Supporting Information

Visible-Light-Driven, Catalyst-Free Intramolecular Crossed and straight [2+2] cycloaddition

Yuan Sang,‡ Xiaoxuan Zhou,‡ Chen Jin, Ling Pan, Qun Liu, Haiyan Yuan,*and Yifei Li*

Jilin Province Key Laboratory of Organic Functional Molecular, Design & Synthesis, Department of Chemistry, Northeast Normal University, Changchun 130024, China
**Corresponding author. E-mail: liyf640@nenu.edu.cn, yuanhy034@nenu.edu.cn*
‡ These authors contributed equally to this work

1. General Information

Materials: All solvents were purchased from commercial sources and used without further purification. The photocatalysts was purchased from Aldrich. The starting materials bis(cinnamoyl)ketenedithioacetals **1** were synthesized according to literature report.[1,2]

Chromatography: Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm Tsingdao silica gel plates (GF-254) using UV light as visualizing agent. Tsingdao silica gel (60, particle size 0.040-0.063 mm) was used for flash column chromatography.

NMR spectra: NMR spectra were recorded on a Brüker Advance 600 (^{1}H: 600 MHz, ^{13}C: 151 MHz and 126 MHz), at ambient temperature. ^{1}H NMR spectra were reported in parts per million (ppm) and the spectra are calibrated to the resonance resulting from incomplete deuteration of the solvent ($CDCl_3$: 7.26 ppm). ^{13}C NMR spectra were reported in ppm with the solvent resonance as the internal standard ($CDCl_3$: 77.0 ppm, t). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

High-resolution mass spectra (HRMS): All compounds were obtained using a Bruker micro TOF II focusspectrometer (ESI). Measured values are reported to 4 decimal places of the calculated value. The calculated values are based on the most abundant isotope.

UV/Vis: UV-vis absorption analysis using Varian cary50 and Cyclic Voltammetry experiments using CH Instruments (CHI 660E).

Photoreactor: The source of the 5w white and blue LED using Wattecs Parallel Light Reactor (white LED Light source, every tube hole groove, 5w). The source of the 40w blue LED (λ = 456 nm) was purchased from Kessil (PR160) with flask (15 mL and 75mL) as the irradiation vessel and the Blue LEDs irradiated at the side with a 5-6 cm distance.

Instruments of Photochemical Reactions

Figure S1. Instruments for photochemical reactions (5w white and blue LEDs and 40w blue LED).

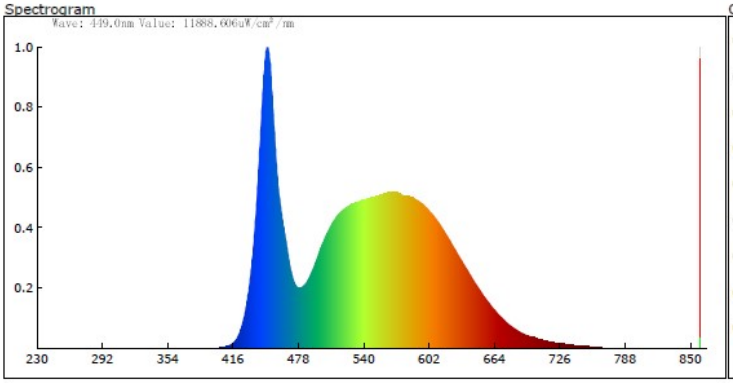
Emission Spectrum

Spectrogram of white light (10W, 6000-6500K)

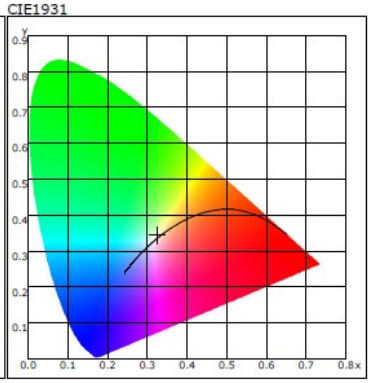
Parameter

Name	Value	Name	Value	Name	Value	Name	Value
FlickerFrequency Hz	324.42	CIE u',v'	0.2017,0.4775	CIE1931 Y	5753834.500		
FluctuateDepth(%)	5.8	Duv y0,dy	0.0000,0.0000	CIE1931 Z	5558575.500		
BinkPercent(%)	3.0	SDCM	9.91	TLCI-2012	61		
BinkExponent	0.02	Ra	80.7	Integral Time(ms)	0		
EffectiveLux(lx)	0.0	Ee(mW/cm²)	1212.417	Peak Signal	62923		
PeakLux(lx)	0.0	S/P	2.075	Dark Signal	2055		
LuxIntgarl(lx.s)	0.0	Dominant(nm)	509.80	Compensate level	2856		
FlashTime(us)	0	Purity(%)	2.3				
E(lx)	3929869.25	HalfWidth(nm)	21.3				
Candle E(fc)	365093.75	Peak(nm)	449.3				
CCT(K)	5792	Center(nm)	450.1				
Duv	0.00387	Centroid(nm)	541.9				
CIE x,y	0.3259,0.3429	Color Ratio(RGB)	13.9,82.8,3.2				
CIE u,v	0.2017,0.3183	CIE1931 X	5469296.000				

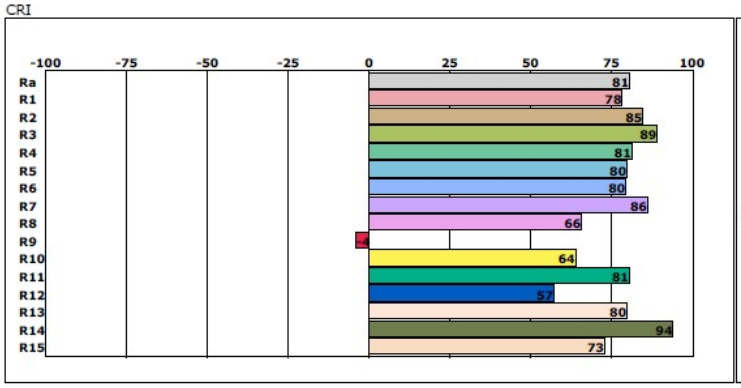
Spectrogram

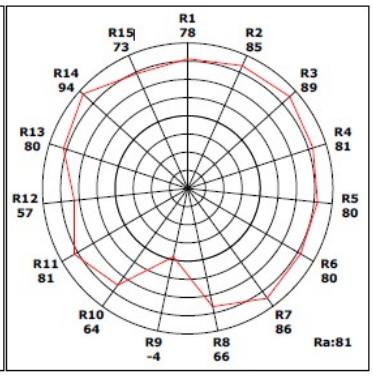


CIE1931



CRI



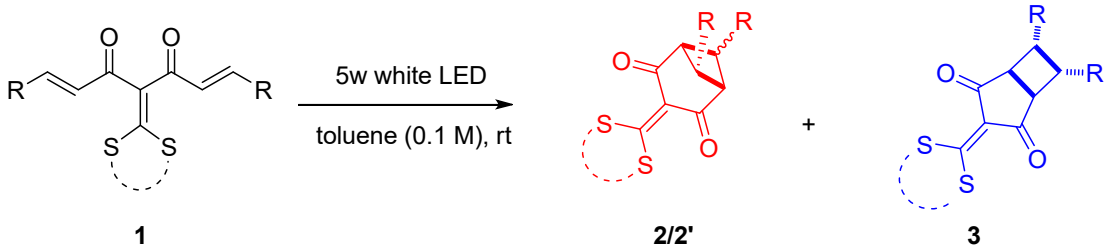


Instrument Status

Type: PCS230850	SN: 0	Scan Range: 230-850nm
Integral Time: 0.413ms	VPeak: 62923	VDark: 2055

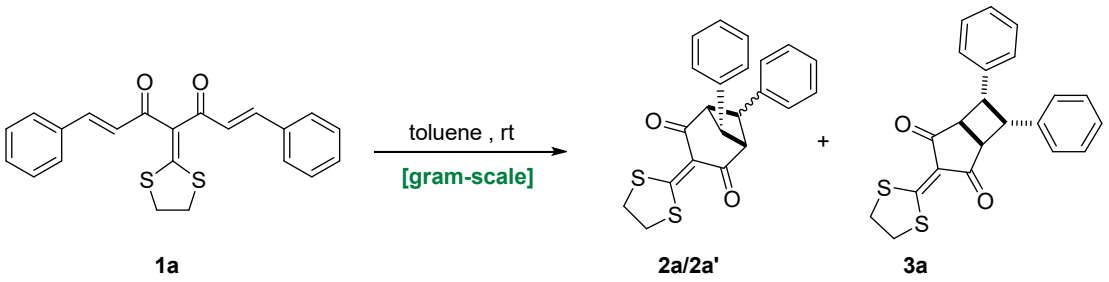
2. Experimental Procedure

2.1 Typical Procedures for Visible-Light-Induced [2+2] cycloaddition



General synthetic procedure (with **2a/2a'**, **3a** as an example): To a 15 mL flask equipped with a stir-bar was added bis(cinnamoyl)ketenedithioacetals **1a** (113.4 mg, 0.3 mmol) and 3 mL toluene. The reaction mixture was stirred for about 2 h at Wattecs Parallel Light Reactor (White LED Light source, every tube hole groove, 5 w) at ambient temperature. After the completion of the reaction as indicated by TLC, the mixture was concentrated by rotary evaporation, then purified by silica gel flash column chromatography (PE/EA = 2/1) to afford mixed crossed products **2a/2a'** (yellow solid, 56.7 mg, 50%) and straight product **3a** (yellow solid, 42.0 mg, 37%).

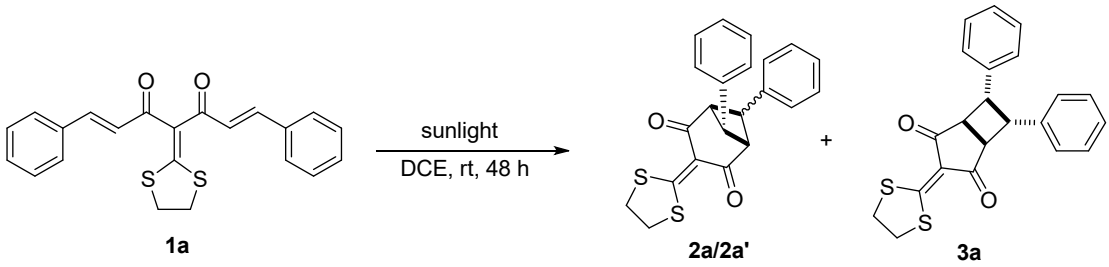
2.2 Gram-scale reaction



Synthetic procedure of white LEDs irradiation:

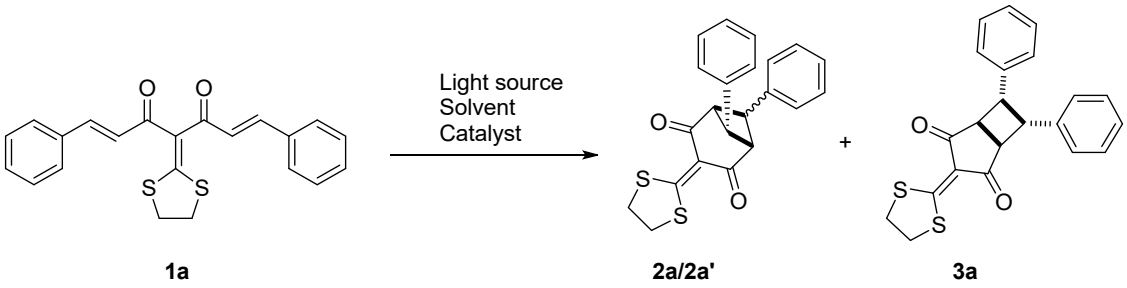
To a 75 mL flask equipped with a stir-bar was added bis(cinnamoyl)ketenedithioacetals **1a** (3 g, 7.9 mmol) and 70 mL toluene. The reaction mixture was stirred for about 30 h under the irradiation of white LED light (10 w) at ambient temperature in a Wattecs Parallel Light Reactor. After the completion of the reaction as indicated by TLC, the solution was concentrated *in vacuo* and then purified by silica gel flash column chromatography (PE/EA = 2/1) to afford **2a/2a'** (1.85 g, 36%) and **3a** (1.70 g, 33%).

2.3 Synthetic procedure of sunlight



To a 15 mL flask was added bis(cinnamoyl)ketenedithioacetals **1a** (113.4 mg, 0.3 mmol) and 3 mL DCE. The reaction mixture was exposed to sunlight for about 48 h at ambient temperature. After the completion of the reaction as indicated by TLC, the solution was concentrated *in vacuo* and then purified by silica gel flash column chromatography (PE/EA = 2/1) to afford **2a**/**2a'** (48.8 mg, 43%) and **3a** (39.7 mg, 35%).

3. Details for Condition Optimizations



1a **2a/2a'** **3a**

3.1 Optimization of Light Source[a]

Entry	Light	Wavelength /nm	Temp (°C)	Solvent	Catalyst	Yield of **2a**/**2a'** (%)	Yield of **3a** (%)
1	5 W	460-465	rt	$CDCl_3$	-	42 (1/0.73)	33
2	40 W	460-465	rt	$CDCl_3$	-	44 (1/0.77)	38
3	100 W	460-465	rt	$CDCl_3$	-	36 (1/0.92)	37

[a] Isolated Yields.

3.2 Optimization of Wavelength[a]

Entry	Light	Wavelength /nm	Temp (°C)	Solvent	Catalyst	Yield of **2a**/**2a'** (%)	Yield of **3a** (%)
1	5 W	435-440	rt	$CDCl_3$	-	40 (1/0.78)	37
2	5 W	460-465	rt	$CDCl_3$	-	42 (1/0.73)	33
3	5 W	490-495	rt	$CDCl_3$	-	37 (1/0.90)	38
4	5 W	525-530	rt	$CDCl_3$	-	not finished	
5	5 W	585-590	rt	$CDCl_3$	-	*N.R.*	
6	5 W	white	rt	$CDCl_3$	-	45 (1/0.61)	37

[a] Isolated Yields.

3.3 Optimization of Temperature[a]

Entry	Light	Wavelength /nm	Temp (°C)	Solvent	Catalyst	Yield of **2a**/**2a'** (%)	Yield of **3a** (%)
1	40 W	460-465	rt	$CDCl_3$	-	44 (1/0.77)	38
2	40 W	460-465	40	$CDCl_3$	-	45 (1/0.60)	40

[a] Isolated Yields.

3.4 Optimization of Solvent[a]

Entry	Light	Wavelength /nm	Temp (℃)	Solvent	Catalyst	Yield of **2a**/**2a'** (%)	Yield of **3a** (%)
1	5 W	white	rt	$CDCl_3$	-	45 (1/0.61)	37
2	5 W	white	rt	DCM	-	35 (1/0.63)	35
3	5 W	white	rt	EtOAc	-	28 (1/0.59)	35
4	5 W	white	rt	MeCN	-	33 (1/0.47)	33
5	5 W	white	rt	Toluene	-	50 (1/0.53)	37
6	5 W	white	rt	1,4-dioxane	-	37 (1/0.58)	41
7	5 W	white	rt	$MeNO_2$	-	39 (1/0.40)	40

[a] Isolated Yields.

3.5 Optimization of Catalyst[a]

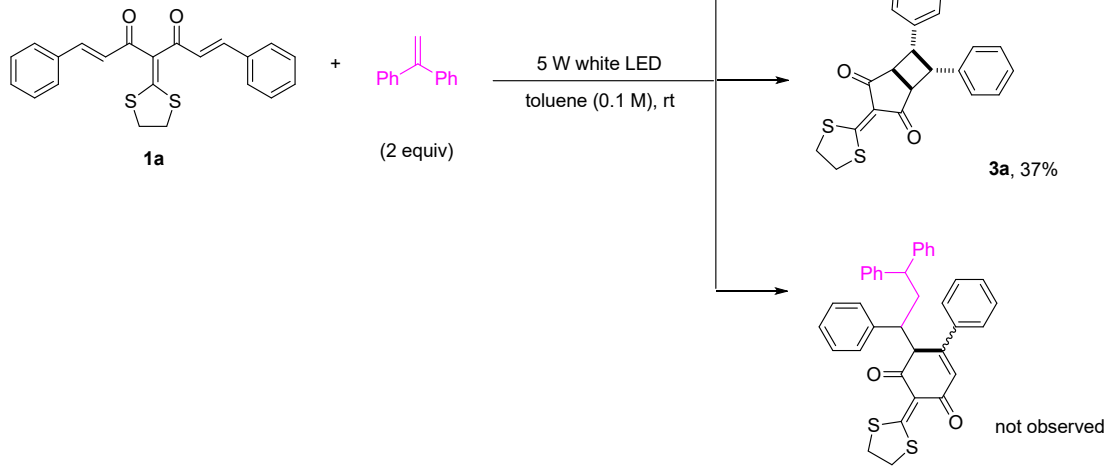
Entry	Light	Wavelength/ nm	Temp (℃)	Solvent	Catalyst	Yield of **2a**/**2a'** (%)	Yield of **3a** (%)
1	5 W	white	rt	Toluene	-	50 (1/0.53)	37
2	5 W	white	rt	Toluene	Acr^+-Mes ClO_4^-	45 (1/0.79)	36
3	5 W	white	rt	Toluene	*fac*-Ir(ppy)$_3$	40 (1/0.99)	40
4	5 W	white	rt	Toluene	$Ru(bpy)_3Cl_2$	49 (1/0.89)	37

[a] Isolated Yields.

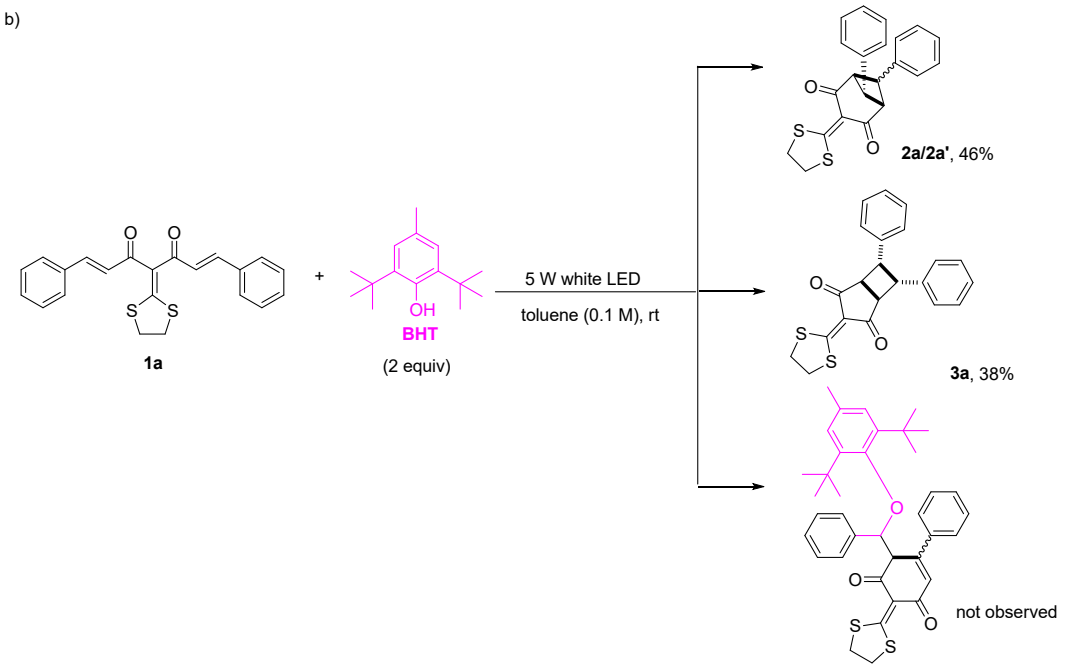
4. Mechanistic Investigations

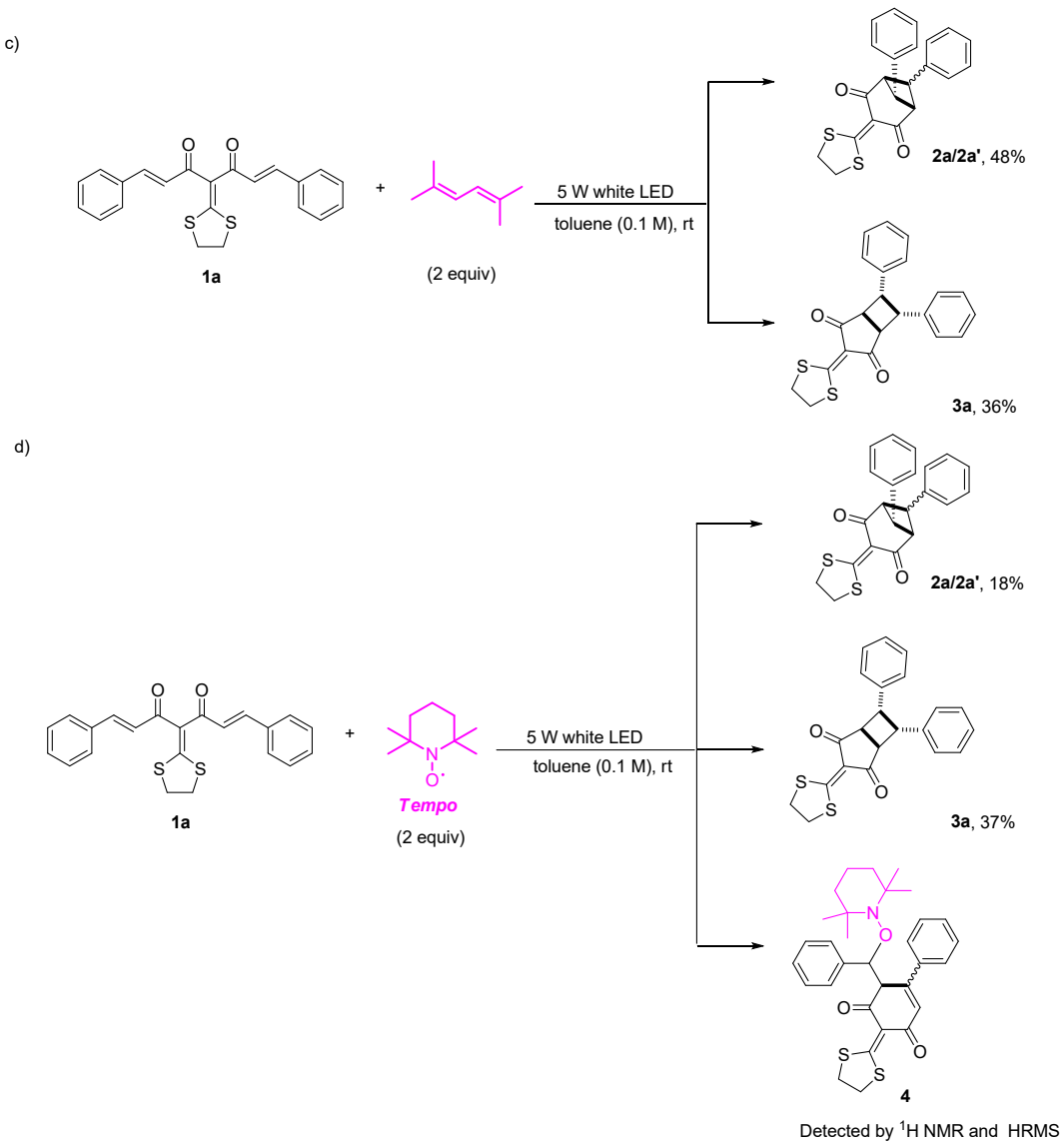
4.1 Radical Trapping Experiment

a)


1a
(2 equiv)
5 W white LED
toluene (0.1 M), rt
2a/2a', 47%
3a, 37%
not observed

b)


1a
BHT
(2 equiv)
5 W white LED
toluene (0.1 M), rt
2a/2a', 46%
3a, 38%
not observed



4.2 Detection of Intermediate 4

4.2.1 ^{1}H NMR of 4

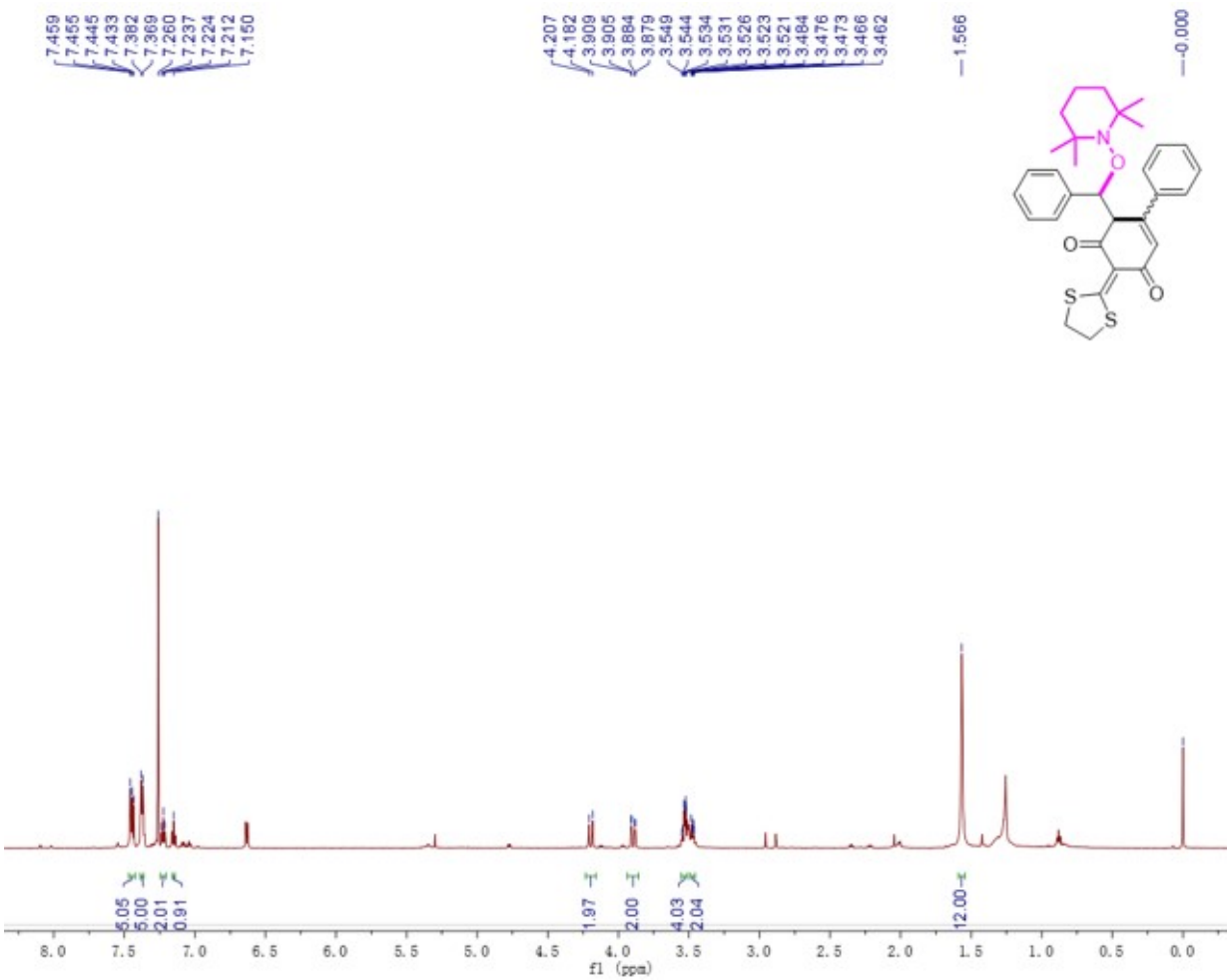


Figure S2. [1]H NMR of **4**

(*R*)-4-(1,3-dithiolan-2-ylidene)-2-((*S*)-phenyl((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-[1,1'-biphenyl]-3,5(2H,4H)-dione 4：

Yellow oil, **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.46-7.43 (m, 5H), 7.38 (d, *J* = 7.8 Hz, 5H), 7.22 (t, *J* = 7.8 Hz, 2H), 7.15 (s, 1H), 4.19 (d, *J* = 15.0 Hz, 2H), 3.91-3.88 (m, 2H), 3.55-3.52 (m, 4H), 3.48-3.46 (m, 2H), 1.57 (s, 12H). **HRMS** (ESI, m/z): Calculated for

$C_{31}H_{35}NO_3S_2$ $[M+H]^+$ 534.2131, found 534.2134.

4.2.2 HRMS of 4

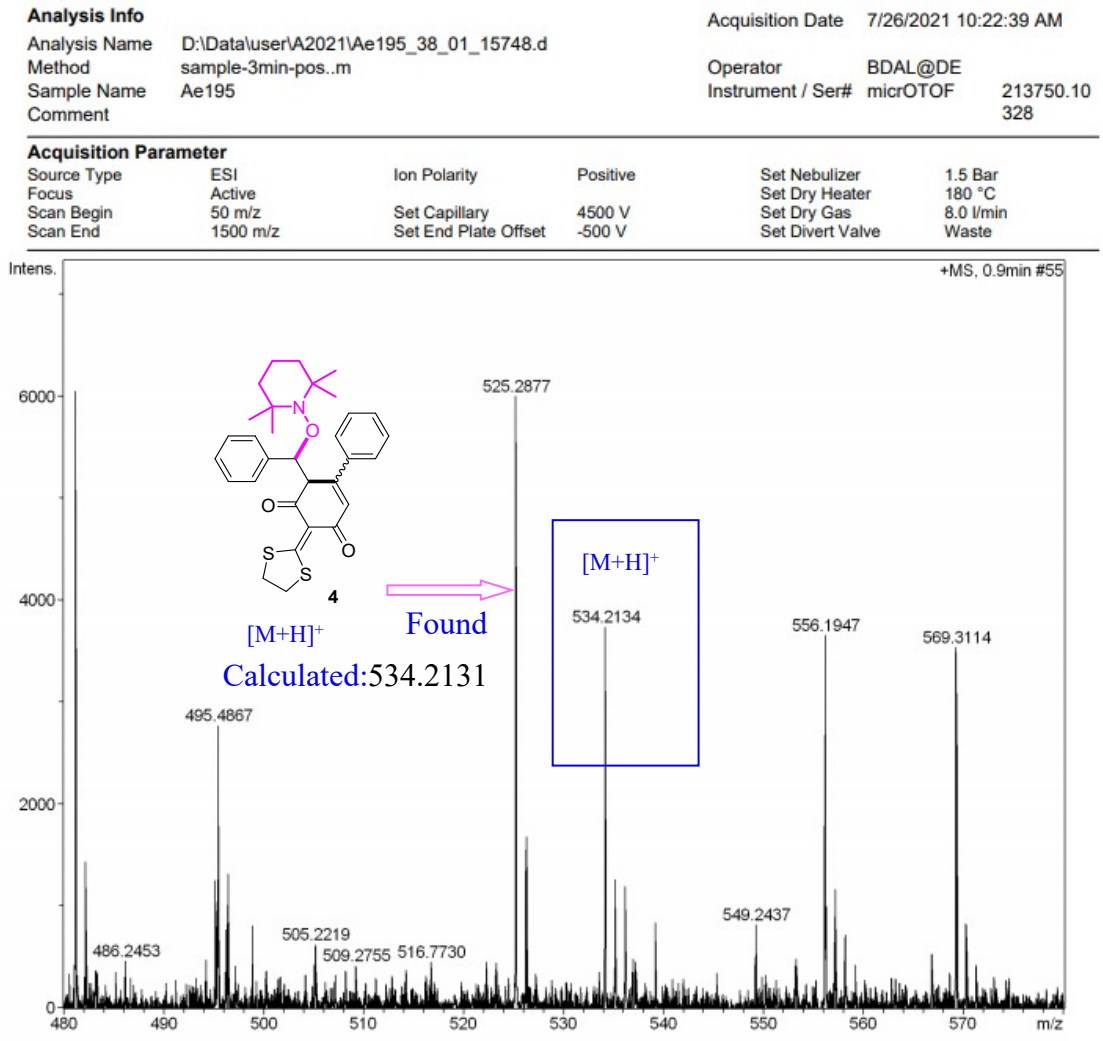


Figure S3. HRMS of **4**

4.3 UV-vis spectrum

UV-vis absorption of four solutions is reported. As follows: ketenedithioacetals **S1a** (2×10^{-5} mol, 2×10^{-4} M in DCE); bis(cinnamoyl)ketenedithioacetals **1** (2×10^{-5} mol, 2×10^{-4} M in DCE) and the other two compounds that cannot go through this cycloaddition reaction.

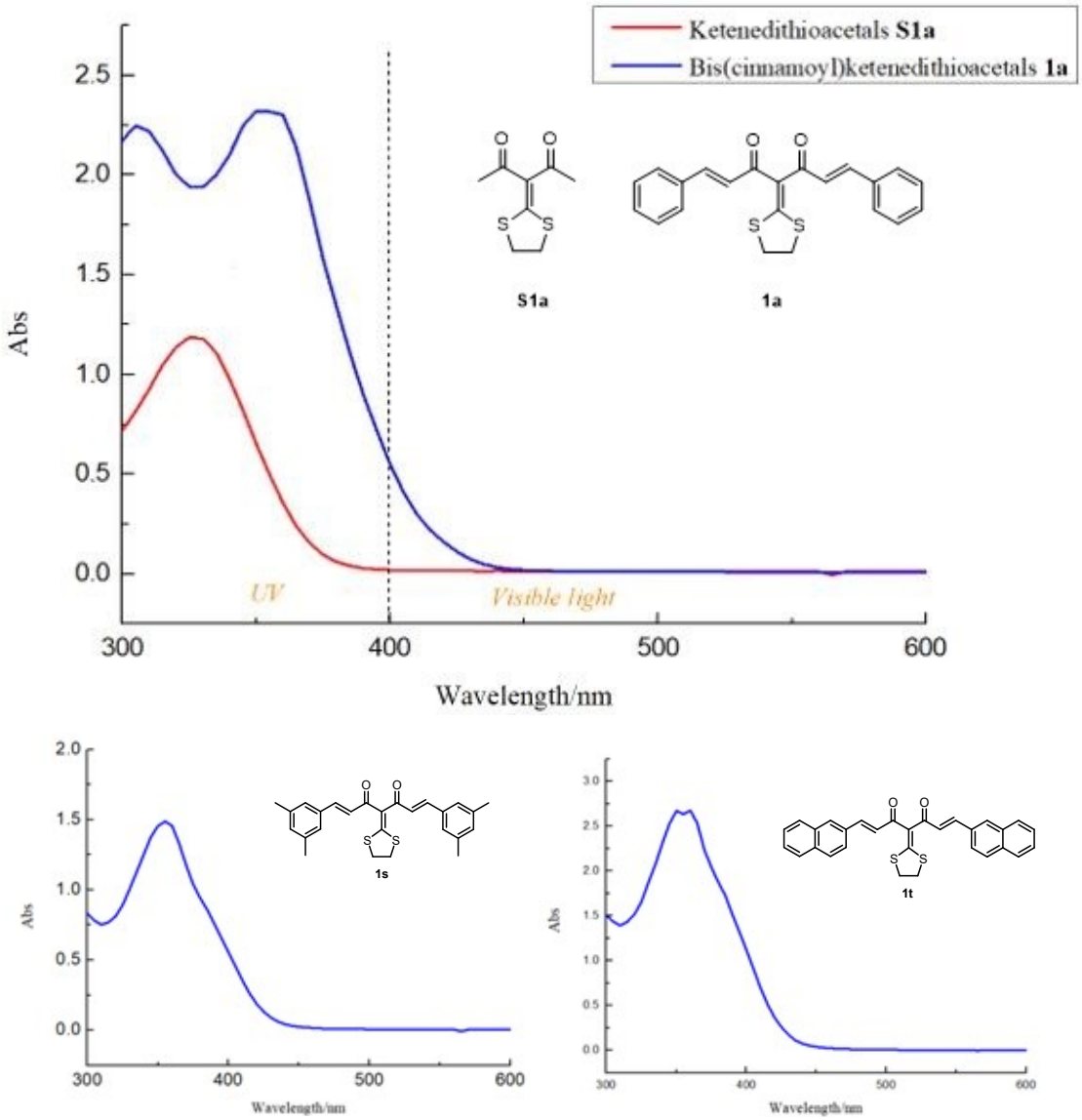


Figure S4. UV-vis spectrum of **S1a**, **1a**, **1s** and **1t**

4.4 Cyclic Voltammetry (CV) Experiments

Cyclic voltammetry (CV) studies were performed in a 150 mL glass beaker, for the electrochemical measurements a three-electrode system connected to an electrochemical station was used. All electrochemical measurements were performed in degassed DMF under dry N_2 atmosphere in room temperature. CV spectra of all compounds is reported at 3 mM in 0.1 M NBu_4PF_6 in degassed DMF with scan rate 100 mV/s. Before the experiment, the glassy carbon electrode was polished with metallographic sandpaper, and then polished to the mirror surface with Al_2O_3 slurry on the suede.

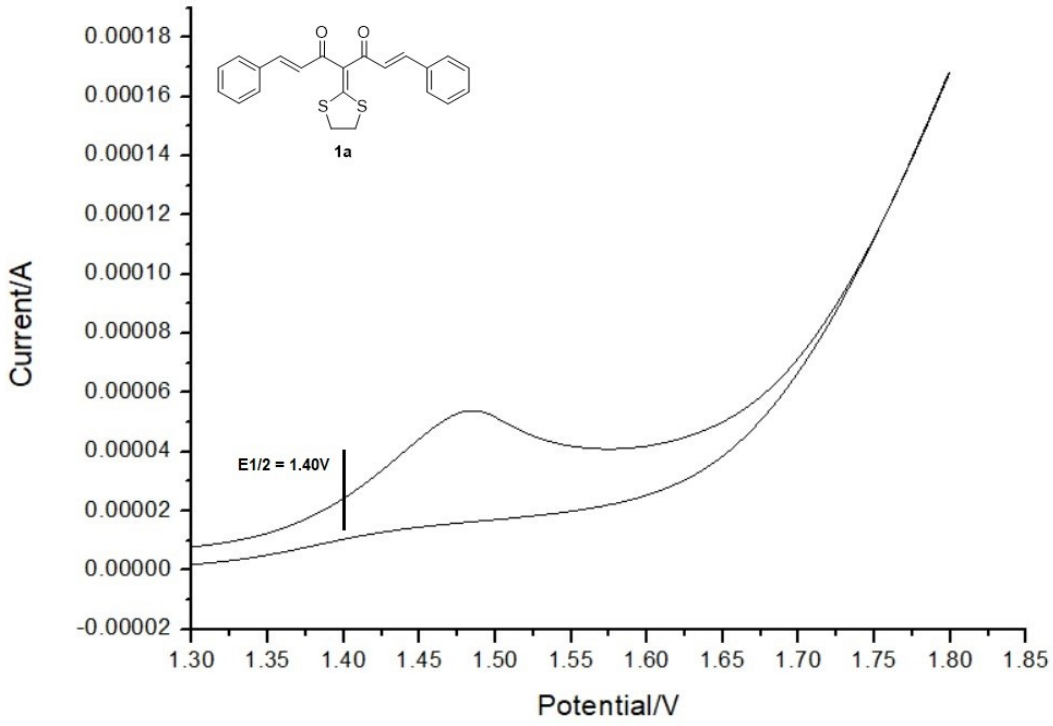


Figure S5. Cyclic voltammogram of bis(cinnamoyl)ketenedithioacetals **1a**. Conditions: DMF (10 mL), NBu_4PF_6 (0.1 M), bis(cinnamoyl)ketenedithioacetals **1a**$^-$ (3 mM). The working electrode is glassy carbon electrode (columniform, 3.0 mm in diameter), the counter electrode is Pt wire and the reference electrode is Ag/AgCl in 0.1 M KCl. Starting point of scan is 1.30 V, scan direction is shown in diagram. The CV experiment began with an initial potential of 1.30 V with switching the potential at 1.85 V (oxidative scan). The oxidation potential $E_{1/2}$ (1.40 V vs. SCE) was converted from internal standard SCE. CV plotting convention (IUPAC).

5. DFT calculations

5.1 Computational studies of 1a

All theoretical calculations were performed with Gaussian 09[3]. All structures were completely optimized by using the (U)B3LYP[4] method and the 6-311+g(2d,p) basis set. Frequency calculations were carried out at the same level to confirm all the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency), and provided the thermal relative Gibbs free energy correction. The searching for minimal energy crossing points was conducted using a modified version of Harvey's code[5] (sobMECP[6]) interfaced with Gaussian 09.

5.1.1 Spin density

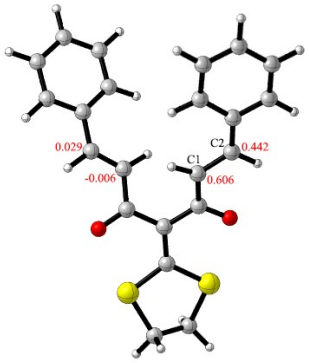
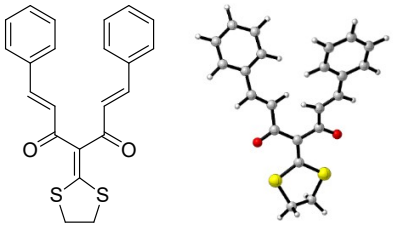


Figure S6. The spin density of **1a-T1**.

Furthermore, our theoretical calculations suggest that the spin density in **1a** is mainly localized on C1 and C2.

5.1.2 Cartesian coordinates and energies of all optimized structures

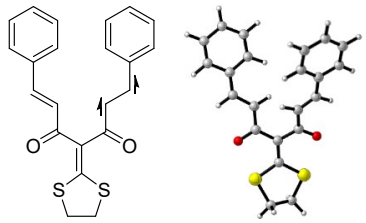


1a

SCF Done: E(UB3LYP) = -1796.31866709 A.U.
Zero-point correction = 0.338302 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -1796.038626

C	5.83671100	-0.39845700	0.64060200
C	5.83697800	0.39753900	-0.63966000
C	3.27733400	-0.00037500	0.00000700
H	6.60070100	-1.17750000	0.64701800
H	5.97516000	0.24159400	1.51351900
H	5.97573400	-0.24251400	-1.51252800
H	6.60100800	1.17654400	-0.64578000
S	4.20989800	-1.24477800	0.81292200
S	4.21028000	1.24393400	-0.81260100
C	1.88872500	-0.00032200	-0.00021800
C	1.19537900	1.23394200	-0.42069500
C	1.19514100	-1.23449600	0.42001500
O	1.78415800	-2.09422000	1.07818200
O	1.78459400	2.09347700	-1.07890500
C	-0.17662800	1.49645600	0.08234300
H	-0.58243500	0.82616300	0.82773300
C	-0.17689100	-1.49673500	-0.08309500
H	-0.58243700	-0.82650300	-0.82868400

C	-0.86392600	2.56995200	-0.33752900
H	-0.37250200	3.19902400	-1.07455200
C	-0.86463000	-2.56979700	0.33716800
H	-0.37359900	-3.19860700	1.07467600
C	-2.19393100	3.00046300	0.08453600
C	-2.71511900	4.18767600	-0.45058300
C	-2.98268600	2.28650600	1.00136400
C	-3.97231600	4.65023800	-0.08349900
H	-2.11920400	4.75029000	-1.16042300
C	-4.23767100	2.74680100	1.36637600
H	-2.61338800	1.36303700	1.42972600
C	-4.73848000	3.93118200	0.82687300
H	-4.35351100	5.57119800	-0.50830500
H	-4.83182200	2.18145300	2.07449100
H	-5.72009400	4.28762800	1.11535500
C	-2.19476500	-3.00002000	-0.08477900
C	-2.71773500	-4.18508800	0.45335400
C	-2.98193900	-2.28788600	-1.00438000
C	-3.97524900	-4.64718300	0.08676400
H	-2.12298300	-4.74636500	1.16522300
C	-4.23720800	-2.74774700	-1.36896000
H	-2.61108700	-1.36629800	-1.43544000
C	-4.73988400	-3.92988300	-0.82627400
H	-4.35786100	-5.56642900	0.51400000
H	-4.83009000	-2.18386100	-2.07930200
H	-5.72170900	-4.28599900	-1.11444300



1a-T1

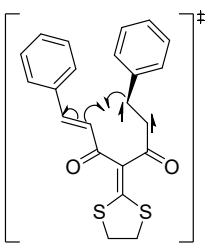
SCF Done: E(UB3LYP) = -1796.23675250 A.U.

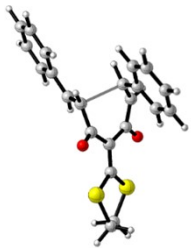
Zero-point correction = 0.334806 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.961140

C	-5.85990500	0.35924800	0.67911400
C	-5.88497700	-0.50961100	-0.55310000
C	-3.31476100	-0.02336100	-0.01333700
H	-6.64605300	1.11598200	0.67118100
H	-5.94691400	-0.23328200	1.59138000
H	-6.07194100	0.07567300	-1.45488800
H	-6.62892300	-1.30504100	-0.48568900
S	-4.25429900	1.25933100	0.73756200
S	-4.24488800	-1.32636800	-0.73749500

C	-1.92991300	-0.00783700	-0.02625400
C	-1.22263000	-1.24941900	-0.39459800
C	-1.23029200	1.23927900	0.34369300
O	-1.82600600	2.15773800	0.95903600
O	-1.78863500	-2.13833300	-1.03375200
C	0.14940400	-1.47157700	0.12931400
H	0.49856000	-0.82189900	0.92125100
C	0.09085200	1.48774000	-0.15329100
H	0.51248000	0.80918400	-0.88032100
C	0.90640900	-2.47943100	-0.33455600
H	0.47155900	-3.08531400	-1.12475400
C	0.81270400	2.70239700	0.20131000
H	0.25755800	3.42536700	0.78505400
C	2.24769400	-2.86059900	0.09690000
C	2.87898400	-3.93640800	-0.54539400
C	2.94395700	-2.20596300	1.12644100
C	4.15436700	-4.34513300	-0.17787000
H	2.35478500	-4.45448900	-1.34061500
C	4.21634900	-2.61390600	1.49349000
H	2.48643000	-1.37334000	1.64612700
C	4.82846600	-3.68493500	0.84350000
H	4.62106800	-5.17949800	-0.68774800
H	4.73635000	-2.09664200	2.29108500
H	5.82320200	-4.00084500	1.13417100
C	2.13191200	2.97181400	-0.13161500
C	2.73522000	4.20929900	0.29247600
C	2.96700600	2.07253800	-0.88636100
C	4.03670000	4.51065800	-0.01117900
H	2.12997300	4.90516400	0.86163200
C	4.27285200	2.39418500	-1.17677000
H	2.56590700	1.12830300	-1.22877700
C	4.82669100	3.60854300	-0.74990900
H	4.46337800	5.45063800	0.31858000
H	4.88010500	1.69914300	-1.74476400
H	5.85408000	3.85313600	-0.98828100





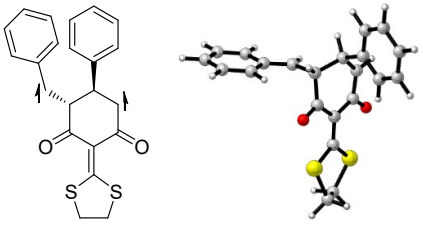
TS1a

SCF Done: E(UB3LYP) = -1796.22691749 A.U.

Zero-point correction = 0.334578 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.948692

C	4.86978600	1.40003900	-1.21558900
C	4.75584600	2.34978100	-0.04965100
C	2.48909800	0.95483700	-0.08944600
H	5.31352900	1.87135600	-2.09385800
H	5.44955900	0.51235600	-0.95795800
H	4.42573900	3.34013500	-0.36719800
H	5.69375200	2.44727900	0.49935500
S	3.18085600	0.85075900	-1.69962400
S	3.51115200	1.68721300	1.13671600
C	1.21669500	0.49201600	0.19425900
C	0.79296500	0.36872600	1.60149600
C	0.32888600	0.10619900	-0.91192600
C	-0.34036900	-0.45728700	1.95115500
C	-1.14490500	0.12693900	-0.69483000
C	-1.12085900	-1.32025300	1.06709200
H	-0.57575300	-0.44437400	3.01298900
O	1.46730500	0.87020500	2.52113800
O	0.75000000	-0.16391500	-2.03220200
C	-1.77116100	1.25674200	-0.22247500
H	-1.15948200	2.01589200	0.25453800
C	-3.19219200	1.52789800	-0.24869800
C	-3.67244300	2.71089500	0.34592300
C	-4.13533300	0.66124900	-0.83611400
C	-5.02535100	3.01226200	0.35822400
H	-2.96418100	3.39304000	0.80297200
C	-5.48697000	0.96545500	-0.82196100
H	-3.80524400	-0.25106500	-1.31686400
C	-5.94162900	2.14040700	-0.22483300
H	-5.36842500	3.92875100	0.82351400
H	-6.19394900	0.28532300	-1.28245800
H	-6.99936100	2.37394500	-0.21700800
H	-1.67668000	-0.56133900	-1.34020900
H	-2.19727700	-1.22673900	1.17744900
C	-0.67315000	-2.61330400	0.61121200
C	-1.60539700	-3.50931600	0.04062300
C	0.67236100	-3.03218800	0.69691900
C	-1.21239000	-4.75236600	-0.42119600
H	-2.64657900	-3.21288400	-0.02691100
C	1.05739700	-4.28028500	0.23525000
H	1.41136700	-2.37323400	1.13445400
C	0.12298200	-5.14705200	-0.32832900
H	-1.94623700	-5.42224900	-0.85383700
H	2.09513500	-4.58207000	0.31424000
H	0.43030900	-6.12035500	-0.69079800



INT1a

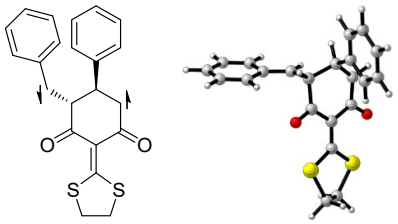
SCF Done: E(UB3LYP) = -1796.26499611 A.U.

Zero-point correction = 0.337811 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.983025

C	4.42160100	-1.57660800	1.48979700
C	4.78381000	-1.82254100	0.04633700
C	2.42291000	-0.59975800	0.02576200
H	4.67013300	-2.42354600	2.13107300
H	4.90469400	-0.68001700	1.88141700
H	4.52864000	-2.83591800	-0.26772300
H	5.84160500	-1.64412700	-0.15272900
S	2.59845800	-1.34043100	1.60357000
S	3.83821400	-0.64166600	-1.00645600
C	1.23488500	-0.01875800	-0.38605700
C	1.18536300	0.73357400	-1.64985400
C	0.03892300	-0.13125500	0.44855900
C	-0.00427100	1.47780900	-1.95261700
C	-1.30899200	0.29046200	-0.16508500
C	-1.20071600	1.54818900	-1.06630200
H	0.03423600	2.08647900	-2.84847000
O	2.17167900	0.79557900	-2.40875300
O	0.05959700	-0.63087400	1.56633300
C	-1.82968500	-0.88436200	-0.94040000
H	-1.56960300	-0.92437200	-1.99373000
C	-2.58546000	-1.95577500	-0.41936100
C	-3.04909800	-2.97417200	-1.29874600
C	-2.92504700	-2.07979300	0.95531700
C	-3.81185600	-4.02812800	-0.83851700
H	-2.79637300	-2.90824700	-2.35128700
C	-3.68750900	-3.14290400	1.40285000
H	-2.55723500	-1.35134700	1.66492700
C	-4.14116100	-4.12174500	0.51667800
H	-4.15480400	-4.78708500	-1.53211900
H	-3.92890400	-3.21831300	2.45679400
H	-4.73864600	-4.95015800	0.87722800
H	-1.96312200	0.50828500	0.67958400
H	-2.08966000	1.56096700	-1.70584600
C	-1.24182500	2.85360800	-0.26630200
C	-2.42695100	3.59013800	-0.21451400

C	-0.13241600	3.32316200	0.44100600
C	-2.50898100	4.75908100	0.53421700
H	-3.29600500	3.24309400	-0.76323000
C	-0.21297600	4.49108200	1.19158300
H	0.80333600	2.77852800	0.40905500
C	-1.40088000	5.21272800	1.24168100
H	-3.43860600	5.31523600	0.56316100
H	0.65699100	4.83869400	1.73604900
H	-1.46165100	6.12355000	1.82518400



INT1a-OSS

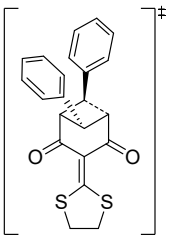
SCF Done: E(UB3LYP) = -1796.26563043 A.U.

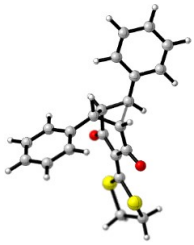
Zero-point correction = 0.337861 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.982622

C	-4.38895000	-1.66411100	-1.47271600
C	-4.75216200	-1.90230600	-0.02822600
C	-2.40400600	-0.65071400	-0.01308600
H	-4.62761300	-2.51848100	-2.10790200
H	-4.88002000	-0.77544000	-1.87228600
H	-4.48756800	-2.91058900	0.29422800
H	-5.81228900	-1.73314600	0.16656700
S	-2.56813200	-1.41181000	-1.58360000
S	-3.82194200	-0.70333300	1.01717900
C	-1.22682600	-0.04618300	0.39241200
C	-1.18304400	0.71002400	1.65456300
C	-0.02996600	-0.14156500	-0.44104400
C	-0.00267500	1.47083900	1.95421600
C	1.31381400	0.32390200	0.15535000
C	1.17845500	1.57977700	1.05594900
H	-0.03992600	2.05927800	2.86353800
O	-2.16581100	0.75712300	2.41817400
O	-0.04087000	-0.65571300	-1.55230100
C	1.90558300	-0.80915700	0.93966100
H	1.73182200	-0.79928100	2.01109800
C	2.64367500	-1.89202800	0.41553200
C	3.18760200	-2.85905700	1.30626200
C	2.89314100	-2.07069000	-0.97213700
C	3.94069400	-3.91848400	0.84257500
H	3.00492200	-2.74927400	2.36955400
C	3.64878600	-3.13752500	-1.42251300

H	2.46192400	-1.38145600	-1.68517500
C	4.18112100	-4.06631900	-0.52630700
H	4.34599800	-4.63855800	1.54390200
H	3.82241400	-3.25570100	-2.48579100
H	4.77165000	-4.89863500	-0.88941900
H	1.94482200	0.55840600	-0.70348400
H	2.07465400	1.61839300	1.68585500
C	1.17888100	2.88393600	0.25151000
C	2.34422300	3.65013600	0.18857700
C	0.05233400	3.32305200	-0.44802500
C	2.39055900	4.81879000	-0.56394500
H	3.22604100	3.32721400	0.73160400
C	0.09740900	4.49031700	-1.20252600
H	-0.86927000	2.75553800	-0.40624900
C	1.26607200	5.24196700	-1.26409600
H	3.30548200	5.39834600	-0.60144900
H	-0.78566700	4.81429000	-1.74044500
H	1.29893000	6.15249300	-1.85029200





TS2a

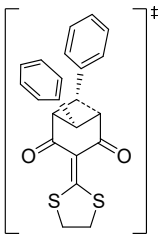
SCF Done: E(UB3LYP) = -1796.27944305 A.U.

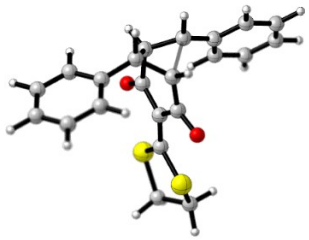
Zero-point correction = 0.339776 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.991690

C	-4.81900400	-1.79978500	-0.79591400
C	-4.49327200	-2.46062500	0.52895800
C	-2.36709300	-1.01937900	-0.09008900
H	-5.30328000	-2.49170700	-1.48659200
H	-5.45849600	-0.92766400	-0.65665000
H	-4.05909100	-3.45154700	0.39244300
H	-5.36378000	-2.53183100	1.18219100
S	-3.24561100	-1.26479000	-1.59488200
S	-3.27201700	-1.38221600	1.37633100
C	-1.05054600	-0.57837200	-0.01936100
C	-0.32618300	-0.50528900	1.21471900
C	-0.28596500	-0.23685800	-1.22674200
C	1.00327000	0.05968800	1.20128400
C	1.17119500	0.17154000	-0.99610800
C	1.24377900	1.17687200	0.18420000
H	1.53533300	0.03775700	2.14758300
O	-0.80437900	-0.86477400	2.35113000

O	-0.74662000	-0.31613900	-2.35397100
C	1.89138000	-0.97281400	-0.26753000
H	1.38016400	-1.92738700	-0.22688100
C	3.33029600	-1.07727000	-0.19214600
C	3.89775500	-2.23000300	0.40115100
C	4.21774500	-0.08453500	-0.66451900
C	5.26711200	-2.37380800	0.52607600
H	3.23789600	-3.01042800	0.76355800
C	5.58879200	-0.23804000	-0.54316600
H	3.82984800	0.80040500	-1.15285000
C	6.12475700	-1.37716000	0.05729500
H	5.67434400	-3.26687300	0.98516700
H	6.24880000	0.53231000	-0.92440400
H	7.19765700	-1.49027900	0.15237700
H	1.60686900	0.47712700	-1.94941800
H	2.27903100	1.50961000	0.29062500
C	0.35382700	2.40233500	0.18863000
C	0.11266200	3.10573600	-0.99318500
C	-0.18766200	2.89146800	1.37907900
C	-0.64961900	4.26934800	-0.98573800
H	0.51221600	2.74112900	-1.93234500
C	-0.94725200	4.05626400	1.38865800
H	-0.02480500	2.35533700	2.30682800
C	-1.18091600	4.74991500	0.20587800
H	-0.83211600	4.79660400	-1.91470000
H	-1.36270300	4.41759400	2.32206900
H	-1.77819300	5.65386200	0.21196200





TS2a'

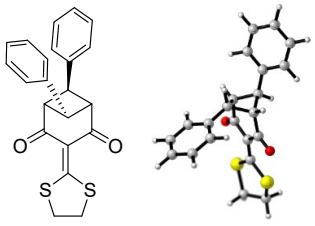
SCF Done: E(UB3LYP) = -1796.27491621 A.U.

Zero-point correction = 0.339834 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.987056

C	0.02418300	4.44757000	-0.61214600
C	-0.60945800	4.27974600	0.75609600
C	0.13055900	1.85853400	0.02385400
H	-0.55751900	5.11620800	-1.24847900
H	1.04292300	4.82776200	-0.53220600
H	-1.68706100	4.12756900	0.68910300
H	-0.40046100	5.12210000	1.41652400
S	0.06490500	2.80760400	-1.45648300

S	0.15867300	2.79398600	1.51509500
C	0.11920900	0.47009800	0.06599000
C	0.02922100	-0.25633500	1.29375400
C	0.11164500	-0.34245000	-1.15340200
C	0.15446700	-1.69130900	1.25080300
C	0.03240400	-1.86054900	-0.95432200
C	1.05713700	-2.25175000	0.14874400
H	0.04476700	-2.20163800	2.20248100
O	-0.07677500	0.29533600	2.45082400
O	0.15028900	0.13985800	-2.27570900
C	-1.17857900	-2.31557900	-0.13539200
H	-1.10880300	-3.36705400	0.13291200
C	-2.53987000	-1.84133700	-0.17545200
C	-3.50784600	-2.54113800	0.58427600
C	-2.97300500	-0.71003000	-0.89892500
C	-4.82544200	-2.12906700	0.62923800
H	-3.19974900	-3.41723700	1.14472400
C	-4.29948600	-0.30635600	-0.85536600
H	-2.28304800	-0.16165700	-1.52356700
C	-5.23155300	-1.00353200	-0.09102900
H	-5.54396800	-2.68301400	1.22167900
H	-4.61016100	0.55865400	-1.42942400
H	-6.26486700	-0.67986000	-0.06065500
H	0.13784500	-2.33634100	-1.93298400
H	1.06120300	-3.34412500	0.22954800
C	2.49477300	-1.78567400	0.04785000
C	3.15280200	-1.78360800	-1.18387400
C	3.21096700	-1.41554000	1.18776100
C	4.49220900	-1.41977000	-1.27419500
H	2.61693500	-2.05758900	-2.08507400
C	4.55148700	-1.05569200	1.09970500
H	2.71791900	-1.39767300	2.15267700
C	5.19708600	-1.05626700	-0.13207500
H	4.98253800	-1.41591900	-2.24051600
H	5.08911700	-0.76750900	1.99541800
H	6.23955700	-0.76945400	-0.20221500



2a

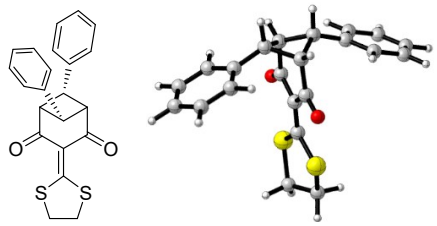
SCF Done: E(UB3LYP) = -1796.32050960 A.U.

Zero-point correction = 0.342162 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1796.031876

C	4.84637100	-1.49358300	0.70174200
C	4.60481500	-2.26184100	-0.57565200
C	2.29495100	-1.11070100	0.06372600
H	5.47988800	-2.04195400	1.40027800
H	5.29061500	-0.51626100	0.50808500
H	4.41413400	-3.31847400	-0.38251000
H	5.43715200	-2.17185400	-1.27509000
S	3.22761400	-1.23438900	1.53993100
S	3.12646800	-1.55168200	-1.41214200
C	0.98239400	-0.68875600	0.06221900
C	0.22681000	-0.52868600	-1.18499600
C	0.27592500	-0.36981800	1.30735400
C	-1.20412700	-0.06261000	-0.99990600
C	-1.15981800	0.09668100	1.12589700
C	-1.24937800	1.15354300	-0.01923300
H	-1.70944800	0.00161600	-1.96102400
O	0.70074000	-0.74241700	-2.29264900
O	0.77618500	-0.49700400	2.41646500
C	-1.86178700	-0.90555500	0.15392900
H	-1.49129400	-1.93141000	0.21859000
C	-3.37339400	-0.94012900	0.12734500
C	-3.99935400	-1.67349700	-0.88774000
C	-4.17753600	-0.30477000	1.07279600
C	-5.38267800	-1.76321600	-0.95873000
H	-3.39229800	-2.18171400	-1.62968400
C	-5.56653000	-0.39338600	1.00485100
H	-3.72751000	0.26206000	1.87806000
C	-6.17424000	-1.12025900	-0.01032800
H	-5.84437900	-2.33710200	-1.75367600
H	-6.17137200	0.10820200	1.75116900
H	-7.25416900	-1.18869200	-0.06300200
H	-1.59485700	0.30789400	2.10004600
H	-2.27088400	1.54328000	-0.03319600
C	-0.28382100	2.30543300	-0.12704400
C	0.22436200	2.92467700	1.01685400
C	0.07361800	2.81581600	-1.37755000
C	1.06709900	4.02674500	0.91403900
H	-0.03125600	2.54066500	1.99771400
C	0.91604300	3.91695500	-1.48184500
H	-0.30128900	2.34446700	-2.27893100
C	1.41545000	4.52723400	-0.33571000
H	1.45495100	4.49110200	1.81316600
H	1.18594700	4.29536000	-2.46082200

H	2.07429700	5.38365600	-0.41643100



2a'

SCF Done: E(UB3LYP) = -1796.32136282 A.U.

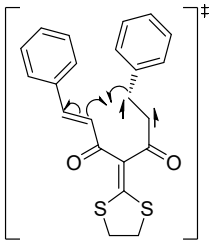
Zero-point correction = 0.342061 (Hartree/Particle)

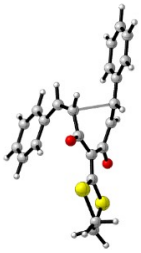
Sum of electronic and thermal Free Energies = -1796.032258

C	0.36235600	4.28716100	-0.66205400
C	-0.36310300	4.28708200	0.66195100
C	-0.00009300	1.73902000	-0.00001600
H	-0.01274500	5.05616500	-1.33884600
H	1.43787700	4.41743500	-0.53410600
H	-1.43865600	4.41708900	0.53399600
H	0.01179800	5.05622200	1.33870300
S	0.07114300	2.66536400	-1.48352800
S	-0.07149100	2.66540600	1.48347800
C	0.00000300	0.36073100	0.00000100
C	0.00135900	-0.40831700	1.24753700
C	-0.00120700	-0.40836100	-1.24751500
C	-0.00800100	-1.91693900	1.06896800
C	0.00823800	-1.91694400	-1.06887000
C	1.06713300	-2.32316200	0.00606000
H	-0.01236800	-2.40672000	2.04056400
O	0.03185100	0.10654600	2.35717900
O	-0.03172300	0.10645300	-2.35717800
C	-1.06688400	-2.32323000	-0.00594200
H	-1.13256700	-3.41613900	-0.00822400
C	-2.46041000	-1.74873500	-0.01330900
C	-3.13167600	-1.49146300	1.18419400
C	-3.13138300	-1.52180300	-1.21723400
C	-4.44042800	-1.02099400	1.17883900
H	-2.62711900	-1.64954900	2.13041300
C	-4.43986600	-1.05113700	-1.22412000
H	-2.62586600	-1.70286000	-2.15878500
C	-5.09981100	-0.80021600	-0.02566200
H	-4.94281100	-0.82224400	2.11828100
H	-4.94187100	-0.87564900	-2.16837000
H	-6.11836000	-0.43065200	-0.03053800
H	0.01265100	-2.40684600	-2.04040500
H	1.13299200	-3.41605300	0.00833800
C	2.46062400	-1.74852600	0.01339600

C	3.13186900	-1.49135200	-1.18416000
C	3.13157700	-1.52136500	1.21727300
C	4.44055400	-1.02075500	-1.17888000
H	2.62729700	-1.64963500	-2.13033800
C	4.44002000	-1.05054800	1.22408400
H	2.62612100	-1.70235400	2.15887300
C	5.09992800	-0.79972700	0.02560300
H	4.94293900	-0.82207500	-2.11833600
H	4.94198400	-0.87487400	2.16832300
H	6.11844600	-0.43007700	0.03038400

TS1b

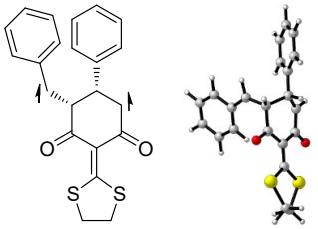




SCF Done: E(UB3LYP) = -1796.21893343 A.U.
Zero-point correction = 0.334417 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -1795.940144

C	4.88531700	-1.95637100	-0.33816600
C	5.05027000	-0.96212500	0.78359400
C	2.46819000	-0.92716400	0.10547500
H	5.71395500	-1.92469600	-1.04734100
H	4.77818800	-2.97512500	0.03745900
H	5.42738300	-0.00462700	0.42072900
H	5.71222900	-1.32904200	1.56947700
S	3.36097500	-1.53397400	-1.28108500
S	3.40817800	-0.66605800	1.56482900
C	1.10968900	-0.66730200	0.05049500
C	0.37749200	-0.35296800	1.29788800
C	0.43590400	-0.67801900	-1.24637500
C	-1.03502700	-0.59597000	1.38460200
C	-0.96337500	-0.16281500	-1.36881400
C	-1.80536700	-1.40363100	0.45011600
H	-1.48983400	-0.25243100	2.30834700
H	-1.32513500	-2.30230400	0.07271100
O	0.98818700	0.00661400	2.32473000
O	0.98483400	-1.07335100	-2.27510700
C	-1.38925500	1.13075500	-1.16007300
H	-2.44725100	1.29553600	-1.34829100
C	-0.67228600	2.31715900	-0.73729300
C	-1.41811100	3.39382700	-0.21529500
C	0.71799100	2.49328400	-0.88247900

C	-0.80254700	4.56584900	0.19078900
H	-2.49350100	3.29062600	-0.12226400
C	1.32881300	3.67117900	-0.48215800
H	1.31613900	1.71974700	-1.34253700
C	0.57774700	4.70880900	0.06496800
H	-1.39729900	5.37260700	0.60239100
H	2.39877500	3.78619400	-0.60754800
H	1.06190300	5.62608300	0.37748500
C	-3.23084700	-1.36697300	0.35343300
C	-3.91677000	-2.38330800	-0.35350000
C	-4.00533800	-0.32646200	0.91818300
C	-5.29319300	-2.36407600	-0.48045000
H	-3.34533100	-3.19313500	-0.79409000
C	-5.38473600	-0.31587800	0.78718500
H	-3.51485700	0.47192200	1.46120800
C	-6.03942900	-1.33027500	0.08989200
H	-5.79428200	-3.15770200	-1.02217400
H	-5.95834200	0.48848300	1.23310000
H	-7.11813400	-1.31808100	-0.00653000
H	-1.58597400	-0.78478200	-2.00113600



INT1b

SCF Done: E(UB3LYP) = -1796.25499222 A.U.

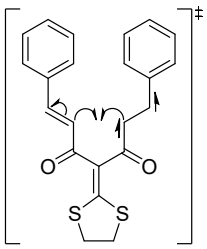
Zero-point correction = 0.337601 (Hartree/Particle)

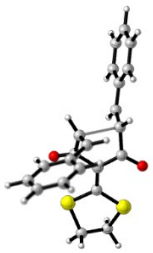
Sum of electronic and thermal Free Energies = -1795.972736

C	-5.25105900	-0.89281600	0.83962600
C	-5.30729800	-0.51132900	-0.61872900
C	-2.72952700	-0.71247000	0.02226400
H	-6.00061000	-0.36956200	1.43515400
H	-5.37029700	-1.96796700	0.98235600
H	-5.45599500	0.56156700	-0.75097600
H	-6.08874700	-1.04764400	-1.15908200
S	-3.60567300	-0.40168500	1.50662300
S	-3.70572000	-0.96727100	-1.40905800
C	-1.34444100	-0.74772200	-0.02070200
C	-0.65461500	-1.11022000	-1.26923600
C	-0.57248500	-0.37183600	1.16279000
C	0.76033000	-1.34785600	-1.20934500
C	0.95981200	-0.39033700	1.10616300
C	1.47408800	-1.47768800	0.08889500

H	1.24612900	-1.60290700	-2.14324300
H	1.14891500	-2.43754600	0.52404500
O	-1.27586200	-1.27786800	-2.33444400
O	-1.11506900	-0.02675100	2.20606400
C	1.63716500	0.94747600	0.94867400
H	2.65232900	0.94023800	1.32993000
C	1.22034400	2.18502800	0.41168600
C	2.15243900	3.26491300	0.45067800
C	-0.04545100	2.46271300	-0.17351700
C	1.84365800	4.51153100	-0.05234800
H	3.12762200	3.08954200	0.89090700
C	-0.34271800	3.71621900	-0.67540100
H	-0.79542900	1.68955900	-0.23731100
C	0.59069500	4.75231300	-0.62227900
H	2.57843400	5.30686600	-0.00349100
H	-1.31701400	3.89211600	-1.11647900
H	0.34671100	5.73064700	-1.01764400
C	2.98455300	-1.54625500	-0.01908000
C	3.70000800	-2.40874700	0.81344300
C	3.69559700	-0.75312600	-0.92273200
C	5.08774200	-2.47850800	0.75027600
H	3.16501100	-3.03914200	1.51635800
C	5.08296800	-0.82238800	-0.99103000
H	3.16354600	-0.07136600	-1.57600400
C	5.78435100	-1.68438400	-0.15412100
H	5.62279300	-3.15802800	1.40311800
H	5.61647300	-0.20046800	-1.70020000
H	6.86499600	-1.73910700	-0.20910800
H	1.24793500	-0.74361700	2.10183200

TS1c





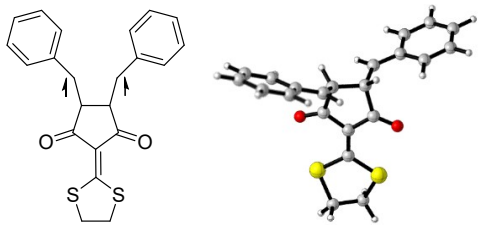
SCF Done: E(UB3LYP) = -1796.22504212 A.U.

Zero-point correction = 0.333735 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.948469

C	3.89195700	3.17711600	-0.57126100
C	3.14500300	4.07077500	0.39349900
C	1.62753200	1.92453700	0.01249300
H	4.38414800	3.74609200	-1.36110500
H	4.63103600	2.55877100	-0.06047900

H	2.59040700	4.85308400	-0.12617000
H	3.80948700	4.52939000	1.12700000
S	2.66690600	2.07677000	-1.38956300
S	1.95413700	3.02861000	1.33225200
C	0.61819500	0.99576000	0.07136400
C	0.39132700	-0.00361100	-0.97789400
C	-0.32858500	0.93344600	1.18155900
C	-0.36874200	-1.19670100	-0.52148300
C	-1.61614800	0.20454400	0.88783100
H	-1.04407600	-1.61198600	-1.26893300
H	-1.89585000	-0.53933400	1.62590300
O	-0.14500400	1.44561900	2.27691400
O	0.78295000	0.11702600	-2.13518300
C	-2.57413000	0.77254700	0.09758900
H	-2.27867900	1.60861400	-0.53114800
C	0.20635400	-2.10463000	0.48068500
H	-0.25832200	-2.16899300	1.46090900
C	-3.95714400	0.35326900	-0.04095500
C	-4.78693700	1.04346200	-0.94233000
C	-4.51786400	-0.71825500	0.67829500
C	-6.11480600	0.68273800	-1.11886300
H	-4.37427700	1.87137100	-1.50813100
C	-5.84352400	-1.07827400	0.49907400
H	-3.91218900	-1.27216000	1.38460400
C	-6.65054300	-0.38107200	-0.39942200
H	-6.73304300	1.23097600	-1.81979600
H	-6.25458300	-1.90699500	1.06348000
H	-7.68684200	-0.66588800	-0.53519300
C	1.31569600	-2.95424300	0.25130700
C	1.99465300	-3.01302100	-0.99577000
C	1.78329800	-3.80111400	1.29299600
C	3.06881600	-3.86496000	-1.17535200
H	1.66713200	-2.37910700	-1.81031800
C	2.85739200	-4.64630500	1.09922200
H	1.28193200	-3.77263700	2.25412500
C	3.51037300	-4.68653100	-0.13606200
H	3.57186300	-3.89368900	-2.13499600
H	3.19554800	-5.28112100	1.91002900
H	4.35301900	-5.35049000	-0.28579600



INT1c

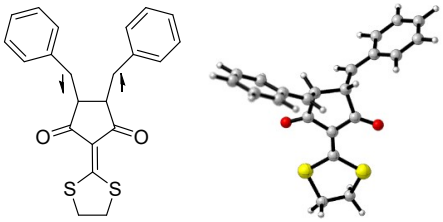
SCF Done: E(UB3LYP) = -1796.27499679 A.U.

Zero-point correction = 0.336857 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.994500

C	-0.73506100	-5.10311900	-0.17142200
C	0.73861100	-5.10265300	0.17156700
C	0.00089400	-2.56153400	-0.00001900
H	-0.98399200	-5.87344600	-0.90217600
H	-1.35687100	-5.23609400	0.71460800
H	1.36050000	-5.23540800	-0.71443900
H	0.98801100	-5.87269400	0.90246000
S	-1.15429600	-3.48234700	-0.93389700
S	1.15687200	-3.48149200	0.93376800
C	0.00035100	-1.18964700	0.00002900
C	-0.94013300	-0.35352400	-0.73320000
C	0.94020800	-0.35279100	0.73321900
C	-0.71525900	1.12102700	-0.29689400
C	0.71429900	1.12157600	0.29673900
H	-0.79130200	1.75497800	-1.18333400
H	0.78982500	1.75567900	1.18312600
O	1.77259600	-0.72435000	1.53889200
O	-1.77223800	-0.72573200	-1.53887100
C	1.75167900	1.49569200	-0.71496300
H	1.46923200	1.40243500	-1.75882500
C	-1.75292000	1.49436700	0.71481100
H	-1.47054200	1.40072800	1.75866400
C	3.06888800	1.91726300	-0.43721800
C	3.92663200	2.28355800	-1.51174200
C	3.59848400	2.01058000	0.87815300
C	5.21456100	2.72399900	-1.28450300
H	3.54886100	2.21620300	-2.52605900
C	4.89129600	2.45218700	1.09134600
H	2.99437300	1.70248400	1.72052400
C	5.70927300	2.81485900	0.01965100
H	5.84460100	2.99945000	-2.12231400
H	5.27452800	2.50921000	2.10360500
H	6.72086900	3.15909300	0.19693200
C	-3.07027600	1.91550400	0.43715100
C	-3.59993400	2.00891800	-0.87819000

C	-3.92817000	2.28115700	1.51177300
C	-4.89291600	2.45007600	-1.09125800
H	-2.99572300	1.70128100	-1.72066600
C	-5.21626800	2.72117100	1.28465700
H	-3.55037000	2.21367000	2.52606900
C	-5.71102600	2.81218300	-0.01946500
H	-5.27617900	2.50719400	-2.10350000
H	-5.84641300	2.99615300	2.12254400
H	-6.72275300	3.15608400	-0.19664300



INT1c-OSS

SCF Done: E(UB3LYP) = -1796.27659634 A.U.

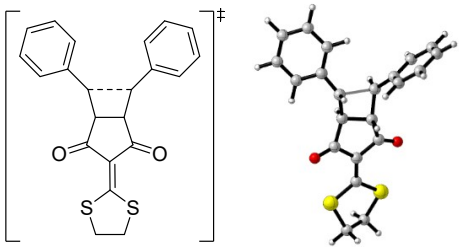
Zero-point correction = 0.336797 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1795.996609

C	0.73885900	5.26720300	-0.16751100
C	-0.73671100	5.26753700	0.16773200
C	0.00047500	2.72585000	-0.00006900
H	0.99218300	6.03793800	-0.89634600
H	1.35582500	5.39930400	0.72203000
H	-1.35361700	5.40009200	-0.72178400
H	-0.98965300	6.03827200	0.89670000
S	1.16047300	3.64691700	-0.92915500
S	-1.15911400	3.64733200	0.92911500
C	0.00018500	1.35462800	-0.00012200
C	0.93693000	0.51841500	-0.73873100
C	-0.93684700	0.51874900	0.73850100
C	0.71436600	-0.95705900	-0.30614200
C	-0.71473100	-0.95682300	0.30599800
H	0.77619700	-1.58830700	-1.19481400
H	-0.77673600	-1.58798000	1.19472600
O	-1.76774000	0.88853500	1.54612500
O	1.76794100	0.88789800	-1.54637800
C	-1.74627900	-1.33825100	-0.69648800
H	-1.53334600	-1.08657100	-1.73096300
C	1.74578000	-1.33870600	0.69639500
H	1.53294800	-1.08678600	1.73083200
C	-2.98793200	-1.95397200	-0.42432300
C	-3.84230000	-2.31004300	-1.50391800
C	-3.44210500	-2.25169700	0.88792800
C	-5.05392500	-2.93430100	-1.28566100

H	-3.52254600	-2.08814700	-2.51610900
C	-4.65830800	-2.87677100	1.09338800
H	-2.84276600	-1.96326600	1.74101000
C	-5.47264700	-3.22705500	0.01505500
H	-5.68258000	-3.19783600	-2.12830700
H	-4.98442800	-3.08891200	2.10499200
H	-6.42389800	-3.71619800	0.18546200
C	2.98722200	-1.95490200	0.42432300
C	3.44130100	-2.25298400	-0.88787600
C	3.84143700	-2.31114400	1.50398100
C	4.65727500	-2.87854900	-1.09322000
H	2.84208400	-1.96446100	-1.74101400
C	5.05282900	-2.93589500	1.28584000
H	3.52174900	-2.08898700	2.51613600
C	5.47146000	-3.22899500	-0.01482600
H	4.98333000	-3.09096000	-2.10478900
H	5.68136600	-3.19954200	2.12853900
H	6.42252600	-3.71852800	-0.18515400

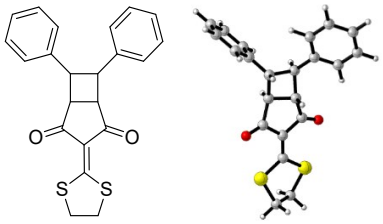
TS2c



SCF Done: E(UB3LYP) = -1796.25438149 A.U.
Zero-point correction = 0.338800 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -1795.969500

C	-5.93940300	-0.51894500	-0.73283300
C	-5.99432700	0.24323400	0.57236900
C	-3.41673500	-0.07673000	-0.01279900
H	-6.69042400	-1.30956800	-0.77320900
H	-6.07023300	0.13994800	-1.58880000
H	-6.13331300	-0.42155800	1.42519500
H	-6.77988000	0.99988400	0.57197200
S	-4.29788400	-1.32614400	-0.87561200
S	-4.39464900	1.12778400	0.79748200
C	-2.05065600	-0.04702500	0.02101800
C	-1.17247500	-1.10165600	-0.56397600
C	-1.24564800	1.05809600	0.62693300
C	0.18381900	-0.74564700	0.01676500
C	0.14152800	0.77332000	0.09091200
H	0.14640200	-1.12564300	1.05114700
H	0.10377800	1.13742300	-0.94634300

O	-1.66781100	1.97616600	1.30456100
O	-1.51875800	-2.03042800	-1.26785700
C	1.64966600	0.90155800	0.55199500
H	1.78452200	0.56995600	1.54576400
C	1.70477400	-0.79268500	-0.43014300
H	1.81452000	-0.42152000	-1.41837200
C	2.52807800	1.91823000	0.05109800
C	3.87161900	1.71710200	-0.26987700
C	2.00584500	3.21539200	-0.01459100
C	4.67720000	2.78657100	-0.64459500
H	4.29920400	0.71547800	-0.22445400
C	2.81153200	4.28544800	-0.38650100
H	0.96256200	3.39216000	0.24089200
C	4.15299700	4.07462500	-0.70125500
H	5.72008200	2.61434800	-0.89139900
H	2.39269700	5.28817300	-0.42322600
H	4.77774800	4.91294600	-0.99393500
C	2.63859600	-1.78414700	0.01501500
C	2.87966800	-2.13170000	1.34809900
C	3.27181200	-2.52602200	-0.99048800
C	3.72377600	-3.18681100	1.66354800
H	2.41534900	-1.56790500	2.15433600
C	4.11173900	-3.58874300	-0.67948200
H	3.09429000	-2.27593800	-2.03098400
C	4.34131500	-3.92276900	0.65594400
H	3.89882500	-3.44230600	2.70907200
H	4.58822400	-4.15237400	-1.47696200
H	5.00039700	-4.74984200	0.90282900



3a

SCF Done: E(UB3LYP) = -1796.28546586 A.U.

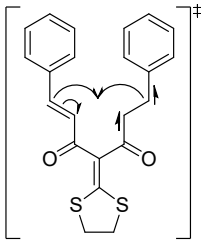
Zero-point correction = 0.341068 (Hartree/Particle)

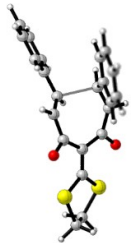
Sum of electronic and thermal Free Energies = -1795.998625

C	-5.96159600	0.50795200	0.71182400
C	-5.99533700	-0.25662200	-0.59291200
C	-3.42838500	0.07305000	0.02413200
H	-6.71337300	1.29759700	0.74192700
H	-6.10162600	-0.15131900	1.56912500
H	-6.13072400	0.40824300	-1.44661700
H	-6.78010200	-1.01404500	-0.60205500

S	-4.32070000	1.32137800	0.87440400
S	-4.39509200	-1.13811500	-0.79848700
C	-2.06233100	0.04490500	0.00481800
C	-1.18994800	1.10765200	0.59569000
C	-1.25151100	-1.05529400	-0.59863000
C	0.17141800	0.75698800	0.01606200
C	0.13618900	-0.76155000	-0.05714600
H	0.12641700	1.13276600	-1.01572200
H	0.10041500	-1.13273400	0.97766700
O	-1.66256300	-1.97481000	-1.27627000
O	-1.54730900	2.03132000	1.29519900
C	1.64317700	-0.72462700	-0.43634000
H	1.76083200	-0.50739300	-1.50226600
C	1.68797500	0.65337200	0.37035400
H	1.80934800	0.41926900	1.43023200
C	2.53049200	-1.87050600	-0.03477600
C	3.85751000	-1.65934000	0.34716400
C	2.04331600	-3.17927000	-0.06677300
C	4.67597800	-2.73034500	0.69096800
H	4.25597900	-0.65180300	0.37512900
C	2.86188700	-4.25084400	0.27421800
H	1.01663000	-3.36071100	-0.36668400
C	4.18120900	-4.02997900	0.65560700
H	5.70225300	-2.54782600	0.98780400
H	2.46655500	-5.25944900	0.24313500
H	4.81847800	-4.86390800	0.92485700
C	2.62981200	1.75900900	-0.01772500
C	2.80685800	2.14944800	-1.34858100
C	3.34782500	2.43886100	0.96908900
C	3.67179100	3.18530800	-1.68067800
H	2.26906400	1.64093200	-2.14081500
C	4.21417900	3.47669900	0.64145900
H	3.22257500	2.15354100	2.00796200
C	4.37973900	3.85358000	-0.68621400
H	3.79455600	3.47043600	-2.71897400
H	4.75852200	3.99072000	1.42495000
H	5.05438900	4.66071200	-0.94541600

TS1d

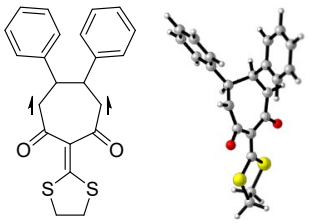




SCF Done: E(UB3LYP) = -1796.21110274 A.U.
Zero-point correction = 0.334915 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -1795.931605

C	5.57874100	-1.01970700	-0.13552300
C	5.52933100	-0.15162000	1.09360700
C	3.05460100	-0.20347300	0.06826900
H	6.49348000	-0.87844500	-0.71396000
H	5.47455300	-2.07779600	0.11179300
H	5.88561000	0.85969900	0.88906100
H	6.09934600	-0.56694000	1.92640000
S	4.17997500	-0.54186500	-1.23813900
S	3.77838700	-0.03188900	1.65851300
C	1.67901200	-0.08869300	-0.14037500
C	1.23468200	0.06420800	-1.54137000
C	0.82618500	-0.06846300	1.07237300
C	-0.09480000	0.41095300	-2.01009000
C	-0.56071000	-0.49358500	1.07775200
C	-1.42357000	0.48518400	-1.39982300
H	-0.06612300	0.60916600	-3.08001900
C	-1.22170500	-1.16422500	0.07129600
H	-1.07570400	-0.23391600	1.99443500
O	2.09441700	-0.00515900	-2.45053300
O	1.32333100	0.24614900	2.16649400
H	-0.61974300	-1.65943700	-0.68282700
C	-2.58128500	-1.71137000	0.21057300
C	-2.97167800	-2.78038600	-0.60779100
C	-3.51299700	-1.20376500	1.12659900
C	-4.24095900	-3.33445900	-0.50710200
H	-2.26418500	-3.18619300	-1.32307100
C	-4.78253000	-1.75724900	1.22620800
H	-3.24859500	-0.36704700	1.76051400
C	-5.15237700	-2.82477900	0.41251300
H	-4.51789300	-4.16590800	-1.14432800
H	-5.48825700	-1.35206100	1.94177200
H	-6.14336900	-3.25481200	0.49431400
H	-2.17560200	-0.07591600	-1.95006600
C	-1.92739900	1.69100500	-0.77574500
C	-3.31763100	1.89748000	-0.66943900
C	-1.06810700	2.66709700	-0.23504900
C	-3.82322100	3.02866800	-0.04984400
H	-3.99491700	1.16026600	-1.08456500
C	-1.58041200	3.79591500	0.38553900
H	0.00447700	2.53637600	-0.30723100
C	-2.95762100	3.98310900	0.48303300

H	-4.89534600	3.17178800	0.01650700
H	-0.90296800	4.53483400	0.79658300
H	-3.35383100	4.86741100	0.96735200



INT1d

SCF Done: E(UB3LYP) = -1796.24069455 A.U.

Zero-point correction = 0.337949 (Hartree/Particle)

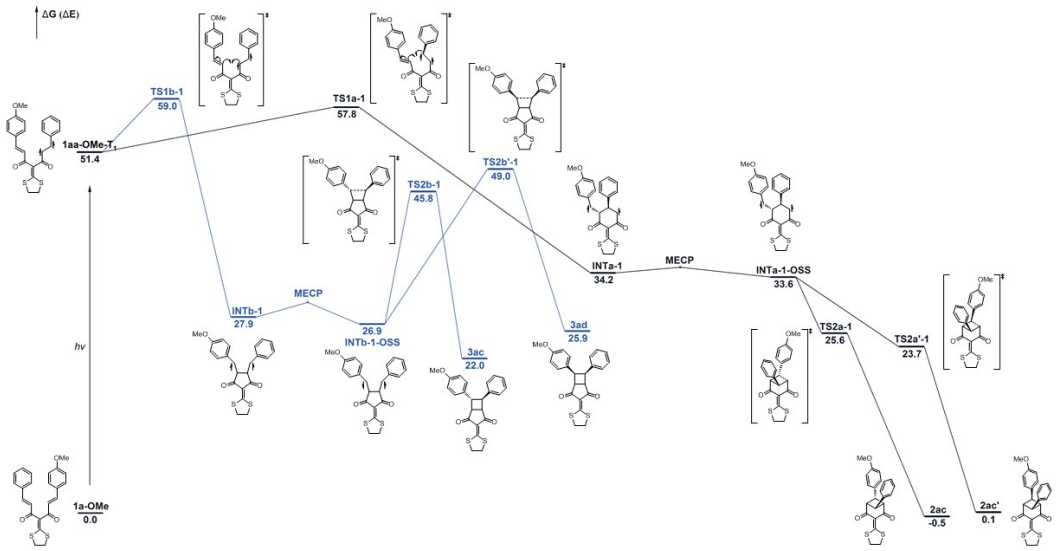
Sum of electronic and thermal Free Energies = -1795.958561

C	-5.73700200	-0.63072300	0.53621100
C	-5.70135400	-0.41296600	-0.95389200
C	-3.20409400	-0.07584300	-0.04788100
H	-6.63525400	-0.21817100	0.99893700
H	-5.65825500	-1.68855600	0.79351200
H	-6.03102700	0.59195900	-1.22358000
H	-6.30143800	-1.14248100	-1.50032500
S	-4.30607100	0.26218600	1.27919800
S	-3.96425800	-0.61601900	-1.53525900
C	-1.82480200	0.06966700	0.07382700
C	-1.32107600	0.77704700	1.26790100
C	-0.98660900	-0.38829300	-1.05095900
C	0.05963000	1.07677700	1.56814600
C	0.41523000	-0.68472200	-0.92309900
C	1.35393000	0.49431000	1.11029000
H	0.13842000	1.82955500	2.34544300
C	1.16690900	-0.86297200	0.34769700
H	0.89201100	-0.91927800	-1.86626200
O	-2.14908500	1.24052000	2.08437200
O	-1.50531700	-0.62191300	-2.16291000
H	0.53780100	-1.45734200	1.02267600
C	2.47318900	-1.62064500	0.18144700
C	2.78754600	-2.64615900	1.07557200
C	3.39005800	-1.31678200	-0.82767400
C	3.98264500	-3.35005200	0.96971300
H	2.08446300	-2.90323800	1.86111000
C	4.58514600	-2.01933000	-0.93762500
H	3.17756400	-0.52255000	-1.53267700
C	4.88650800	-3.03796900	-0.03960200
H	4.20264600	-4.14604200	1.67133000
H	5.28264600	-1.76859200	-1.72808200
H	5.81636800	-3.58686800	-0.12883800

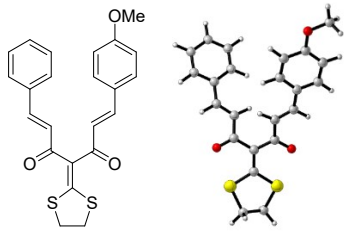
H	1.90553400	0.23972700	2.02453400
C	2.20078900	1.53933300	0.38742000
C	3.51835800	1.76860000	0.78689800
C	1.68379100	2.29352100	-0.66993200
C	4.30744400	2.71272700	0.13800000
H	3.93440700	1.19724600	1.60905800
C	2.47201400	3.23390100	-1.32396600
H	0.65700700	2.15230400	-0.98475000
C	3.78747600	3.44601800	-0.92278900
H	5.32897100	2.87342800	0.46189100
H	2.05410400	3.80672900	-2.14328100
H	4.40015300	4.18197300	-1.42962100

5.2 Computational studies of unsymmetrical bis(cinnamoyl)ketenedithioacetal

5.2.1 Computational analysis of 1a-OMe



5.2.2 Cartesian coordinates and energies of all optimized structures



1a-OMe

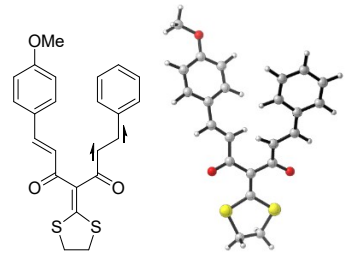
SCF Done: E(RB3LYP) = -1910.87992309 A.U.

Zero-point correction= 0.370758 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.570475

C	6.21272900	-1.25486700	-0.76876100
C	6.01657800	-1.97066500	0.54335300
C	3.68551000	-0.80887000	-0.03660000
H	7.18134600	-0.75618200	-0.83103900

H	6.10744600	-1.93284300	-1.61734400
H	6.38419800	-1.37956900	1.38378400
H	6.49894200	-2.94932700	0.56006900
S	4.92709300	0.05458200	-0.92820100
S	4.21521700	-2.25917800	0.79890600
C	2.36895100	-0.37294700	0.00464300
C	1.33956000	-1.31573300	0.49358500
C	2.07982100	1.00362100	-0.44394900
O	2.87840100	1.61658000	-1.15532500
O	1.65897700	-2.29350600	1.17426900
C	-0.05853500	-1.14989900	0.03547200
H	-0.26369600	-0.39648300	-0.71260000
C	0.88073600	1.69671100	0.09153300
H	0.32762600	1.21236800	0.88460500
C	-1.03156300	-1.95482300	0.49665700
H	-0.73271700	-2.69698900	1.23203800
C	0.52803800	2.90831000	-0.36454700
H	1.14277000	3.32451100	-1.15783300
C	-2.43815600	-1.95701400	0.12507700
C	-3.28978100	-2.91060800	0.69320700
C	-3.00590700	-1.04347000	-0.78466100
C	-4.64324400	-2.97209600	0.38080300
H	-2.88122700	-3.62613100	1.39804900
C	-4.34531100	-1.08936700	-1.10357500
H	-2.38741100	-0.28354900	-1.24574200
C	-5.17894900	-2.05656100	-0.52429400
H	-5.26139500	-3.72811500	0.84397600
H	-4.77925900	-0.38473900	-1.80189200
C	-0.58823900	3.73810600	0.08137900
C	-0.79542900	4.97670700	-0.54330200
C	-1.46962100	3.36031000	1.10751600
C	-1.84055300	5.80850000	-0.16191400
H	-0.12317400	5.28404700	-1.33652500
C	-2.51229600	4.18983700	1.48816300
H	-1.33912800	2.41094000	1.61184700
C	-2.70336100	5.41786300	0.85579100
H	-1.98049500	6.76118900	-0.65868200
H	-3.18175700	3.88052600	2.28206200
H	-3.51970200	6.06343700	1.15694200
O	-6.48236000	-2.01624800	-0.90602400
C	-7.38185200	-2.97079600	-0.35623600
H	-7.44773300	-2.87343600	0.73124500
H	-8.35154600	-2.75314000	-0.79802600
H	-7.08495400	-3.99107800	-0.61560000



1aa-OMe-T_1

SCF Done: E(UB3LYP) = -1910.79798597 A.U.

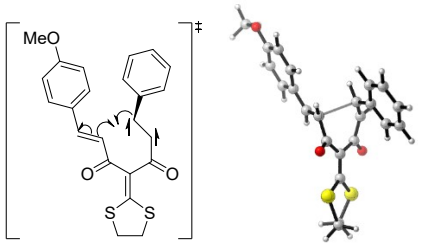
Zero-point correction= 0.367144 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.493822

C	6.26388100	-1.07886900	-0.80915600
C	6.10123000	-1.87013300	0.46405400
C	3.74247300	-0.71720500	-0.02469900
H	7.22710100	-0.56875300	-0.86285900
H	6.14665800	-1.70928900	-1.69221100
H	6.47764600	-1.32223100	1.32945900
H	6.59684000	-2.84119700	0.41620700
S	4.96542900	0.22626800	-0.86638100
S	4.30939500	-2.19788600	0.73454300
C	2.41823200	-0.31897900	0.02994900
C	1.41019400	-1.30357500	0.47392000
C	2.07490800	1.06048800	-0.37198500
O	2.86937100	1.75372800	-1.05329200
O	1.73614200	-2.28670500	1.14328900
C	0.01663300	-1.15736900	-0.00834300
H	-0.17090200	-0.45022800	-0.80564600
C	0.90122600	1.68138100	0.16808100
H	0.34614400	1.16669100	0.93889000
C	-0.96865500	-1.92321400	0.49482300
H	-0.68253200	-2.61656300	1.28123200
C	0.52988400	3.04152500	-0.20089200
H	1.25306400	3.57970600	-0.80029700
C	-2.37129000	-1.93951800	0.11231500
C	-3.24169900	-2.82449000	0.75896500
C	-2.91817600	-1.10735900	-0.88472100
C	-4.59316200	-2.89530800	0.44163900
H	-2.84876800	-3.47727400	1.53036600
C	-4.25540900	-1.16453400	-1.21061400
H	-2.28383300	-0.40530500	-1.41115600
C	-5.10796900	-2.06100400	-0.55035900
H	-5.22615800	-3.59619800	0.96705900
H	-4.67318400	-0.52412300	-1.97725700
C	-0.66405000	3.66220400	0.13649700
C	-0.91350100	5.01236300	-0.29781100

C	-1.70400700	3.02976100	0.90648500
C	-2.08175300	5.65828800	0.01162400
H	-0.14789700	5.51295200	-0.87901300
C	-2.87113600	3.69605500	1.20238500
H	-1.56948500	2.01516400	1.25630300
C	-3.07922900	5.01114500	0.76596900
H	-2.24089000	6.67564000	-0.32615400
H	-3.63856600	3.19676400	1.78230500
H	-3.99951000	5.52724400	1.00875700
O	-6.40722800	-2.03851800	-0.94637000
C	-7.32541400	-2.92650300	-0.32063800
H	-7.40015400	-2.72842000	0.75248600
H	-8.28762700	-2.73751000	-0.79097800

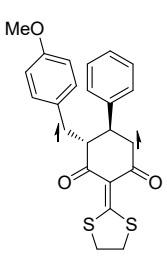
TS1a-1

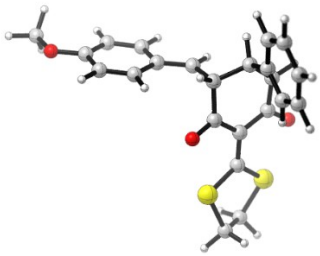


SCF Done: E(UB3LYP) = - -1910.78783466 A.U.
Zero-point correction= 0.367021 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -1910.479932

C	-5.06006700	-2.28643900	-1.21772200
C	-4.74447600	-3.20363600	-0.06261000
C	-2.82001200	-1.36435600	-0.09211400
H	-5.39958200	-2.83100300	-2.10011700
H	-5.81197800	-1.54313200	-0.94823800
H	-4.21702200	-4.10003200	-0.39264800
H	-5.63878400	-3.50071400	0.48751100
S	-3.52585800	-1.38982700	-1.69970100
S	-3.65938900	-2.30945500	1.12795700
C	-1.67354900	-0.64649000	0.19389600
C	-1.27662200	-0.45139600	1.60114900
C	-0.89385500	-0.06688400	-0.90975600
C	-0.34932500	0.59861200	1.95427300
C	0.54724300	0.23520200	-0.69121400
C	0.20141200	1.62852600	1.07648000
H	-0.09329400	0.61536500	3.01122900
O	-1.81584400	-1.10231500	2.51681000
O	-1.36901700	0.11506000	-2.02663300
C	1.40854800	-0.73514200	-0.22912000
H	0.97760300	-1.61268200	0.24254400
C	2.85025900	-0.69177600	-0.26296800

C	3.58634200	-1.74753500	0.30044500
C	3.58764000	0.36922400	-0.83463600
C	4.97401700	-1.76102100	0.30630700
H	3.05245500	-2.57892500	0.74718900
C	4.96529700	0.36818200	-0.83482900
H	3.06962200	1.20192500	-1.29358000
C	5.67540100	-0.69661200	-0.26340900
H	5.49406200	-2.59655400	0.75327800
H	5.52489000	1.18302400	-1.27710500
H	0.91363700	1.02486000	-1.33583200
O	7.03039300	-0.59957500	-0.31533700
C	7.80923000	-1.64885300	0.24553900
H	7.61663400	-2.59984200	-0.25948300
H	8.84714700	-1.36222500	0.09237300
H	7.61640900	-1.75697400	1.31681400
C	-0.54072400	2.78229700	0.62942100
C	-1.94564400	2.87755200	0.73028900
C	0.15046200	3.87039900	0.04990800
C	-2.61568200	4.00068400	0.27289800
H	-2.50657600	2.06652400	1.17666700
C	-0.52606400	4.98664300	-0.40789100
H	1.23137800	3.82493200	-0.02878900
C	-1.91556500	5.05992700	-0.30128700
H	-3.69432700	4.05236800	0.36354500
H	0.02733800	5.80772100	-0.84851900
H	-2.44512200	5.93363300	-0.66099000





INTa-1

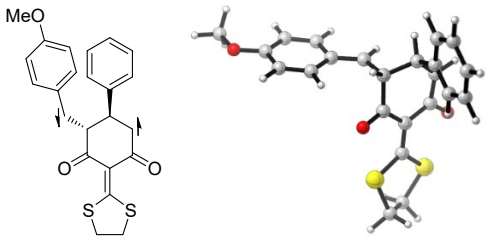
SCF Done: E(UB3LYP) = -1910.82545241A.U.

Zero-point correction= 0.370096 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.514500

C	-2.50383400	-4.21744100	-1.50780600
C	-2.61970500	-4.63604200	-0.06332600
C	-1.85577800	-2.08995400	-0.04166600
H	-2.05027000	-4.99053600	-2.12987600
H	-3.47282900	-3.94500600	-1.92911400
H	-1.72185200	-5.15192000	0.28080000
H	-3.48713000	-5.27298500	0.11661000
S	-1.40185500	-2.74415400	-1.60283700

S	-2.84489200	-3.12615300	0.96930900
C	-1.45174800	-0.83324200	0.37442700
C	-1.99232400	-0.26386400	1.61894100
C	-0.50694900	-0.06190800	-0.43591200
C	-1.68979900	1.10496500	1.92854300
C	0.13145700	1.18308300	0.20162700
C	-0.86074600	1.99843700	1.06955700
H	-2.17942300	1.51059400	2.80618700
O	-2.75720800	-0.91722000	2.35467100
O	-0.13911300	-0.42843500	-1.54537500
C	1.29544900	0.70120100	1.01875800
H	1.09536900	0.47714400	2.06193100
C	2.59874900	0.45839100	0.54272200
C	3.60732300	0.02415700	1.44265700
C	2.99178700	0.63048300	-0.81607900
C	4.90932900	-0.20472100	1.03822100
H	3.34562600	-0.12785600	2.48388600
C	4.28612800	0.40199200	-1.22002600
H	2.25567000	0.91852300	-1.55398700
C	5.26294300	-0.01315700	-0.30254400
H	5.63957000	-0.53169100	1.76545000
H	4.57527600	0.52959900	-2.25600800
H	0.47603100	1.80199700	-0.62750200
O	6.51125800	-0.20637300	-0.81081000
C	7.54323100	-0.63329800	0.06742900
H	7.31222200	-1.60720000	0.50916900
H	8.43849200	-0.71827000	-0.54463500
H	7.71589000	0.09719400	0.86342700
C	-1.72888400	2.95315500	0.24481700
C	-2.81537400	2.50049400	-0.50789600
C	-1.42246400	4.31514300	0.22068300
C	-3.56496100	3.38612600	-1.27443700
H	-3.08408300	1.45121800	-0.49798100
C	-2.17226200	5.20288400	-0.54341200
H	-0.58620700	4.68494700	0.80429900
C	-3.24666900	4.73992300	-1.29533700
H	-4.40254000	3.01615300	-1.85389200
H	-1.91702500	6.25608600	-0.54925600
H	-3.83344400	5.42917600	-1.89066700



INTa-1-OSS

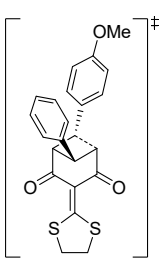
SCF Done: E(UB3LYP) = -1910.82639432 A.U.

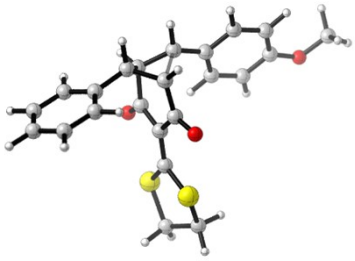
Zero-point correction= 0.370167 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.514185

C	-2.38319800	-4.26133100	-1.48582800
C	-2.49591700	-4.68389900	-0.04223500
C	-1.76937500	-2.12341400	-0.01789100
H	-1.92020500	-5.02807100	-2.10890700
H	-3.35487400	-3.99926800	-1.90743800
H	-1.59264900	-5.19046500	0.30149400
H	-3.35620400	-5.33128700	0.13488600
S	-1.29705100	-2.77668400	-1.57587700
S	-2.74068600	-3.17932200	0.99310500
C	-1.39800500	-0.85610200	0.39155600
C	-1.94145900	-0.29377100	1.63958400
C	-0.47886000	-0.06192000	-0.42178600
C	-1.67699900	1.08449600	1.93906000
C	0.10472400	1.22783800	0.18702300
C	-0.91739200	2.00723400	1.05326300
H	-2.14552300	1.46926300	2.83736000
O	-2.67496700	-0.96692500	2.38842200
O	-0.08781800	-0.43071800	-1.52264200
C	1.30037000	0.86574800	1.01769400
H	1.14098800	0.79402400	2.08882300
C	2.59387400	0.58189800	0.53776400
C	3.63507800	0.28715800	1.45650900
C	2.94397200	0.58483000	-0.84342600
C	4.92939000	0.02964300	1.04615900
H	3.40507400	0.26712000	2.51597400
C	4.23146400	0.33097800	-1.25287800
H	2.17882700	0.76018000	-1.58706500
C	5.24119600	0.05333600	-0.31868100
H	5.68639700	-0.18802900	1.78668500
H	4.49006700	0.33045400	-2.30462300
H	0.40540600	1.84045700	-0.66537900
O	6.47743000	-0.18257200	-0.83438500
C	7.54179300	-0.48314100	0.05835400
H	7.33898400	-1.39660400	0.62501800
H	8.41968700	-0.63315900	-0.56609100

H	7.72584400	0.34376500	0.75049500
C	-1.83718100	2.90681100	0.22069700
C	-2.92035000	2.39629800	-0.49861600
C	-1.58136900	4.27778100	0.15705400
C	-3.71575000	3.23482000	-1.27199800
H	-3.15130300	1.33896600	-0.45594500
C	-2.37718400	5.11846400	-0.61384300
H	-0.74911000	4.69219600	0.71599600
C	-3.44768000	4.59833100	-1.33302400
H	-4.55056300	2.82035400	-1.82475300
H	-2.16089300	6.17976700	-0.65005300
H	-4.07069600	5.25066700	-1.93311300
H	-0.33946100	2.68497400	1.69278200





TS2a-1

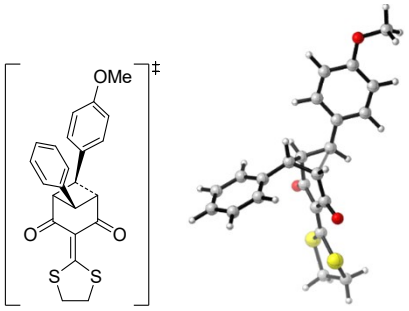
SCF Done: E(UB3LYP) = -1910.83906224 A.U.

Zero-point correction= 0.372071 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.522479

C	1.24851800	4.41199300	-0.59500100
C	0.52264500	4.37452100	0.73535600
C	0.86539100	1.84908300	0.03624000
H	0.84691300	5.18092100	-1.25701500
H	2.31685700	4.58183800	-0.45707500
H	-0.55882900	4.43353000	0.60738200
H	0.85192100	5.16599700	1.40997200
S	1.00627700	2.79551600	-1.44456300
S	0.94909100	2.77619700	1.53210200
C	0.67733000	0.46697700	0.05932100
C	0.46950700	-0.26686500	1.26729400
C	0.61301900	-0.32200600	-1.17010000
C	0.43402900	-1.71529700	1.19204900
C	0.37816200	-1.82990800	-1.00257900
C	1.32421600	-2.34678400	0.11884800
H	0.23445100	-2.22253700	2.13116700
O	0.40705900	0.24573600	2.43913600
O	0.71785400	0.16187500	-2.28926000
C	-0.89420200	-2.17194200	-0.22008400
H	-0.94444000	-3.23217500	0.01878800
C	-2.19315400	-1.55980500	-0.27901600

C	-3.25518500	-2.18000400	0.41896700
C	-2.49184500	-0.35125000	-0.95474700
C	-4.52554200	-1.64118300	0.46395700
H	-3.06326100	-3.10995600	0.94292600
C	-3.75814800	0.19031200	-0.92113100
H	-1.73453100	0.15062300	-1.53847400
C	-4.78750200	-0.43897800	-0.20804300
H	-5.30174300	-2.15381000	1.01432900
H	-3.98313700	1.10809300	-1.44972100
H	0.45775700	-2.29741100	-1.98766900
H	1.21896800	-3.43593800	0.17533800
C	2.80176700	-2.01997900	0.07465900
C	3.49859900	-2.07416500	-1.13429200
C	3.51033600	-1.72781100	1.24148600
C	4.86920200	-1.84210200	-1.17630700
H	2.96882700	-2.28759800	-2.05530200
C	4.88162900	-1.49883200	1.20152400
H	2.98826200	-1.66531300	2.18908400
C	5.56622300	-1.55541400	-0.00765400
H	5.39050200	-1.87970300	-2.12557700
H	5.41315500	-1.26806100	2.11727200
H	6.63335800	-1.37057300	-0.04007500
O	-5.99257500	0.18064500	-0.23449100
C	-7.08213700	-0.40633100	0.46887100
H	-6.86951600	-0.47702200	1.53906500



TS2a'-1

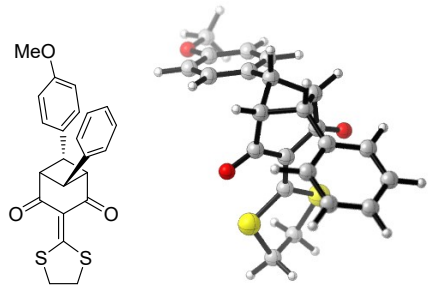
SCF Done: E(UB3LYP) = -1910.84215754 A.U.

Zero-point correction= 0.372048 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.525546

C	-5.17598700	-2.30081900	-0.74507100
C	-4.74645300	-2.95733800	0.55151200
C	-2.81305600	-1.26164700	-0.06642300
H	-5.60277700	-3.02084800	-1.44510100
H	-5.89963700	-1.50526300	-0.56447000
H	-4.21226100	-3.89138600	0.37352000
H	-5.58772100	-3.14277800	1.22070800
S	-3.68933500	-1.58119400	-1.56181500

S	-3.62863900	-1.77910300	1.40707100
C	-1.56259900	-0.64556700	-0.01877600
C	-0.82392100	-0.47700100	1.19651800
C	-0.88614500	-0.18989600	-1.23750500
C	0.42652300	0.26045000	1.14723200
C	0.50870900	0.41525900	-1.04103700
C	0.47824000	1.41526500	0.14561700
H	0.98289100	0.29760500	2.07921100
O	-1.21102900	-0.87833500	2.34808700
O	-1.35563500	-0.31320300	-2.35836900
C	1.39600100	-0.62419600	-0.33794500
H	1.01671800	-1.63822600	-0.29001900
C	2.83299600	-0.53813500	-0.30443400
C	3.57215400	-1.61114500	0.24426600
C	3.57616800	0.57427300	-0.77310300
C	4.95137800	-1.58433200	0.33916500
H	3.03763800	-2.48312100	0.60394900
C	4.94909500	0.60721300	-0.69053100
H	3.06488300	1.41152100	-1.23057500
C	5.65548700	-0.46718100	-0.12682700
H	5.47012700	-2.43037900	0.76763200
H	5.51131100	1.45438700	-1.06308500
H	0.87309000	0.77973200	-2.00364500
H	1.45931800	1.89035000	0.22594300
C	-0.57438200	2.50258800	0.19571400
C	-0.97313400	3.15862600	-0.97041100
C	-1.11712200	2.91600300	1.41408500
C	-1.89074600	4.20305000	-0.92044100
H	-0.57704300	2.84728100	-1.92993800
C	-2.03222000	3.96150700	1.46583800
H	-0.83437500	2.41038300	2.33015500
C	-2.42198800	4.60969200	0.29834000
H	-2.19436300	4.69411400	-1.83748400
H	-2.44723300	4.26396400	2.42014100
H	-3.13976400	5.42037100	0.33762100
O	7.00374800	-0.33042300	-0.08626000
C	7.78299200	-1.38324600	0.47171700
H	7.65633800	-2.31068800	-0.09343800
H	8.81708400	-1.05453600	0.40147100



2ac

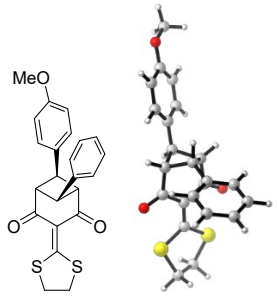
SCF Done: E(RB3LYP) = -1910.88074840 A.U.

Zero-point correction= 0.374336 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.562829

C	0.95571700	4.28714700	-0.68465300
C	0.18383200	4.29973800	0.61300100
C	0.53752800	1.74514600	-0.03035100
H	0.61428800	5.05897500	-1.37590200
H	2.02753800	4.40472400	-0.51887400
H	-0.88462300	4.44373300	0.44624300
H	0.54453900	5.06581700	1.30087600
S	0.67346100	2.66701300	-1.51247500
S	0.42457000	2.67670600	1.44787000
C	0.51991400	0.36744300	-0.02733800
C	0.46441000	-0.39918300	1.22040400
C	0.55280300	-0.40460700	-1.27282400
C	0.44249600	-1.90787200	1.04413700
C	0.53715300	-1.91203000	-1.09120000
C	1.55069000	-2.32959000	0.02216300
H	0.39655400	-2.39509900	2.01604400
O	0.45858200	0.11800000	2.32962800
O	0.56840000	0.10876500	-2.38348900
C	-0.58193400	-2.30409800	-0.06733100
H	-0.65509900	-3.39668300	-0.07208800
C	-1.96595100	-1.71142700	-0.12453600
C	-2.66885800	-1.40985100	1.03804400
C	-2.61326700	-1.51082000	-1.34956300
C	-3.97508200	-0.92481600	0.99823600
H	-2.19702000	-1.54223500	2.00489800
C	-3.90959200	-1.02956800	-1.40747200
H	-2.09285200	-1.72422700	-2.27626300
C	-4.60255200	-0.73422200	-0.23092000
H	-4.48072700	-0.69699300	1.92599300
H	-4.40403700	-0.86928300	-2.35745500
H	0.57086600	-2.40393500	-2.06119100
H	1.60199500	-3.42320400	0.02851300
C	2.95076900	-1.77442400	0.08170100

C	3.66716100	-1.51643700	-1.08918100
C	3.58282600	-1.56860700	1.31024400
C	4.98190700	-1.06612000	-1.03358300
H	3.19373900	-1.65810900	-2.05389000
C	4.89724000	-1.11836200	1.36744200
H	3.04201500	-1.75101400	2.23173900
C	5.60232500	-0.86675200	0.19507600
H	5.51974000	-0.86645300	-1.95301700
H	5.36852700	-0.95946500	2.33029200
H	6.62555100	-0.51296000	0.23869400
O	-5.87428900	-0.26249400	-0.38902900
C	-6.62324200	0.05406400	0.77457400
H	-6.14202300	0.84676800	1.35580000
H	-7.59093900	0.40351100	0.42073200



2ac'

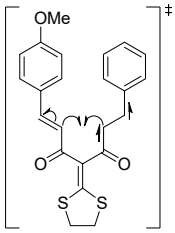
SCF Done: E(RB3LYP) = -1910.87982819 A.U.

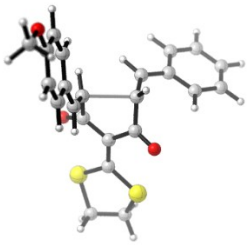
Zero-point correction= 0.374449 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.561995

C	-5.30676900	-1.87014700	-0.64773700
C	-4.95753000	-2.65237800	0.59584300
C	-2.78758200	-1.26203400	-0.06033200
H	-5.90485000	-2.45414700	-1.34868400
H	-5.83643000	-0.94678100	-0.40921200
H	-4.67206100	-3.67878700	0.36107200
H	-5.77481000	-2.66557800	1.31829200
S	-3.74466500	-1.42975800	-1.51664100
S	-3.53074900	-1.82981600	1.41980800
C	-1.52288000	-0.71411700	-0.07728900
C	-0.75266700	-0.51710100	1.15589200
C	-0.88435200	-0.29189800	-1.32878000
C	0.62044400	0.09008000	0.95106900
C	0.50516400	0.30244600	-1.16770400
C	0.52504400	1.33101800	0.00636100
H	1.14419900	0.17546900	1.90068900
O	-1.17409300	-0.80984400	2.26706600
O	-1.40152100	-0.43326200	-2.42845100
C	1.32461900	-0.65580300	-0.24428500

H	1.04580000	-1.70864800	-0.32952500
C	2.83193400	-0.54760700	-0.26293300
C	3.56633700	-1.31062100	0.64524900
C	3.54822700	0.26057500	-1.15028100
C	4.95639000	-1.27371300	0.68613000
H	3.04418100	-1.95653500	1.34369400
C	4.93367800	0.31028500	-1.12578200
H	3.02656800	0.86168100	-1.88450000
C	5.65014900	-0.45526700	-0.20594700
H	5.48015400	-1.88406700	1.40844600
H	5.48034200	0.93814400	-1.81832300
H	0.89419100	0.57979400	-2.14495400
H	1.50535100	1.81489300	0.00897500
C	-0.54021100	2.38499900	0.16738800
C	-1.11397600	2.99633500	-0.94957200
C	-0.92983500	2.81567500	1.43798400
C	-2.05009800	4.01454900	-0.80120400
H	-0.83522500	2.67122300	-1.94537700
C	-1.86596900	3.83297900	1.58791400
H	-0.50580100	2.34770800	2.31907900
C	-2.42872800	4.43734800	0.46842200
H	-2.48694100	4.47390600	-1.68020900
H	-2.15898000	4.15019900	2.58189900
H	-3.15991800	5.22847100	0.58487200
O	7.00847100	-0.33985700	-0.25823200
C	7.78600000	-1.10229900	0.65335800
H	7.62816900	-2.17580400	0.51146000
H	8.82373400	-0.85916700	0.43545400
H	7.56175300	-0.83489400	1.69052300





TS1b-1

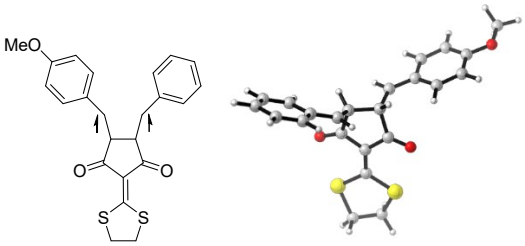
SCF Done: E(UB3LYP) = -1910.78585231 A.U.

Zero-point correction= 0.366065 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.480444

C	-4.55326400	-3.10363800	-0.71253600
C	-3.88028800	-4.00239300	0.30101600
C	-2.29658700	-1.89363000	-0.01850900
H	-5.01568900	-3.67080400	-1.52148100
H	-5.30388700	-2.46275800	-0.24855700

H	-3.31600200	-4.80252000	-0.17968800
H	-4.59415400	-4.43814300	1.00137700
S	-3.26009300	-2.04211400	-1.47535400
S	-2.72025000	-2.97509800	1.29334500
C	-1.27412100	-0.98563700	0.08658700
C	-0.96722500	0.00028800	-0.95701500
C	-0.38648900	-0.92866700	1.24597700
C	-0.21915300	1.18217600	-0.46038200
C	0.92923800	-0.23250300	1.00767500
H	0.49538300	1.59286400	-1.17325800
H	1.19457800	0.50368000	1.75880000
O	-0.64258400	-1.41838600	2.33729600
O	-1.28287300	-0.13108700	-2.13663300
C	1.91081300	-0.83147300	0.26713100
H	1.62130500	-1.65986300	-0.37460800
C	-0.83199400	2.09633900	0.51394200
H	-0.41334900	2.15813900	1.51497100
C	3.30664700	-0.45544700	0.19608700
C	4.16300500	-1.15704800	-0.66515600
C	3.87273800	0.59542000	0.94849000
C	5.51099100	-0.84376100	-0.78462700
H	3.75982800	-1.96955900	-1.25941300
C	5.20735200	0.91828700	0.83893000
H	3.25558800	1.16542500	1.63159300
C	6.04273500	0.20185200	-0.02952500
H	6.12966600	-1.41391500	-1.46308700
H	5.63685000	1.72544500	1.41913700
C	-1.92059200	2.95715600	0.23245400
C	-2.54187200	3.01932600	-1.04416400
C	-2.42613300	3.81220500	1.24949900
C	-3.59772500	3.88190600	-1.27458000
H	-2.18426600	2.37958500	-1.84132900
C	-3.48123100	4.66817100	1.00499300
H	-1.96943400	3.78106400	2.23258500
C	-4.07723600	4.71148500	-0.25867300
H	-4.05642300	3.91284500	-2.25616600
H	-3.84895800	5.30897600	1.79807600
H	-4.90510800	5.38384700	-0.44819600
O	7.34251800	0.59997800	-0.06150100
C	8.24283600	-0.08850000	-0.91989300
H	7.93935700	0.00011200	-1.96711100
H	9.20933700	0.39097300	-0.78224400



INTb-1

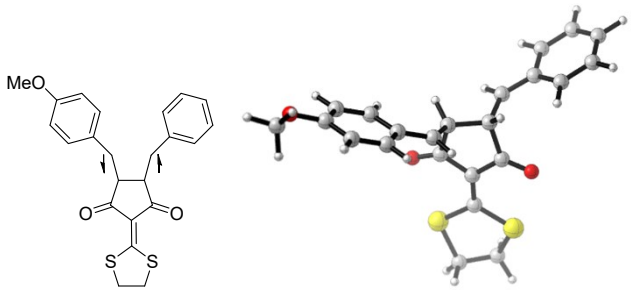
SCF Done: E(UB3LYP) = -1910.83538196 A.U.

Zero-point correction= 0.369111 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.526444

C	-2.78610000	-4.75084300	-0.20054900
C	-1.37858100	-5.17757200	0.15457400
C	-1.34785600	-2.53088800	-0.01145600
H	-3.24148200	-5.41554800	-0.93556200
H	-3.42715900	-4.69808200	0.68016200
H	-0.81392500	-5.48190700	-0.72743400
H	-1.36928400	-5.98887600	0.88337100
S	-2.70985500	-3.07790500	-0.96179600
S	-0.51678600	-3.74864800	0.92896000
C	-0.95300500	-1.21794100	-0.00296200
C	-1.60437200	-0.14344000	-0.74011400
C	0.17419800	-0.68619600	0.75270300
C	-0.97368300	1.20246100	-0.28646700
C	0.38734300	0.78972900	0.32373400
H	-0.85142800	1.83711500	-1.16724300
H	0.63179300	1.37586400	1.21307300
O	0.85077600	-1.28455500	1.56885900
O	-2.49635000	-0.25718800	-1.55977400
C	1.50029300	0.84633700	-0.67659200
H	1.21421400	0.84929900	-1.72342900
C	-1.87555900	1.85135300	0.71589500
H	-1.64726600	1.67372200	1.76205700
C	2.87700200	0.85266200	-0.37959500
C	3.82749200	0.95611900	-1.42861000
C	3.39775100	0.77553300	0.94412900
C	5.18853000	0.99962000	-1.18890300
H	3.47137300	1.00965300	-2.45148000
C	4.75098100	0.81752800	1.18409500
H	2.72035700	0.64914600	1.77748800
C	5.66436800	0.93419900	0.12580900
H	5.87023400	1.08420800	-2.02382600
H	5.13865300	0.75206800	2.19332900
C	-3.01018900	2.63785500	0.42627600
C	-3.47086700	2.88854200	-0.89454600
C	-3.74005200	3.23156200	1.49362900

C	-4.57515600	3.68973100	-1.11949600
H	-2.97121900	2.42103600	-1.73202900
C	-4.84010400	4.02989400	1.25469400
H	-3.41321700	3.05117600	2.51182200
C	-5.26710300	4.26964800	-0.05454500
H	-4.91042900	3.86141300	-2.13584000
H	-5.37494100	4.47209500	2.08729800
H	-6.13118600	4.89571200	-0.24082400
O	6.97961900	0.96932200	0.47755300
C	7.95427900	1.08574400	-0.54929800
H	7.82862000	2.01463500	-1.11359700
H	8.91797200	1.09781200	-0.04478400
H	7.91456100	0.23384400	-1.23470100



INTb-1-OSS

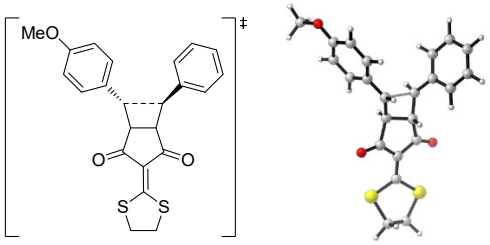
SCF Done: E(UB3LYP) = -1910.83707966 A.U.

Zero-point correction= 0.369148 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.527658

C	3.12527600	4.67514200	-0.20118600
C	1.74780500	5.19032800	0.15500900
C	1.54776100	2.55116000	-0.01331700
H	3.62209800	5.31057300	-0.93527200
H	3.76162400	4.58054300	0.67944500
H	1.20300300	5.52919000	-0.72689600
H	1.79057000	6.00122700	0.88312000
S	2.94127200	3.01208600	-0.96546000
S	0.79925900	3.81943900	0.93171800
C	1.06864400	1.26750800	-0.00678300
C	1.63900000	0.15660300	-0.75831600
C	-0.08248200	0.80647600	0.75962800
C	0.92929700	-1.14863500	-0.30228200
C	-0.39923300	-0.64939700	0.32434900
H	0.75744100	-1.77424800	-1.18079200
H	-0.67432800	-1.22478500	1.21178700
O	-0.71246400	1.43991600	1.58609300
O	2.52743300	0.21325300	-1.58730100
C	-1.50872800	-0.62674600	-0.66976200
H	-1.22510800	-0.53599900	-1.71355100

C	1.78552400	-1.84605600	0.69627100
H	1.66635400	-1.54410100	1.73225300
C	-2.88645300	-0.66000600	-0.37198800
C	-3.83788000	-0.68655700	-1.42371400
C	-3.40465100	-0.67422500	0.95392200
C	-5.19892900	-0.74199500	-1.18575700
H	-3.48319900	-0.66919100	-2.44830200
C	-4.75761600	-0.72865300	1.19334500
H	-2.72638400	-0.61003500	1.79384400
C	-5.67273800	-0.76761900	0.13097100
H	-5.88192700	-0.76470900	-2.02351400
H	-5.14358300	-0.73171900	2.20529200
C	2.76728700	-2.82207200	0.41633400
C	3.10201900	-3.23895800	-0.89950600
C	3.46672300	-3.43806800	1.49039600
C	4.05858000	-4.21454600	-1.11315200
H	2.62380000	-2.76912200	-1.74839000
C	4.41876800	-4.41156500	1.26386000
H	3.23565700	-3.13310300	2.50511800
C	4.72238300	-4.81182200	-0.04023100
H	4.29961800	-4.51137000	-2.12736200
H	4.93309300	-4.86620600	2.10263600
H	5.47060300	-5.57474300	-0.21730900
O	-6.98699300	-0.82203200	0.48160800
C	-7.96481800	-0.85753800	-0.54855300
H	-7.84605100	-1.74339100	-1.17953200
H	-8.92725600	-0.90096300	-0.04344700
H	-7.92156700	0.04210200	-1.16968000



TS2b-1

SCF Done: E(UB3LYP) = -1910.80688136 A.U.

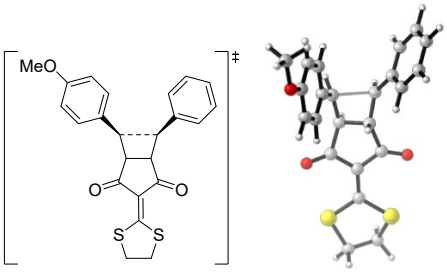
Zero-point correction= 0.370989 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.492478

C	6.14365700	-1.49155500	0.85764700
C	6.56708900	-0.59463500	-0.29452200
C	3.89565300	-0.59219100	-0.13574300
H	6.81168700	-2.34538100	0.97894500
H	6.08513600	-0.93853000	1.79579400
H	6.86392800	-1.18579700	-1.16106400
H	7.39149800	0.06227400	-0.01152900

S	4.47775900	-2.14202800	0.44667100
S	5.15051700	0.48415800	-0.77365900
C	2.53130200	-0.20275000	-0.04805700
C	1.51695500	-0.98292800	0.58012900
C	1.97970400	0.99054200	-0.68168100
C	0.15203900	-0.36210400	0.06271000
C	0.54287600	1.09428200	-0.11768400
H	0.02134300	-0.81362300	-0.92468600
H	0.69173200	1.52839800	0.87620900
O	2.52176200	1.79786700	-1.41650100
O	1.55181400	-2.02508700	1.23420900
C	-0.82978900	1.47630700	-0.57878600
H	-1.14519800	1.03219000	-1.51764900
C	-1.19608200	-0.08460100	0.63534100
H	-1.19357000	0.46934200	1.56970300
C	-1.53662700	2.70395100	-0.22694300
C	-1.01107900	3.65844900	0.65876200
C	-2.80249300	2.94369100	-0.79036700
C	-1.72397100	4.80924900	0.96236800
H	-0.03060700	3.51317400	1.09423700
C	-3.51464300	4.09180000	-0.48101700
H	-3.22025900	2.21877700	-1.47983200
C	-2.97852200	5.02923600	0.39894700
H	-1.29693500	5.54207600	1.63634800
H	-4.48629600	4.26121100	-0.92930800
H	-3.53216900	5.92880700	0.63932700
C	-2.39455600	-0.87261800	0.41655500
C	-3.57085900	-0.55615800	1.12833700
C	-2.45357900	-1.94401900	-0.48709800
C	-4.73619400	-1.26698900	0.94607000
H	-3.55424100	0.26387200	1.83719900
C	-3.61792800	-2.67323400	-0.67502900
H	-1.57028600	-2.23339600	-1.04221600
C	-4.77163500	-2.33619700	0.04024000
H	-5.63580400	-1.02440100	1.49732200
H	-3.61614300	-3.50149100	-1.36924000
O	-5.95911800	-2.97831500	-0.06826600
C	-6.06193200	-4.08682700	-0.95724800
H	-7.08719100	-4.43855400	-0.87213300

TS2b'-1



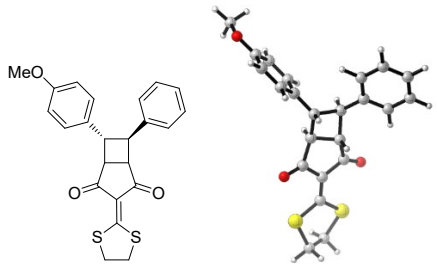
SCF Done: E(UB3LYP) = -1910.80187820 A.U.

Zero-point correction= 0.371008 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.487380

C	-6.25103300	-1.19886300	-0.48510100
C	-6.31942100	0.31599300	-0.59585100
C	-3.79031500	-0.20012700	-0.16234500
H	-7.05096800	-1.59400800	0.14359800
H	-6.30780800	-1.66487700	-1.46896700
H	-6.51225700	0.78018900	0.37194800
H	-7.07570200	0.63990300	-1.31217100
S	-4.65420600	-1.67573000	0.30281300
S	-4.68864500	0.88135100	-1.21615000
C	-2.47667800	0.08903200	0.29269200
C	-1.63340800	-0.85916300	1.01866700
C	-1.79010300	1.30464200	0.03256900
C	-0.44248500	-0.01669900	1.51591200
C	-0.26621700	1.00296200	0.40218800
H	-0.83871200	0.49845300	2.39571800
H	0.11248100	0.49573700	-0.48735600
O	-2.11443100	2.35641000	-0.52240000
O	-1.84113200	-2.03551900	1.26494100
C	0.86005400	1.74303200	1.03011100
H	0.62306700	2.21986000	1.97749100
C	1.05202800	-0.12587700	1.72836700
C	1.96793200	2.37132000	0.32120100
C	2.82098700	3.24052600	1.02424800
C	2.23342000	2.13877200	-1.03782200
C	3.89061000	3.85789700	0.39554300
H	2.62655700	3.43743900	2.07305900
C	3.30163400	2.76164700	-1.66712000
H	1.59476700	1.48014700	-1.61166500
C	4.13476800	3.62058100	-0.95544800
H	4.53032300	4.53099300	0.95367200
H	3.48351000	2.57960900	-2.71946100
C	1.95262300	-0.96226600	0.94881200
C	3.33328300	-0.89254900	1.18582600
C	1.50269900	-1.86681900	-0.03249500

C	4.23752300	-1.67125400	0.48104900
H	3.70799700	-0.20898000	1.93938600
C	2.39210300	-2.65009100	-0.73857600
H	0.44230600	-1.99039300	-0.20924000
C	3.76812900	-2.55669600	-0.49406200
H	5.29310800	-1.58515100	0.69567000
H	2.04424600	-3.35904300	-1.47910200
H	1.39563200	0.07035700	2.73987300
H	4.96651900	4.10617300	-1.45152900
O	4.55732300	-3.36616000	-1.24219100
C	5.96504500	-3.33522600	-1.03361300
H	6.38267300	-4.05738100	-1.73108800



3ac

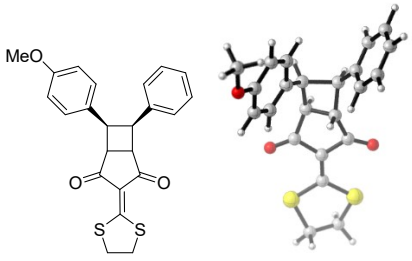
SCF Done: E(UB3LYP) = -1910.84491666 A.U.

Zero-point correction= 0.373285 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.529587

C	6.19025100	-1.61815100	0.61835000
C	6.33056600	-1.00278100	-0.75631500
C	3.80103900	-0.63446900	-0.01611700
H	6.72993300	-2.56246500	0.69981500
H	6.53571300	-0.94084900	1.40008600
H	6.25169900	-1.75297500	-1.54387700
H	7.27286100	-0.46503500	-0.86857200
S	4.41411300	-1.98586300	0.91981000
S	4.98087700	0.22349700	-0.99149300
C	2.48430500	-0.27132700	0.01244700
C	1.41609200	-1.03030200	0.73595500
C	1.93011900	0.93826700	-0.66726100
C	0.14871000	-0.40538200	0.17466000
C	0.54729400	1.04524100	-0.05026800
H	0.04054100	-0.86926500	-0.81594000
H	0.73222600	1.48465800	0.94101700
O	2.51156600	1.66405100	-1.44777400
O	1.58024400	-1.95027600	1.50868900
C	-0.94227500	1.34831900	-0.37241500
H	-1.16870100	1.07213700	-1.40691800
C	-1.27516200	0.10063900	0.56821700
H	-1.27173500	0.45129100	1.60278600

C	-1.50230500	2.70877200	-0.06060500
C	-0.71277200	3.84894300	-0.22696300
C	-2.82241900	2.86601100	0.36913200
C	-1.22907400	5.11496100	0.02905300
H	0.31242200	3.74469800	-0.56608300
C	-3.33862000	4.13149200	0.62797400
H	-3.45267400	1.99431800	0.50159900
C	-2.54402000	5.26075400	0.45857900
H	-0.60137600	5.98802200	-0.10641100
H	-4.36399500	4.23428300	0.96379200
H	-2.94592100	6.24633600	0.66151000
C	-2.48181600	-0.76178400	0.32887300
C	-3.28206700	-1.16431900	1.40481800
C	-2.84526100	-1.20507400	-0.94105800
C	-4.39150700	-1.97182200	1.22288400
H	-3.02611800	-0.83998600	2.40765300
C	-3.95792700	-2.01746200	-1.14588300
H	-2.25923100	-0.91677200	-1.80669600
C	-4.73917300	-2.40576800	-0.05791300
H	-5.00377800	-2.27984800	2.06127300
H	-4.20212700	-2.33493400	-2.14989000
O	-5.84867700	-3.19494600	-0.14092200
C	-6.24358000	-3.67267700	-1.41853100
H	-7.13337600	-4.27523800	-1.24909100
H	-6.48851600	-2.84809400	-2.09506700



3ad

SCF Done: E(UB3LYP) = -1910.83872257 A.U.

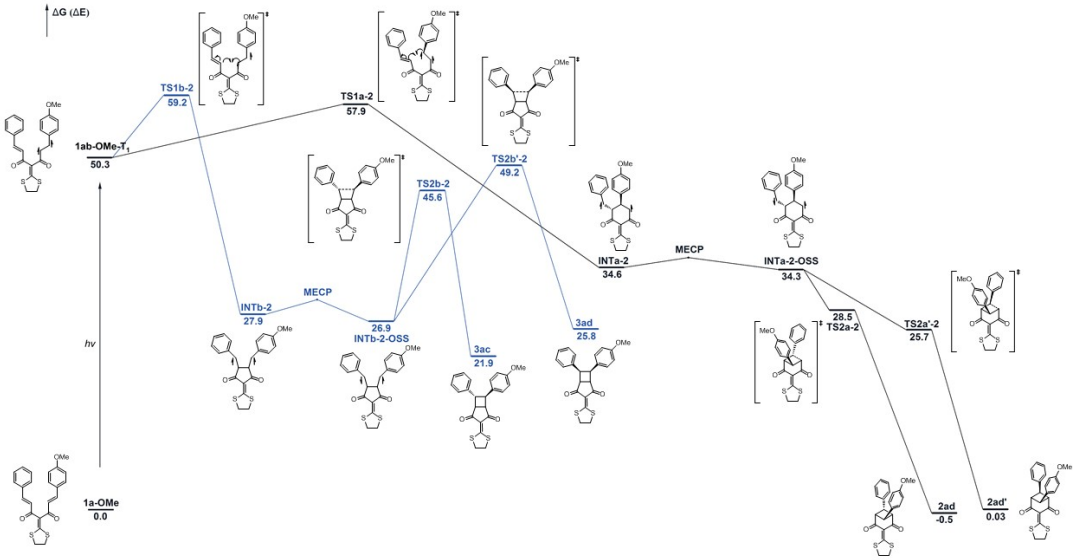
Zero-point correction= 0.373627 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.522464

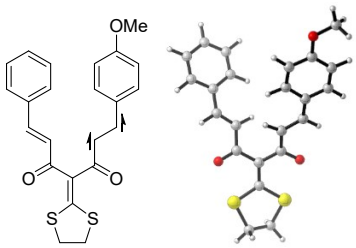
C	-6.02870000	-1.37812200	-0.84579500
C	-6.36418200	0.08846900	-0.69238600
C	-3.78707400	-0.16376400	-0.08440900
H	-6.82222800	-2.02126900	-0.46322700
H	-5.82722000	-1.63948900	-1.88519400
H	-6.82471400	0.29758200	0.27375500
H	-7.02339100	0.44205300	-1.48619000
S	-4.52027600	-1.74135500	0.14176800
S	-4.80932700	1.06282900	-0.81087000

C	-2.49680700	0.09679200	0.28387500
C	-1.62255600	-0.86947000	1.01220800
C	-1.79109500	1.38584300	0.01557100
C	-0.46422500	0.01571600	1.45489700
C	-0.34835600	1.03650500	0.33346600
H	-0.89094200	0.54279800	2.32027800
H	0.00181400	0.48932000	-0.55102600
O	-2.28865800	2.40586700	-0.41424100
O	-1.87244800	-2.03560400	1.23989900
C	0.90477900	1.61071700	1.03660800
H	0.59854400	2.24832500	1.86882200
C	1.08302500	0.11254700	1.66191900
C	2.00180000	2.29612400	0.27717700
C	2.77749200	3.26177300	0.92711500
C	2.29515300	2.00773400	-1.05771600
C	3.81455100	3.91461700	0.27133100
H	2.55869800	3.51087200	1.96035400
C	3.32806000	2.66232300	-1.71988800
H	1.71495700	1.26790600	-1.59459500
C	4.09371900	3.61622600	-1.05837600
H	4.39780500	4.66267000	0.79560700
H	3.53338300	2.42602200	-2.75738800
C	1.99132900	-0.83570900	0.92533900
C	3.37128000	-0.62996400	0.95909400
C	1.52349900	-1.95945200	0.23555200
C	4.25983200	-1.48976400	0.32158200
H	3.77235800	0.22445900	1.49210600
C	2.39474600	-2.82486800	-0.40826900
H	0.46621600	-2.18908400	0.22310700
C	3.76982300	-2.59487000	-0.37442900
H	5.32025800	-1.28680400	0.37463900
H	2.02435500	-3.69599800	-0.93423000
H	1.37071700	0.14853100	2.71367100
H	4.89620600	4.12786000	-1.57640900
O	4.54657400	-3.50116500	-1.03779300
C	5.95447200	-3.32143700	-1.02156000
H	6.36689000	-4.14456600	-1.60138500
H	6.24189500	-2.37259800	-1.48509800

5.2.3 Computational analysis of 1a-OMe’



5.2.4 Cartesian coordinates and energies of all optimized structures



1ab-OMe-T_1

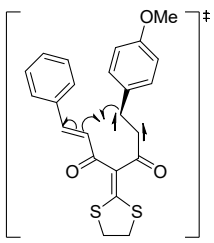
SCF Done: E(UB3LYP) = -1910.79978774 A.U.

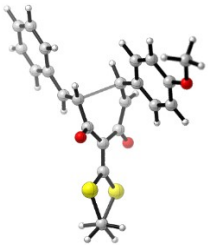
Zero-point correction= 0.367504 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.494488

C	6.06470500	-1.81534800	0.56727800
C	6.26450400	-1.09294500	-0.74111000
C	3.70659400	-0.74039400	-0.05589100
H	6.59075100	-2.77092600	0.60010000
H	6.38258400	-1.20616500	1.41513300
H	6.20810500	-1.77606200	-1.59023800
H	7.21405000	-0.55645600	-0.77968800
S	4.27207900	-2.18582100	0.77251600
S	4.93256100	0.16412600	-0.93401500
C	2.38171300	-0.34113400	-0.01421100
C	2.05581900	1.02791200	-0.45675300
C	1.36787100	-1.29255800	0.48770300
O	1.70454000	-2.29354000	1.16892300
O	2.81632400	1.65750900	-1.19529400
C	0.85421700	1.69291000	0.10986800
H	0.36774200	1.22146400	0.95374100
C	0.00675200	-1.17277700	0.05607800
H	-0.23948400	-0.43306800	-0.69180500

C	0.42303800	2.86596700	-0.38122900
H	0.97795500	3.26930200	-1.22381200
C	-1.01181800	-2.08852200	0.52154900
H	-0.68000700	-2.84921700	1.21650000
C	-0.70409100	3.66834900	0.08490300
C	-0.99584200	4.86777400	-0.58180100
C	-1.51639500	3.30324000	1.17126000
C	-2.05442600	5.67355700	-0.18296400
H	-0.37786400	5.16568400	-1.42136900
C	-2.57264000	4.10707900	1.56941100
H	-1.32001300	2.38432400	1.70958400
C	-2.84752900	5.29613900	0.89491000
H	-2.25908800	6.59639500	-0.71260500
H	-3.18694000	3.80813400	2.41055300
H	-3.67380100	5.92196300	1.21033100
C	-2.34718900	-2.05284300	0.15029300
C	-3.26938000	-3.01864000	0.69113100
C	-2.91004500	-1.08785000	-0.76414700
C	-4.60020900	-3.02578900	0.36311700
H	-2.88525000	-3.76185600	1.37964700
C	-4.23831200	-1.09919700	-1.08489800
H	-2.27345000	-0.33443900	-1.20724500
C	-5.10919400	-2.06223400	-0.53286500
H	-5.24968200	-3.77401400	0.79640100
H	-4.65265300	-0.37017900	-1.77050500
O	-6.40303000	-1.97840600	-0.92355700
C	-7.34281600	-2.91811900	-0.41063500
H	-7.41991900	-2.84486900	0.67735800
H	-8.29735100	-2.65568300	-0.86029800
H	-7.07455100	-3.93916800	-0.69434800





TS1a-2

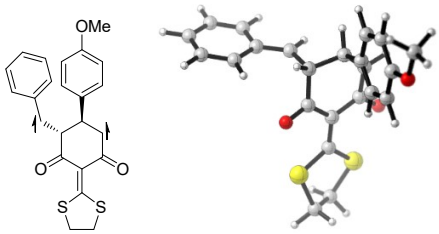
SCF Done: E(UB3LYP) = -1910.78758543 A.U.

Zero-point correction= 0.367052 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.479882

C	-4.08419400	-3.16189700	-1.28792300
C	-3.66656900	-4.12346500	-0.20350400
C	-1.91721100	-2.11913400	-0.12359200
H	-4.38676200	-3.67348200	-2.20288300

H	-4.89627800	-2.51137000	-0.95956300
H	-3.06385200	-4.94147000	-0.60128900
H	-4.52051300	-4.54009600	0.33300700
S	-2.64670100	-2.09634500	-1.72090000
S	-2.64923400	-3.21668100	1.03647300
C	-0.83237500	-1.32526900	0.19849500
C	-0.42622400	-1.19553900	1.61047400
C	-0.12353300	-0.60470800	-0.87036500
C	0.42472700	-0.10185600	2.02049600
C	1.29631700	-0.21464100	-0.65200500
C	0.87346000	1.02284300	1.20233500
H	0.70022800	-0.13319700	3.07214600
O	-0.89724400	-1.94541300	2.48676000
O	-0.63685400	-0.37214000	-1.96039000
C	2.23384100	-1.15038700	-0.27385600
H	1.87837500	-2.09066900	0.13509400
C	3.67064600	-0.99530800	-0.32045400
C	4.48682300	-2.04287600	0.15044200
C	4.31119800	0.16066300	-0.81067000
C	5.86898300	-1.94245900	0.13440800
H	4.01652100	-2.94211600	0.53264900
C	5.69335800	0.25794100	-0.82452500
H	3.72132300	0.98440200	-1.19294500
C	6.48205400	-0.79040700	-0.35266300
H	6.47221800	-2.76378200	0.50299100
H	6.16297000	1.15585600	-1.20908600
H	1.59308200	0.64203800	-1.24461500
C	0.03321900	2.14153600	0.85912700
C	-1.37580300	2.12109400	0.98991000
C	0.61135200	3.32280200	0.35240300
C	-2.14394800	3.20765100	0.63459900
H	-1.86443700	1.23918300	1.38358700
C	-0.15410000	4.41836700	-0.01187200
H	1.68951100	3.37797400	0.24810200
C	-1.54488100	4.36709400	0.12540900
H	-3.22146300	3.18668700	0.73966000
H	0.33546600	5.30232500	-0.39594800
H	1.92748800	1.26403500	1.30494200
H	7.56218900	-0.70980800	-0.36667100
O	-2.39239300	5.37940400	-0.20036100
C	-1.84663200	6.57873700	-0.73356900
H	-1.31326500	6.39023200	-1.66979500
H	-2.69541500	7.23094500	-0.92646300



INTa-2

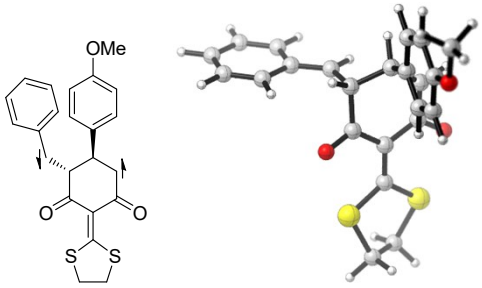
SCF Done: E(UB3LYP) = -1910.82478590 A.U.

Zero-point correction= 0.370094 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.513473

C	3.30031700	-3.65874000	-1.66930000
C	3.78875600	-3.92460900	-0.26715500
C	1.90263200	-2.05803700	-0.06244700
H	4.11398800	-3.63548900	-2.39577900
H	2.56097300	-4.39581500	-1.98655800
H	4.70162600	-3.36964300	-0.04495000
H	3.96394100	-4.98568800	-0.08302900
S	2.50685500	-1.99722000	-1.70705400
S	2.48639100	-3.38721900	0.92123700
C	1.01935200	-1.11487200	0.43305100
C	0.42241600	-1.29478200	1.76685900
C	0.65974400	0.04825200	-0.37637200
C	-0.62043700	-0.39728400	2.17512100
C	-0.12879700	1.19031000	0.29620600
C	-1.17573400	0.69026700	1.32416900
H	-1.07437400	-0.60801600	3.13635600
O	0.75547500	-2.24190300	2.50433100
O	1.03492300	0.18549500	-1.53397500
C	0.85419200	2.10661700	0.96192500
H	1.03285200	1.93879800	2.01946300
C	1.58812900	3.13888000	0.33920400
C	2.45407000	3.94884100	1.12571300
C	1.50516300	3.43190800	-1.04904200
C	3.17210700	4.98616600	0.56623200
H	2.54175400	3.74032300	2.18631500
C	2.23074300	4.47414900	-1.59614200
H	0.89098600	2.81412500	-1.68974700
C	3.06533100	5.26079800	-0.80002800
H	3.82234800	5.58856400	1.18992100
H	2.15451400	4.67576500	-2.65834900
H	-0.63866500	1.70865000	-0.51733000
C	-2.50389300	0.27654100	0.68488100
C	-2.63042400	-0.88324000	-0.09102300
C	-3.63498900	1.06758200	0.85753400
C	-3.83463700	-1.22203800	-0.68075700

H	-1.77880800	-1.53614000	-0.23913000
C	-4.85759100	0.73973200	0.27352100
H	-3.57093100	1.96823900	1.45878800
C	-4.96031300	-0.41247400	-0.50323400
H	-3.92820600	-2.11702600	-1.28299000
H	-5.70948200	1.38572500	0.43272700
H	-1.41233100	1.53815700	1.97725400
H	3.63038800	6.07415900	-1.23876200
O	-6.09957100	-0.83310300	-1.12208600
C	-7.27519300	-0.04920100	-0.97819800
H	-7.13534800	0.95694300	-1.38502600
H	-8.04725700	-0.56342300	-1.54637100
H	-7.58218500	0.02029600	0.06980700



INTa-2-OSS

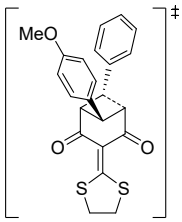
SCF Done: E(UB3LYP) = -1910.82529479 A.U.

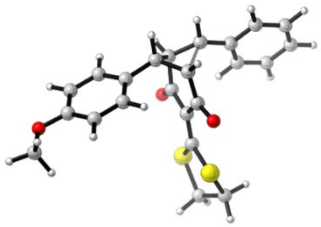
Zero-point correction= 0.370094 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.513473

C	-3.34628900	3.62622200	-1.67565300
C	-3.84520600	3.87322500	-0.27375700
C	-1.92361900	2.04591800	-0.07195500
H	-4.15671300	3.58912800	-2.40514900
H	-2.62218700	4.38107200	-1.98631100
H	-4.74596000	3.29647600	-0.05757600
H	-4.04476300	4.92897700	-0.08399000
S	-2.51524300	1.98301500	-1.72008700
S	-2.53491700	3.35783100	0.91616800
C	-1.02869600	1.11318800	0.42496900
C	-0.43517300	1.30463900	1.75837100
C	-0.65195000	-0.04332900	-0.38787200
C	0.62209200	0.42456300	2.16579900
C	0.13205400	-1.17958300	0.29522400
C	1.17680600	-0.67205400	1.32160400
H	1.09045700	0.65561400	3.11534400
O	-0.78161500	2.24967300	2.49334700
O	-1.01396200	-0.17793900	-1.55003600
C	-0.87832900	-2.07325500	0.95260000
H	-1.12207200	-1.84957400	1.98675900

C	-1.57183900	-3.13873200	0.34073000
C	-2.47628400	-3.91730500	1.11613600
C	-1.41711400	-3.49331300	-1.02704400
C	-3.16188500	-4.98159000	0.56686200
H	-2.61954800	-3.66239900	2.16042200
C	-2.11259500	-4.56061700	-1.56477300
H	-0.77128700	-2.90341700	-1.66289700
C	-2.98532600	-5.31557500	-0.77888000
H	-3.84193600	-5.55875700	1.18263600
H	-1.98189200	-4.80752900	-2.61203100
H	0.64527500	-1.70934400	-0.50779700
C	2.50428100	-0.25540000	0.68518200
C	2.62666000	0.89970600	-0.09867400
C	3.64058800	-1.03678100	0.86965400
C	3.83153000	1.24347900	-0.68406900
H	1.77085900	1.54484000	-0.25652400
C	4.86374700	-0.70395900	0.29027400
H	3.57971300	-1.93373800	1.47676100
C	4.96220700	0.44373700	-0.49406100
H	3.92180500	2.13448100	-1.29266400
H	5.71957900	-1.34238200	0.45851700
H	1.41336400	-1.51428800	1.98050800
H	-3.52571400	-6.14957300	-1.20980700
O	6.10166200	0.86823400	-1.10936000
C	7.28306500	0.09561000	-0.95142200
H	7.15478900	-0.91466800	-1.35168900
H	8.05454300	0.61234800	-1.51808200





TS2a-2

SCF Done: E(UB3LYP) = -1910.83456537 A.U.

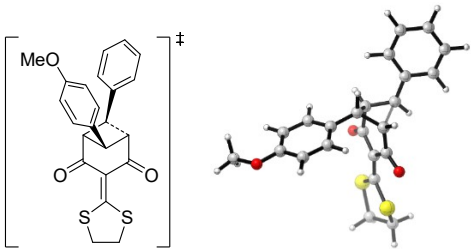
Zero-point correction= 0.372129 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.517884

C	-0.67577500	4.44843900	-0.68733900
C	-1.29124300	4.27755000	0.68858400
C	-0.46571400	1.87490600	-0.01388700
H	-1.28737200	5.08525400	-1.32832900
H	0.32842500	4.86810600	-0.62177800
H	-2.36269600	4.08314100	0.63322300
H	-1.10954900	5.13726800	1.33458300

S	-0.58013600	2.79870200	-1.50795200
S	-0.46042300	2.83368600	1.46292100
C	-0.42505100	0.48739700	0.04756100
C	-0.46987300	-0.22549100	1.28473300
C	-0.41385000	-0.34223500	-1.16056600
C	-0.28899600	-1.65626200	1.25882800
C	-0.43613200	-1.85807300	-0.93989600
C	0.61953900	-2.19896600	0.15441500
H	-0.36494100	-2.15577100	2.21974700
O	-0.57346400	0.33525600	2.43763200
O	-0.40321800	0.12528100	-2.28956900
C	-1.61732700	-2.34554000	-0.09725900
H	-1.50594800	-3.39090500	0.18088500
C	-2.99565000	-1.92138100	-0.12043700
C	-3.92776300	-2.65487700	0.65212800
C	-3.47914900	-0.80773800	-0.83958500
C	-5.25917600	-2.29200000	0.71256500
H	-3.58096600	-3.51833300	1.20955300
C	-4.81895700	-0.45323200	-0.78008400
H	-2.81782700	-0.23461600	-1.47294900
C	-5.71531500	-1.18335800	-0.00388600
H	-5.94946500	-2.87144400	1.31412900
H	-5.16829700	0.39895400	-1.35108200
H	-0.32543200	-2.34325800	-1.91341200
H	0.65711500	-3.28976800	0.24774500
C	2.03723300	-1.68598400	0.02024300
C	2.73283200	-1.85167100	-1.18388300
C	2.71565000	-1.10438500	1.08595700
C	4.04943100	-1.44834100	-1.31579700
H	2.23629500	-2.29626500	-2.03895400
C	4.04406000	-0.69571300	0.97199600
H	2.20906000	-0.95052900	2.03133400
C	4.71745800	-0.86680700	-0.23498600
H	4.58014700	-1.56974300	-2.25180900
H	4.53027900	-0.24385900	1.82510500
H	-6.75948600	-0.89814100	0.03861600
O	6.01247200	-0.50050900	-0.46156100
C	6.73604800	0.10465000	0.59942800
H	6.82109100	-0.56744300	1.45897800

TS2a'-2



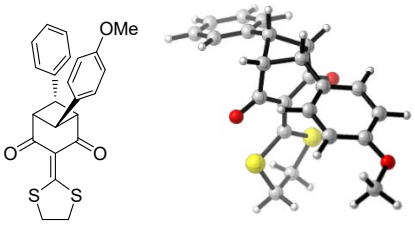
SCF Done: E(UB3LYP) = -1910.83891983 A.U.

Zero-point correction= 0.371941 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.522420

C	-3.49209600	-3.81481500	-0.81069000
C	-2.91881400	-4.34227200	0.48966400
C	-1.49431100	-2.19571200	-0.09512500
H	-3.69474600	-4.61792800	-1.52086500
H	-4.40898200	-3.25023600	-0.63883300
H	-2.14844000	-5.09466900	0.31788700
H	-3.68768600	-4.75241500	1.14554800
S	-2.24793400	-2.70676700	-1.60148300
S	-2.17353700	-2.90973400	1.36424600
C	-0.43436600	-1.29913600	-0.01975400
C	0.23303800	-0.99357700	1.21069000
C	0.12644000	-0.66527500	-1.22078700
C	1.26038900	0.02276700	1.20351700
C	1.33609200	0.24393800	-0.98854900
C	1.05352100	1.17687000	0.21997000
H	1.78198500	0.17330700	2.14402600
O	-0.05775400	-1.53056700	2.34015500
O	-0.29609700	-0.87467800	-2.34656500
C	2.43810400	-0.57365900	-0.29963900
H	2.31261700	-1.64986300	-0.28455100
C	3.81661500	-0.14713500	-0.23416000
C	4.77544100	-1.03368500	0.31165200
C	4.27322500	1.11750100	-0.66894600
C	6.10472300	-0.67221100	0.42795900
H	4.45189000	-2.01366000	0.64436300
C	5.60746200	1.47102700	-0.55575100
H	3.58127800	1.81688200	-1.12073000
C	6.53185200	0.58534200	-0.00189700
H	6.81707400	-1.37104000	0.85035700
H	5.93461300	2.44269600	-0.90679800
H	1.61270900	0.71195400	-1.93546900
H	1.89703000	1.86265100	0.32970100
C	-0.22858400	1.98017200	0.26957300
C	-0.76743100	2.54500400	-0.88198800

C	-0.87476100	2.23288300	1.48509500
C	-1.91285400	3.33901600	-0.84069300
H	-0.30329200	2.36331500	-1.84441500
C	-2.01076700	3.02052600	1.54472600
H	-0.49149400	1.79873600	2.40140700
C	-2.54004900	3.58070800	0.37927500
H	-2.30244600	3.74939600	-1.76161900
H	-2.51148400	3.20807100	2.48641000
H	7.57335000	0.86869200	0.08728800
O	-3.66558500	4.33617800	0.53827700
C	-4.25654800	4.91421600	-0.61597600
H	-5.13066400	5.45738800	-0.26302500
H	-3.57180000	5.61151400	-1.10863200
H	-4.57042400	4.14680400	-1.33018100



2ad

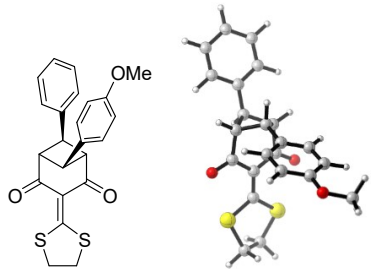
SCF Done: E(UB3LYP) = -1910.88074840 A.U.

Zero-point correction= 0.374336 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.562829

C	0.95571700	4.28714700	-0.68465300
C	0.18383200	4.29973800	0.61300100
C	0.53752800	1.74514600	-0.03035100
H	0.61428800	5.05897500	-1.37590200
H	2.02753800	4.40472400	-0.51887400
H	-0.88462300	4.44373300	0.44624300
H	0.54453900	5.06581700	1.30087600
S	0.67346100	2.66701300	-1.51247500
S	0.42457000	2.67670600	1.44787000
C	0.51991400	0.36744300	-0.02733800
C	0.46441000	-0.39918300	1.22040400
C	0.55280300	-0.40460700	-1.27282400
C	0.44249600	-1.90787200	1.04413700
C	0.53715300	-1.91203000	-1.09120000
C	1.55069000	-2.32959000	0.02216300
H	0.39655400	-2.39509900	2.01604400
O	0.45858200	0.11800000	2.32962800
O	0.56840000	0.10876500	-2.38348900
C	-0.58193400	-2.30409800	-0.06733100
H	-0.65509900	-3.39668300	-0.07208800

C	-1.96595100	-1.71142700	-0.12453600
C	-2.66885800	-1.40985100	1.03804400
C	-2.61326700	-1.51082000	-1.34956300
C	-3.97508200	-0.92481600	0.99823600
H	-2.19702000	-1.54223500	2.00489800
C	-3.90959200	-1.02956800	-1.40747200
H	-2.09285200	-1.72422700	-2.27626300
C	-4.60255200	-0.73422200	-0.23092000
H	-4.48072700	-0.69699300	1.92599300
H	-4.40403700	-0.86928300	-2.35745500
H	0.57086600	-2.40393500	-2.06119100
H	1.60199500	-3.42320400	0.02851300
C	2.95076900	-1.77442400	0.08170100
C	3.66716100	-1.51643700	-1.08918100
C	3.58282600	-1.56860700	1.31024400
C	4.98190700	-1.06612000	-1.03358300
H	3.19373900	-1.65810900	-2.05389000
C	4.89724000	-1.11836200	1.36744200
H	3.04201500	-1.75101400	2.23173900
C	5.60232500	-0.86675200	0.19507600
H	5.51974000	-0.86645300	-1.95301700
H	5.36852700	-0.95946500	2.33029200
H	6.62555100	-0.51296000	0.23869400
O	-5.87428900	-0.26249400	-0.38902900
C	-6.62324200	0.05406400	0.77457400
H	-6.14202300	0.84676800	1.35580000
H	-7.59093900	0.40351100	0.42073200
H	-6.76583000	-0.82604100	1.40923300



2ad’

SCF Done: E(UB3LYP) = -1910.87987897 A.U.

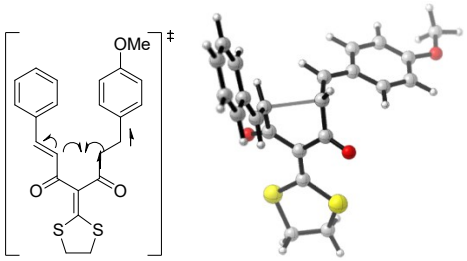
Zero-point correction= 0.374451 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.562355

C	3.45697300	-3.83315800	-0.75479000
C	3.80840700	-3.33922900	0.62818900
C	1.54486200	-2.12489600	-0.05226000
H	4.33351900	-3.91531100	-1.39904800
H	2.94635500	-4.79668600	-0.72284500

H	4.53489300	-2.52611000	0.59444000
H	4.19356200	-4.13594700	1.26613000
S	2.32999900	-2.60774800	-1.54120400
S	2.27453300	-2.70913700	1.42796400
C	0.41887400	-1.33015200	-0.04583500
C	-0.26271500	-0.97075400	1.20270700
C	-0.15156400	-0.79254500	-1.28561700
C	-1.47731600	-0.07950300	1.02624600
C	-1.39773200	0.05648400	-1.09903100
C	-2.36254200	-0.68809600	-0.12146900
H	-1.93133500	0.13079000	1.99200700
O	0.08525200	-1.38131700	2.30169000
O	0.33386300	-0.99085700	-2.39114600
C	-1.16665000	1.09420400	0.04676600
H	-1.75175800	0.39412000	-2.07002100
C	-3.81534400	-0.26208500	-0.10323700
C	-4.58269600	-0.51560800	1.03892700
C	-4.44459800	0.31988500	-1.20395100
C	-5.93200900	-0.18908600	1.08276200
H	-4.11890600	-0.97776600	1.90343300
C	-5.79737700	0.64901800	-1.16296000
H	-3.88409500	0.51735000	-2.10902100
C	-6.54574700	0.39845700	-0.01991500
H	-6.50546200	-0.39400600	1.97923100
H	-6.26407300	1.10244600	-2.02962300
H	-7.59748000	0.65639500	0.01289500
H	-2.31916500	-1.77857100	-0.18807900
C	0.09611700	1.90912900	0.14822200
C	0.72235200	2.41120400	-0.98891100
C	0.64153000	2.24060700	1.39406500
C	1.85489100	3.21932500	-0.90409300
H	0.33444000	2.16726200	-1.97135500
C	1.76579200	3.04160400	1.49661000
H	0.18601900	1.86055700	2.30141500
C	2.38129000	3.53918600	0.34569000
H	2.31281600	3.58189900	-1.81363400
H	2.18829900	3.29042500	2.46213600
H	-2.03325100	1.76168600	0.05735100
O	3.48598500	4.31645000	0.54786500
C	4.15273800	4.84606800	-0.58784200
H	4.98998700	5.42278600	-0.20028100
H	4.53072500	4.04991200	-1.23672300
H	3.49637900	5.50436200	-1.16547100

TS1b-2



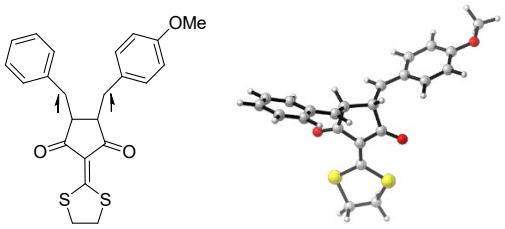
SCF Done: E(UB3LYP) = -1910.78559047 A.U.

Zero-point correction= 0.366026 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.480314

C	1.32837800	4.88025100	-0.55724200
C	0.25703100	5.28221300	0.43157700
C	-0.01995200	2.67146600	0.03020900
H	1.46291000	5.62498100	-1.34291100
H	2.28530600	4.70054700	-0.06574100
H	-0.62085200	5.69350700	-0.06821800
H	0.62320900	6.00320800	1.16374800
S	0.78683900	3.32777000	-1.38075700
S	-0.24602000	3.78064900	1.36785100
C	-0.45132500	1.37014500	0.08196000
C	-0.19048100	0.39700600	-0.98447200
C	-1.23265100	0.84431100	1.19873100
C	-0.28944800	-1.01908200	-0.54641900
C	-2.03251100	-0.39656600	0.89062700
H	-0.69902600	-1.69317300	-1.29877300
H	-1.92669300	-1.19842300	1.61286300
O	-1.29055100	1.35842800	2.30687200
O	0.08354500	0.70581900	-2.14128400
C	-3.15338800	-0.32420300	0.11322900
H	-3.28268500	0.56200100	-0.50291000
C	0.65698500	-1.56026700	0.43945600
H	0.28254800	-1.87466800	1.40971800
C	-4.18858300	-1.33208500	-0.02762000
C	-5.24214500	-1.09972200	-0.92960500
C	-4.19629300	-2.54124400	0.69202100
C	-6.25589500	-2.02991300	-1.10744100
H	-5.25516800	-0.17445000	-1.49490900
C	-5.20868100	-3.46958400	0.51188700
H	-3.40618800	-2.75482500	1.40111400
C	-6.24450400	-3.22101700	-0.38801700
H	-7.05624000	-1.82638100	-1.80900200
H	-5.19447200	-4.39407500	1.07712600
C	2.03515000	-1.76195000	0.19815400
C	2.66387400	-1.43874600	-1.03873000

C	2.86189900	-2.32061800	1.20621300
C	4.00657000	-1.65978900	-1.23546200
H	2.07519400	-1.00617800	-1.83793700
C	4.21229900	-2.54419900	1.00882000
H	2.41896100	-2.57817700	2.16185000
C	4.79899200	-2.21384600	-0.21837800
H	4.47868700	-1.41138200	-2.17811600
H	4.80028200	-2.97216500	1.80892100
O	6.11514900	-2.38878000	-0.52054900
C	6.97000300	-2.94868100	0.46654800
H	7.95747600	-2.99587900	0.01267700
H	7.01132500	-2.31936700	1.36059400
H	6.64980500	-3.95729900	0.74425200
H	-7.03456900	-3.94951500	-0.52444500



INTb-2

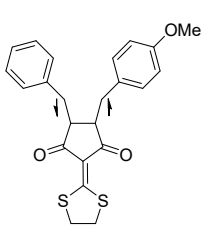
SCF Done: E(UB3LYP) = -1910.83538197 A.U.

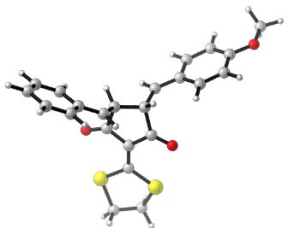
Zero-point correction= 0.369107 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.526458

C	-1.37965700	5.17746100	-0.15454100
C	-2.78709400	4.75040500	0.20053200
C	-1.34837700	2.53075400	0.01147300
H	-1.37052900	5.98874600	-0.88336100
H	-0.81510900	5.48195300	0.72748000
H	-3.42810100	4.69749900	-0.68020800
H	-3.24265000	5.41501500	0.93552300
S	-0.51748200	3.74872400	-0.92886600
S	-2.71049000	3.07750700	0.96179800
C	-0.95323900	1.21789800	0.00300800
C	0.17410000	0.68639900	-0.75262100
C	-1.60440400	0.14324100	0.74015400
C	0.38755200	-0.78947800	-0.32368900
C	-0.97337600	-1.20251900	0.28651800
H	0.63212600	-1.37553800	-1.21304900
H	-0.85098700	-1.83714300	1.16729100
O	-2.49643400	0.25678400	1.55976400
O	0.85058000	1.28493400	-1.56873700
C	-1.87514900	-1.85155400	-0.71584800
H	-1.64684700	-1.67385700	-1.76199800

C	1.50052900	-0.84591700	0.67662200
H	1.21445700	-0.84876000	1.72346200
C	-3.00968500	-2.63820000	-0.42628500
C	-3.73953600	-3.23183400	-1.49368600
C	-3.47028200	-2.88912200	0.89452700
C	-4.83949400	-4.03031300	-1.25480900
H	-3.41278600	-3.05125600	-2.51187100
C	-4.57446200	-3.69046600	1.11941800
H	-2.97064900	-2.42166800	1.73204700
C	-5.26639700	-4.27031200	0.05441600
H	-5.37434800	-4.47243500	-2.08744400
H	-4.90966500	-3.86234300	2.13575200
C	2.87722500	-0.85216300	0.37960300
C	3.39795200	-0.77499200	-0.94412600
C	3.82772900	-0.95557800	1.42861300
C	4.75117900	-0.81693300	-1.18410900
H	2.72053200	-0.64861700	-1.77746800
C	5.18876500	-0.99902400	1.18888700
H	3.47161000	-1.00911700	2.45148200
C	5.66458300	-0.93358800	-0.12583100
H	5.13884700	-0.75144400	-2.19334300
H	5.87048200	-1.08358300	2.02380000
O	6.97983700	-0.96862100	-0.47760300
C	7.95451000	-1.08565200	0.54916500
H	8.91816700	-1.09809500	0.04459100
H	7.91523700	-0.23383100	1.23469700
H	7.82845500	-2.01456300	1.11333800
H	-6.13038600	-4.89651900	0.24064300





INTb-2-OSS

SCF Done: E(UB3LYP) = -1910.83707965 A.U.

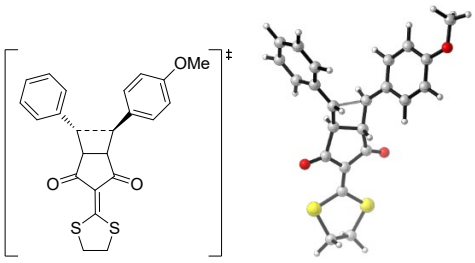
Zero-point correction= 0.369148 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.527652

C	1.74789300	5.19032200	0.15500100
C	3.12536100	4.67511500	-0.20118000
C	1.54780700	2.55115900	-0.01332500
H	1.79066400	6.00122400	0.88310700
H	1.20310200	5.52918500	-0.72691000
H	3.76170200	4.58051500	0.67945500

H	3.62219500	5.31053600	-0.93526700
S	0.79932600	3.81944900	0.93171100
S	2.94134300	3.01205600	-0.96544600
C	1.06866900	1.26751500	-0.00679100
C	-0.08247100	0.80650500	0.75961200
C	1.63901300	0.15659800	-0.75831600
C	-0.39923700	-0.64936700	0.32434400
C	0.92928500	-1.14862700	-0.30228400
H	-0.67433800	-1.22474500	1.21178800
H	0.75742000	-1.77423600	-1.18079500
O	2.52745200	0.21323200	-1.58729600
O	-0.71245000	1.43996100	1.58606700
C	1.78549700	-1.84606600	0.69626900
H	1.66634000	-1.54410000	1.73225000
C	-1.50873300	-0.62671500	-0.66976500
H	-1.22511400	-0.53597600	-1.71355500
C	2.76722900	-2.82211300	0.41633500
C	3.46665600	-3.43811800	1.49039800
C	3.10193800	-3.23902600	-0.89950300
C	4.41867000	-4.41164700	1.26386600
H	3.23560800	-3.13313300	2.50511900
C	4.05846800	-4.21464500	-1.11314500
H	2.62372600	-2.76918600	-1.74838900
C	4.72226200	-4.81192800	-0.04022300
H	4.93298800	-4.86629300	2.10264300
H	4.29948900	-4.51148800	-2.12735400
C	-2.88645800	-0.65996700	-0.37198900
C	-3.40465500	-0.67418000	0.95392100
C	-3.83788700	-0.68651600	-1.42371500
C	-4.75762000	-0.72860000	1.19334500
H	-2.72638800	-0.60999200	1.79384200
C	-5.19893600	-0.74194600	-1.18575600
H	-3.48320700	-0.66915300	-2.44830300
C	-5.67274400	-0.76756500	0.13097300
H	-5.14358600	-0.73166300	2.20529300
H	-5.88193300	-0.76465800	-2.02351300
O	-6.98699900	-0.82197000	0.48161300
C	-7.96483000	-0.85747800	-0.54854100
H	-8.92726600	-0.90089900	-0.04343000
H	-7.92158100	0.04215900	-1.16967200
H	-7.84607000	-1.74333400	-1.17951700
H	5.47045700	-5.57487400	-0.21729800

TS2b-2



SCF Done: E(UB3LYP) = -1910.80723510 A.U.

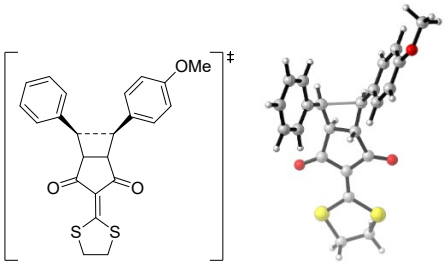
Zero-point correction= 0.370904 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.493092

C	6.38131000	-0.59336000	-0.92639500
C	6.37830400	-1.63604200	0.17986000
C	3.97677800	-0.45967900	0.09801900
H	7.35518900	-0.11408200	-1.03530000
H	6.07716000	-1.02195100	-1.88201800
H	6.90994900	-1.27352800	1.05989300
H	6.83033000	-2.57351700	-0.14882500
S	5.17472100	0.70218900	-0.44471000
S	4.63587700	-2.00764600	0.65454300
C	2.57975000	-0.20316600	0.04124300
C	2.00756700	0.97289200	-0.52768400
C	1.56601200	-1.05559400	0.65258200
C	0.51850800	1.00276100	0.02245600
C	0.22470900	-0.48210800	0.13947700
H	0.62520300	1.41686300	1.02879800
H	0.14527400	-0.89090500	-0.87304300
O	1.70335900	-2.05501300	1.33709300
O	2.49279400	1.91405400	-1.15416500
C	-1.16652100	-0.24267400	0.64354200
H	-1.22952200	0.25493400	1.60620400
C	-0.82703000	1.37343700	-0.49852900
H	-1.08988700	0.93119900	-1.45517500
C	-2.34210000	-1.02365300	0.29438400
C	-3.56499400	-0.74218500	0.92273900
C	-2.32356200	-2.06014800	-0.65949600
C	-4.71885600	-1.45378900	0.63225700
H	-3.60857200	0.04970400	1.66193700
C	-3.46231600	-2.77758000	-0.95586200
H	-1.39905100	-2.32246200	-1.15781300
C	-4.67319200	-2.48126300	-0.31480300
H	-5.63746000	-1.20944000	1.14633000
H	-3.44315900	-3.58540400	-1.67632600
C	-1.55498100	2.59838600	-0.19124000
C	-1.10648900	3.53295300	0.75730800

C	-2.76535100	2.85808200	-0.85886900
C	-1.83958200	4.67999900	1.02234300
H	-0.16937000	3.37368000	1.27534400
C	-3.49947800	4.00204000	-0.58700800
H	-3.12123800	2.15171300	-1.60038100
C	-3.03969900	4.91798500	0.35629900
H	-1.47116300	5.39638600	1.74672900
H	-4.42703600	4.18627000	-1.11573500
H	-3.60905500	5.81544700	0.56596600
O	-5.73282100	-3.24444000	-0.67566500
C	-6.99121800	-3.01173500	-0.05086000
H	-7.35311700	-2.00025300	-0.25479700
H	-7.67522500	-3.73580000	-0.48681300
H	-6.93091600	-3.17168600	1.02903000

TS2b'-2



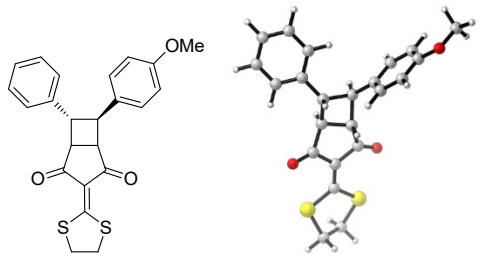
SCF Done: E(UB3LYP) = -1910.80158972 A.U.

Zero-point correction= 0.371006 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.486985

C	6.50056200	-0.44277100	-0.55525200
C	6.07770400	-1.88314200	-0.31563000
C	3.86018800	-0.50554500	-0.13007100
H	7.40398000	-0.18870900	0.00211100
H	6.67246400	-0.25819600	-1.61582600
H	6.13908200	-2.14794300	0.74047700
H	6.67005100	-2.58642500	-0.90263200
S	5.16457100	0.68351800	0.03188900
S	4.33503400	-2.02775500	-0.86858500
C	2.53583000	-0.24877000	0.31415500
C	2.06554800	1.05557100	0.77555400
C	1.48541700	-1.20452000	0.29243700
C	0.67663700	0.77519600	1.38499300
C	0.15307700	-0.35277700	0.51104500
H	0.90583500	0.36834400	2.37421800
H	-0.06067800	0.03906100	-0.48532700
O	1.43487000	-2.40014400	-0.00173500
O	2.65110100	2.12550900	0.77280300
C	-1.13917100	-0.54450000	1.22466100

H	-1.04561000	-0.84719300	2.26426500
C	-0.69475200	1.39958700	1.49315200
C	-2.39926100	-0.92681000	0.61627700
C	-3.45893400	-1.34776500	1.43489000
C	-2.63043900	-0.88370000	-0.77319200
C	-4.68796700	-1.71962900	0.91347800
H	-3.30944300	-1.39520300	2.50814800
C	-3.84572800	-1.25387500	-1.30654900
H	-1.84402700	-0.56510000	-1.44455400
C	-4.88829800	-1.67436600	-0.46981800
H	-5.47261200	-2.04658000	1.58075000
H	-4.01866900	-1.22943800	-2.37489300
C	-1.30188600	2.27676600	0.49439200
C	-2.63996700	2.67427200	0.65803000
C	-0.59207000	2.76040400	-0.61568200
C	-3.25021900	3.51517500	-0.25908000
H	-3.19957600	2.31317100	1.51366700
C	-1.20608800	3.60562700	-1.53059000
H	0.45441300	2.51400900	-0.73775000
C	-2.53529500	3.98168300	-1.36011200
H	-4.28275300	3.81073200	-0.11667000
H	-0.63907800	3.98261800	-2.37316300
H	-1.06054000	1.56120500	2.50305400
H	-3.00962000	4.64228700	-2.07592000
O	-6.04261700	-2.01396100	-1.09159100
C	-7.14206800	-2.45991400	-0.30394200
H	-7.46839600	-1.68415100	0.39421000
H	-7.94228300	-2.67296400	-1.00852800
H	-6.88997500	-3.37012900	0.24681000



3ac

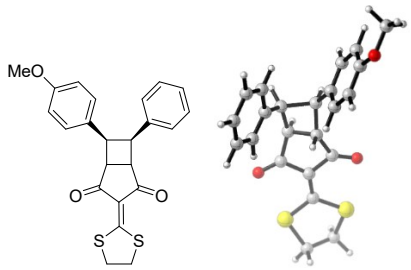
SCF Done: E(UB3LYP) = -1910.84510068 A.U.

Zero-point correction= 0.373291 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.530218

C	6.36822500	-1.01487900	-0.64646200
C	6.16789700	-1.71343800	0.68002500
C	3.81485500	-0.66502400	0.01430600
H	7.31957300	-0.48303600	-0.68848200

H	6.31222500	-1.71322000	-1.48217700
H	6.48783300	-1.09040500	1.51589700
H	6.69528300	-2.66718900	0.72296500
S	5.04103700	0.24043000	-0.85521500
S	4.37775400	-2.07893900	0.88726600
C	2.50084500	-0.29106300	0.01083600
C	1.98554000	0.96496900	-0.61279000
C	1.39676400	-1.08426200	0.63705600
C	0.57709000	1.04461200	-0.05225300
C	0.15942600	-0.41355400	0.06181800
H	0.72035000	1.41706300	0.97290700
H	0.09127000	-0.81262200	-0.95997900
O	1.52043900	-2.05241000	1.35681400
O	2.60672400	1.73469300	-1.31676400
C	-1.27561200	0.07982400	0.42826100
H	-1.31249600	0.36510400	1.48208900
C	-0.89468800	1.38257900	-0.41743600
H	-1.07947700	1.17502000	-1.47589000
C	-2.47724100	-0.75307500	0.08587600
C	-3.32902200	-1.20085400	1.09188000
C	-2.78310100	-1.12461200	-1.23023600
C	-4.44525300	-1.98994900	0.81889800
H	-3.12022100	-0.93436200	2.12236500
C	-3.88639000	-1.90589400	-1.52253500
H	-2.15232700	-0.79689800	-2.04895200
C	-4.72850400	-2.34672700	-0.49735200
H	-5.07512500	-2.31528300	1.63487900
H	-4.11797600	-2.18774400	-2.54214400
C	-1.45860500	2.72496400	-0.04133000
C	-0.64469000	3.85976000	-0.05303700
C	-2.80659200	2.87193400	0.29661800
C	-1.16331000	5.11053400	0.26629400
H	0.40171400	3.76468700	-0.32261400
C	-3.32525000	4.12161300	0.61853000
H	-3.45591000	2.00420400	0.30727500
C	-2.50547400	5.24573200	0.60474000
H	-0.51619300	5.97977800	0.25080500
H	-4.37248200	4.21667700	0.88127100
H	-2.90966500	6.21899500	0.85665600
O	-5.79009000	-3.11045800	-0.88515500
C	-6.67518500	-3.59090600	0.11609500
H	-7.15446400	-2.76668500	0.65320800
H	-7.43339700	-4.16826600	-0.40854400
H	-6.15609400	-4.23797800	0.82968600



3ad

SCF Done: E(UB3LYP) = -1910.83885888 A.U.

Zero-point correction= 0.373577 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1910.522327

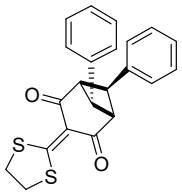
C	6.31828200	-0.32593700	-0.98967800
C	6.16392800	-1.75132500	-0.50802900
C	3.83815300	-0.54139400	-0.05223400
H	7.29443700	0.08812900	-0.73412600
H	6.16728700	-0.24579800	-2.06674200
H	6.57540900	-1.88542300	0.49297900
H	6.63455800	-2.46463200	-1.18581600
S	5.05619900	0.71719500	-0.15266600
S	4.37258200	-2.16334200	-0.45357900
C	2.54903600	-0.27618000	0.31651700
C	2.06739700	1.06007400	0.77549300
C	1.44865200	-1.28701200	0.31030300
C	0.69601600	0.72858200	1.34943000
C	0.21351900	-0.41981500	0.47701100
H	0.95076700	0.29707500	2.32809100
H	0.03814500	-0.00227500	-0.52295900
O	1.56776400	-2.48273900	0.14117700
O	2.69626300	2.09845000	0.75289200
C	-1.14108200	-0.37486600	1.22690500
H	-1.04333400	-0.87716100	2.19178600
C	-0.78766000	1.19593700	1.50387300
C	-2.41970200	-0.81351500	0.57951600
C	-3.41974500	-1.39462700	1.35668700
C	-2.67505600	-0.66392500	-0.78960400
C	-4.63322100	-1.81116700	0.81339800
H	-3.25151600	-1.53741100	2.41917000
C	-3.87104700	-1.07550900	-1.34960700
H	-1.93060500	-0.21775100	-1.43704300
C	-4.86295500	-1.65103600	-0.55160800
H	-5.37536000	-2.26140600	1.45758100
H	-4.05964600	-0.95964800	-2.40957600
C	-1.35982000	2.20513700	0.54435900
C	-2.73122000	2.48425400	0.59545800

C	-0.57742000	2.90841200	-0.37333000
C	-3.30329400	3.42271200	-0.25222900
H	-3.35722800	1.95600500	1.30540300
C	-1.15060600	3.84830500	-1.22734200
H	0.49284800	2.75318100	-0.40588400
C	-2.51416200	4.10683900	-1.17327600
H	-4.36735600	3.62032400	-0.19508500
H	-0.52206100	4.38534800	-1.92807600
H	-1.03875400	1.49147400	2.52358700
H	-2.95910000	4.83993600	-1.83565300
O	-6.00696900	-2.02233100	-1.19605000
C	-7.04601400	-2.61851900	-0.43424700
H	-7.41272700	-1.93882400	0.34127700
H	-7.84886300	-2.82855800	-1.13775900
H	-6.71572900	-3.55382100	0.02800600

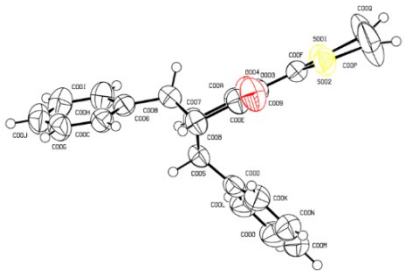
6. X-Ray Structures of Compounds 2a and 2g'

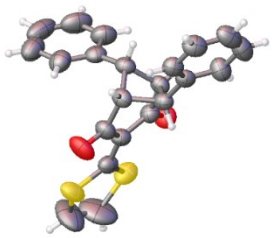
Single-crystal X-ray diffraction data was collected at room temperature on a Oxford Diffraction Gemini R Ultra diffractometer, the X-ray generator using Mo-Kα (λ=0.71073 Å) radiation with a ω scan technique. The crystal structures were solved by direct method of SHELXS-97 1 and refined by full-matrix least-squares techniques using the SHELXL-97 program. Drawing of the compound shows ellipsoid contour at the 30% probability level. Non-hydrogen atoms were refined anisotropic. CCDC deposition number: 2120337 (**2a**) and 2120342 (**2g'**). The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

6.1 Crystal data of 2a



2a

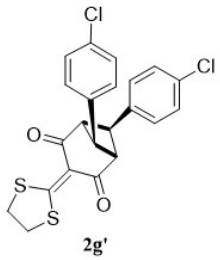




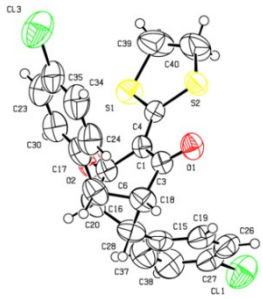
Empirical formula	$C_{22}H_{16}O_2S_2$
Formula weight	378.07
Crystal system	Monoclinic
Space group	-C 1
a (Å)	28.151(2)
b (Å)	8.7194(6)
c (Å)	16.9591(13)

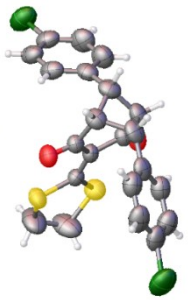
a (Å)	90
β (deg)	115.173(4)
γ (deg)	90
Volume ($Å^3$)	3767.5(5)
Z	1 c
Calculated density (mg/m^3)	1.3128
Absorption coefficient (mm^{-1})	1.114
F(000)	1568.0
Theta range for data collection (deg)	3.470 to 63.639
Reflections collected/unique	4434/5989
Goodness-of-fit on F^2	7.4990
Final R indices [$I> 2\sigma(I)$]	R1=0.4375, WR2=0.7739
R indices (all data)	R1=0.4734, WR2=0.8022

6.2 Crystal data of 2g'



2g'





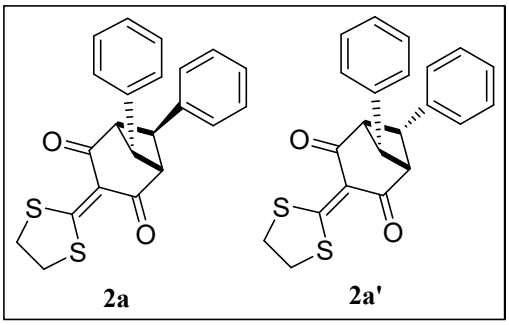
Empirical formula	$C_{22}H_{16}Cl_2O_2S_2$
Formula weight	446.00
Crystal system	Monoclinic
Space group	P -1
a (Å)	12.9787(15)
b (Å)	13.8453(17)
c (Å)	14.023(2)
α (Å)	75.109(12)
β (deg)	71.440(13)
γ (deg)	70.545(11)
Volume ($Å^3$)	2220.0(6)
Z	1
Calculated density (mg/m^3)	1.337
Absorption coefficient (mm^{-1})	0.495
F(000)	918.0
Theta range for data collection (deg)	4.216 to 25.663
Reflections collected/unique	5533/8662

Goodness-of-fit on F^2	1.088
Final R indices [$I > 2\sigma(I)$]	R1=0.0618, WR2=0.1539
R indices (all data)	R1=0.0989, WR2=0.1751

7. Characterization data for the products

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2a)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2a')



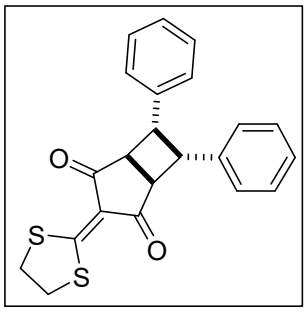
2a/2a' (56.7 mg, 50% yield) as yellow oil, cannot be separated by column chromatography.

2a, **^{1}H NMR** (600 MHz, $CDCl_3$), δ 7.47 (d, *J* = 7.8 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.22 (d, J = 7.2 Hz, 2H), 7.12 (d, J = 7.2 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 2H), 4.40 (t, *J* = 6.0 Hz, 1H), 3.92 (d, *J* = 6.0 Hz, 2H), 3.83 (s, 1H), 3.34-3.28 (m, 4H).

2a', **^{1}H NMR** (600 MHz, $CDCl_3$), δ 7.18 (t, *J* = 7.2 Hz, 5H), 7.09 (d, *J* = 7.8 Hz, 5H), 4.23 (t, *J* = 6.6 Hz, 2H), 4.17 (t, *J* = 5.4 Hz, 2H), 3.10 (s, 4H).

2a/2a', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.2, 194.0, 182.1, 179.6, 138.7, 138.3, 137.9, 128.9, 128.4, 128.4, 127.0, 127.0, 126.4, 126.3, 126.1, 125.7, 120.4, 119.2, 55.4, 55.0, 46.5, 46.0, 46.0, 37.5, 37.1. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{18}O_2S_2$ $[M+Na]^+$ 401.0640, found 401.0645.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-diphenylbicyclo[3.2.0]heptane-2,4-dione (3a)



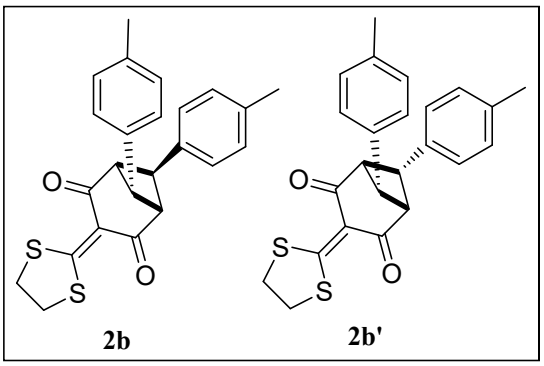
3a (42.0 mg, 37% yield) as yellow solid. mp: 203-204 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.10 (t, *J* = 7.2 Hz, 4H), 7.03 (t, *J* = 7.2 Hz, 2H), 6.98 (d, *J* = 7.8 Hz, 4H), 4.06 (d, *J* = 3.6 Hz, 2H), 3.65 (d, *J* = 4.2 Hz, 2H), 3.56 (s, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 200.6, 183.9, 139.2, 128.0, 127.9, 126.2, 121.3, 48.0, 47.2, 37.6. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{18}O_2S_2$ $[M+Na]^+$ 401.0640, found 4 01.0638.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-p-tolylbicyclo[3.1.1]heptane-2,4-dione (2b)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-p-tolylbicyclo[3.1.1]heptane-2,4-di one (2b')



2b/2b' (51.2 mg, 42% yield) as yellow oil, cannot be separated by column chromatogr aphy.

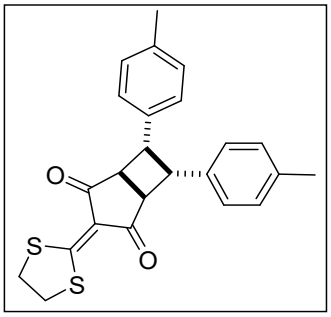
2b, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.8 Hz, 2H), 6.96 (t, *J* = 5.4 Hz, 5H), 6.8 7 (s, 1H), 4.35 (t, *J* = 6.0 Hz, 1H), 3.86 (d, *J* = 6.0 Hz, 2H), 3.77 (s, 1H), 3.31-3.26 (m, 4H), 2.36 (s, 3H), 2.32 (s, 1H), 2.21 (s, 5H).

2b', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.22 (t, *J* = 8.4 Hz, 3H), 6.99 (d, *J* = 8.4 Hz, 4H), 6.86 (s, 1H), 4.16 (t, *J* = 6.0 Hz, 2H), 4.11 (t, *J* = 6.0 Hz, 2H), 3.09 (s, 4H), 2.22 (s, 6 H).

2b/2b', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 194.2, 181.6, 179.0, 136.6, 135.8, 135. 7, 135.5, 135.2, 134.8, 129.7, 129.4, 129.0, 128.5, 126.9, 125.9, 125.5, 120.5, 119.3, 5 5.4, 55.0, 46.3, 45.9, 45.8, 37.4, 37.0, 21.0, 21.0. **HRMS** (ESI, m/z): Calculated for C_{24}

$H_{22}O_2S_2$ $[M+Na]^+$ 429.0953, found 429.0955.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-p-tolylbicyclo[3.2.0]heptane-2,4-dione (3b)

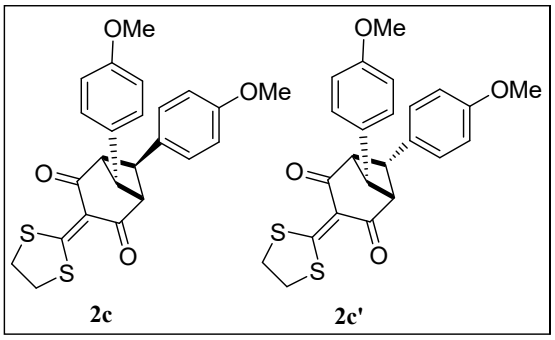


3b (51.2 mg, 42% yield) as brown oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.91 (d, *J* = 8.0 Hz, 4H), 6.87 (d, *J* = 8.0 Hz, 4H), 3.98 (d, *J* = 3.5 Hz, 2H), 3.58 (d, *J* = 4.0 Hz, 2H), 3.52 (s, 4H), 2.20 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.6, 183.5, 136.2, 135.5, 128.5, 127.8, 121.3, 48.4, 46.9, 37.5, 20.9. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_2$ $[M+Na]^+$ 429.0953, found 429.0944.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-methoxyphenyl)bicyclo[3.1.1]heptane-2,4-dione (2c)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-methoxyphenyl)bicyclo[3.1.1]heptane-2,4-dione (2c')



2c/2c' (53.9 mg, 41% yield) as yellow oil, cannot be separated by column chromatography.

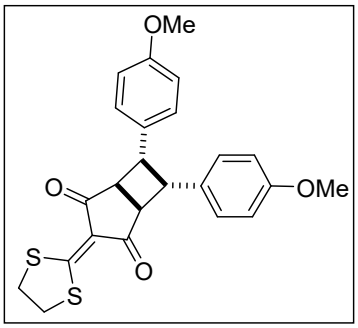
2c, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.71 (d, *J* = 9.0 Hz, 2H), 4.34 (t, *J* = 6.6 Hz, 1H), 3.83 (s, 2H), 3.82 (s, 3H), 3.76 (s, 1H), 3.71 (s, 3H), 3.34-3.29 (m, 4H).

2c', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 6.99 (d, *J* = 8.4 Hz, 4H), 6.73 (d, *J* = 8.4 Hz, 4H), 4.15 (t, *J* = 6.0 Hz, 2H), 4.08 (t, *J* = 5.4 Hz, 2H), 3.71 (s, 6H), 3.13 (s, 4H).

2c/2c', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 194.3, 181.7, 179.1, 158.5, 157.9, 157.8, 130.7, 130.2, 130.0, 128.1, 127.2, 126.8, 120.5, 119.3, 114.2, 113.8, 55.5, 55.3, 55.1,

55.1, 45.9, 45.5, 45.5, 37.4, 37.0. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_4S_2$ [M+Na]$^+$ 461.0852, found 461.0845.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-methoxyphenyl)bicyclo[3.2.0]heptane-2,4-dione (3c)

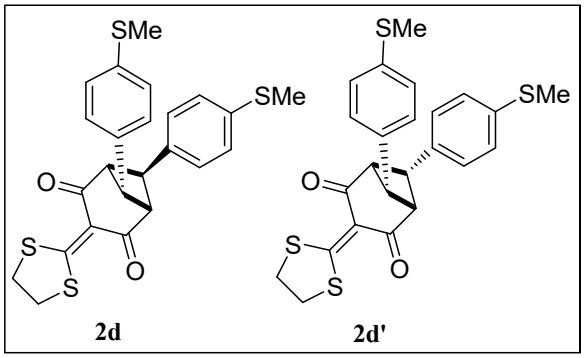


3c (53.9 mg, 41% yield) as yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.89 (d, *J* = 8.0 Hz, 4H), 6.66 (d, *J* = 8.5 Hz, 4H), 3.96 (d, *J* = 3.5 Hz, 2H), 3.71 (s, 6H), 3.56 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.7, 183.6, 157.8, 131.4, 129.0, 127.5, 113.3, 55.1, 48.3, 46.6, 37.5. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_4S_2$ [M+Na]$^+$ 461.0852, found 461.0861.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-(methylthio)phenyl)bicyclo[3.1.1]heptane-2,4-dione (2d)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-(methylthio)phenyl)bicyclo[3.1.1]heptane-2,4-dione (2d')



2d/2d' (57.8 mg, 41% yield) as yellow solid. mp: 105-106 ℃, cannot be separated by column chromatography.

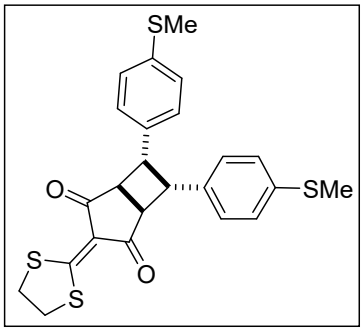
2d, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.06 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 7.8 Hz, 2H), 4.32 (t, *J* = 6.0 Hz, 1H), 3.84 (d, *J* = 6.0 Hz, 2H), 3.78 (s, 1H), 3.34 (s, 4H), 2.50 (s, 3H), 2.40 (s, 3H).

2d', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.09 (d, *J* = 8.4 Hz, 4H), 7.00 (d, *J* = 8.4 Hz, 4H), 4.16 (t, *J* = 6.0 Hz, 2H), 4.10 (t, *J* = 6.0 Hz, 2H), 3.16 (s, 4H), 2.41 (s, 6H).

2d/2d', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.0, 193.9, 136.4, 134.7, 127.6, 127.1, 126.6,

126.6, 126.6, 126.5, 126.3, 120.2, 55.4, 55.0, 46.2, 45.8, 45.7, 37.5, 37.2, 15.9, 15.7, 1 5.6. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_4$ $[M+Na]^+$ 493.0395, found 493.039 1.

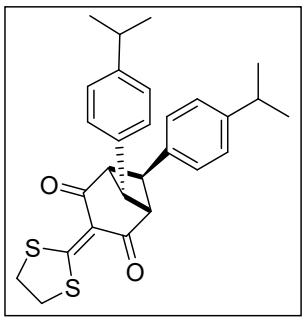
(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-(methylthio)phenyl)bicyclo[3.2.0] heptane-2,4-dione (3d)



3d (57.8 mg, 41% yield) as yellow solid. mp: 143-144 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.02 (d, *J* = 8.5 Hz, 4H), 6.90 (d, *J* = 8.5 Hz, 4H), 3.99 (d, *J* = 4.0 Hz, 2H), 3.57 (s, 2H), 3.57 (s, 4H), 2.40 (s, 6H). **^{13}C NMR** (151 MHz, CD Cl_3) δ 200.3, 136.1, 136.0, 128.4, 128.1, 126.9, 126.2, 48.1, 46.7, 37.6, 15.8. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_4$ $[M+Na]^+$ 493.0395, found 493.0402.

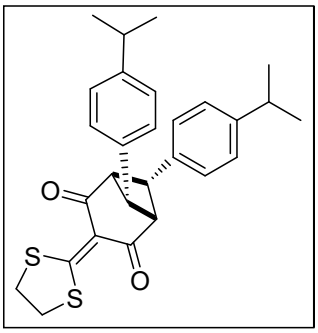
(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-isopropylphenyl)bicyclo[3.1.1] heptane-2,4-dione (2e)



2e (33.2 mg, 24% yield) as yellow solid. mp: 198-200 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 7.5 Hz, 2H), 6.90 (d, *J* = 8.0 Hz, 2H), 4.38 (t, *J* = 6.5 Hz, 1H), 3.88 (d, *J* = 6.5 Hz, 2H), 3.78 (s, 1H), 3.35-3.30 (m, 2H), 3.30-3.25 (m, 2H), 2.97-2.89 (m, 1H), 2.82-2.74 (m, 1H), 1.27 (d, *J* = 7.0 Hz, 6H), 1.15 (d, *J* = 7.0 Hz, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.5, 181.5, 147.7, 146.6, 135.9, 135.6, 127.0, 126.8, 126.4, 125.6, 119.5, 55.5, 46.4, 45.9, 37.4, 33.7, 33.5, 23.9, 23.8. **HRMS** (ESI, m/z): Calculated for $C_{28}H_{30}O_2S_2$ $[M+Na]^+$ 485.1579, found 485.1587.

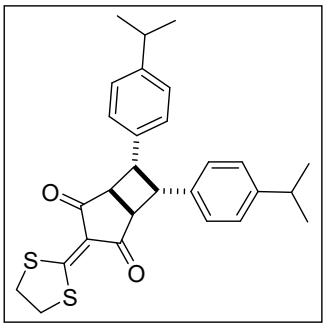
(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-isopropylphenyl)bicyclo[3.1.1] heptane-2,4-dione (2e')



2e' (29.2 mg, 21% yield) as white solid. mp: 125-127 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.4 Hz, 4H), 6.99 (d, *J* = 7.8 Hz, 4H), 4.18 (t, *J* = 6.6 Hz, 2H), 4.12 (t, *J* = 6.0 Hz, 2H), 3.07 (s, 4H), 2.82-2.76 (m, 2H), 1.15 (d, *J* = 6.6 Hz, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.4, 178.8, 146.8, 135.2, 126.4, 12 6.0, 120.9, 55.2, 46.0, 37.1, 33.6, 23.8. **HRMS** (ESI, m/z): Calculated for $C_{28}H_{30}O_2S_2$ [M+Na]$^+$ 485.1579, found 485.1571.

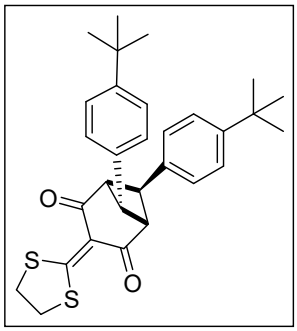
(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-isopropylphenyl)bicyclo[3.2.0]he ptane-2,4-dione (3e)



3e (56.8 mg, 41% yield) as brown oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 6.93 (d, *J* = 7.8 Hz, 4H), 6.87 (d, *J* = 8.4 Hz, 4H), 3.99 (d, *J* = 3.6 Hz, 2H), 3.62 (d, *J* = 4.2 Hz, 2H), 3.50 (s, 4H), 2.78-2.71 (m, 2H), 1.12 (d, *J* = 7.2 Hz, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.6, 183.4, 146.6, 136.4, 127.8, 1 25.6, 121.3, 47.9, 47.0, 37.5, 33.4, 23.8. **HRMS** (ESI, m/z): Calculated for $C_{28}H_{30}O_2S_2$ [M+Na]$^+$ 485.1579, found 485.1568.

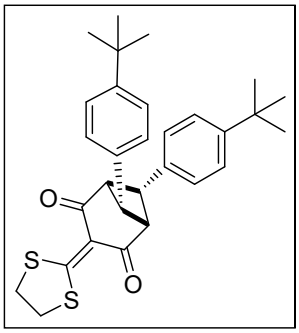
(1*R*,5*S*,6*R*,7*S*)-6,7-bis(4-(*tert*-butyl)phenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1. 1]heptane-2,4-dione (2f)



2f (43.7 mg, 30% yield) as yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 8.4 Hz, 2H), 4.38 (t, *J* = 6.0 Hz, 1H), 3.88 (d, *J* = 6.6 Hz, 2H), 3.78 (s, 1H), 3.34-3.31 (m, 2H), 3.30-3.27 (m, 2H), 1.34 (s, 9H), 1.22 (s, 9H).**^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.6, 181.5, 150.0, 148.9, 135.6, 135.3, 126.8, 125.7, 125.4, 125.3, 119.6, 55.5, 46.3, 45.9, 37.5, 34.5, 34.3, 31.3, 31.2. **HRMS** (ESI, m/z): Calculated for $C_{30}H_{34}O_2S_2$ $[M+Na]^+$ 513.1892, found 513.1899.

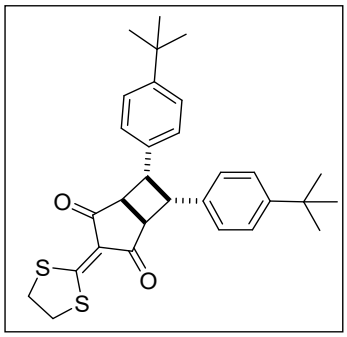
(1*r*,5*s*,6*R*,7*S*)-6,7-bis(4-(*tert*-butyl)phenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]heptane-2,4-dione (2f')



2f' (25.4 mg, 17% yield) as yellow solid. mp: 199-201 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.4 Hz, 4H), 7.00 (d, *J* = 8.4 Hz, 4H), 4.19 (t, *J* = 6.0 Hz, 2H), 4.13 (t, *J* = 6.0 Hz, 2H), 3.08 (s, 4H), 1.23 (s, 18H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.6, 178.7, 149.1, 134.8, 125.8, 125.3, 121.0, 55.2, 46.0, 37.1, 34.4, 31.2. **HRMS** (ESI, m/z): Calculated for $C_{30}H_{34}O_2S_2$ $[M+Na]^+$ 513.1892, found 513.1883.

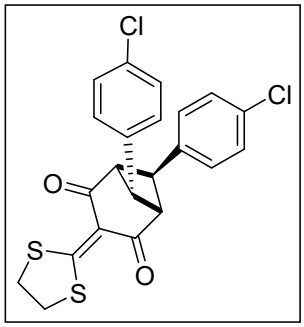
(1*R*,5*S*,7*S*)-6,7-bis(4-(*tert*-butyl)phenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.2.0]heptane-2,4-dione (3f)



3f (66.2 mg, 45% yield) as yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.4 Hz, 4H), 6.86 (d, *J* = 8.4 Hz, 4H), 3.99 (d, *J* = 4.2 Hz, 2H), 3.63 (d, *J* = 4.2 Hz, 2H), 3.54 (s, 4H), 1.19 (s, 18H). **^{13}C NMR** (1 51 MHz, $CDCl_3$) δ 200.8, 183.3, 148.9, 136.1, 127.6, 124.5, 121.4, 47.8, 47.0, 37.5, 3 4.2, 31.2. **HRMS** (ESI, m/z): Calculated for $C_{30}H_{34}O_2S_2$ $[M+Na]^+$ 513.1892, found 51 3.1893.

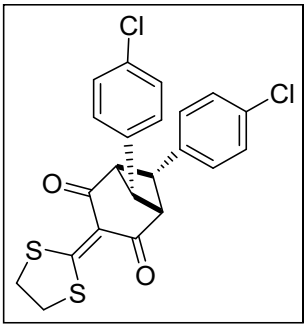
(1*R*,5*S*,6*R*,7*S*)-6,7-bis(4-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]he ptane-2,4-dione (2g)



2g (24.7 mg, 18% yield) as yellow solid. mp: 225-227 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41-7.37 (m, 4H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.93-6.91 (m, 2H),4.28 (t, *J* = 6.0 Hz, 1H), 3.84 (d, *J* = 6.0 Hz, 2H), 3.78 (s, 1H), 3.35(d, *J* = 1.8 Hz, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.4, 183.1, 136.9, 136.5, 133.0, 132.3, 129.0 , 128.6, 128.4, 127.2, 118.7, 55.2, 45.9, 45.4, 37.5. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{16}Cl_2O_2S_2$ $[M+Na]^+$ 468.9861, found 468.9865.

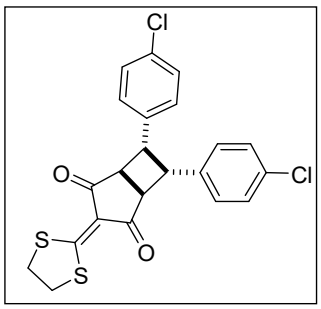
(1*r*,5*s*,6*R*,7*S*)-6,7-bis(4-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]hep tane-2,4-dione (2g')



2g' (26.2 mg, 20% yield) as yellow solid. mp: 151-152 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.4 Hz, 4H), 7.01 (d, *J* = 7.8 Hz, 4H), 4.16 (t, *J* = 5.4 Hz, 2H), 4.11 (t, *J* = 5.4 Hz, 2H), 3.18 (s, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 193.4, 181.0, 136.3, 132.4, 128.7, 127.6, 119.9, 54.9, 45.4, 37.3. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{16}Cl_2O_2S_2$ $[M+Na]^+$ 468.9861, found 468.9868.

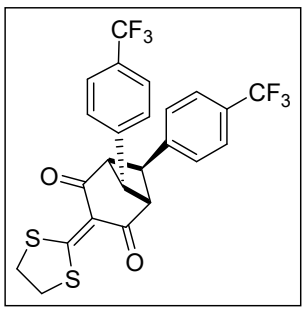
(1*R*,5*S*,7*S*)-6,7-bis(4-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.2.0]hepta ne-2,4-dione (3g)



3g (52.2 mg, 39% yield) as yellow solid. mp: 166-168 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.10 (d, *J* = 8.4 Hz, 4H), 6.90 (d, *J* = 8.4 Hz, 4H), 4.00 (d, *J* = 4.2 Hz, 2H), 3.57, (s, 4H), 3.56, (s, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 199.9, 184.6, 137.4, 132.2, 129.2, 128.2, 121.0, 47.9, 46.4, 37.6. **HRMS** (ESI, m/z): Calculat ed for $C_{22}H_{16}Cl_2O_2S_2$ $[M+Na]^+$ 468.9861, found 468.9857.

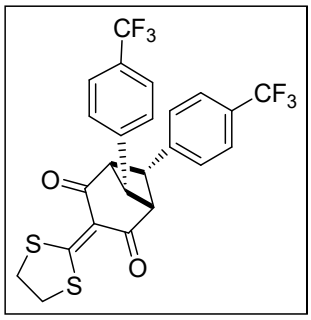
(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-(trifluoromethyl)phenyl)bicyc lo[3.1.1]heptane-2,4-dione (2h)



2h (28.7 mg, 19% yield) as yellow solid. mp: 189-191 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.8 Hz, 2H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.46 (d, *J* = 7.8 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 4.35 (t, *J* = 6.6 Hz, 1H), 3.95 (d, *J* = 6.6 Hz, 2H), 3.89 (s, 1H), 3.38-3.34 (m, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.0, 184. 0, 142.4, 142.1, 129.7 (q, *J* =33.2 Hz), 128.8 (q, *J* =31.7 Hz), 127.5, 126.2, 126.0 (q, *J* =4.5 Hz), 125.5 (q, *J* =4.5 Hz), 118.5, 55.2, 46.4, 45.8, 37.6. **HRMS** (ESI, m/z): Calc ulated for $C_{24}H_{16}F_6O_2S_2$ $[M+Na]^+$ 537.0388, found 537.0381.

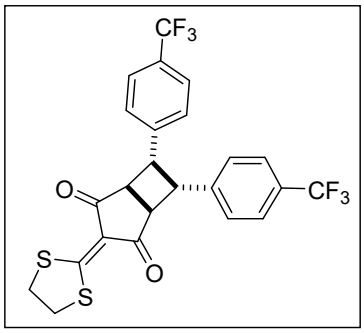
(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-(trifluoromethyl)phenyl)bicycl o[3.1.1]heptane-2,4-dione (2h')



2h' (20.6 mg, 13% yield) as yellow solid. mp: 197-199 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.0 Hz, 4H), 7.20 (d, *J* = 8.0 Hz, 4H), 4.27 (t, *J* = 5.0 Hz, 2H), 4.23-4.20 (m, 2H), 3.16 (s, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 1 93.0, 181.9, 141.7, 128.9 (q, *J* =32.8 Hz), 126.5, 125.5 (q, *J* =3.8 Hz), 124.0 (q, *J* =27 2.2 Hz), 119.6, 54.9, 45.7, 37.2. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{16}F_6O_2S_2$ $[M+N a]^+$ 537.0388, found 537.0385.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(4-(trifluoromethyl)phenyl)bicyclo[3.2 .0]heptane-2,4-dione (3h)



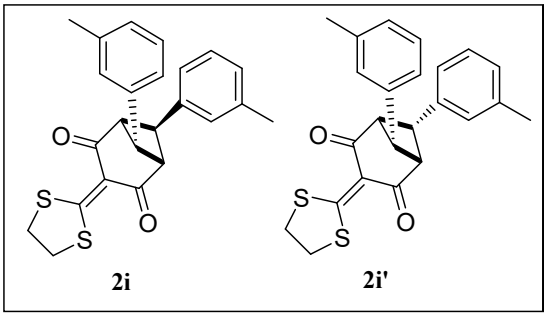
3h (80.2 mg, 52% yield) as yellow solid. mp: 237-238 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.8 Hz, 4H), 7.10 (d, *J* = 8.4 Hz, 4H), 4.14 (d, *J* = 3.6 Hz, 2H), 3.66 (d, *J* = 4.2 Hz, 2H), 3.60 (s, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$)

δ 199.5, 185.2, 142.8, 128.7 (q, *J* = 33.2 Hz) 128.2, 125.0 (q, *J* = 4.5 Hz), 123.9 (q, *J* = 271.8 Hz), 120.8, 47.7, 46.7, 37.7. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{16}F_6O_2S_2$ [M +Na]$^+$ 537.0388, found 537.0384.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-m-tolylbicyclo[3.1.1]heptane-2,4-dione (2i)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-m-tolylbicyclo[3.1.1]heptane-2,4-dione (2i')



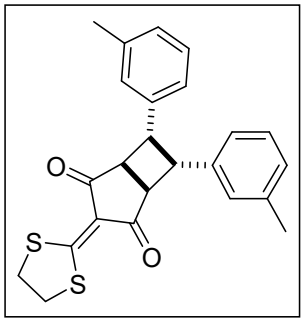
2i/**2i'** (51.2 mg, 42% yield) as yellow solid. mp: 118-119 ℃, cannot be separated by c olumn chromatography.

2i, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.22 (t, *J* = 9.0 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 7. 08 (d, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 3.5 Hz, 1H), 7.04 (d, *J* = 7.5 Hz, 1H), 6.86 (s, 1H), 6.81 (s, 1H), 6.78 (d, *J* = 8.0 Hz, 1H), 4.35 (t, *J* = 6.0 Hz, 1H), 3.88 (d, *J* = 6.5 Hz, 2H), 3.76 (s, 1H), 3.31-3.25 (m, 4H), 2.39 (s, 3H), 2.22 (s, 3H).

2i', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.5 Hz, 2H), 6.91 (s, 1H), 6.88 (d, *J* = 7.5 Hz, 5H), 4.15 (t, *J* = 5.5 Hz, 2H), 4.11(t, *J* = 5.5 Hz, 2H), 3.07 (s, 4H), 2.24 (s, 6H).

2i/2i', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.2, 194.0, 181.7, 179.1, 145.1, 138.6, 138.4, 138.2, 137.8, 137.8, 128.6, 128.2, 128.1, 127.8, 127.7, 127.1, 127.1, 126.8, 126.4, 123.9 , 123.1, 122.7, 120.5, 119.2, 55.4, 55.0, 46.5, 46.0, 45.9, 37.4, 37.0, 21.4, 21.3, 21.3. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_2$ [M+Na]$^+$ 429.0953, found 429.0962.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-m-tolylbicyclo[3.2.0]heptane-2,4-dione (3i)

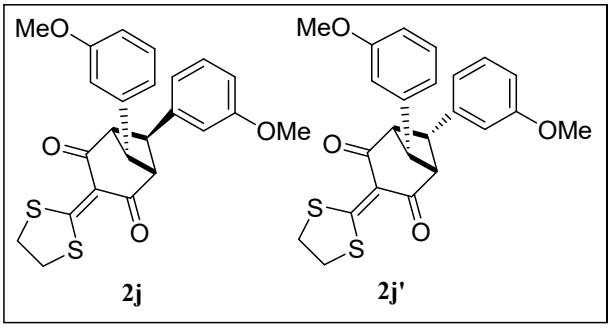


3i (52.4 mg, 43% yield) as yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.97 (t, *J* = 7.5 Hz, 2H), 6.83 (t, *J* = 7.5 Hz, 4H), 6.74 (d, *J* = 7.5 Hz, 2H), 3.99 (d, *J* = 4.0 Hz, 2H), 3.62 (d, *J* = 4.0 Hz, 2H), 3.53 (s, 4H), 2.18 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.7, 183.7, 139.0, 137.2, 128.8, 127.6, 126.8, 125.0, 121.3, 48.0, 47.1, 37.5, 21.2. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_2$ $[M+Na]^+$ 429.0953, found 429.0961.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-methoxyphenyl)bicyclo[3.1.1]heptane-2,4-dione (2j)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-methoxyphenyl)bicyclo[3.1.1]heptane-2, 4-dione (2j')



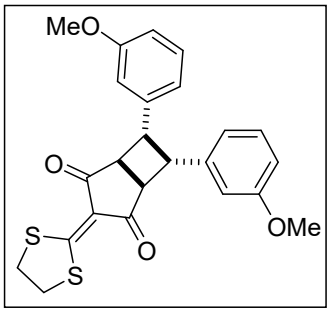
2j **2j'** (43.4 mg, 33% yield) as yellow oil, cannot be separated by column chromatography.

2j, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (t, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H) 7.05 (d, *J* = 7.5 Hz, 1H), 6.98 (s, 1H), 6.86-6.84 (m, 1H), 6.58 (d, *J* = 7.0 Hz, 1H), 6.52 (s, 1H), 4.38 (t, *J* = 6.0 Hz, 1H), 3.89 (d, *J* = 6.5 Hz, 2H), 3.84 (s, 3H), 3.79 (s, 1H), 3.71 (s, 3H), 3.35-3.30 (m, 4H).

2j', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.10 (d, *J* = 3.0 Hz, 1H), 6.68-6.63 (m, 5H), 6.61 (s, 2H), 4.19 (t, *J* = 6.0 Hz, 2H), 4.13 (t, *J* = 6.0 Hz, 2H), 3.73 (s, 6H), 3.13 (s, 4H).

2j/2j', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.1, 193.8, 182.0, 179.5, 160.1, 159.5, 140.2, 139.9, 139.4, 129.9, 129.5, 129.5, 120.5, 119.2, 119.2, 118.6, 118.2, 113.0, 112.8, 112.8, 112.5, 111.2, 110.7, 55.5, 55.3, 55.2, 55.2, 55.1, 46.5, 46.2, 46.0, 37.5, 37.1. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_4S_2$ $[M+Na]^+$ 461.0852, found 461.0854.

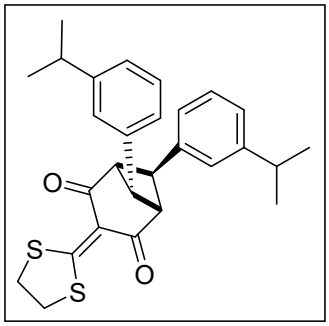
(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-methoxyphenyl)bicyclo[3.2.0]heptane-2,4-dione (3j)



3j (44.5 mg, 34% yield) as yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.04 (t, *J* = 7.8 Hz, 2H), 6.63 (d, *J* = 7.8 Hz, 2H), 6.61-6.60 (m, 2H), 6.50 (s, 2H), 4.01 (d, *J* = 3.6 Hz, 2H), 3.63 (s, 6H), 3.62 (d, *J* = 4.2 Hz, 2H), 3.57 (s, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.3, 183.9, 159.1, 140.8, 128.8, 1 21.1, 120.4, 113.6, 111.9, 55.0, 48.0, 47.1, 37.5. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_4S_2$ $[M+Na]^+$ 461.0852, found 461.0852.

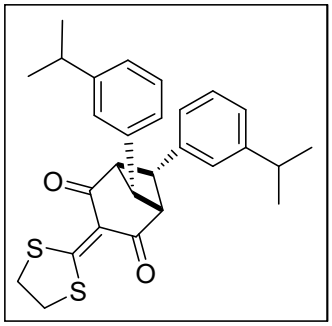
(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-isopropylphenyl)bicyclo[3.1.1] heptane-2,4-dione (2k)



2k (34.7 mg, 25% yield) as yellow solid. mp: 149-150 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 9.5 Hz, 2H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.85 (s, 1H), 6.8 2 (d, *J* = 7.0 Hz, 1H), 4.41 (t, *J* = 6.5 Hz, 1H), 3.91 (d, *J* = 6.5 Hz, 2H), 3.80 (s, 1H), 3.3 5-3.24 (m, 4H), 2.98-2.90 (m, 1H), 2.82-2.74 (m, 1H), 1.28 (d, *J* = 7.0 Hz, 6H), 1.15 (d, *J* = 7.0 Hz, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 181.5, 149.6, 148.8, 138.7, 138.3, 128.8, 128.3, 125.4, 125.1, 124.4, 124.3, 124.0, 123.3, 119.5, 55.6, 46.5, 46.2, 37.4, 34.2, 34.0, 24.0, 23.9. **HRMS** (ESI, m/z): Calculated for $C_{28}H_{30}O_2S_2$ $[M+Na]^+$ 4 85.1579, found 485.1586.

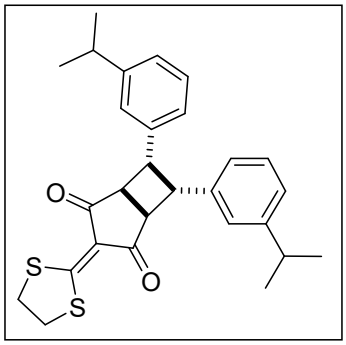
(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-isopropylphenyl)bicyclo[3.1.1] heptane-2,4-dione (2k')



2k' (33.3 mg, 24% yield) as yellow solid. mp: 156-157 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (t, *J* = 7.5 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.93 (s, 2H), 6.90 (d, *J* = 8.0 Hz, 2H), 4.21 (t, *J* = 6.0 Hz, 2H), 4.14 (t, *J* = 6.0 Hz, 2H), 3.06 (s, 4H), 2.84-2.76 (m, 2H), 1.16 (d, *J* = 7.0 Hz, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.0, 178.8, 148.8, 137.9, 128.3, 124.4, 124.4, 123.7, 120.8, 55.3, 46.1, 37.0, 34.0, 23.8. **HRMS** (ESI, m/z): Calculated for $C_{28}H_{30}O_2S_2$ $[M+Na]^+$ 485.1579, found 485.1583.

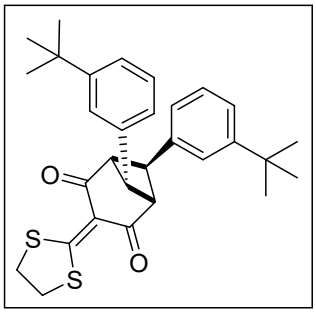
(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-isopropylphenyl)bicyclo[3.2.0]heptane-2,4-dione (3k)



3k (63.8 mg, 46% yield) as brown oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.03 (t, *J* = 7.2 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 4H), 6.67 (s, 2H), 4.02 (d, *J* = 4.2 Hz, 2H), 3.64 (d, *J* = 4.2 Hz, 2H), 3.51 (s, 4H), 2.70-2.63 (m, 2H), 1.03-1.01 (m, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.6, 183.6, 148.1, 139.0, 127.7, 126.3, 125.2, 124.0, 121.2, 47.9, 47.2, 37.5, 33.8, 23.7. **HRMS** (ESI, m/z): Calculated for $C_{28}H_{30}O_2S_2$ $[M+Na]^+$ 485.1579, found 485.1582.

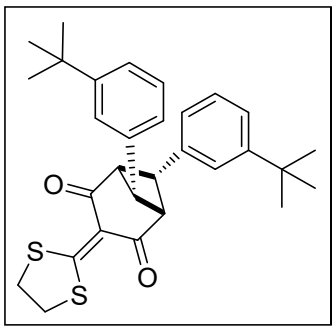
(1*R*,5*S*,6*R*,7*S*)-6,7-bis(3-(*tert*-butyl)phenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]heptane-2,4-dione (2l)



2l (28.7 mg, 19% yield) as yellow solid. mp: 174-175 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.36 (d, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 6.0 Hz, 2H), 7.01 (s, 1H), 6.82 (d, *J* = 6.0 Hz, 1H), 4.44 (t, *J* = 6. 0 Hz, 1H), 3.92 (d, *J* = 6.0 Hz, 2H), 3.82 (s, 1H), 3.33-3.29 (m, 2H), 3.28-3.24 (m, 2H), 1.35 (s, 9H), 1.22 (s, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 181.4, 151.8, 151.0, 138.3, 138.0, 128.4, 128.1, 124.2, 124.0, 123.9, 123.2, 123.0, 123.0, 119.5, 55.6, 46.6, 46.3, 37.4, 34.8, 34.6, 31.4, 31.2. **HRMS** (ESI, m/z): Calculated for $C_{30}H_{34}O_2S_2$ $[M+Na]^+$ 513.1892, found 513.1880.

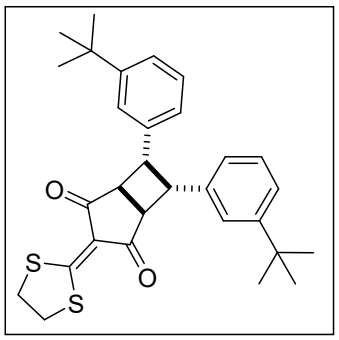
(1*r*,5*s*,6*R*,7*S*)-6,7-bis(3-(*tert*-butyl)phenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]heptane-2,4-dione (2l')



2l' (39.0 mg, 26% yield) as yellow solid. mp: 191-192 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.15-7.11 (m, 4H), 7.08 (s, 2H), 6.91 (d, *J* = 6.5 Hz, 2 H), 4.23 (t, *J* = 5.5 Hz, 2H), 4.15 (t, *J* = 6.0 Hz, 2H), 3.04 (s, 4H), 1.23 (s, 18H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.0, 178.7, 151.0, 137.5, 128.1, 123.5, 123.4, 123.1, 12 0.8, 55.3, 46.2, 37.0, 34.6, 31.2. **HRMS** (ESI, m/z): Calculated for $C_{30}H_{34}O_2S_2$ $[M+Na]^+$ 513.1892, found 513.1885.

(1*R*,5*S*,7*S*)-6,7-bis(3-(*tert*-butyl)phenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.2.0]heptane-2,4-dione (3l)

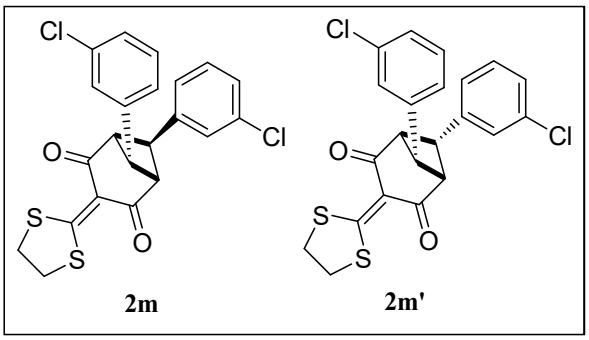


3l (66.2 mg, 45% yield) as yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.09-7.03 (m, 4H), 6.91 (d, *J* = 7.0 Hz, 2H), 6.76 (s, 2 H), 4.06 (d, *J* = 4.0 Hz, 2H), 3.65 (d, *J* = 4.0 Hz, 2H), 3.57 (s, 4H), 1.07 (s, 18H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.8, 183.5, 150.4, 138.9, 127.6, 125.5, 124.9, 123.0, 12 1.5, 48.3, 47.4, 37.6, 34.3, 31.2. **HRMS** (ESI, m/z): Calculated for $C_{30}H_{34}O_2S_2$ [M+Na] $^+$ 513.1892, found 513.1890.

(1*R*,5*S*,6*R*,7*S*)-6,7-bis(3-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]he ptane-2,4-dione (2m)

(1*r*,5*s*,6*R*,7*S*)-6,7-bis(3-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]hep tane-2,4-dione (2m')



2m/**2m'** (45.5 mg, 34% yield) as yellow solid. mp: 215-216 ℃, cannot be separated b y column chromatography.

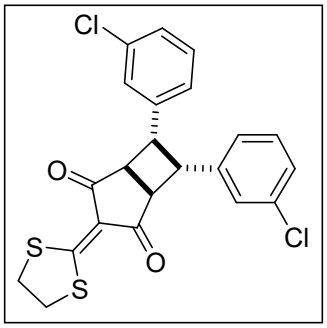
2m, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.30 (m, 3H), 7.17-7.07 (m, 5H), 4.30 (t, *J* = 6.5 Hz, 1H), 3.79 (s, 1H), 3.36 (d, *J* = 3.5 Hz, 4H), 3.17 (s, 2H).

2m', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.44 (s, 2H), 7.00 (s, 2H), 6.96 (d, *J* = 7.5 Hz, 2H), 6.88 (d, *J* = 7.5 Hz, 2H), 4.16 (t, *J* = 5.5 Hz, 2H), 4.11 (t, *J* = 5.5 Hz, 2H), 3.87 (d, *J* = 6.5 Hz, 4H).

2m/2m', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.2, 193.0, 183.3, 181.1, 140.4, 140.1, 139.7 , 135.0, 134.4, 130.2, 129.8, 127.5, 127.3, 127.0, 126.9, 126.4, 126.0, 125.2, 124.4, 12 4.0, 118.7, 55.2, 54.8, 46.2, 45.6, 45.5, 37.6, 37.2. **HRMS** (ESI, m/z): Calculated for C_{22}

$H_{16}Cl_2O_2S_2$ $[M+Na]^+$ 468.9861, found 468.9857.

(1*R*,5*S*,7*S*)-6,7-bis(3-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.2.0]heptane-2,4-dione (3m)

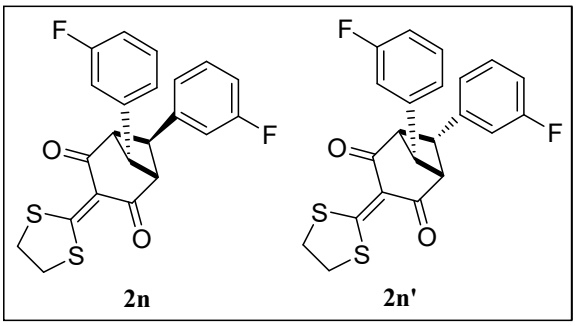


3m (50.8 mg, 38% yield) as yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.07-7.03 (m, 4H), 7.00 (s, 2H), 6.85-6.82 (m, 2H), 4.00 (d, *J* = 4.0 Hz, 2H), 3.61 (d, *J* = 4.0 Hz, 2H), 3.58 (s, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 199.8, 184.8, 140.8, 133.9, 129.2, 128.0, 126.6, 126.1, 120.9, 47.5, 46.7, 37.7. **HR MS** (ESI, m/z): Calculated for $C_{22}H_{16}Cl_2O_2S_2$ $[M+Na]^+$ 468.9861, found 468.9851.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-fluorophenyl)bicyclo[3.1.1]heptane-2,4-dione (2n)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-fluorophenyl)bicyclo[3.1.1]heptane-2,4-dione (2n')



2n/**2n'** (36.0 mg, 29% yield) as yellow solid. mp: 182-183 ℃, cannot be separated by column chromatography.

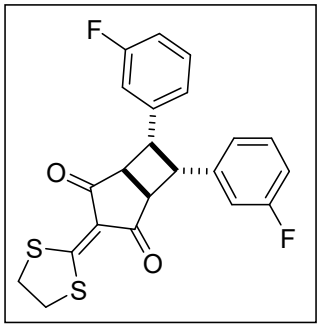
2n, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.42-7.38 (m, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.02 (t, *J* = 8.5 Hz, 1H), 6.81-6.77 (m, 4H), 6.71 (d, *J* = 9.0 Hz, 1H), 4.32 (t, *J* = 6.0 Hz, 1H), 3.87 (d, *J* = 6.5 Hz, 2H), 3.80 (s, 1H), 3.36-3.31 (m, 4H).

2n', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.20-7.13 (m, 5H), 6.86 (d, *J* = 7.5 Hz, 2H), 6.77 (s, 1H), 4.19 (t, *J* = 6.0 Hz, 2H), 4.12 (t, *J* = 5.5 Hz, 2H), 3.15 (s, 4H).

2n/2n', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.2, 193.1, 183.1, 180.8, 163.1, 162.6, 141.0, 140.9, 140.6, 140.2, 130.4, 130.0, 122.6, 121.8, 121.5, 119.8, 118.7, 114.2, 114.1, 1

13.6, 113.6, 113.2, 112.9, 55.2, 54.8, 46.1, 45.7, 45.4, 37.5, 37.1. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{16}F_2O_2S_2$ $[M+Na]^+$ 437.0452, found 437.0452.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-fluorophenyl)bicyclo[3.2.0]hepta ne-2,4-dione (3n)

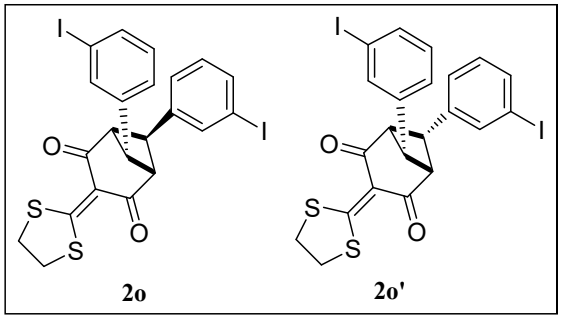


3n (38.5 mg, 31% yield) as yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.11-7.06 (m, 2H), 6.78-6.74 (m, 4H), 6.70 (t, *J* = 2.0 Hz, 1H), 6.68 (t, *J* = 2.0 Hz, 1H), 4.03 (d, *J* = 4.5 Hz, 2H), 3.61 (d, *J* = 4.5 Hz, 2H), 3. 58 (s, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 199.8, 184.7, 162.5, 141.4, 129.5, 123.6, 1 21.0, 114.8, 113.3, 47.6, 46.8, 37.6. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{16}F_2O_2S_2$ [$M+Na]^+$ 437.0452, found 437.0459.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-iodophenyl)bicyclo[3.1.1]hept ane-2,4-dione(2o)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-iodophenyl)bicyclo[3.1.1]hepta ne-2,4-dione (2o')



2o/**2o'** (45.4 mg, 24% yield) as yellow solid. mp: 151-153 ℃, cannot be separated by column chromatography.

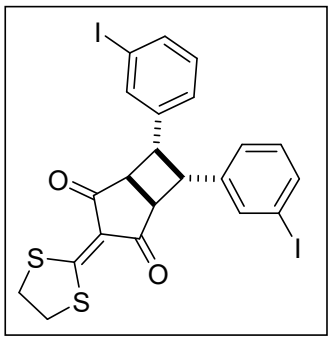
2o, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 8.5 Hz, 1H), 7.41 (d, *J* = 7.0 Hz, 1H), 7.35 (s, 1H), 7.16 (t, *J* = 8.0 Hz, 1H), 6.96 (d, *J* = 7.5 Hz, 1H), 6.92 (t, *J* = 8.0 Hz, 1H), 4.28 (t, *J* = 6.5 Hz, 1H), 3.84 (d, *J* = 6.5 Hz, 2 H), 3.76 (s, 1H), 3.37-3.34 (m, 4H).

2o', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.60 (s, 1H),

7.05-7.02 (m, 5H), 4.08 (t, *J* = 6.0 Hz, 4H), 3.73 (s, 4H).

2o/2o', **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.2, 183.3, 140.7, 140.5, 136.3, 136.2, 136.1, 135.8, 135.8, 135.2, 134.9, 130.6, 130.1, 126.3, 125.5, 125.1, 118.7, 94.9, 94.5, 60.4, 55.1, 54.8, 46.0, 45.4, 45.3, 37.6, 37.3, 21.0, 15.2, 14.2. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{17}I_2O_2S_2$ $[M+Na]^+$ 630.8754, found 630.8760.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(3-iodophenyl)bicyclo[3.2.0]heptane-2,4-dione (3o)

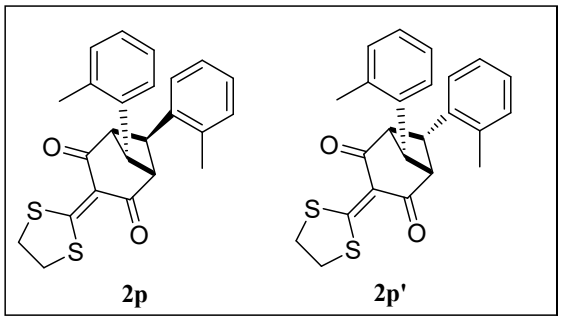


3o (62.4 mg, 33% yield) as yellow solid. mp: 198-200 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.5 Hz, 2H), 7.34 (s, 2H), 6.89 (d, *J* = 7.5 Hz, 2H), 6.85 (t, *J* = 7.5 Hz, 2H), 3.95 (d, *J* = 4.0 Hz, 2H), 3.58 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 199.8, 184.7, 141.0, 137.0, 135.5, 129.6, 127.2, 121.0, 94.0, 47.3, 46.6, 37.7. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{17}I_2O_2S_2$ $[M+Na]^+$ 630.8754, found 630.8758.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-o-tolylbicyclo[3.1.1]heptane-2,4-dione (2p)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-o-tolylbicyclo[3.1.1]heptane-2,4-dione (2p')

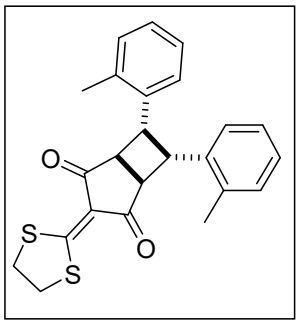


2p/**2p'** (34.1 mg, 28% yield) as yellow solid. mp: 88-90 ℃, cannot be separated by column chromatography.

2p, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.2 Hz, 1H), 7.26 (d, *J* = 3.0 Hz, 2H),

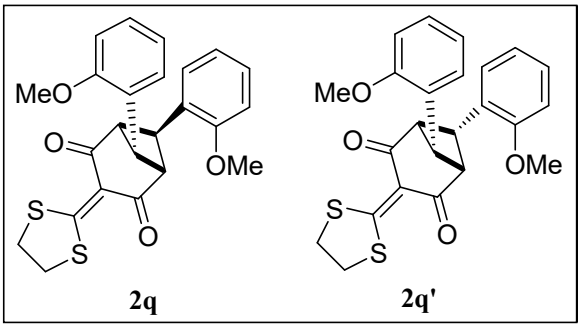
7.04 (s, 1H), 7.02 (t, *J* = 4.8 Hz, 3H), 6.94 (d, *J* = 7.8 Hz, 1H), 4.46 (t, *J* = 6.0 Hz, 1H), 3.89 (d, *J* = 6.0 Hz, 2H), 3.76 (s, 1H), 3.35-3.29 (m, 4H), 2.30 (s, 3H), 2.25 (s, 3H).
2p', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.05 (d, *J* = 3.0 Hz, 4H), 7.00-6.98 (m, 4H), 4.25 (t, *J* = 5.4 Hz, 2H), 4.16 (t, *J* = 5.4 Hz, 2H), 3.13 (s, 4H), 2.36 (s, 6H).
2p/2p', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 194.2, 181.9, 179.5, 137.5, 136.6, 136. 3, 136.0, 135.9, 135.8, 130.9, 130.6, 130.5, 127.3, 127.0, 126.8, 126.4, 126.2, 125.6, 1 25.5, 125.4, 120.0, 118.9, 56.1, 54.9, 47.2, 46.0, 45.7, 43.4, 37.5, 37.1, 20.2, 20.1, 19. 3. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_2$ $[M+Na]^+$ 429.0953, found 429.0950.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di-o-tolylbicyclo[3.2.0]heptane-2,4-dion e (3p)



3p (48.7 mg, 40% yield) as yellow solid. mp: 235-236 ℃.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21-7.19 (m, 2H), 7.03-6.97 (m, 4H), 6.95-6.93 (m, 2 H), 4.22 (d, *J* =4.5 Hz, 2H), 3.63 (d, *J* =4.5 Hz, 2H), 3.56 (s, 4H), 2.08 (s, 6H). **^{13}C N MR** (151 MHz, $CDCl_3$) δ 200.8, 183.7, 137.4, 135.9, 130.0, 126.9, 126.4, 125.5, 121. 5, 48.1, 44.3, 37.6, 19.6. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_2$ $[M+Na]^+$ 429. 0953, found 429.0944.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(2-methoxyphenyl)bicyclo[3.1.1] heptane-2,4-dione (2q)
(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(2-methoxyphenyl)bicyclo[3.1.1]h eptane-2,4-dione (2q')



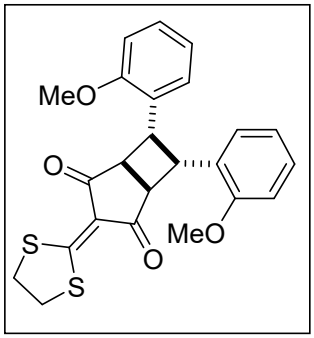
2q/**2q'** (31.5 mg, 24% yield) as yellow solid. mp: 218-219 ℃, cannot be separated by column chromatography.

2q, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.0 Hz, 1H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.05-7.01 (m, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.72 (d, *J* = 8.0 Hz, 2H), 4.35 (t, *J* = 6.5 Hz, 1H), 3.86 (d, *J* = 6.5 Hz, 6H), 3.76 (s, 3H), 3.32-3.25 (m, 4H).

2q', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.10 (t, *J* = 7.5 Hz, 2H), 6.96 (d, *J* = 7.0 Hz, 2H), 6.75 (t, *J* = 7.5 Hz, 4H), 4.20 (t, *J* = 6.0 Hz, 2H), 4.13 (t, *J* = 5.5 Hz, 2H), 3.83 (s, 6H), 3.10 (s, 4H).

2q/**2q'**, **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.0, 194.9, 177.6, 158.2, 157.6, 157.4, 128.2, 127.8, 127.8, 127.6, 127.4, 127.2, 127.0, 126.6, 126.6, 126.2, 120.8, 120.2, 120.0, 120.0, 119.6, 110.4, 110.3, 110.2, 56.0, 55.4, 55.3, 55.2, 54.7, 45.0, 44.1, 43.7, 37.3, 37.0. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_4S_2$ $[M+Na]^+$ 461.0852, found 461.0847.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-bis(2-methoxyphenyl)bicyclo[3.2.0]heptane-2,4-dione (3q)

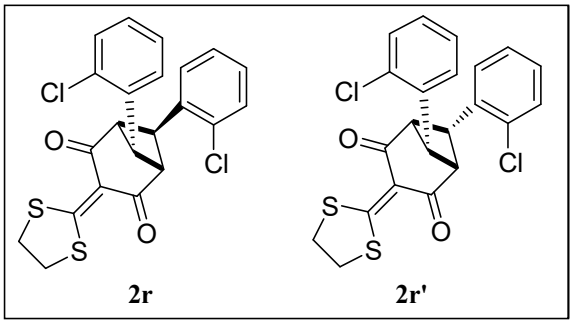


3q (53.9 mg, 41% yield) as yellow solid. mp: 218-219 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14-7.12 (m, 2H), 7.00-6.96 (m, 2H), 6.74 (t, *J* = 7.5 Hz, 2H), 6.48 (d, *J* = 8.0 Hz, 2H), 4.25 (d, *J* = 4.0 Hz, 2H), 3.73 (d, *J* = 4.0 Hz, 2H), 3.52 (s, 4H), 3.49 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 201.6, 182.8, 156.7, 128.6, 127.8, 127.2, 121.8, 119.3, 109.2, 54.6, 46.7, 43.0, 37.4. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_4S_2$ $[M+Na]^+$ 461.0852, found 461.0848.

(1*R*,5*S*,6*R*,7*S*)-6,7-bis(2-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]heptane-2,4-dione (2r)

(1*r*,5*s*,6*R*,7*S*)-6,7-bis(2-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]heptane-2,4-dione (2r')



2r **2r'**

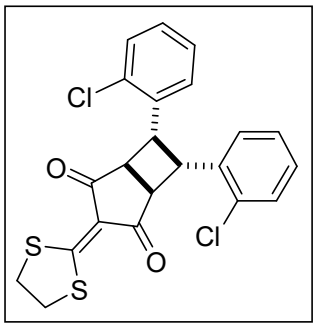
2r/**2r'** (49.5 mg, 37% yield) as yellow solid. mp: 210-211 ℃, cannot be separated by column chromatography.

2r, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.99 (d, *J* = 16.2 Hz, 0.5H), 7.67 (d, *J* = 7.8 Hz, 0.5 H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.2 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1.5H), 7.03 (d, *J* = 7.2 Hz, 1.5H), 6.96 (d, *J* = 15.6 Hz, 1H), 4.40 (t, *J* = 6.0 Hz, 1H), 4.05 (d, *J* = 6.0 Hz, 2H), 3.90 (s, 1H), 3.38-3.32 (m, 4H).

2r', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.8 Hz, 2H), 7.12-7.07 (m, 6H), 4.45 (t, *J* = 5.4 Hz, 2H), 4.22 (t, *J* = 5.4 Hz, 2H), 3.18 (s, 4H).

2r/2r', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.4, 193.5, 180.6, 135.1, 133.6, 130.2, 129.9, 129.8, 128.7, 128.4, 128.4, 128.4, 128.0, 127.2, 127.1, 126.5, 126.4, 119.8, 60.4, 55.7, 54.3, 46.7, 46.0, 45.6, 37.9, 37.6, 37.2, 14.2. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{16}Cl_2O_2S_2$ $[M+Na]^+$ 468.9861, found 468.9861.

(1*R*,5*S*,7*S*)-6,7-bis(2-chlorophenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.2.0]hepta ne-2,4-dione (3r)



3r (57.5 mg, 43% yield) as yellow solid. mp: 171-173 ℃.

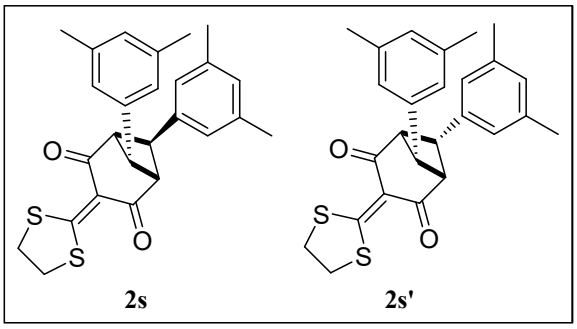
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23-7.22 (m, 2H), 7.14-7.12 (m, 2H), 7.07-7.04 (m, 2 H), 7.01-6.98 (m, 2H), 4.54 (d, *J* = 4.2 Hz, 2H), 3.65 (d, *J* =3.6 Hz, 2H), 3.58 (s, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 200.0, 184.8, 136.2, 134.4, 129.3, 128.6, 127.8, 126.0, 121.1, 46.9, 44.2, 37.7. **HRMS** (ESI, m/z): Calculated for $C_{22}H_{16}Cl_2O_2S_2$ $[M+Na]^+$ 46 8.9861, found 468.9861.

(1*R*,5*S*,6*R*,7*S*)-6,7-bis(3,5-dimethylphenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.

1]heptane-2,4-dione (2s)

(1*r*,5*s*,6*R*,7*S*)-6,7-bis(3,5-dimethylphenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.1.1]heptane-2,4-dione (2s')



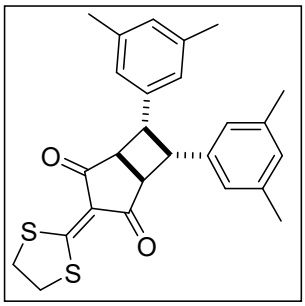
2s/**2s'** (40.4 mg, 31% yield) as yellow solid. mp: 209-210 ℃, cannot be separated by column chromatography.

2s, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.06 (s, 2H), 6.93 (s, 1H), 6.71 (s, 1H), 6.61 (s, 2H), 4.31 (t, *J* = 6.0 Hz, 1H), 3.86 (d, *J* = 6.0 Hz, 2H), 3.71 (s, 1H), 3.32-3.27 (m, 4H), 2.20 (s, 12H).

2s', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 6.73 (s, 2H), 6.68 (s, 4H), 4.09 (t, *J* = 4.8 Hz, 2H), 4.06 (t, *J* = 4.8 Hz, 2H), 3.09 (s, 4H), 2.34 (s, 6H), 2.18 (s, 6H).

2s/2s', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 194.0, 181.4, 178.6, 138.6, 138.3, 138.2, 137.8, 137.7, 128.6, 128.1, 128.0, 125.0, 124.8, 123.9, 123.5, 120.6, 119.3, 55.5, 55.1, 46.5, 46.0, 45.9, 37.4, 37.0, 21.3, 21.2, 21.2. **HRMS** (ESI, m/z): Calculated for $C_{26}H_{26}O_2S_2$ $[M+Na]^+$ 457.1266, found 457.1274.

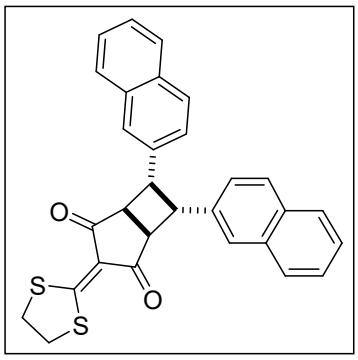
(1*R*,5*S*,7*S*)-6,7-bis(3,5-dimethylphenyl)-3-(1,3-dithiolan-2-ylidene)bicyclo[3.2.0]heptane-2,4-dione (3s)



3s (57.3 mg, 44% yield) as yellow solid. mp: 241-243 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.66 (s, 2H), 6.59 (s, 4H), 3.93 (d, *J* = 4.0 Hz, 2H), 3.61 (d, *J* = 3.5 Hz, 2H), 3.55 (s, 4H), 2.14 (s, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.8, 183.3, 139.0, 136.9, 127.6, 126.0, 121.5, 48.0, 47.2, 37.5, 21.1. **HRMS** (ESI, m/z): Calculated for $C_{26}H_{26}O_2S_2$ $[M+Na]^+$ 457.1266, found 457.1254.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di(naphthalen-2-yl)bicyclo[3.2.0]hepta ne-2,4-dione (3t)

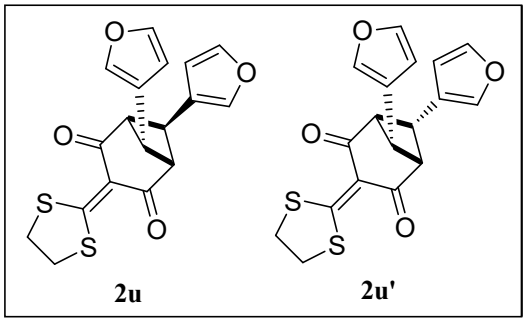


3t (43.0 mg, 30% yield) as yellow solid. mp: 157-159 ℃.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.8 Hz, 2H), 7.66 (s, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.38-7.36 (m, 2H), 7.35-7.32 (m, 2H), 7.00 (d, *J* = 1.8 Hz, 1H), 6.99 (d, *J* = 1.8 Hz, 1H), 4.31 (d, *J* = 3.6 Hz, 2H), 3.82 (d, *J* = 4.2 Hz, 2H), 3.59 (s, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.5, 184.1, 136.9, 133.1, 131.9, 127.6, 127.6, 127.4, 126.5, 126.2, 125.8, 125.4, 121.4, 48.4, 47.4, 37.6. **HRMS** (ESI, m/z): Calculated for $C_{30}H_{22}O_2S_2$ $[M+Na]^+$ 501.0953, found 501.0955.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di(furan-3-yl)bicyclo[3.1.1]heptane-2,4-dione (2u)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di(furan-3-yl)bicyclo[3.1.1]heptane-2,4-dione (2u')



2u/**2u'** (46.2 mg, 43% yield) as yellow solid. mp 174-175 ℃.

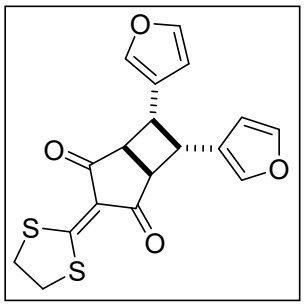
2u, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.46 (s, 1H), 7.23 (s, 1H), 7.06 (s, 1H), 6.42 (s, 1H), 6.10 (s, 1H), 4.28 (t, *J* = 6.0 Hz, 1H), 3.60 (s, 1H), 3.51 (d, *J* = 6.0 Hz, 2 H),3.40 (s, 4H).

2u', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.24 (s, 2H), 7.08 (s, 2H), 6.15 (s, 2H), 3.94 (t, *J* =6.0 Hz, 2H), 3.78 (t, *J* = 6.0 Hz, 2H), 3.30 (s, 4H).

2u//2u', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.9, 194.0, 182.1, 179.4, 143.7, 143.0, 143. 0, 139.6, 139.2, 139.0, 123.2, 122.1, 121.5, 120.7, 119.2, 110.2, 109.6, 109.4, 56.0, 55.8

, 40.1, 40.0, 39.8, 37.6, 37.3. **HRMS** (ESI, m/z): Calculated for $C_{18}H_{14}O_4S_2$ $[M+Na]^+$ 381.0226, found 381.0227.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di(furan-3-yl)bicyclo[3.2.0]heptane-2,4-dione (3u)

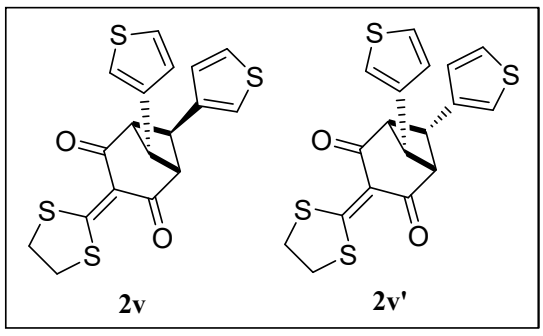


3u (44.0 mg, 41% yield) as yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 (t, *J* = 1.8 Hz, 2H), 7.20 (s, 2H), 6.05-6.04 (m, 2 H), 3.76 (d, *J* = 4.2 Hz, 2H), 3.57 (s, 4H), 3.36 (d, *J* = 4.2 Hz, 2H). **^{13}C NMR** (151 M Hz, $CDCl_3$) δ 200.1, 184.1, 142.9, 139.6, 123.9, 121.0, 110.5, 48.5, 38.2, 37.6. **HRMS** (ESI, m/z): Calculated for $C_{18}H_{14}O_4S_2$ $[M+Na]^+$ 381.0226, found 381.0226.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di(thiophen-3-yl)bicyclo[3.1.1]heptane-2,4-dione (2v)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di(thiophen-3-yl)bicyclo[3.1.1]heptane-2,4-dione (2v')



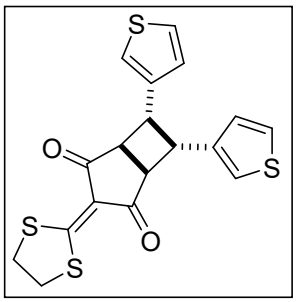
2v/**2v'** (49.1 mg, 42% yield) as yellow solid. mp: 177-178 ℃, cannot be separated by column chromatography.

2v, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.39-7.38 (m, 1H), 7.28 (t, *J* = 1.2 Hz, 1H), 7.14 (d, *J* = 3.0 Hz, 2H), 7.11 (d, *J* = 4.8 Hz, 1H), 6.76 (d, *J* = 4.8 Hz, 1H) 4.38 (t, *J* = 6.6 Hz, 1H), 3.76 (s, 1H), 3.74 (d, *J* = 6.0 Hz, 2H), 3.37-3.32 (m, 4H).

2v', **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.16-7.15 (m, 2H), 6.87 (s, 2H), 6.82 (d, *J* = 4.2 H z, 2H), 4.11 (t, *J* = 5.4 Hz, 2H), 3.98 (t, *J* = 5.4 Hz, 2H), 3.19 (s, 4H).

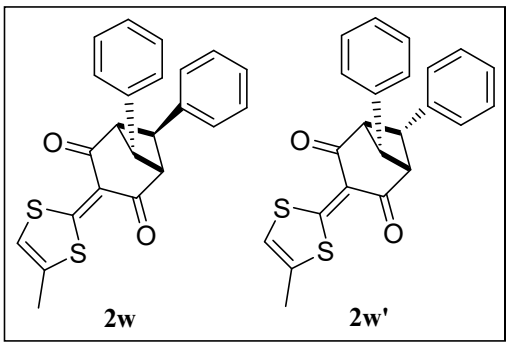
2v/2v', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.0, 194.1, 182.0, 179.3, 139.3, 139.1, 138.3, 127.2, 126.6, 126.3, 126.0, 125.9, 121.3, 120.9, 120.6, 120.5, 119.2, 56.4, 56.0, 43.7, 43.7, 43.4, 37.5, 37.2. **HRMS** (ESI, m/z): Calculated for $C_{18}H_{14}O_2S_4$ $[M+Na]^+$ 412.97 69, found 412.9789.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6,7-di(thiophen-3-yl)bicyclo[3.2.0]heptane-2,4-dione (3v)



3v (56.2 mg, 48% yield) as yellow solid. mp: 111-112 ℃.
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.07-7.06 (m, 2H), 6.88 (d, *J* = 1.2 Hz, 2H), 6.60 (d, *J* = 5.4 Hz, 2H), 4.00 (d, *J* = 3.0 Hz, 2H), 3.55 (s, 4H), 3.54 (s, 2H). **^{13}C NMR** (151 M Hz, $CDCl_3$) δ 200.2, 184.0, 140.4, 127.4, 125.2, 121.3, 121.3, 48.8, 42.9, 37.6. **HRMS** (ESI, m/z): Calculated for $C_{18}H_{14}O_2S_4$ $[M+Na]^+$ 412.9769, found 412.9774.

(1*R*,5*S*,6*R*,7*R*,*Z*)-3-(4-methyl-1,3-dithiol-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2w)
(1*r*,5*s*,6*R*,7*S*,*Z*)-3-(4-methyl-1,3-dithiol-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2w')

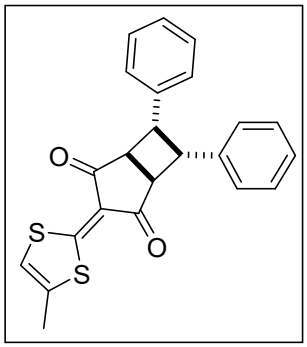


2w/**2w'** (43.3 mg, 37% yield) as brown oil, cannot be separated by column chromatography.
2w, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.0 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 5H), 6.80 (s, 1H), 4.46 (t, *J* = 6.5 Hz, 1H), 3.95-3.90 (m, 3H), 2.39 (s, 3H).

2w', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.13 (d, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 7.5 Hz, 4H), 7.07-7.04 (m, 3H), 7.01 (t, *J* = 8.0 Hz, 2H), 6.59 (s, 1H), 4.30 (t, *J* = 5.5 Hz, 2H), 4.17-4.15 (m, 2H), 2.24 (s, 3H).

2w/2w', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.5, 194.2, 193.0, 192.7, 174.1, 172.1, 139.1, 139.0, 138.8, 138.3, 138.3, 128.8, 128.3, 128.2, 127.0, 127.0, 126.2, 126.1, 126.1, 125.7, 120.0, 119.4, 115.1, 114.0, 55.0, 54.9, 54.5, 54.4, 48.8, 48.0, 48.0, 15.2, 15.0. **HR MS** (ESI, m/z): Calculated for $C_{23}H_{18}O_2S_2$ $[M+Na]^+$ 413.0640, found 413.0636.

(1*R*,5*S*,7*S*,*Z*)-3-(4-methyl-1,3-dithiol-2-ylidene)-6,7-diphenylbicyclo[3.2.0]heptane-2,4-dione (3w)

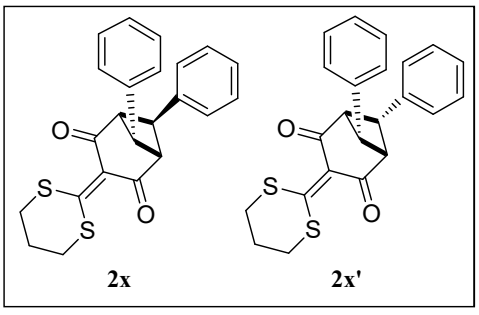


3w (29.2 mg, 25% yield) as yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.11 (t, *J* = 7.8 Hz, 4H), 7.08 (d, *J* = 1.2 Hz, 1H), 7.03 (t, *J* = 7.2 Hz, 2H), 7.00-6.99 (m, 4H), 4.05 (d, *J* = 4.8 Hz, 2H), 3.69 (d, *J* = 3.0 Hz, 2H), 2.57 (d, *J* = 1.2 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 199.9, 199.6, 175.0, 139.8, 139.5, 128.1, 127.8, 126.0, 120.2, 117.1, 48.2, 48.1, 47.1, 47.0, 15.6. **HRMS** (ESI, m/z): Calculated for $C_{23}H_{18}O_2S_2$ $[M+Na]^+$ 413.0640, found 413.0649.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithian-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2x)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithian-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2x')



2x/**2x'** (42.3 mg, 36% yield) as yellow oil, cannot be separated by column chromatography.

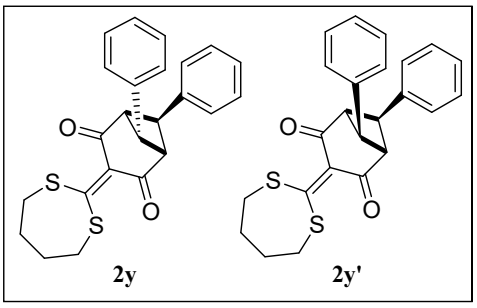
2x, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.0 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.14 (d, *J* = 7.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 4.34 (t, *J* = 6.0 Hz, 1H), 3.86 (d, *J* = 6.0 Hz, 2H), 3.81 (s, 1H), 2.88-2.83 (m, 2H), 2.81-2.75 (m, 2H), 2.26-2.19 (m, 2H).

2x', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.20 (t, *J* = 7.5 Hz, 5H), 7.10 (d, *J* = 7.5 Hz, 5H), 4.18 (t, *J* = 6.0 Hz, 2H), 4.10 (t, *J* = 5.5 Hz, 2H), 2.57 (t, *J* = 7.0 Hz, 4H), 2.08-2.02 (m, 2H).

2x/2x', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 194.3, 186.1, 183.2, 138.8, 138.3, 138.0, 128.8, 128.4, 128.3, 127.0, 127.0, 126.3, 126.3, 126.2, 125.9, 124.9, 56.2, 55.9, 46.3, 46.0, 45.9, 30.5, 30.2, 23.4, 23.3. **HRMS** (ESI, m/z): Calculated for $C_{23}H_{20}O_2S_2$ $[M+Na]^+$ 415.0797, found 415.0786.

(1*R*,5*S*,6*R*,7*S*)-3-(1,3-dithiepan-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2y)

(1*r*,5*s*,6*R*,7*S*)-3-(1,3-dithiepan-2-ylidene)-6,7-diphenylbicyclo[3.1.1]heptane-2,4-dione (2y')



2y/**2y'** (52.4 mg, 43% yield) as yellow oil, cannot be separated by column chromatography.

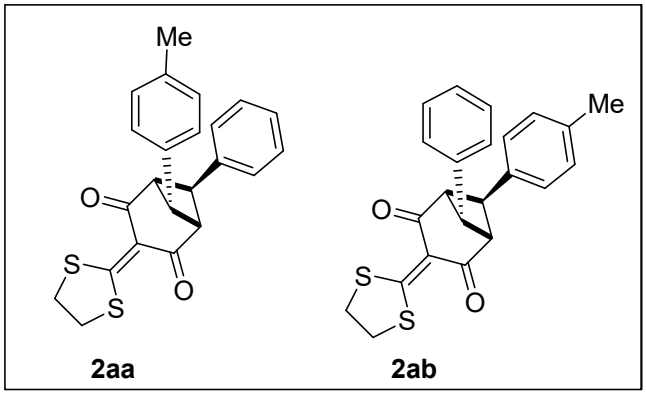
2y, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.0 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.23-7.20 (m, 2H), 7.14-7.12 (m, 1H), 7.00 (d, *J* = 8.0 Hz, 2H), 4.32 (t, *J* = 6.5 Hz, 1H), 3.89 (d, *J* = 6.0 Hz, 2H), 3.79 (s, 1H), 3.08-3.03 (m, 2H), 2.97-2.92 (m, 2H), 2.02-1.93 (m, 4H).

2y', **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.0 Hz, 5H), 7.10 (d, *J* = 7.5 Hz, 5H), 4.18-4.13 (m, 4H), 2.73 (s, 4H), 1.82 (s, 4H).

2y/2y', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 194.5, 185.1, 138.8, 138.2, 137.9, 128.8, 128.4, 128.3, 127.8, 127.1, 127.0, 127.0, 126.8, 126.4, 126.3, 126.2, 125.9, 56.6, 56.4, 45.8, 45.6, 45.5, 38.6, 38.0, 28.4, 28.3. **HRMS** (ESI, m/z): Calculated for $C_{24}H_{22}O_2S_2$ $[M+Na]^+$ 429.0953, found 429.0959.

(1*S*,5*S*,6*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6-phenyl-7-(*p*-tolyl)bicyclo[3.1.1]heptan e-2,4-dione (2aa)

(1*R*,5*R*,6*R*,7*R*)-3-(1,3-dithiolan-2-ylidene)-6-phenyl-7-(*p*-tolyl)bicyclo[3.1.1]hepta ne-2,4-dione (2ab)

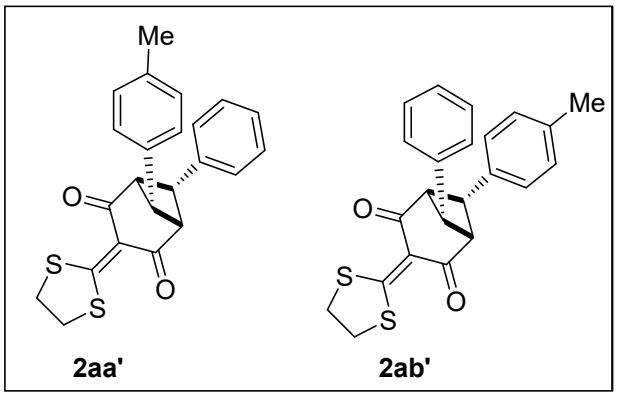


2aa/**2ab**/**2aa'**/**2ab**' (41.2 mg, 35% yield) as yellow oil, cannot be separated by column chromatography.

2aa/**2ab**, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.43-7.36 (m, 4H), 7.14-7.10 (m, 4H), 7.05-7.0 3 (m, 4H), 6.91-6.88 (m, 4H), 6.81-6.79 (m, 2H), 4.33 (t, *J* = 6.0 Hz, 1H), 4.29 (t, *J* = 6.0 Hz, 1H), 3.84 (dd, *J* = 14.0 Hz, 6.0 Hz, 2H), 3.81 (dd, *J* = 14.0 Hz, 6.0 Hz, 2H), 3. 75 (d, *J* = 7.5 Hz, 1H), 3.72 (d, *J* = 7.5 Hz, 1H), 3.33-3.23 (m, 8H), 2.31 (d, *J* = 7.5 H z, 3H), 2.26 (d, *J* = 6.0 Hz, 3H).

(1*S*,5*S*,6*R*,7*R*)-3-(1,3-dithiolan-2-ylidene)-6-phenyl-7-(*p*-tolyl)bicyclo[3.1.1]heptan e-2,4-dione (2aa')

(1*R*,5*R*,6*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6-phenyl-7-(*p*-tolyl)bicyclo[3.1.1]heptan e-2,4-dione (2ab')



2aa/**2ab**/**2aa'**/**2ab**'(41.2 mg, 35% yield) as yellow oil, cannot be separated by column chromatography.

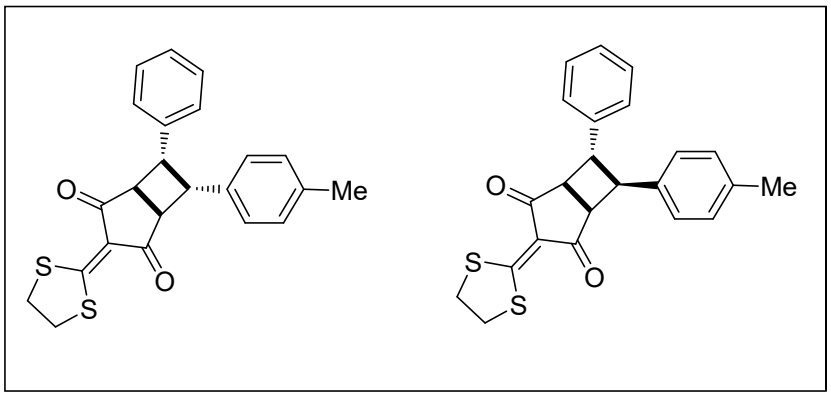
2aa'/**2ab'**, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36-7.34 (m, 2H), 7.29-7.25 (m, 2H), 7.17-7.

14 (m, 4H), 7.03-7.00 (m, 4H), 6.95-6.93 (m, 6H), 4.17-4.05 (m, 8H), 3.05-3.03 (m, 8 H), 2.17 (s, 6H), 2.16 (d, J = 6.0 Hz, 6H).

2aa/**2ab**/**2aa'**/**2ab'**, **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.5, 195.4, 195.3, 195.2, 194.3, 194.2, 194.2, 194.0, 182.1, 181.9, 181.8, 181.6, 179.6, 179.3, 179.3, 179.1, 144.0, 143.9, 143.7, 143.6, 138.8, 138.7, 138.4, 138.3, 138.0, 137.9, 136.8, 136.7, 135.9, 135.9, 135.8, 135.7, 135.6, 135.5, 135.3, 135.2, 134.8, 134.7, 129.8, 129.6, 129.5, 129.1, 129.1, 128.9, 128.9, 128.5, 128.4, 128.4, 127.1, 127.0, 126.4, 126.4, 126.3, 126.3, 126.1, 126.1, 126.0, 126.0, 125.8, 125.6, 120.6, 120.5, 120.4, 119.4, 119.3, 119.3, 119.3, 55.5, 55.5, 55.1, 55.1, 46.6, 46.6, 46.4, 46.3, 46.1, 46.1, 46.0, 45.9, 45.9, 45.8, 37.5, 37.1, 21.0, 21.0. **HRMS** (ESI, m/z): Calculated for $C_{23}H_{20}NaO_2S_2$ $[M+Na]^+$ 415.0797, found415.0791.

(1*R*,5*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6-phenyl-7-(*p*-tolyl)bicyclo[3.2.0]heptane-2,4-dione (3aa)

(1*R*,5*S*,7*R*)-3-(1,3-dithiolan-2-ylidene)-6-phenyl-7-(*p*-tolyl)bicyclo[3.2.0]heptane-2,4-dione (3ab)

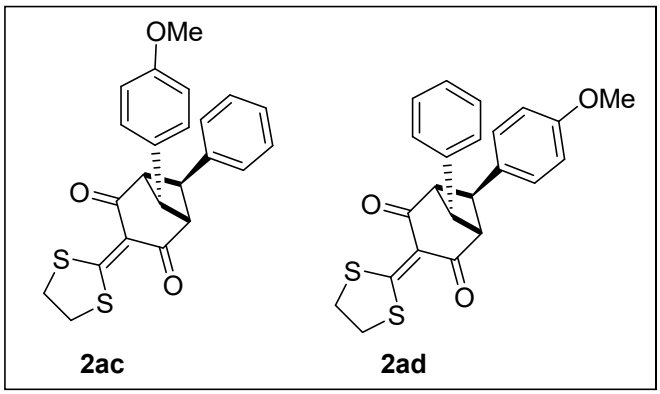


3aa/**3ab** (49.5 mg, 42% yield) as yellow oil, cannot be separated by column chromato graphy.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.11 (dd, J = 16 Hz, 6 Hz, 6H), 7.04 (d, J = 6.5 Hz, 2H), 6.99 (t, J = 7.0 Hz, 4H), 6.91 (t, J = 7.5 Hz, 3H), 6.88-6.85 (m, 3H), 4.06-3.98 (m, 4H), 3.65-3.58 (m, 4H), 3.54-3.53 (m, 8H), 2.21 (s, 3H), 2.20 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.8, 200.7, 200.7, 200.6, 184.0, 183.8, 183.6, 139.3, 139.1, 136.3, 136.1, 135.6, 135.5, 129.3, 129.2, 129.2, 129.1, 128.6, 128.5, 128.0, 127.9, 127.8, 127.7, 127.6, 126.1, 126.1, 121.3, 121.3, 121.3, 48.4, 48.3, 48.1, 48.0, 47.2, 47.2, 46.9, 46.9, 37.6, 37.6, 37.5, 22.6, 20.9, 20.9. **HRMS** (ESI, m/z): Calculated for $C_{23}H_{20}NaO_2S_2$ $[M+Na]^+$ 415.0797, found 415.0805.

(1*S*,5*S*,6*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6-(4-methoxyphenyl)-7phenylbicyclo

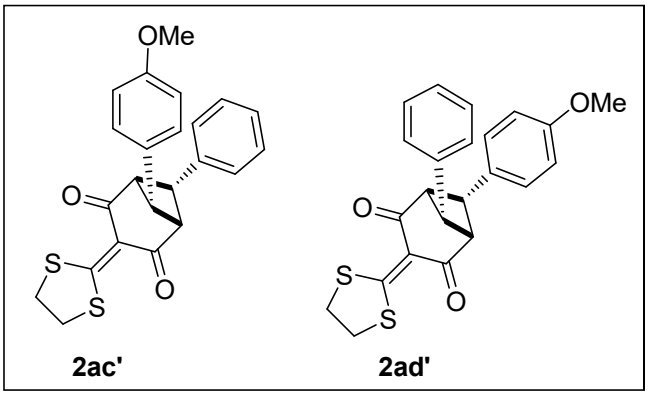
[3.1.1]heptane-2,4-dione (2ac)
(1*R*,5*R*,6*R*,7*R*)-3-(1,3-dithiolan-2-ylidene)-6-(4-methoxyphenyl)-7-phenylbicyclo [3.1.1]heptane-2,4-dione (2ad)



2ac/**2ad**/**2ac'**/**2ad**'(46.6 mg, 38% yield) as yellow oil, cannot be separated by column chromatography.

2ac/**2ad**, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.46-7.40 (m, 4H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 7.0 Hz, 2H), 6.99 (d, *J* = 9.0 Hz, 4H), 6.73 (d, *J* = 9.0 Hz, 4H), 4.38 (t, *J* = 6.0 Hz, 1H), 4.33 (t, *J* = 6.0 Hz, 1H), 3.86 (t, *J* = 5.5 Hz, 2H),3.70 (s, 3H), 3.33-3.30 (m, 4H).

(1*S*,5*S*,6*R*,7*R*)-3-(1,3-dithiolan-2-ylidene)-6-(4-methoxyphenyl)-7-phenylbicyclo [3.1.1]heptane-2,4-dione (2ac')
(1*R*,5*R*,6*S*,7*S*)-3-(1,3-dithiolan-2-ylidene)-6-(4-methoxyphenyl)-7-phenylbicyclo [3.1.1]heptane-2,4-dione (2ad')



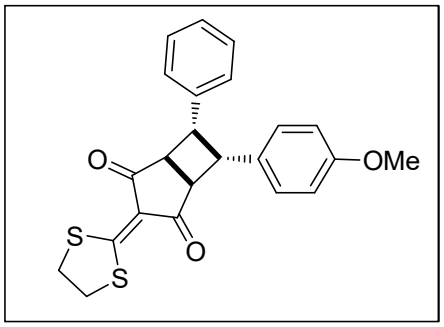
2ac/**2ad**/**2ac'**/**2ad**'(46.6 mg, 38% yield) as yellow oil, cannot be separated by column chromatography.

2ac'/**2ad'**, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.37 (t, *J* = 9.0 Hz, 2H), 7.21-7.18 (m, 4H),7.07 (d, *J* = 8.0 Hz, 4H), 6.98 (d, *J* = 6.0 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* =8.5 Hz, 2H), 6.71 (d, *J* =8.5 Hz, 2H), 4.18 (dd, *J* = 12.5 Hz, 6.0 Hz, 4H), 4.12 (t, *J* = 6.0 Hz, 4H), 3.71 (s, 3H), 3.13-3.08 (m, 4H).

2ac/**2ad**/**2ac'**/**2ad**', **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.4, 195.3, 194.2, 181.9, 181.9,

179.4, 158.6, 158.0, 157.9, 138.8, 138.4, 138.0, 130.7, 130.2, 130.0, 128.8, 128.4, 128.1 , 127.3, 127.1, 127.0, 126.9, 126.4, 126.3, 126.1, 125.7, 120.5, 119.3, 114.3, 113.9, 58.4 , 55.6, 55.4, 55.3, 55.1, 55.1, 46.5, 46.1, 46.0, 46.0, 45.6, 45.5, 37.5, 37.1.0. **HRMS** (ESI, m/z): Calculated for $C_{23}H_{20}NaO_3S_2$ $[M+Na]^+$ 431.0746, found 431.0738.

(1*S*,5*R*,6*S*)-3-(1,3-dithiolan-2-ylidene)-6-(4-methoxyphenyl)-7-phenylbicyclo[3.2.0]heptane-2,4-dione (3ac)

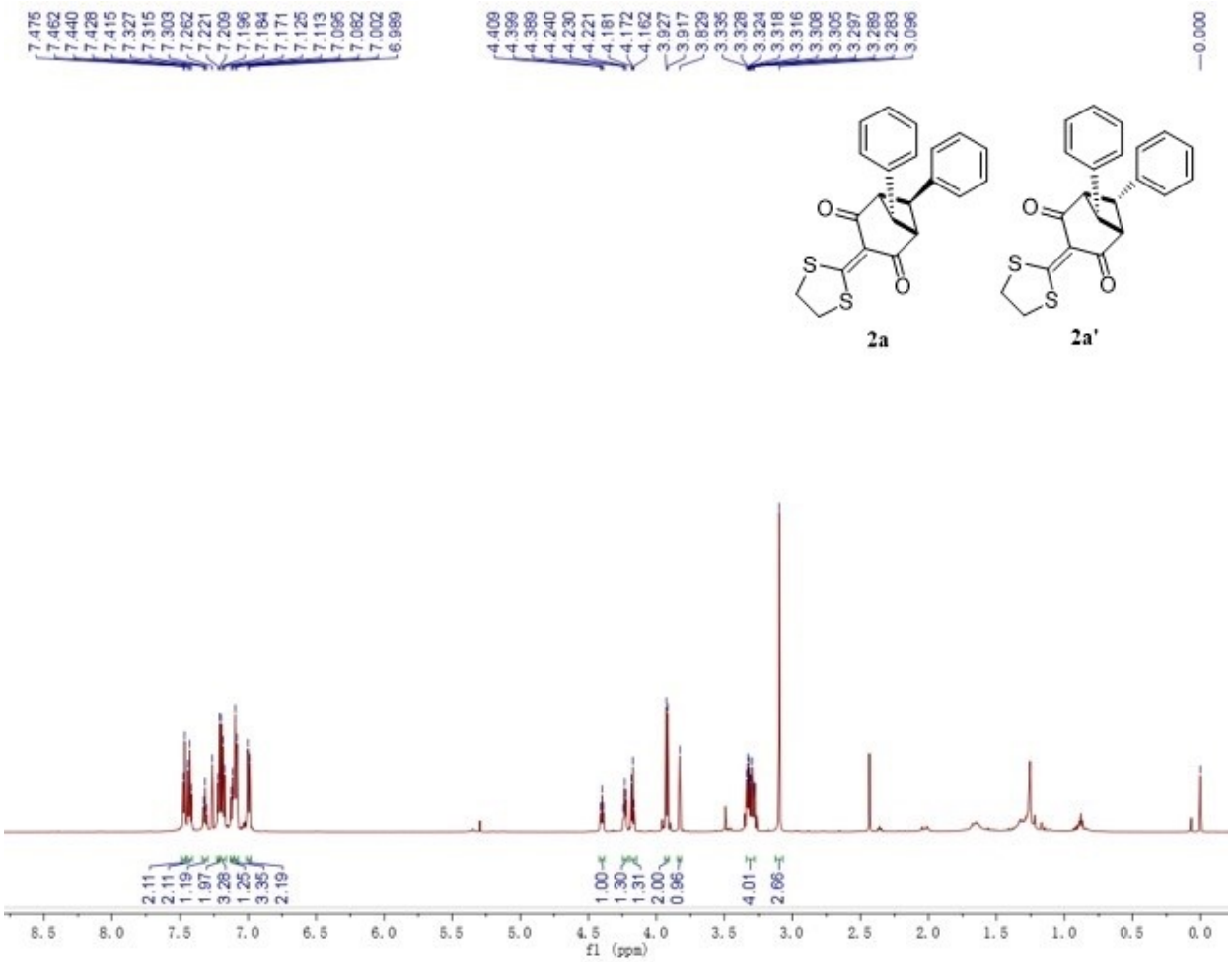


3ac/3ad (57.6 mg, 47% yield) as yellow oil, cannot be separated by column chromato graphy.

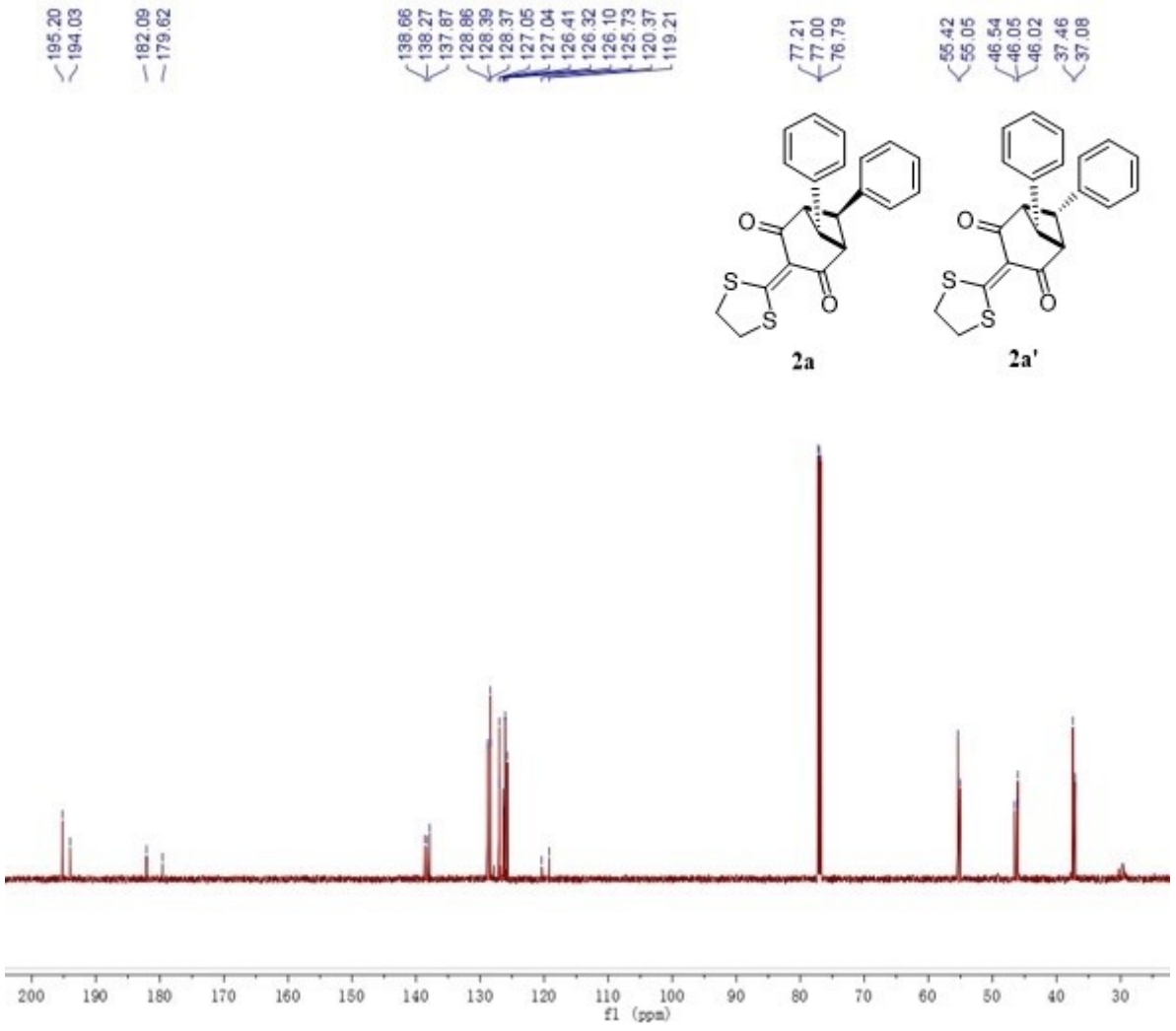
3ac, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.11 (d, *J* = 7.5 Hz, 2H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.98(d, *J* = 7.5 Hz, 2H), 6.88 (t, *J* = 8.5 Hz, 2H), 6.64 (d, *J* = 8.5 Hz, 2H), 4.04-3.98 (m, 1H), 3.77 (d, *J* = 8.5 Hz, 1H), 3.69 (s, 3H), 3.65-3.63 (m, 1H), 3.59-3.56 (m, 1H), 3.55(s, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ200.7, 200.6, 183.7, 157.9, 139.2, 131.3, 129.0, 128.0, 127.9, 126.1, 113.3, 55.1, 48.5, 47.9, 47.3, 46.7, 37.6. **HRMS** (ESI, m/z): Calculated for $C_{23}H_{20}NaO_3S_2$ $[M+Na]^+$ 431.0746, found 431.0754.

8. Copies of ^{1}H NMR and ^{13}C NMR spectra

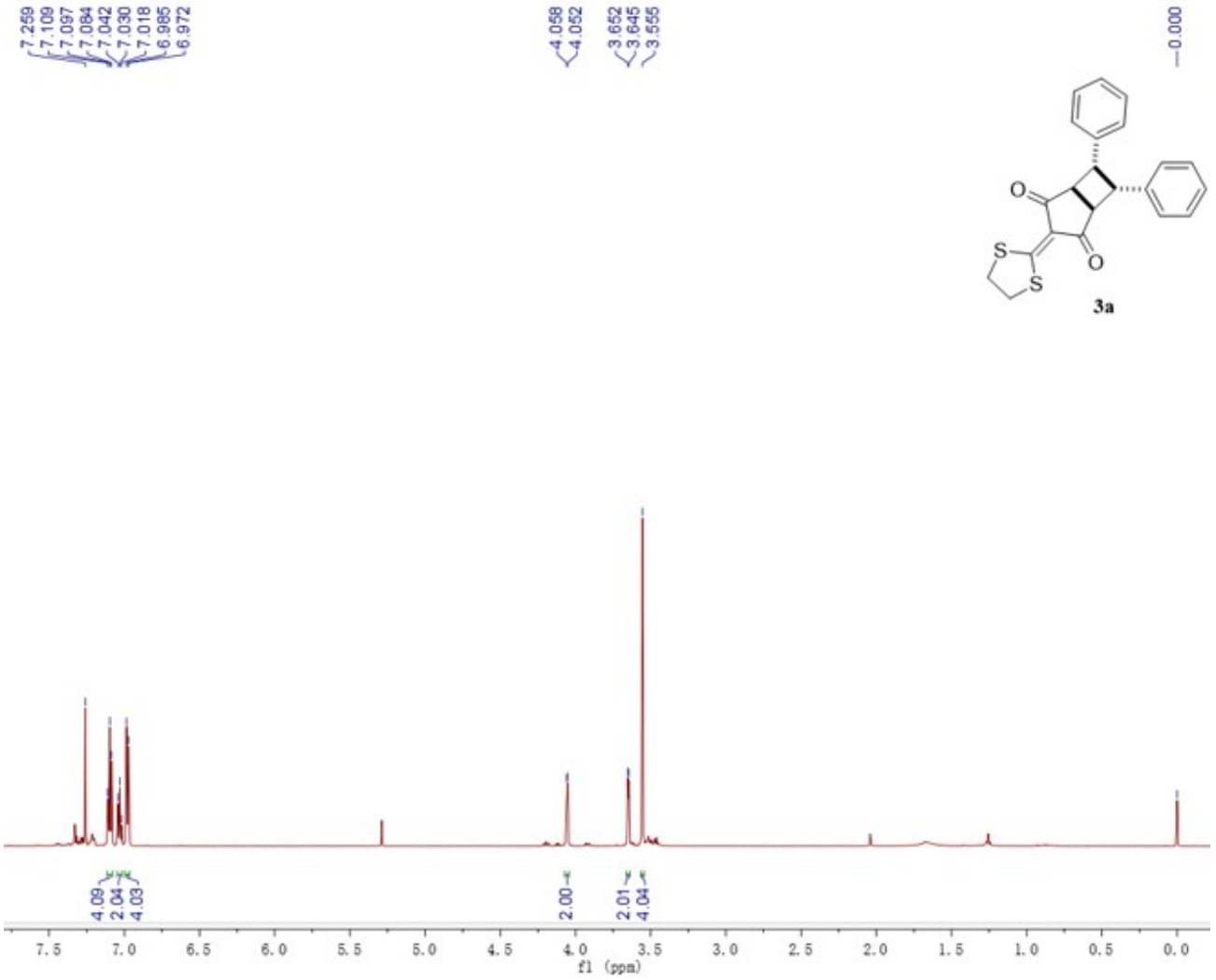
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2a/2a'



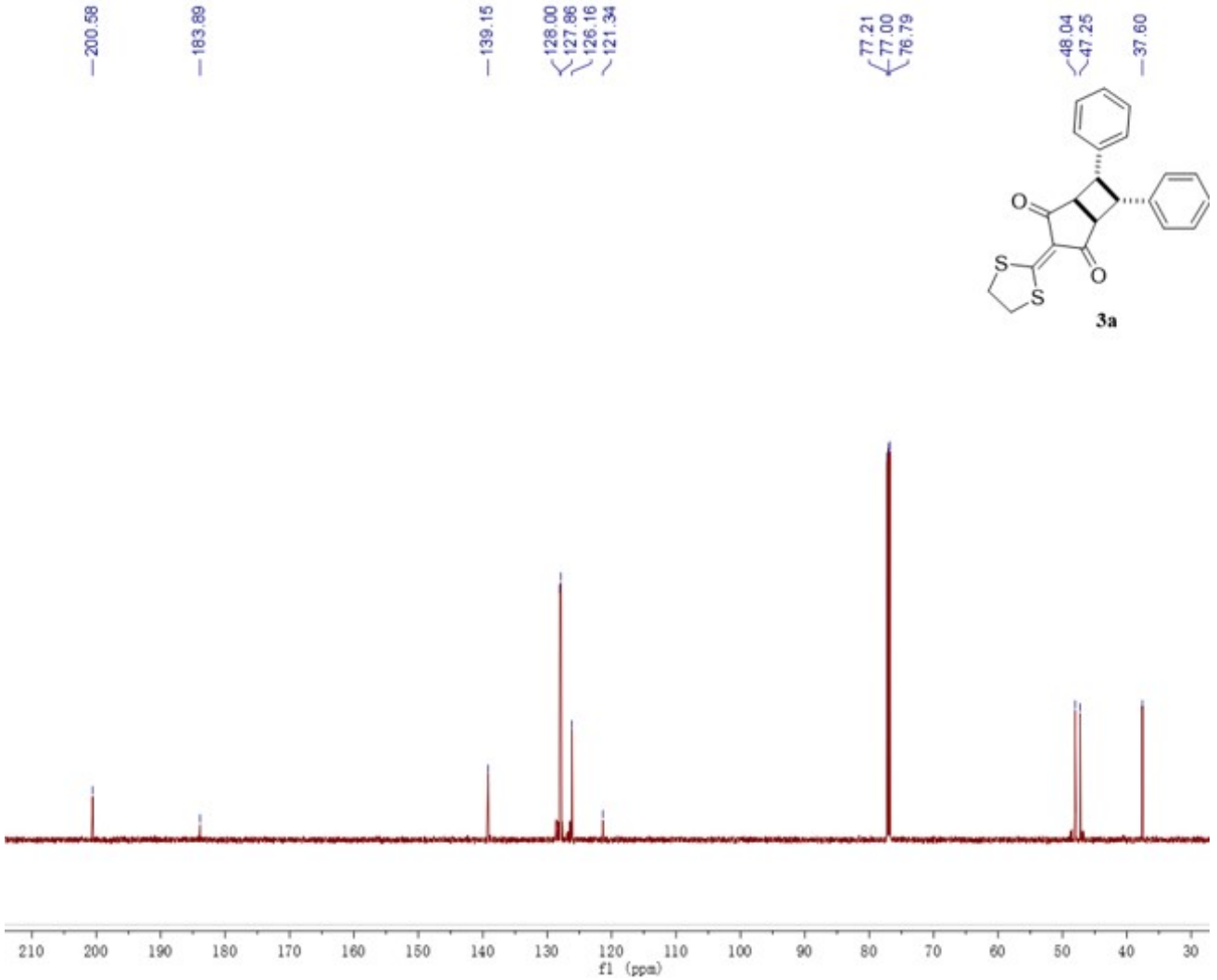
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2a/2a'



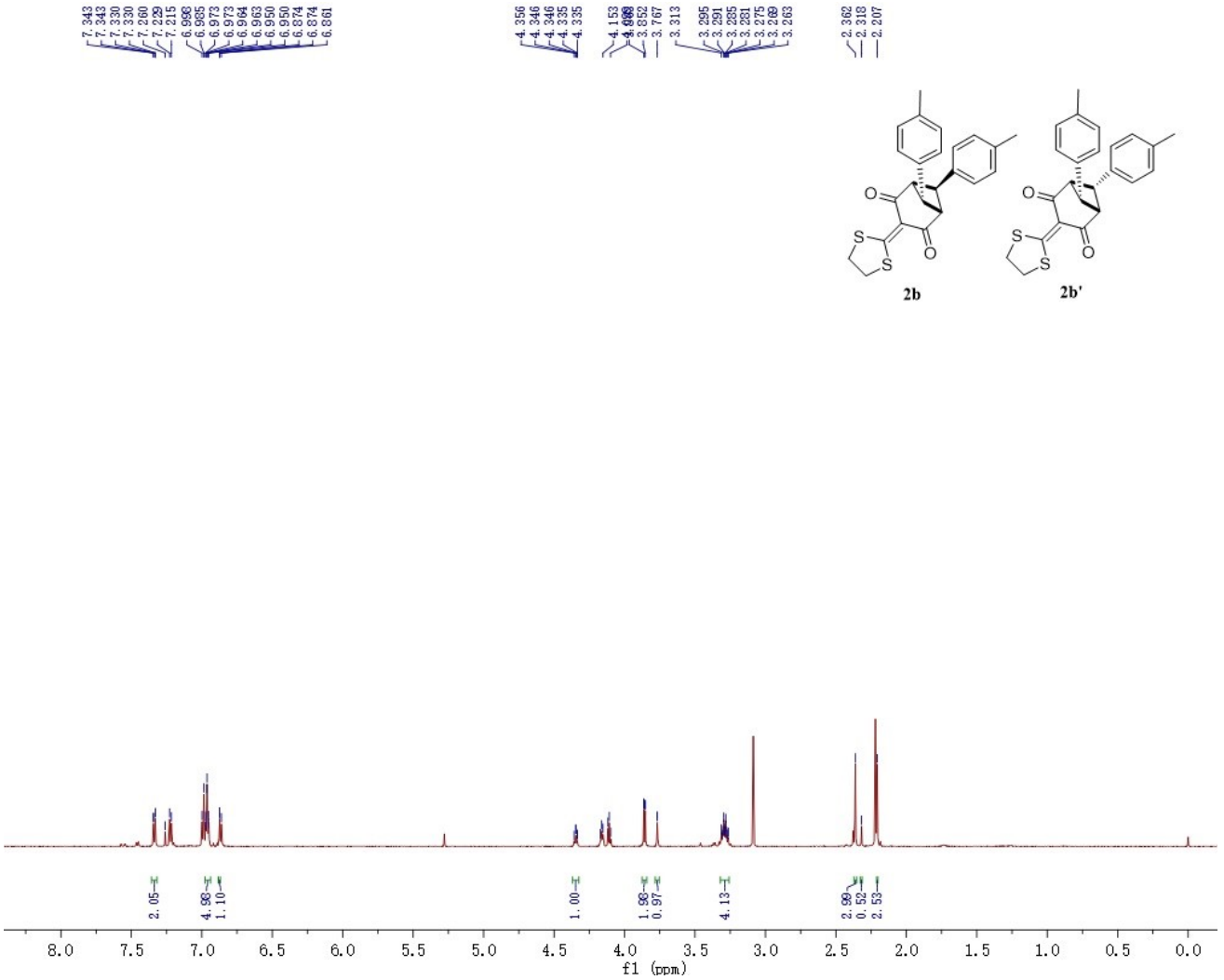
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3a



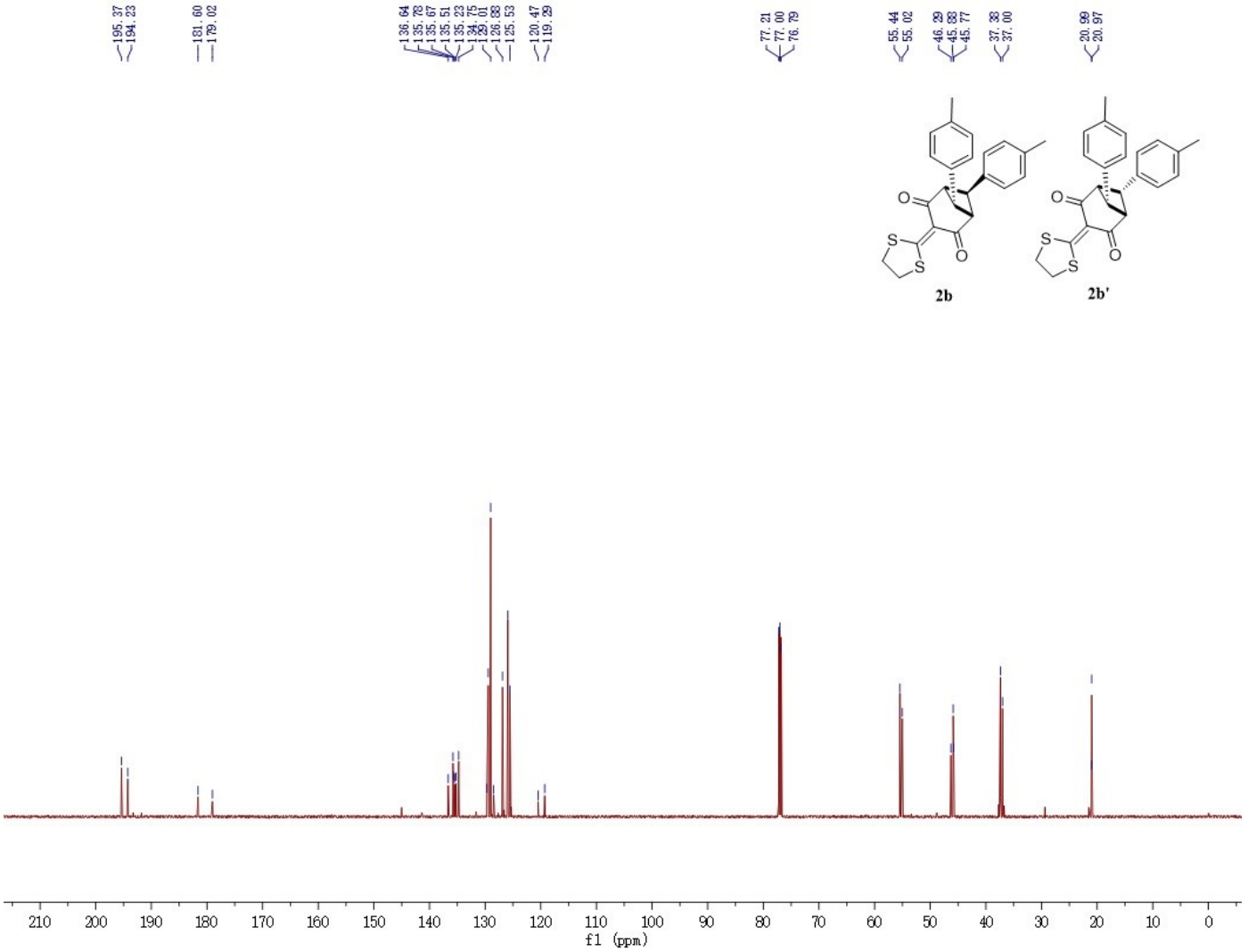
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3a



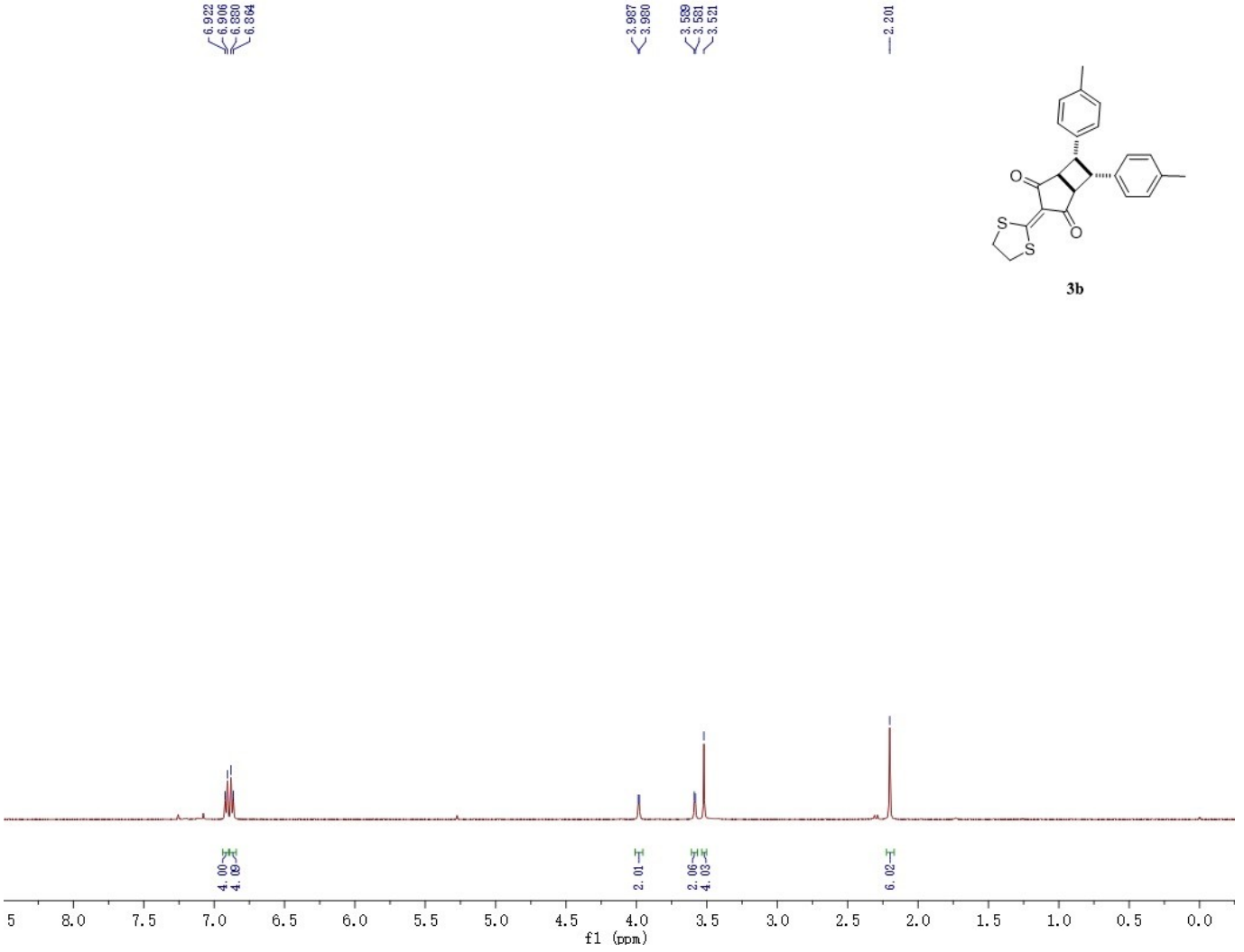
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2b/2b'



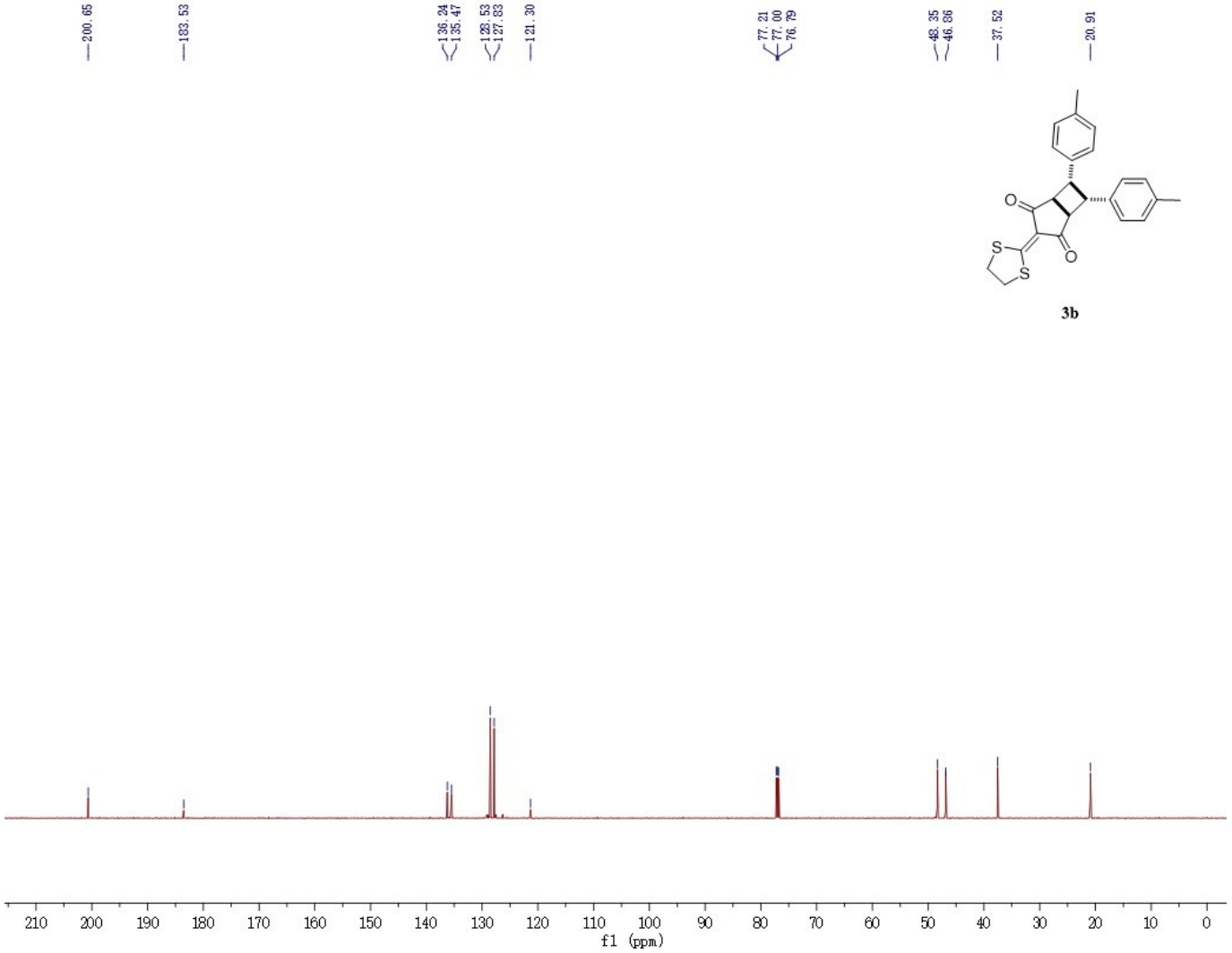
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2b/2b'



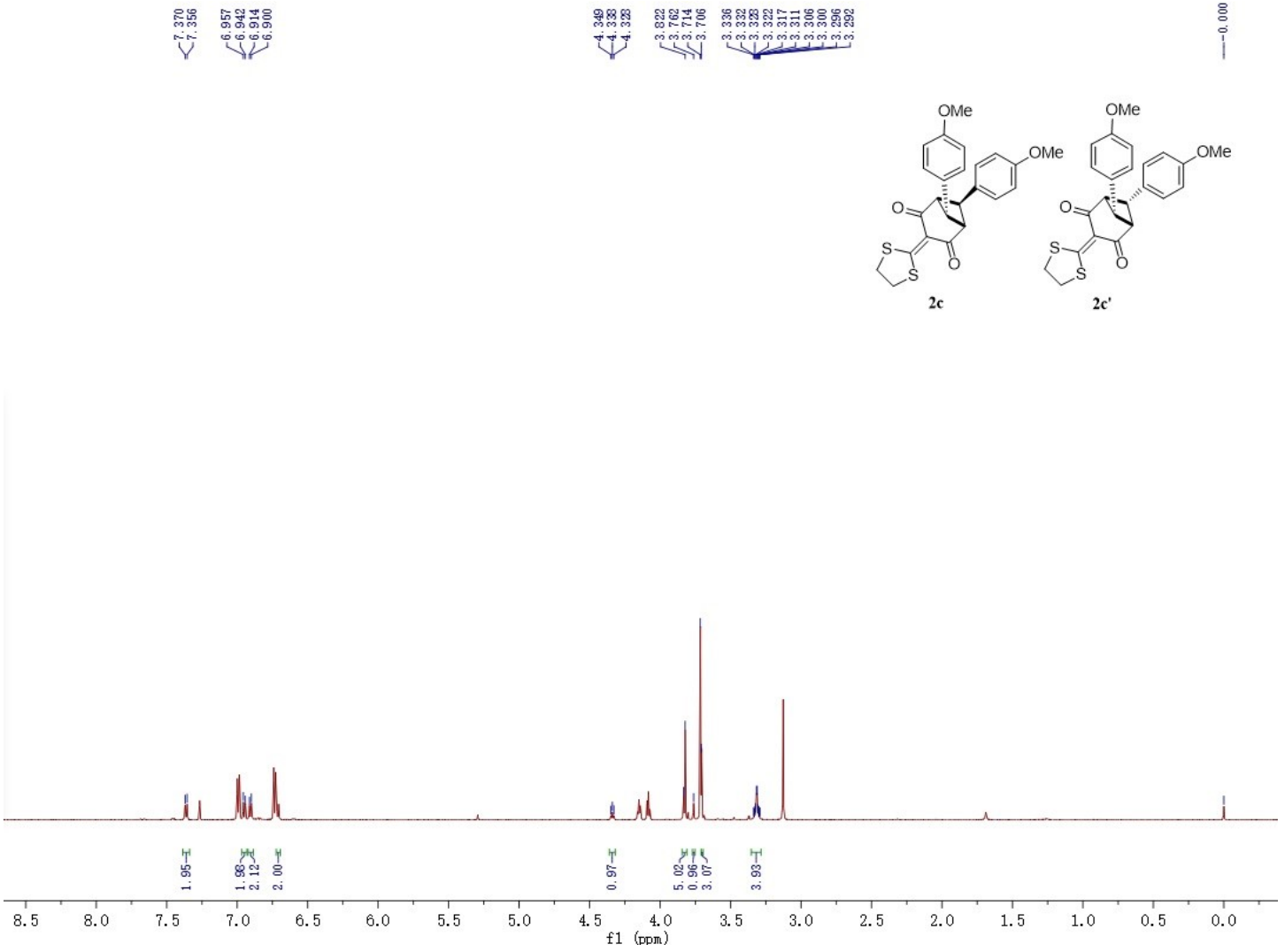
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3b



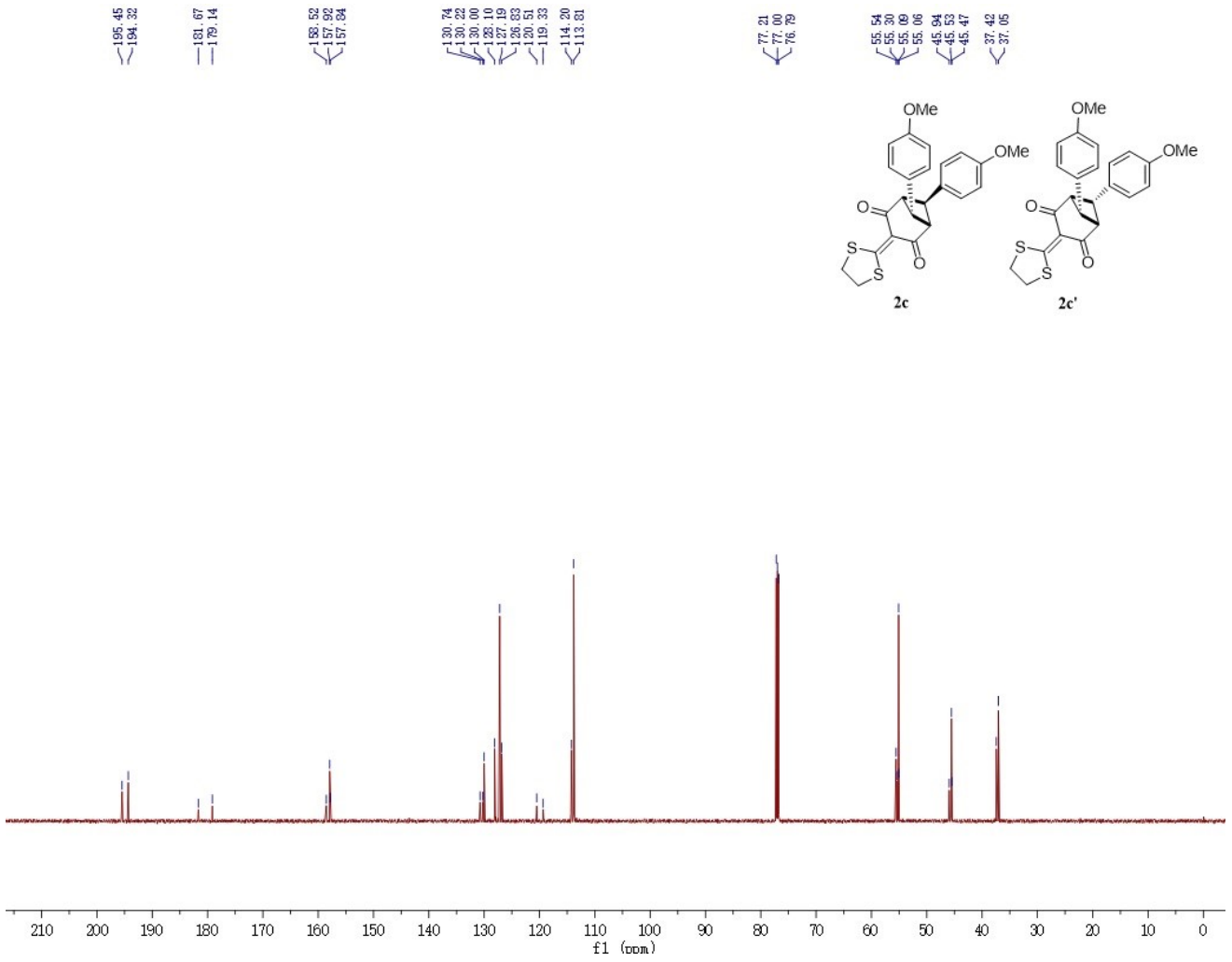
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3b



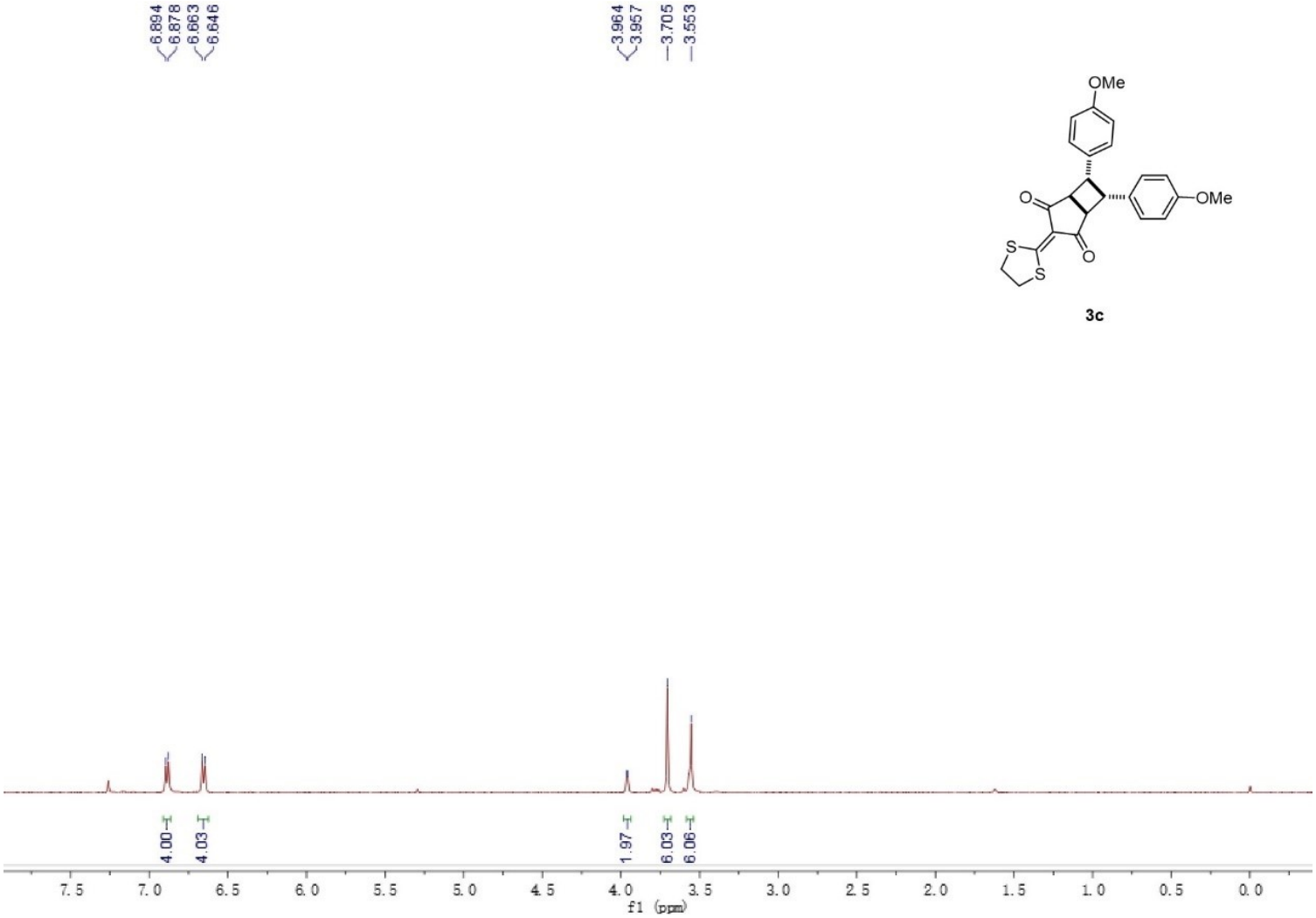
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2c/2c'



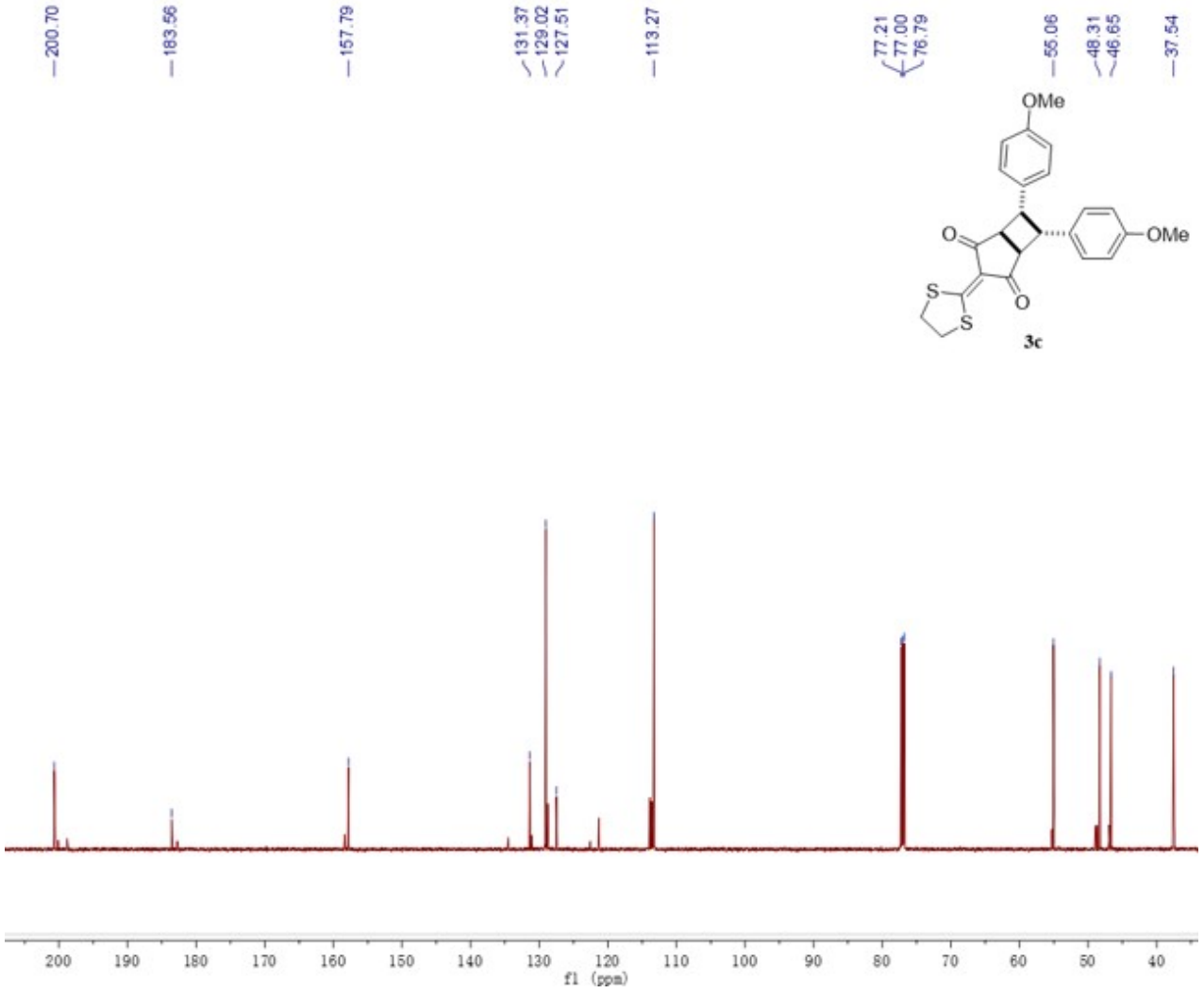
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2c/2c'



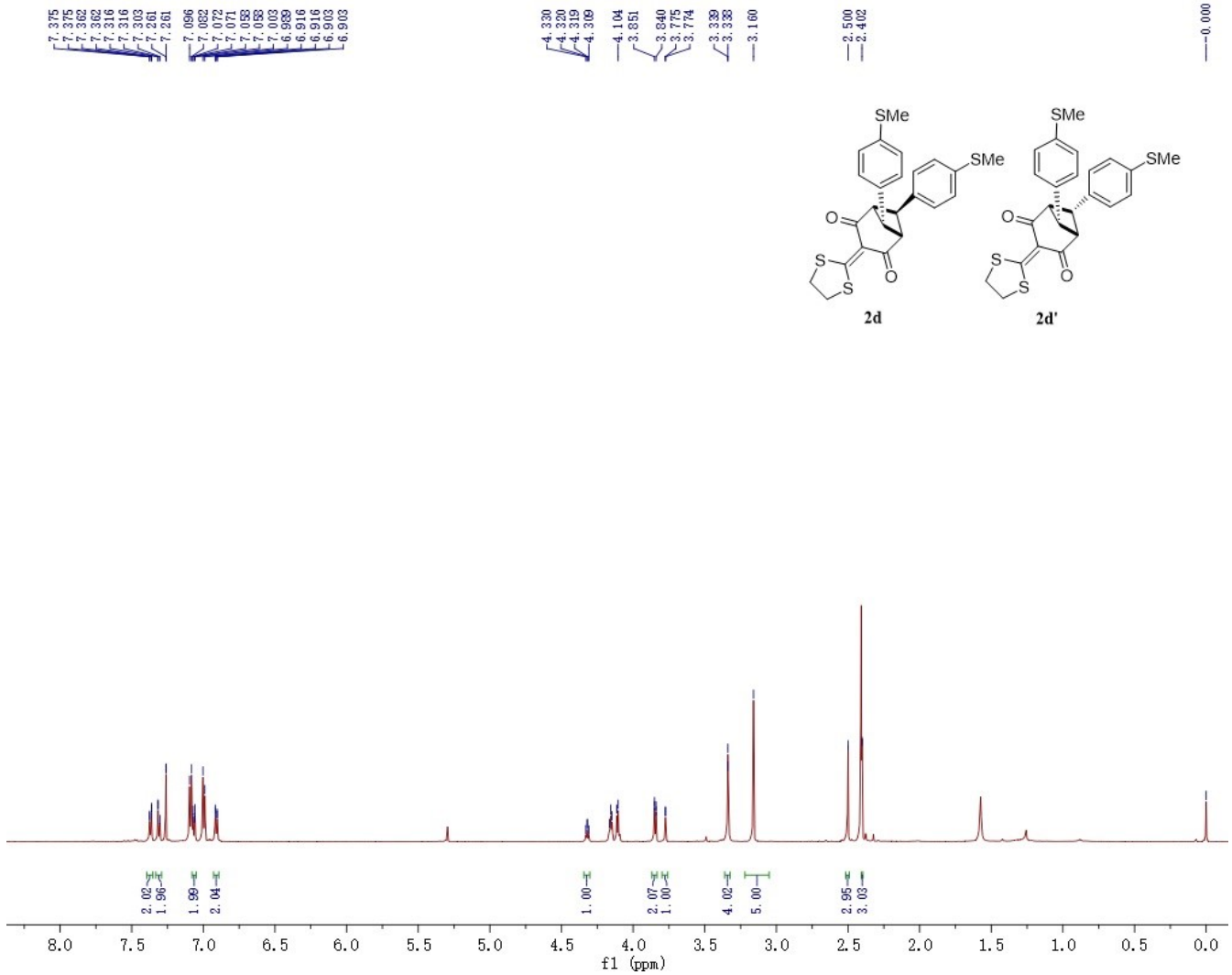
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3c



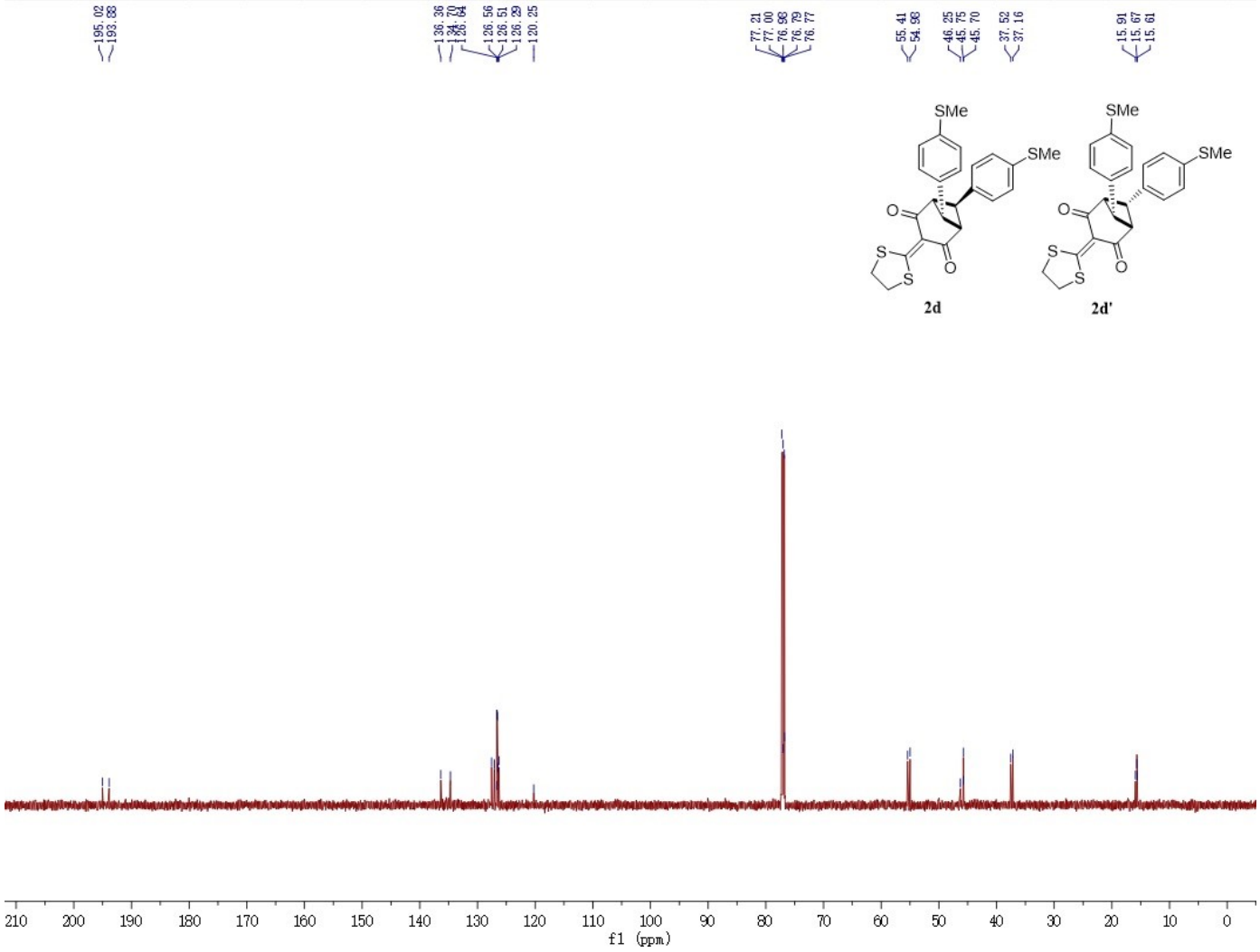
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3c



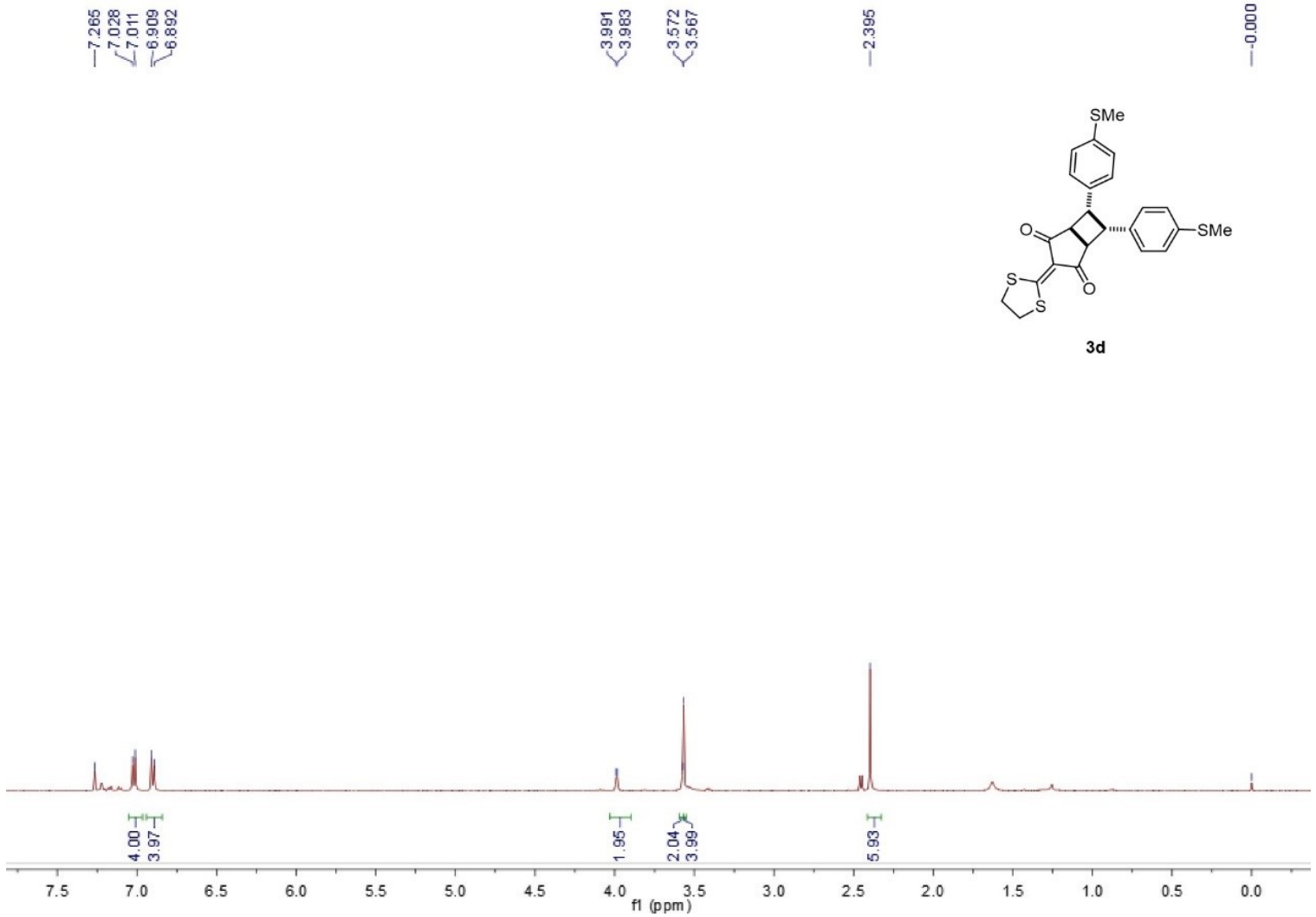
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2d/2d'



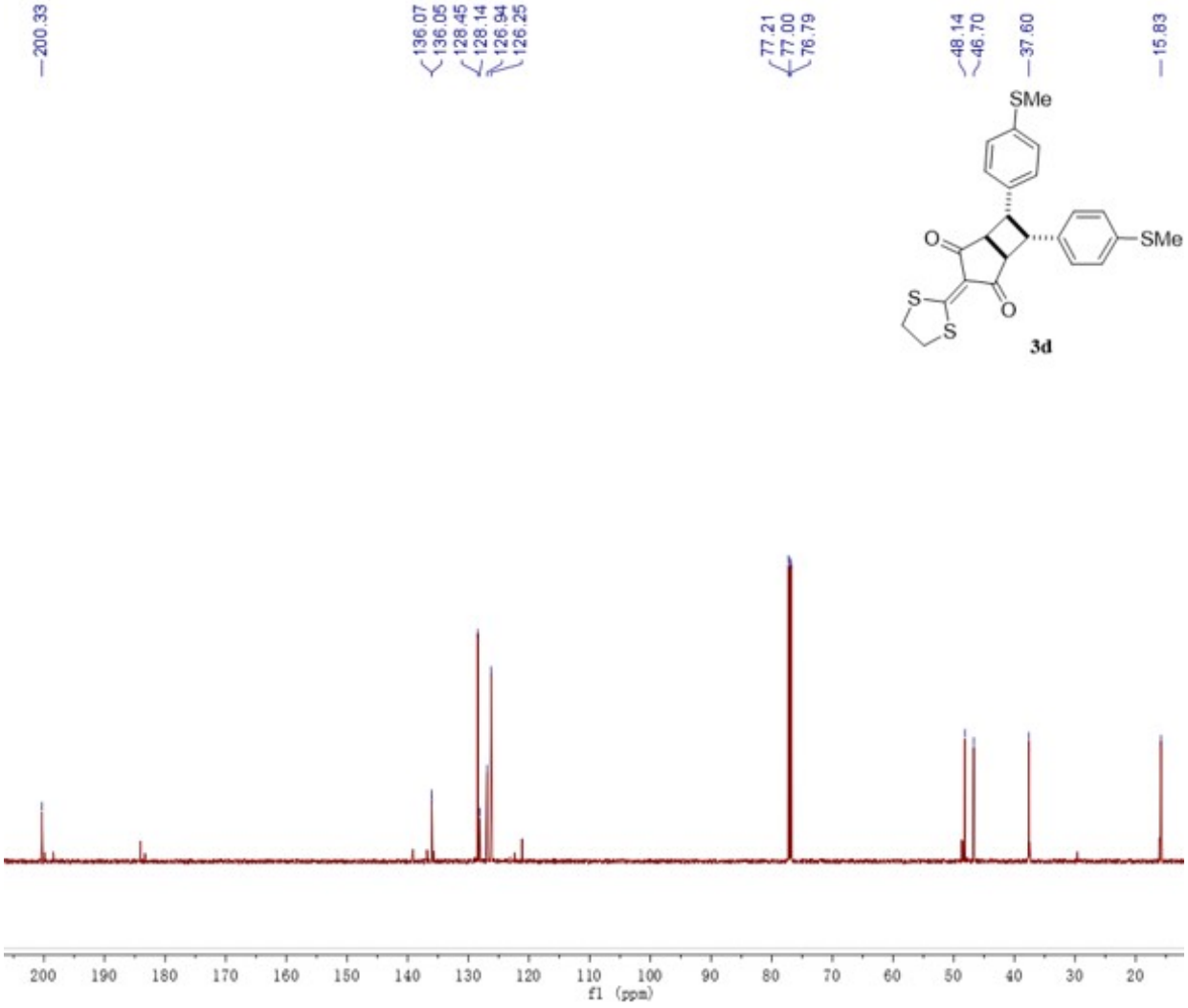
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2d/2d'



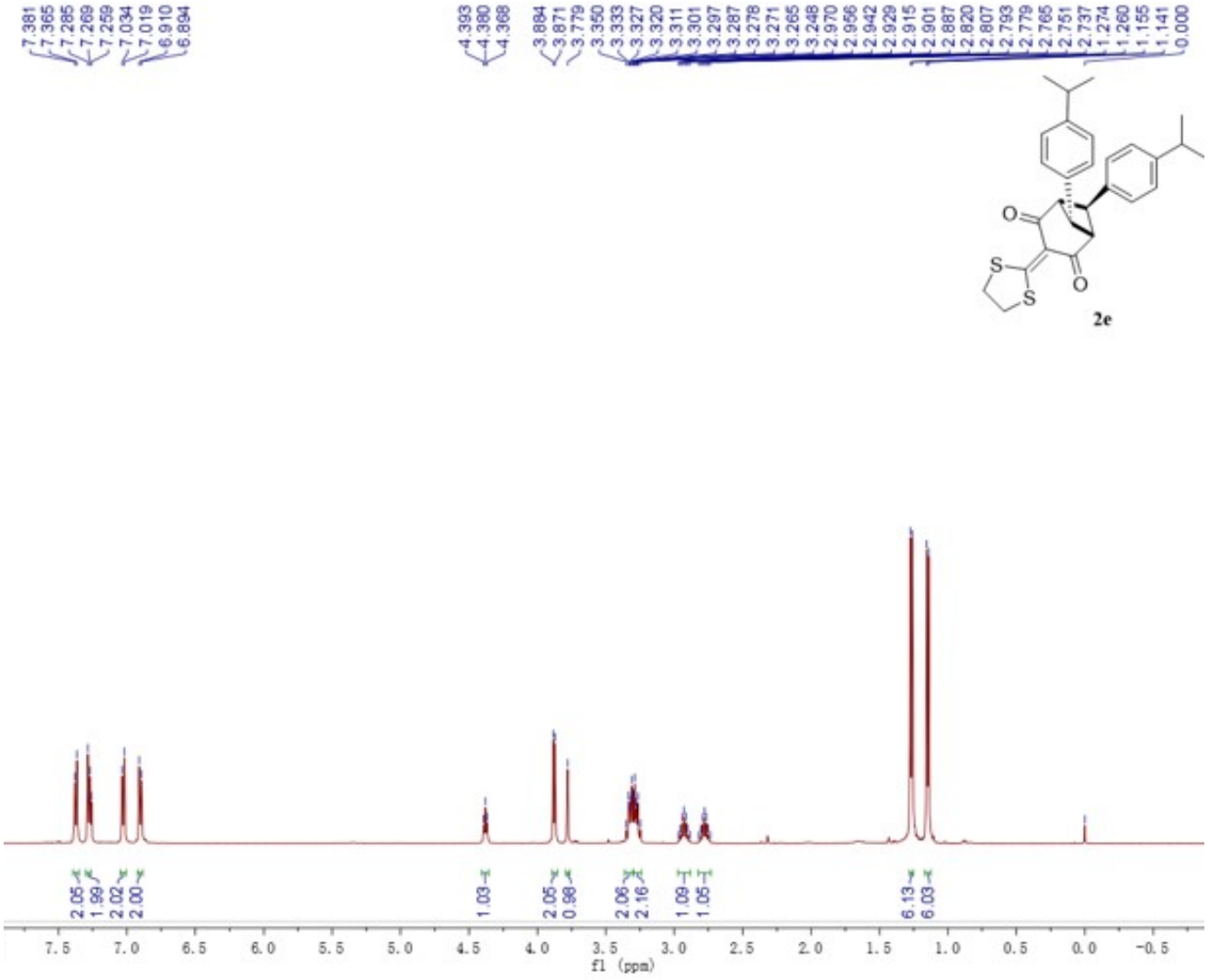
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3d



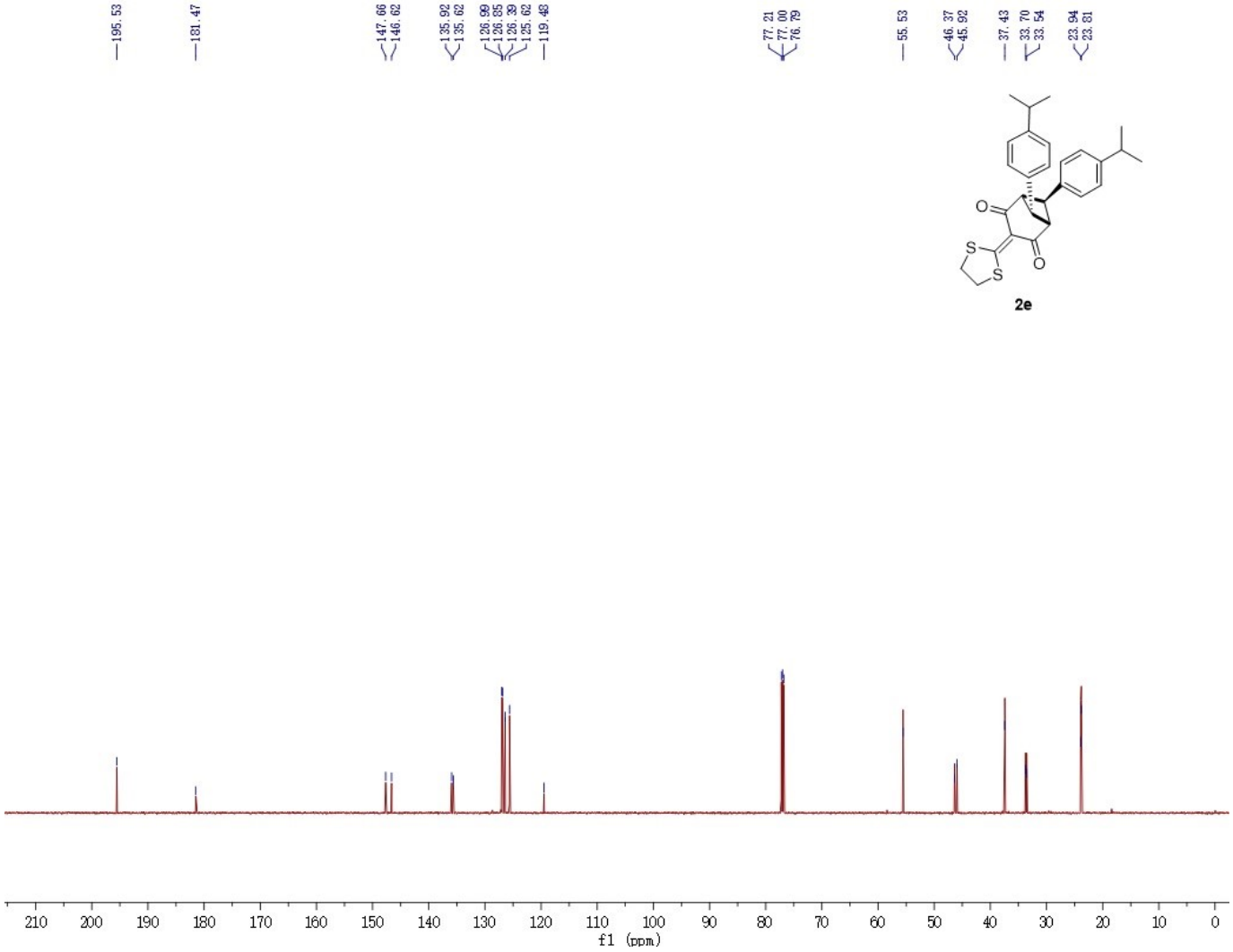
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3d



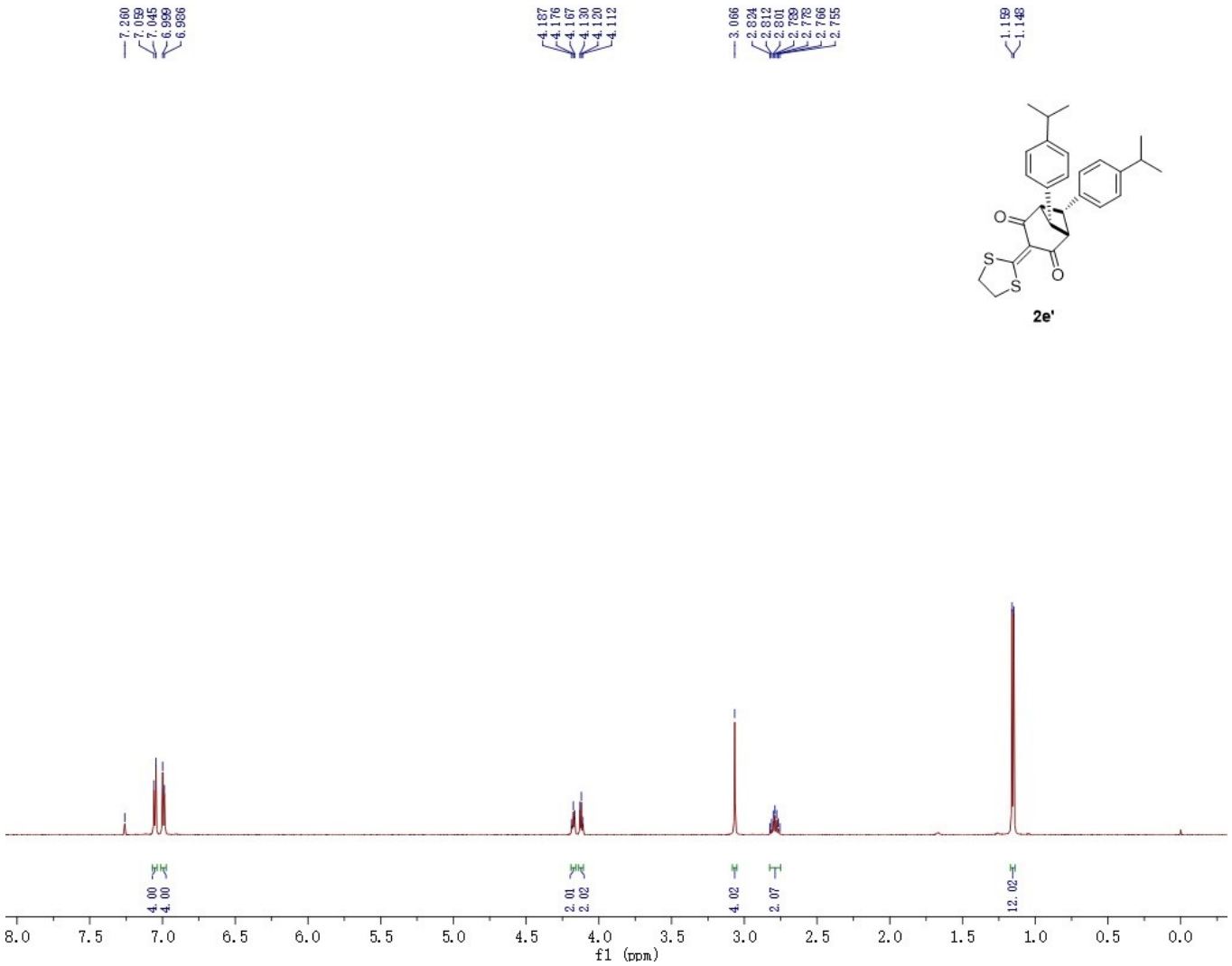
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2e



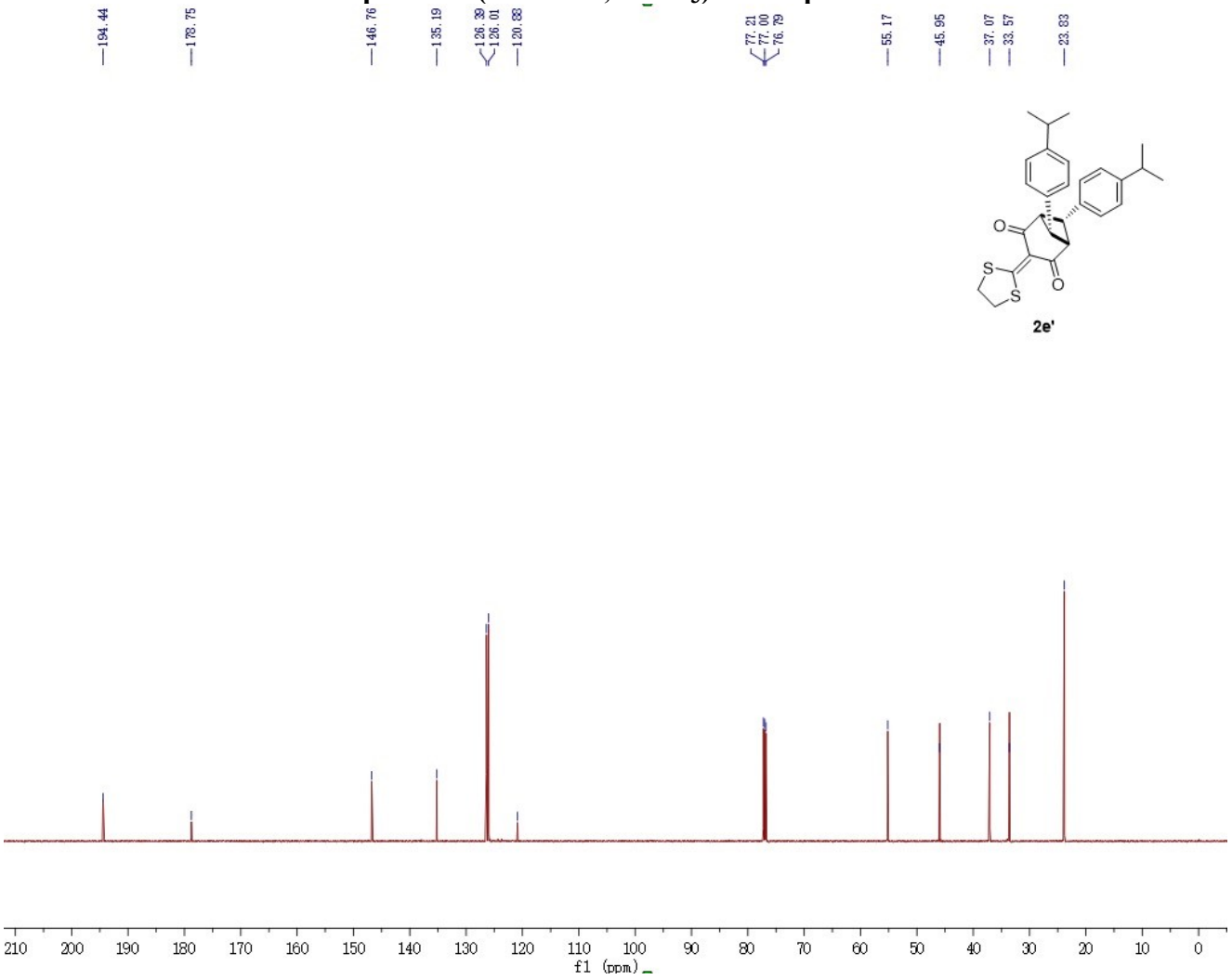
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2e



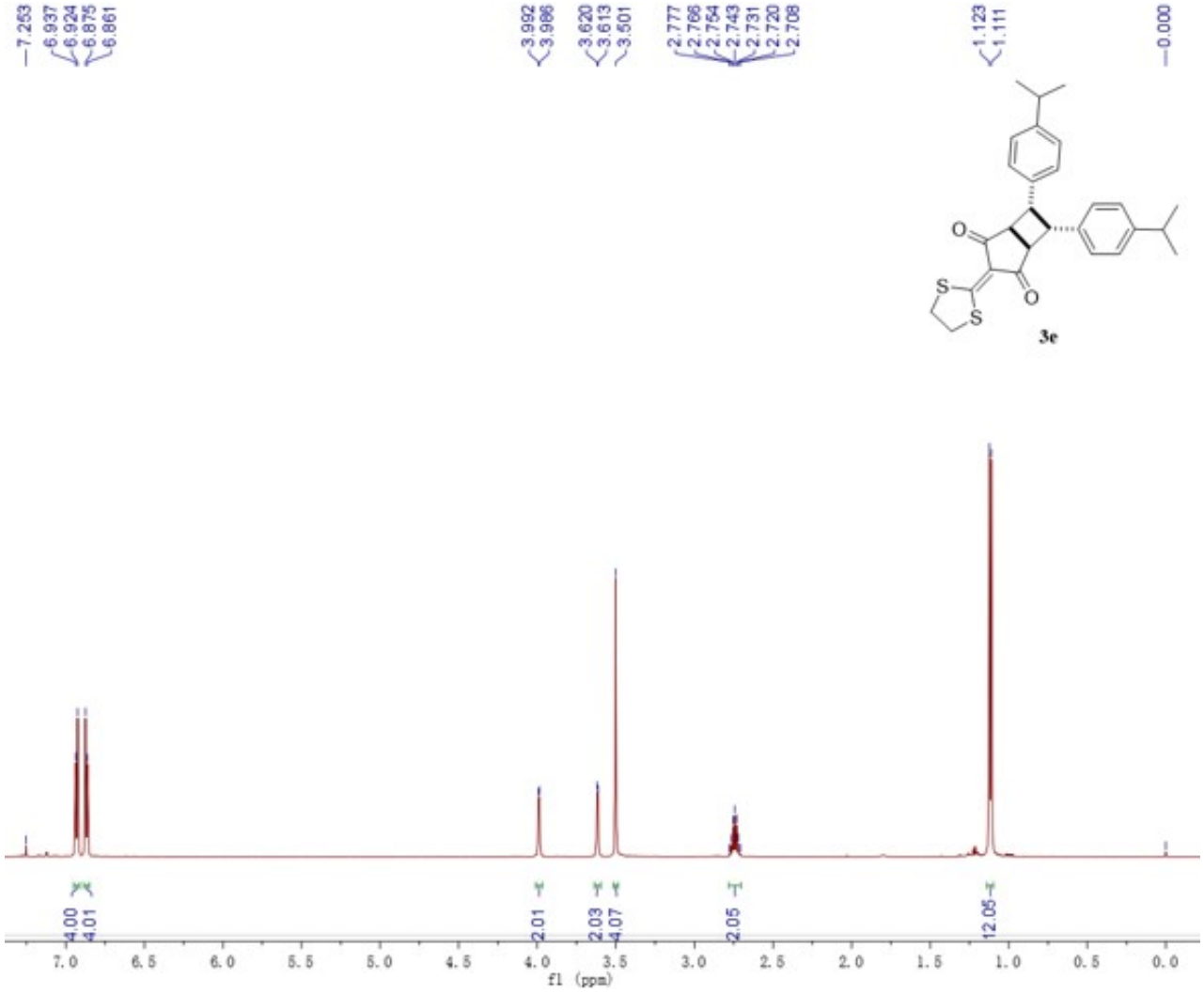
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2e'



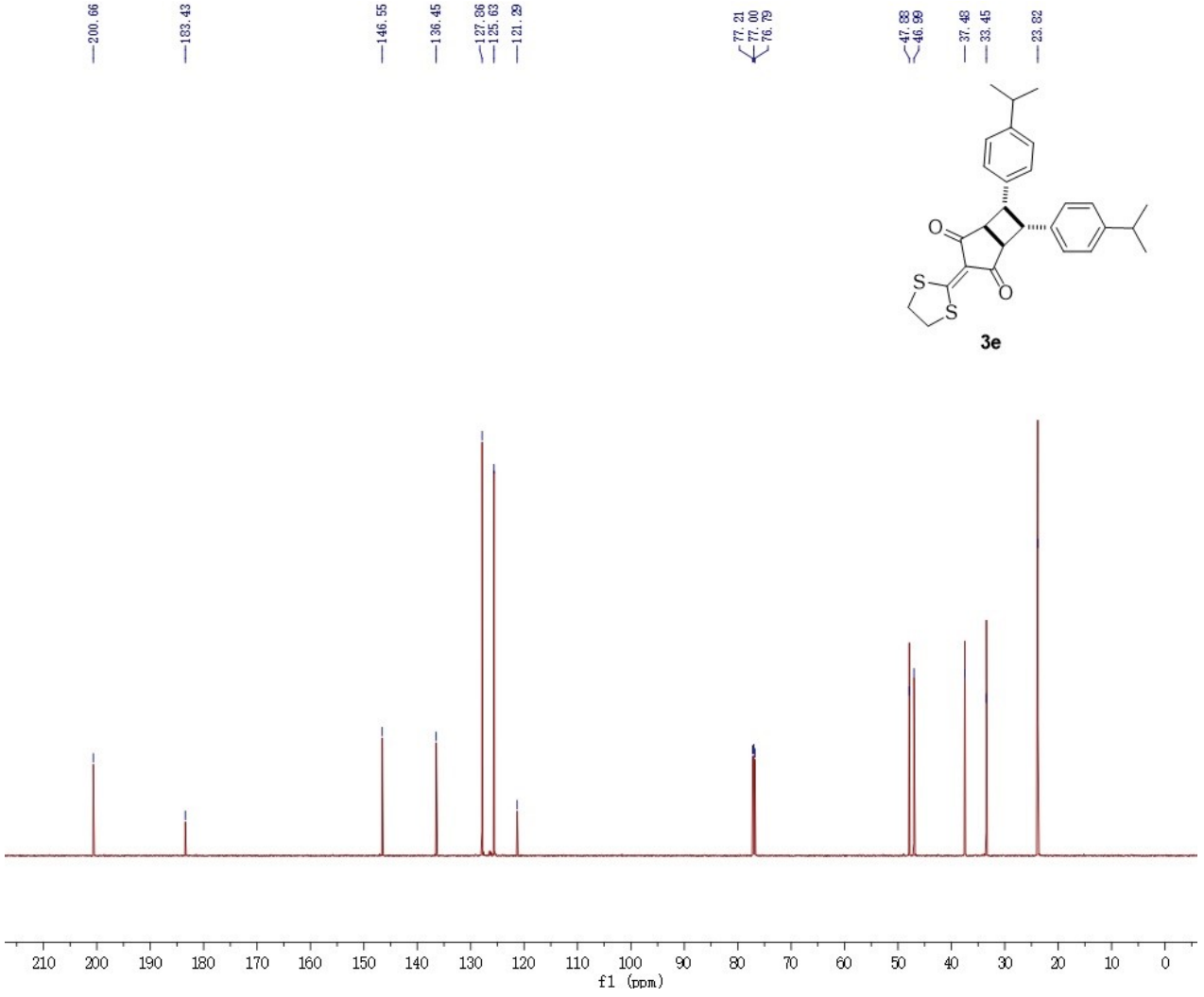
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2e'



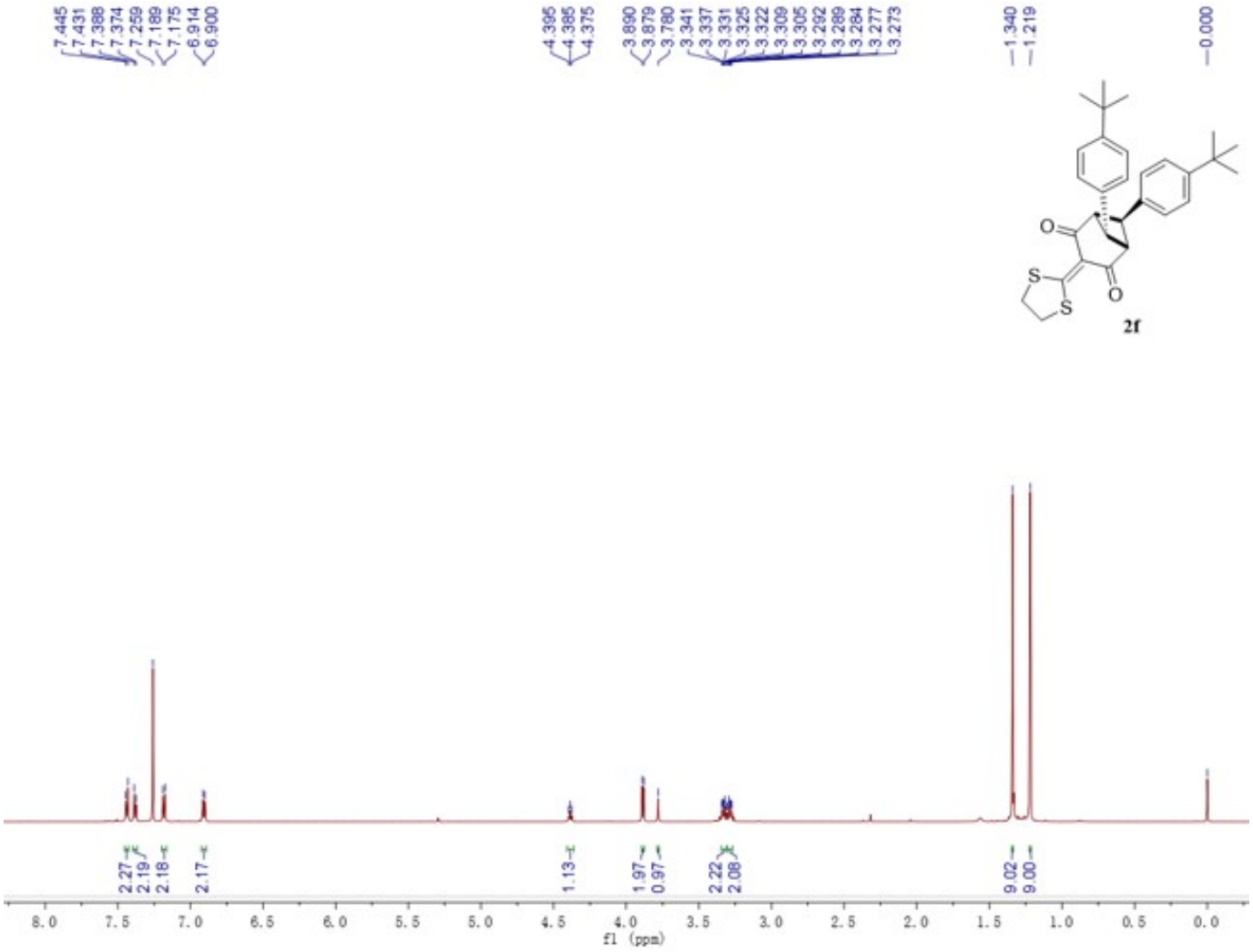
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3e



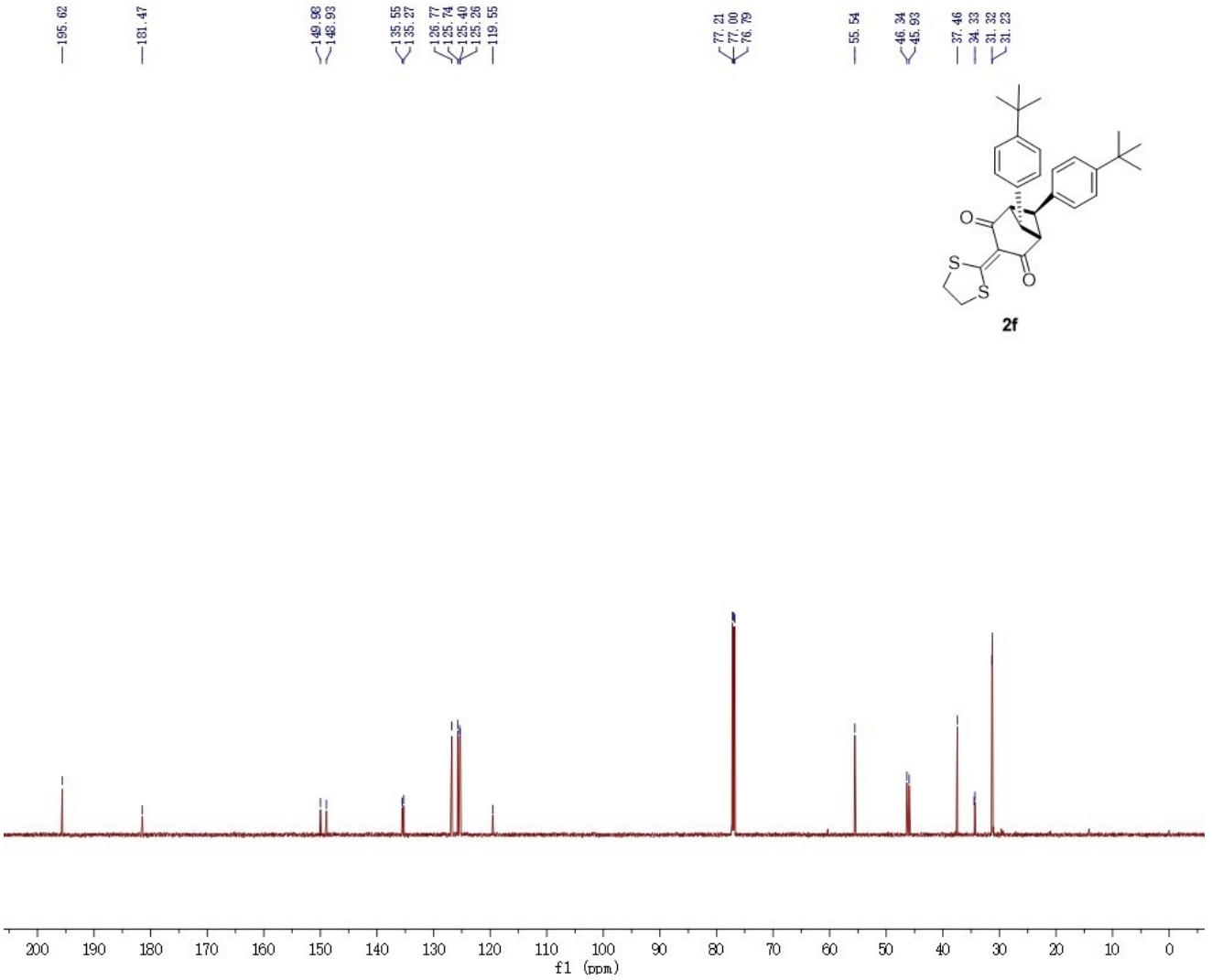
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3e



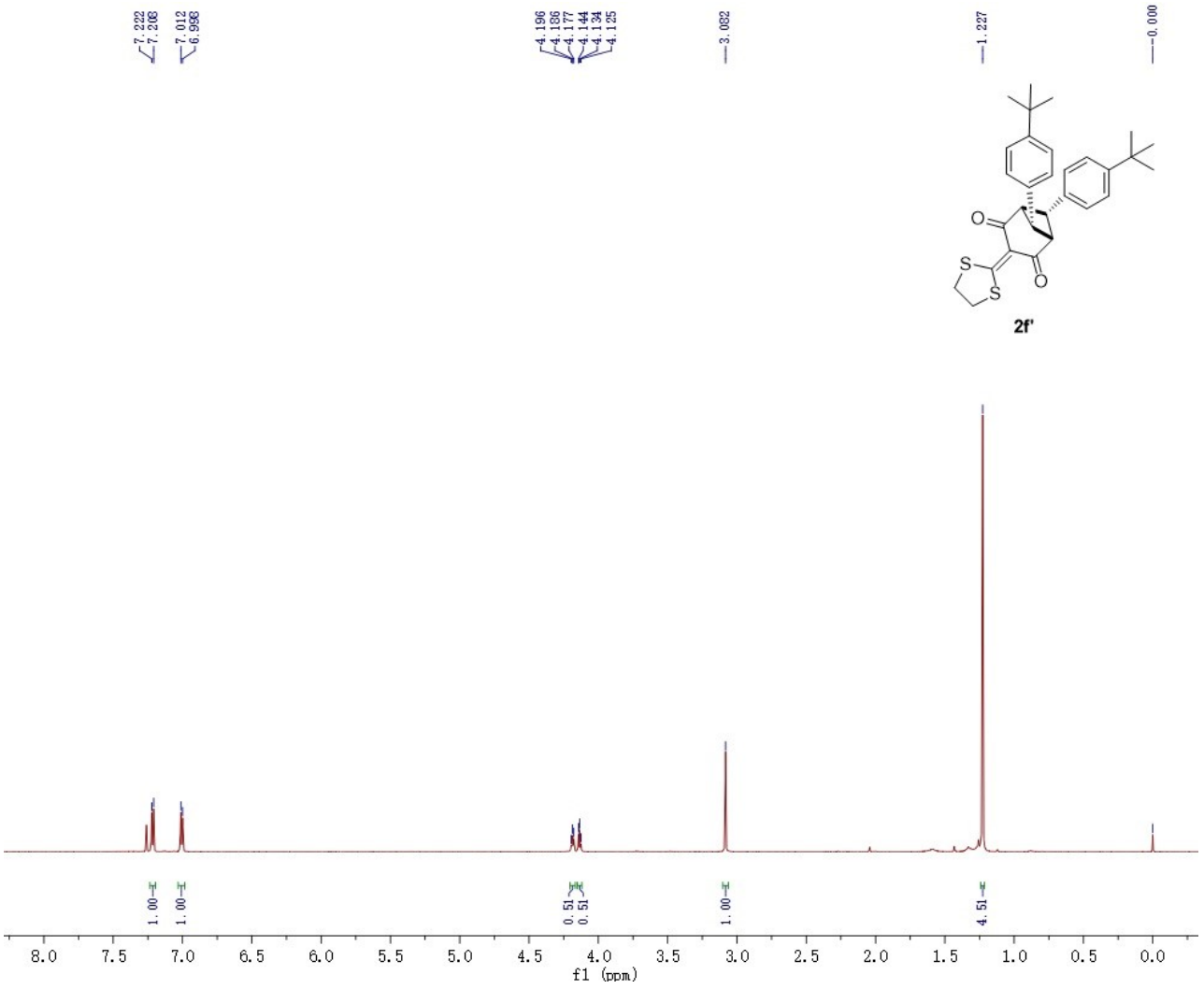
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2f



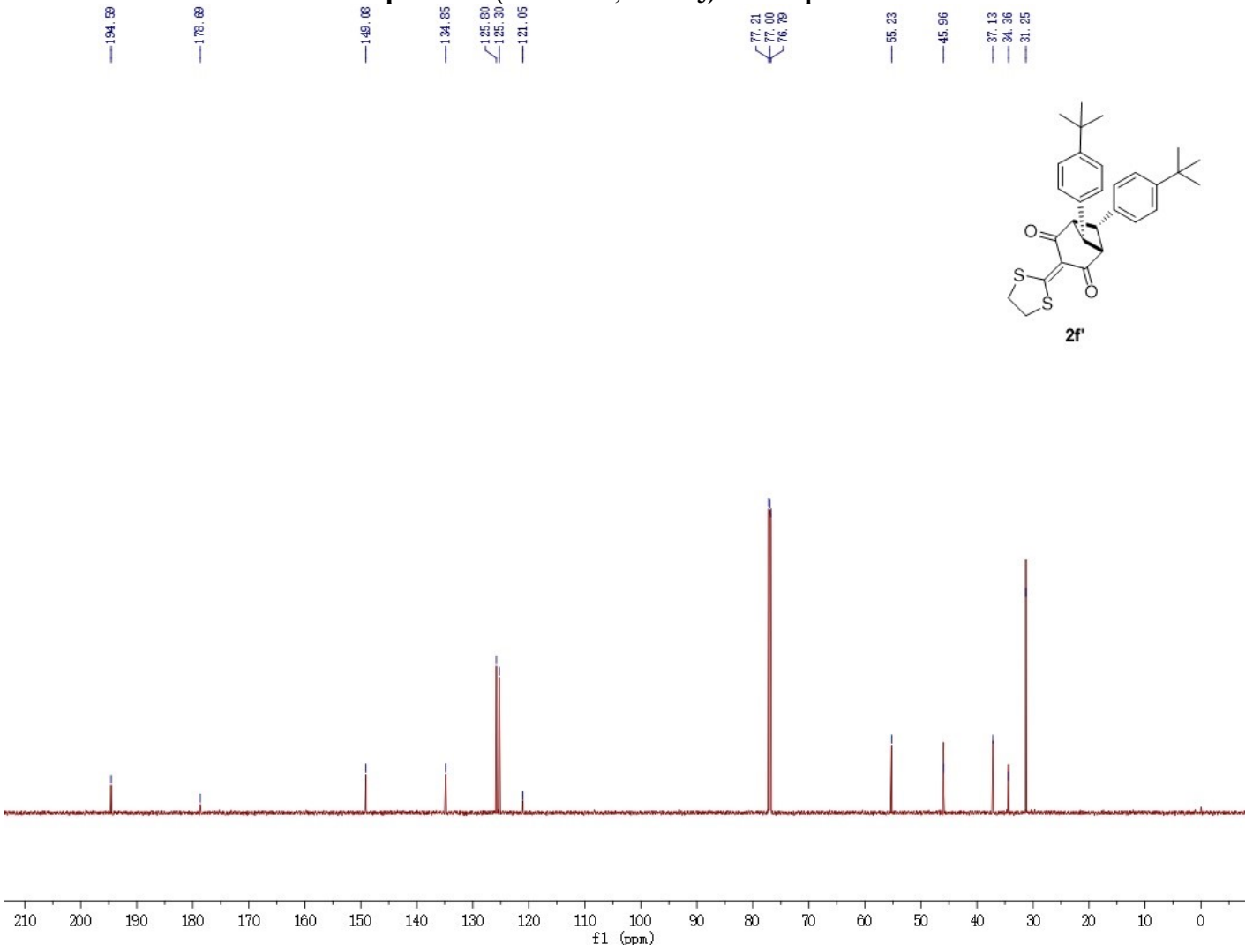
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2f



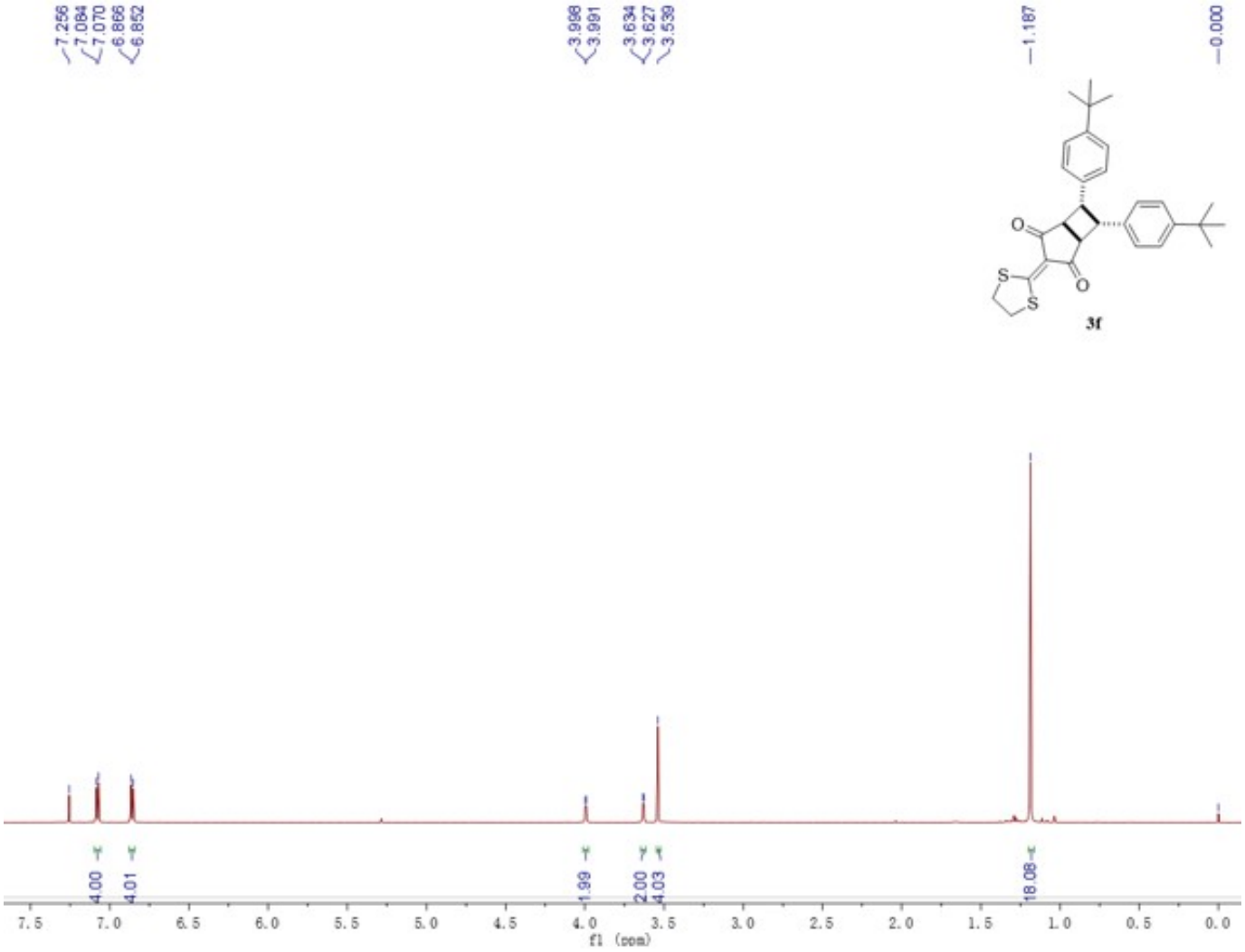
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2f'



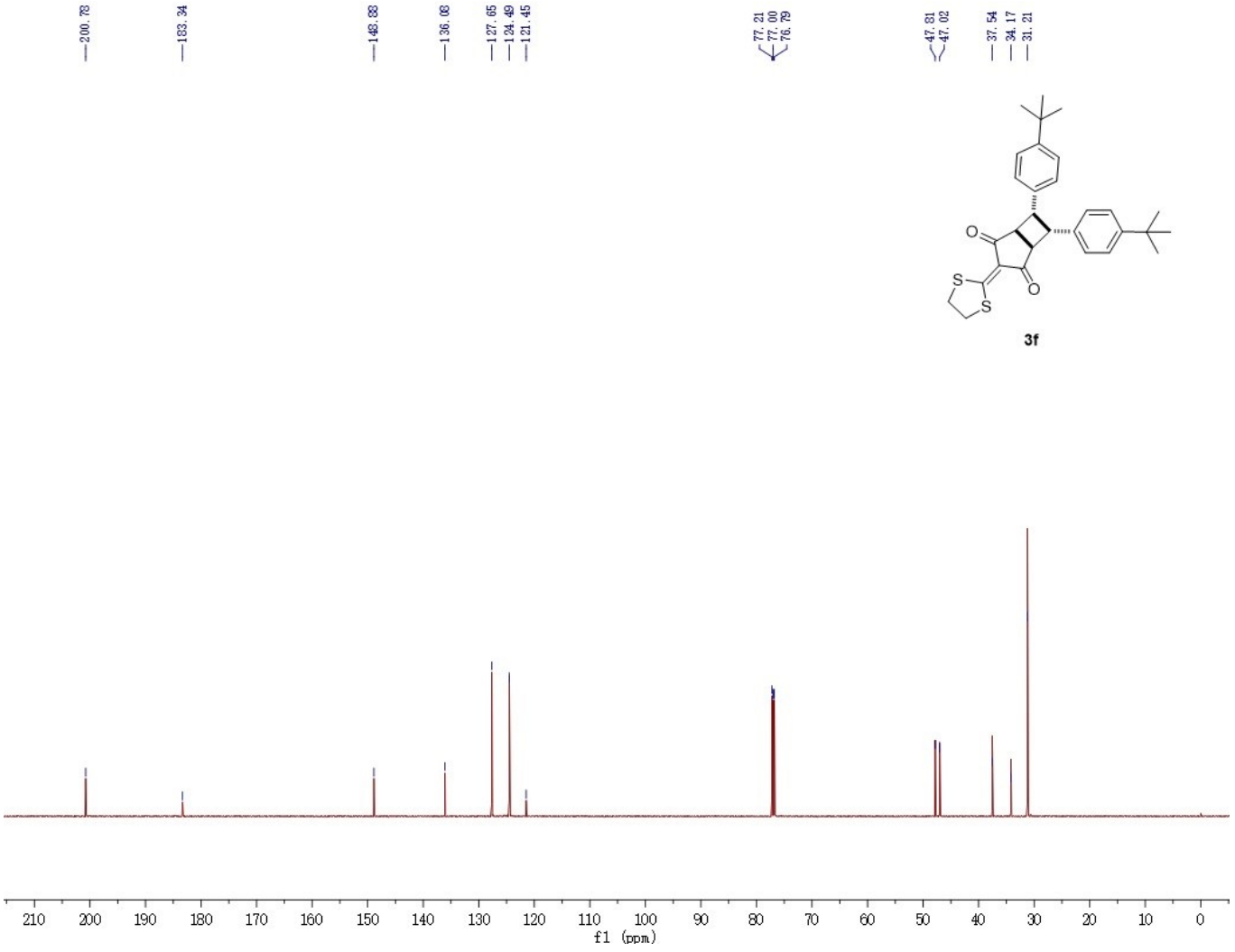
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2f'



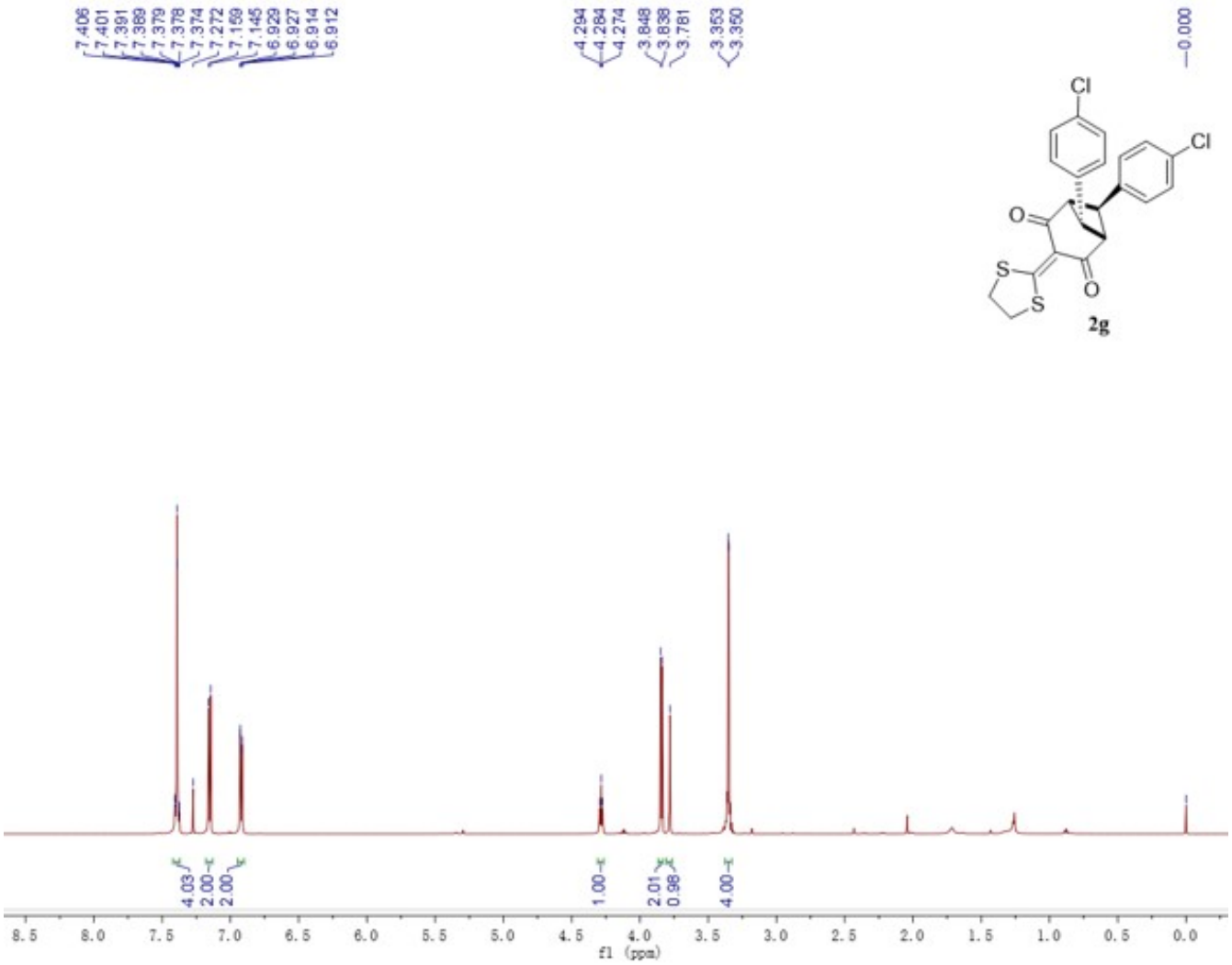
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3f



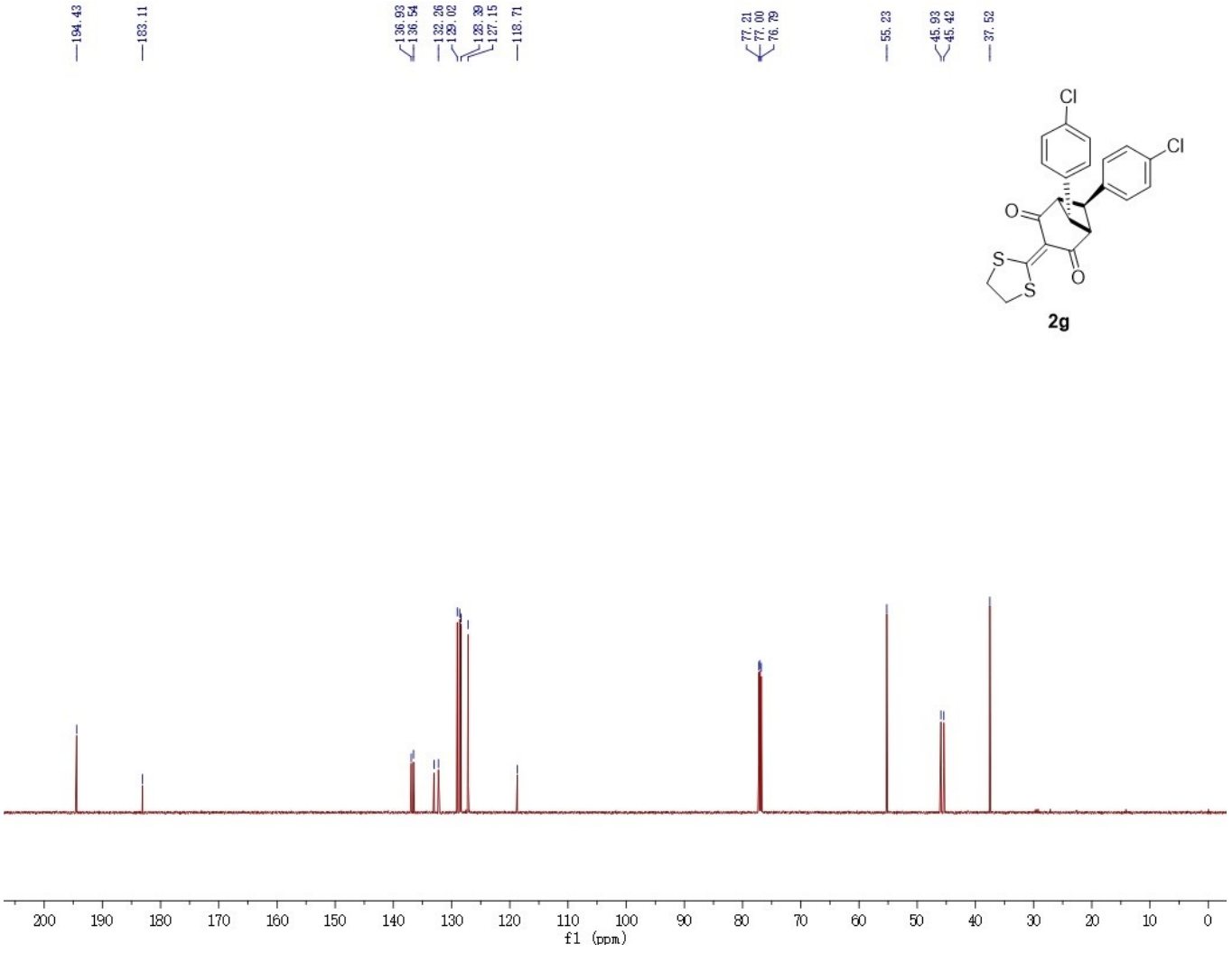
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3f



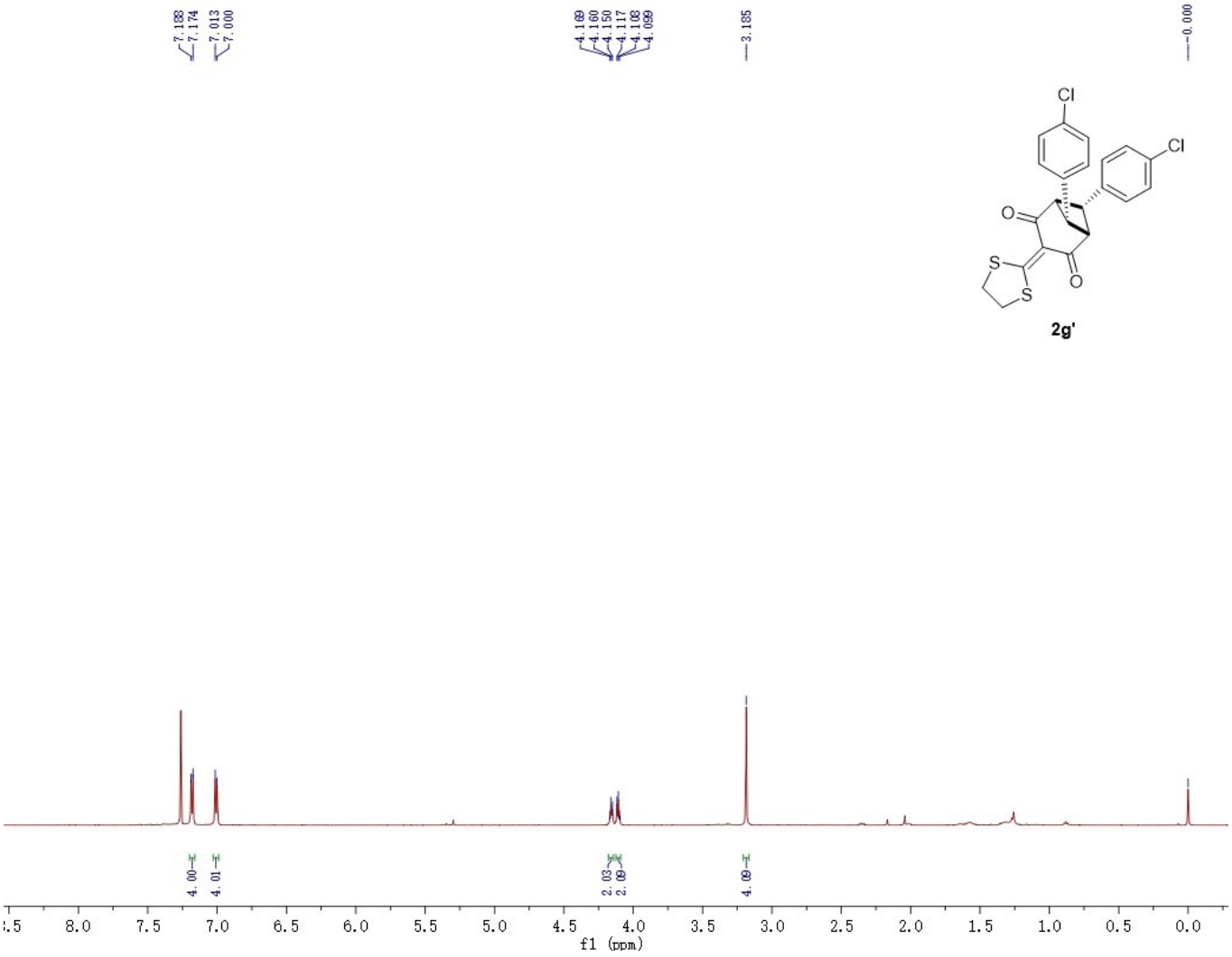
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2g



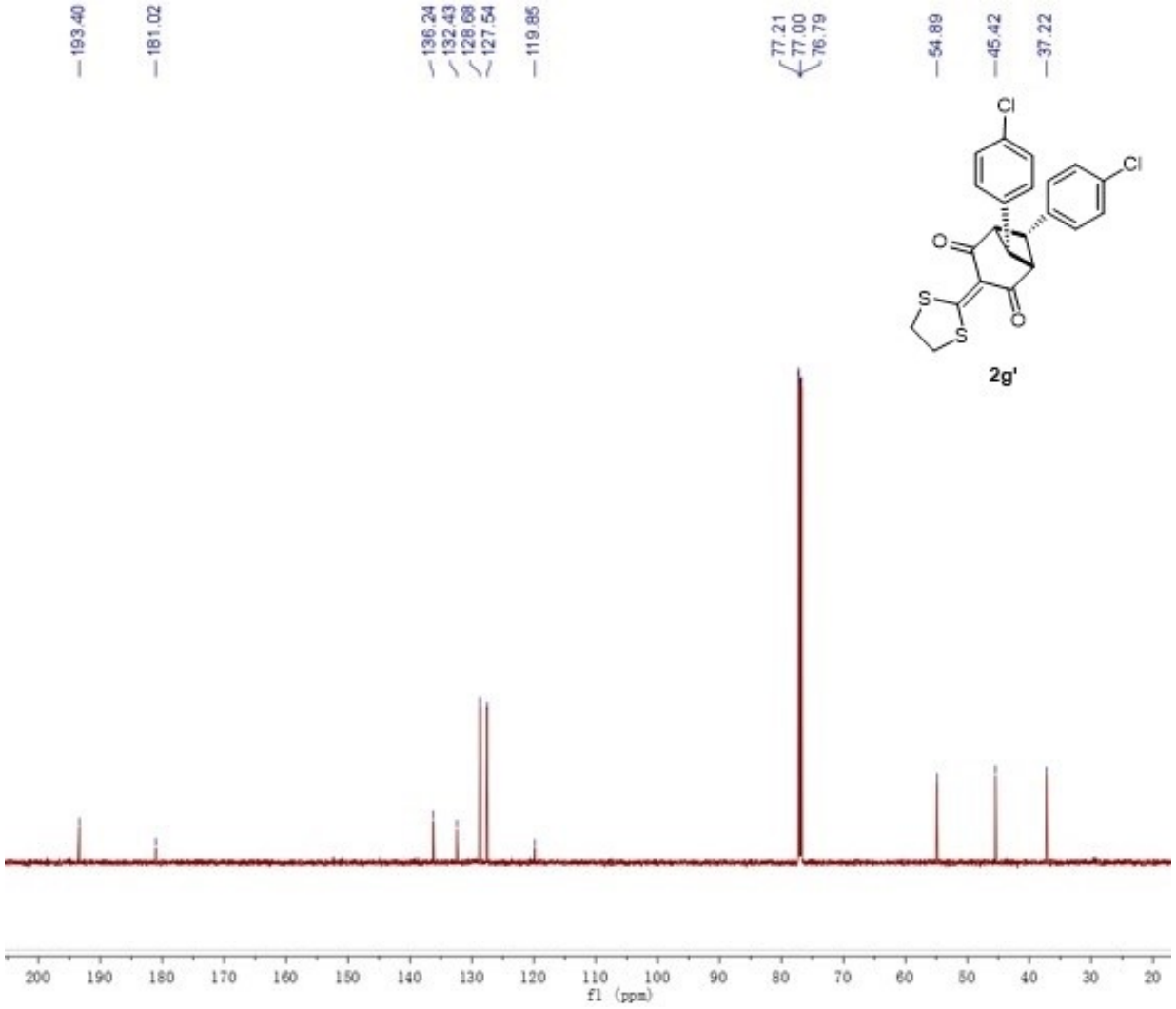
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2g



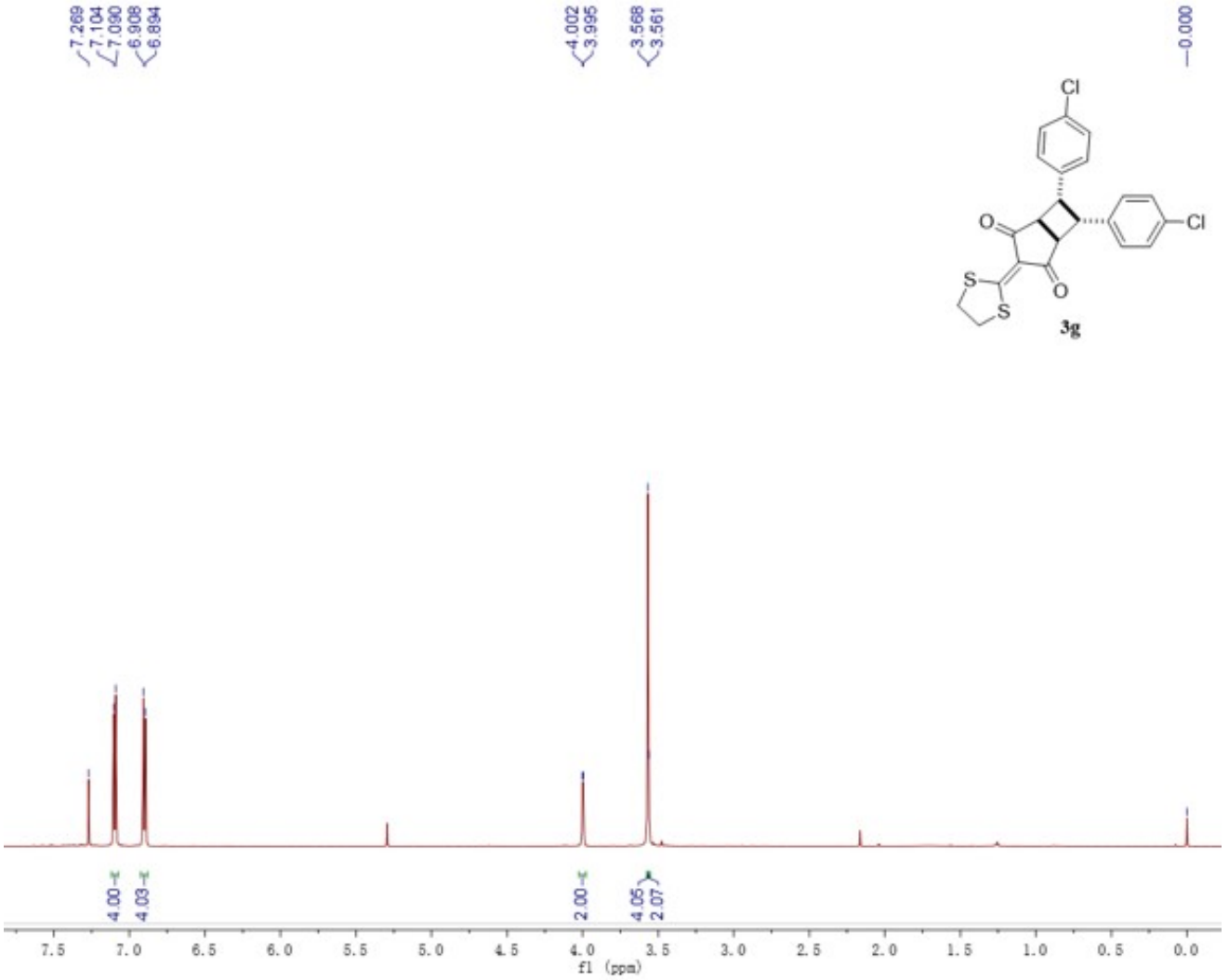
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2g'



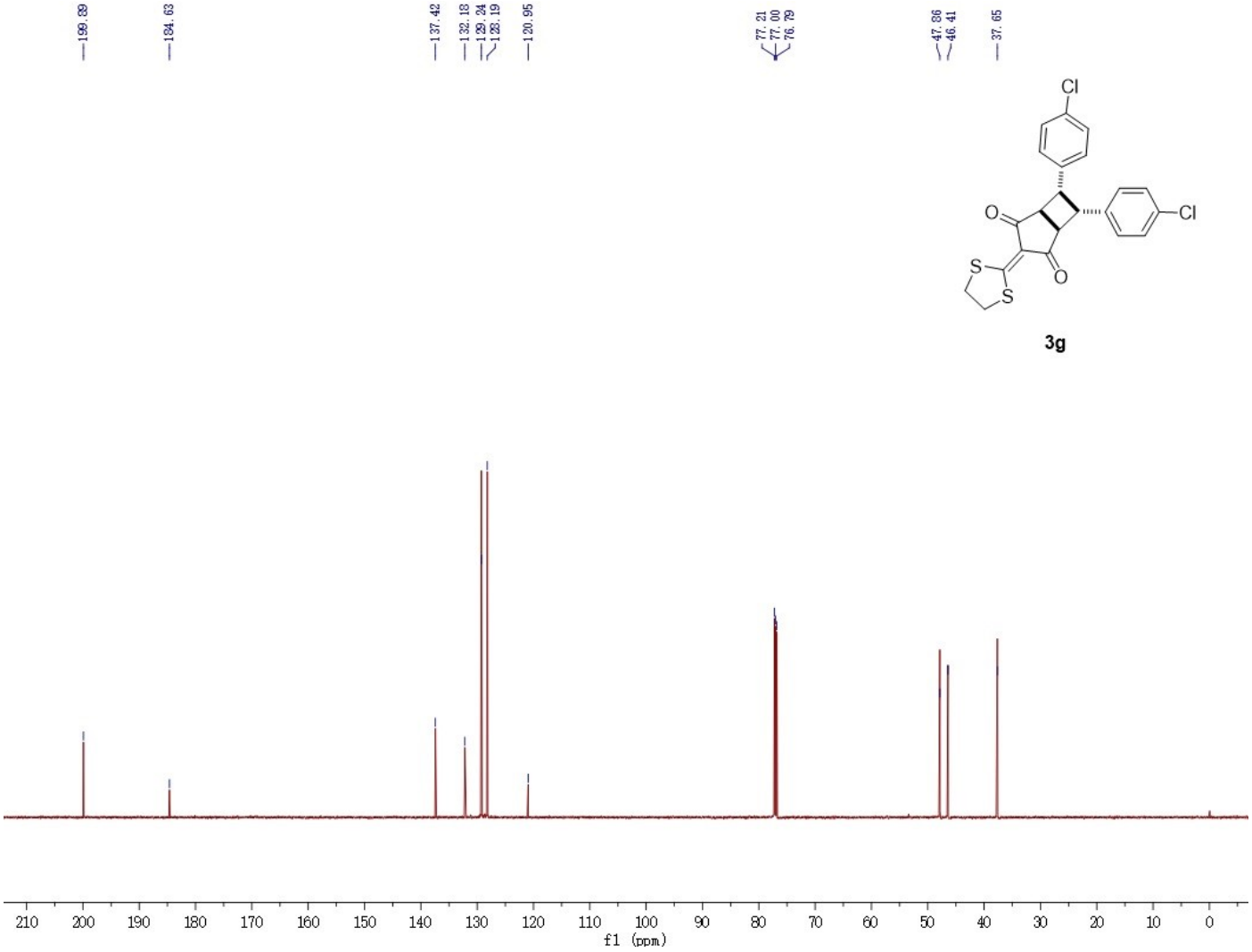
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2g'



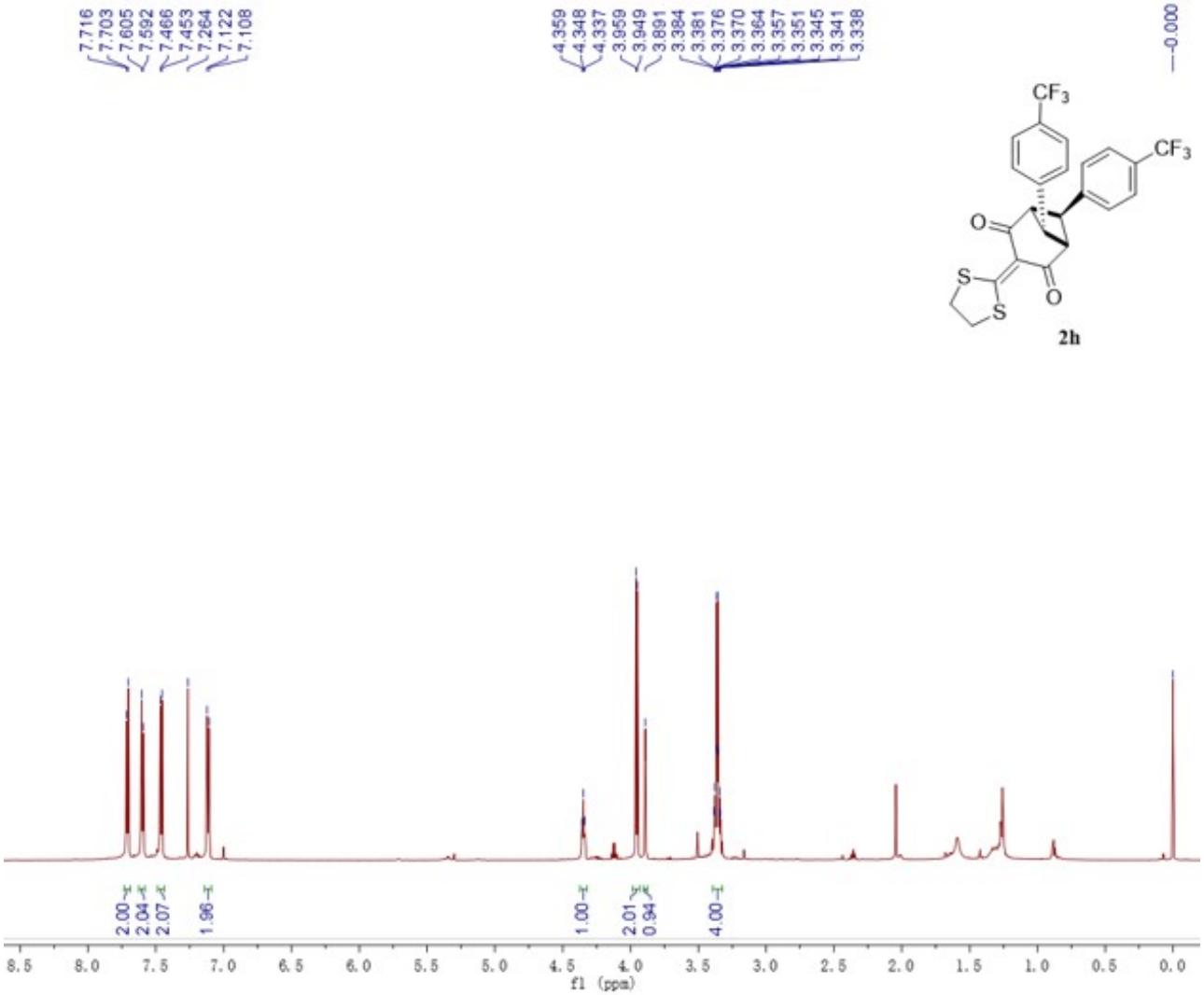
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3g



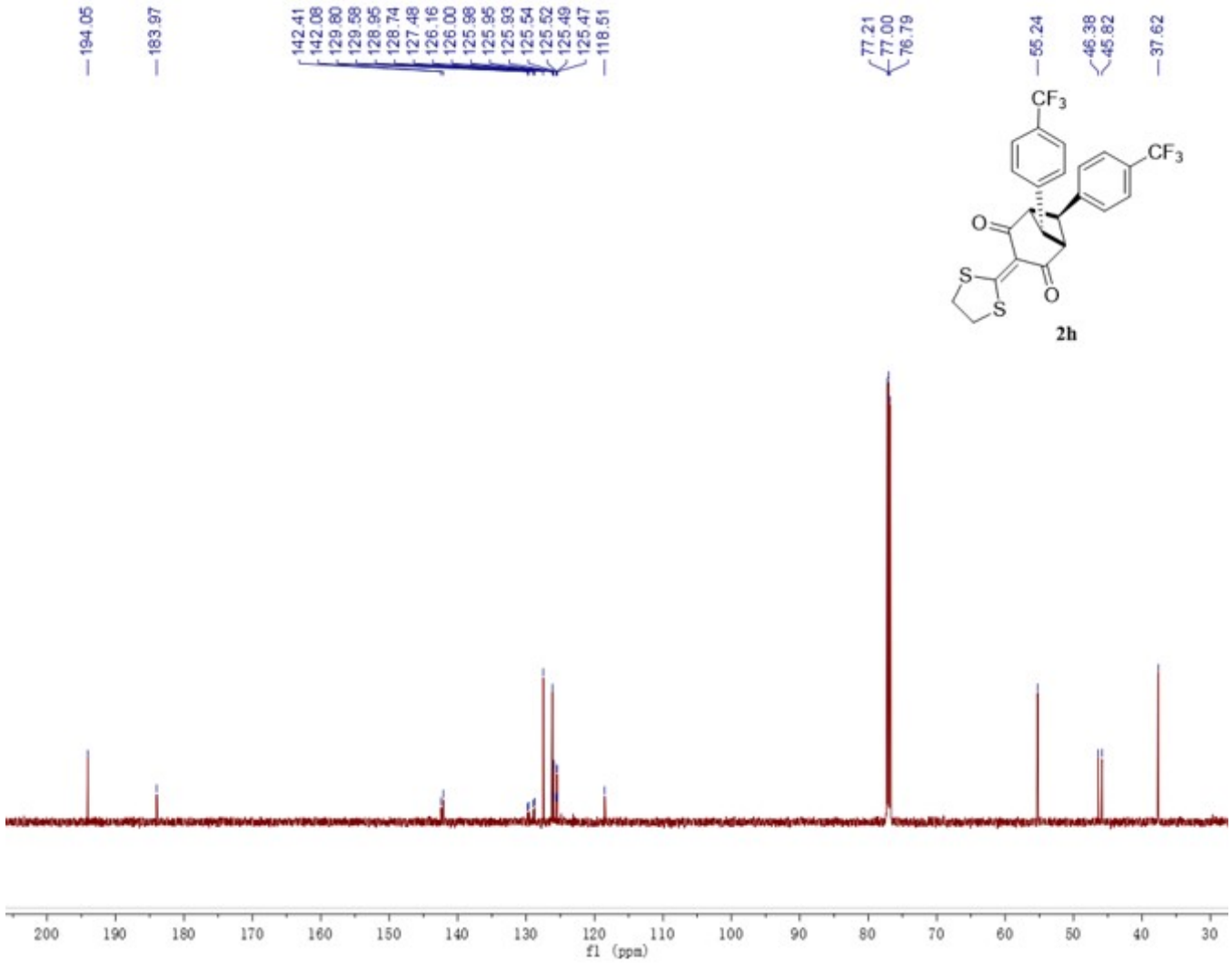
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3g



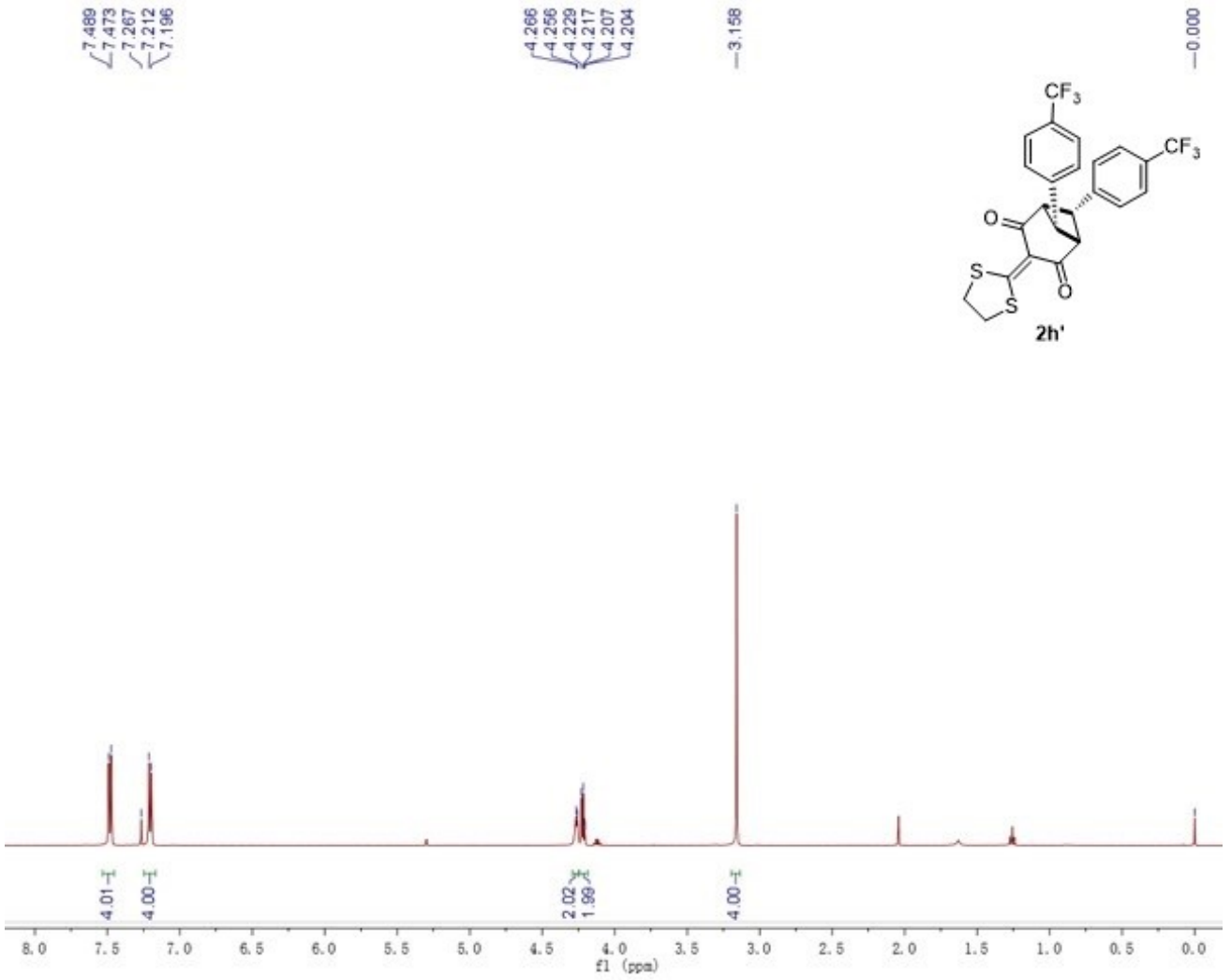
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2h



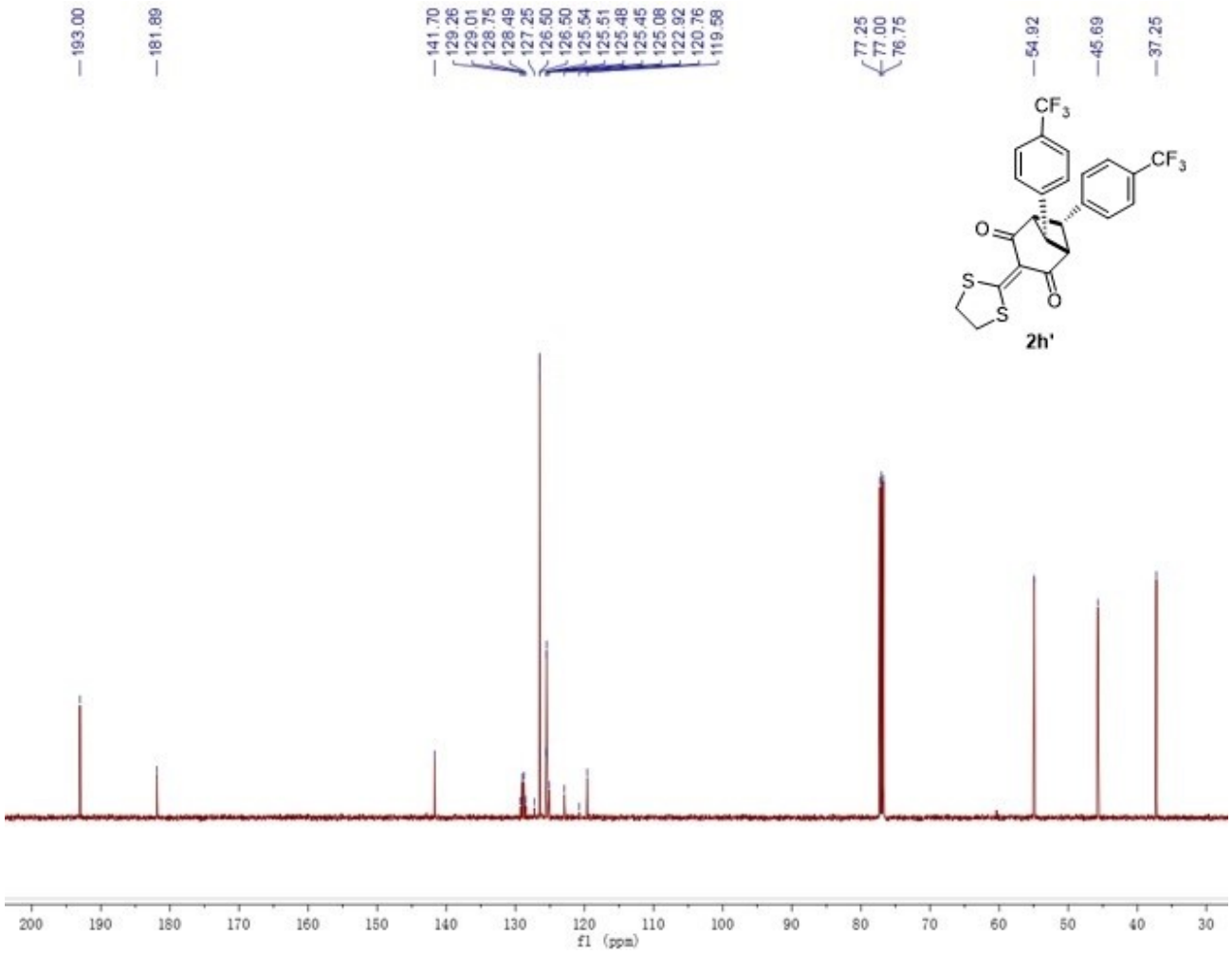
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2h



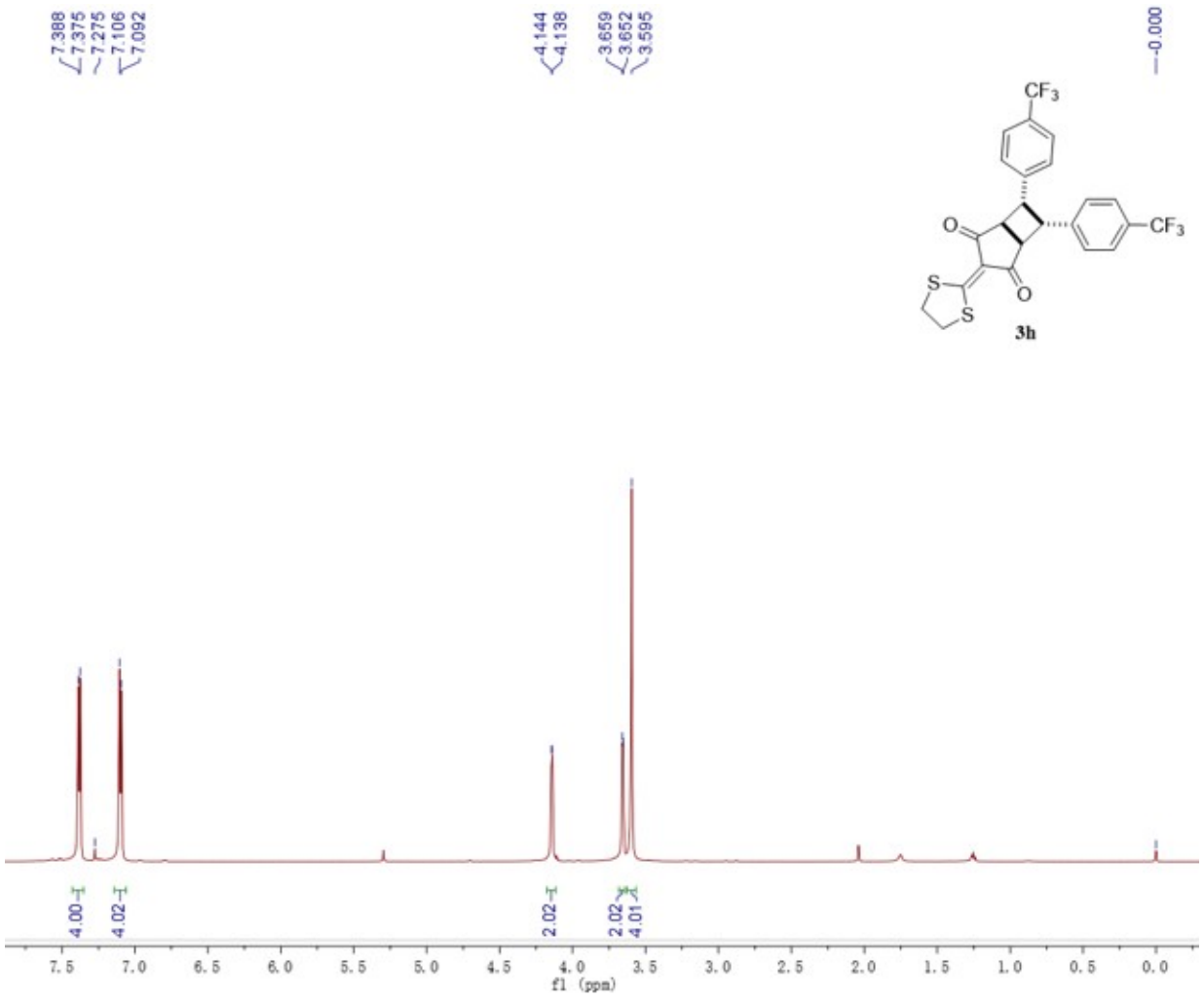
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2h'



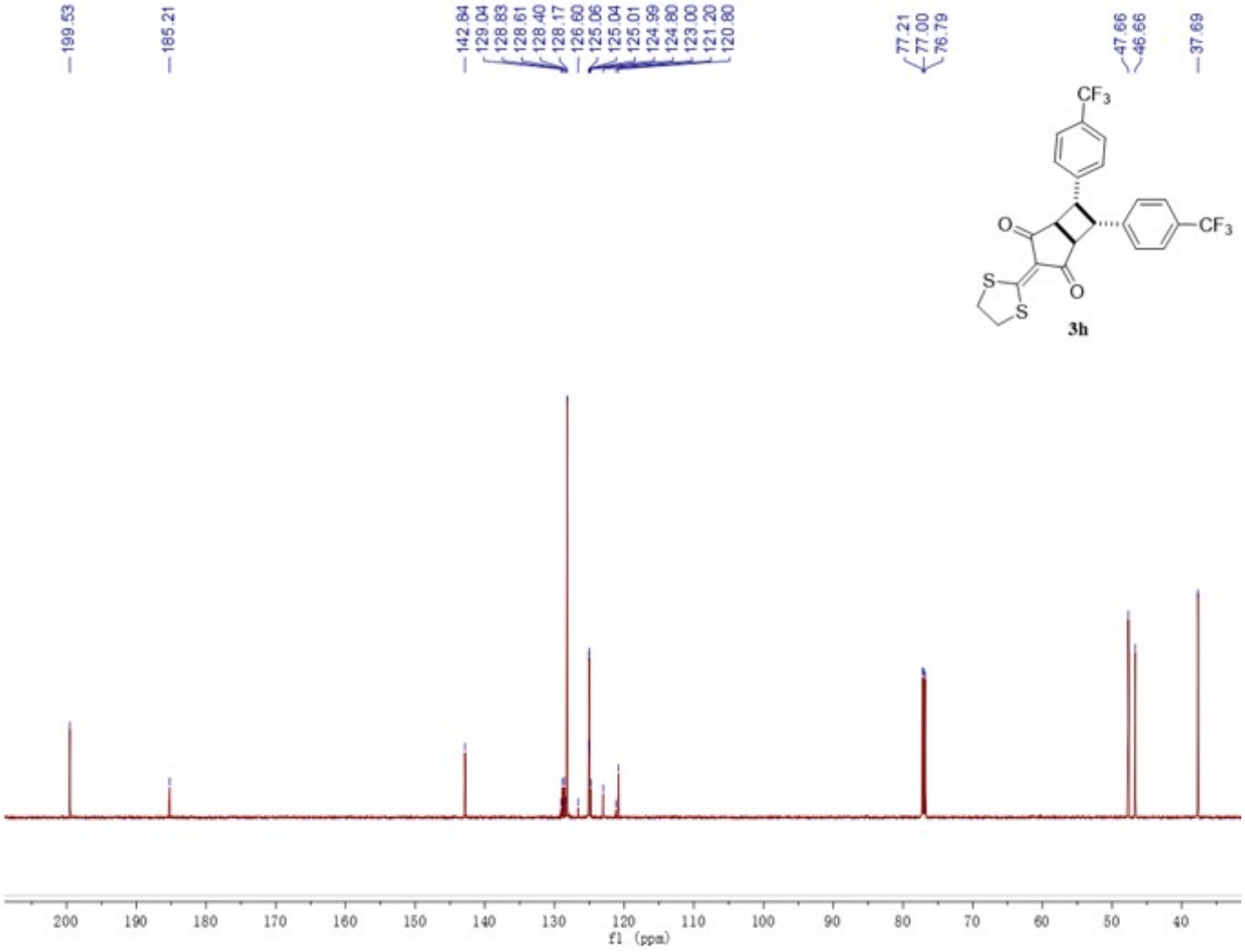
^{13}C spectrum (126 MHz, $CDCl_3$) of compound 2h'



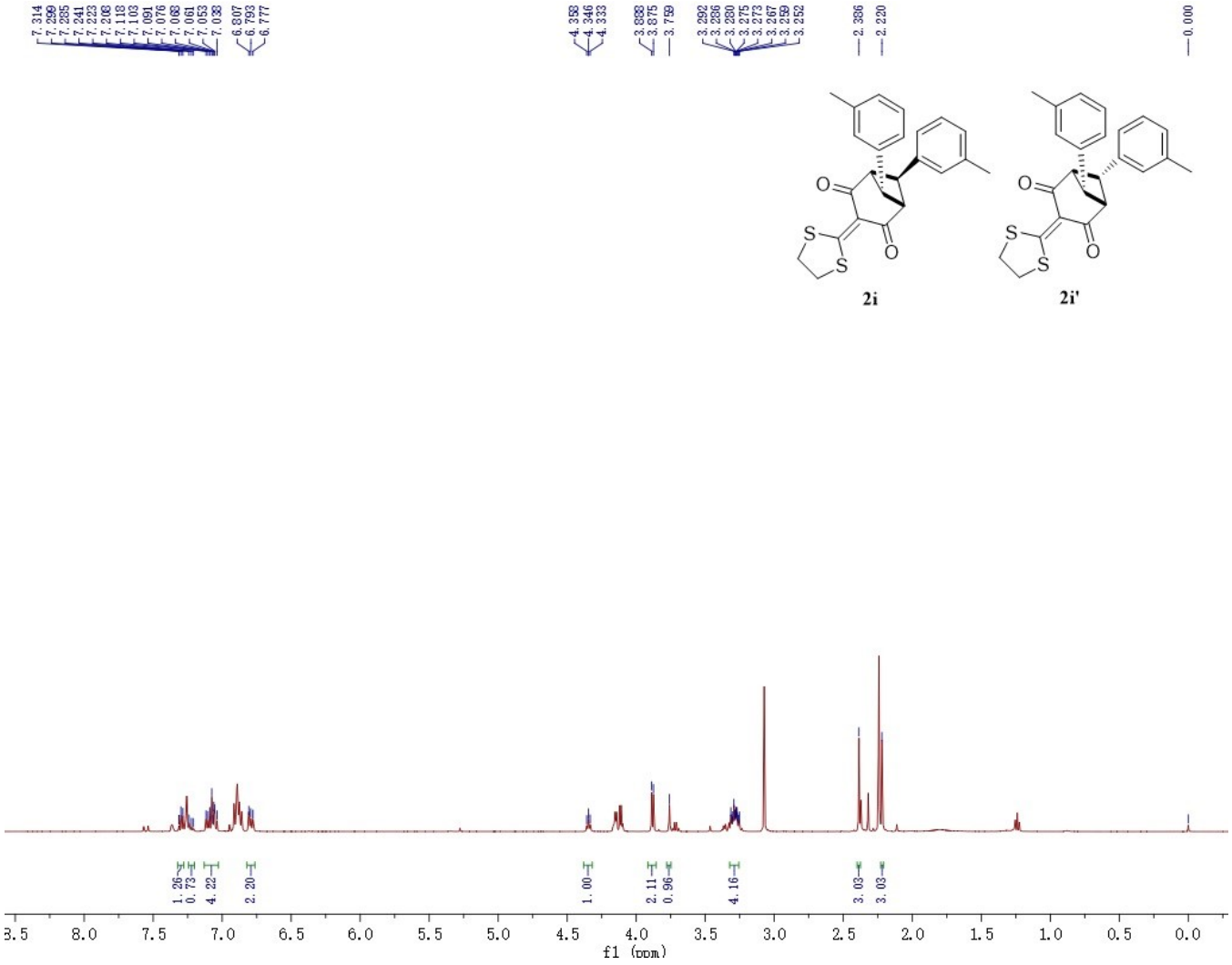
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3h



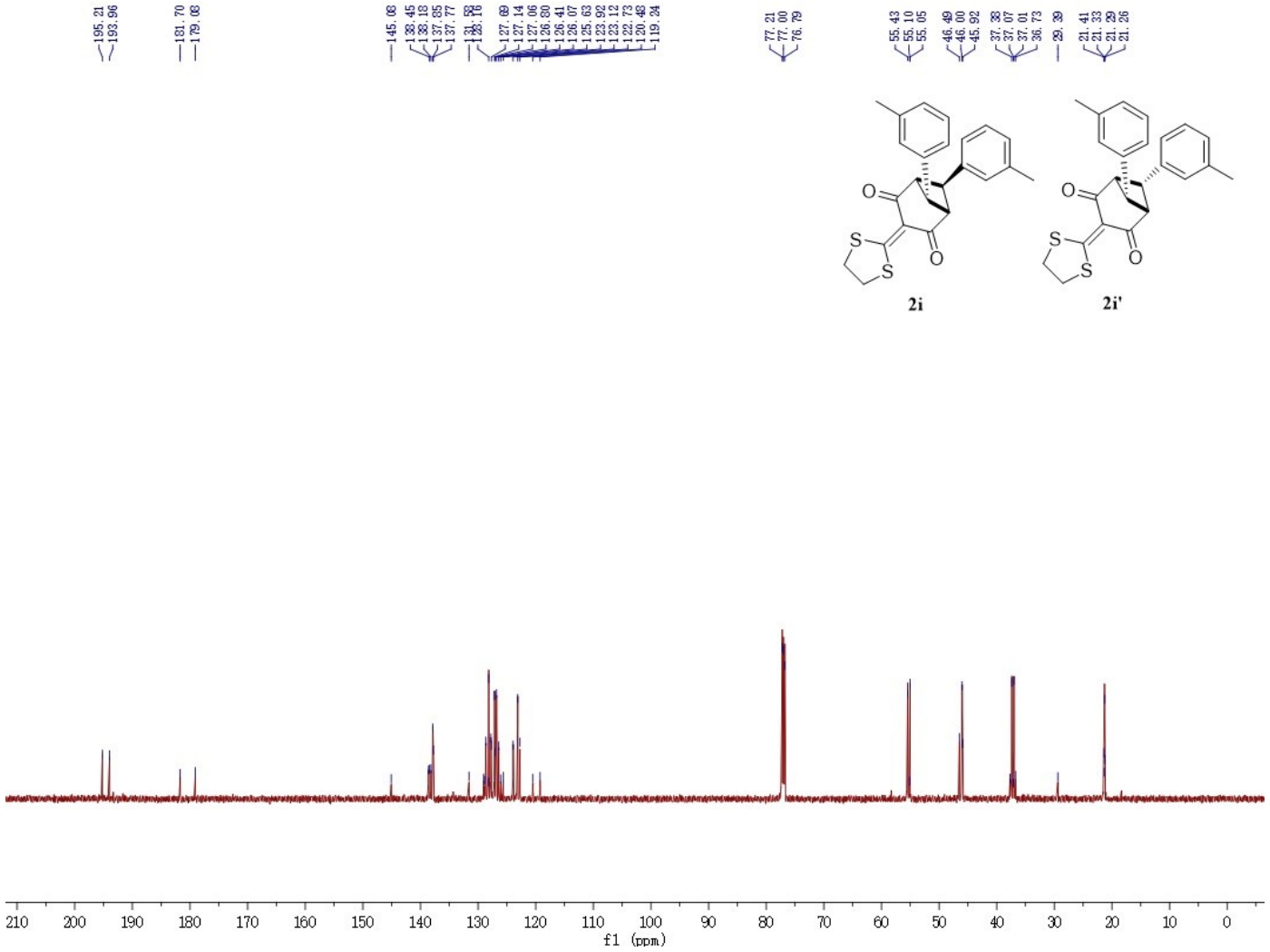
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3h



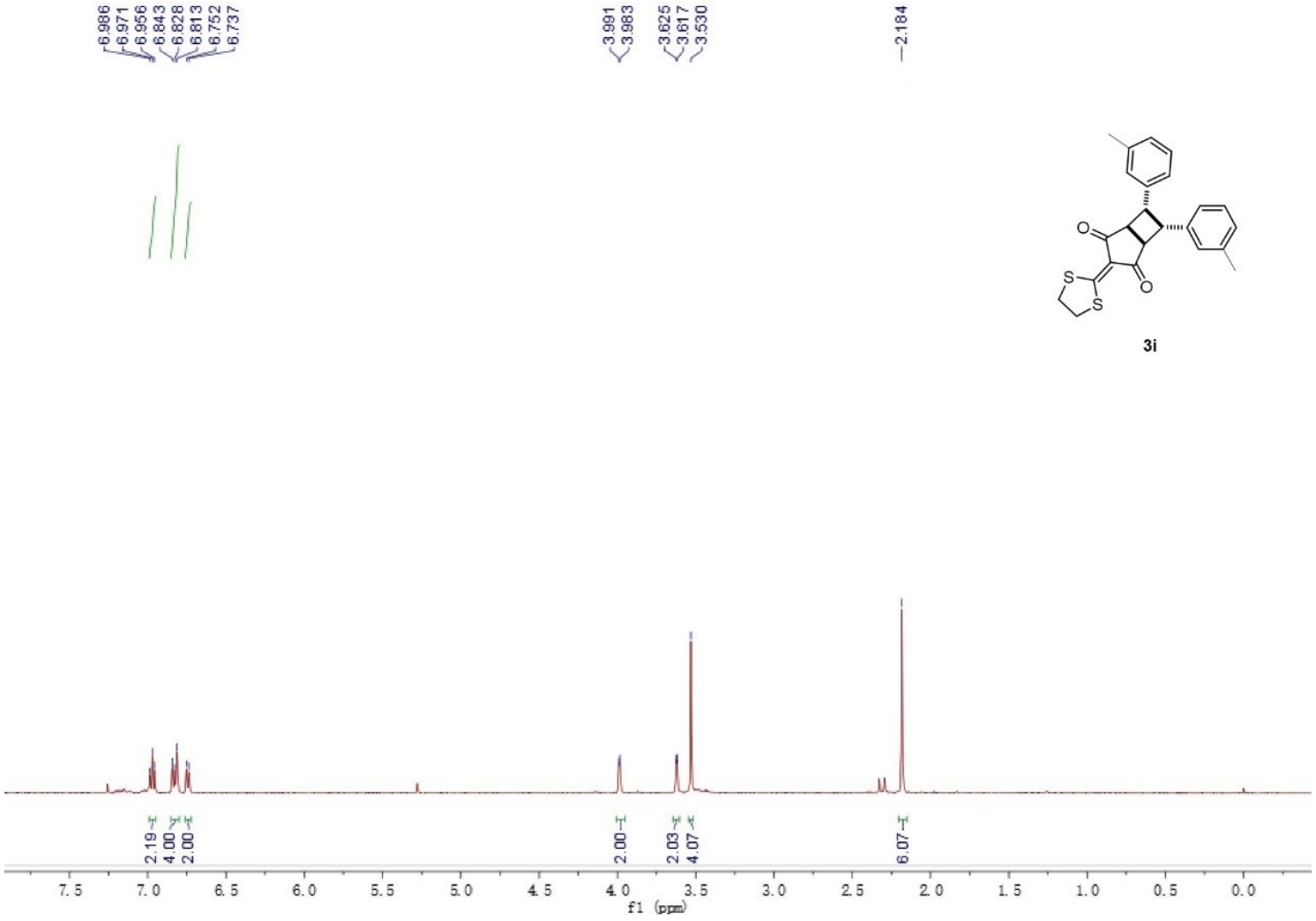
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2i/2i'



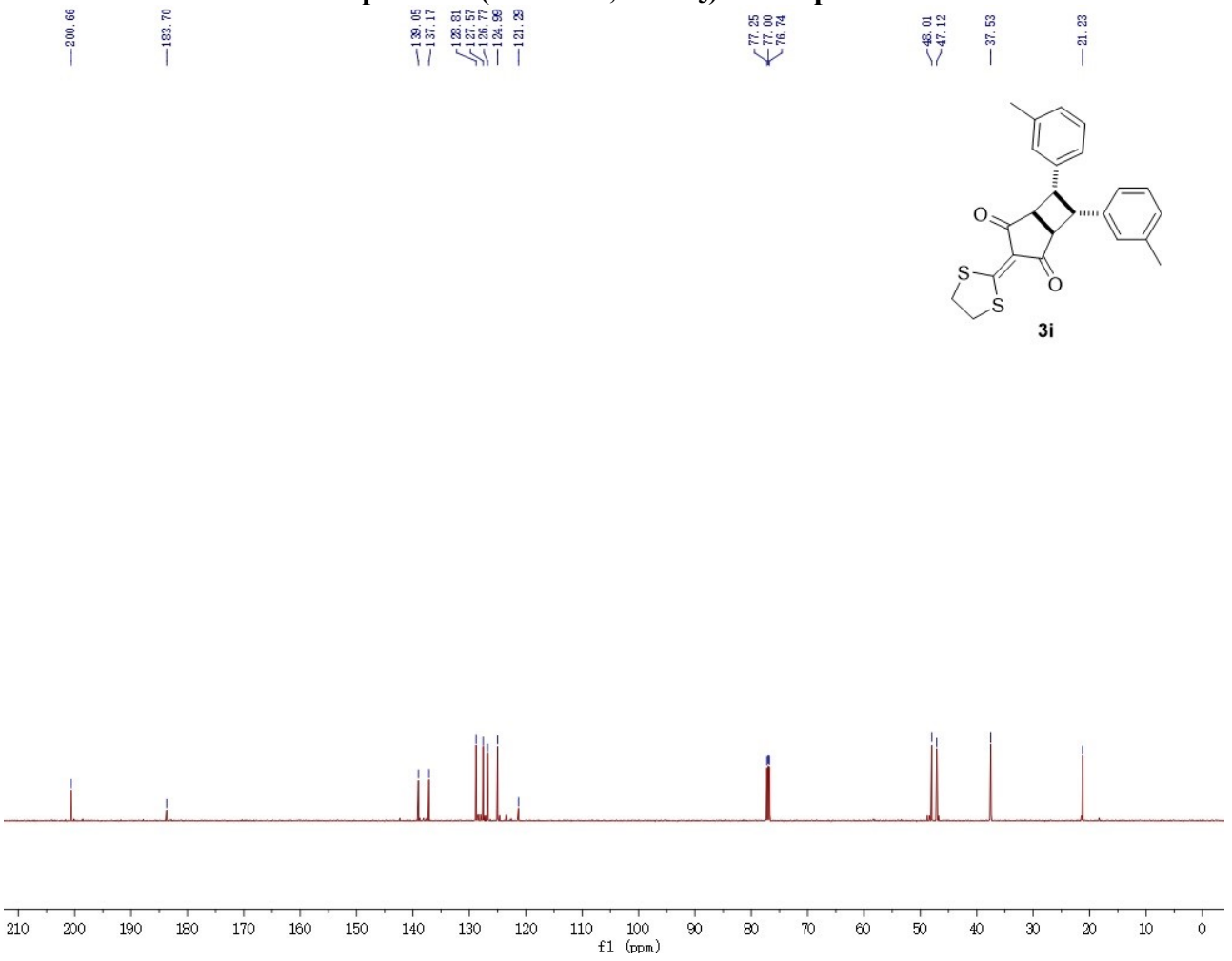
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2i/2i'



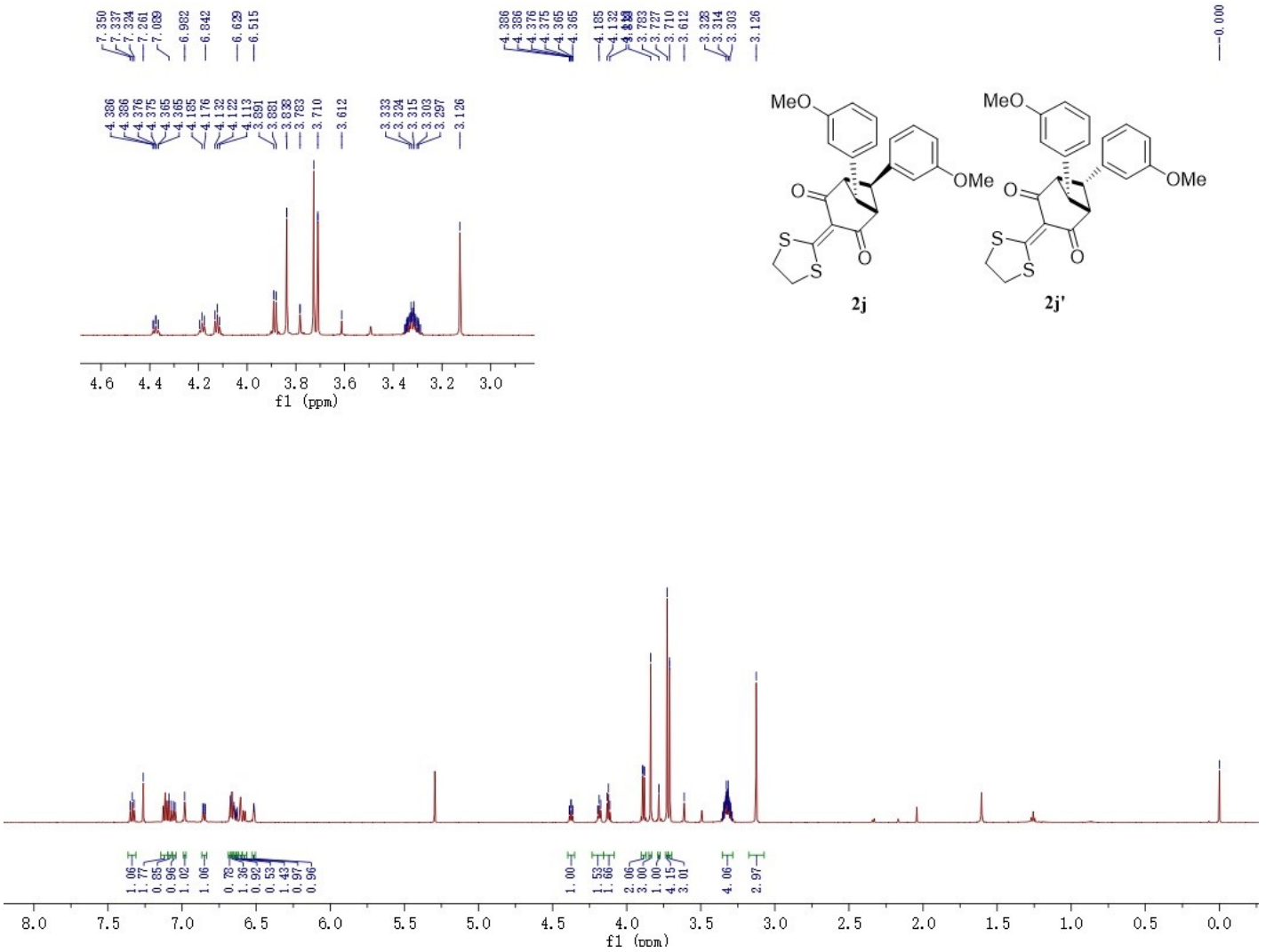
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3i



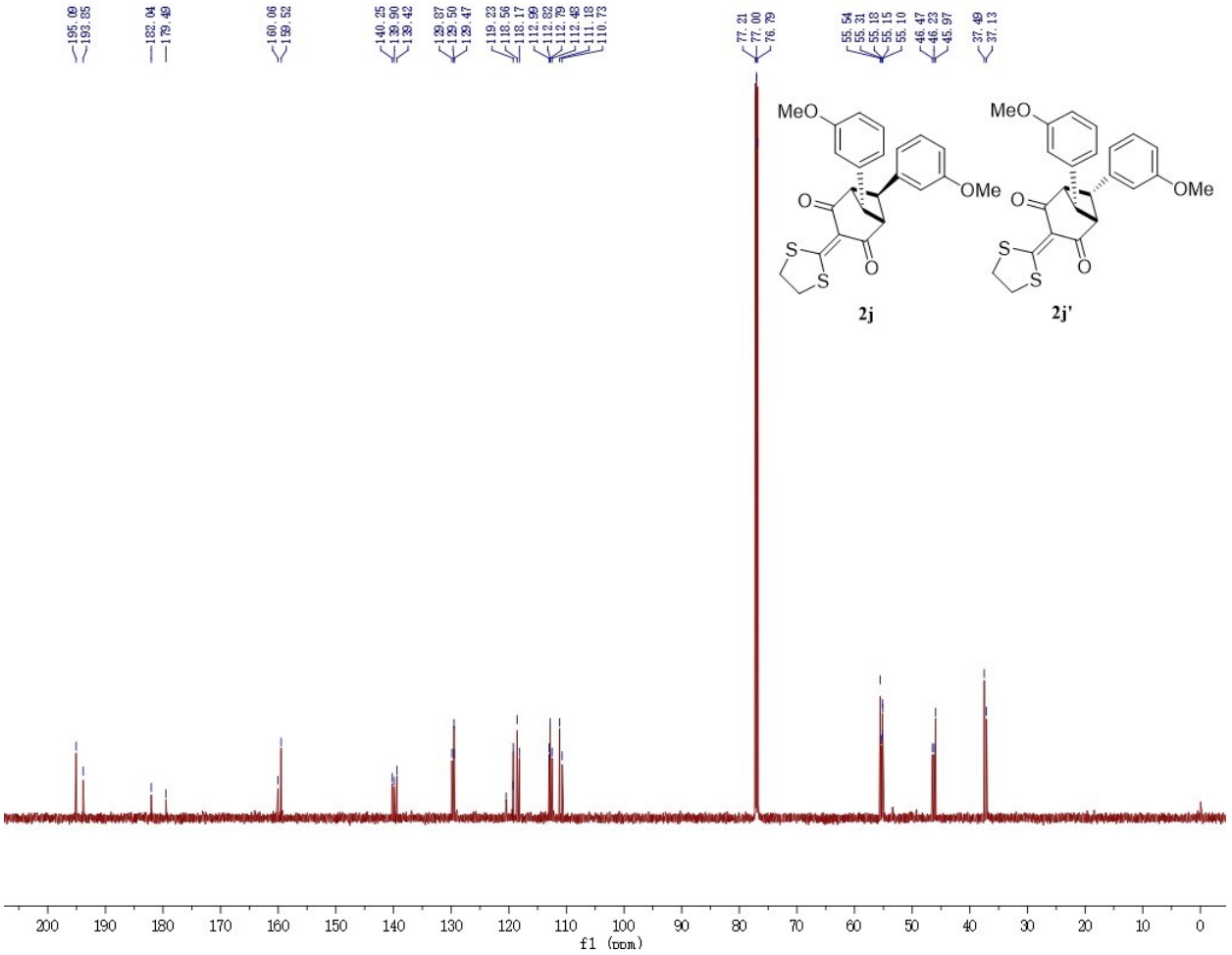
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3i



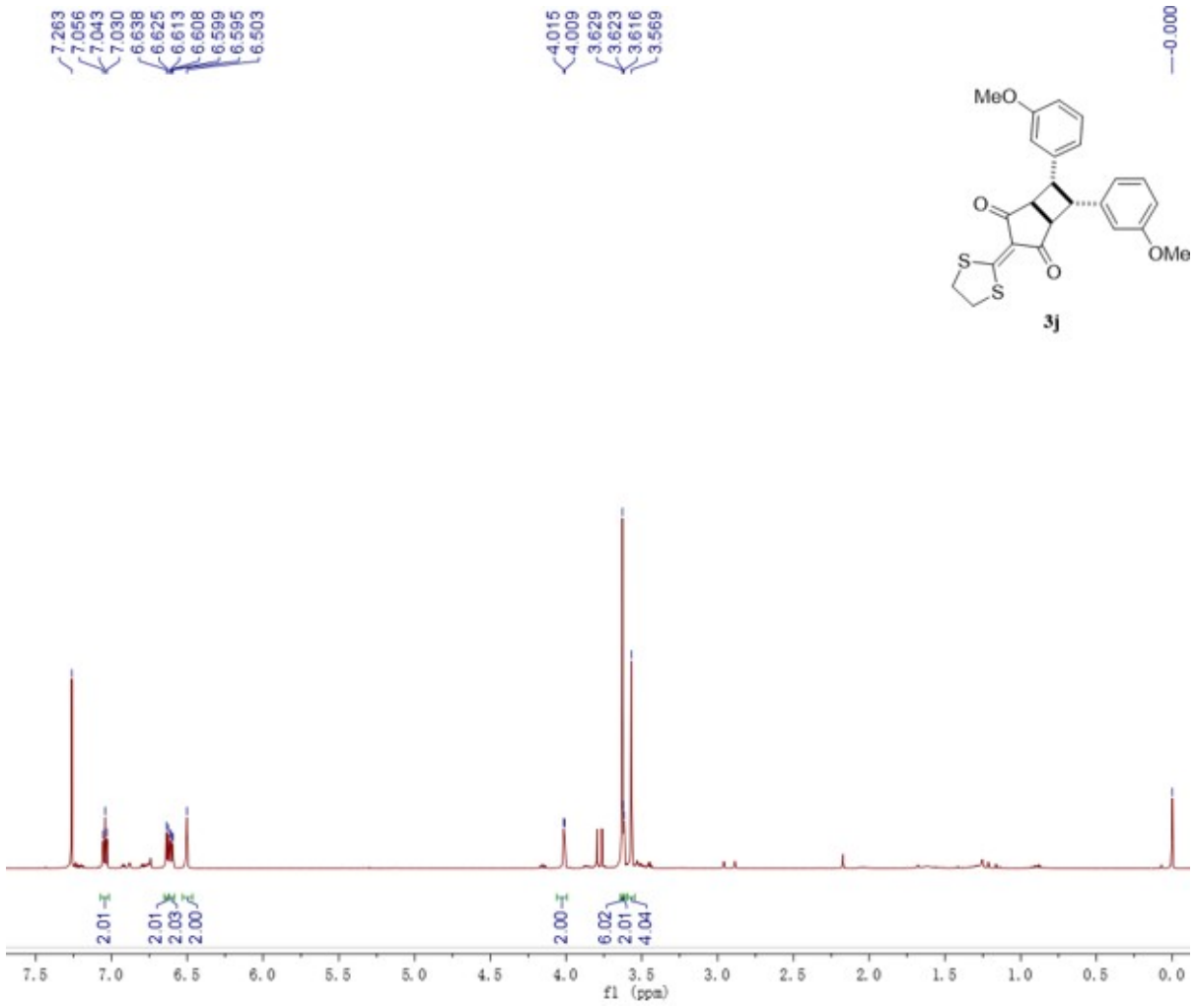
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2j/2j'



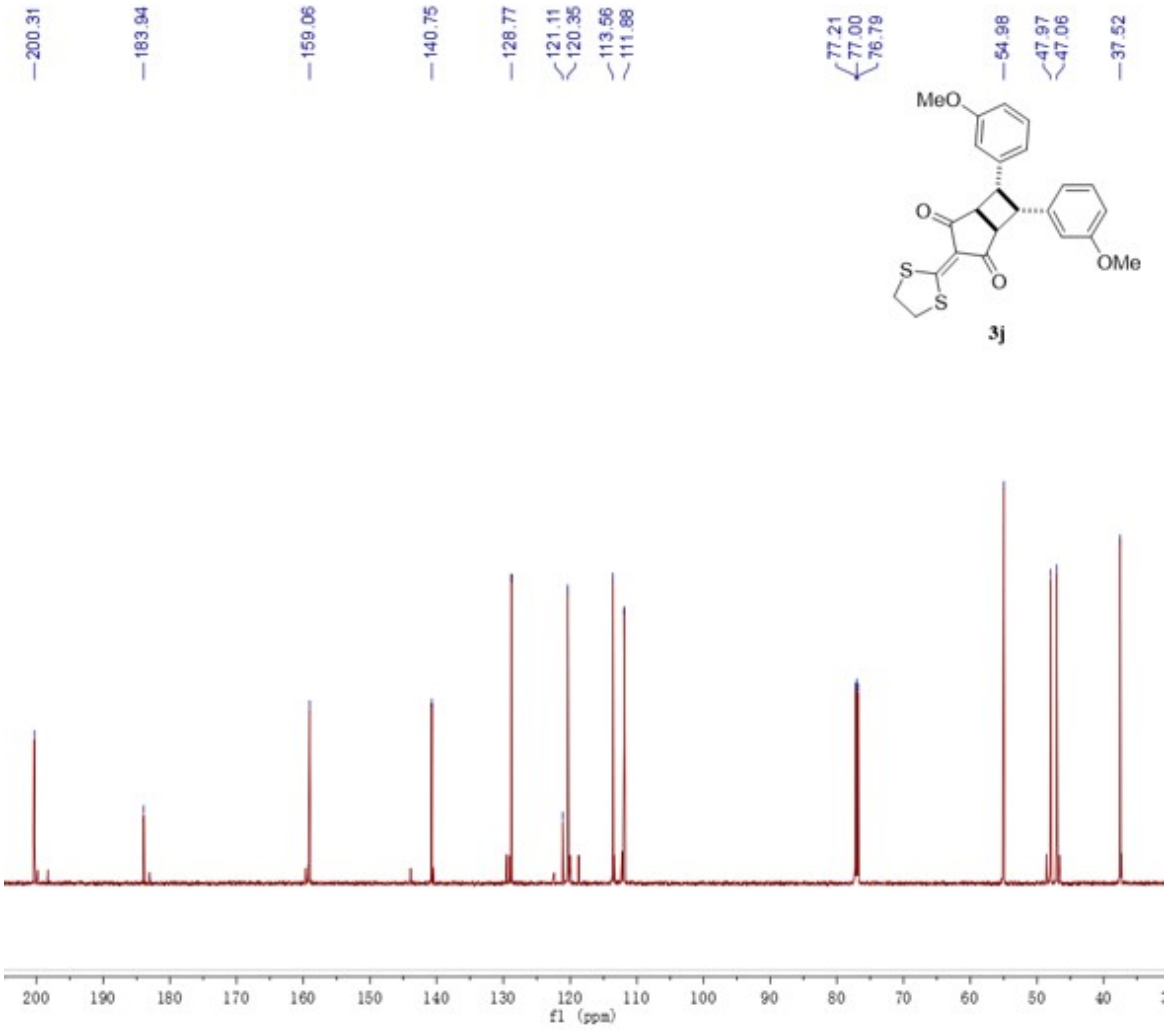
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2j/2j'



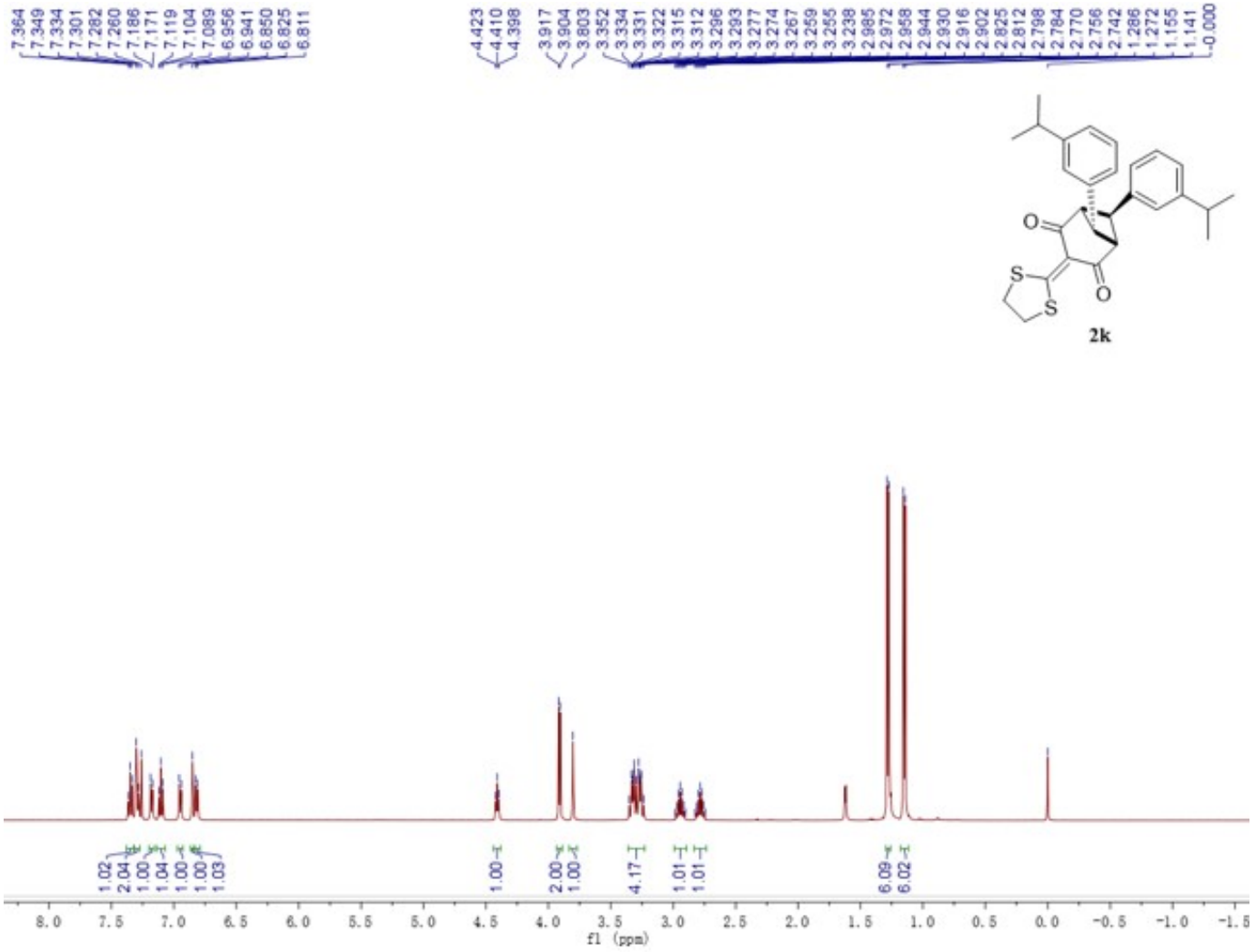
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3j



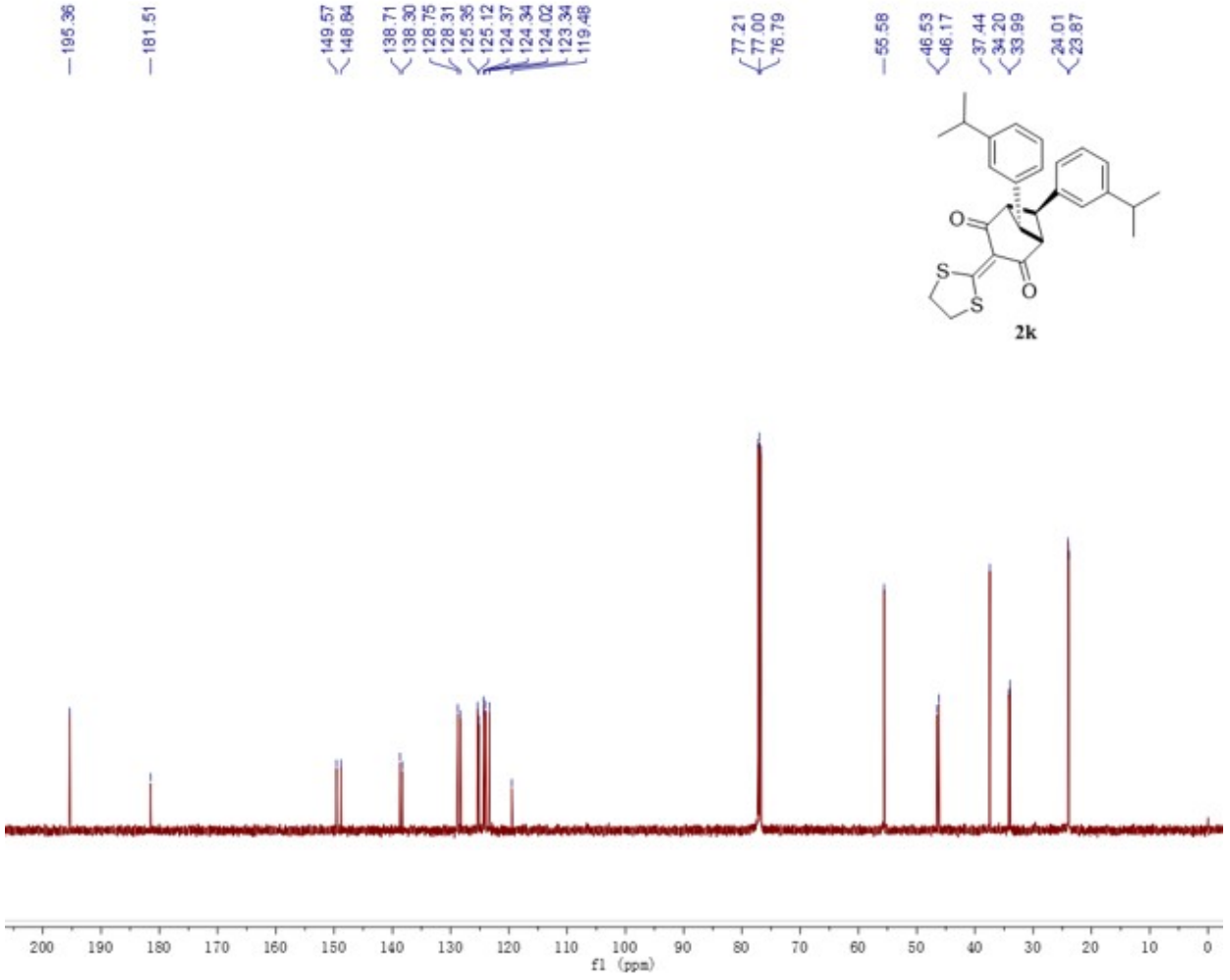
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3j



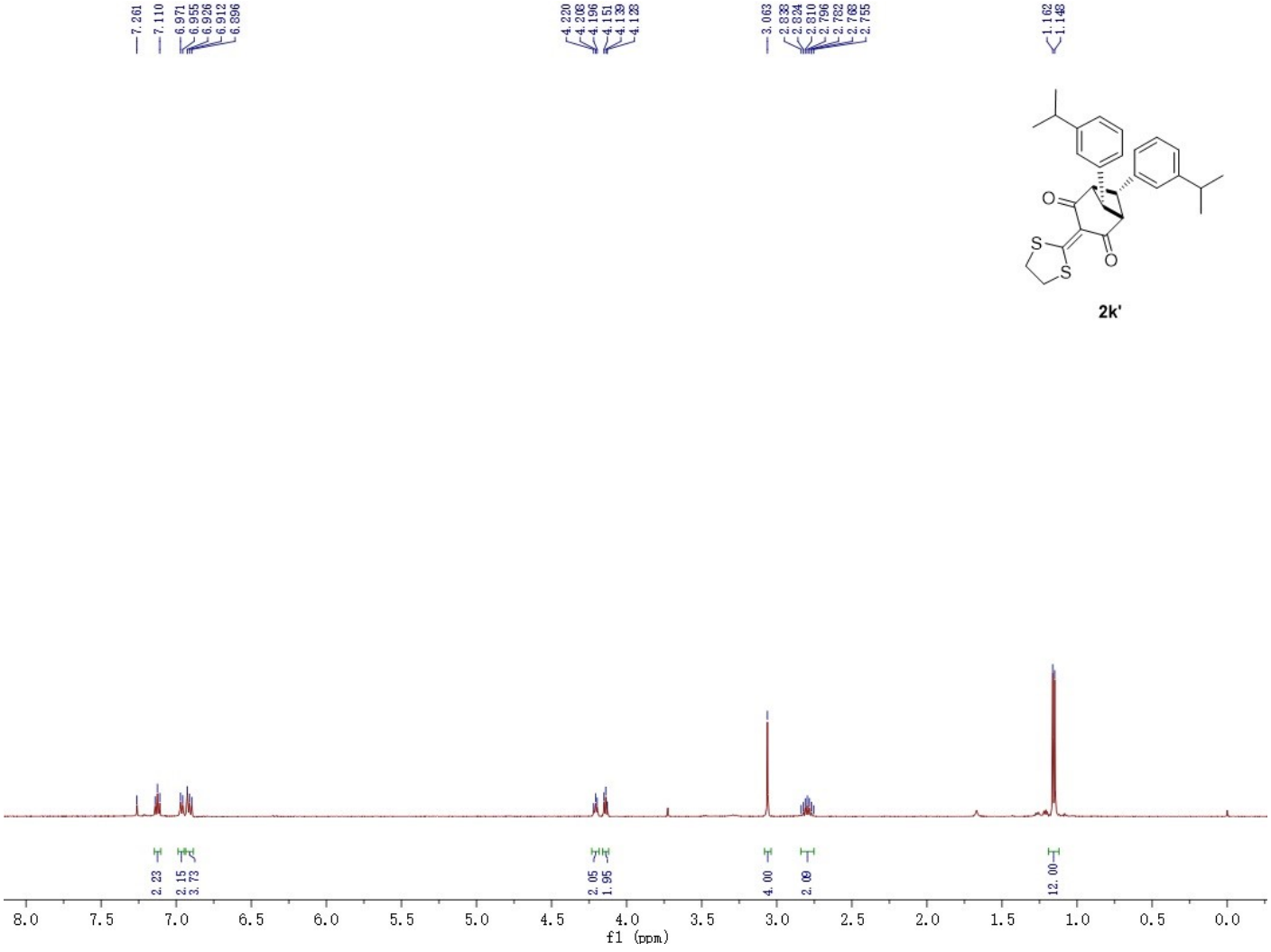
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2k



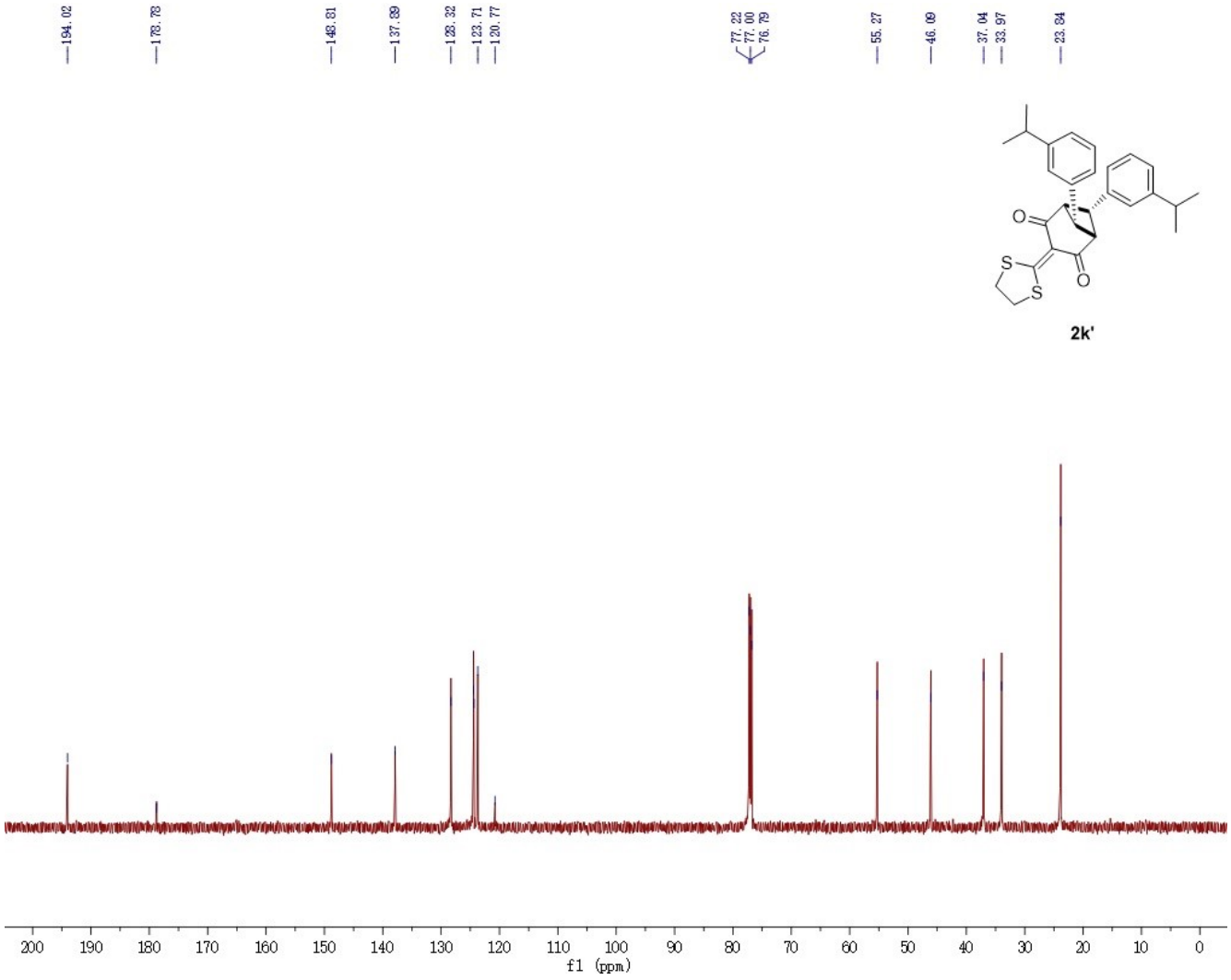
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2k



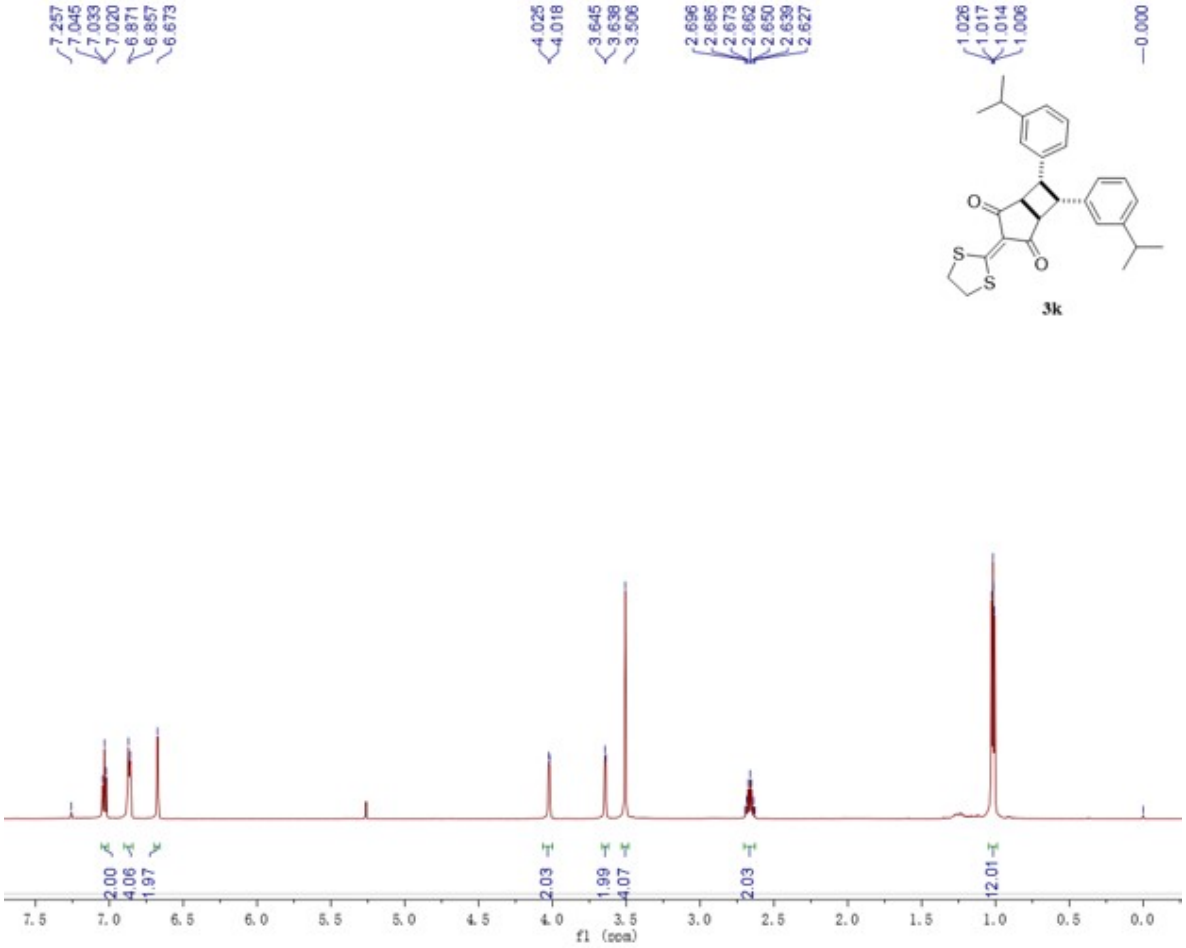
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2k'



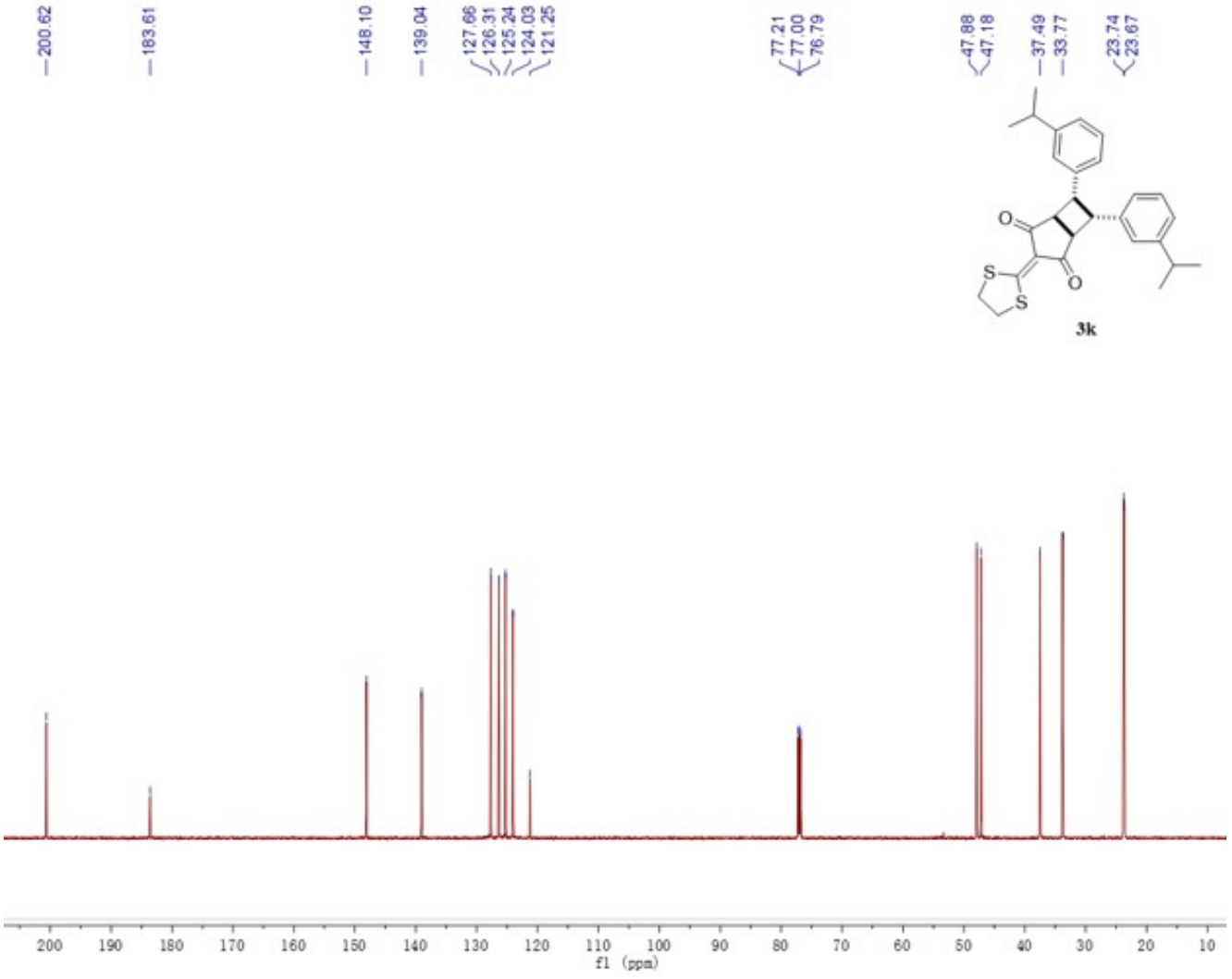
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2k'



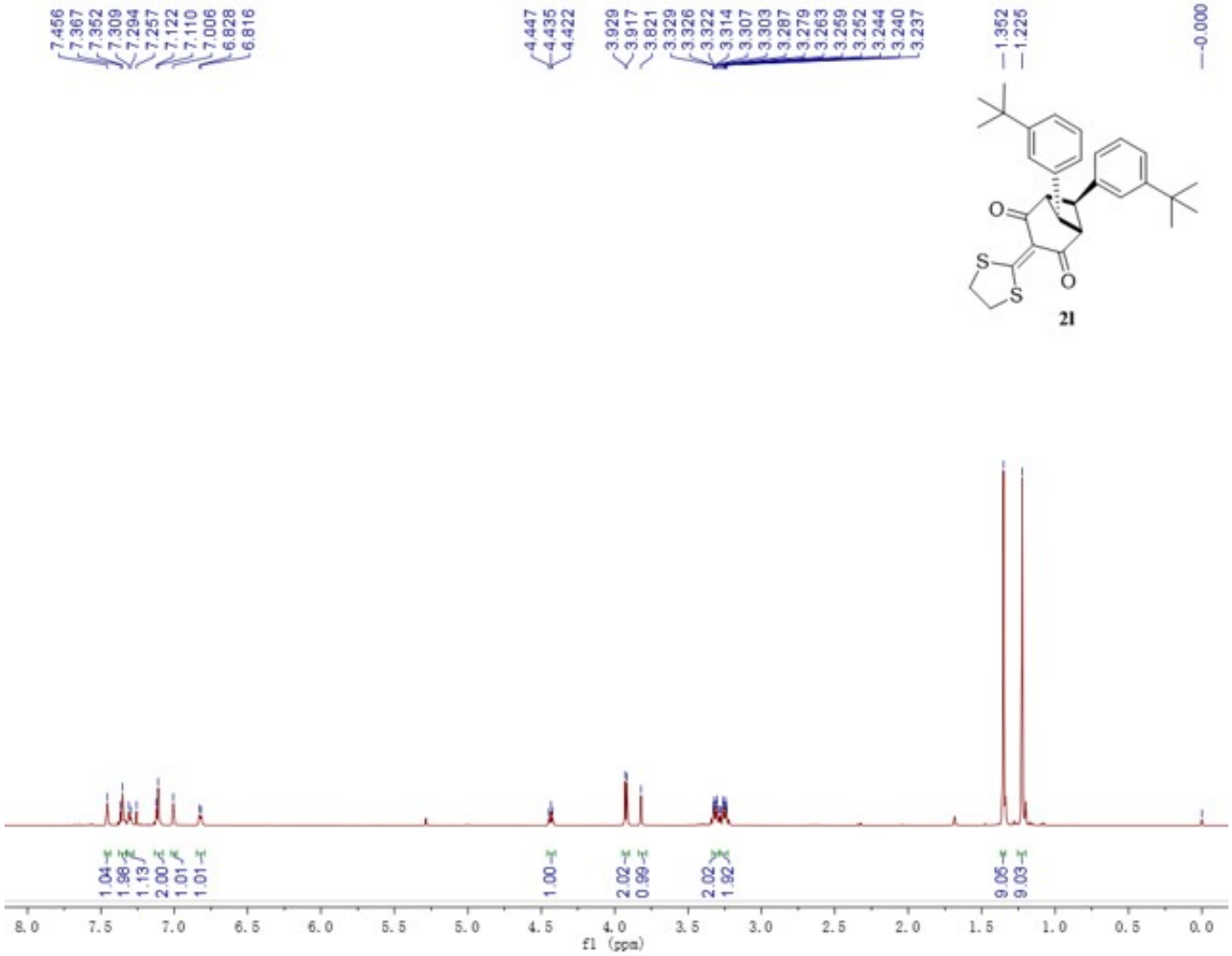
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3k



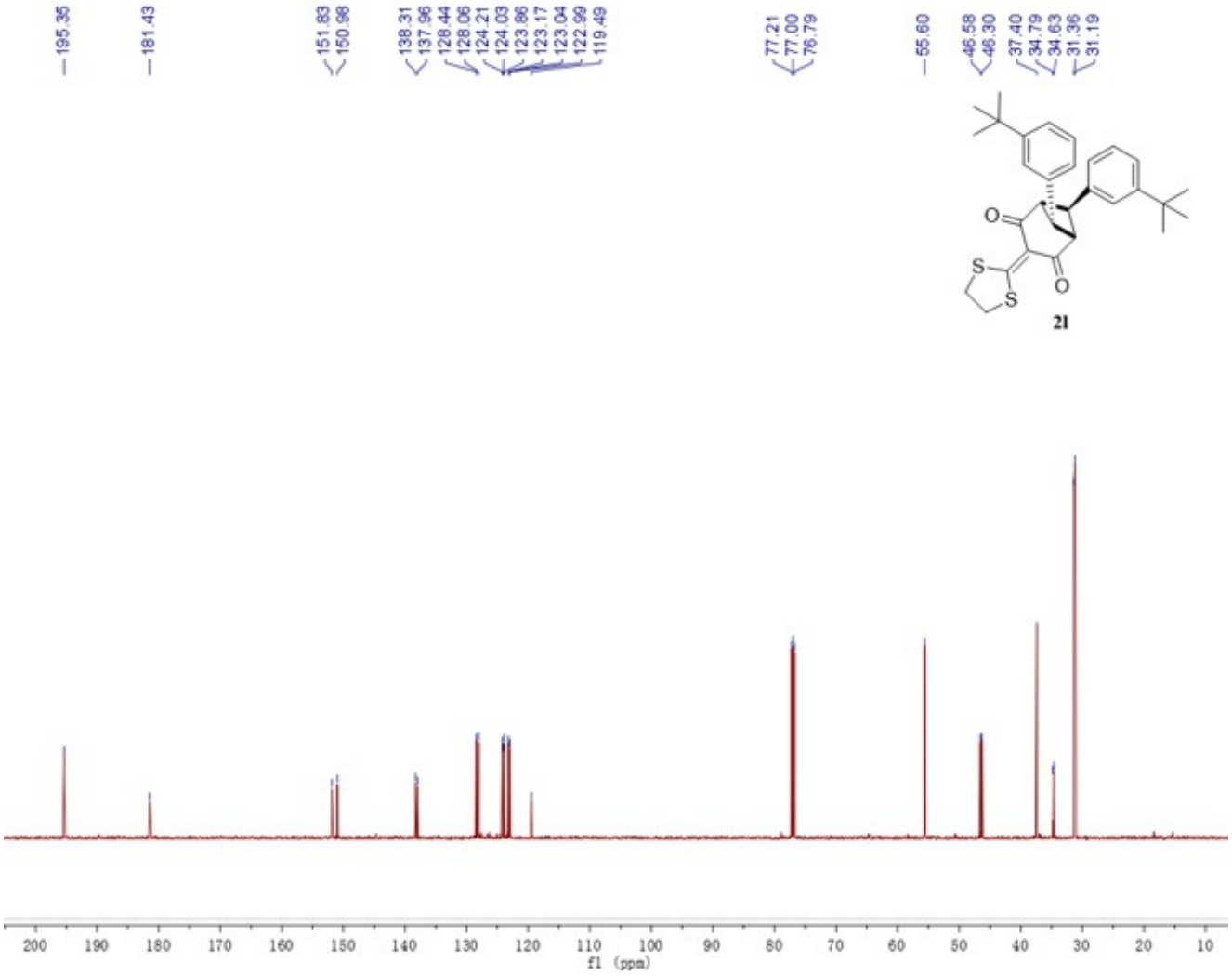
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3k



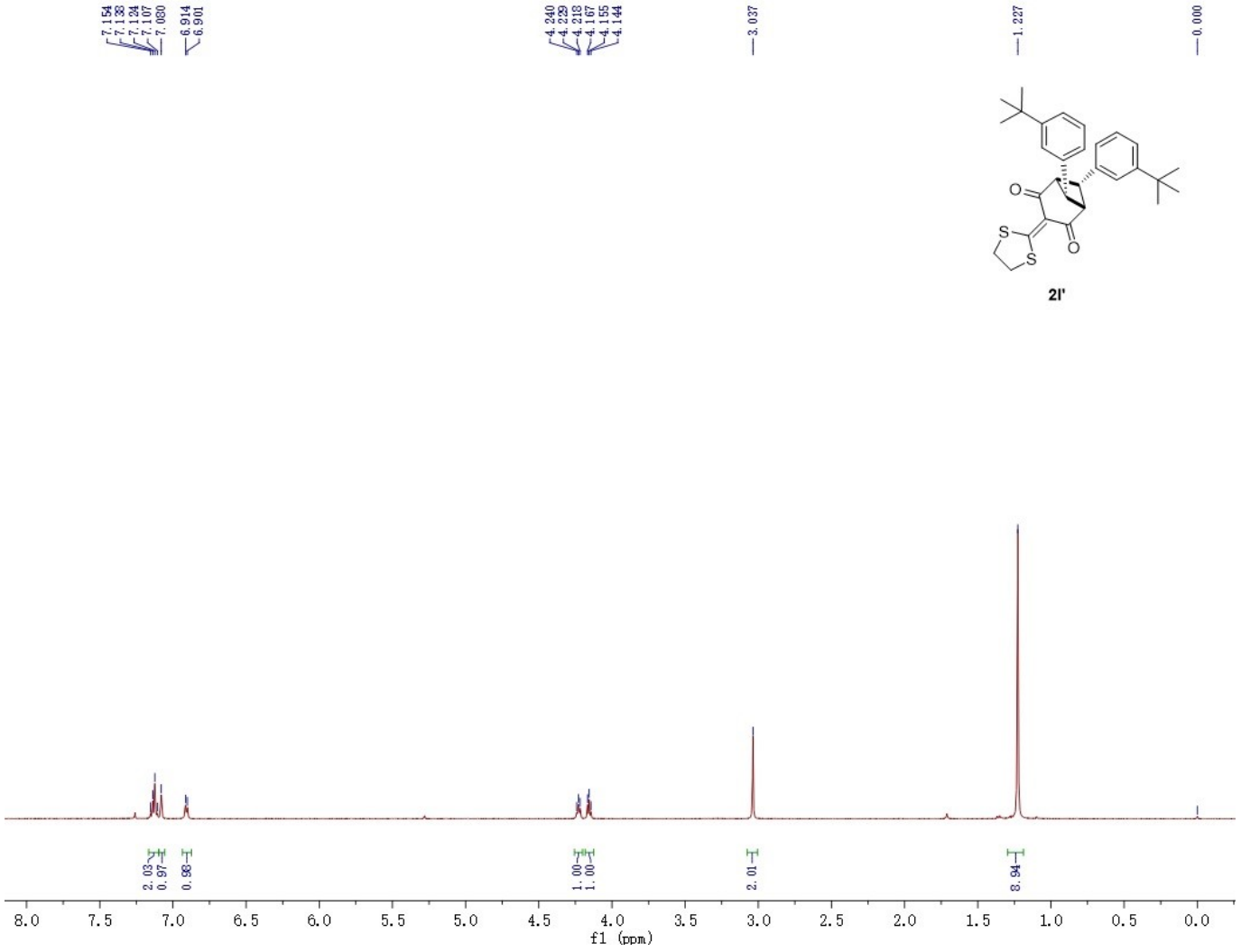
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2l



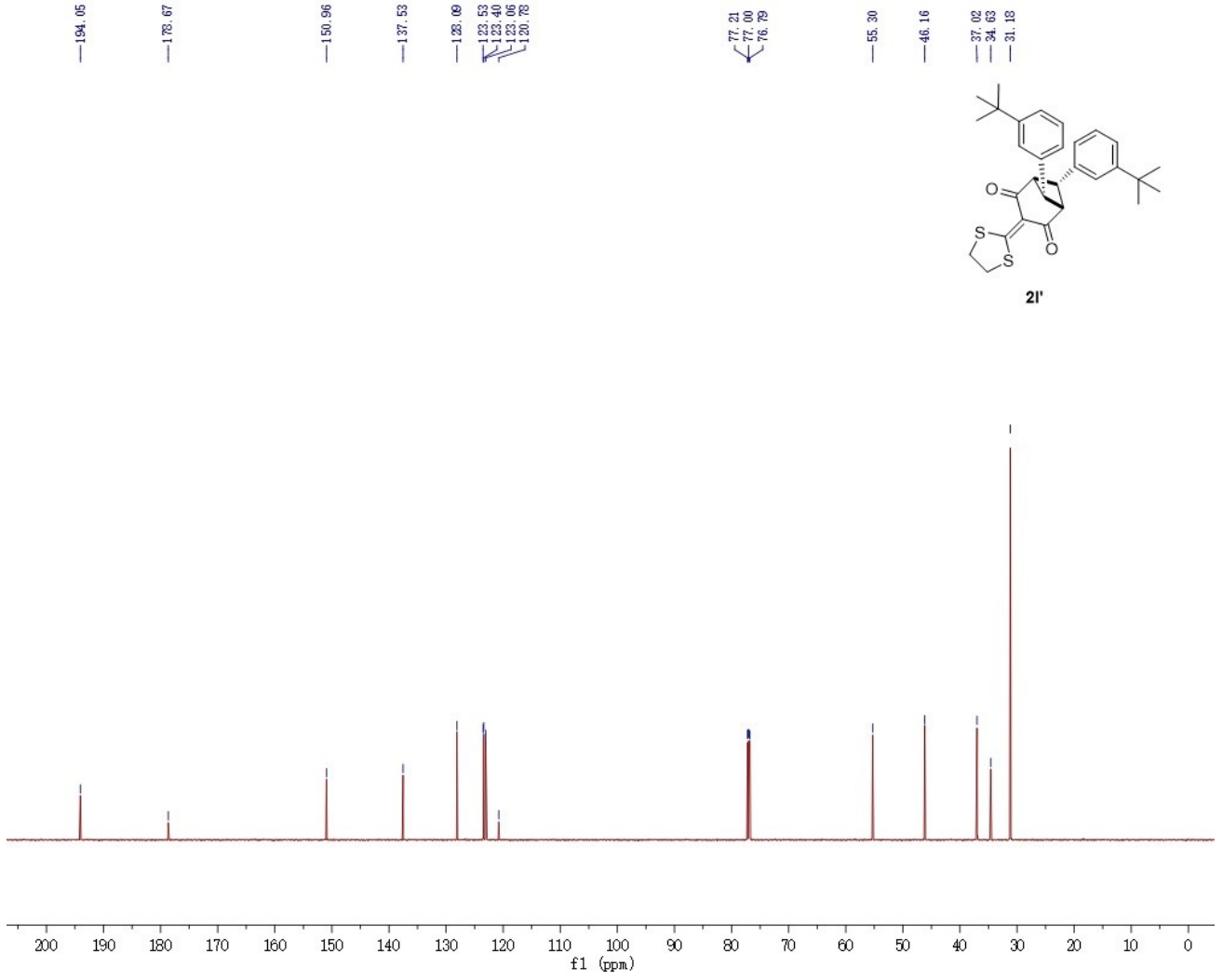
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2l



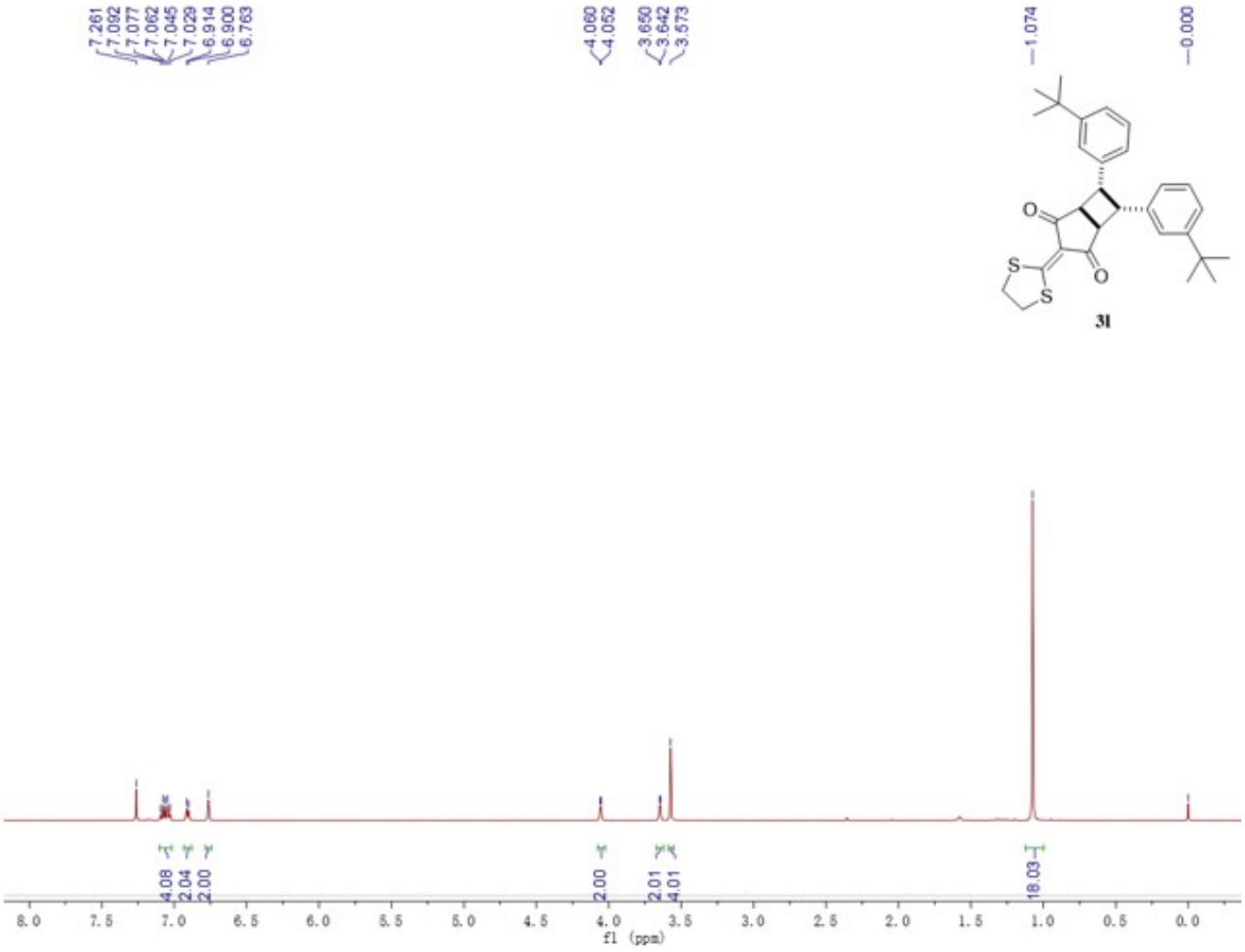
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2l'



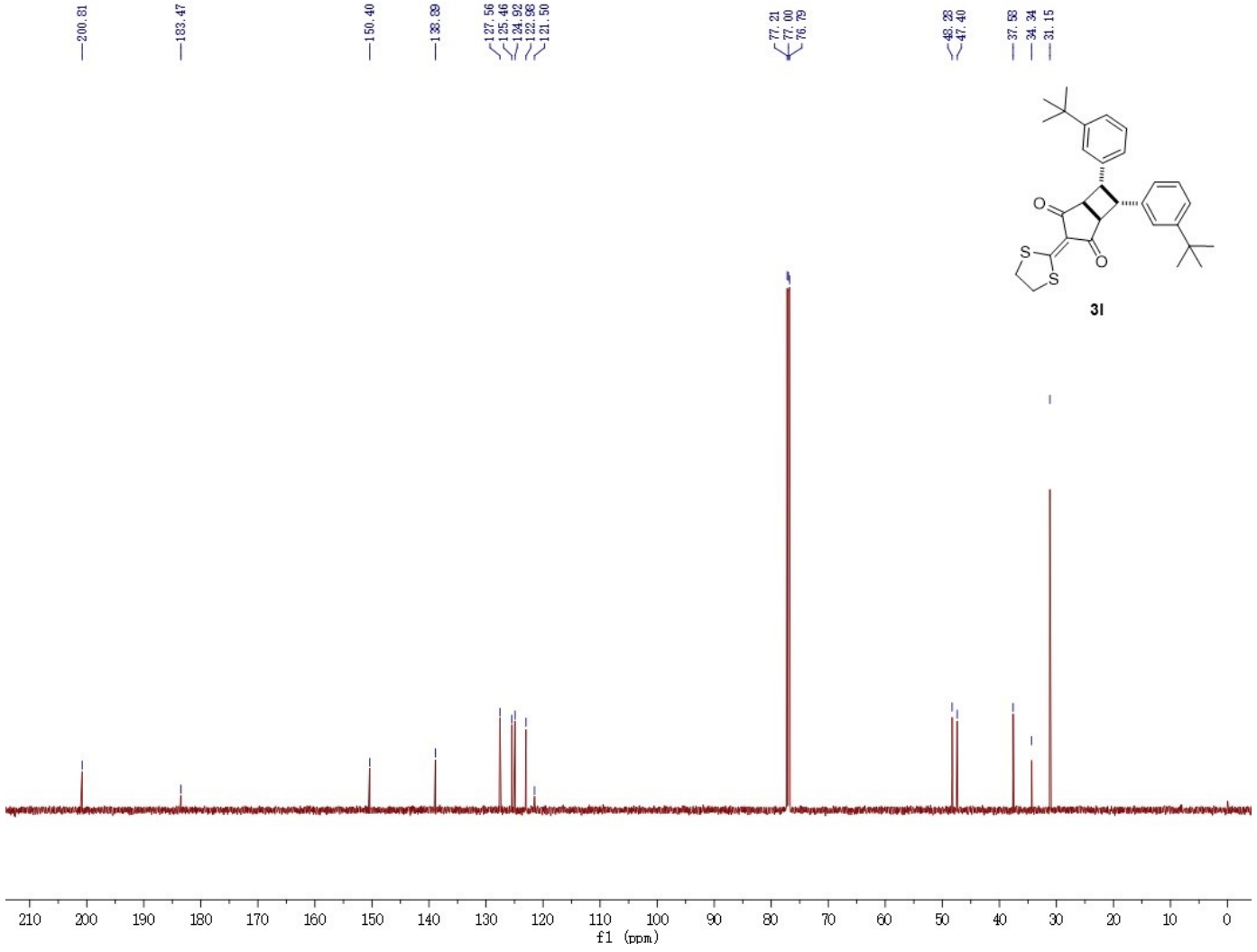
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2l'



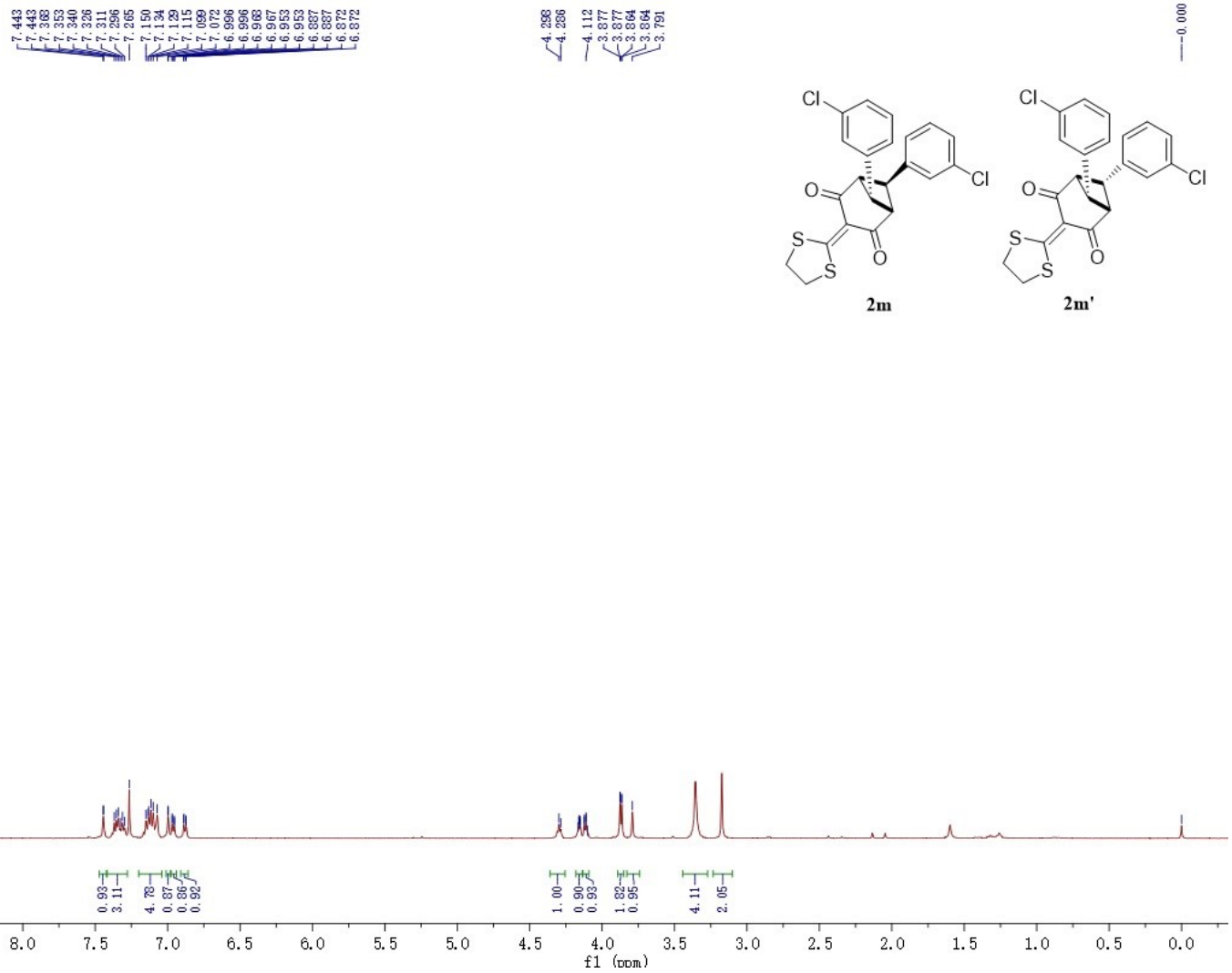
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3l



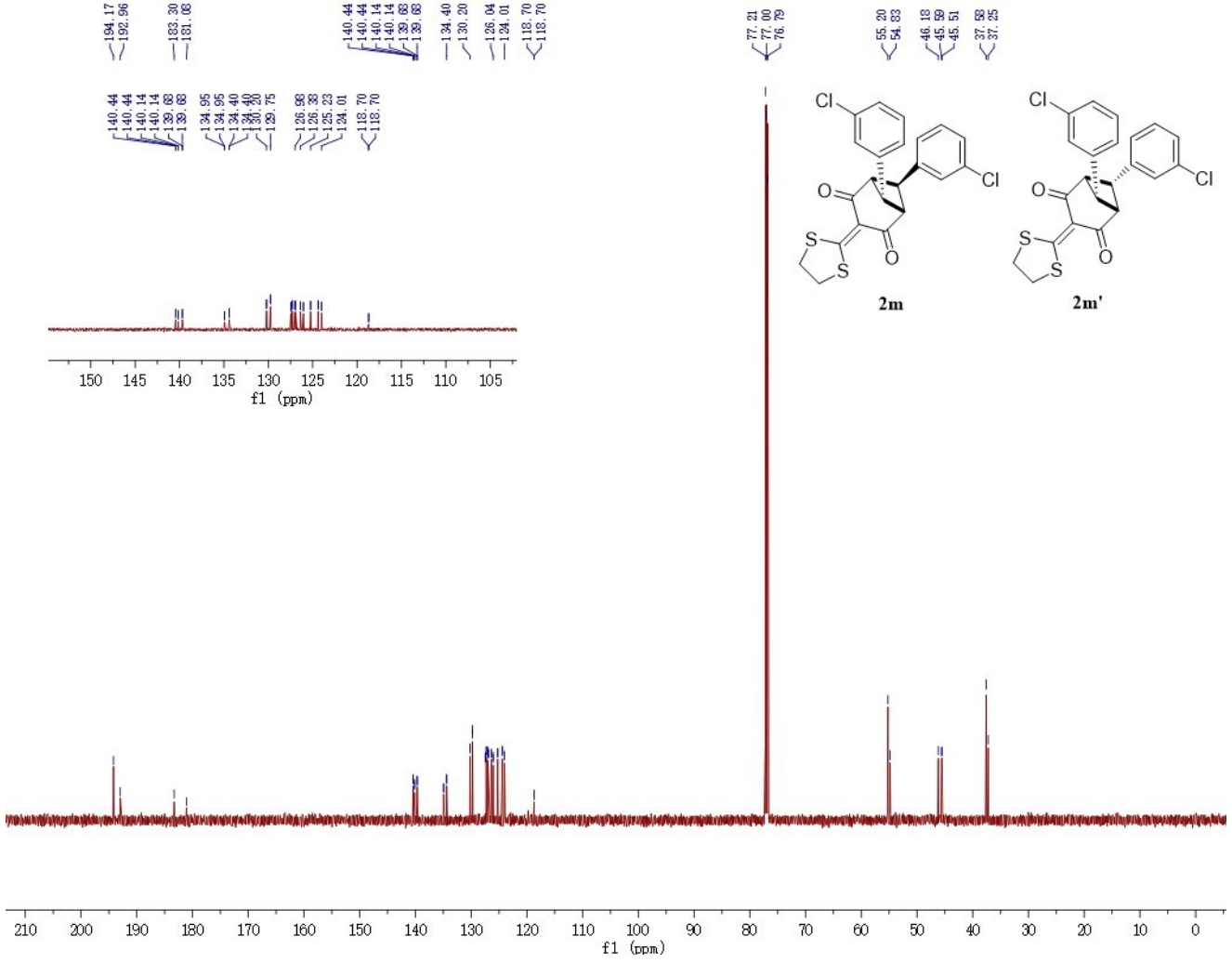
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3l



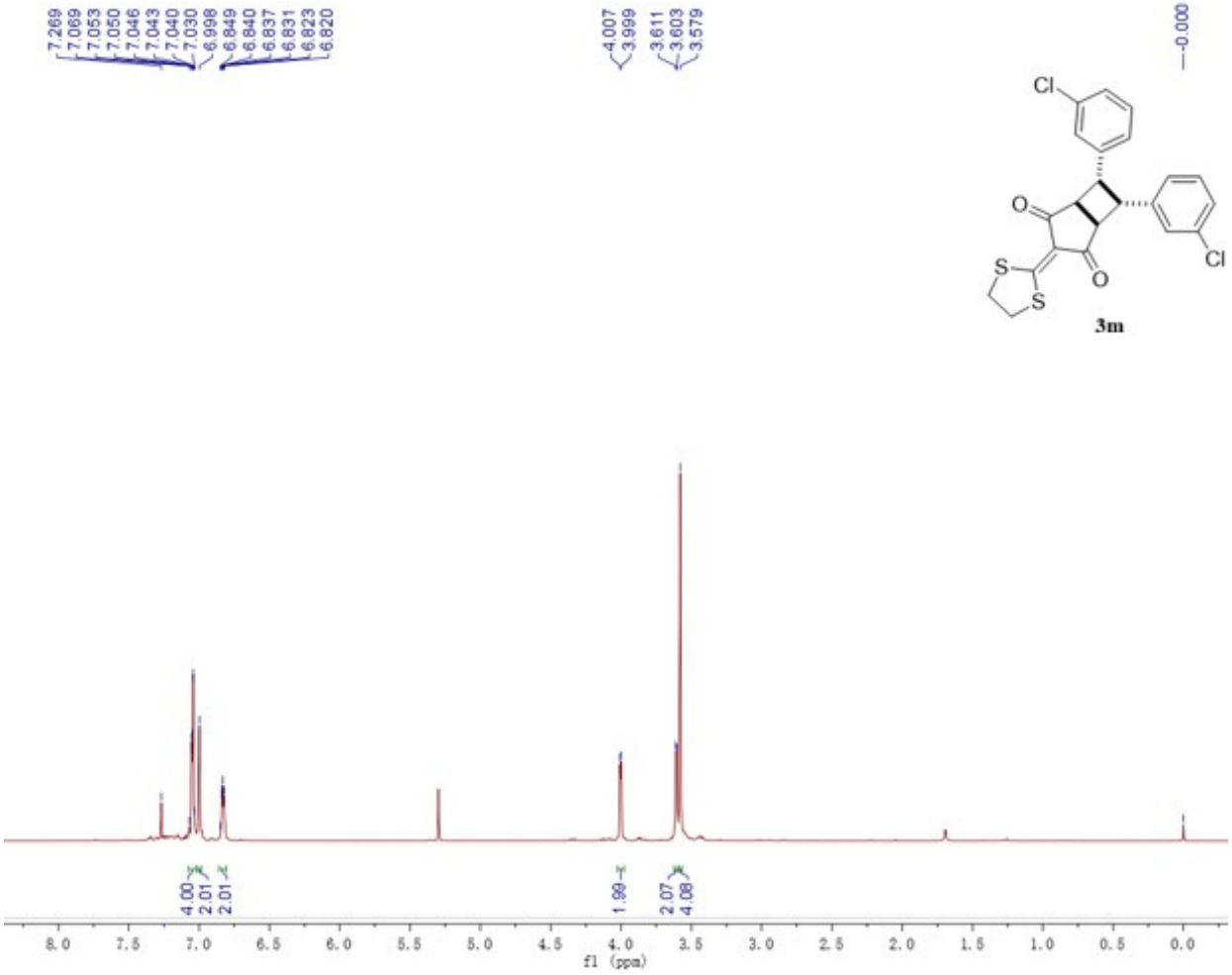
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2m/2m'



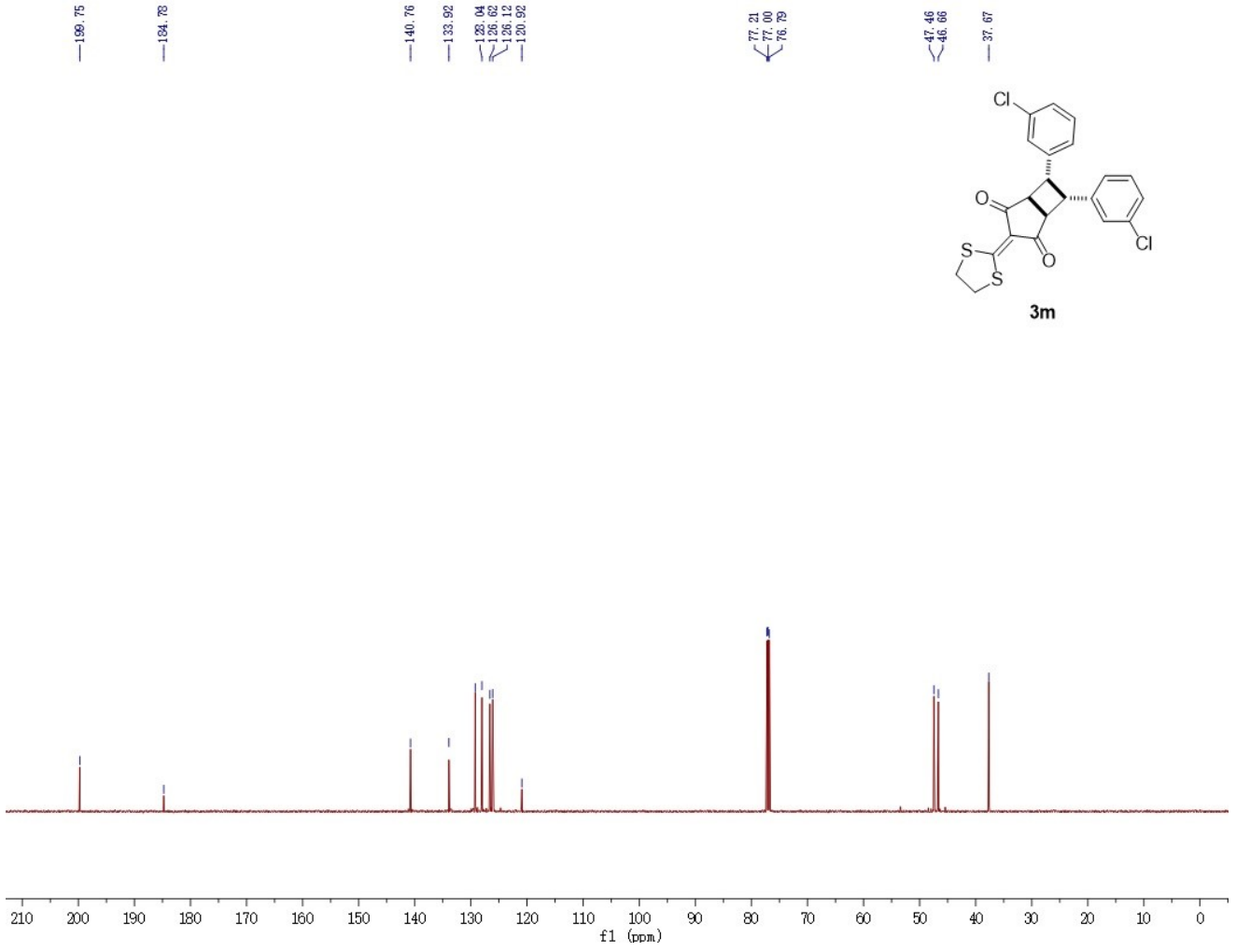
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2m/2m'



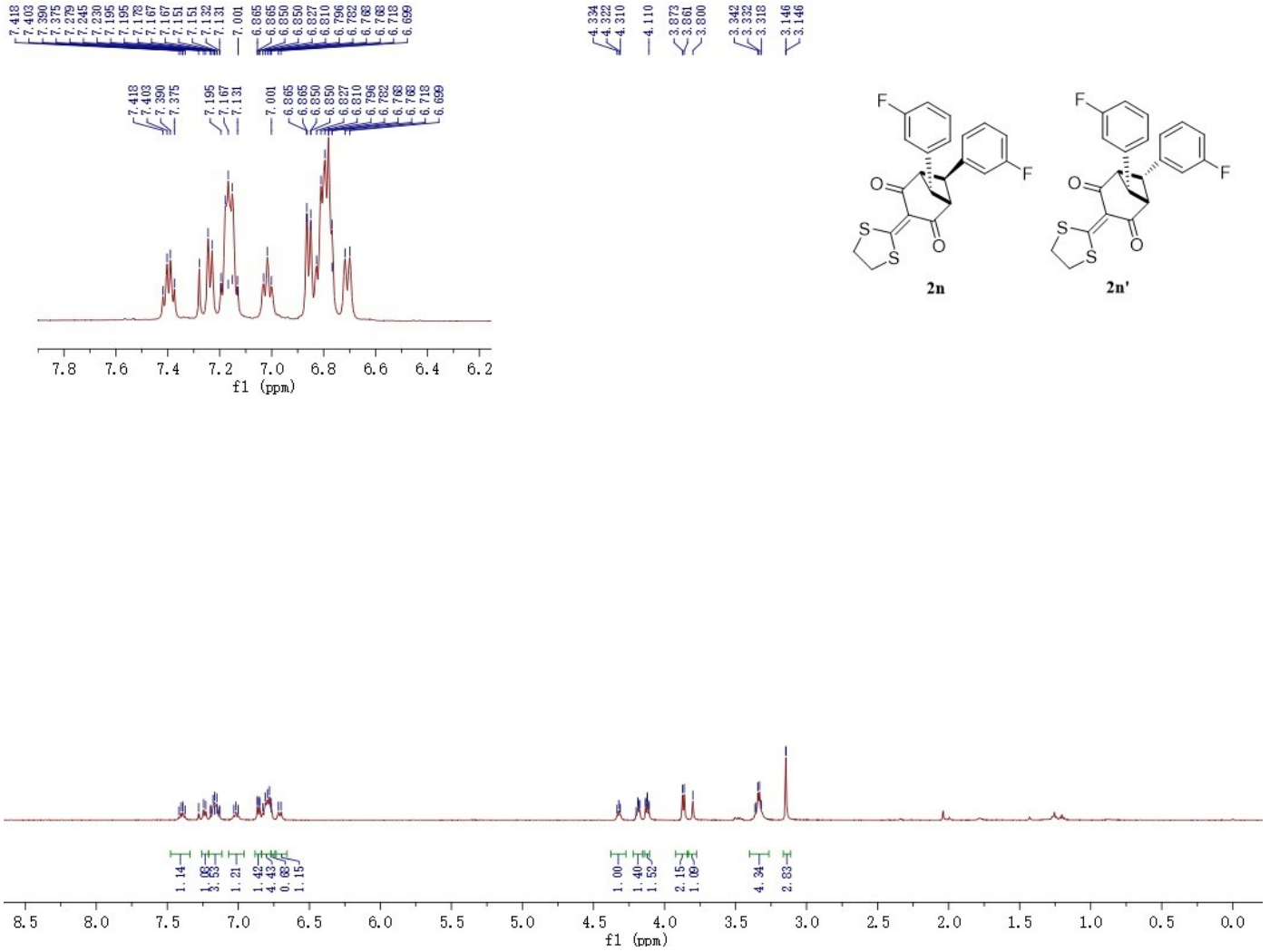
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3m



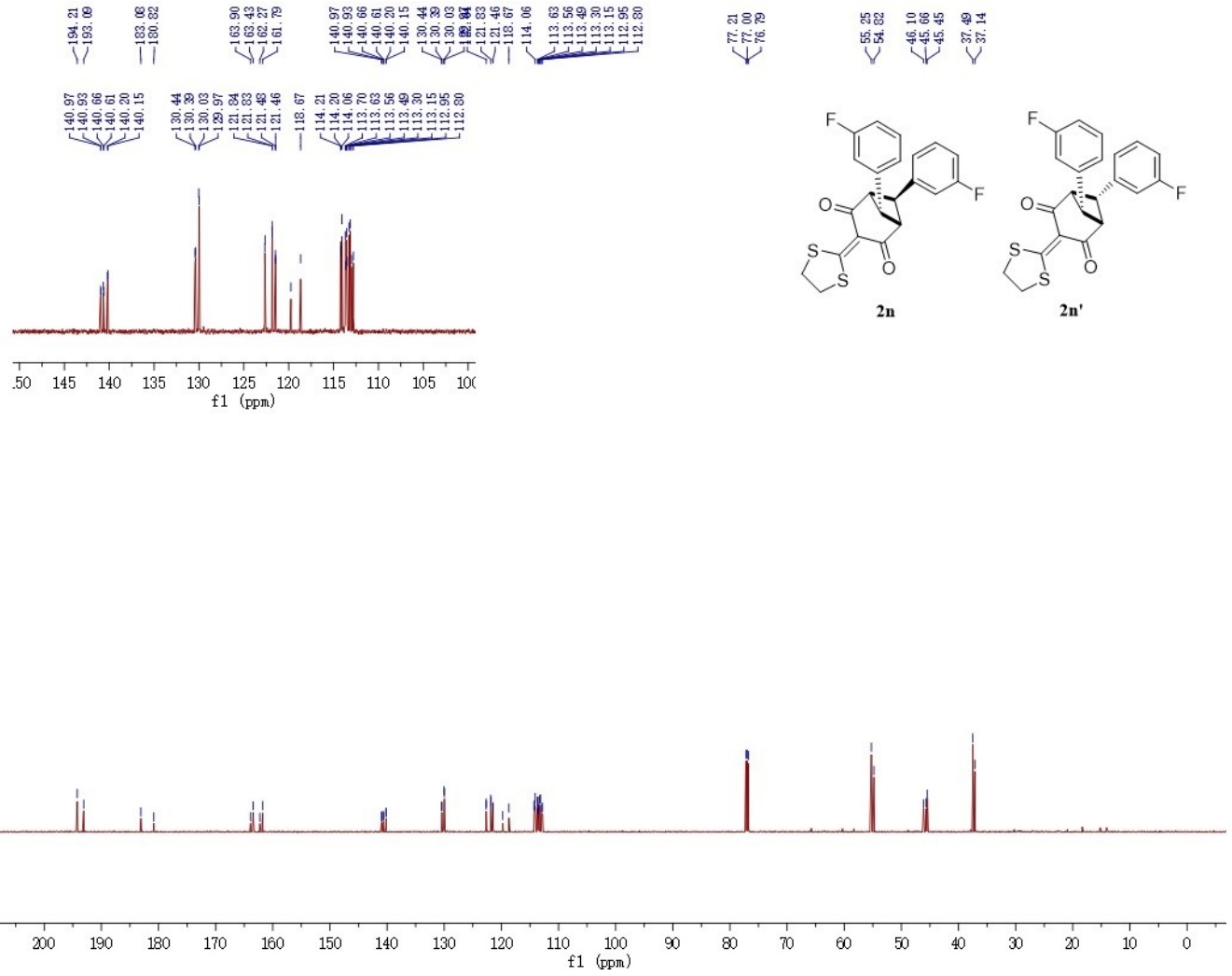
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3m



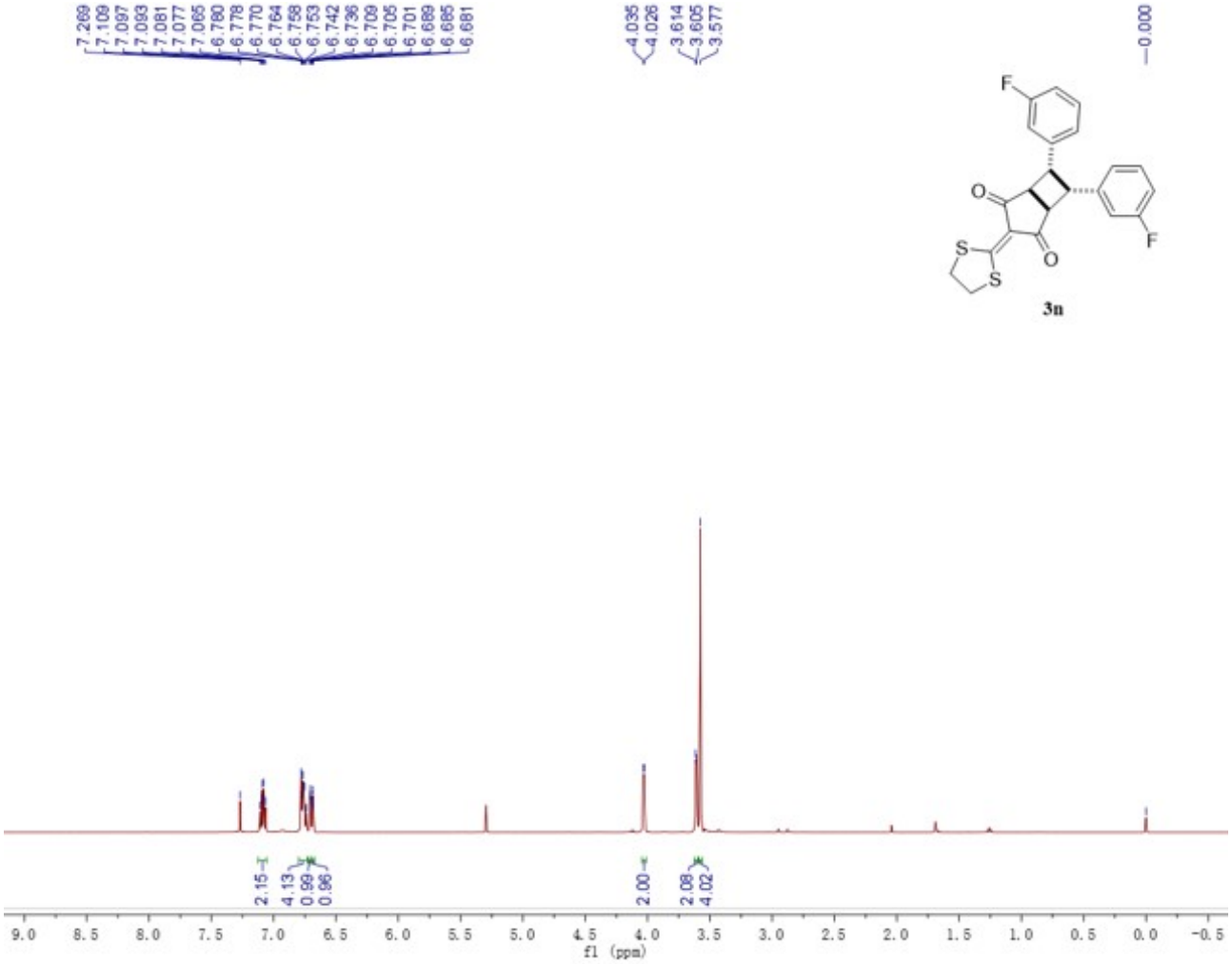
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2n/2n'



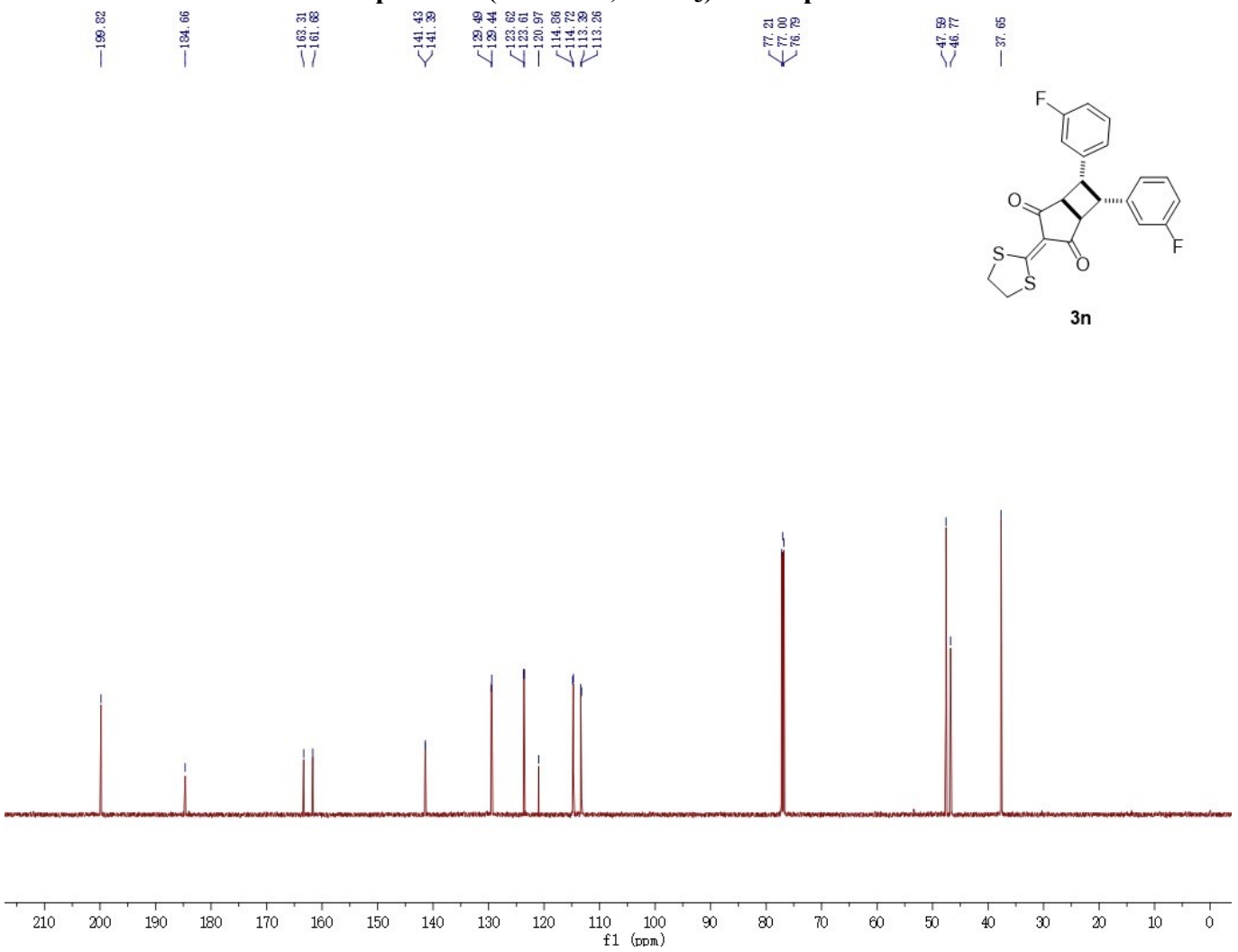
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2n/2n'



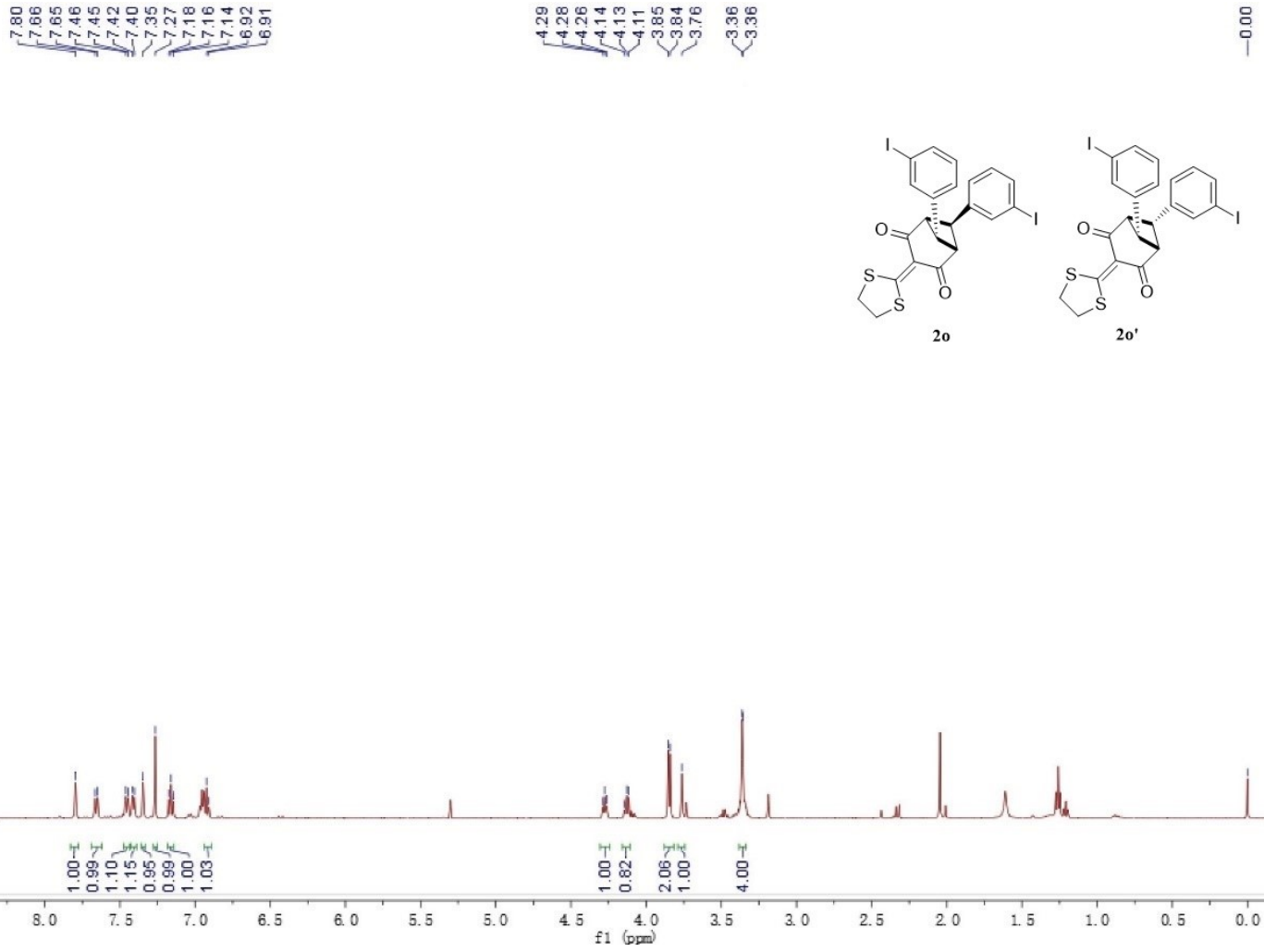
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3n



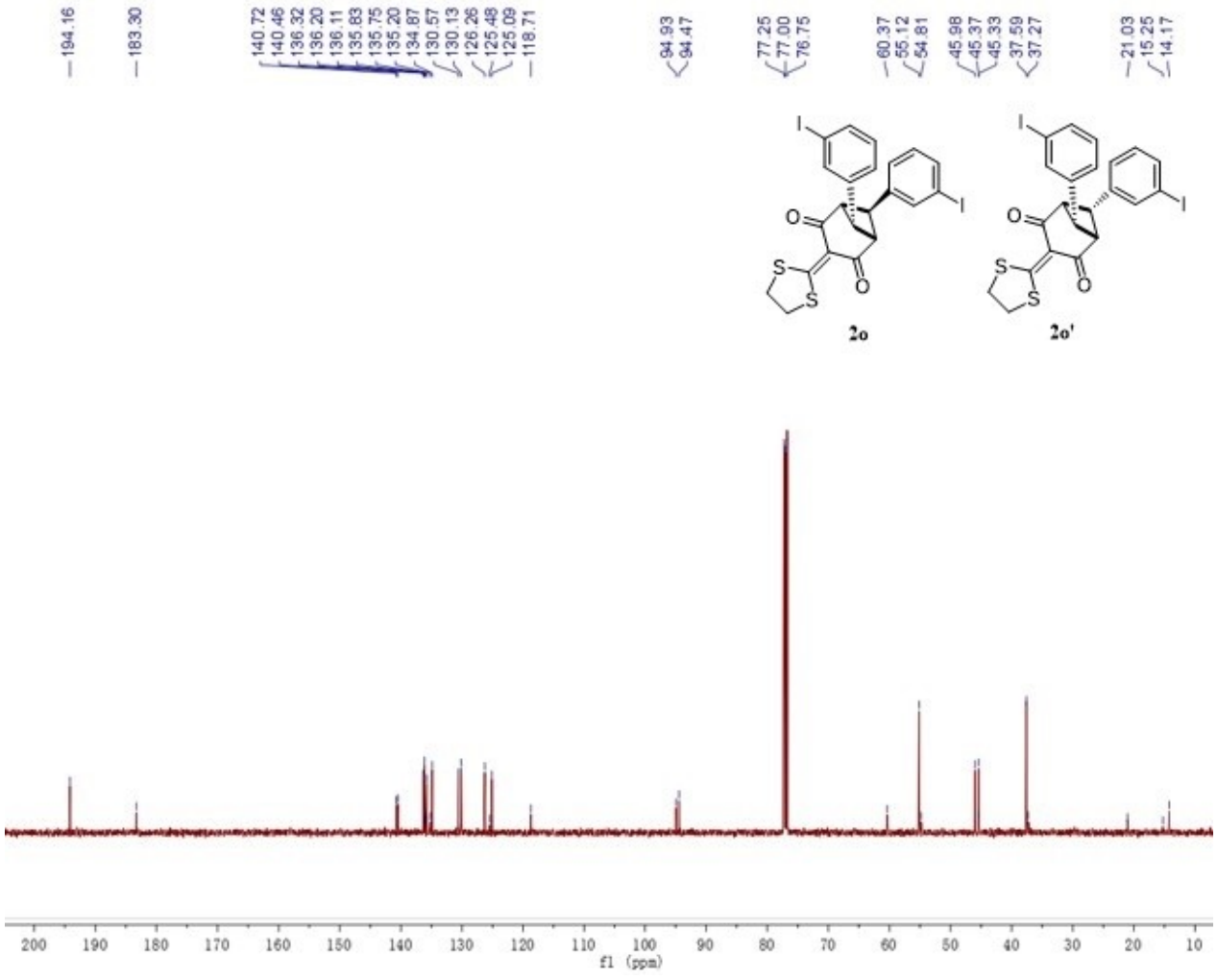
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3n



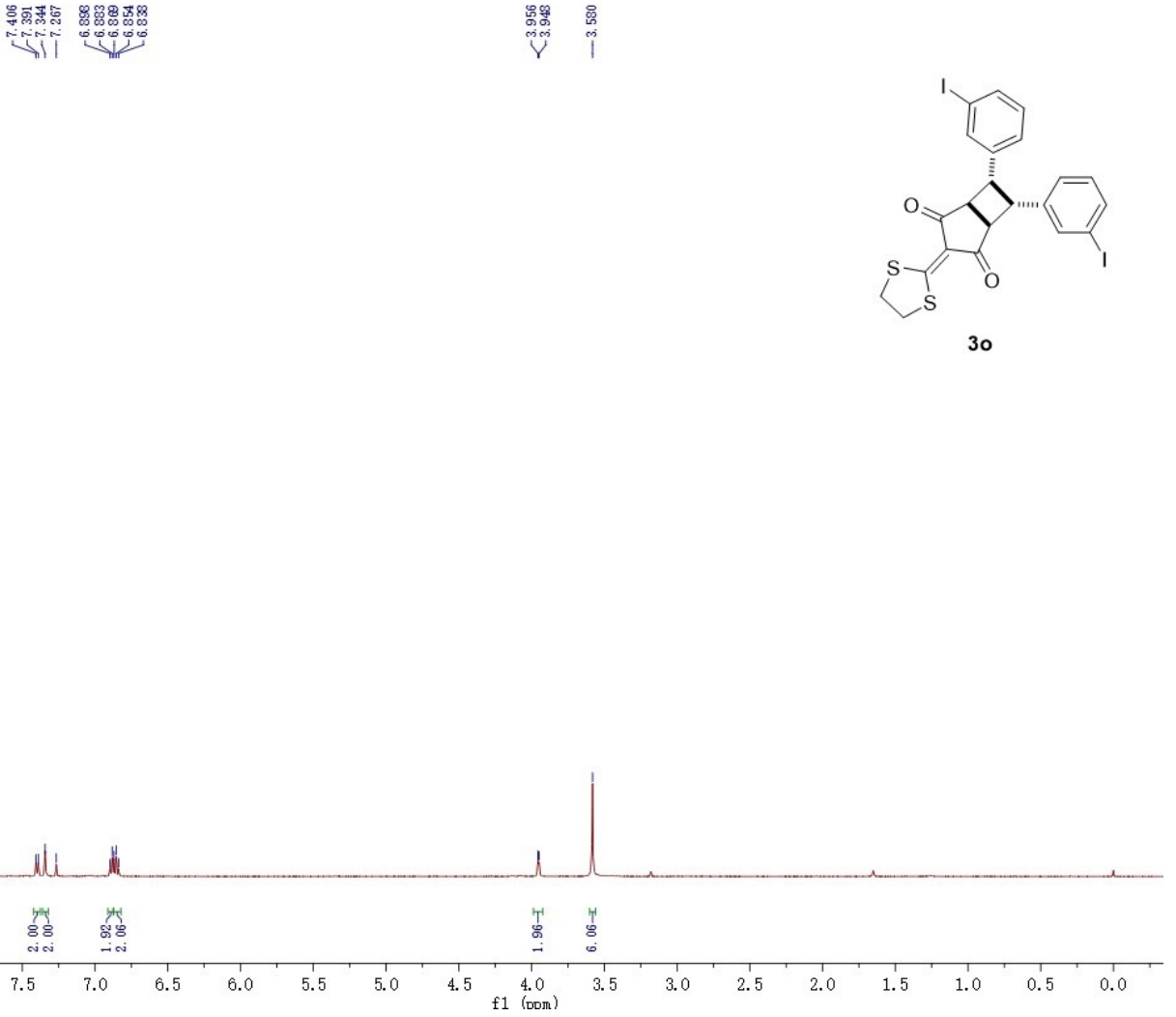
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2o/2o'



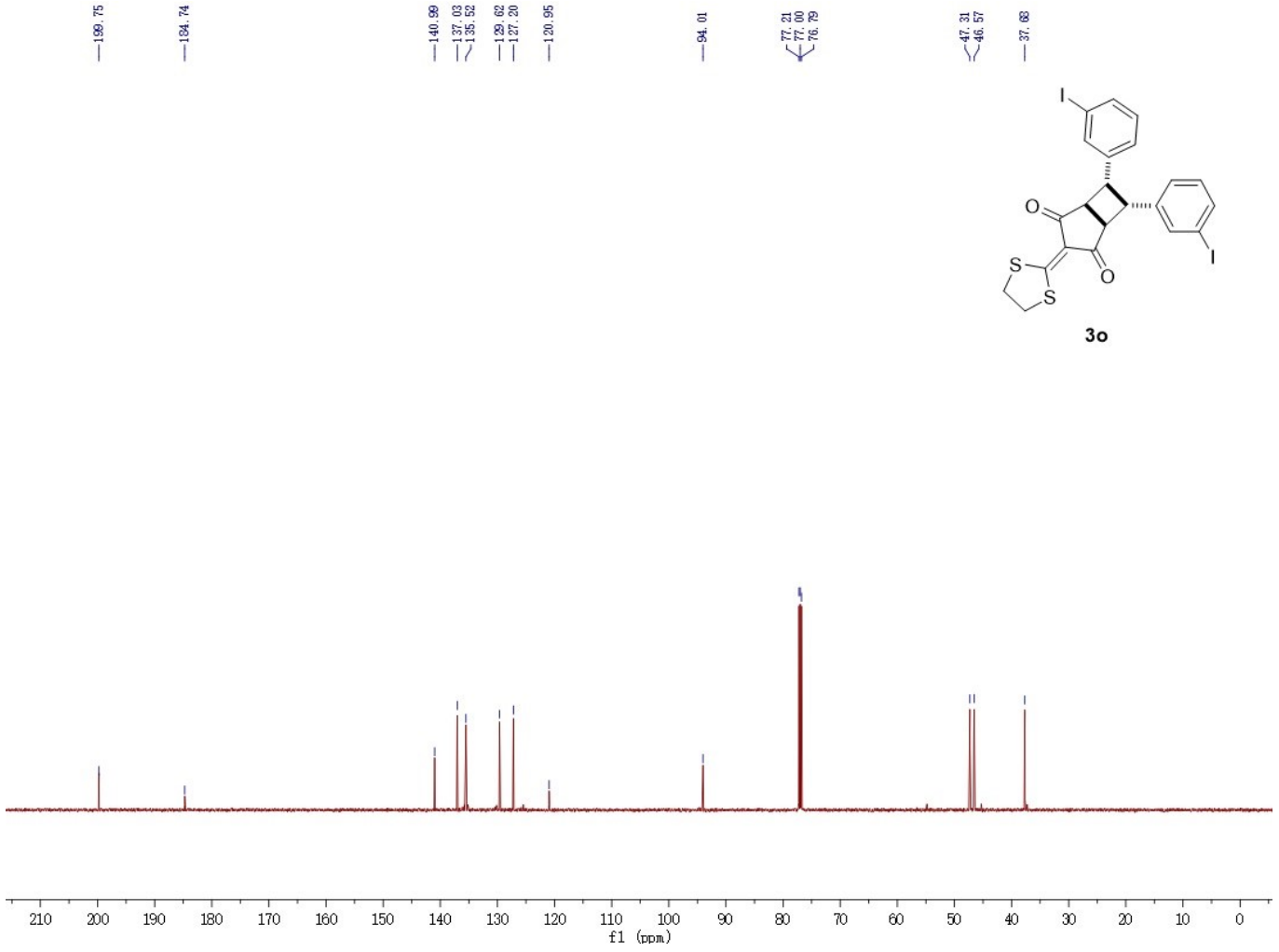
^{13}C spectrum (126 MHz, $CDCl_3$) of compound 2o/2o'



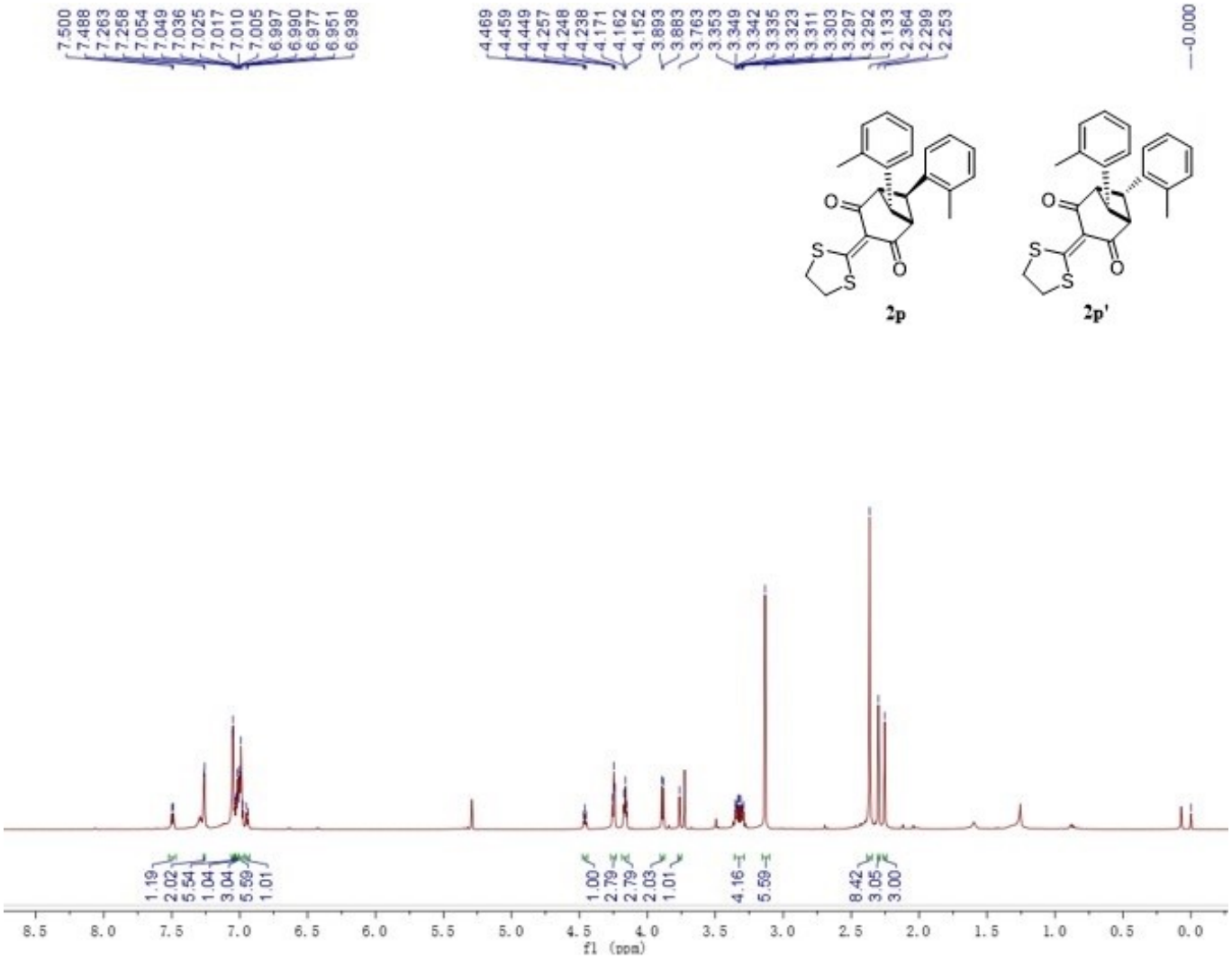
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3o



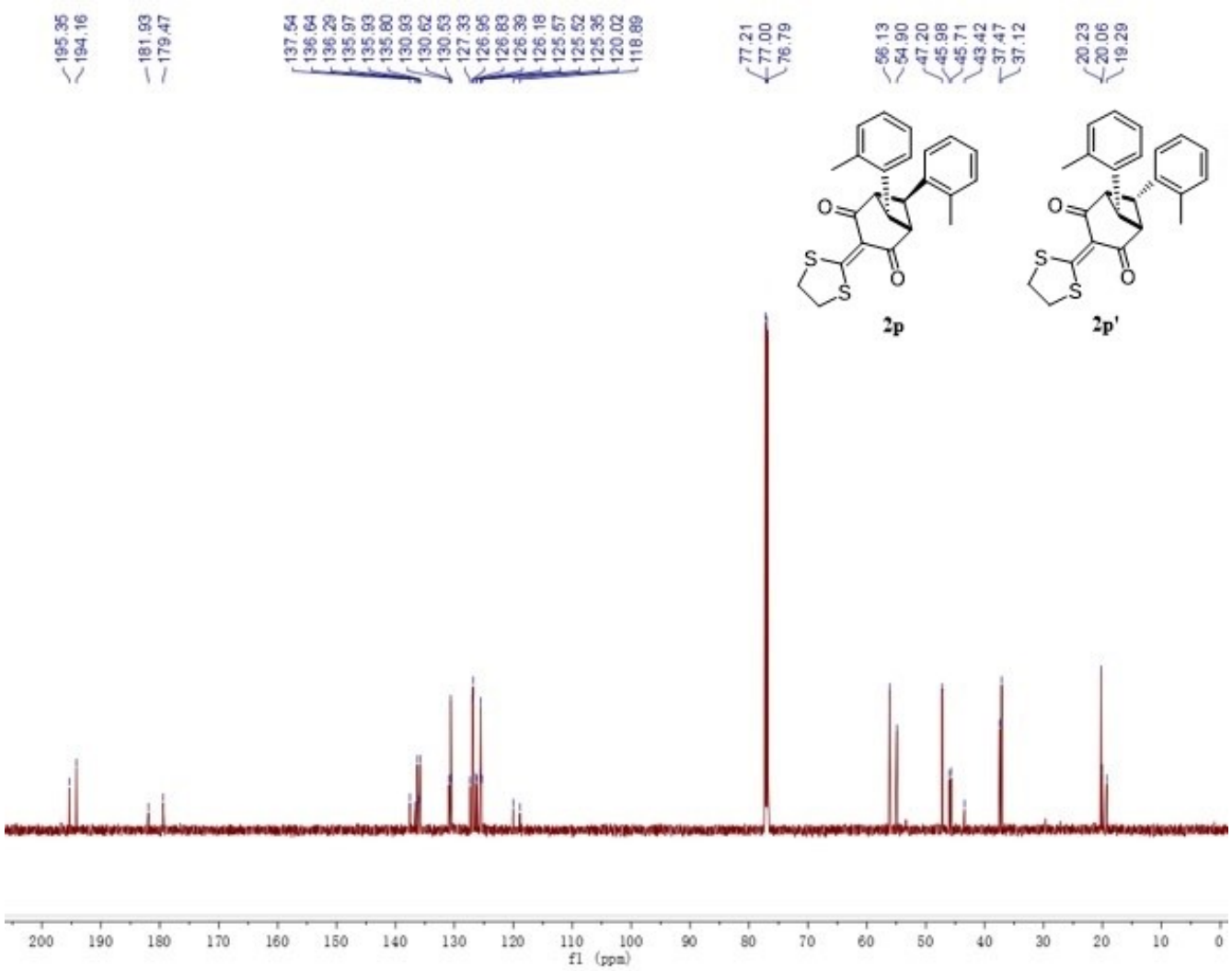
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3o



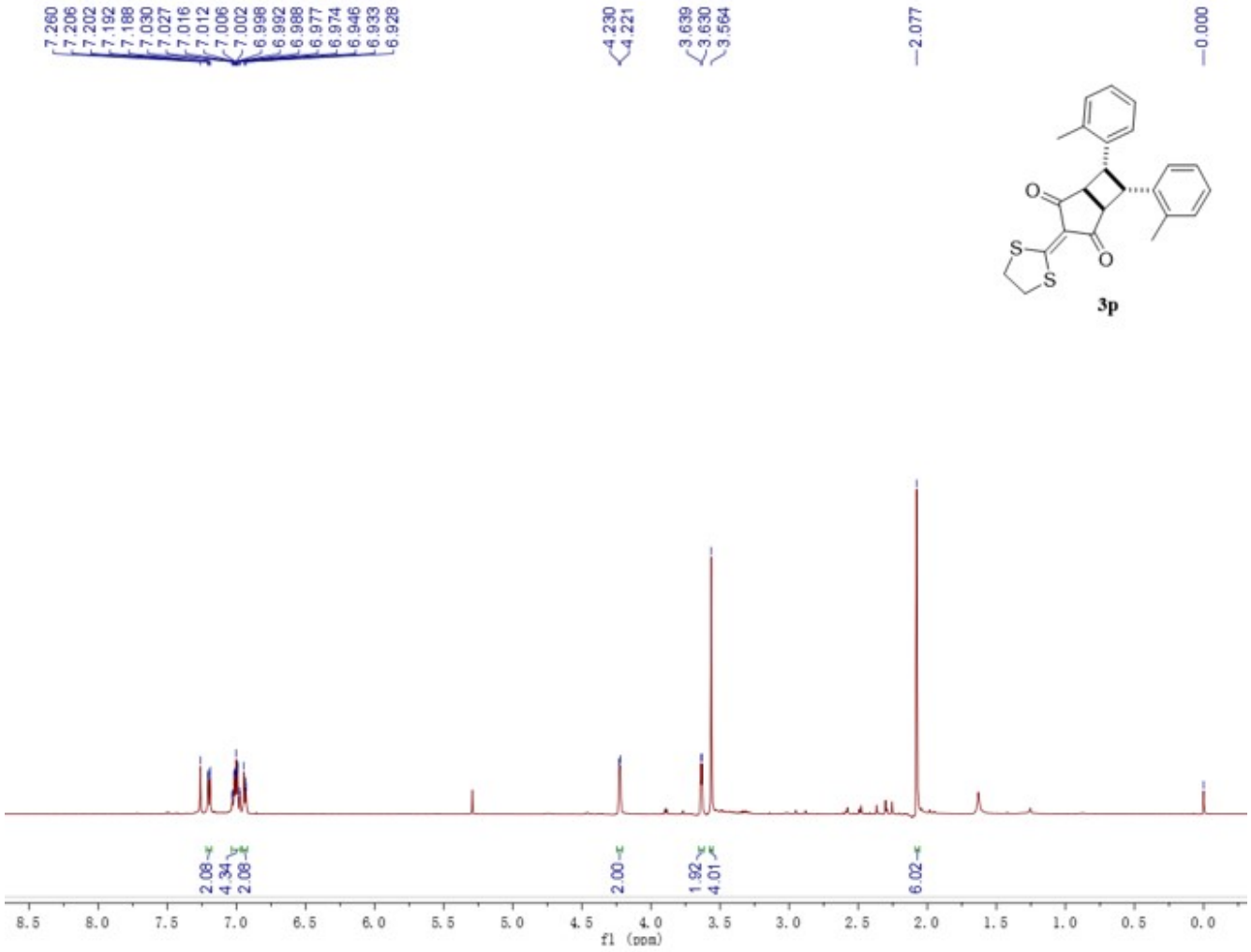
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2p/2p'



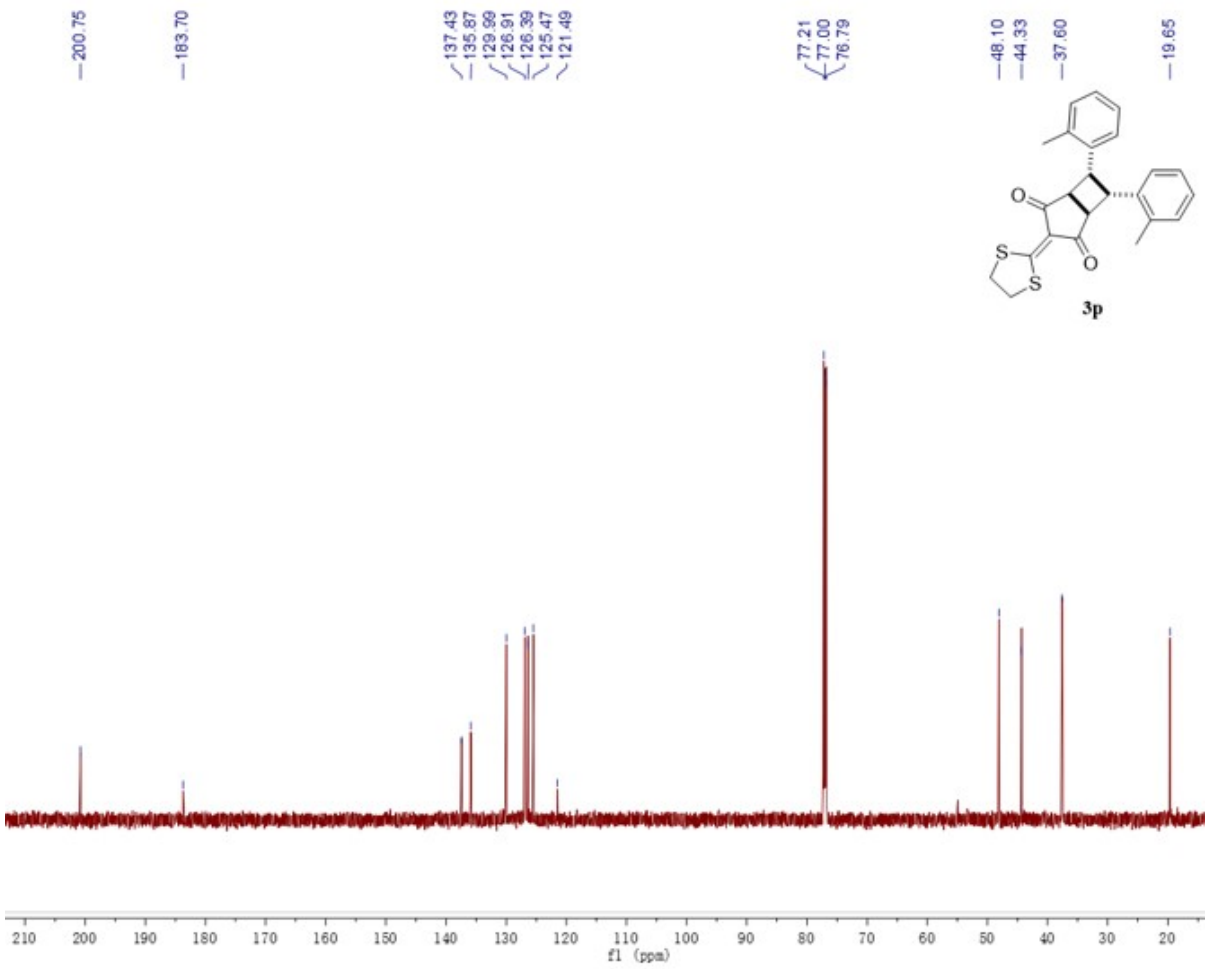
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2p/2p'



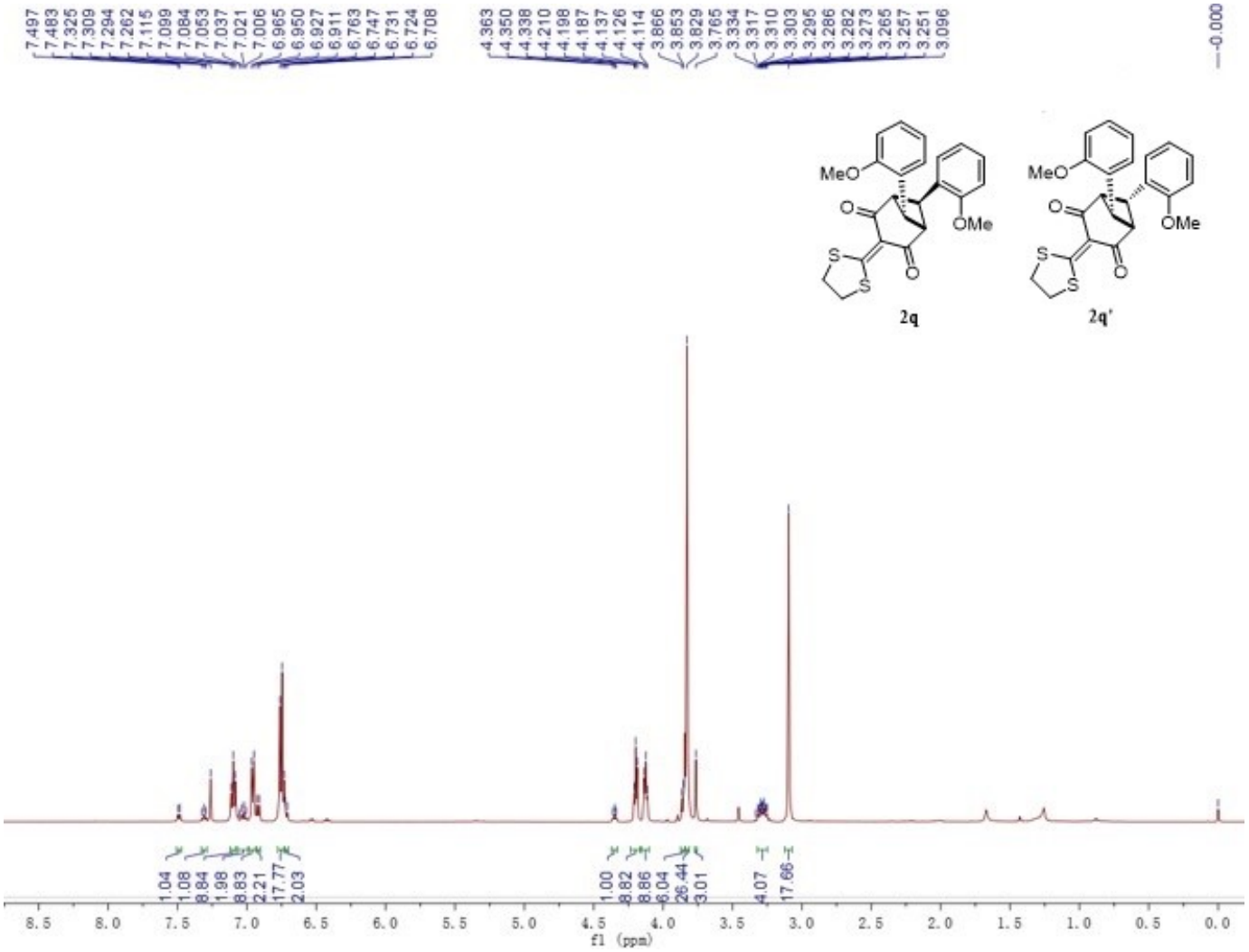
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3p



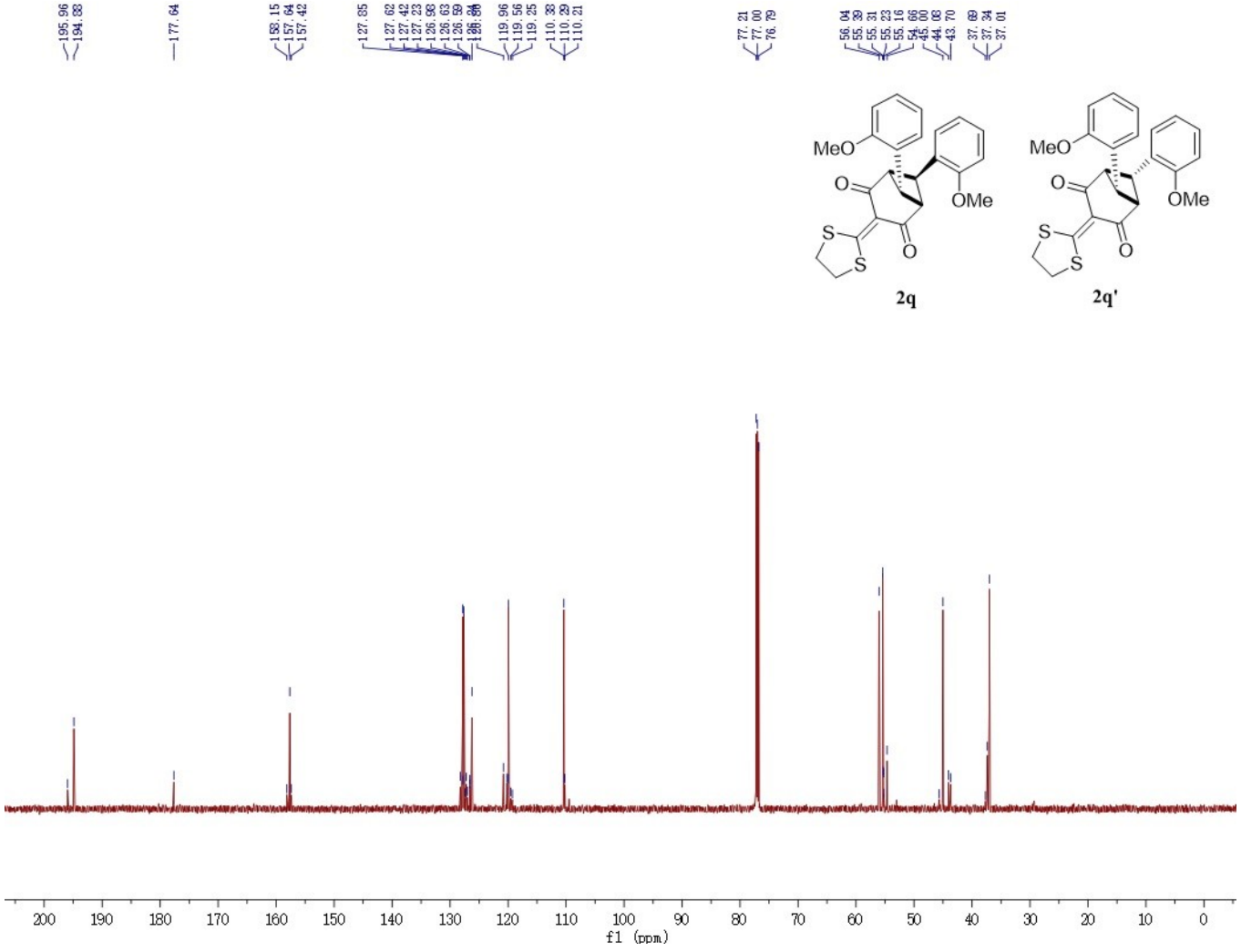
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3p



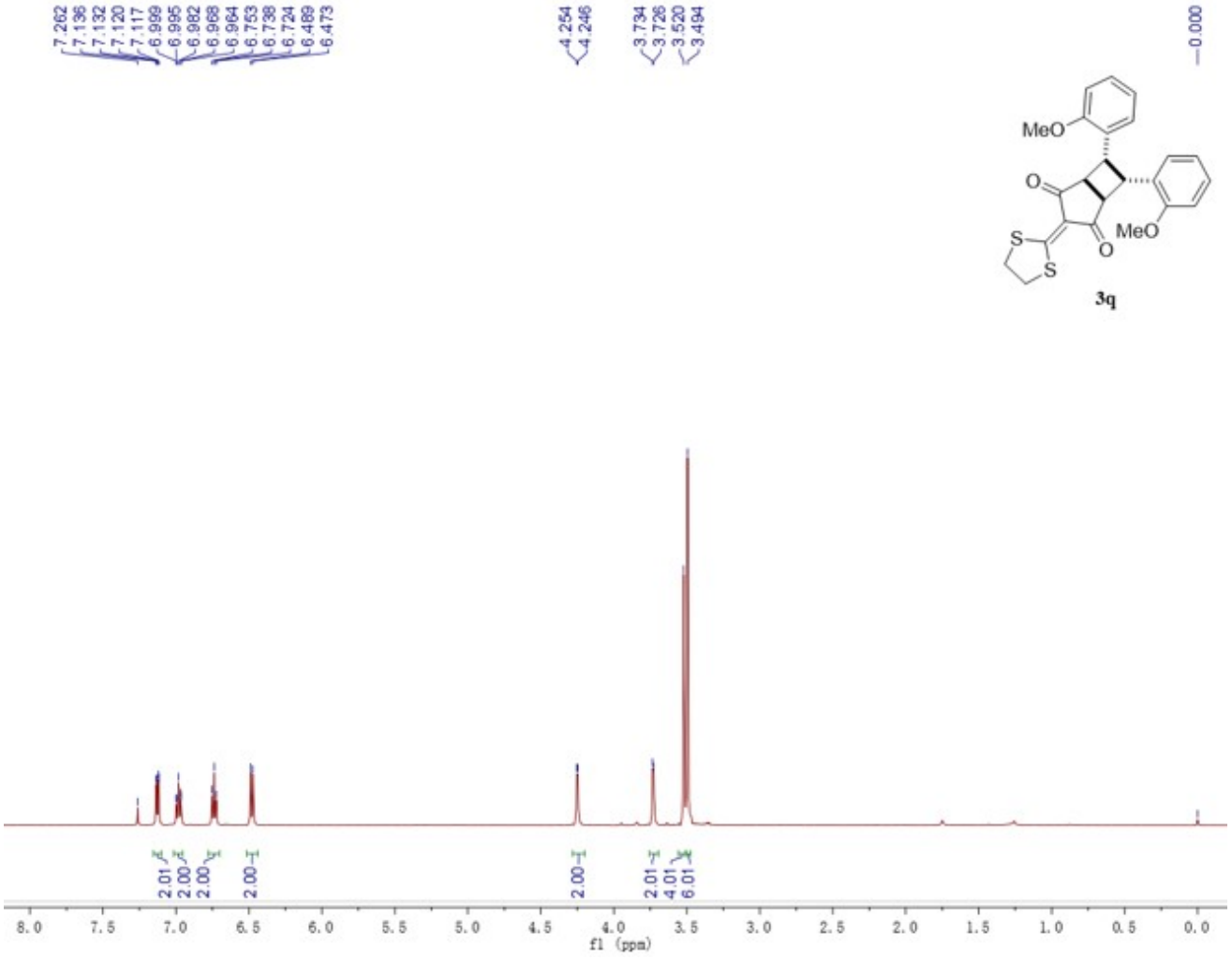
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2q/2q'



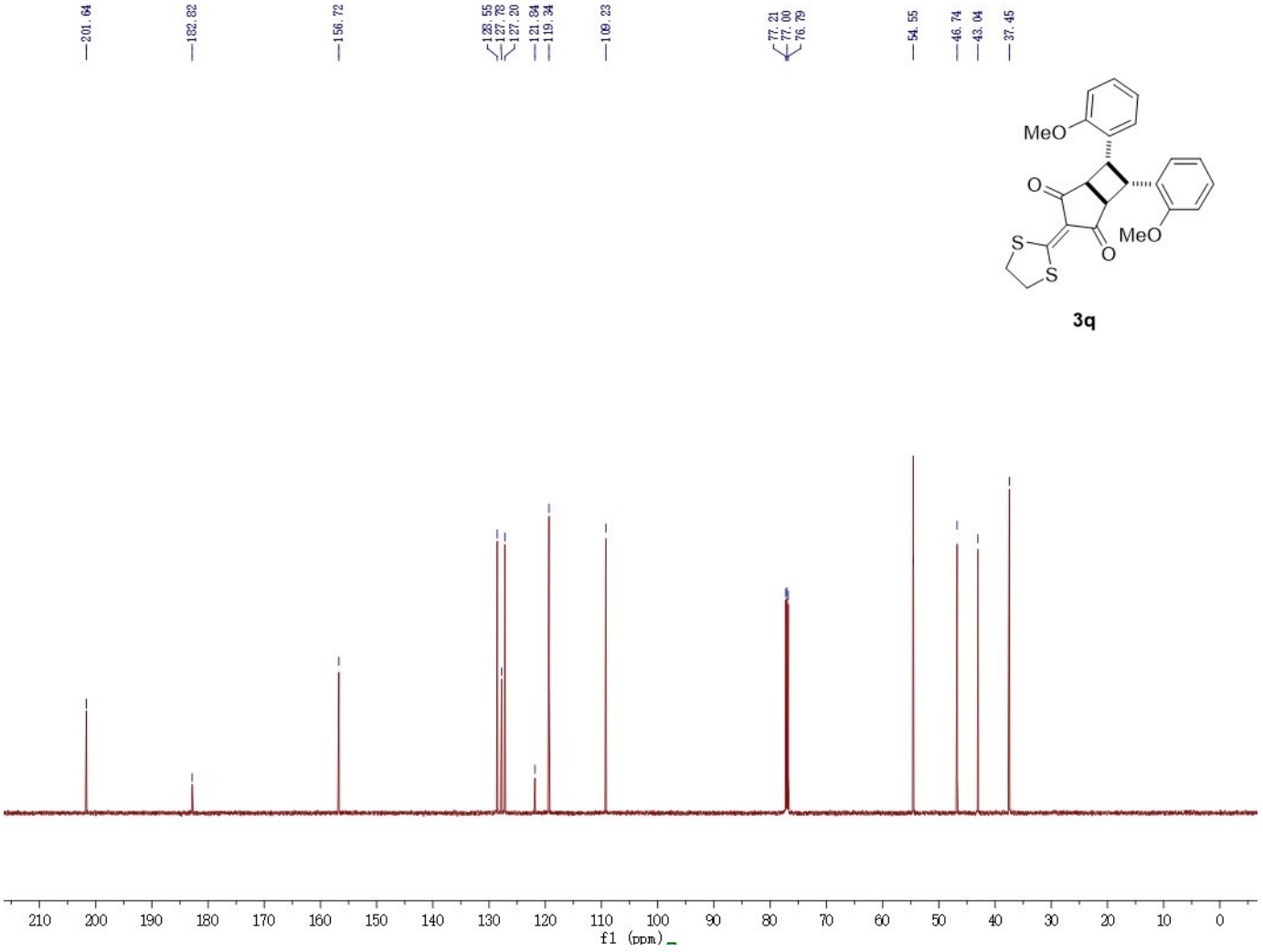
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2q/2q'



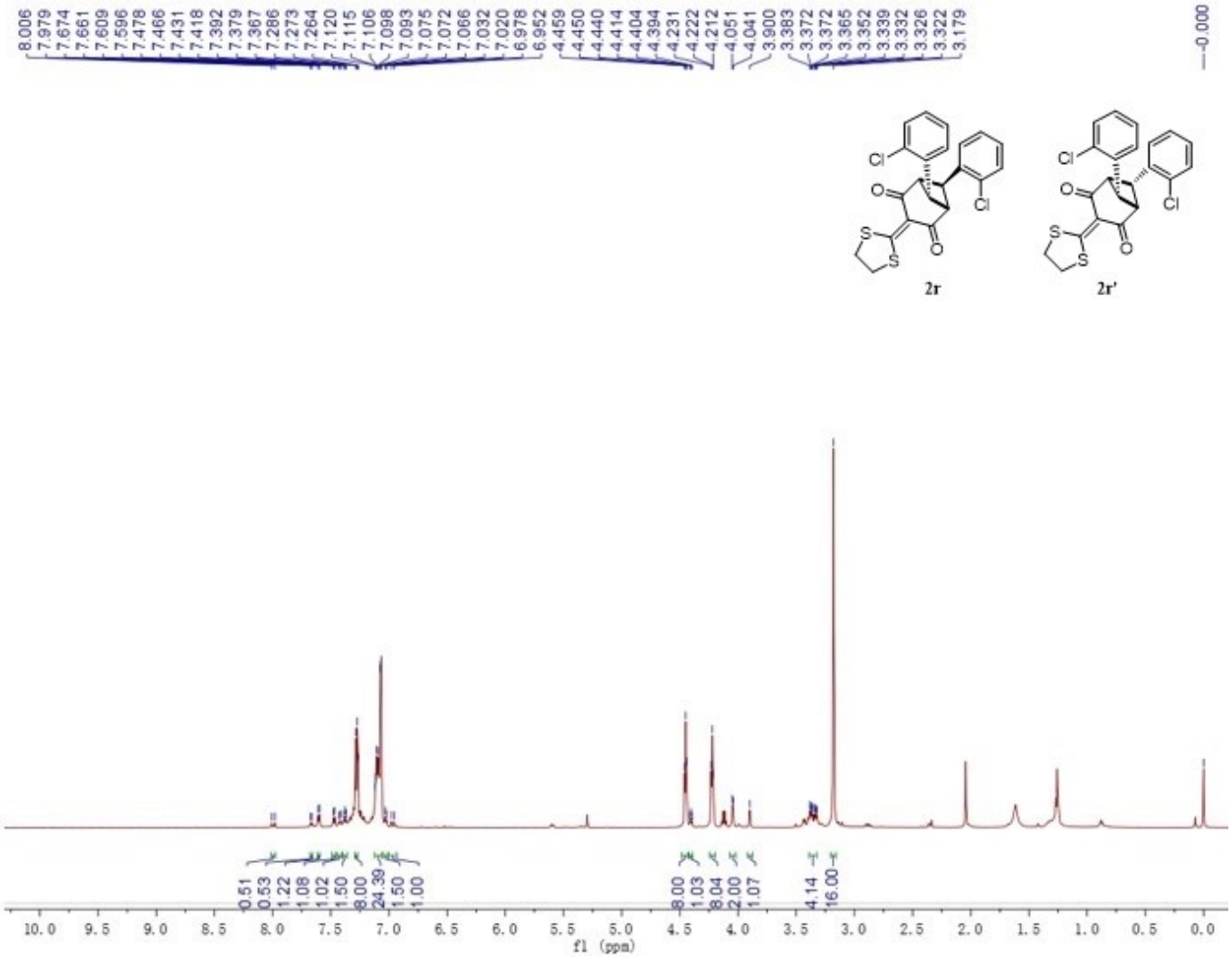
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3q



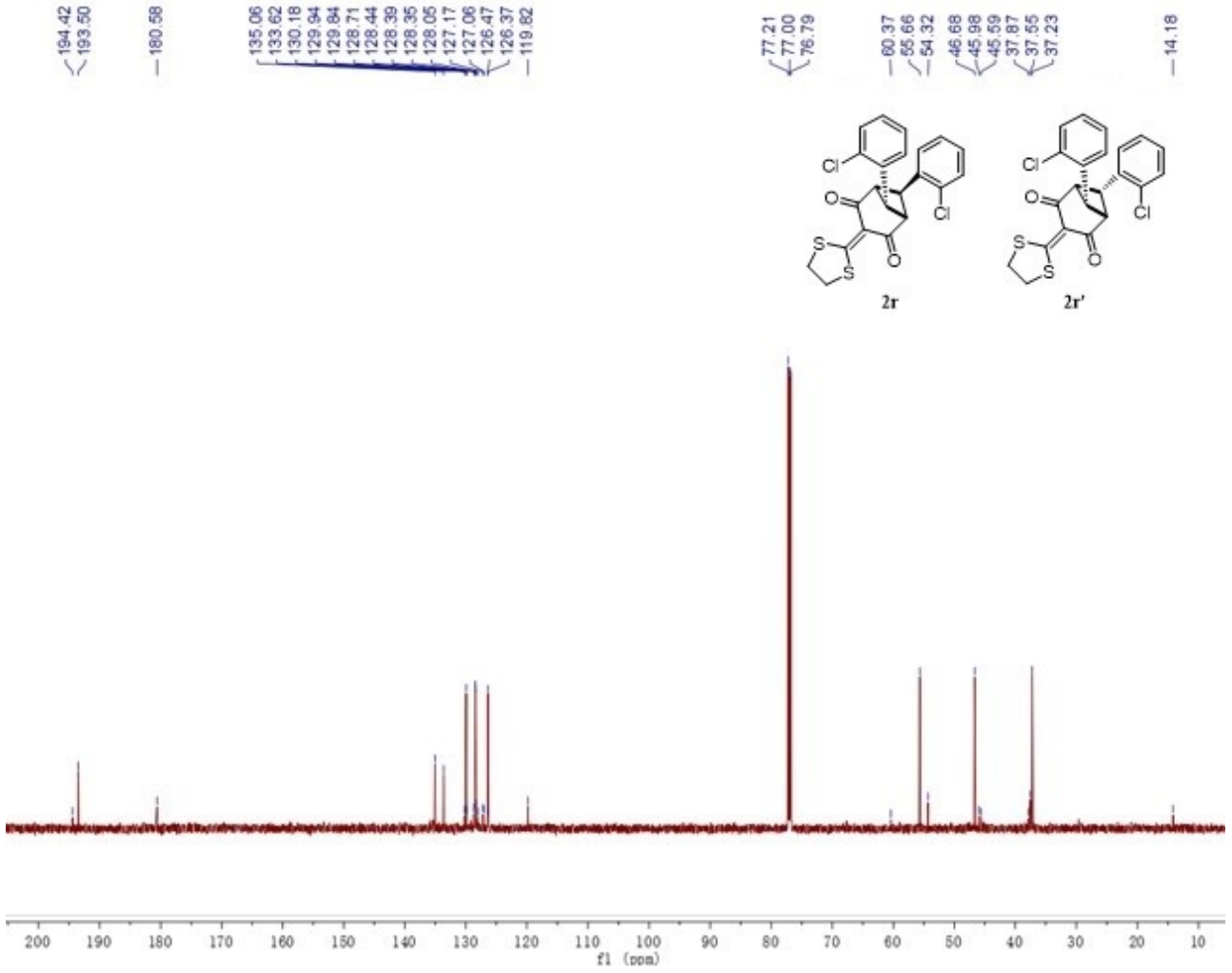
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3q



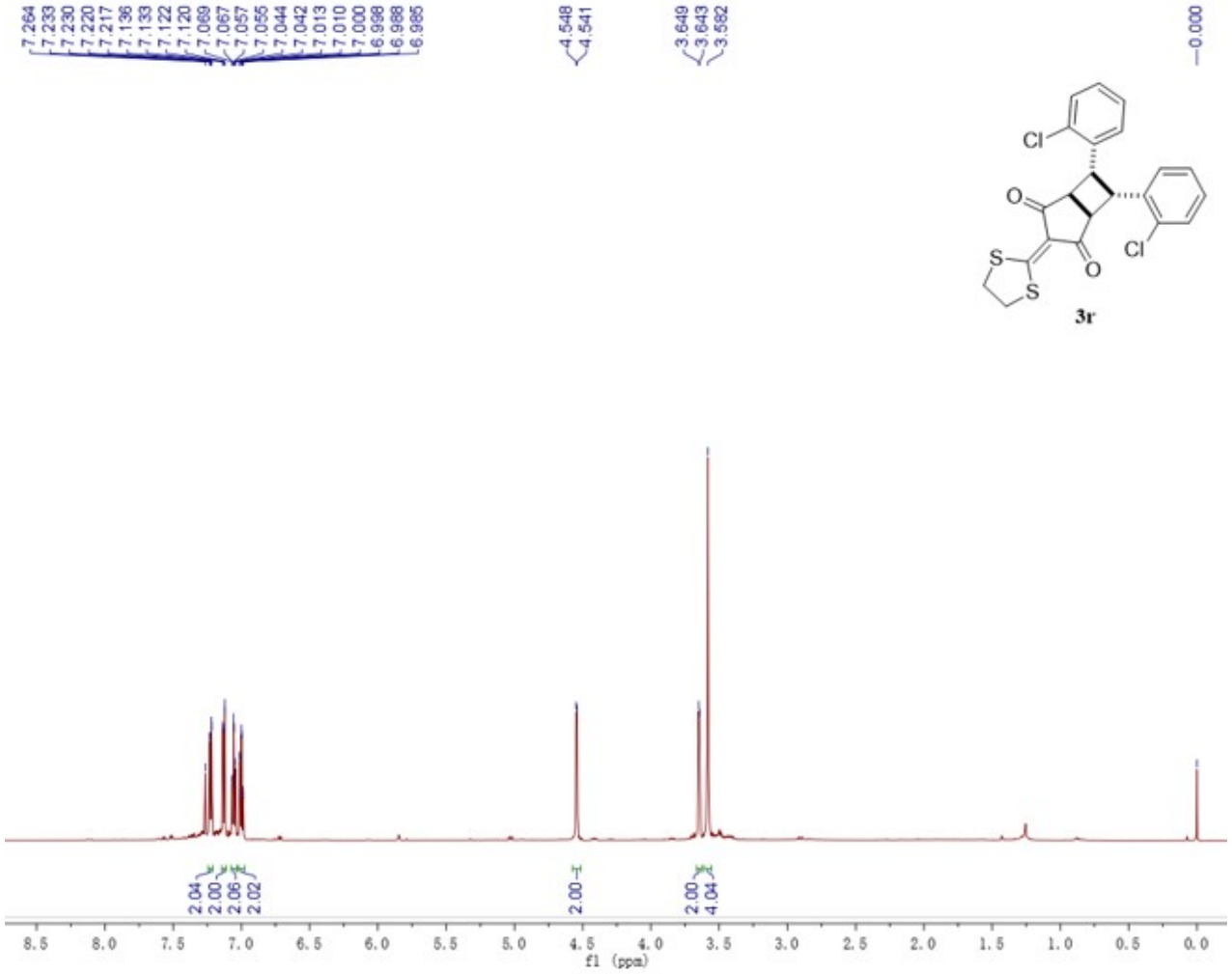
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2r/2r'



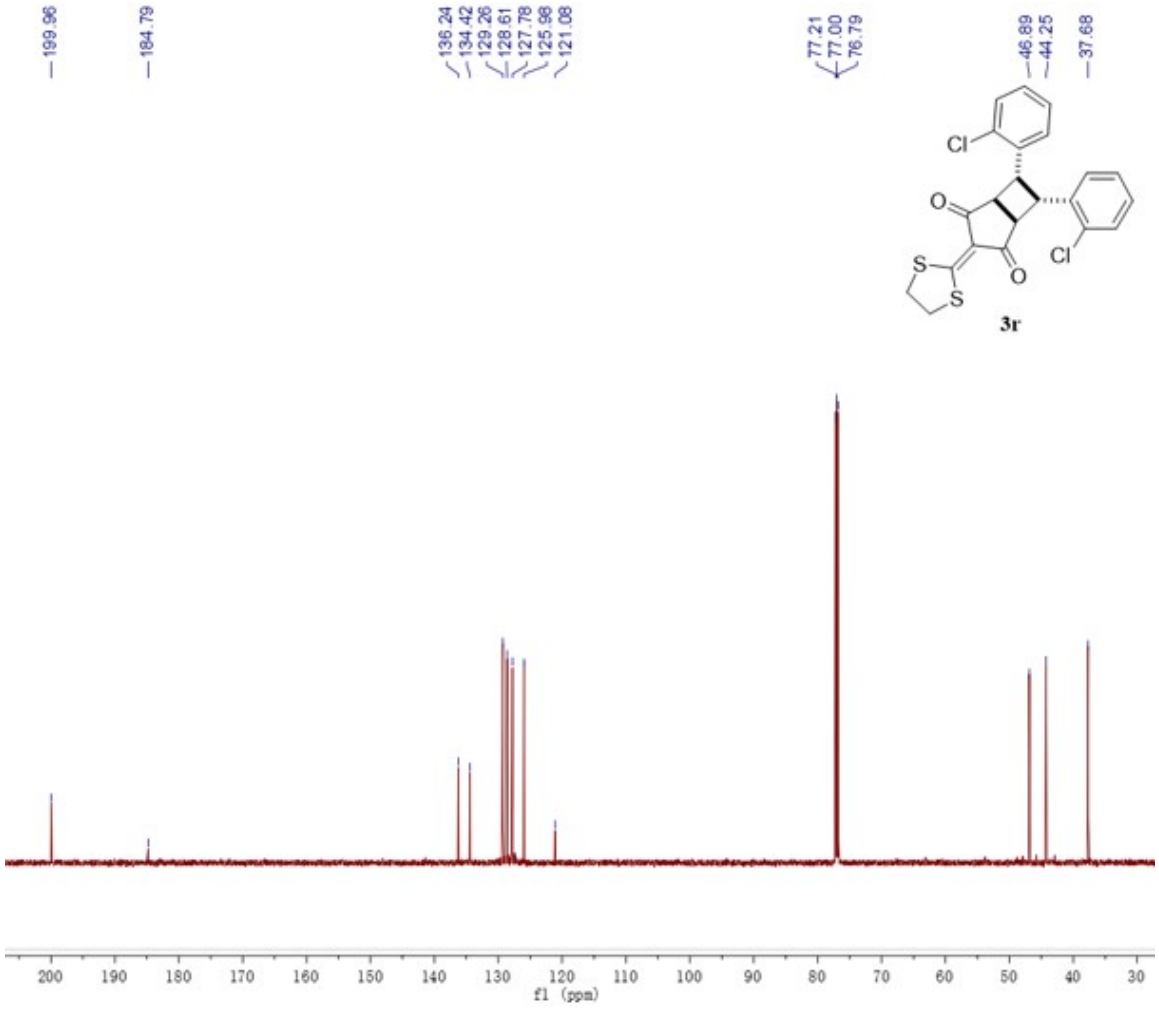
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2r/2r'



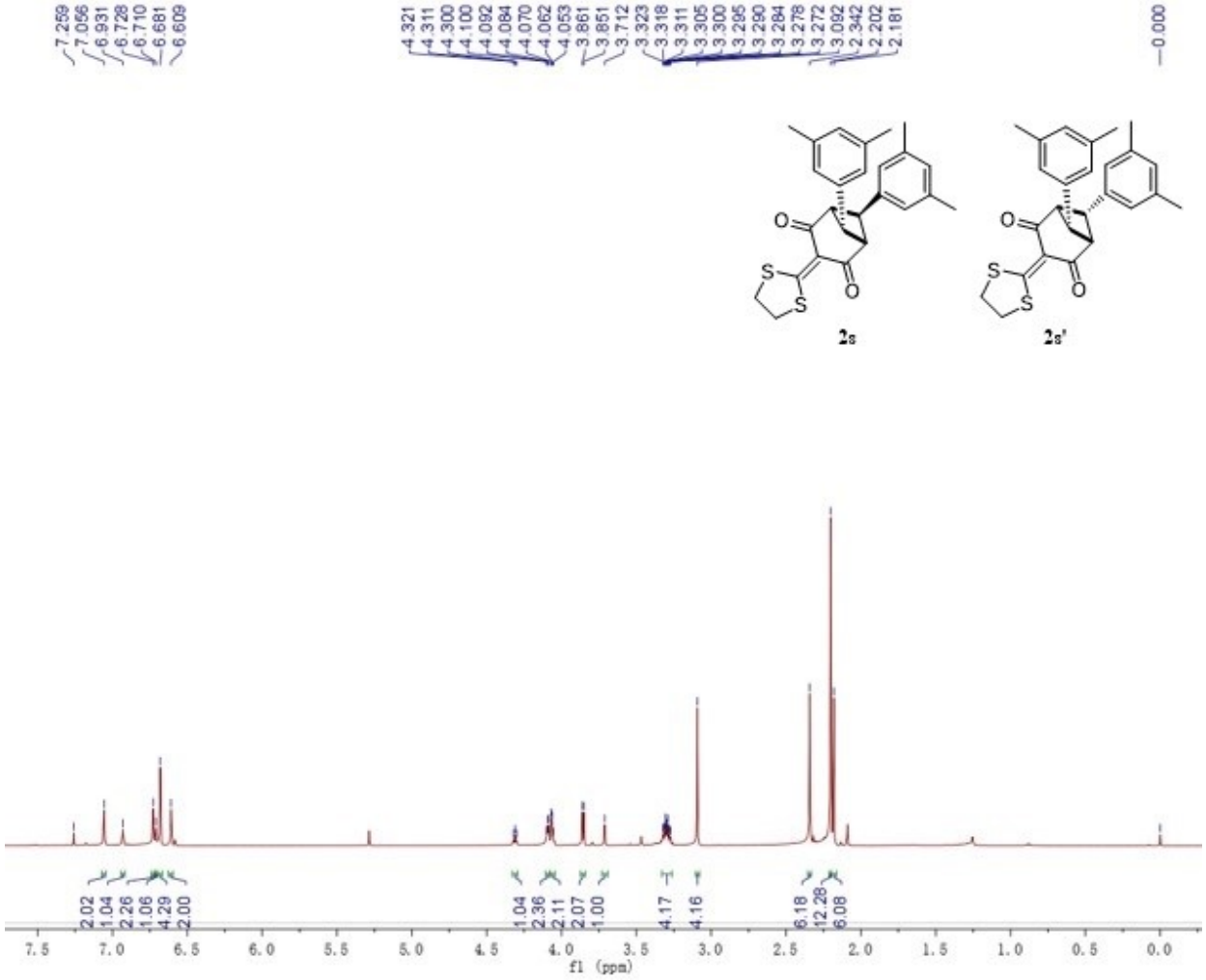
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3r



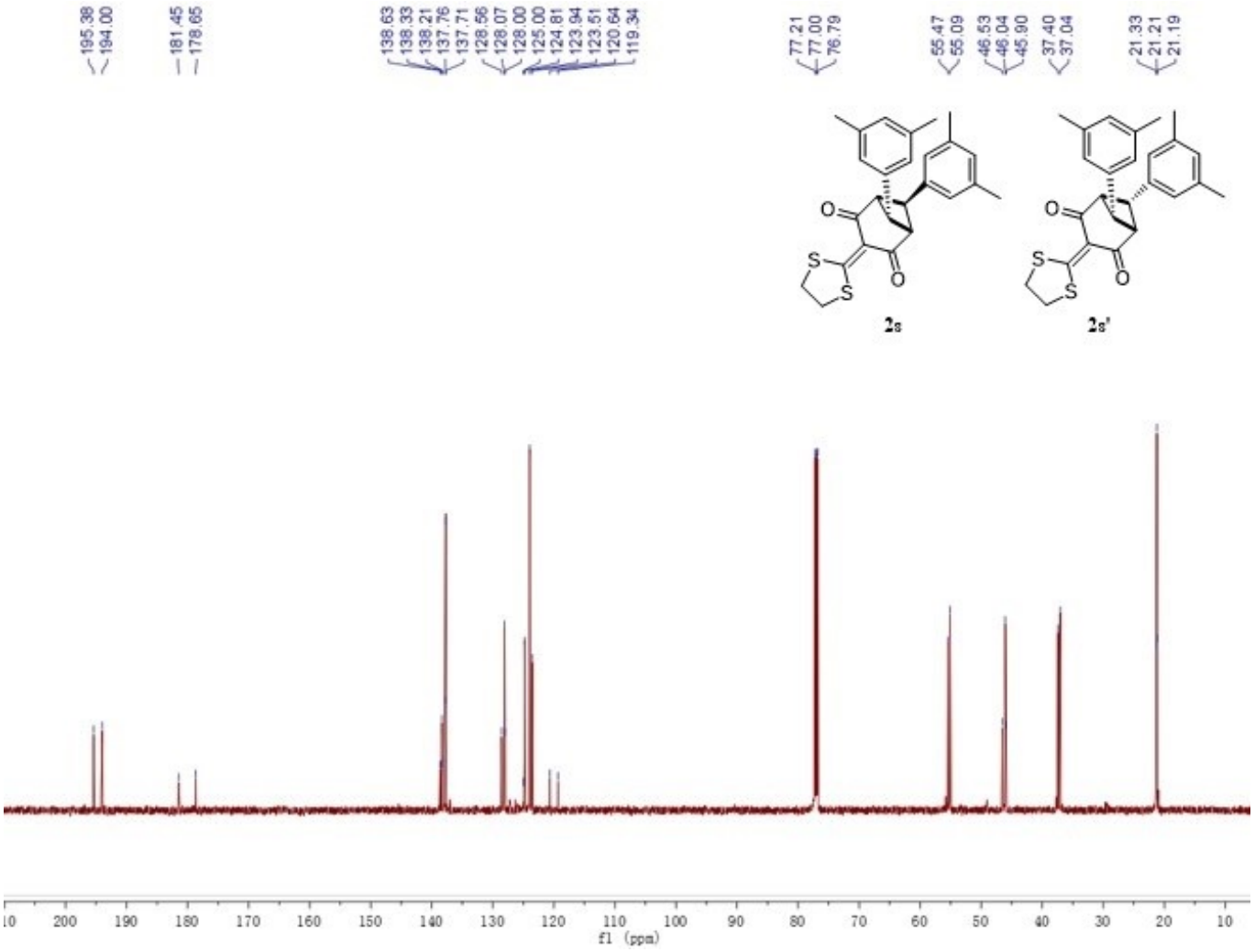
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3r



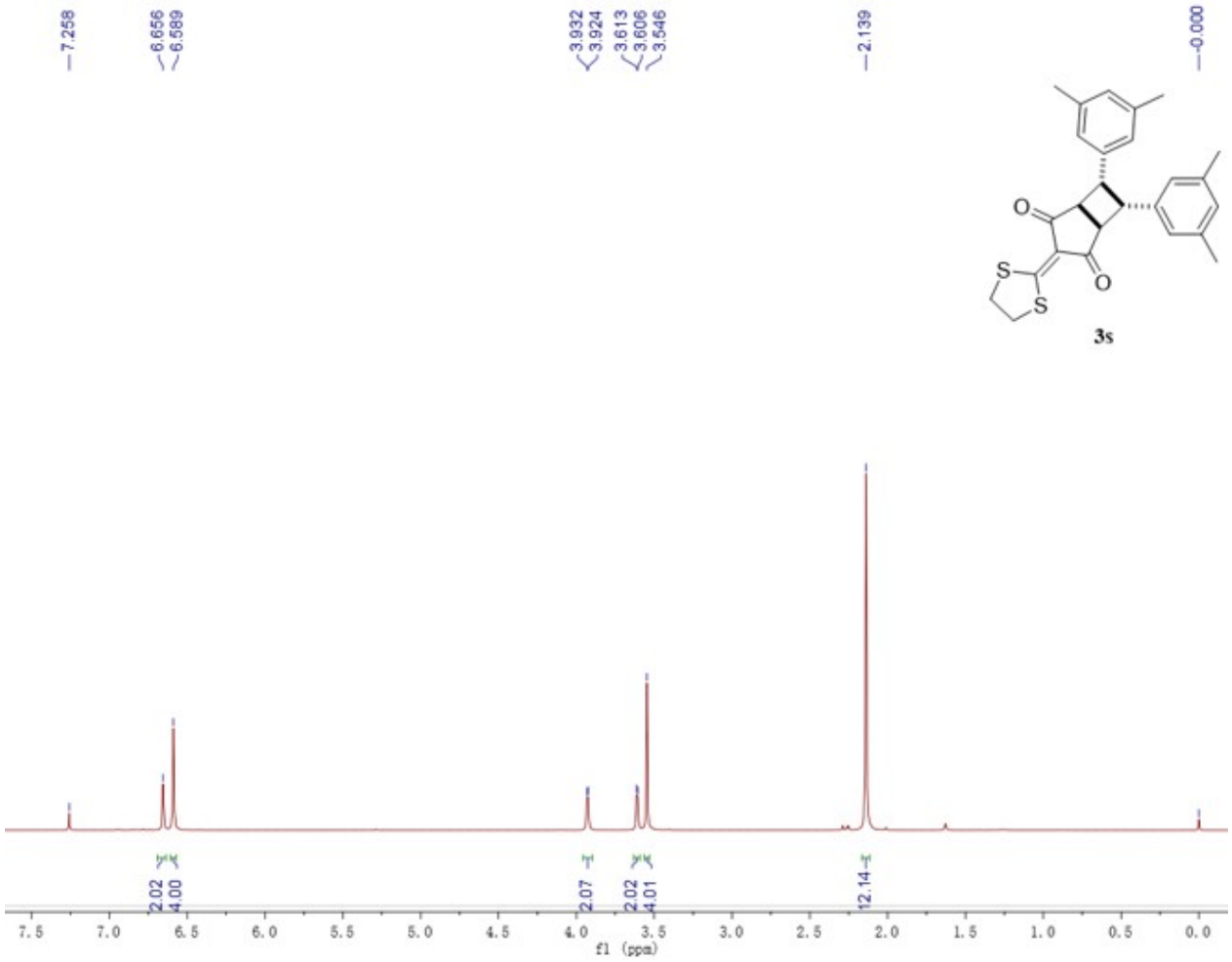
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2s/2s'



^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2s/2s'



^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3s



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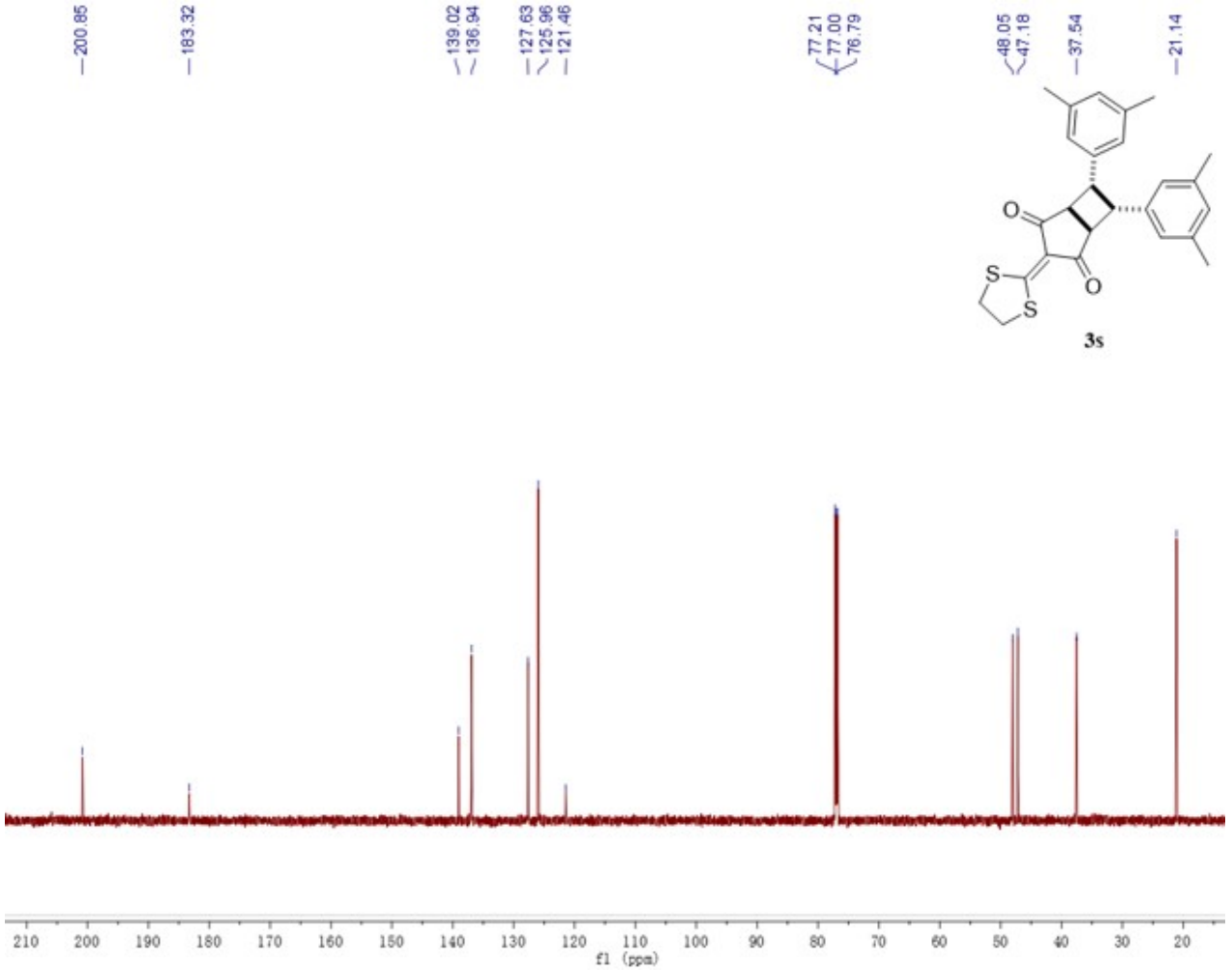
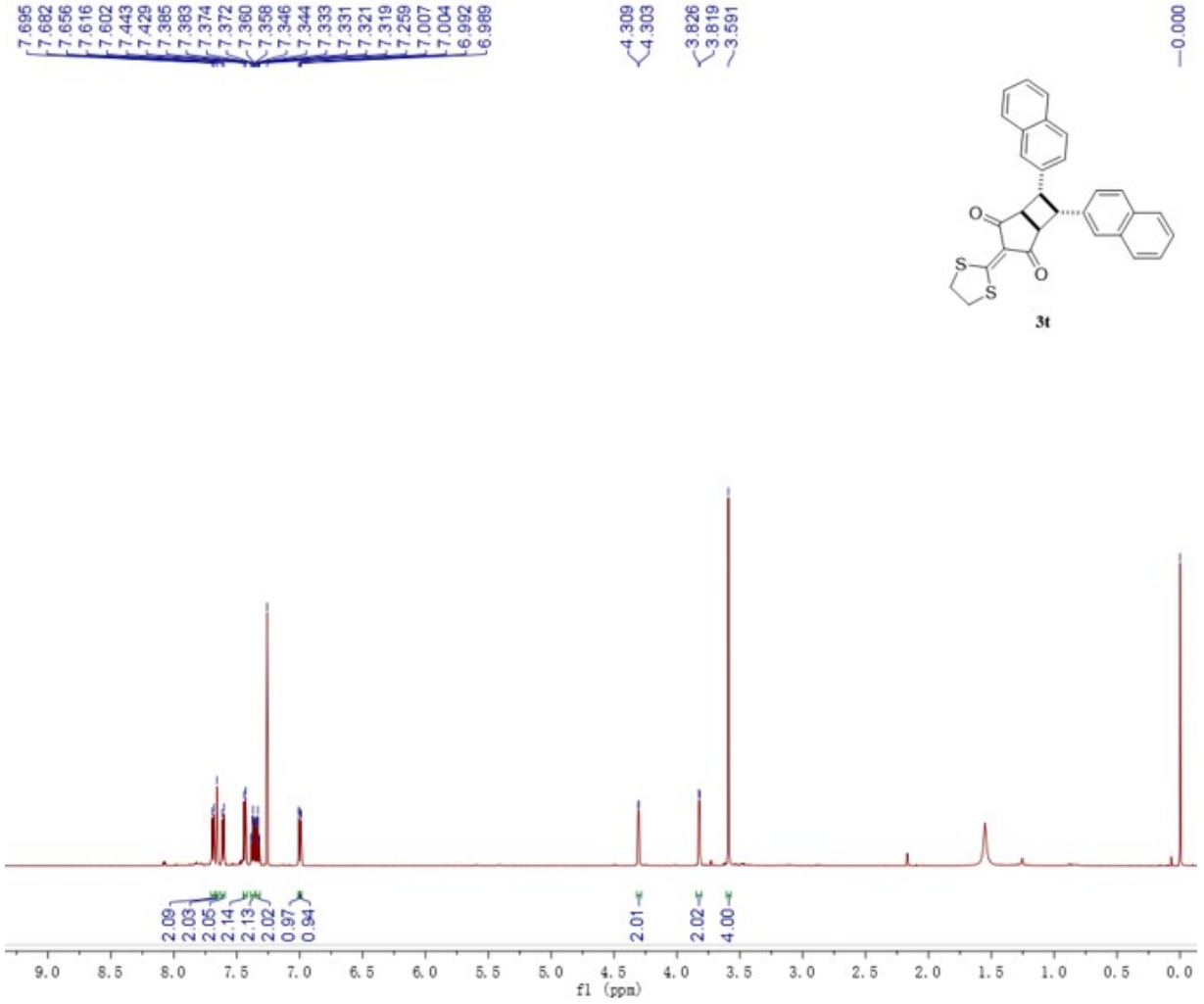
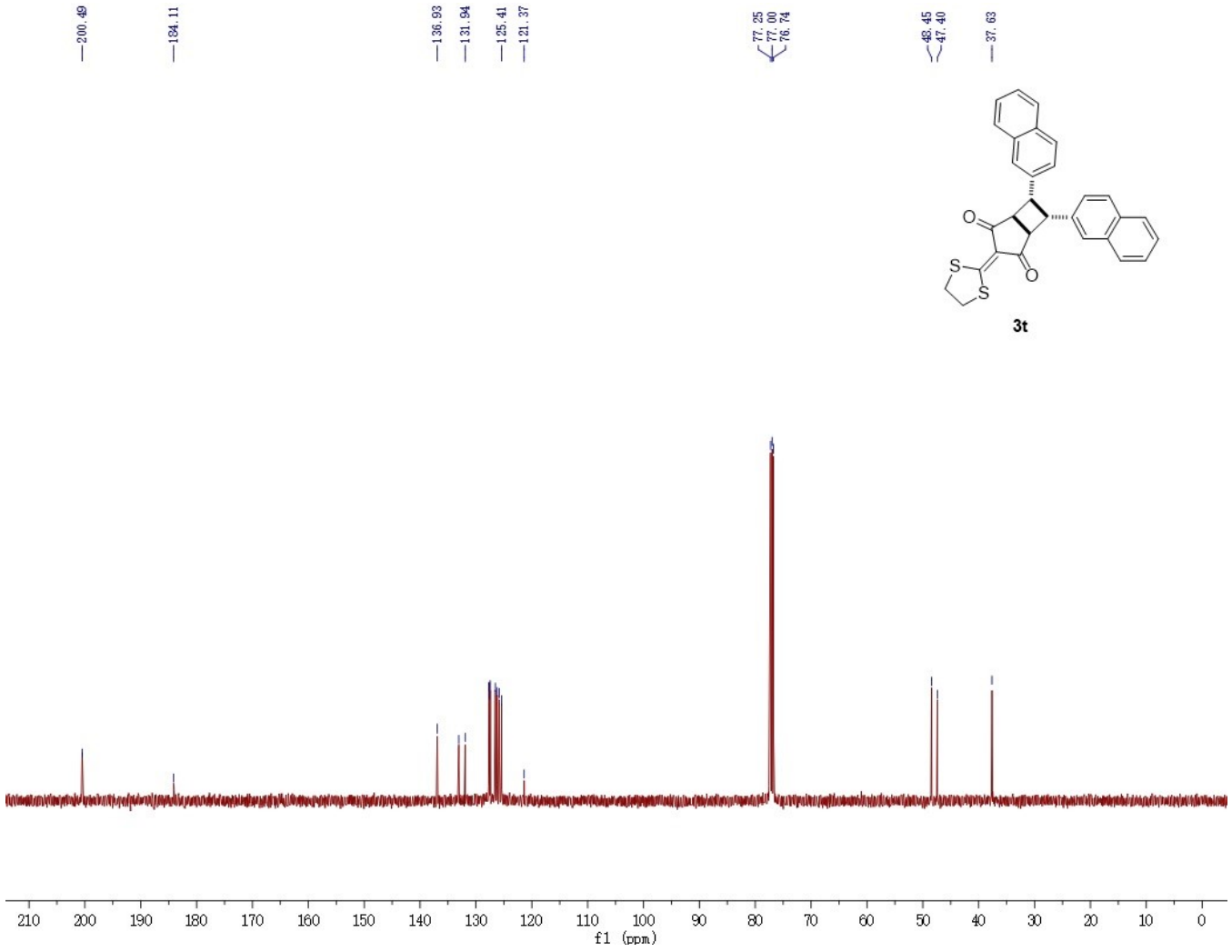


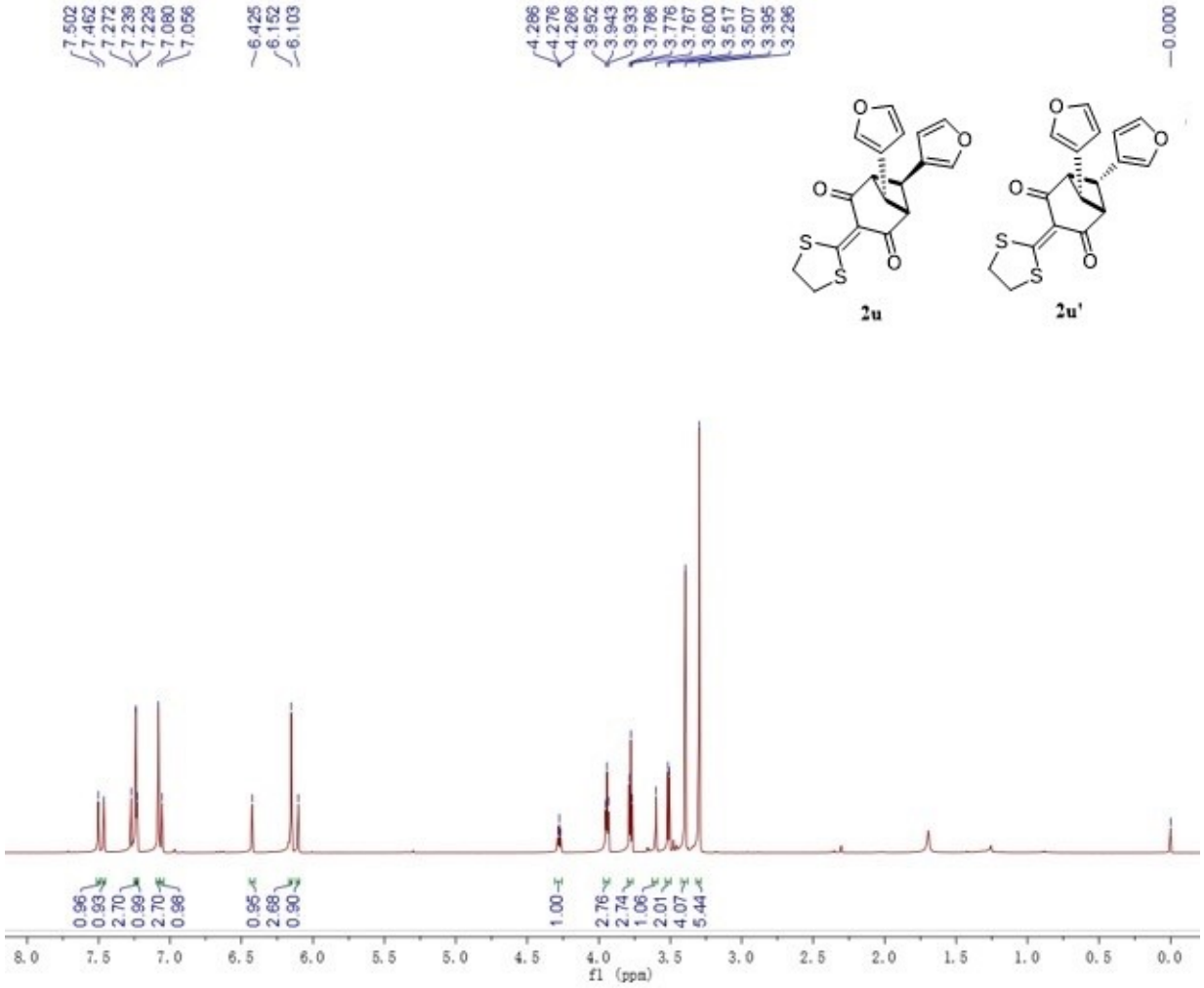
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3t



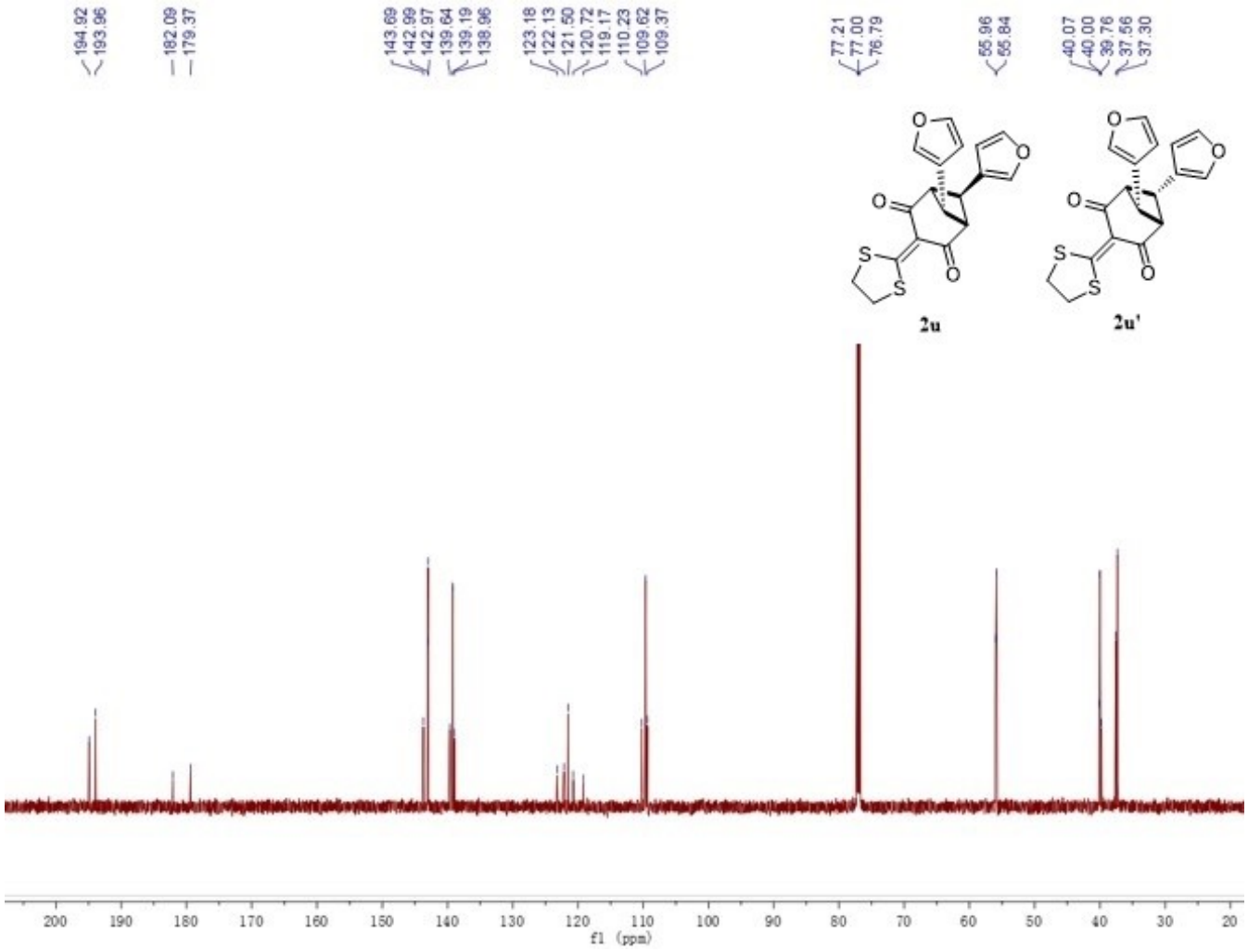
^{13}C spectrum (126 MHz, $CDCl_3$) of compound 3t



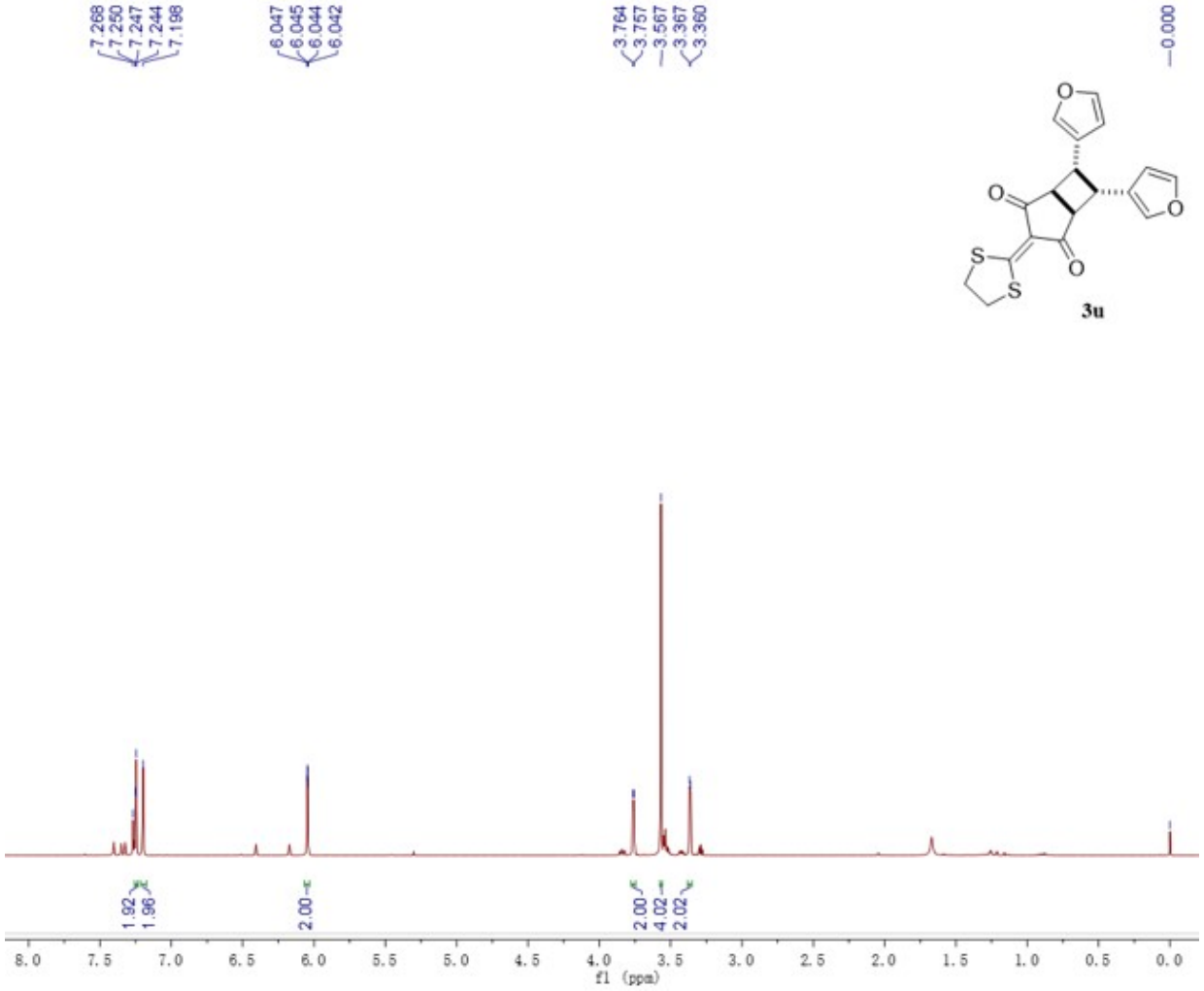
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2u/2u'



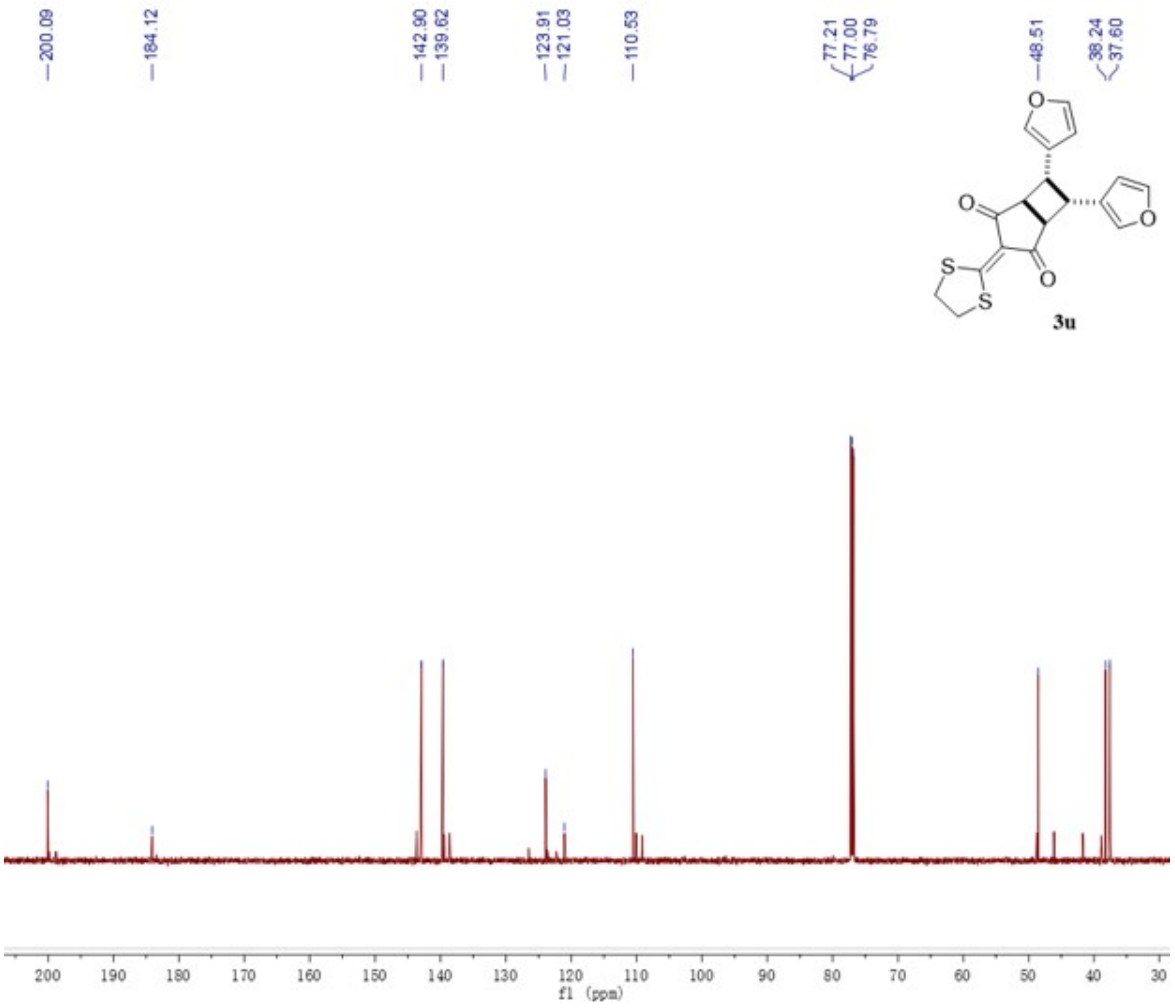
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2u/2u'



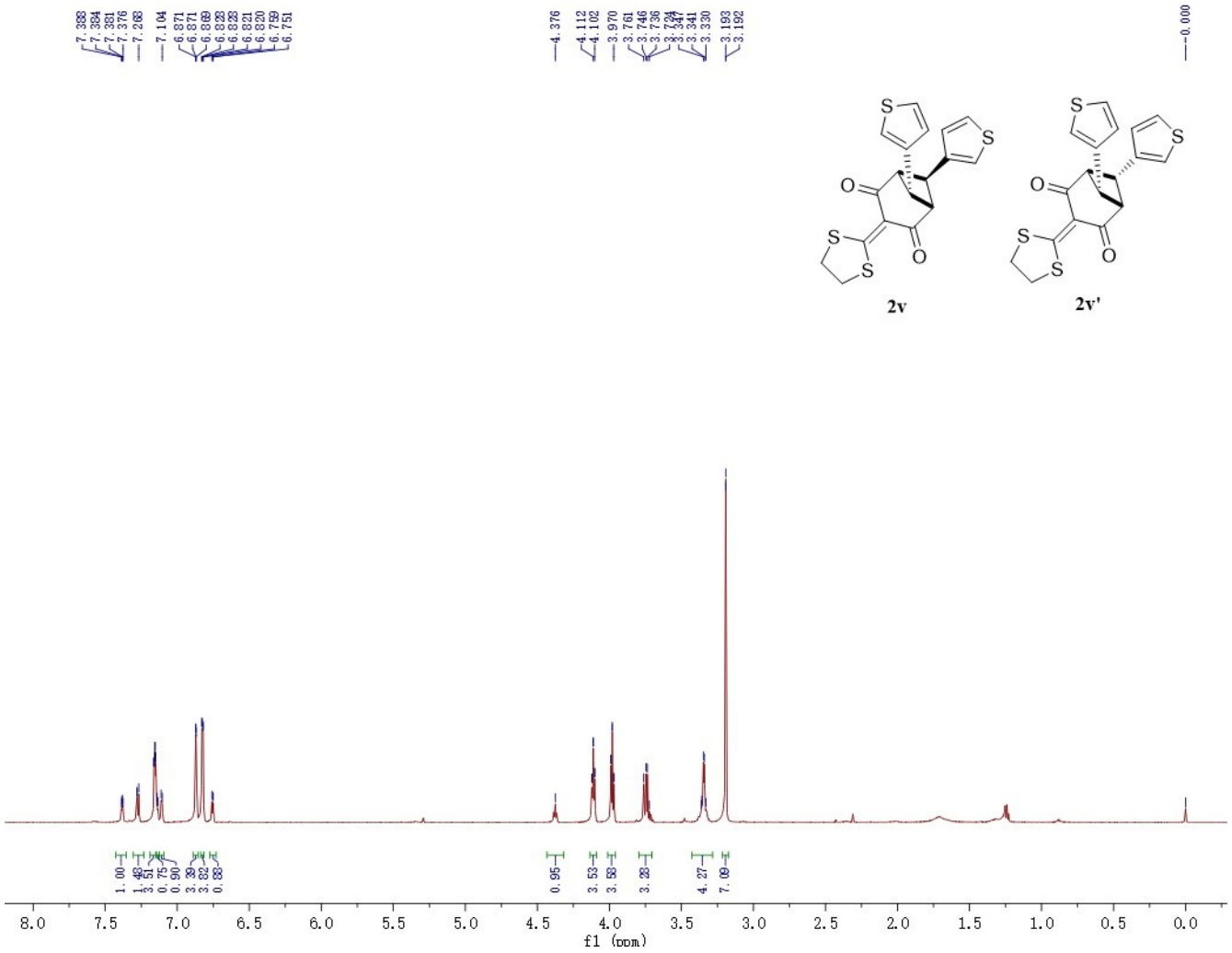
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3u



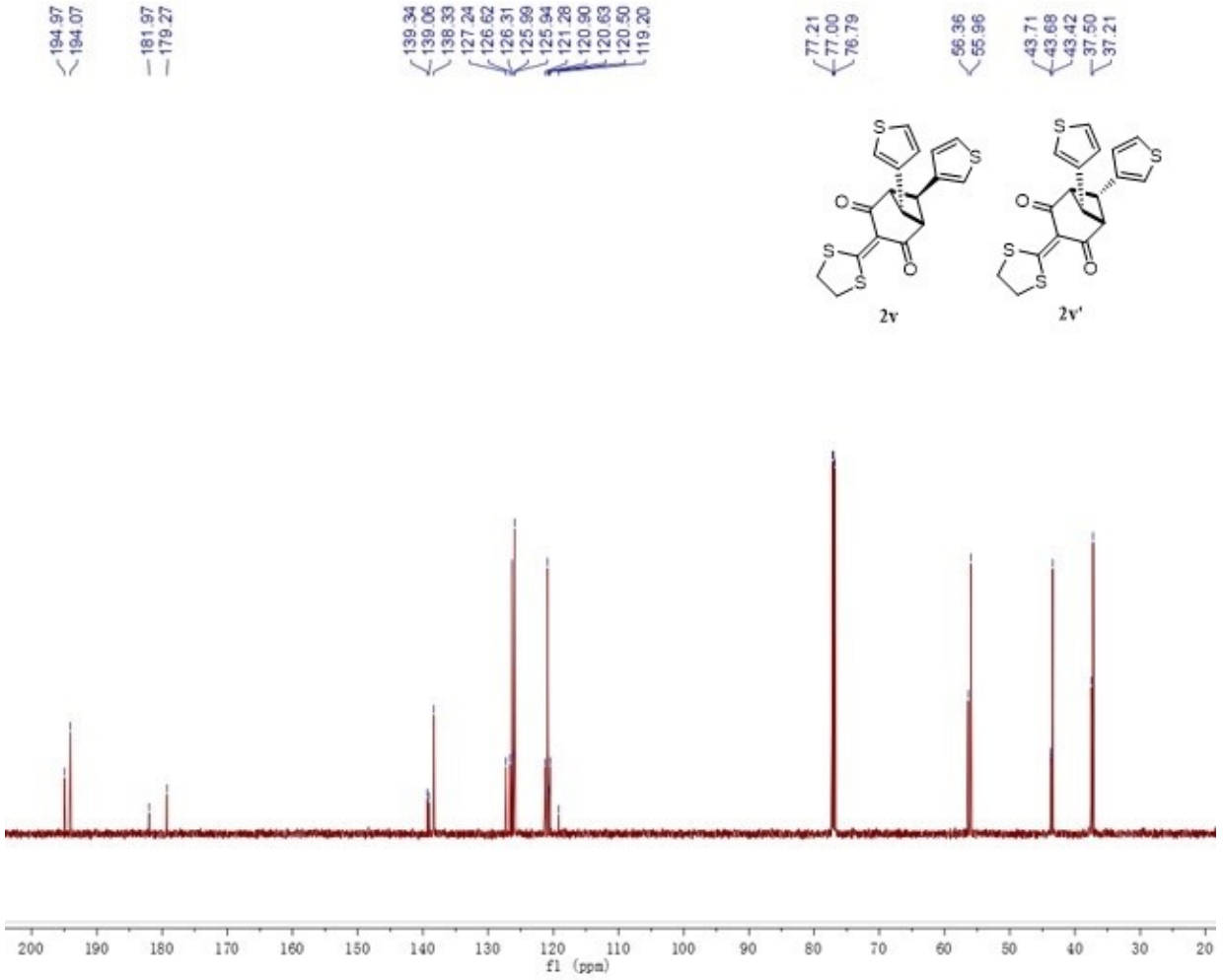
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3u



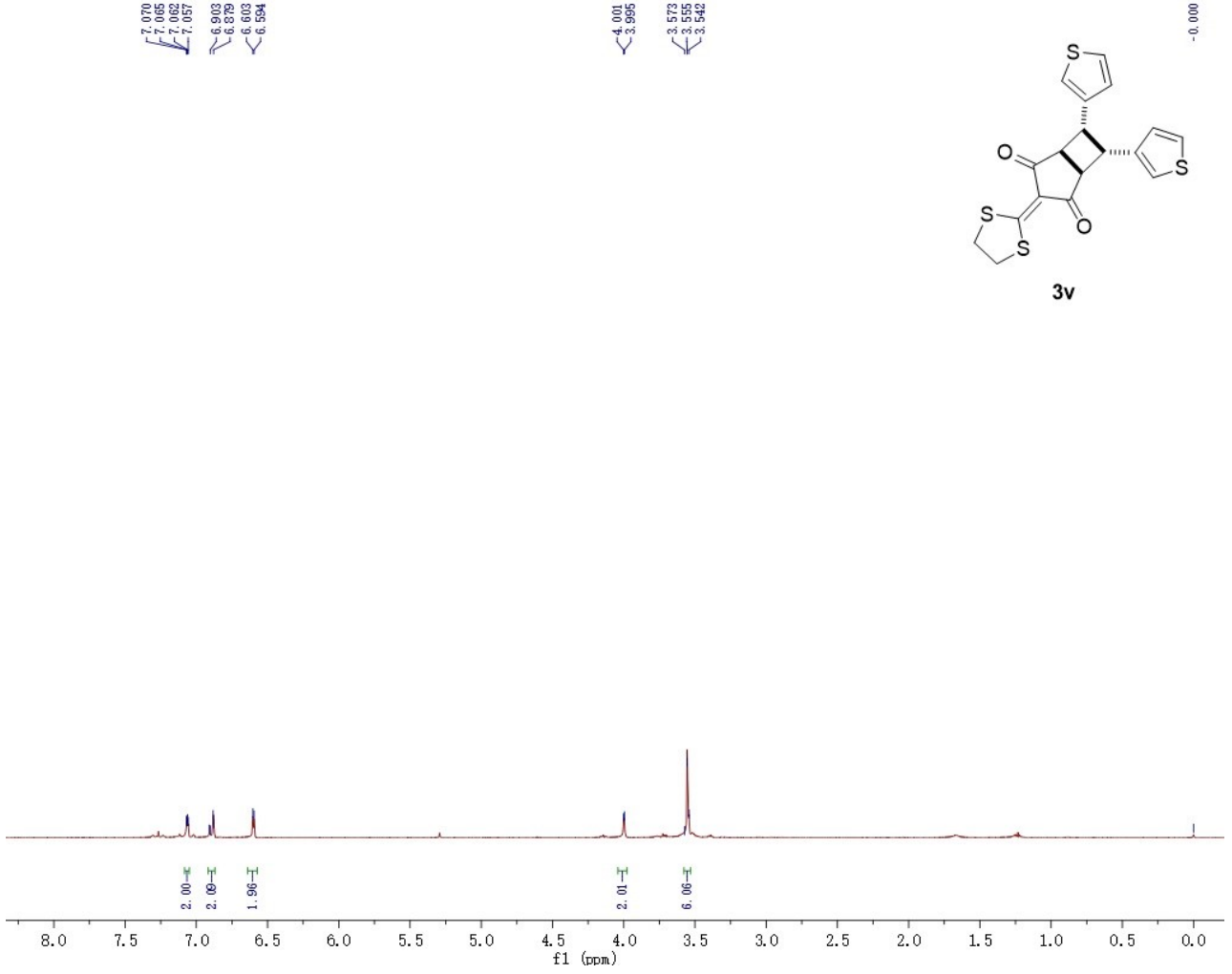
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 2v/2v'



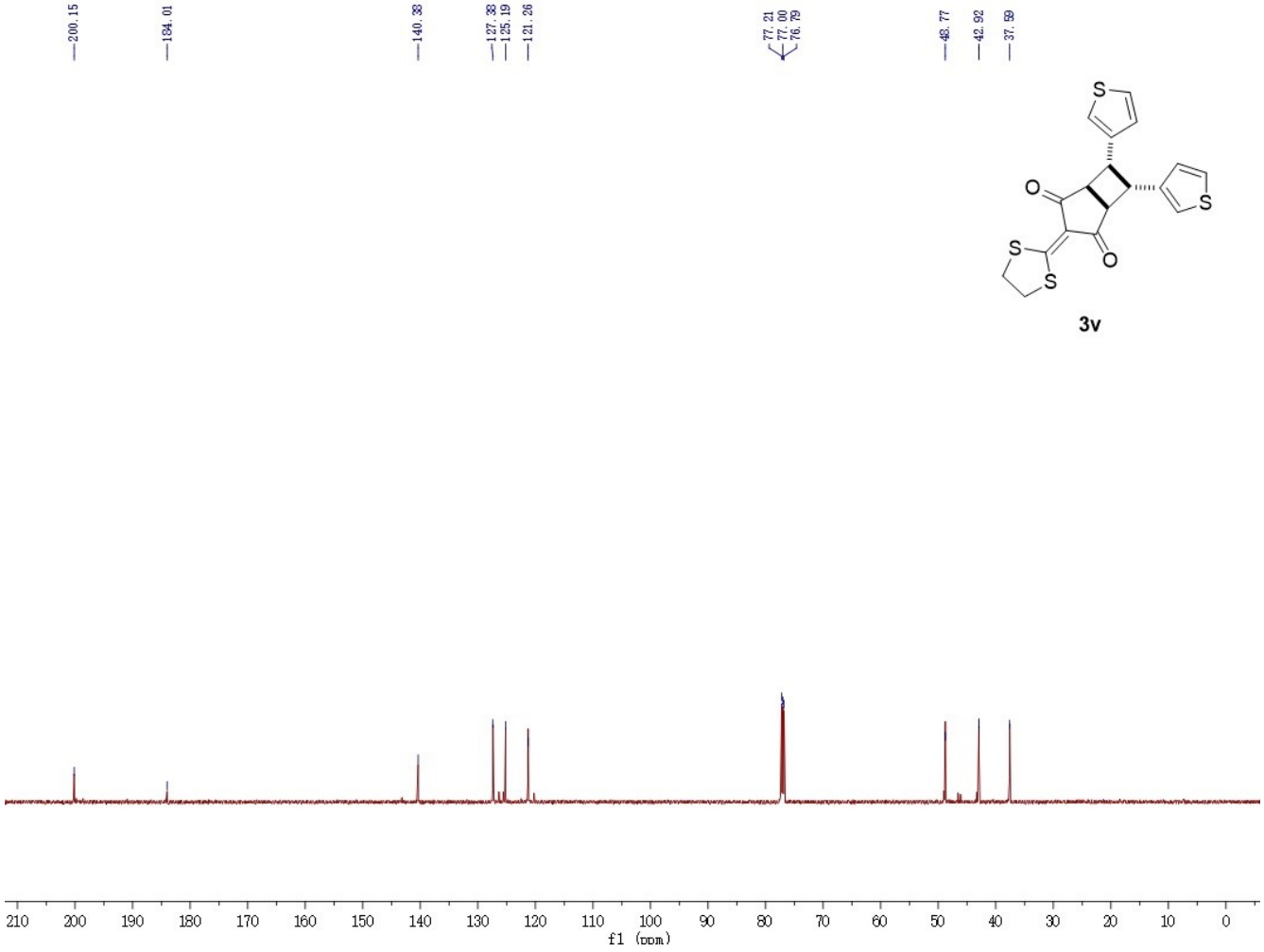
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2v/2v'



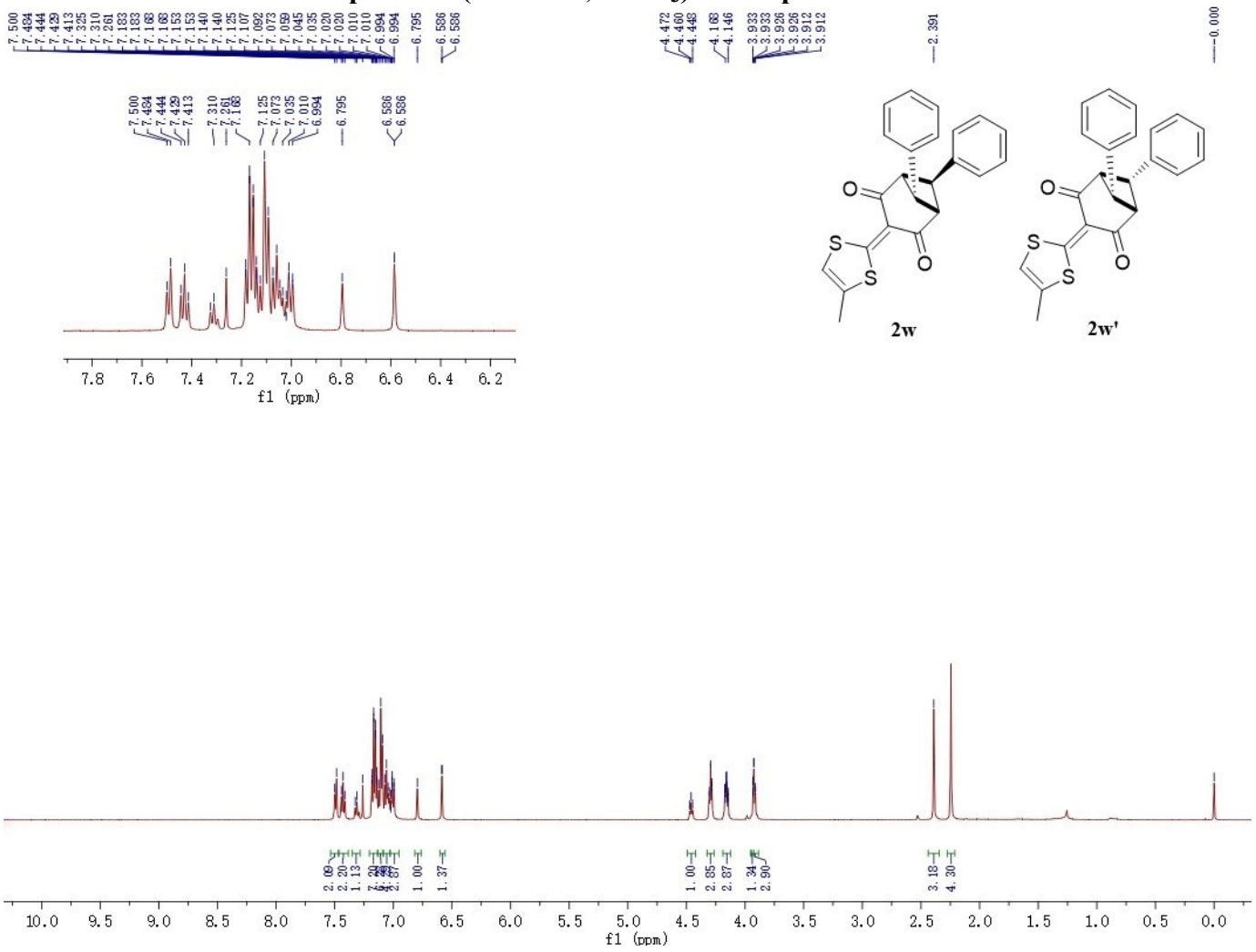
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3v



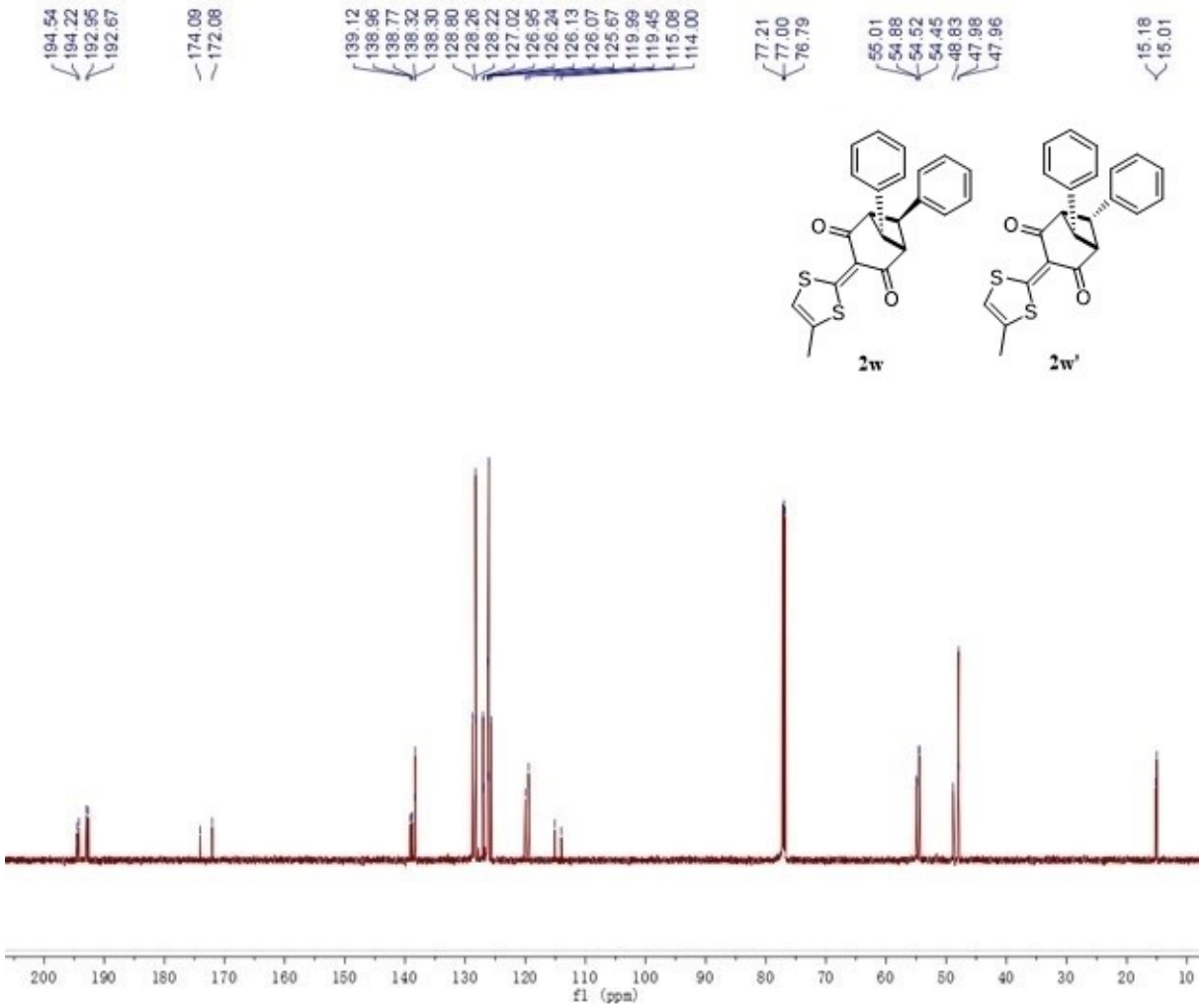
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3v



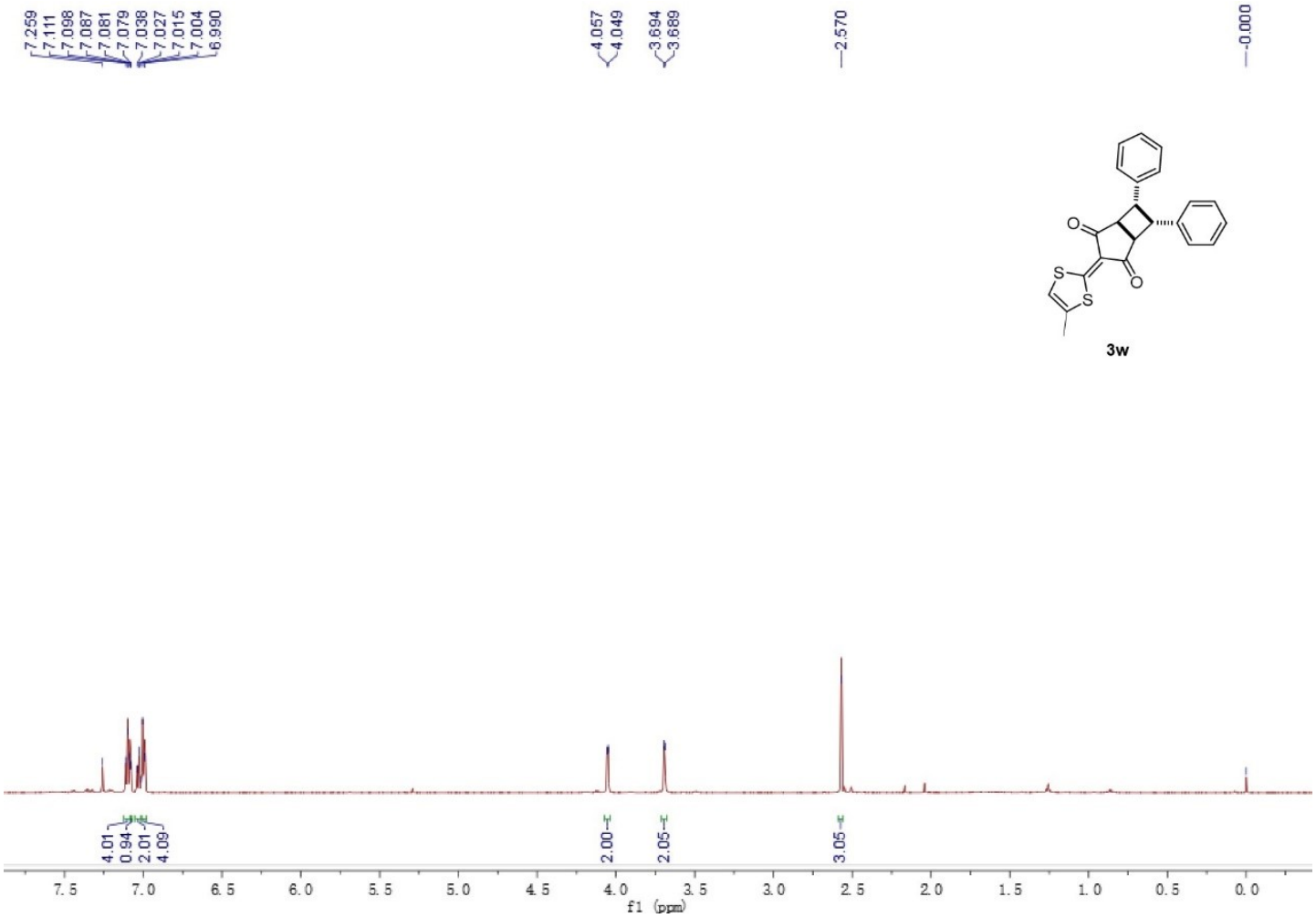
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2w/2w'



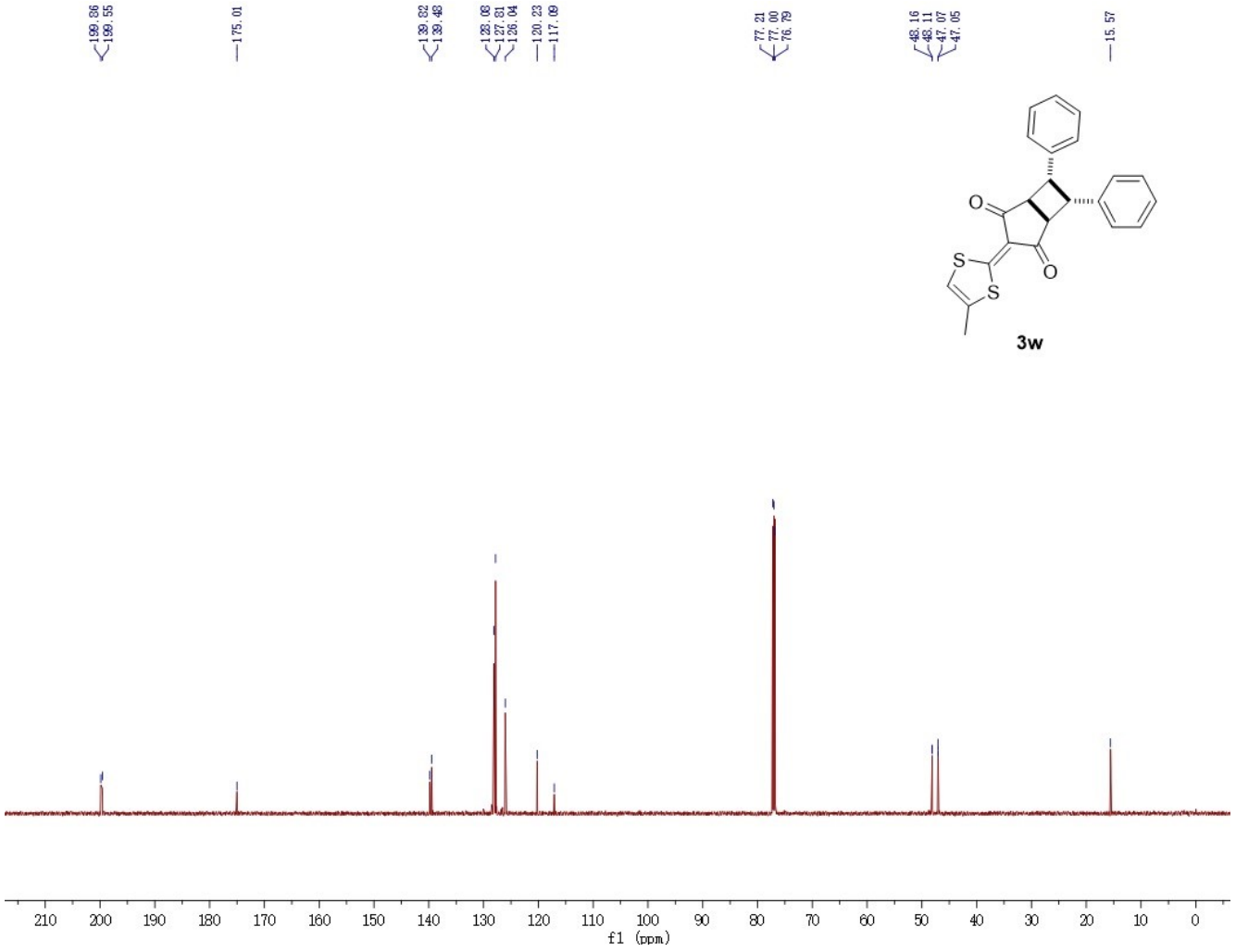
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2w/2w'



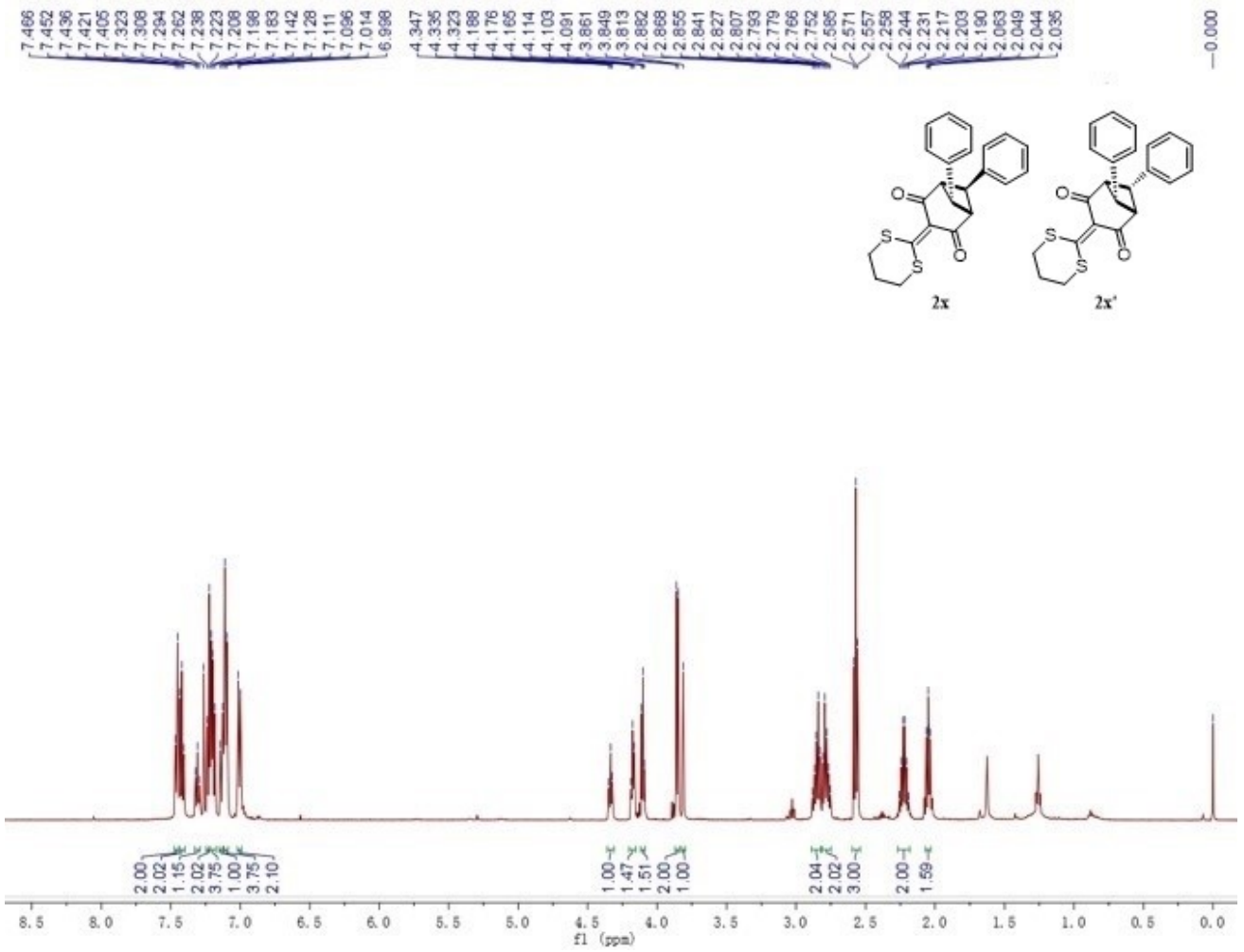
^{1}H spectrum (600 MHz, $CDCl_3$) of compound 3w



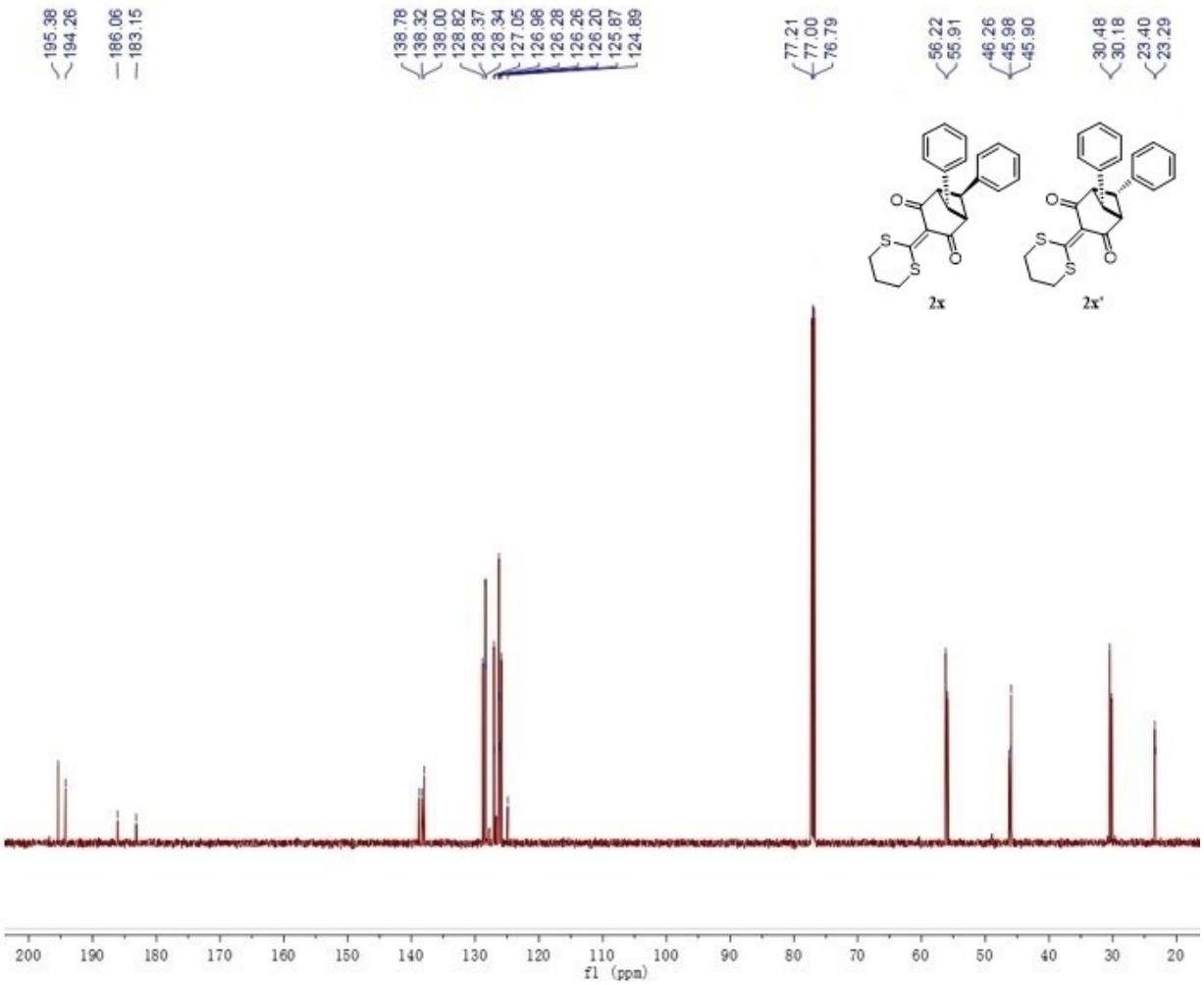
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3w



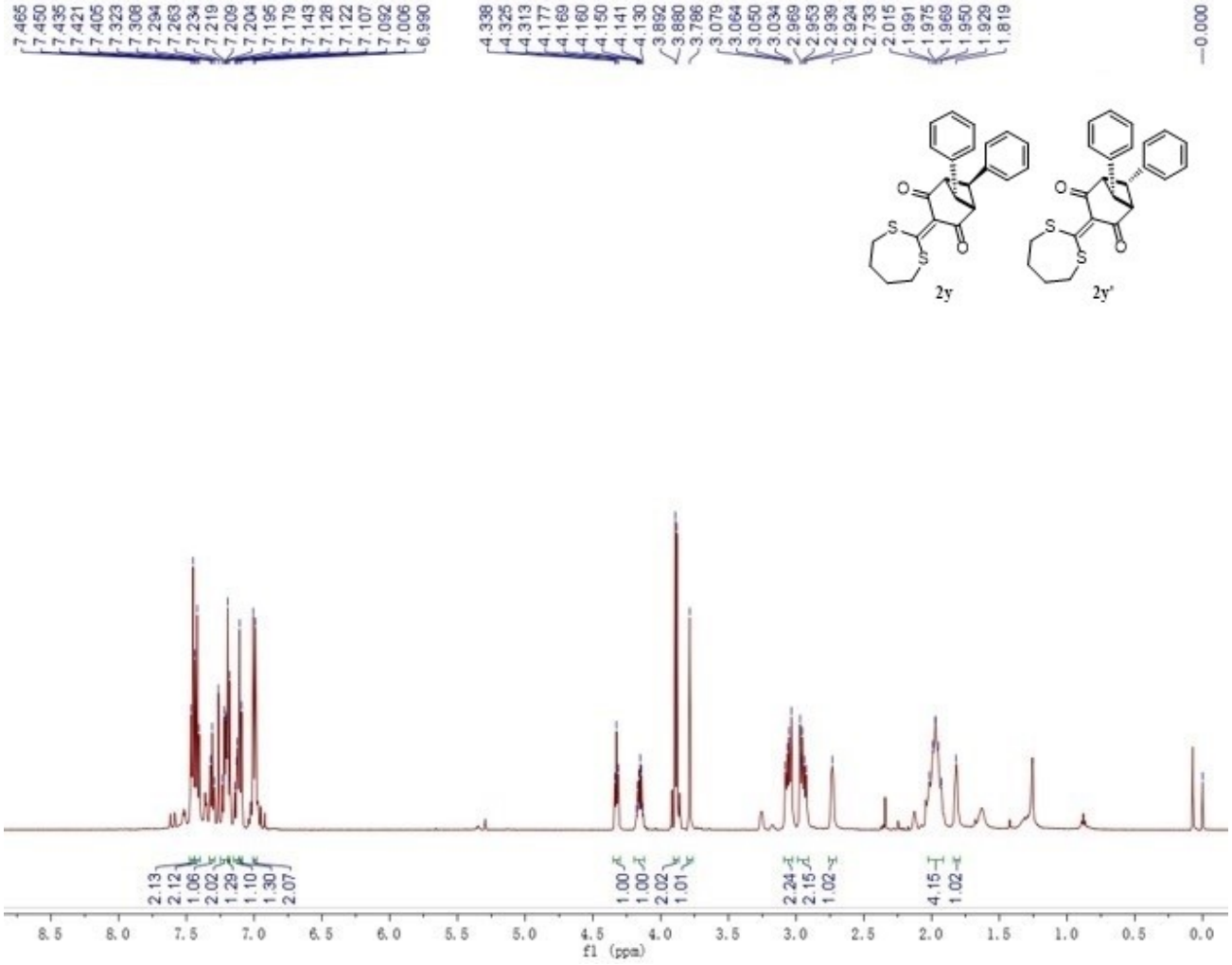
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2x/2x'



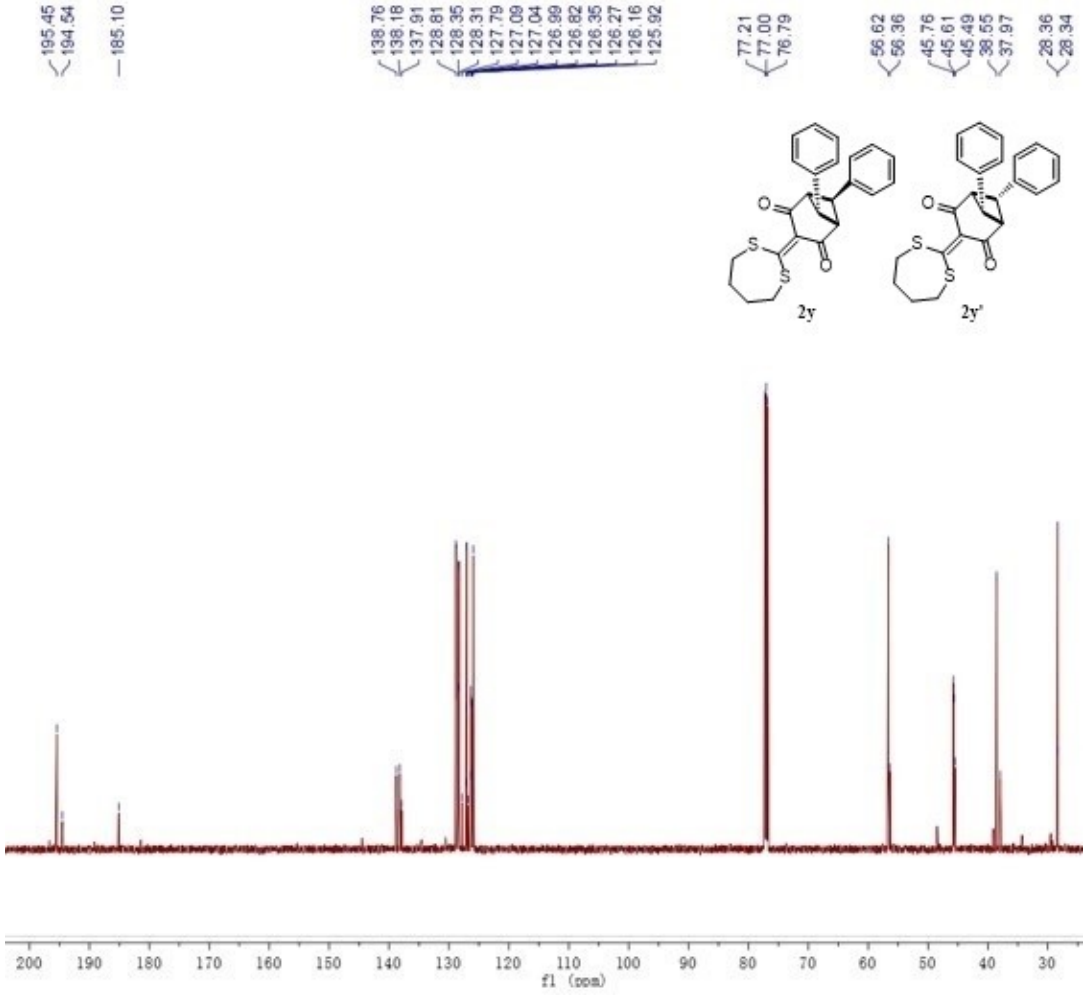
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2x/2x'



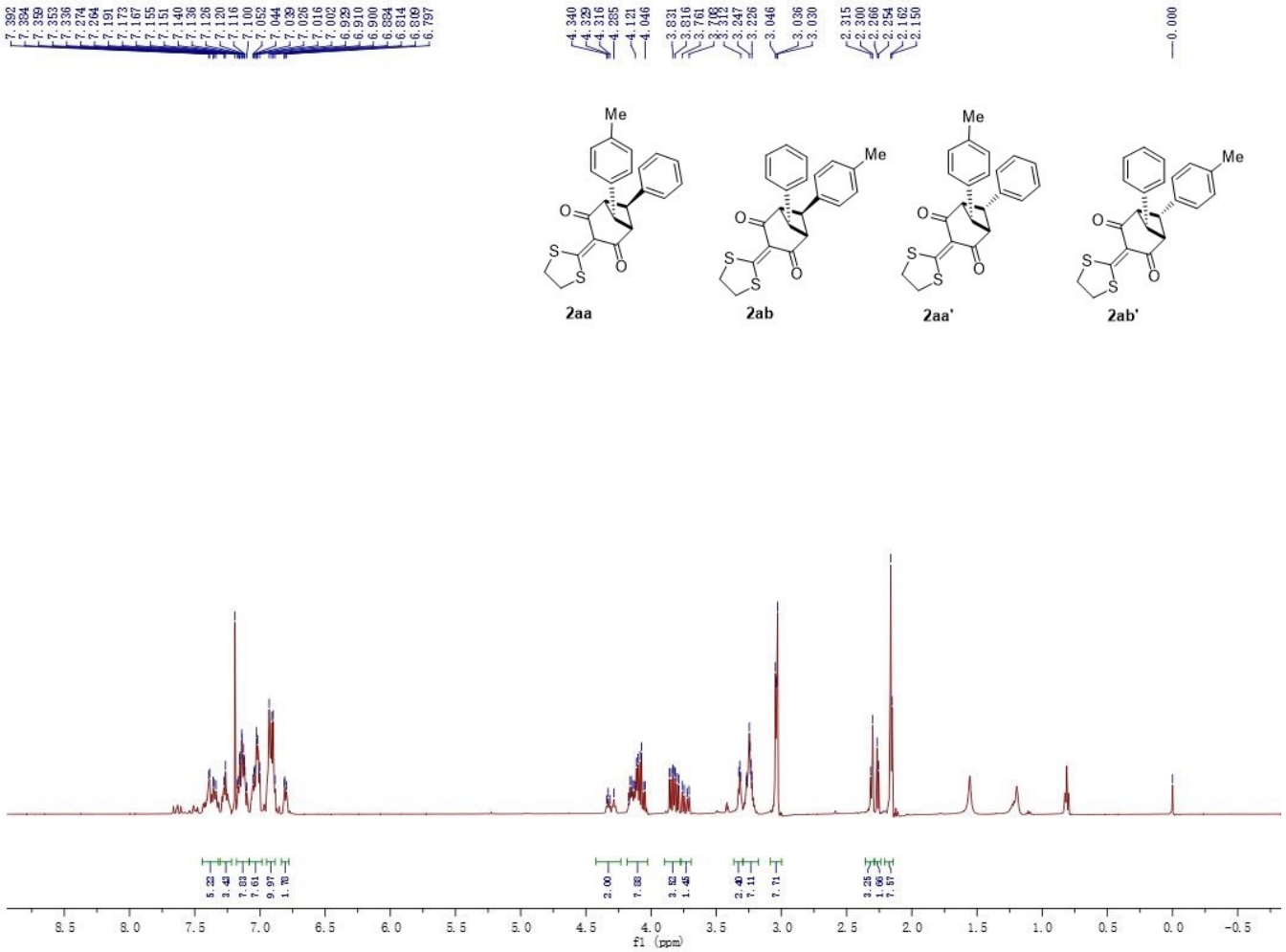
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2y/2y'



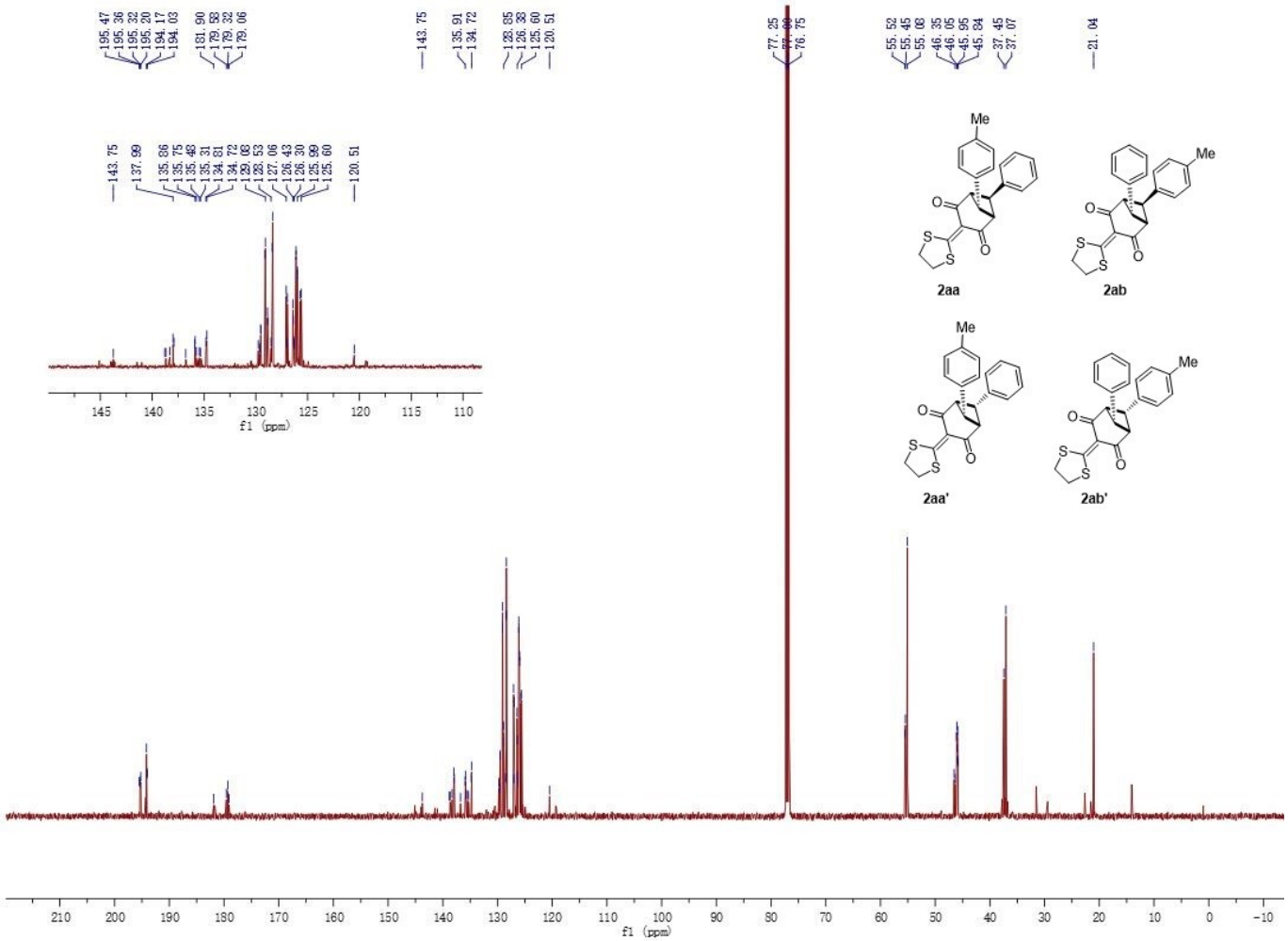
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2y/2y'



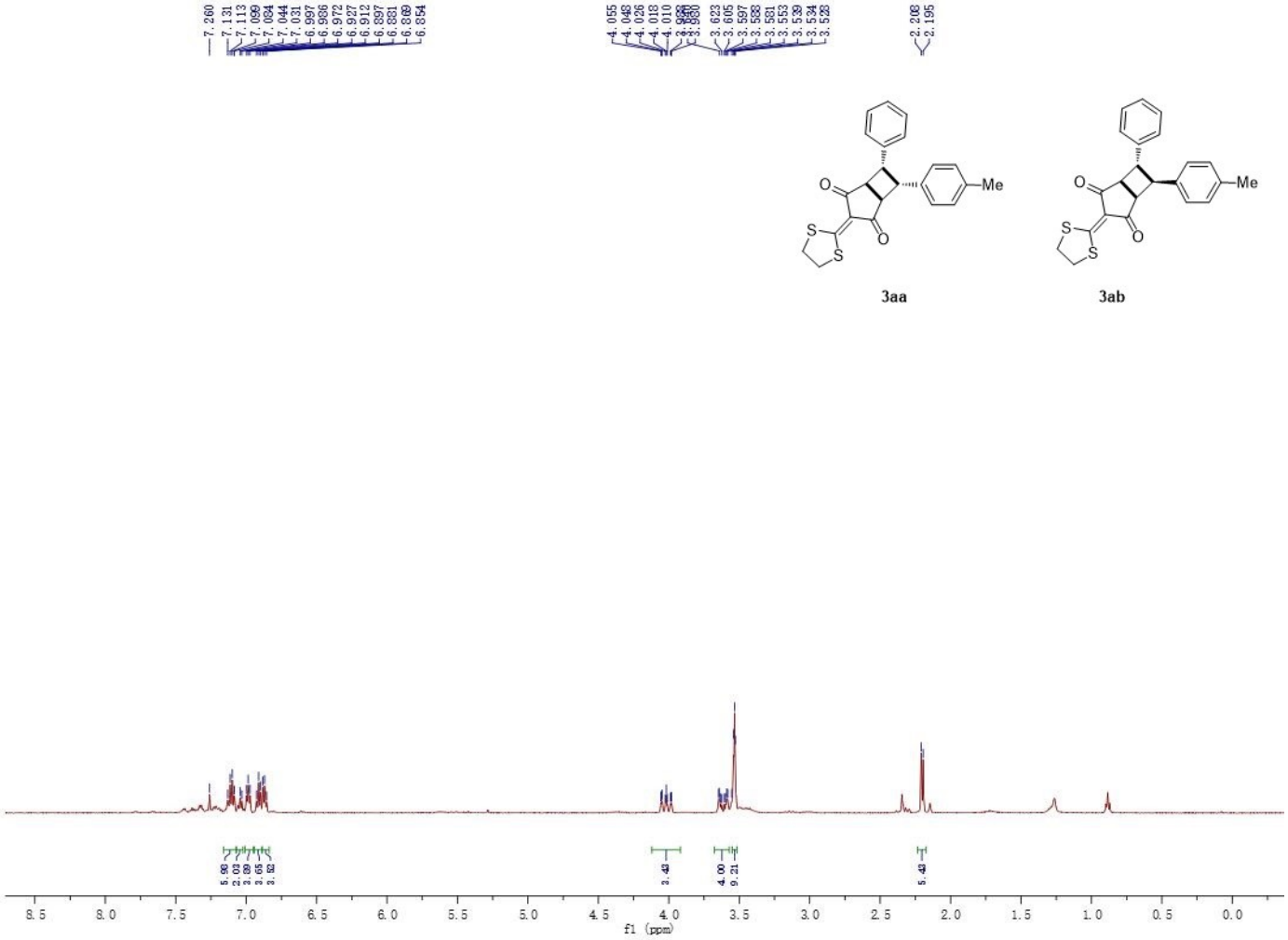
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2aa/2ab/2aa'/2ab'



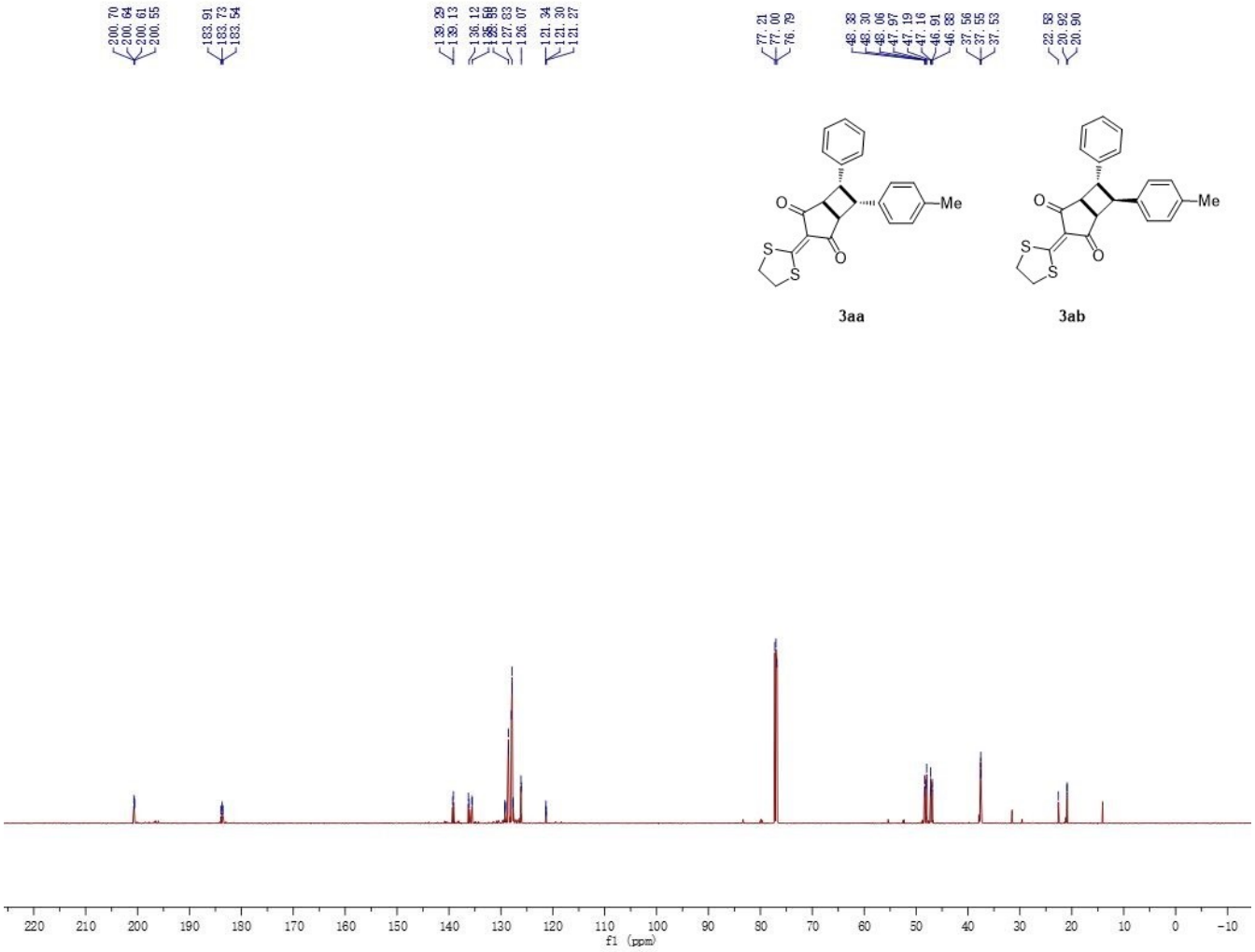
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2aa/2ab/2aa'/2ab'



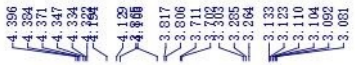
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3aa/3ab

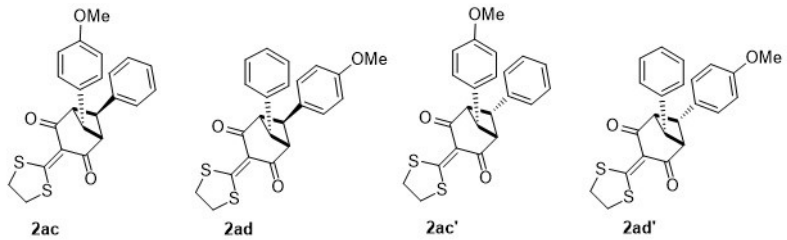


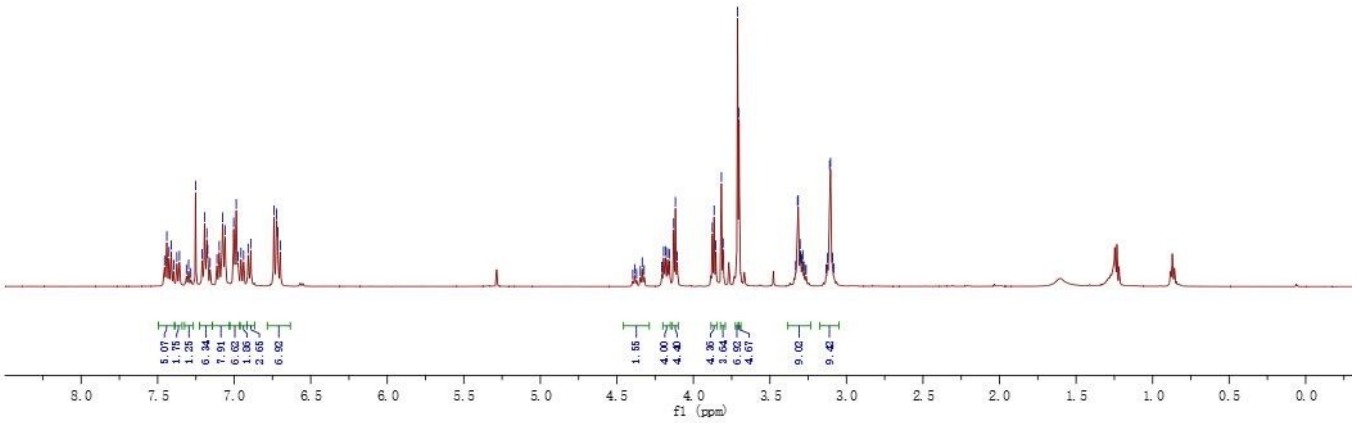
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3aa/3ab



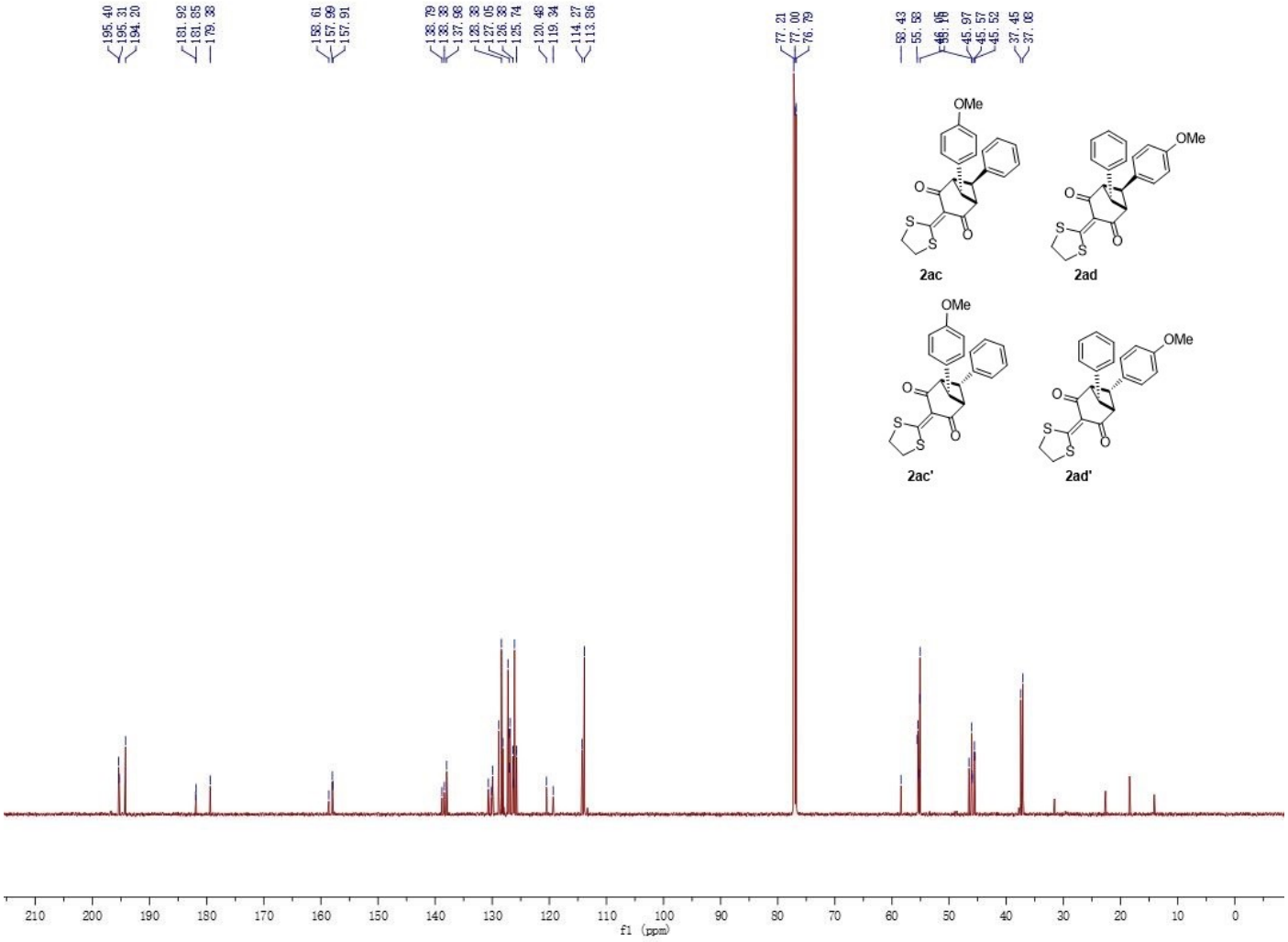
^{1}H spectrum (500 MHz, $CDCl_3$) of compound 2ac/2ad/2ac'/2ad'



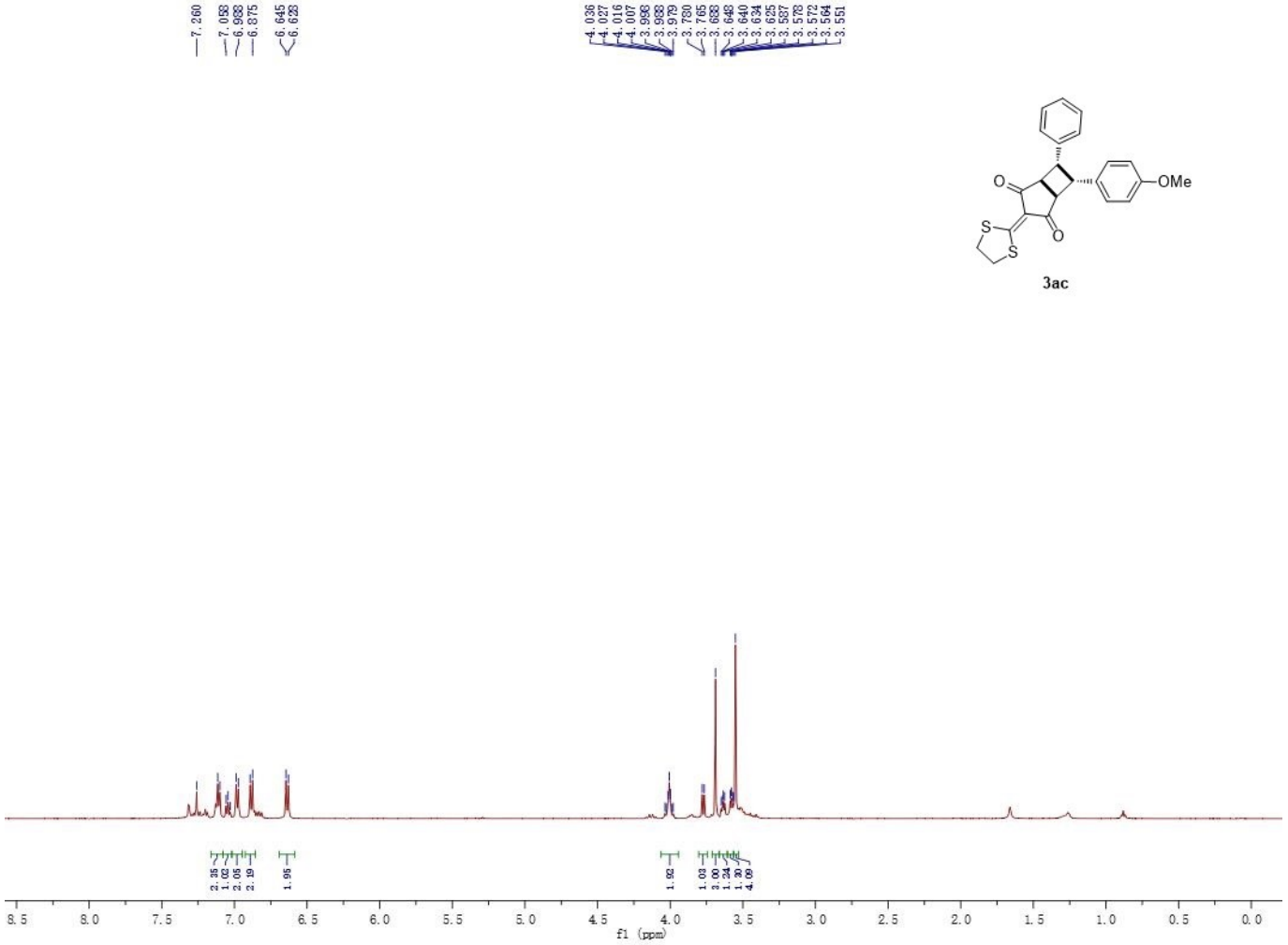




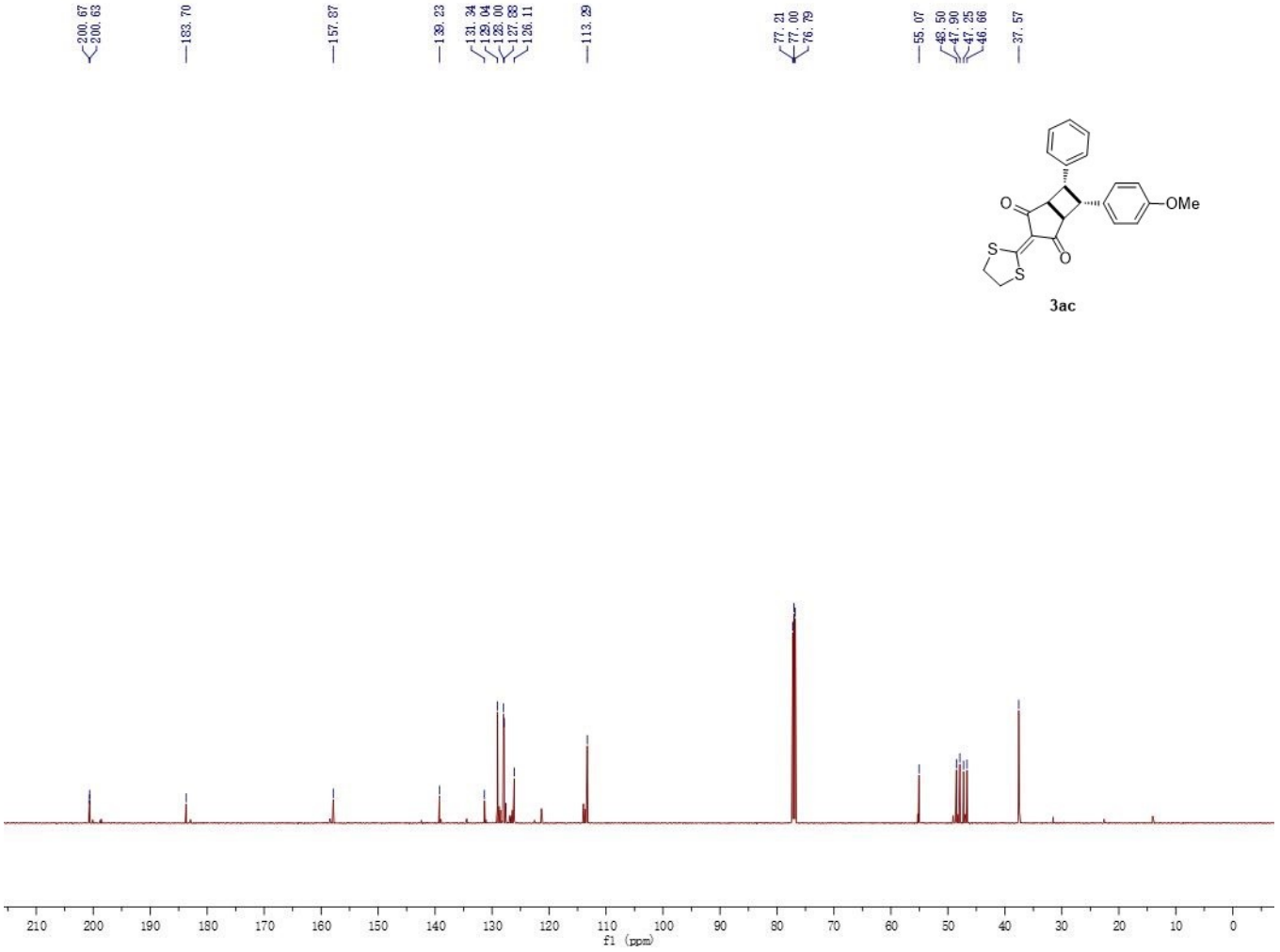
^{13}C spectrum (151 MHz, $CDCl_3$) of compound 2ac/2ad/2ac'/2ad'



^{1}H spectrum (500 MHz, $CDCl_3$) of compound 3ac



^{13}C spectrum (151 MHz, $CDCl_3$) of compound 3ac



9. References

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