2.40098	-3.95949	1.89809
C	-3.01006	-4.79016	0.95771
C	-3.2514	-4.35409	-0.34831
C	-1.97101	-0.88556	-0.40336
H	-1.53633	-1.98913	2.2651
H	-2.22406	-4.32625	2.90397
H	-3.30311	-5.79679	1.23968
H	-3.72357	-4.99732	-1.08341
H	-3.35707	-2.80216	-2.73924
S	-0.0547	-0.96617	-0.61373
C	-2.49543	-1.11547	-1.83684
O	-2.44897	-0.33697	-2.76833
N	-2.986	-2.39435	-1.88991
C	2.21275	2.21963	0.65189
O	2.78582	3.22422	0.9703
S	0.43576	0.83205	-1.4354
C	-3.46748	2.29012	0.93744
C	-3.41566	1.32739	-0.12044
C	-4.30468	1.51555	-1.19352
C	-5.16847	2.61192	-1.20318
C	-5.18532	3.54169	-0.15922
C	-4.3257	3.38109	0.93005
C	-2.42845	0.34858	0.26322
H	-4.31889	0.82108	-2.02468
H	-5.84396	2.74094	-2.04453
H	-5.86566	4.38705	-0.19027
H	-4.3252	4.08439	1.75832
H	-2.35348	2.40716	2.75266
S	0.52396	2.2899	0.05694
C	-1.9084	0.72444	1.53821
O	-1.02901	0.19741	2.25893
N	-2.55725	1.90864	1.8986



TS17-isoindigo

C	3.91017	-0.66691	-0.32641
C	4.14952	1.30925	-1.75816
H	4.60051	2.27095	-1.50709
H	4.51363	0.99872	-2.74228
N	4.63566	0.33885	-0.76006
N	2.66777	-0.88187	-0.80939
C	2.63736	1.38519	-1.71352
H	2.27348	2.00354	-2.53629
H	2.31216	1.83627	-0.7714
C	2.05421	-0.00533	-1.84038
H	2.27719	-0.43881	-2.82135
H	0.97084	-0.00233	-1.69136
C	5.93445	0.64055	-0.13301
H	6.46466	-0.29649	0.03982
H	6.50941	1.21362	-0.8615
C	5.73729	1.41063	1.17309
H	5.50268	2.45794	0.95793
H	6.69056	1.3916	1.71118
C	4.62716	0.79422	2.02766
H	3.64829	1.08991	1.62894
H	4.6785	1.20605	3.03934
C	4.69675	-0.73318	2.11832
H	3.95386	-1.06624	2.84658
H	5.67761	-1.02934	2.50263
C	4.44202	-1.52176	0.79612
H	3.74303	-2.33036	0.99604
H	5.36114	-1.99271	0.43722
C	-2.83057	3.1478	0.72462
C	-2.3832	2.27474	-0.28461
C	-2.17451	2.77488	-1.56566
C	-2.42754	4.12719	-1.81654
C	-2.87262	4.97314	-0.80123

C	-3.08098	4.49218	0.49287
C	-2.23401	0.91468	0.32507
H	-1.81049	2.11218	-2.341
H	-2.26856	4.52311	-2.81444
H	-3.05963	6.02119	-1.01404
H	-3.4282	5.13916	1.29172
H	-3.2345	2.85815	2.80572
S	-0.05103	1.0895	0.7431
C	-2.65566	1.11956	1.78164
O	-2.67753	0.3006	2.68093
N	-2.97536	2.44692	1.91826
C	2.05128	-2.16582	-0.6532
O	2.60342	-3.18235	-0.97291
S	0.35934	-0.75047	1.48276
C	-3.16193	-2.43144	-0.99831
C	-3.23652	-1.51086	0.08573
C	-3.99196	-1.90112	1.20119
C	-4.60294	-3.15614	1.22695
C	-4.49171	-4.04446	0.15482
C	-3.76748	-3.68053	-0.98109
C	-2.52102	-0.31087	-0.33669
H	-4.08969	-1.24032	2.05176
H	-5.17495	-3.44454	2.10415
H	-4.97126	-5.01735	0.19921
H	-3.67649	-4.34688	-1.83384
H	-2.12235	-2.31654	-2.85783
S	0.36284	-2.17998	-0.05786
C	-1.98488	-0.58624	-1.65776
O	-1.21437	0.07948	-2.36894
N	-2.42923	-1.85006	-2.01586



Isoindigo

H	-2.04603	2.3482	-0.00002
H	-4.82806	-1.78486	0.00001
H	-5.90302	0.47503	-0.00001
H	-4.49161	2.51098	-0.00002
O	0.10955	-2.68947	0.00001
C	-0.60878	-0.3097	0. 00000
C	-0.75183	-1.83029	0. 00000
C	-2.63312	1.44603	-0.00001
C	-2.00657	0.19282	0. 00000

C	-2.85099	-0.94308	0. 00000
C	-4.23418	-0.87707	0. 00000
C	-4.82111	0.387	-0.00001
C	-4.02615	1.53102	-0.00001
N	-2.08854	-2.09983	0.00001
H	-2.45526	-3.04308	0.00002
H	2.04601	-2.3482	-0.00001
H	4.82808	1.78484	0. 00000
H	5.903	-0.47505	-0.00001
H	4.4916	-2.51098	-0.00001
O	-0.10953	2.68947	0.00001
C	0.60879	0.3097	0. 00000
C	0.75185	1.8303	0.00001
C	2.6331	-1.44604	-0.00001
C	2.00657	-0.19282	0. 00000
C	2.85099	0.94308	0. 00000
C	4.23418	0.87707	0. 00000
C	4.82109	-0.38701	-0.00001
C	4.02613	-1.53103	-0.00001
N	2.08855	2.09982	0.00001
H	2.45528	3.04307	0.00001