

Supporting Information for

Synthesis of Sulfur-Containing Benzo[*b*]pyrrolo[2,1-*c*][1,4]oxazine-3,9-diones: Blue Light Promoted Radical Cyclization Process

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1. The details information of the crystal of 3k	S3-S6
2. Copies of the Products ^1H NMR, $^{13}\text{C}\{^1\text{H}\}$ NMR	S7-S27

1. The details information of the crystal of 3k

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20210608

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 20210608

Bond precision: C-C = 0.0066 Å Wavelength=0.71073

Cell: a=9.3901(8) b=15.1733(8) c=16.2514(7)
alpha=73.186(4) beta=77.982(5) gamma=87.462(5)

Temperature: 293 K

	Calculated	Reported
Volume	2167.6(2)	2167.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H20 Br N O3 S	C24 H20 Br N O3 S
Sum formula	C24 H20 Br N O3 S	C24 H20 Br N O3 S
Mr	482.37	482.38
Dx, g cm ⁻³	1.478	1.478
Z	4	4
Mu (mm ⁻¹)	2.018	2.018
F000	984.0	984.0
F000'	983.73	
h, k, lmax	11, 18, 19	11, 18, 19
Nref	7637	7620
Tmin, Tmax	0.817, 0.817	0.516, 1.000
Tmin'	0.817	

Correction method= # Reported T Limits: Tmin=0.516 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.000

R(reflections)= 0.0507(4496) wR2(reflections)=
S = 0.944 Npar= 543 0.1053(7620)

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta (Min). 17 Note

Author Response: Theta min = 3.11 deg. The theta value of the missing reflections are less than 3.11 deg. and therefore reflections were excluded.

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for O4 --C23 . 5.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C12 --C17 . 6.0 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S4 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C30 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C30 -C52 1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C15 -C22 1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0066 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C24 H20 Br N O3 S
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.682 Check

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C24 H20 Br N O3 S
PLAT793_ALERT_4_G Model has Chirality at C6 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C14 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C27 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C31 (Centro SPGR) R Verify
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

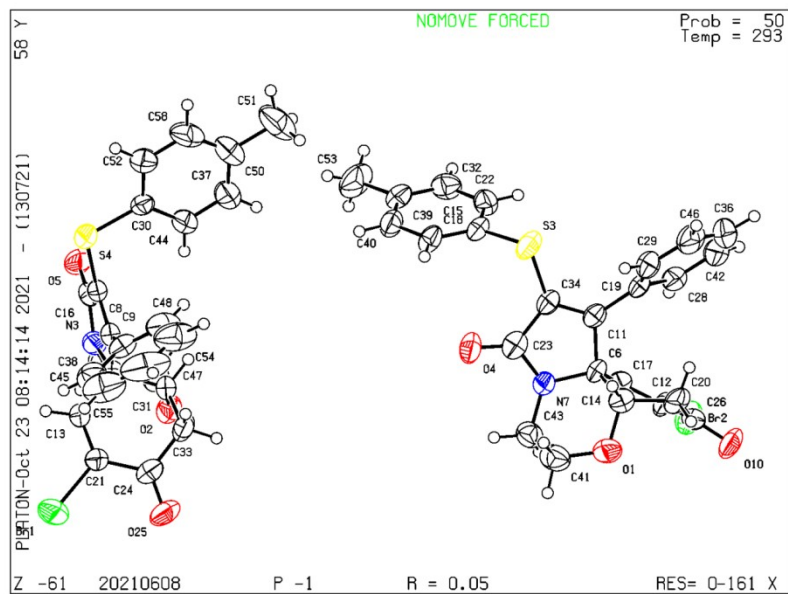
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that [full publication checks](#) are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/07/2021; check.def file version of 13/07/2021



2. Copies of the Products ^1H NMR, $^{13}\text{C}\{^1\text{H}\}$ NMR

Figure S1 ^1H -NMR spectrum (400 MHz, CDCl_3) of **3a**

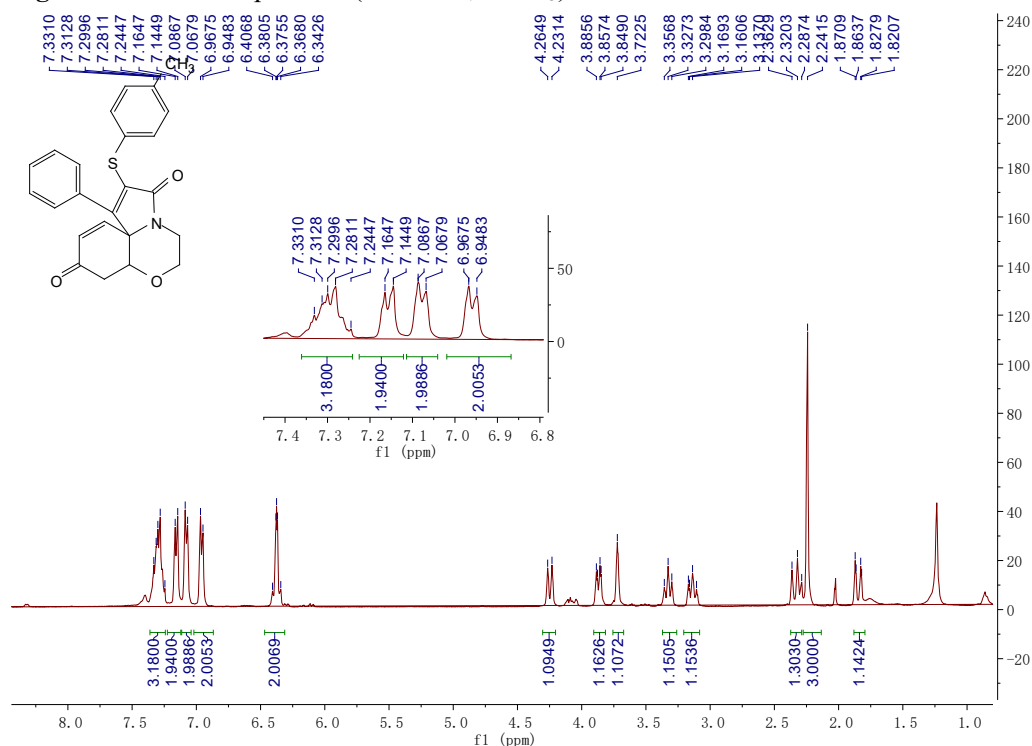


Figure S2 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3a**

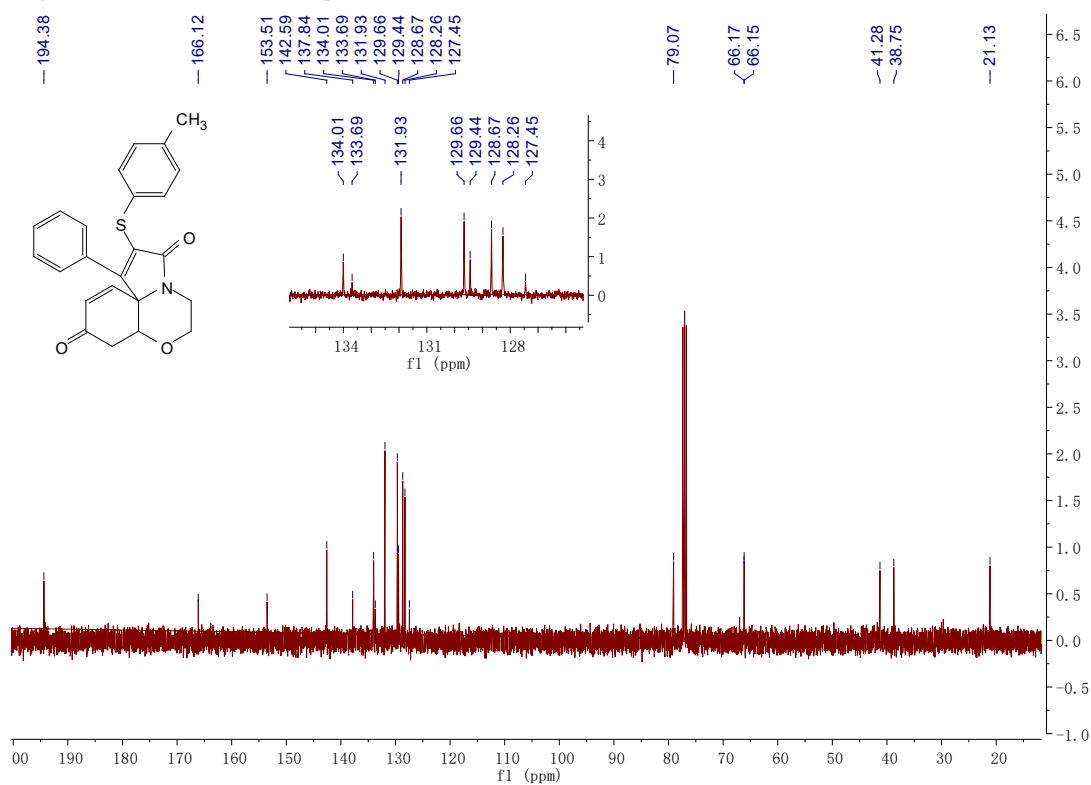


Figure S3 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3b**

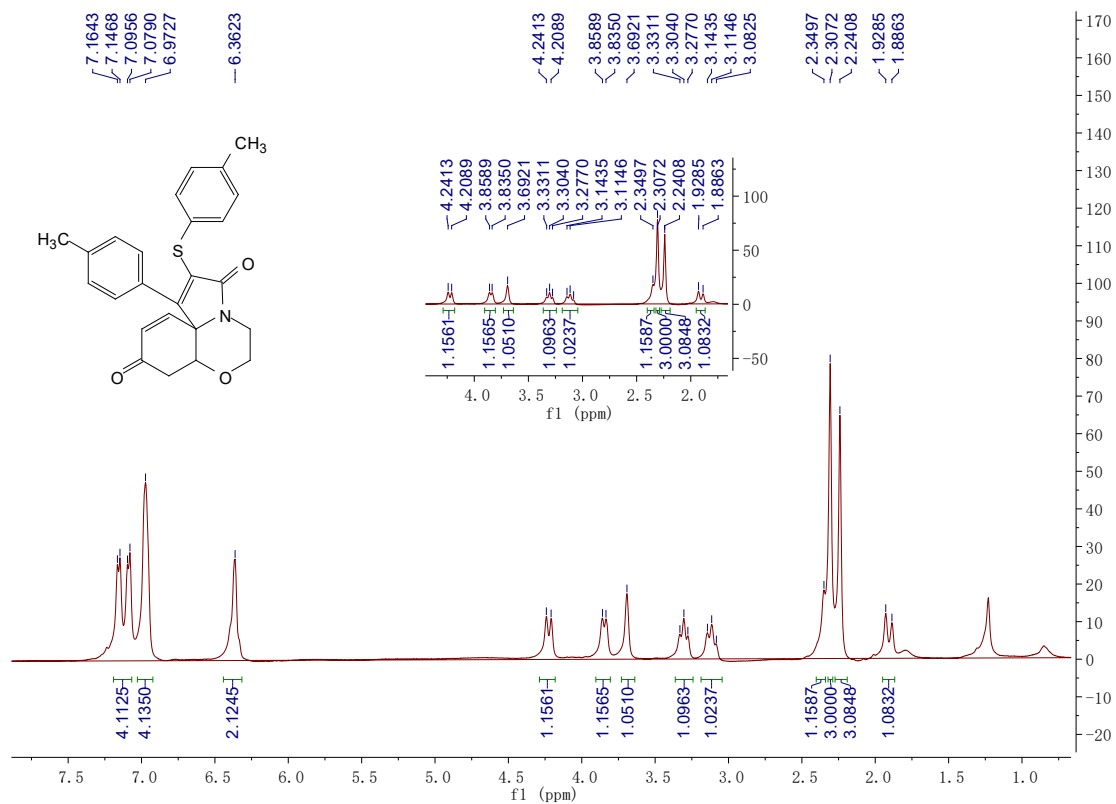


Figure S4 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3b**

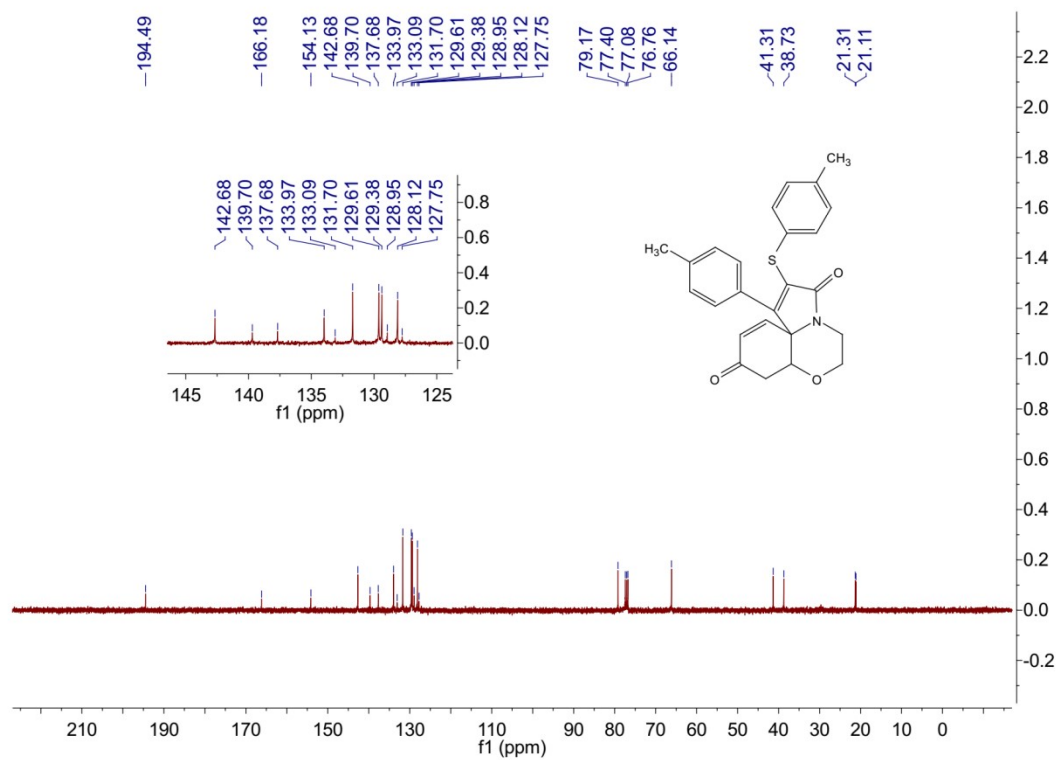


Figure S5 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3c**

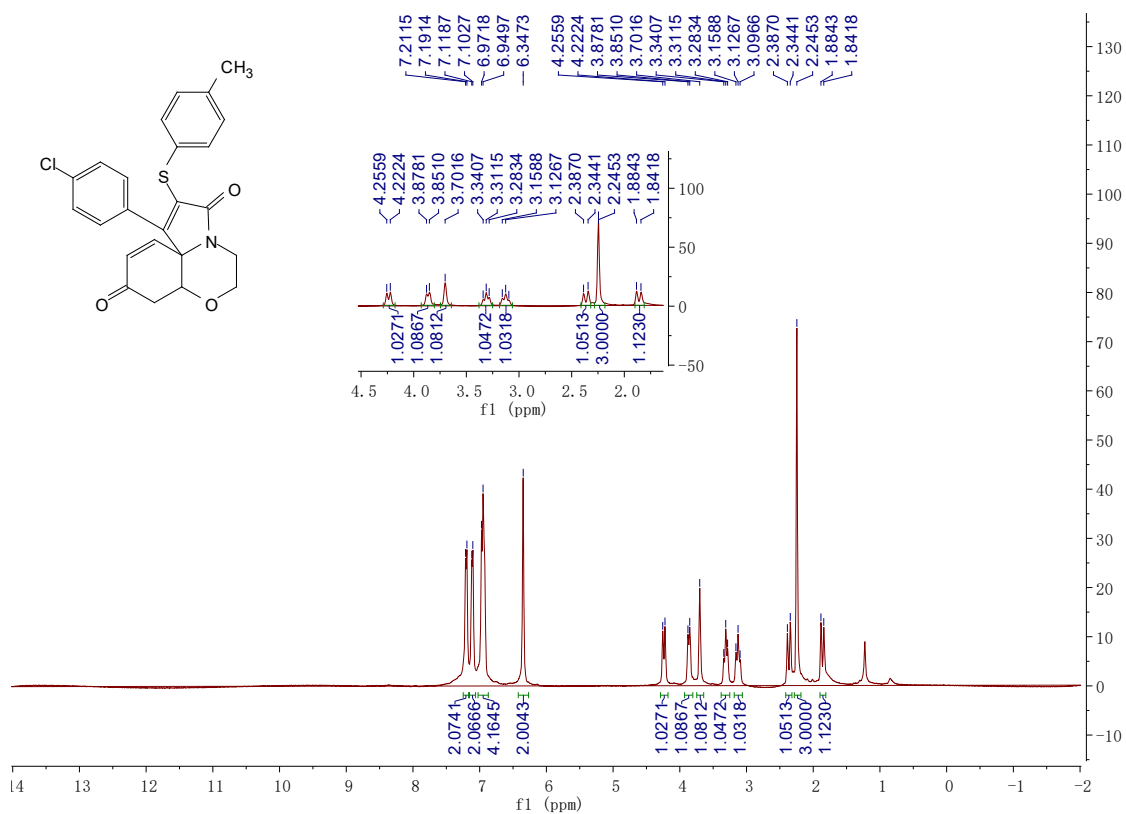


Figure S6 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3c**

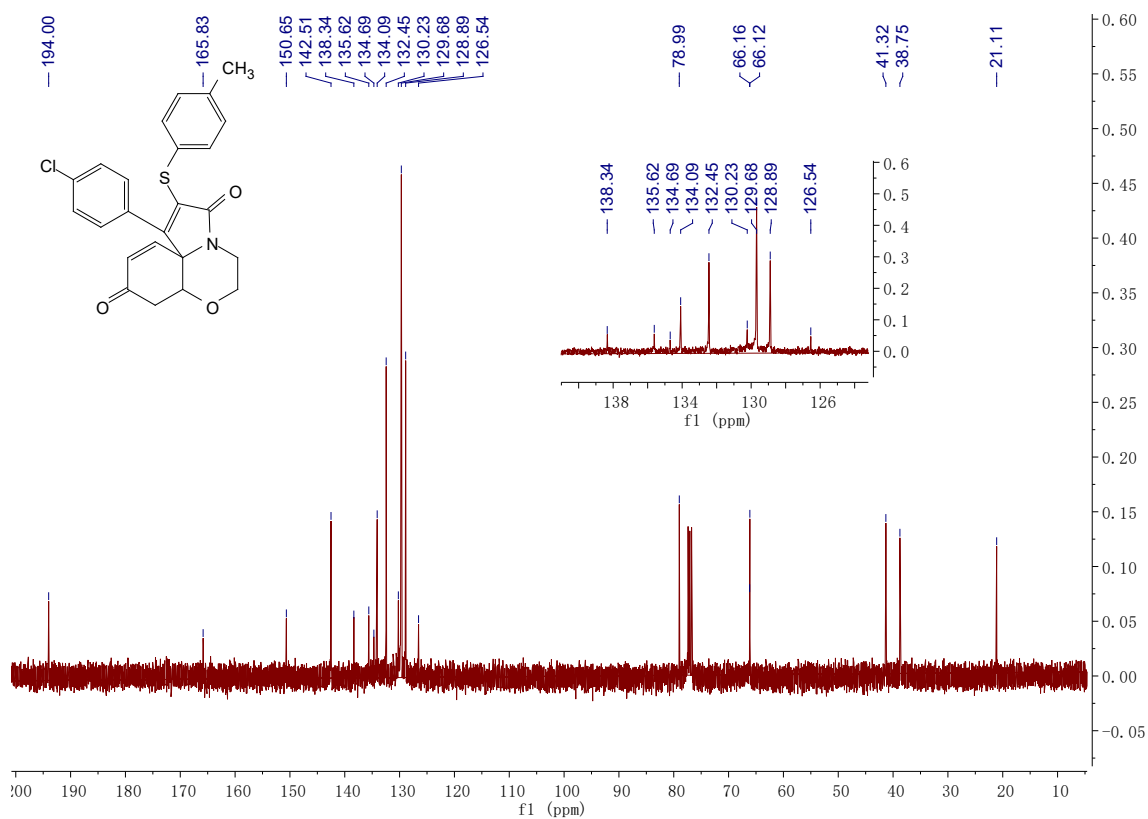


Figure S9 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3e**

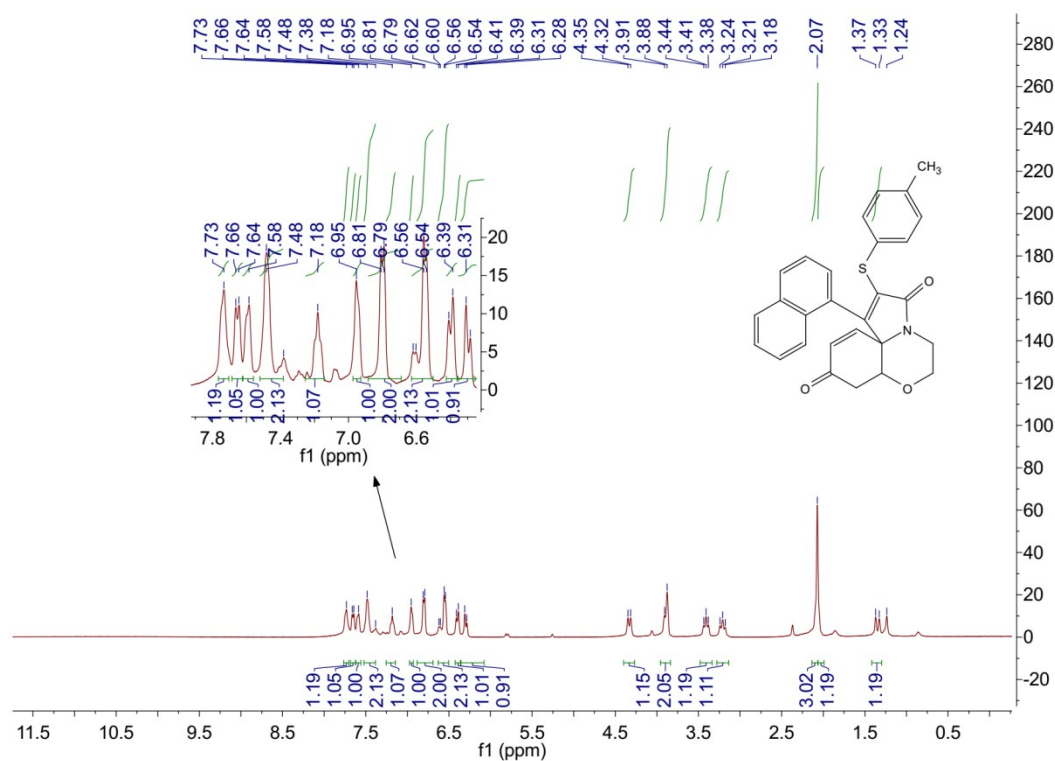


Figure S10 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3e**

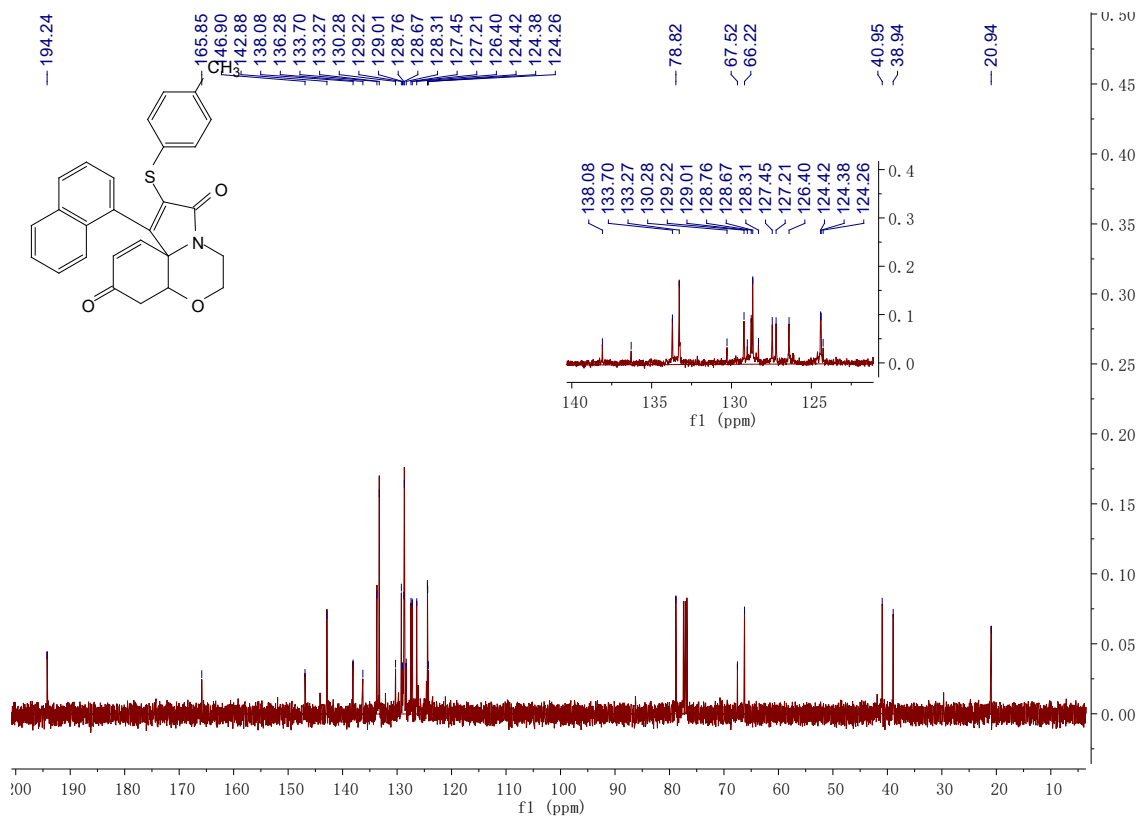


Figure S11 ^1H -NMR spectrum (400 MHz, CDCl_3) of **3f**

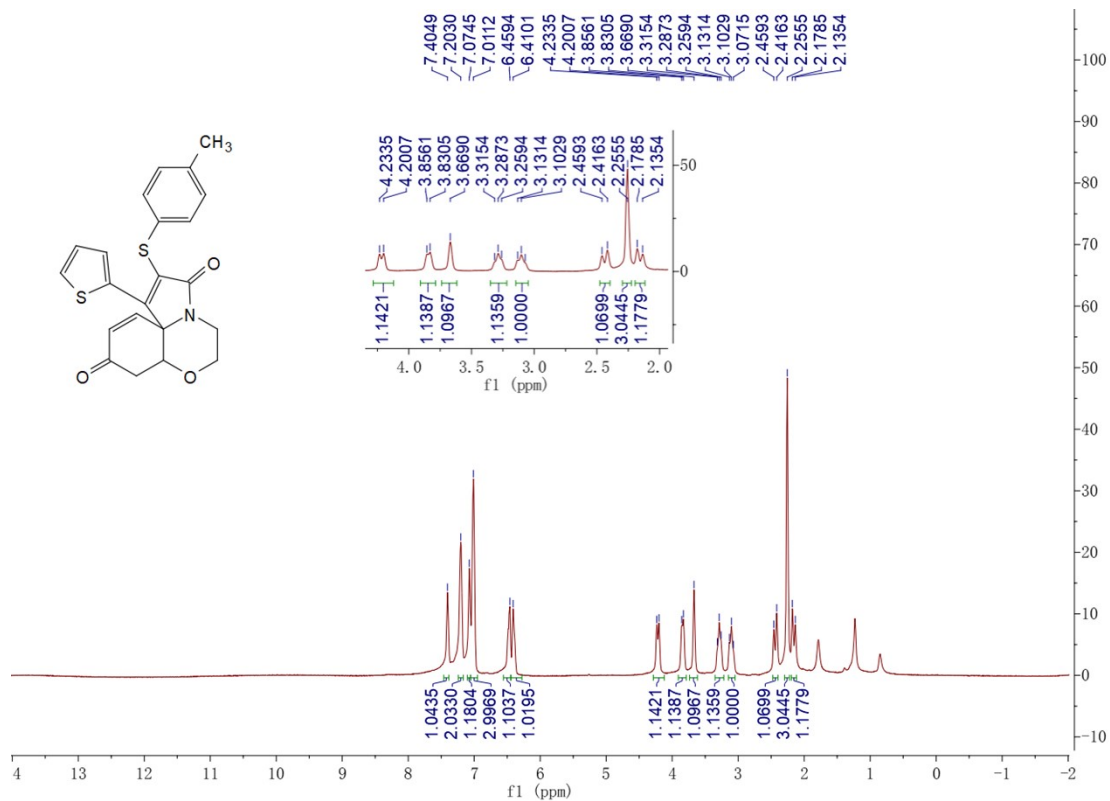


Figure S12 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3f**

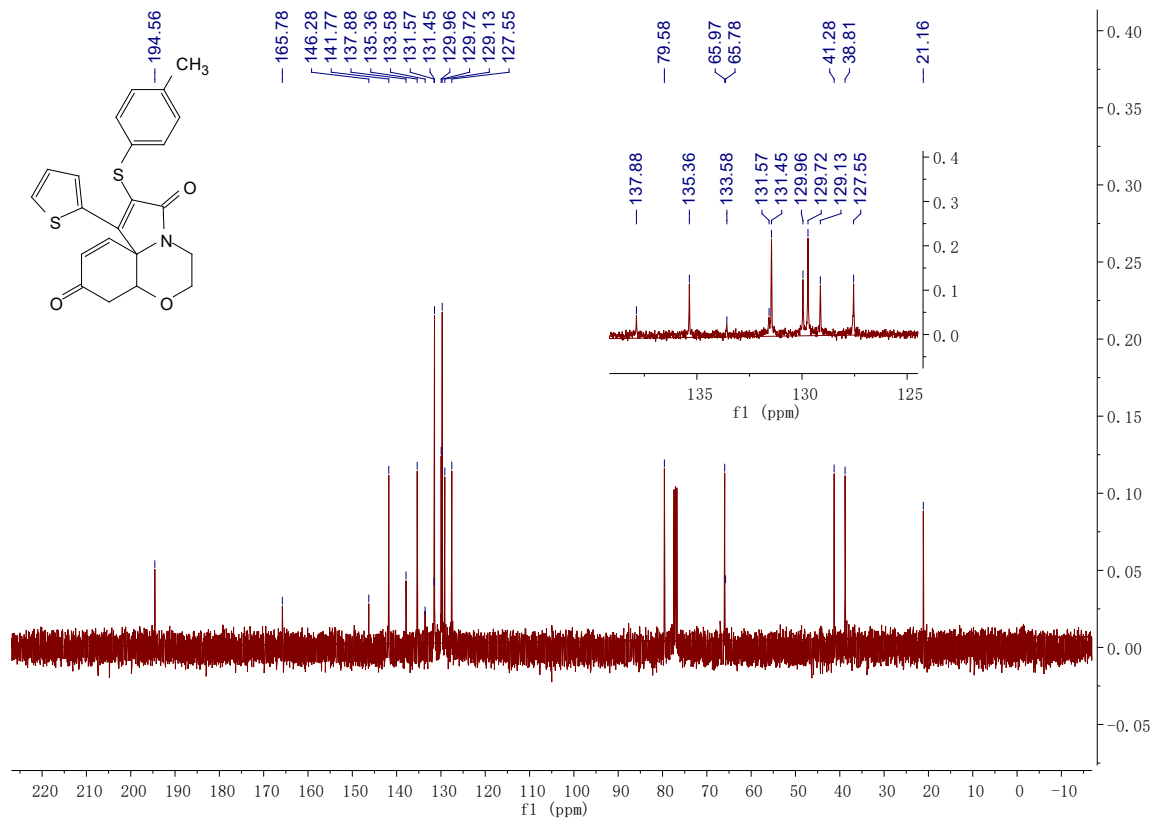


Figure S13 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3g**

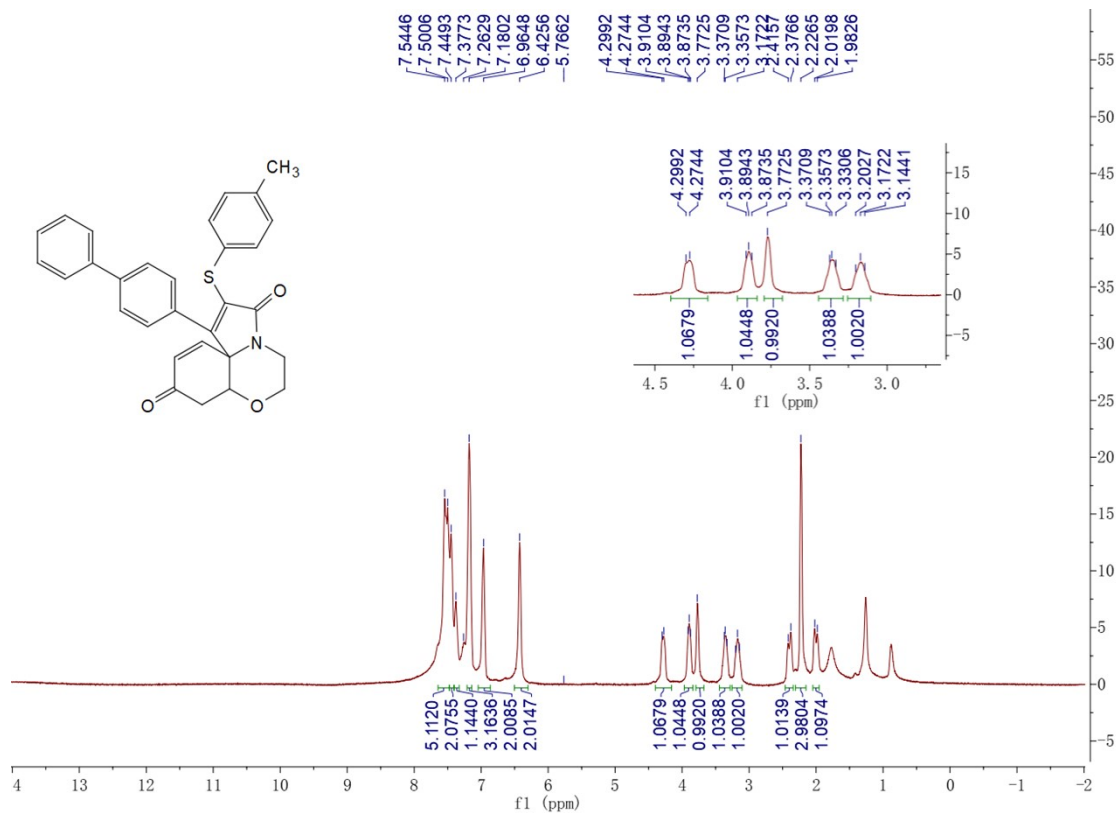


Figure S14 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3g**

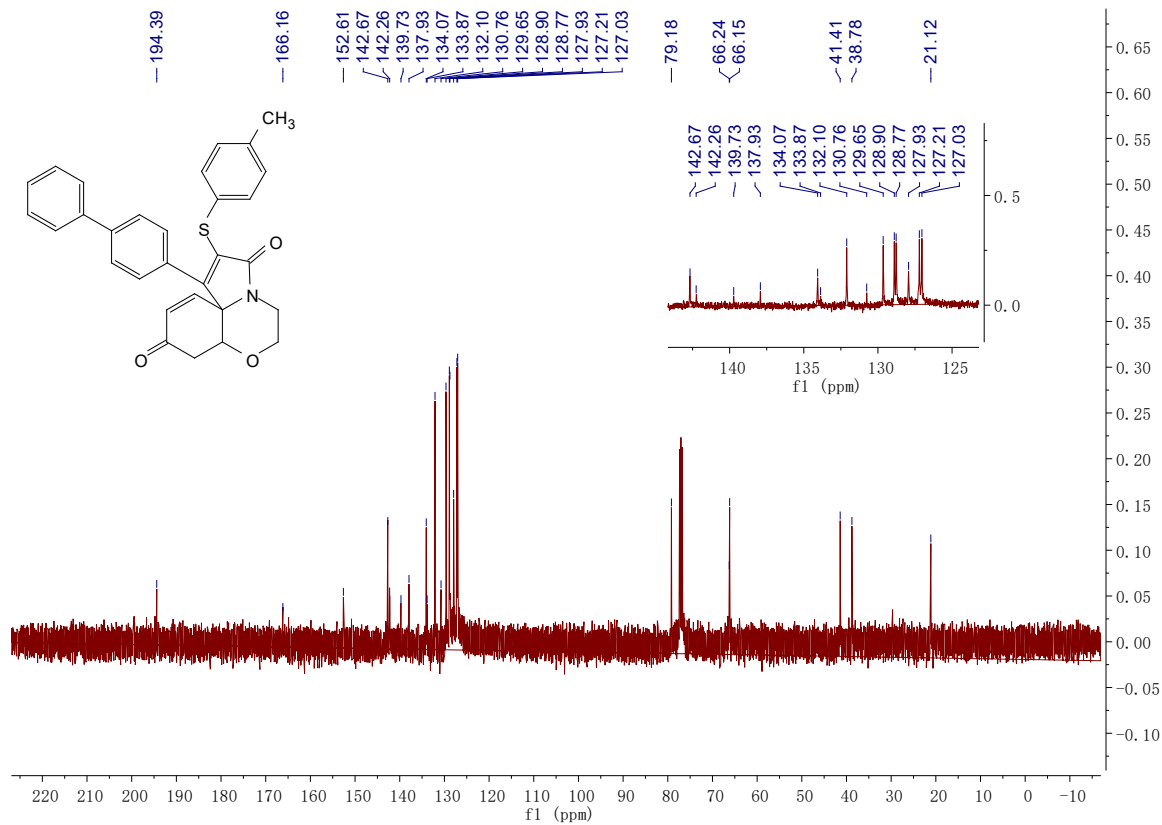


Figure S15 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3h**

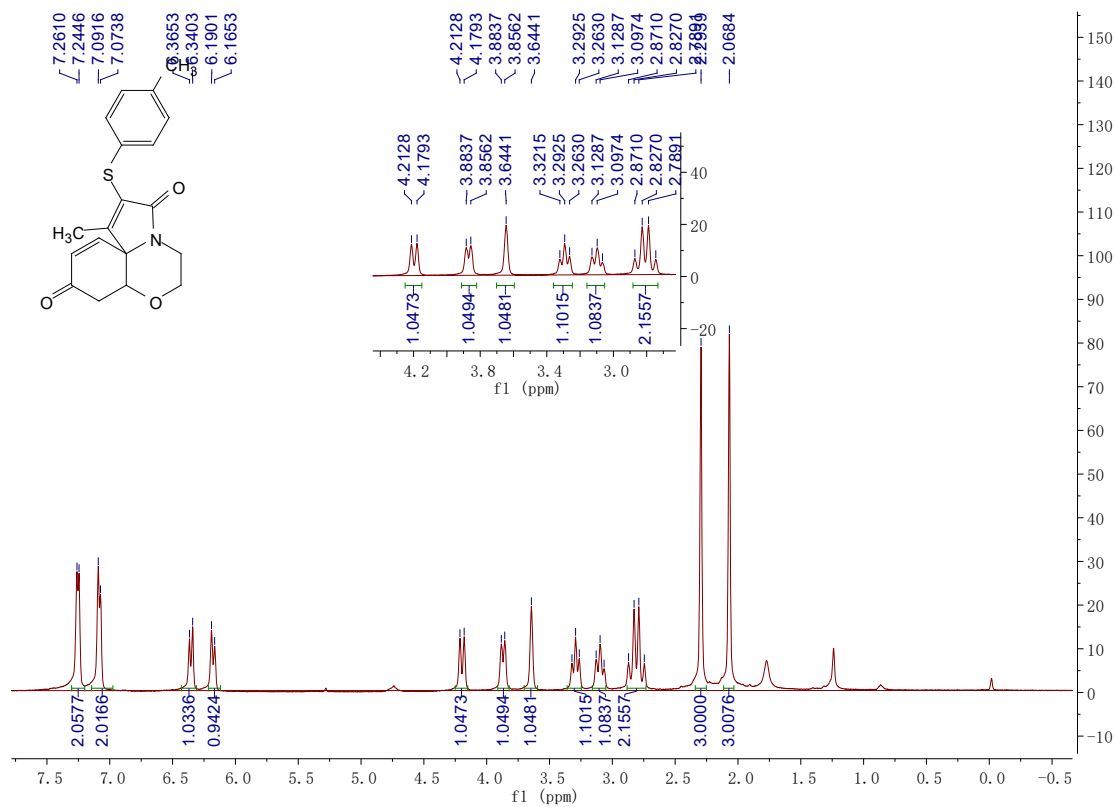


Figure S16 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3h**

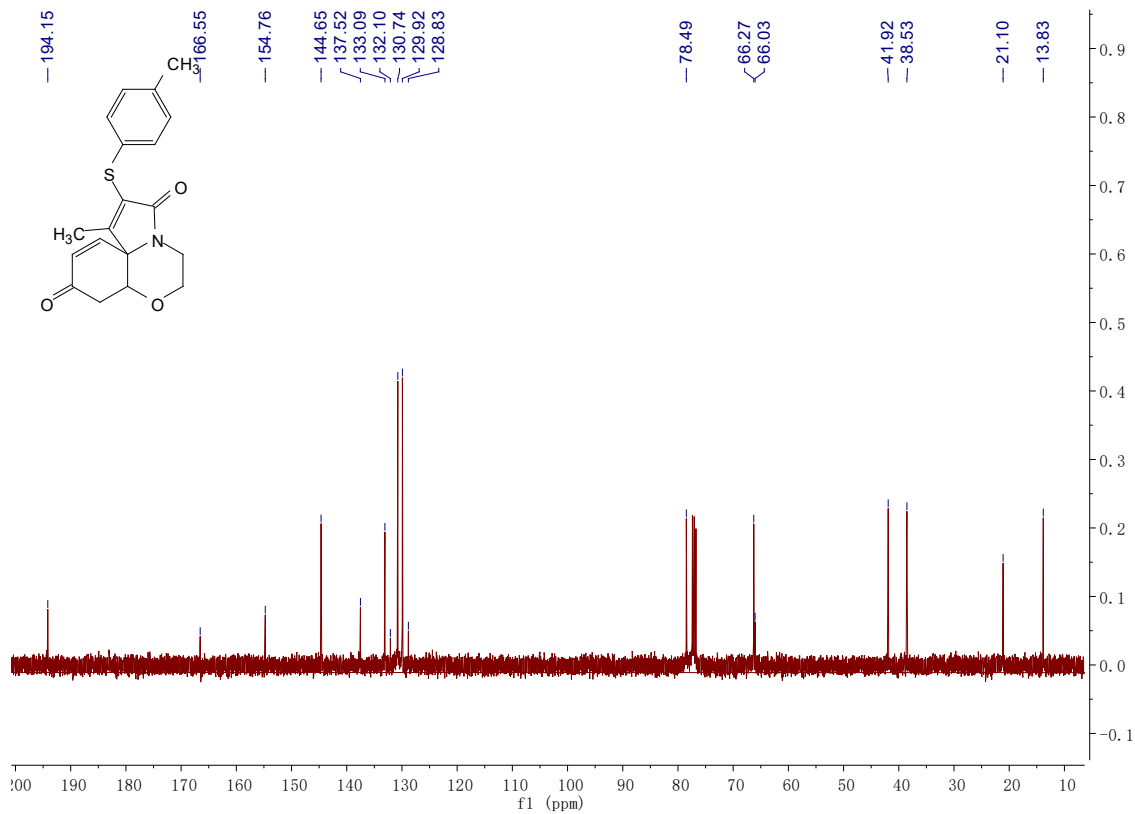


Figure S17 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3i**

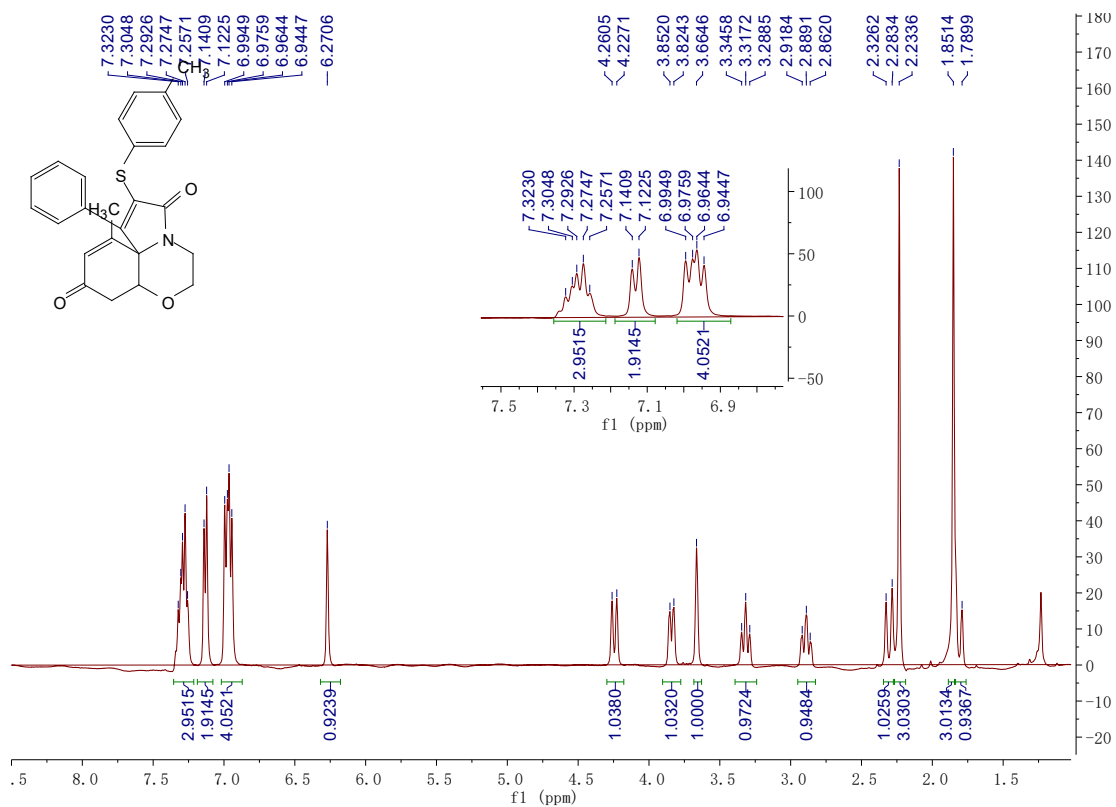


Figure S18 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3i**

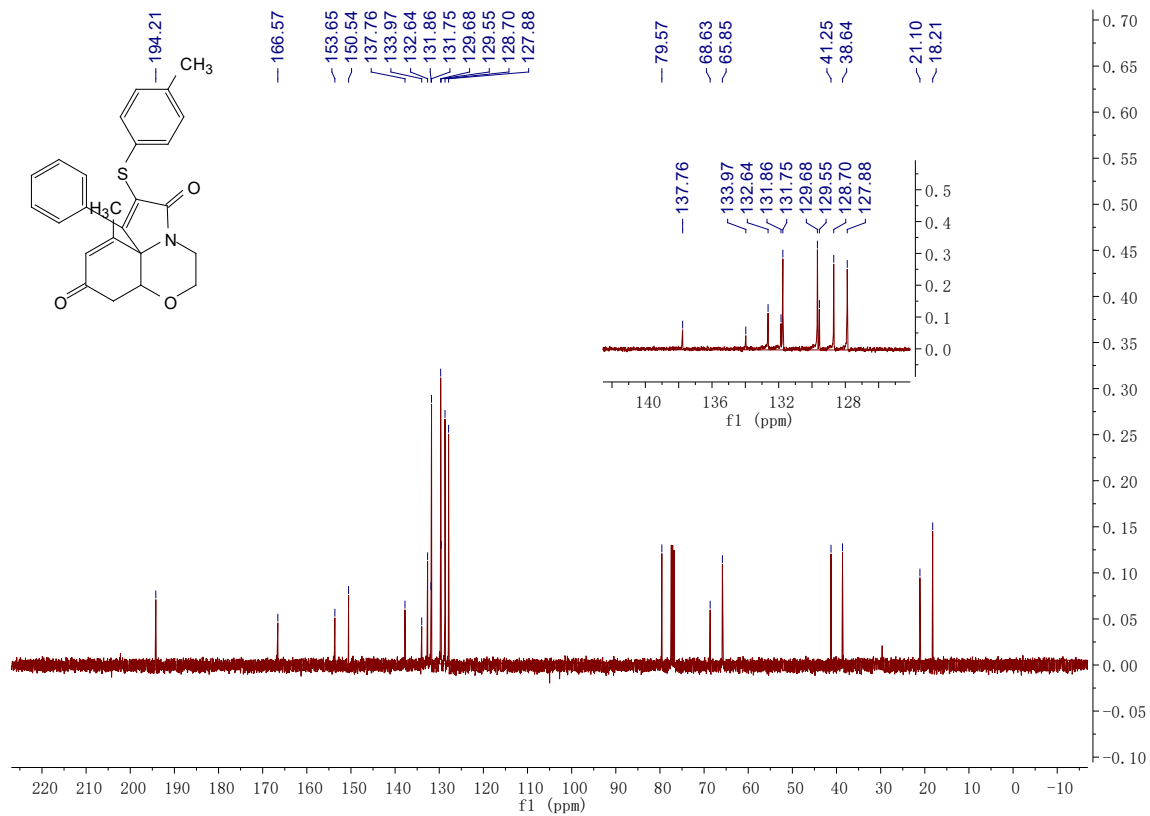


Figure S19 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3j**

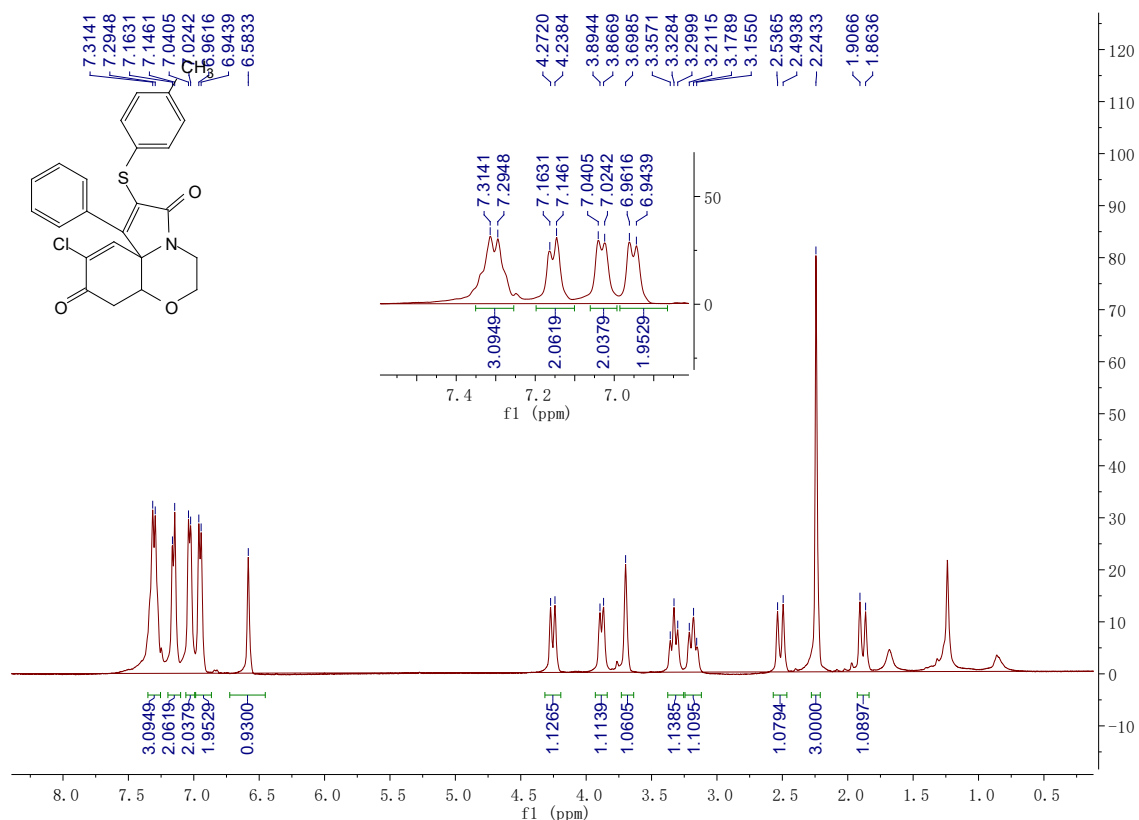


Figure S20 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3j**

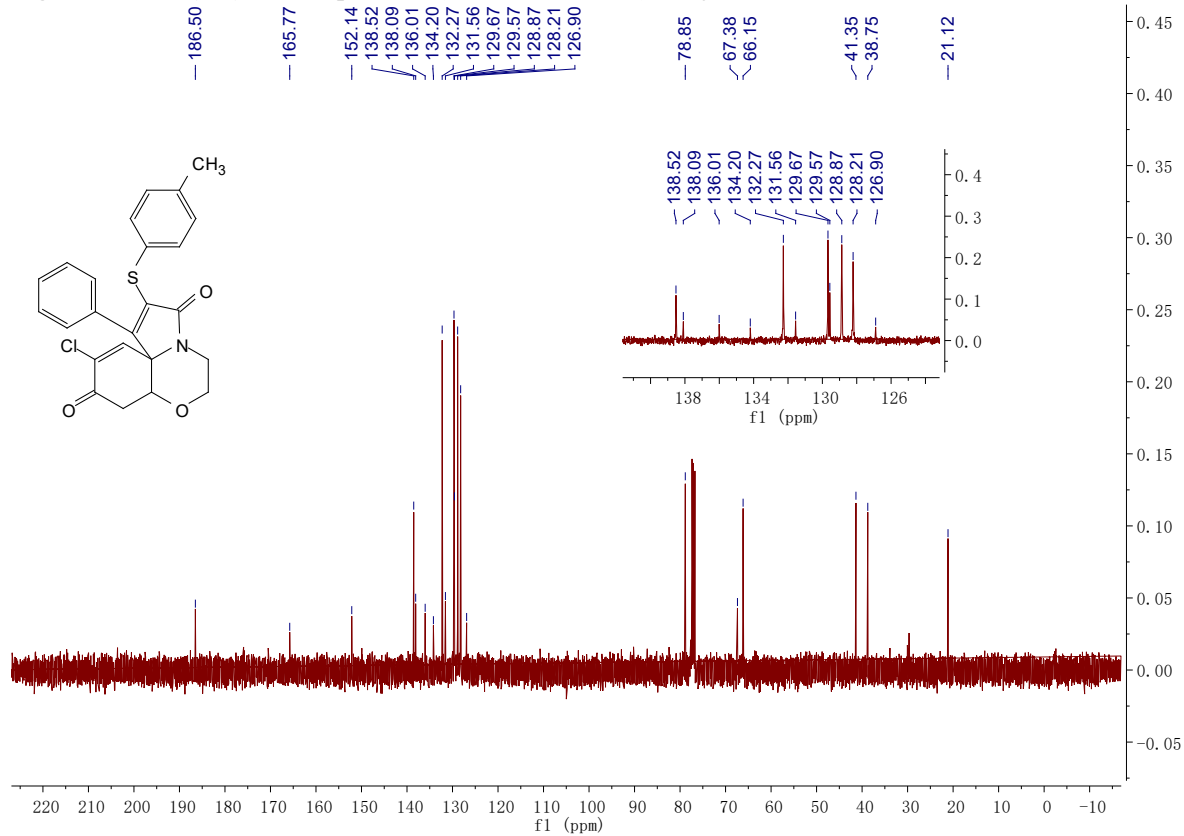


Figure S21 ¹H-NMR spectrum (400 MHz, CDCl₃) of **3k**

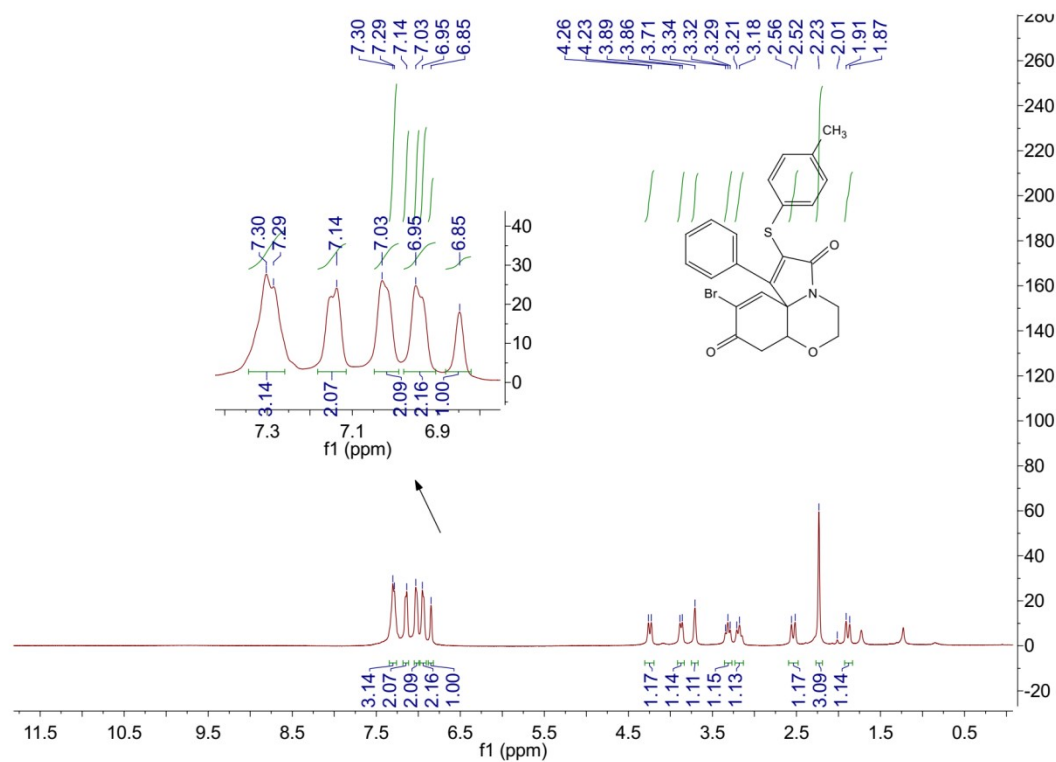


Figure S22 ¹³C{¹H}-NMR spectrum (100 MHz, CDCl₃) of **3k**

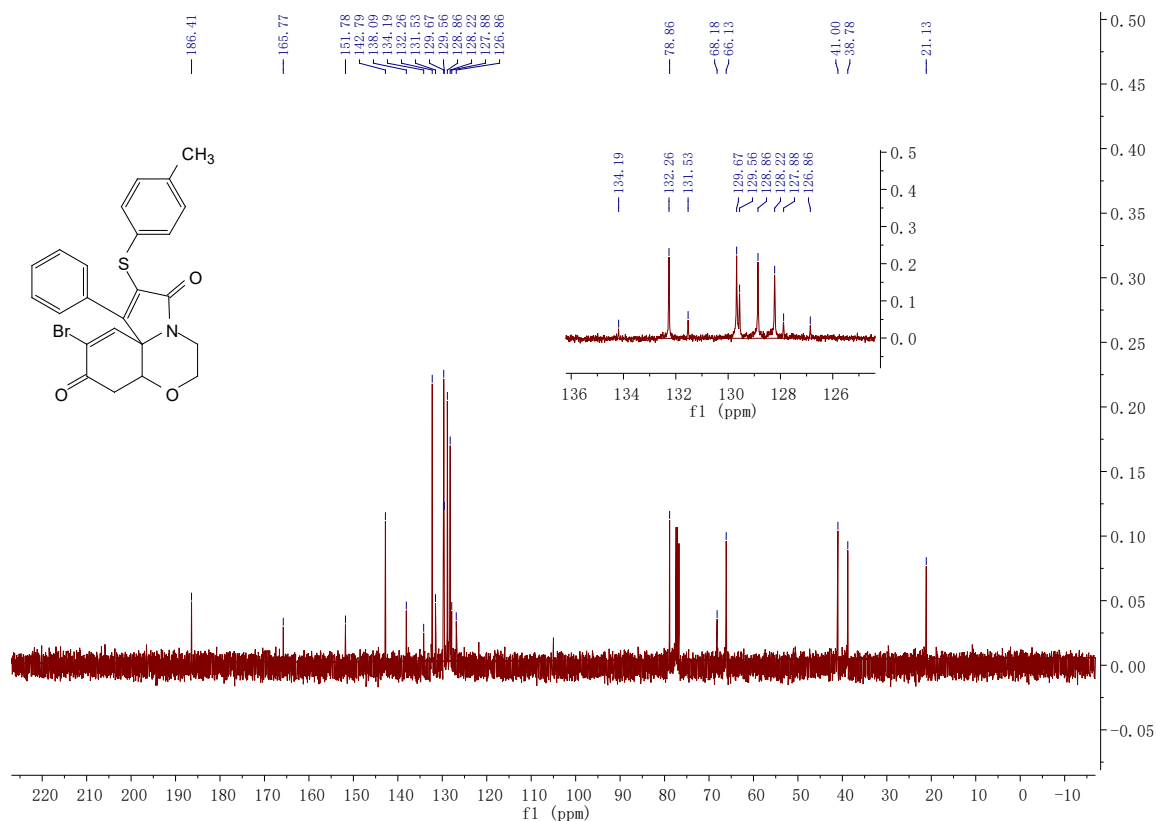


Figure S23 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **31**

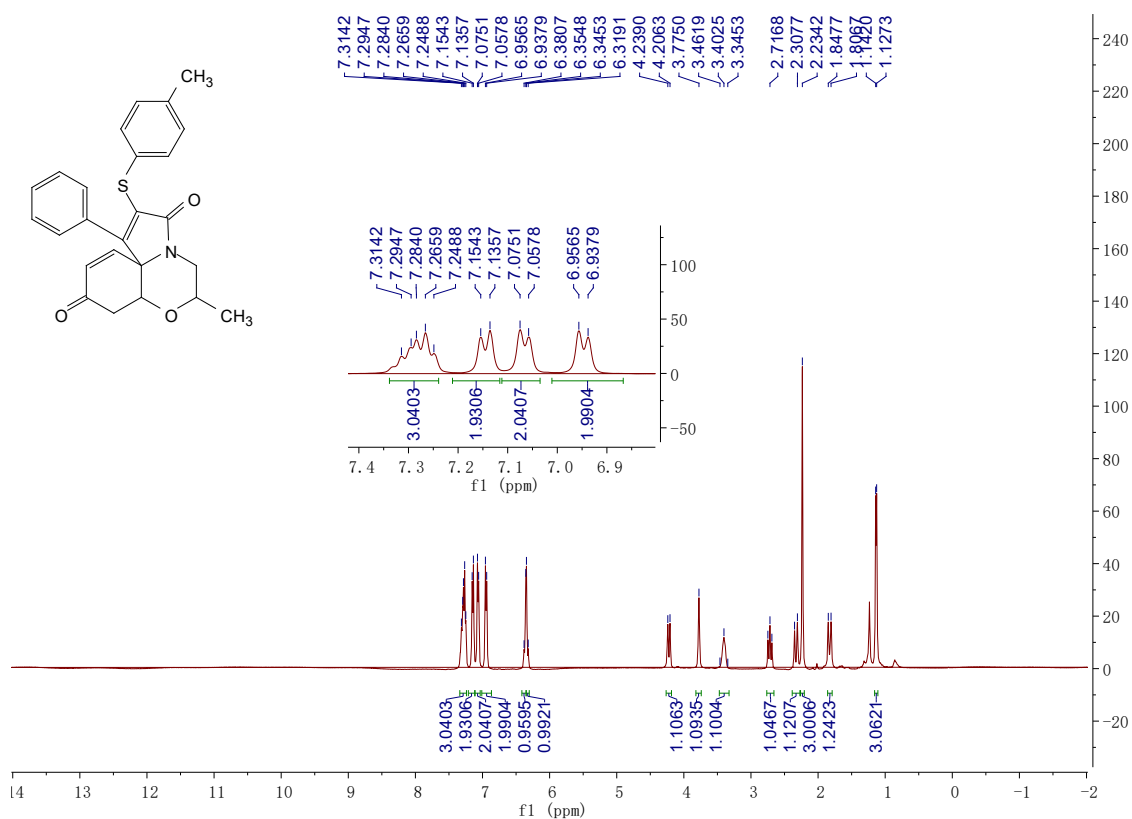


Figure S24 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **31**

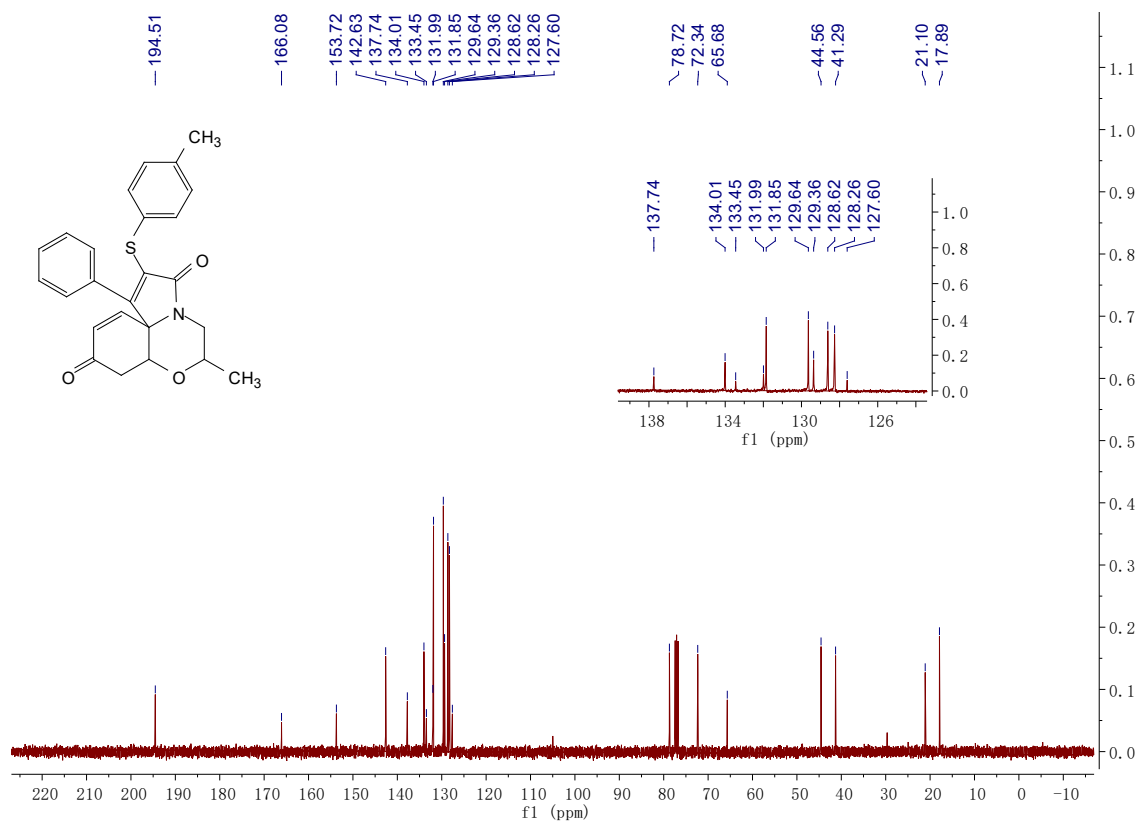


Figure S25 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3m**

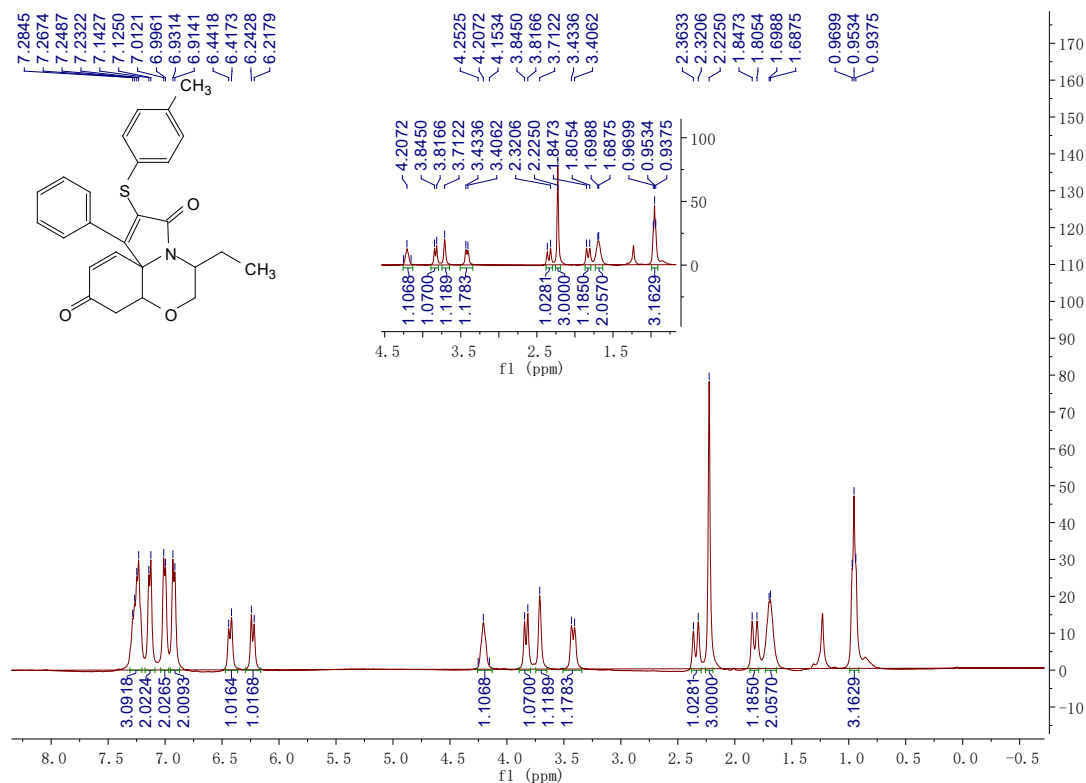


Figure S26 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3m**

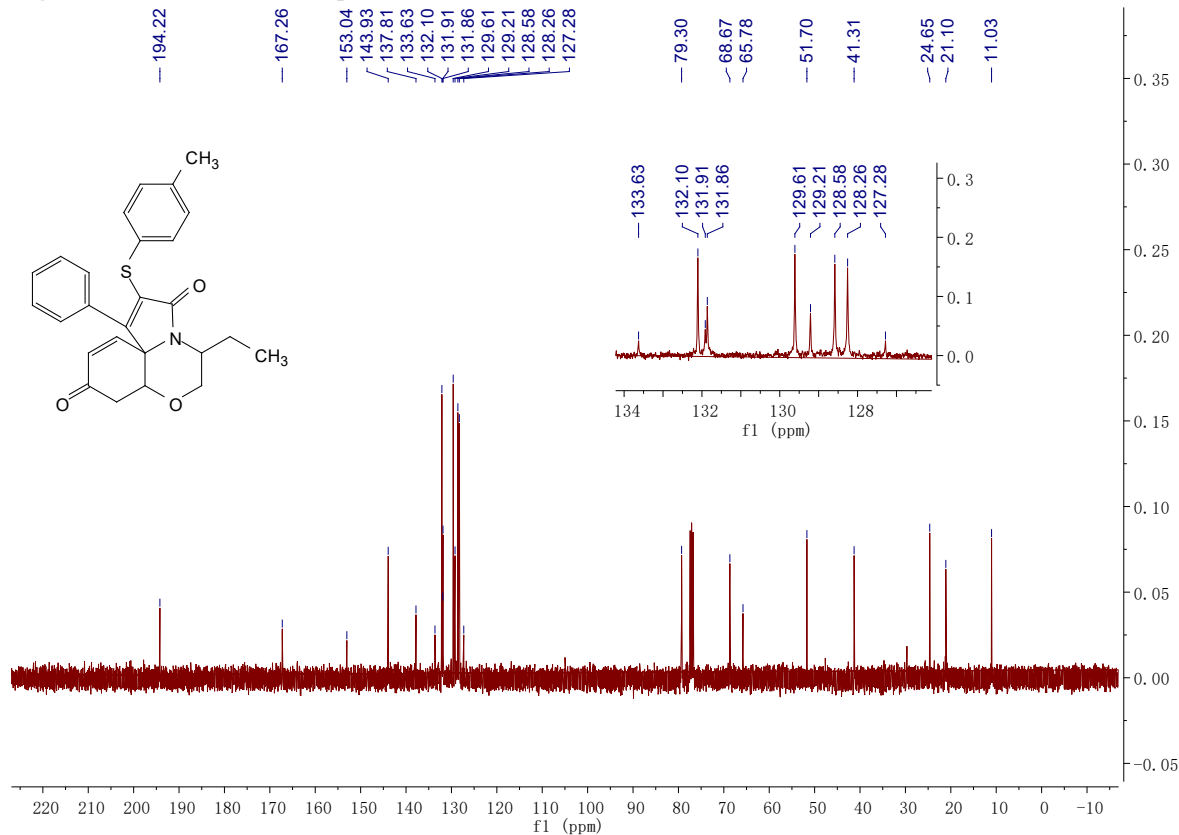


Figure S27 ¹H-NMR spectrum (400 MHz, CDCl₃) of **3n**

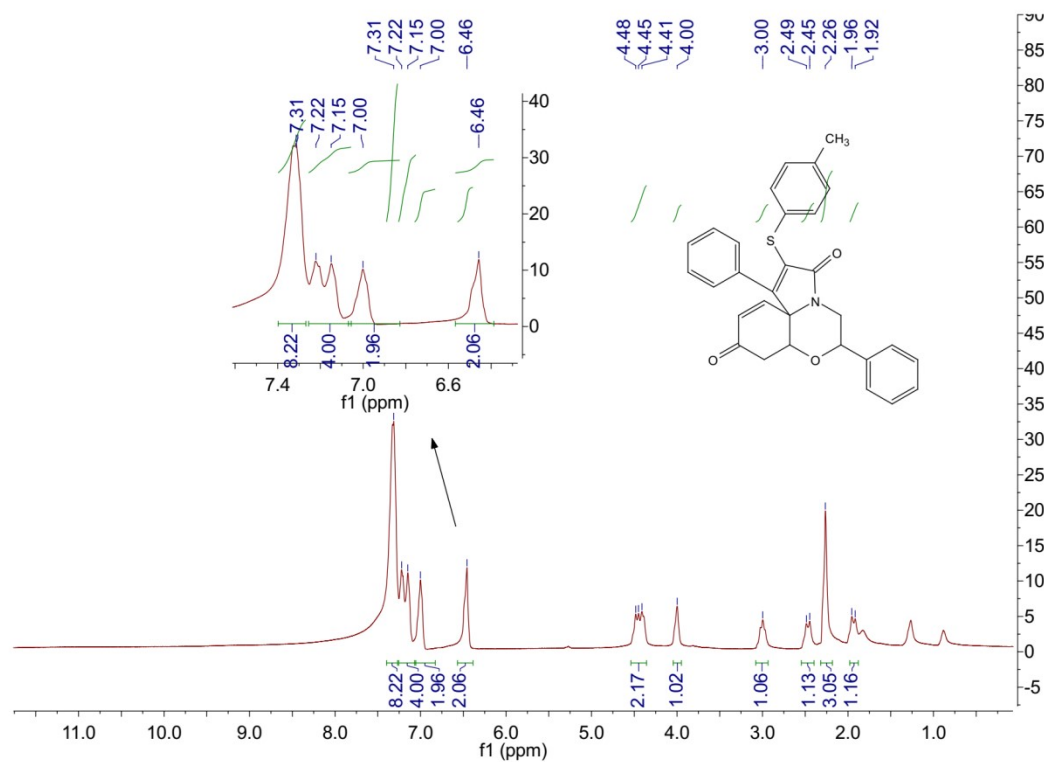


Figure S28 ¹³C{¹H}-NMR spectrum (100 MHz, CDCl₃) of **3n**

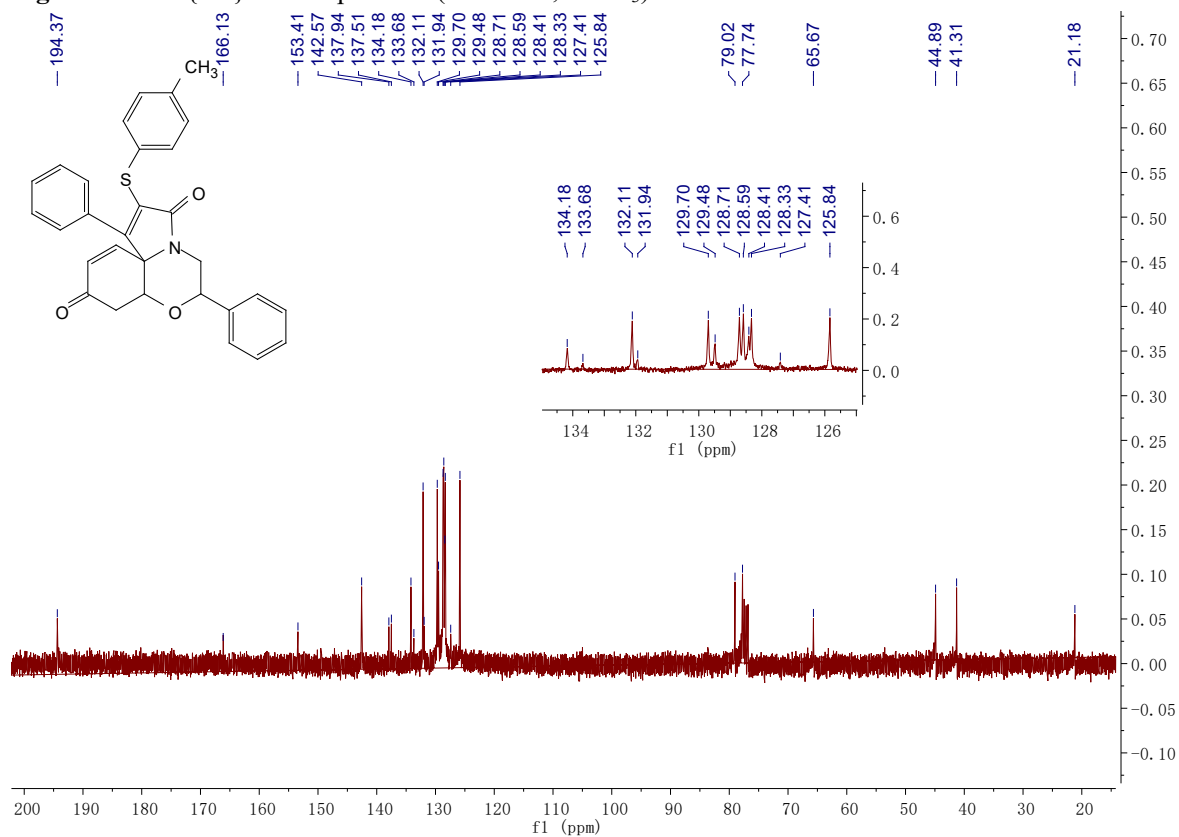


Figure S29 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3o**

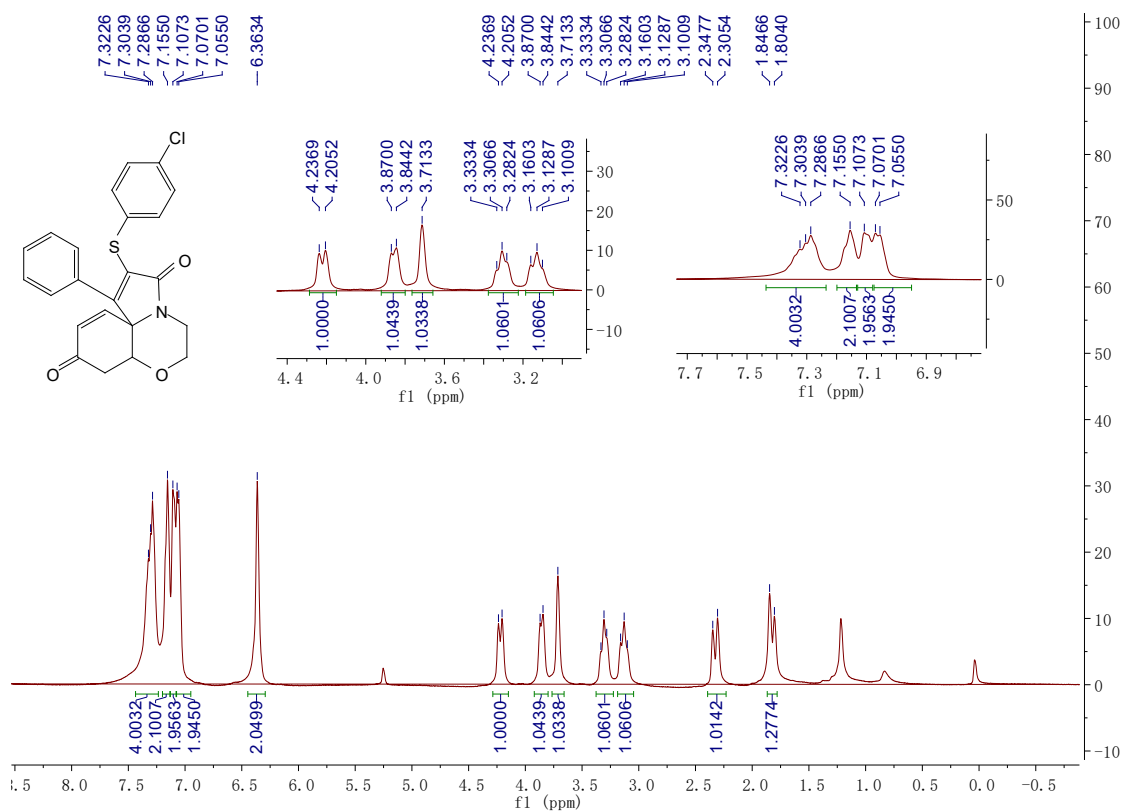


Figure S30 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3o**

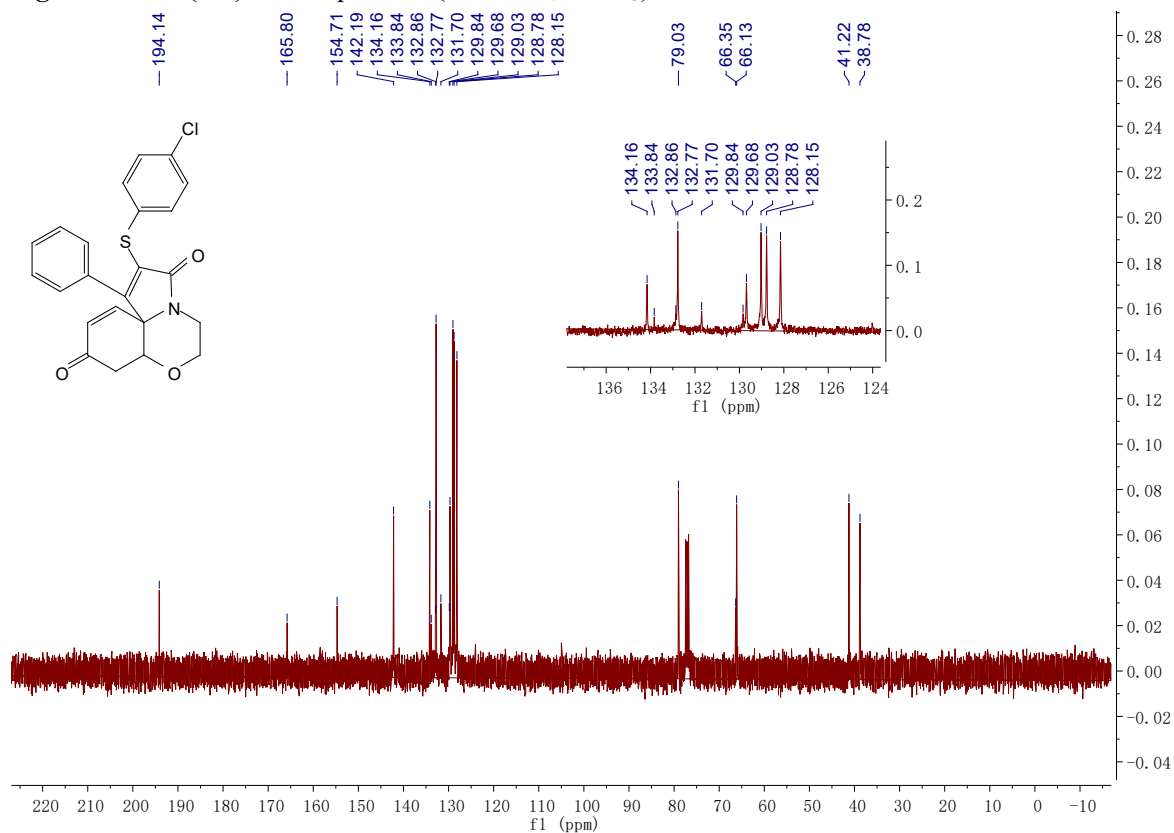


Figure S31 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3p**

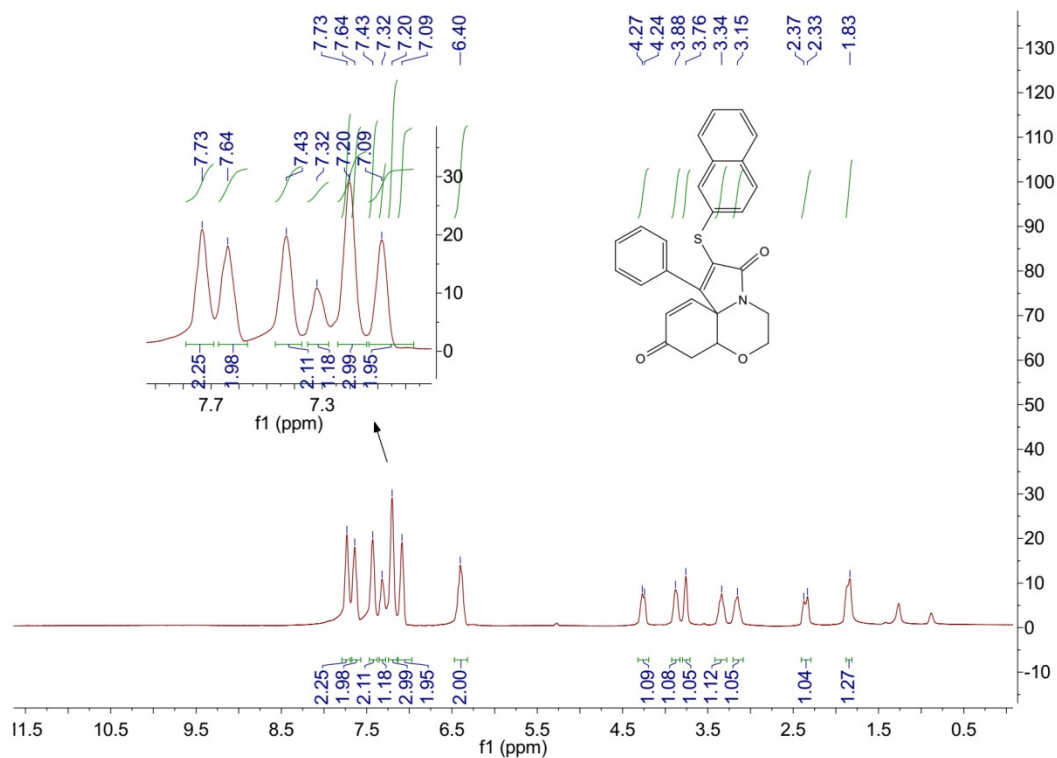


Figure S32 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3p**

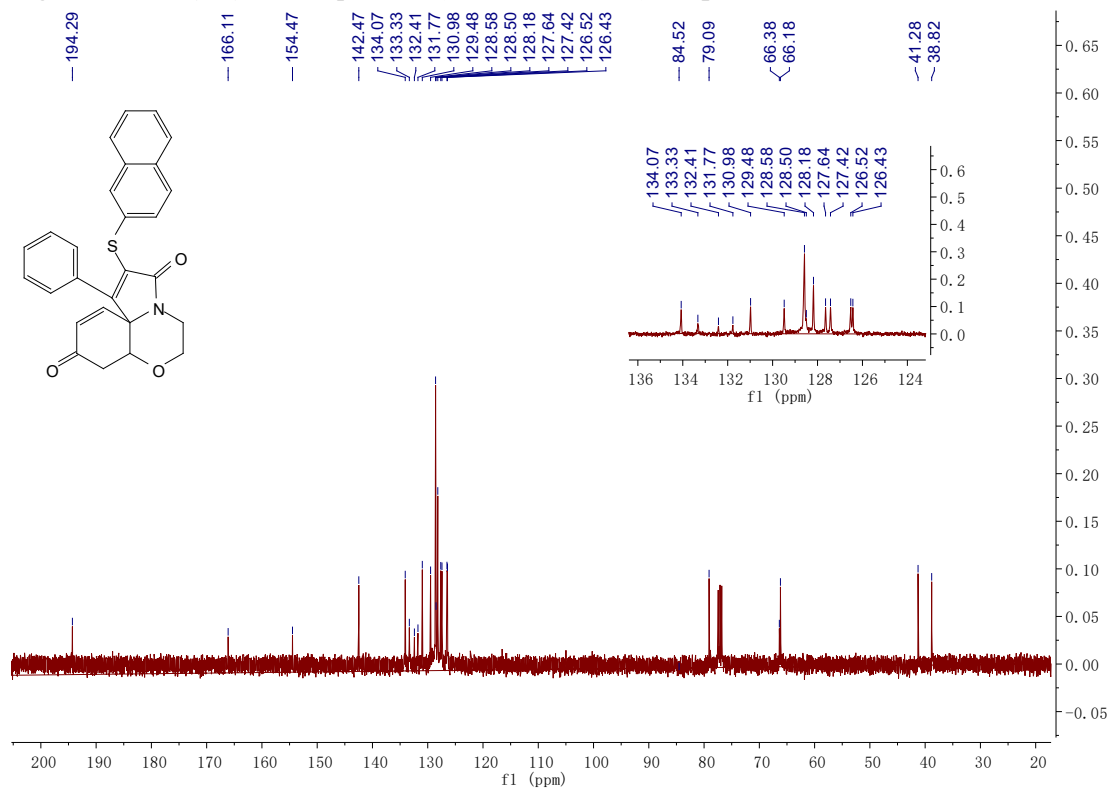


Figure S33 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3q**

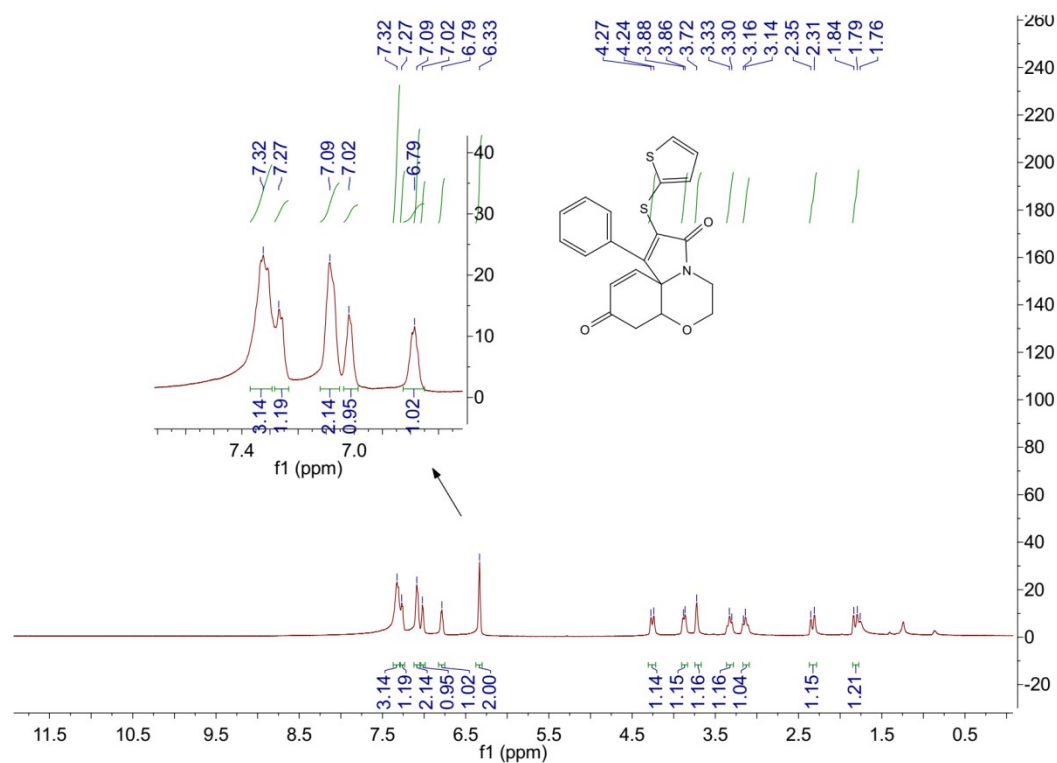


Figure S34 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3q**

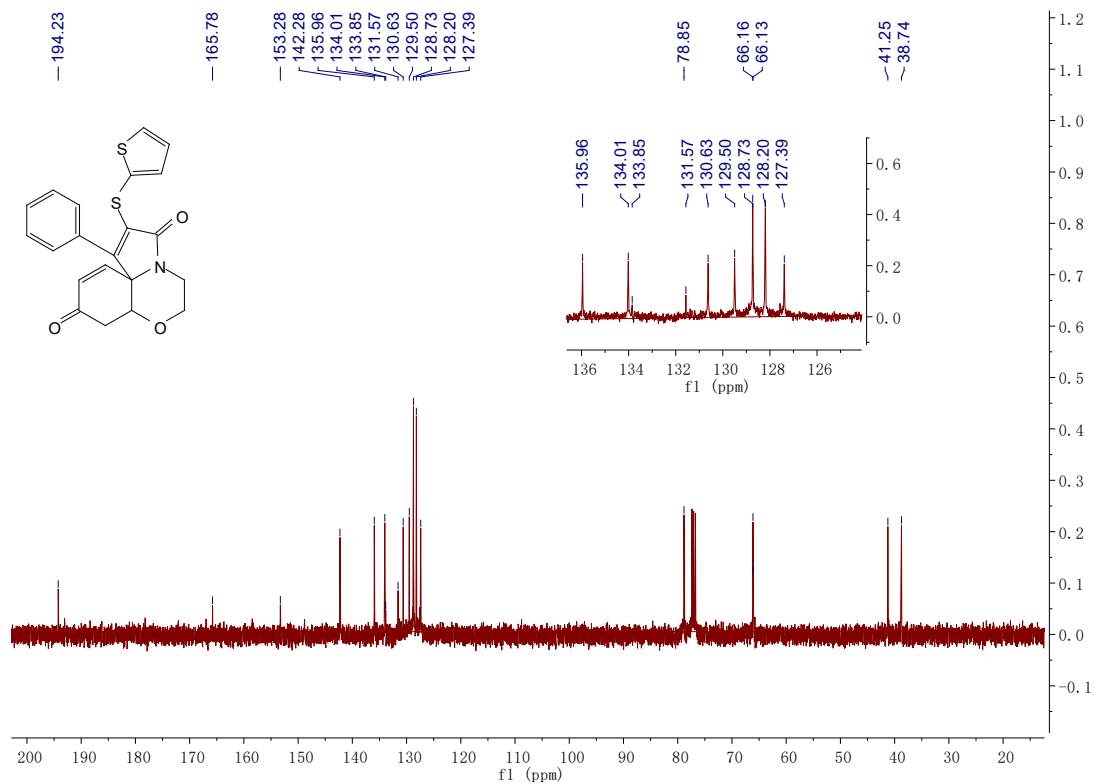


Figure S35 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3r**

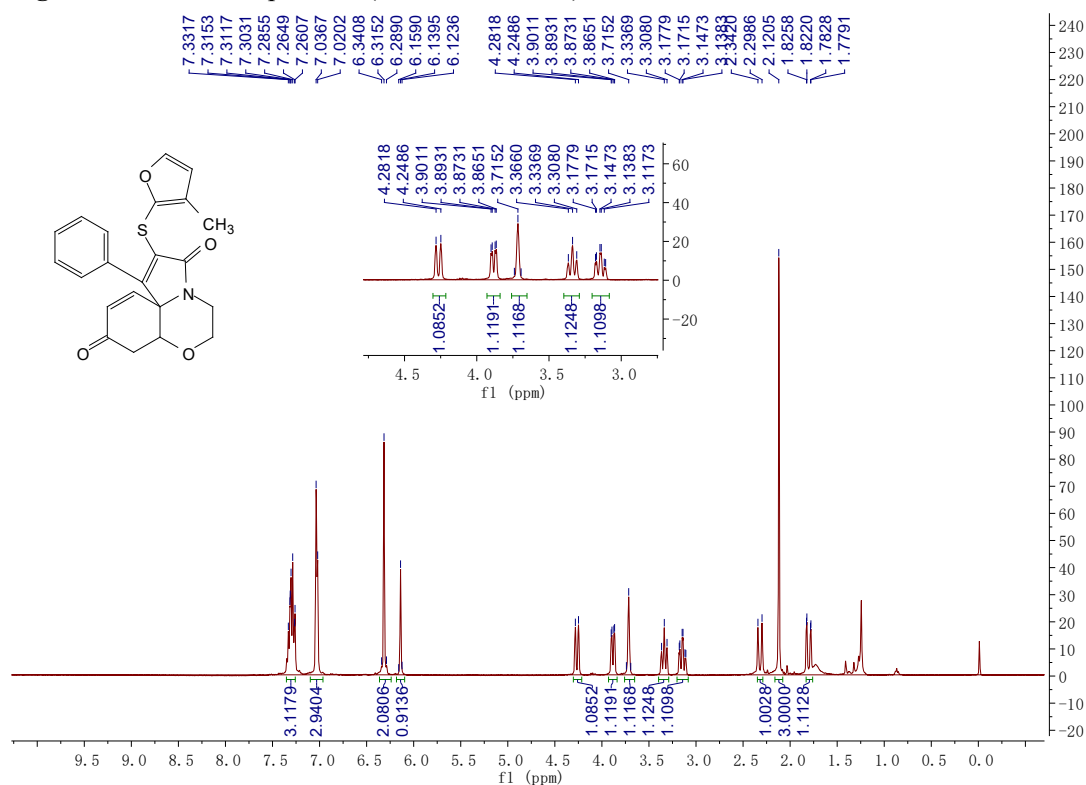


Figure S36 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3r**

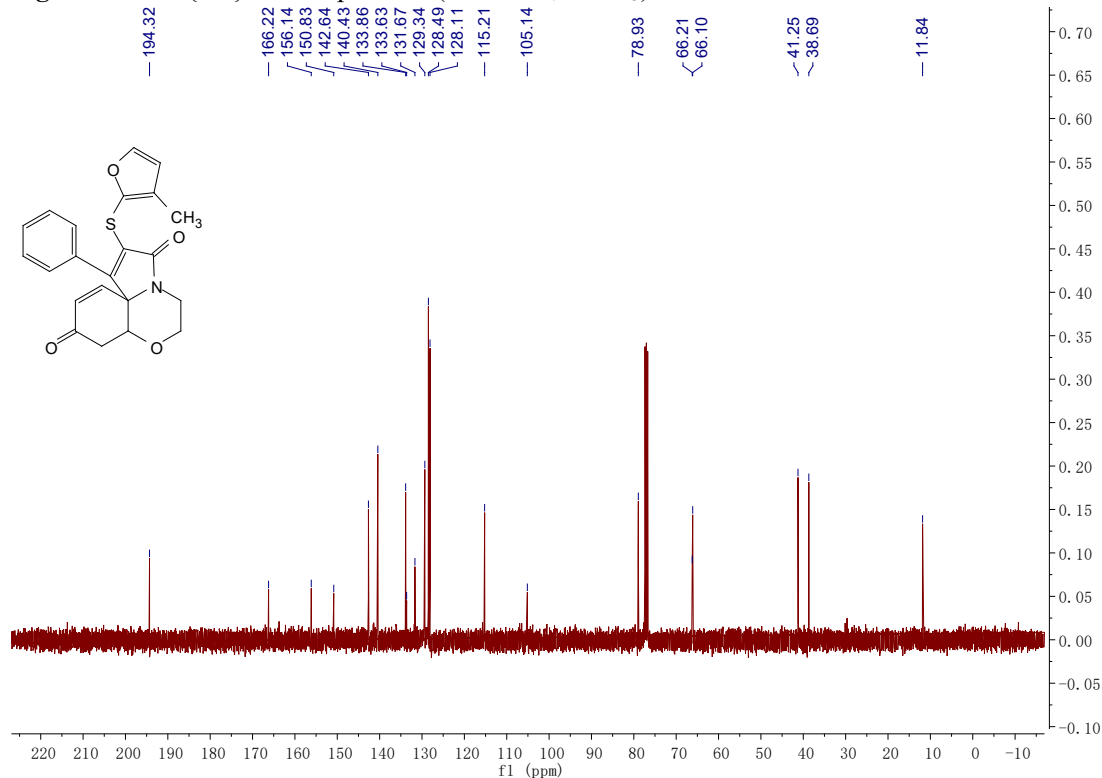


Figure S37 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3s**

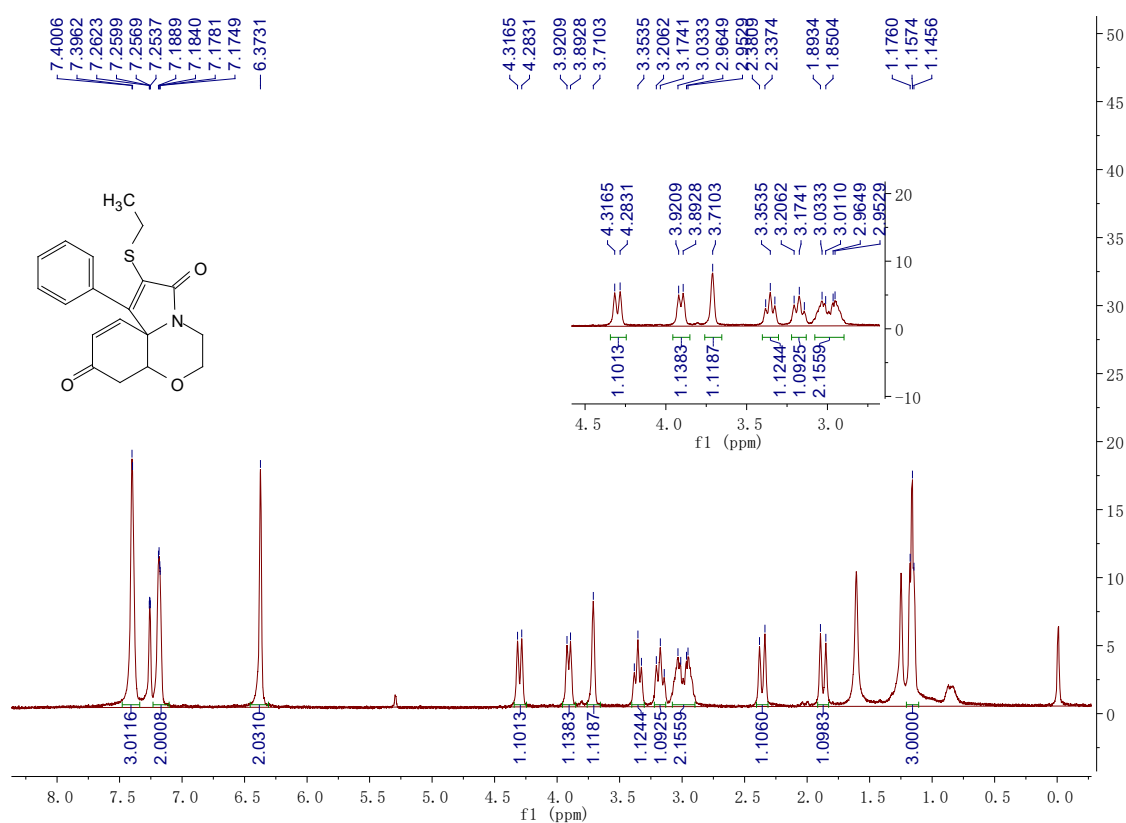


Figure S38 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3s**

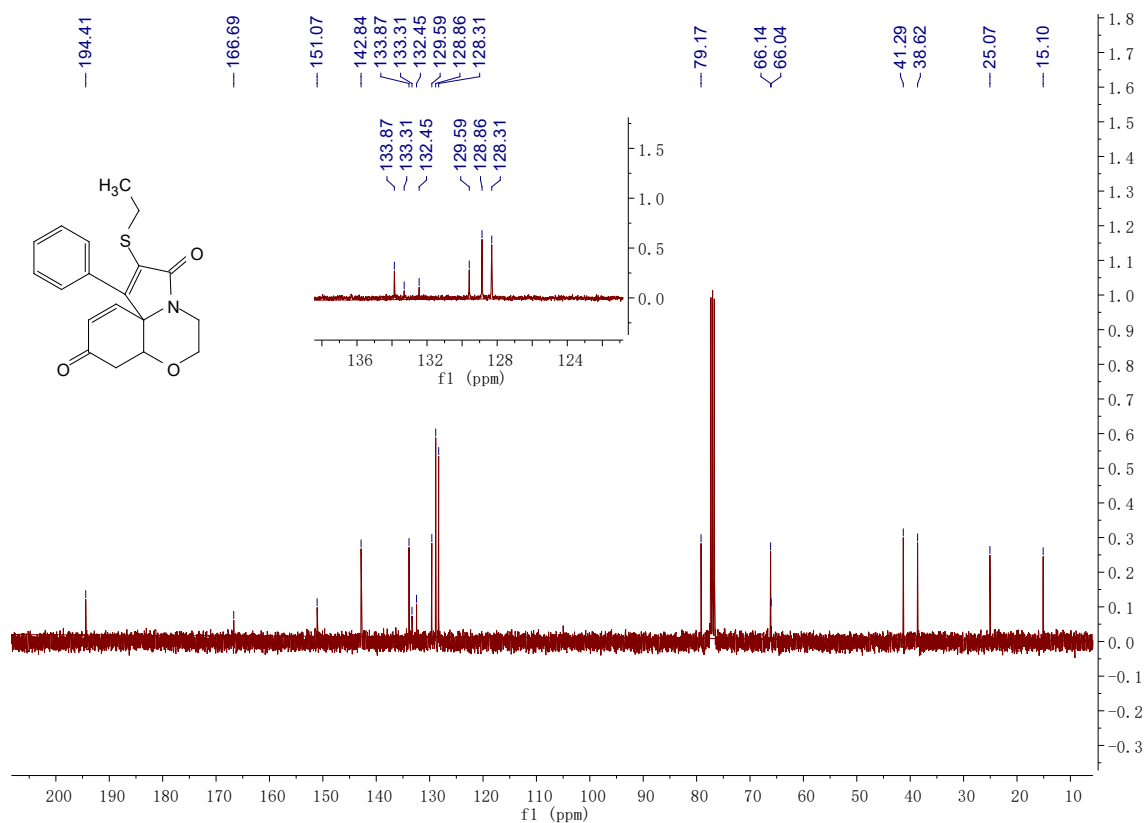


Figure S39 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3t**

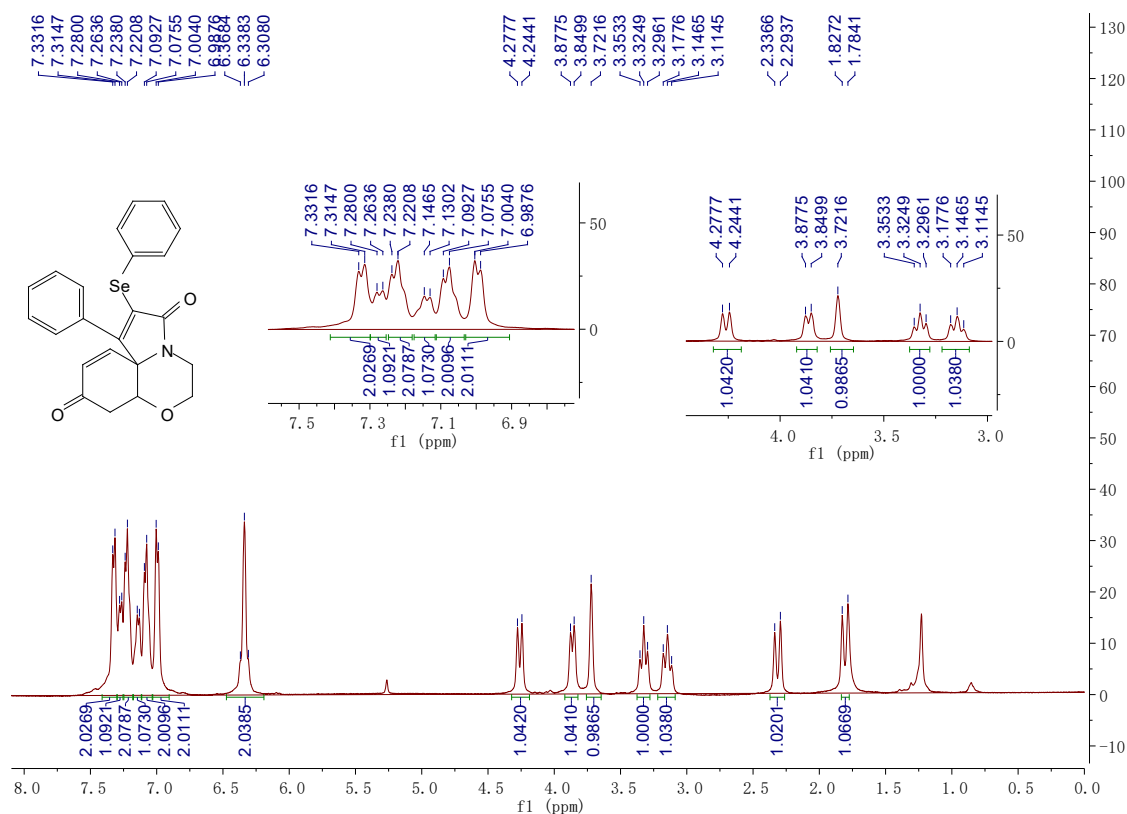


Figure S40 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3t**

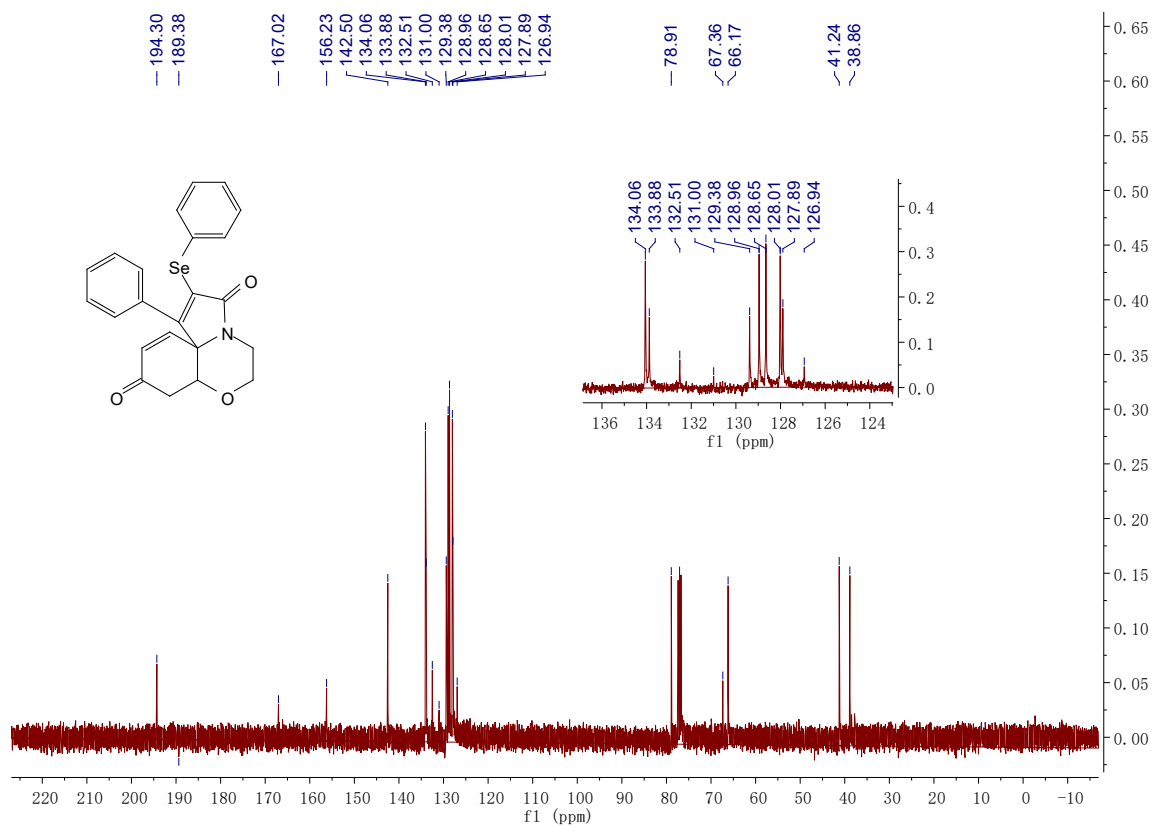


Figure S43 $^1\text{H-NMR}$ spectrum (400 MHz, CDCl_3) of **3v**

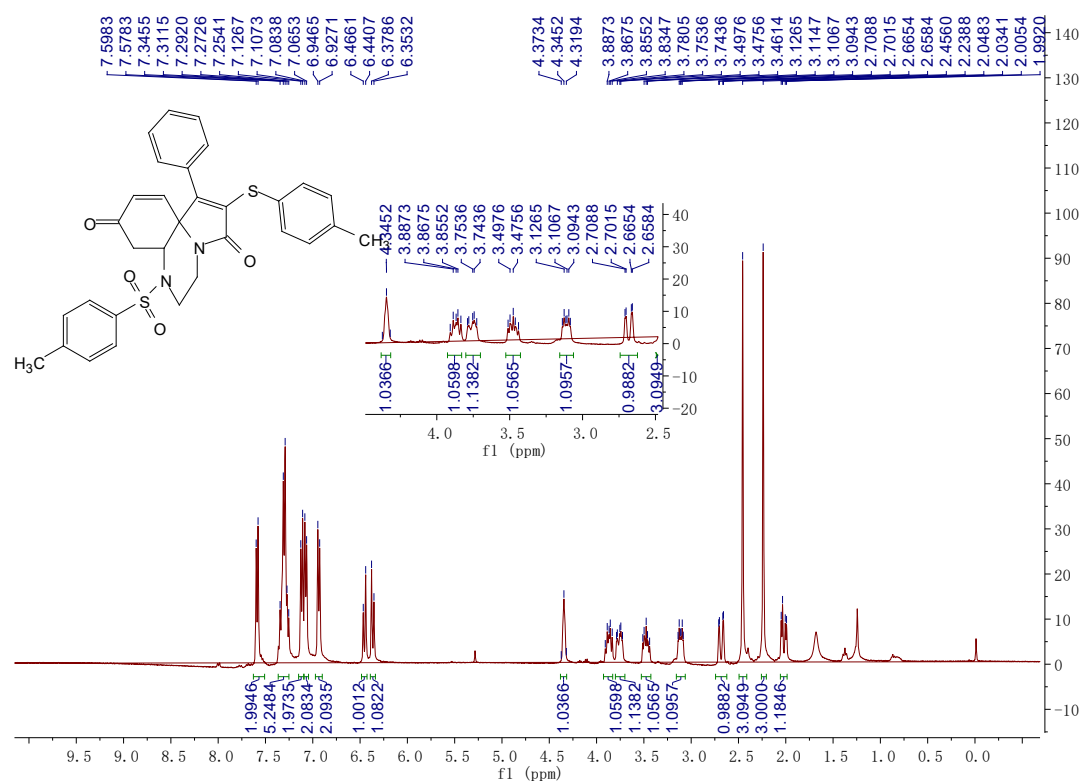


Figure S44 $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100 MHz, CDCl_3) of **3v**

