Synthesis and biological evaluation of dithiocarbamate esters of partenolide as potential anti-acute myelogenous leukemia agents

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SUPPLEMENTARY DATA

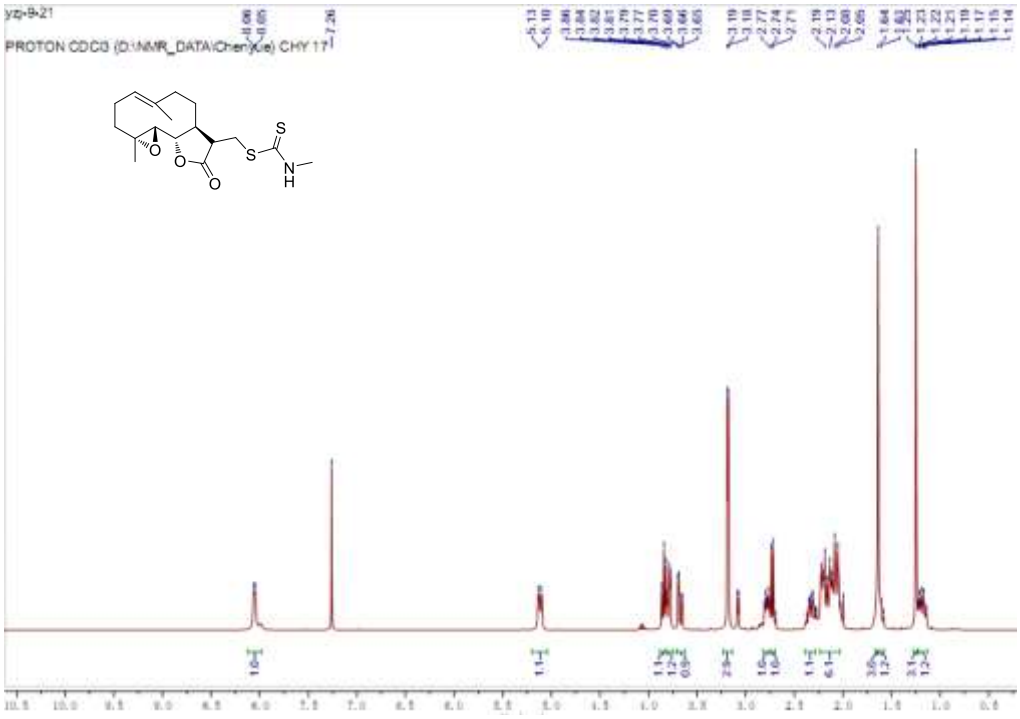
1. NMR spectra of compounds (compound 7a-7o, 8, 10, 11 and 12)·····S2

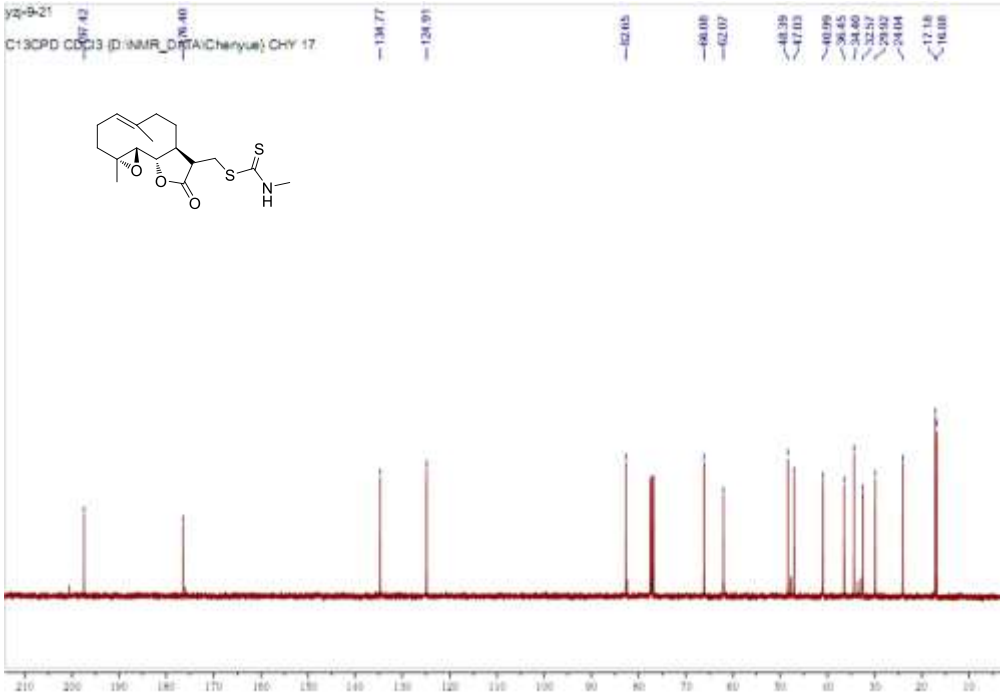
2. X-ray data of compound 7c·····S22

3. 2D NMR spectra of 7l·····S23

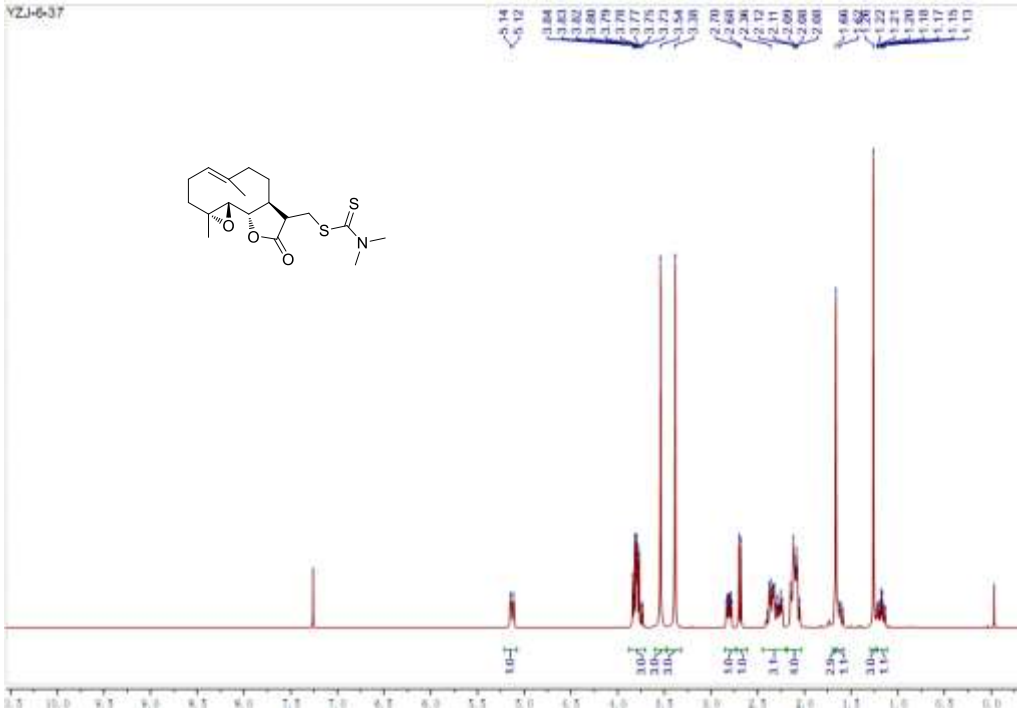
1. NMR spectra of compounds (compound 7a-7o, 8, 10, 11 and 12)

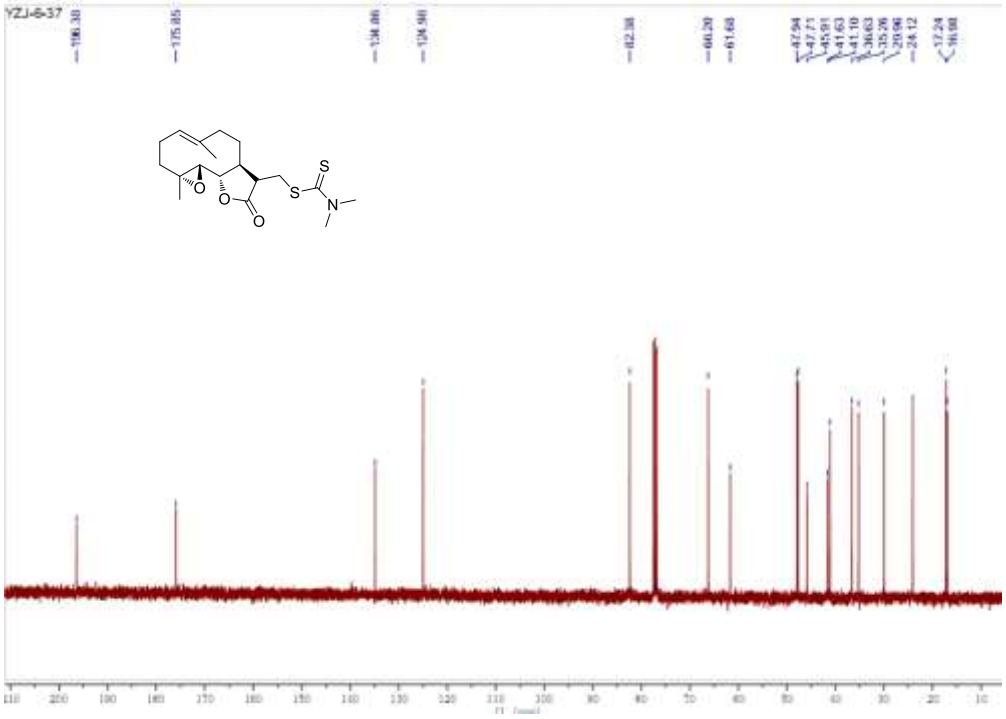
NMR spectra of **7a** in $CDCl_3$



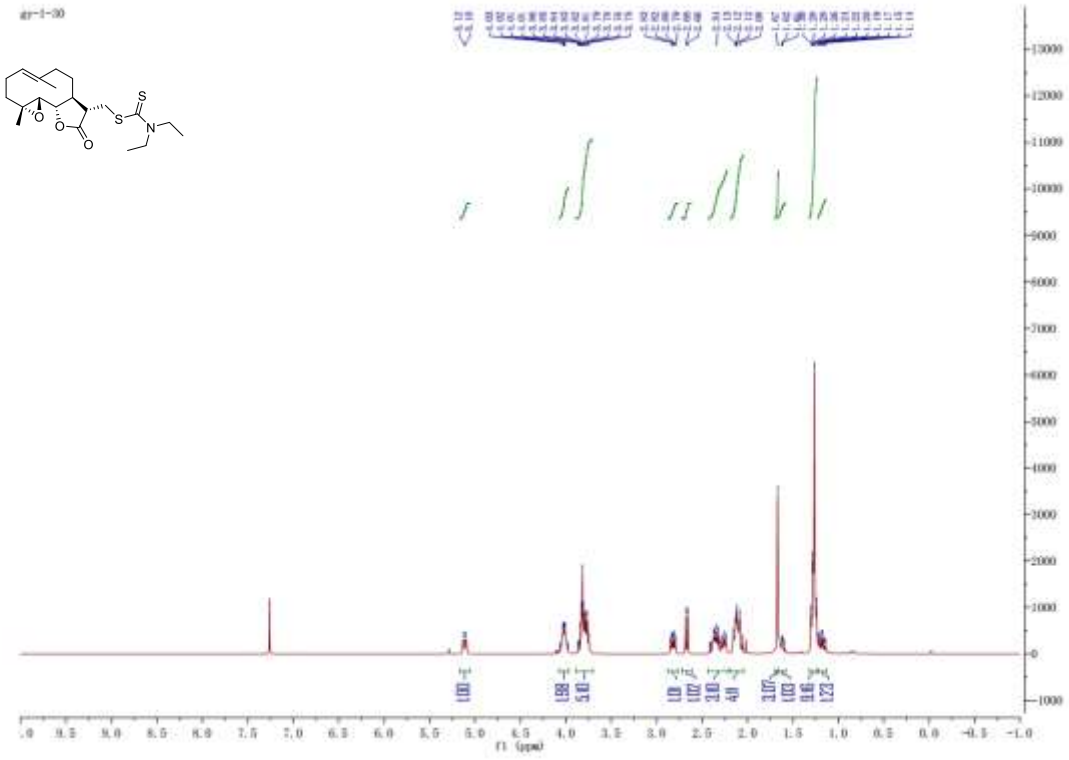


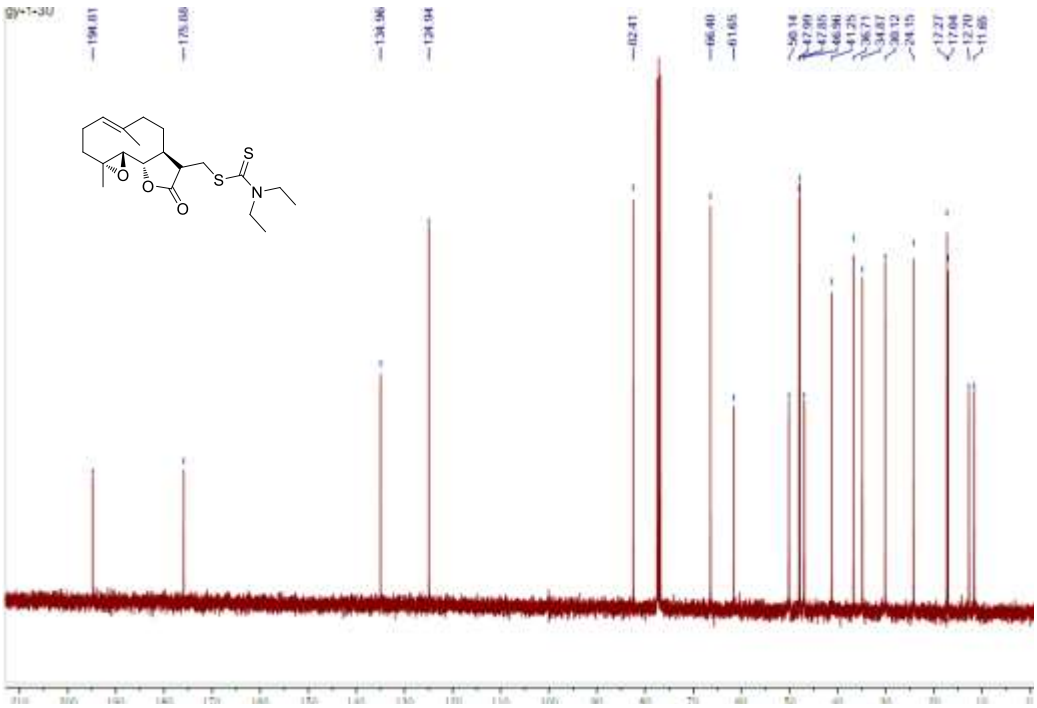
NMR spectra of **7b** in $CDCl_3$



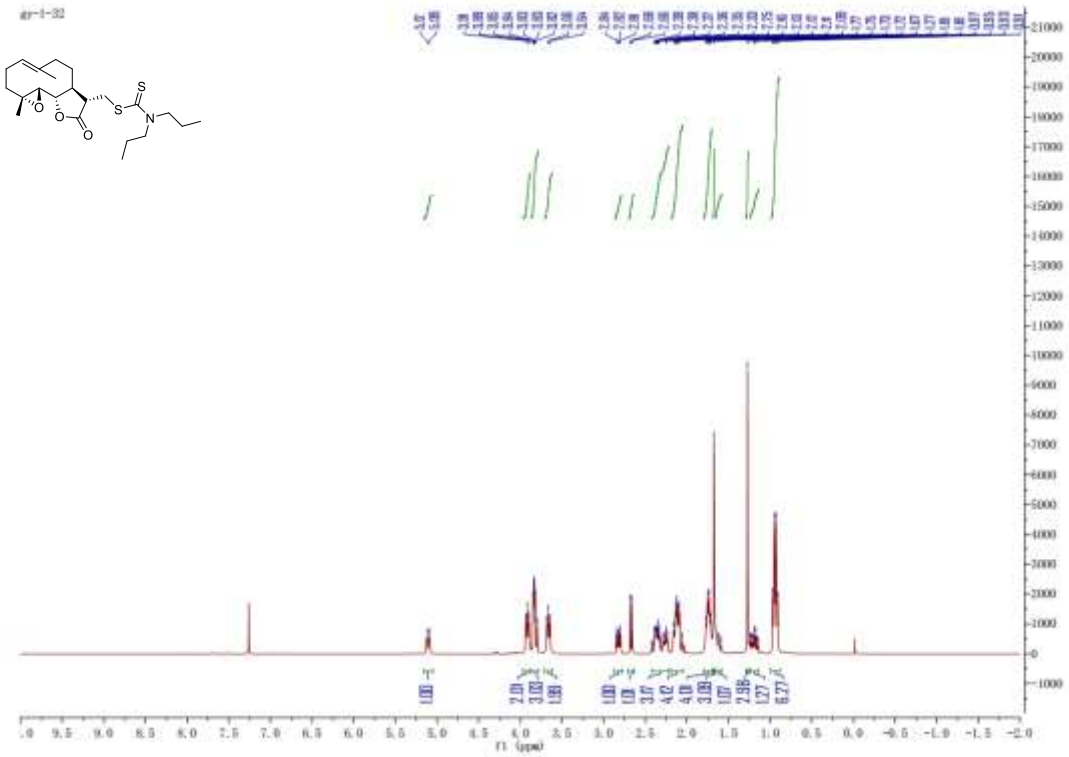


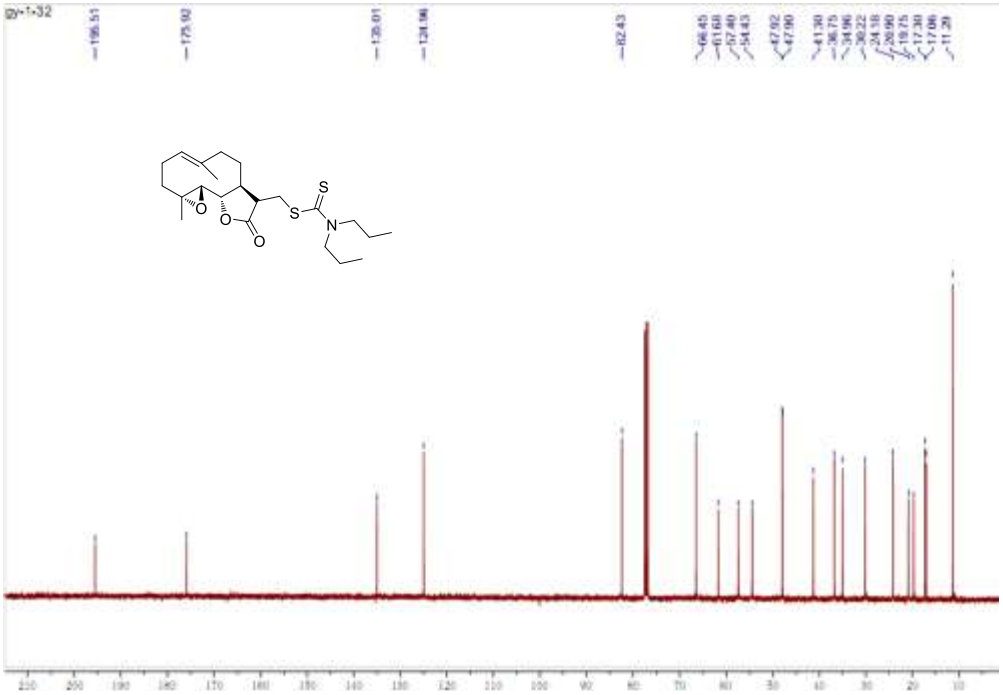
NMR spectra of **7c** in $CDCl_3$



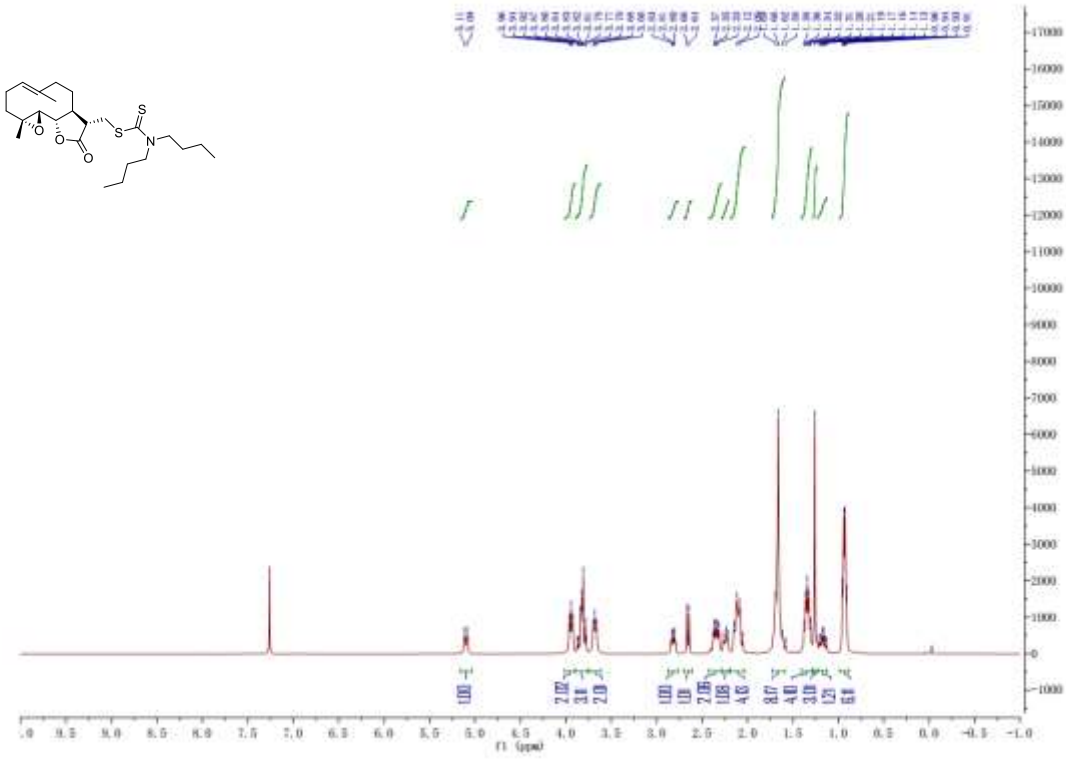


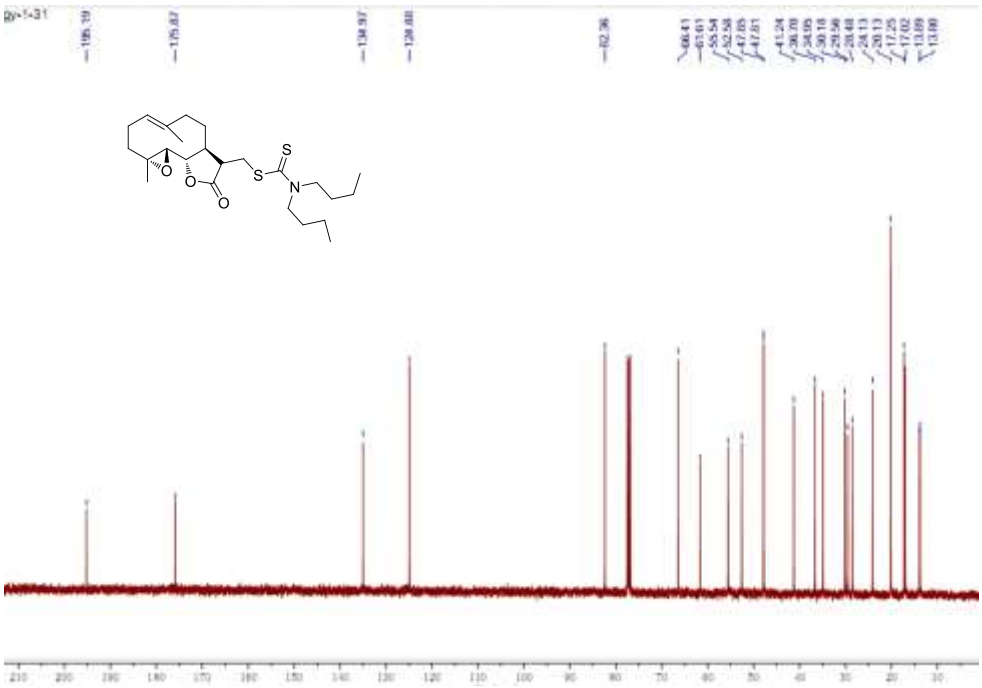
NMR spectra of **7d** in $CDCl_3$



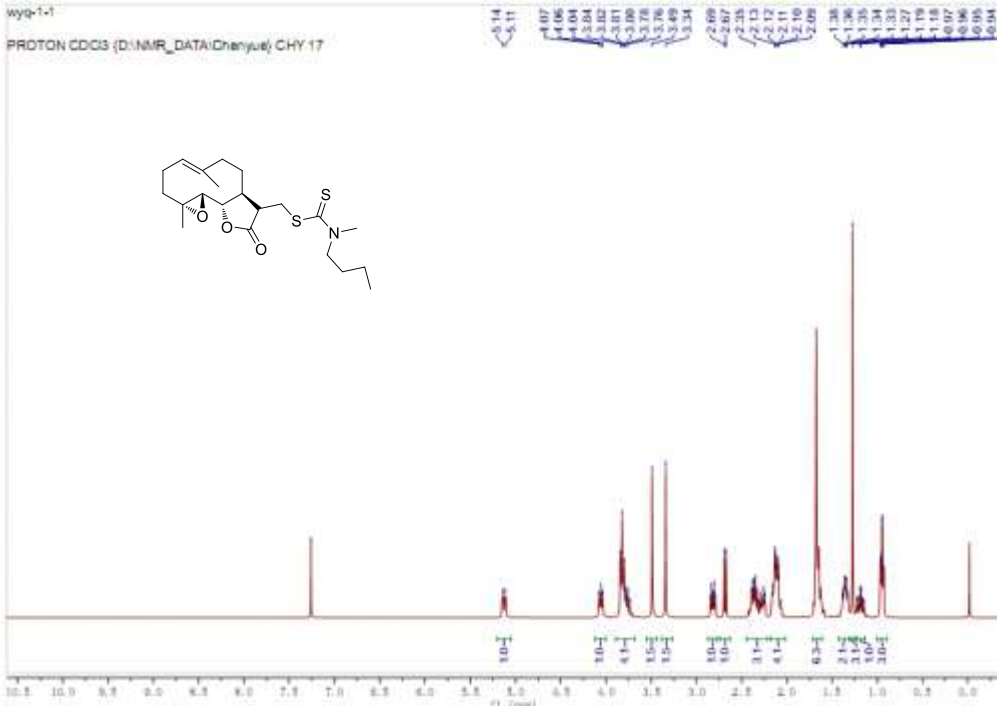


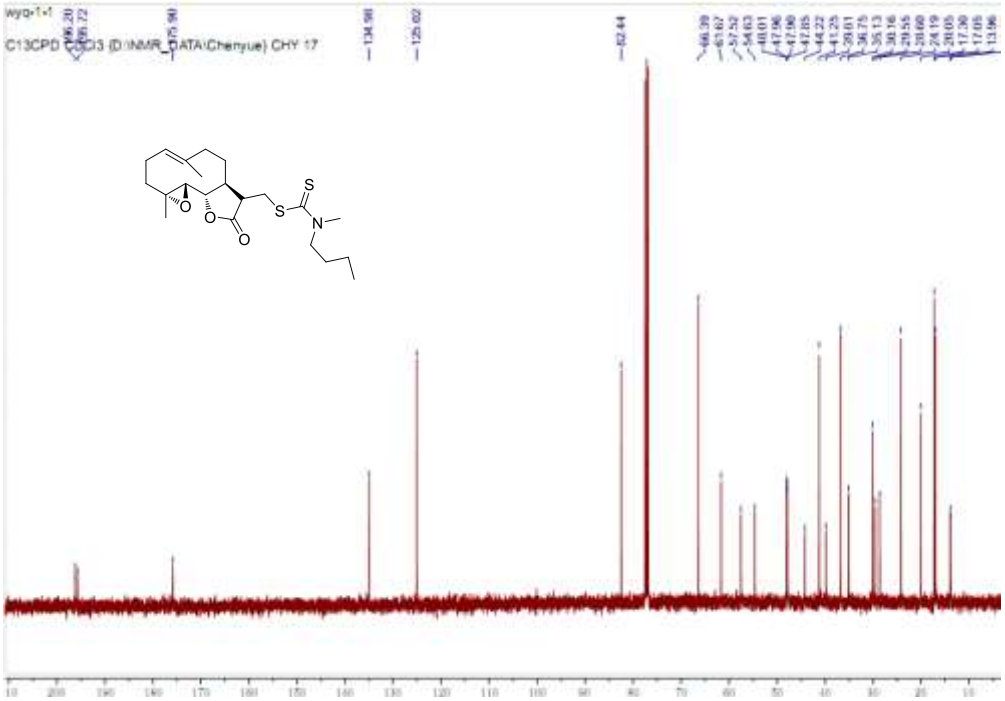
NMR spectra of **7e** in $CDCl_3$



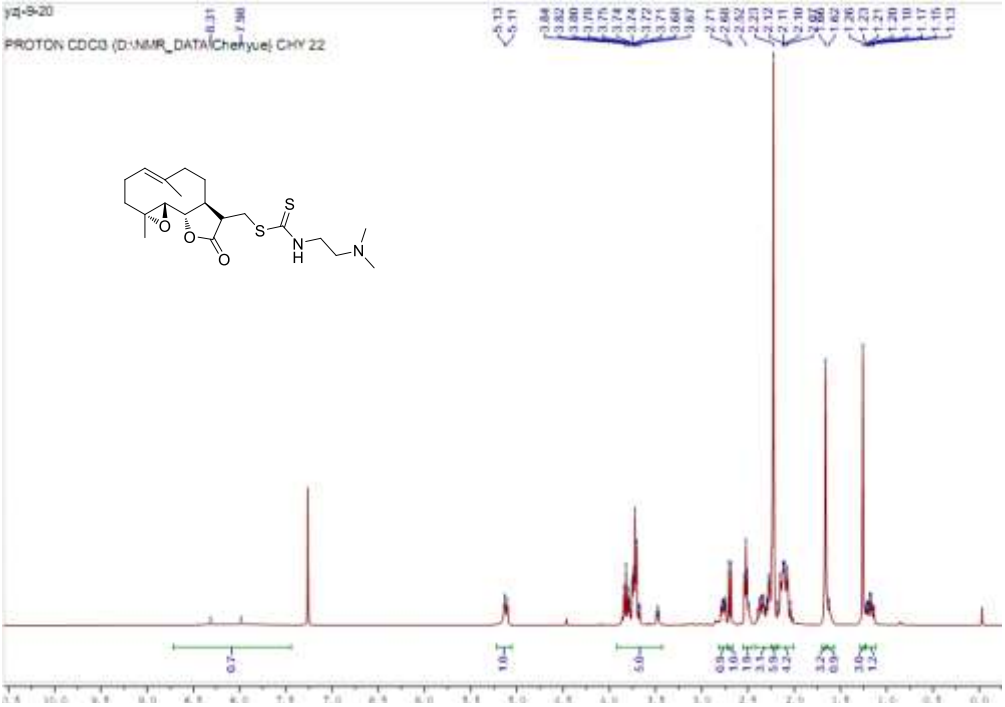


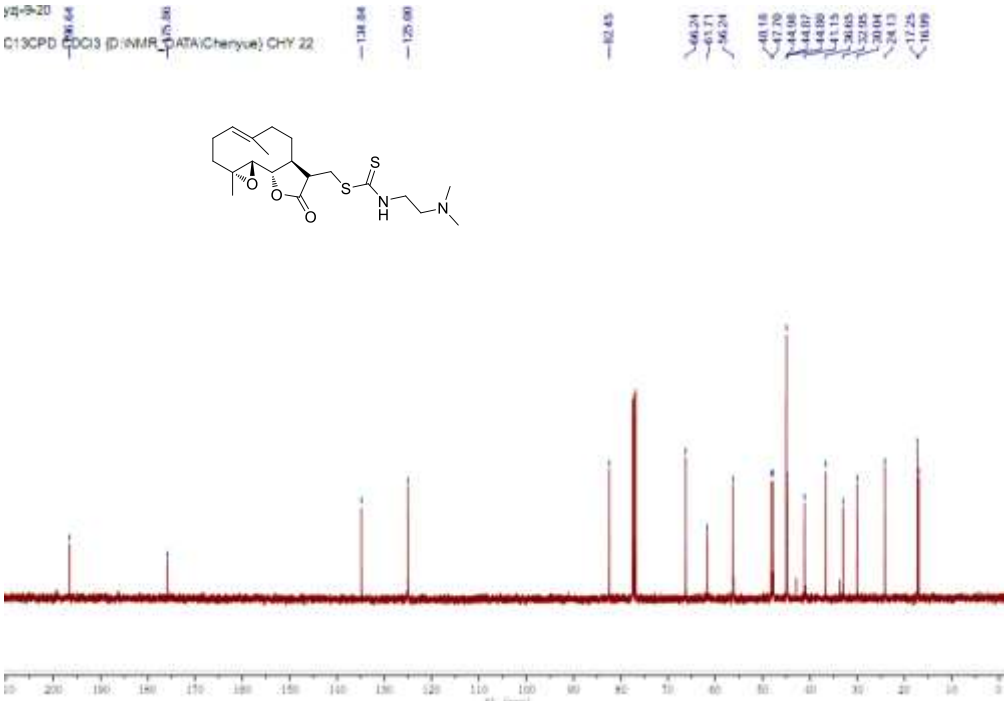
NMR spectra of **7f** in $CDCl_3$



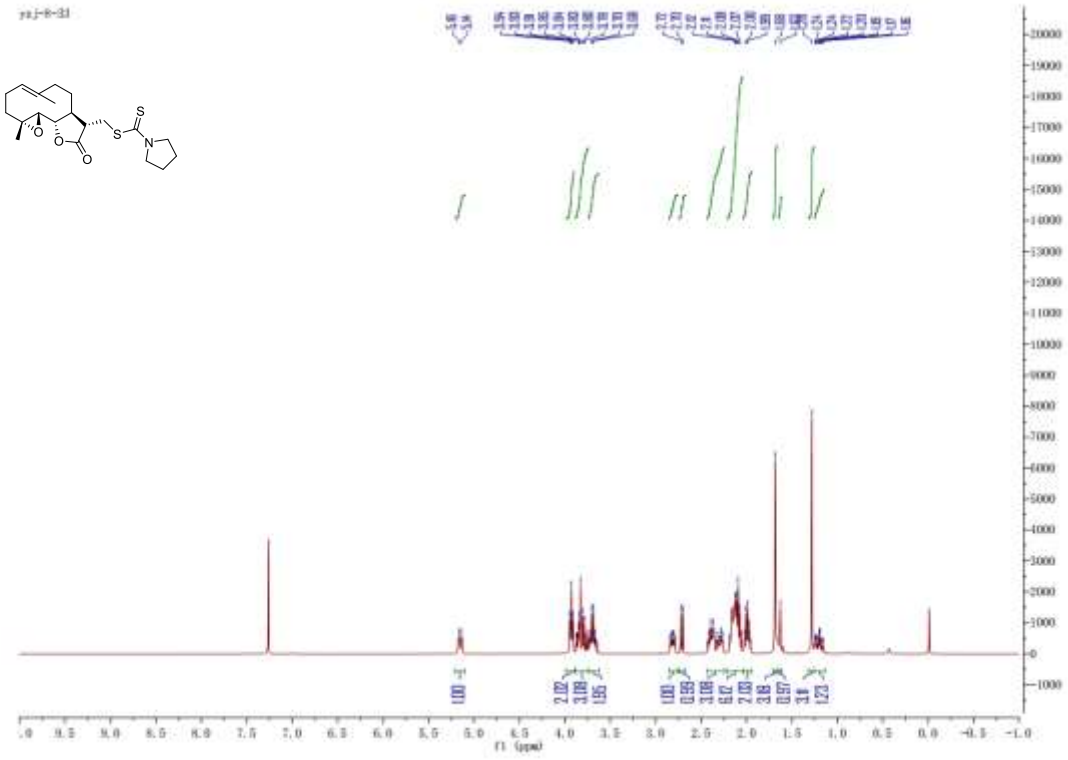


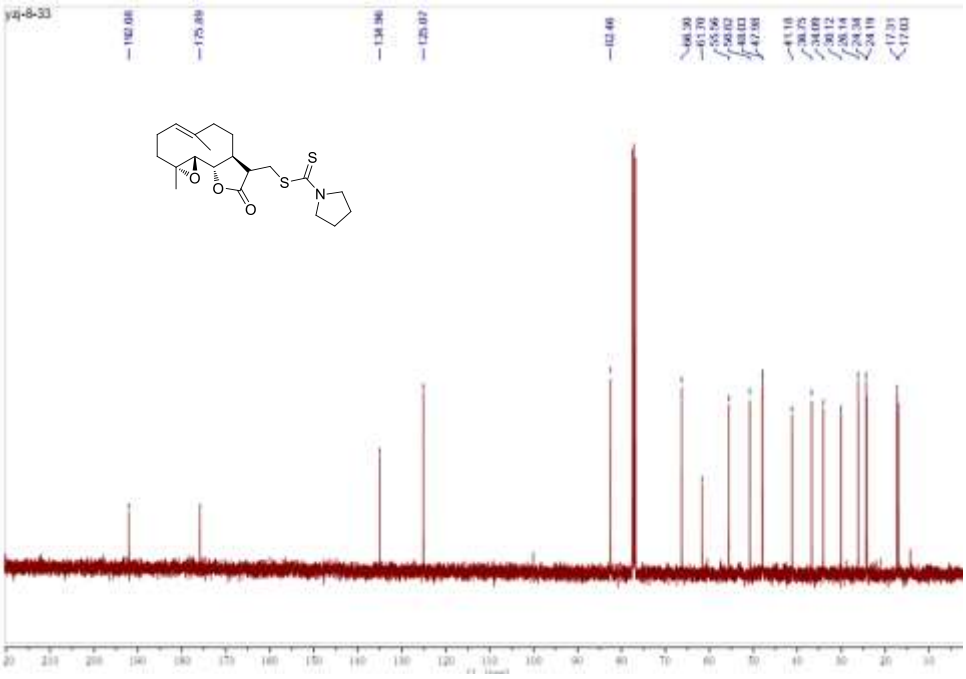
NMR spectra of **7g** in $CDCl_3$



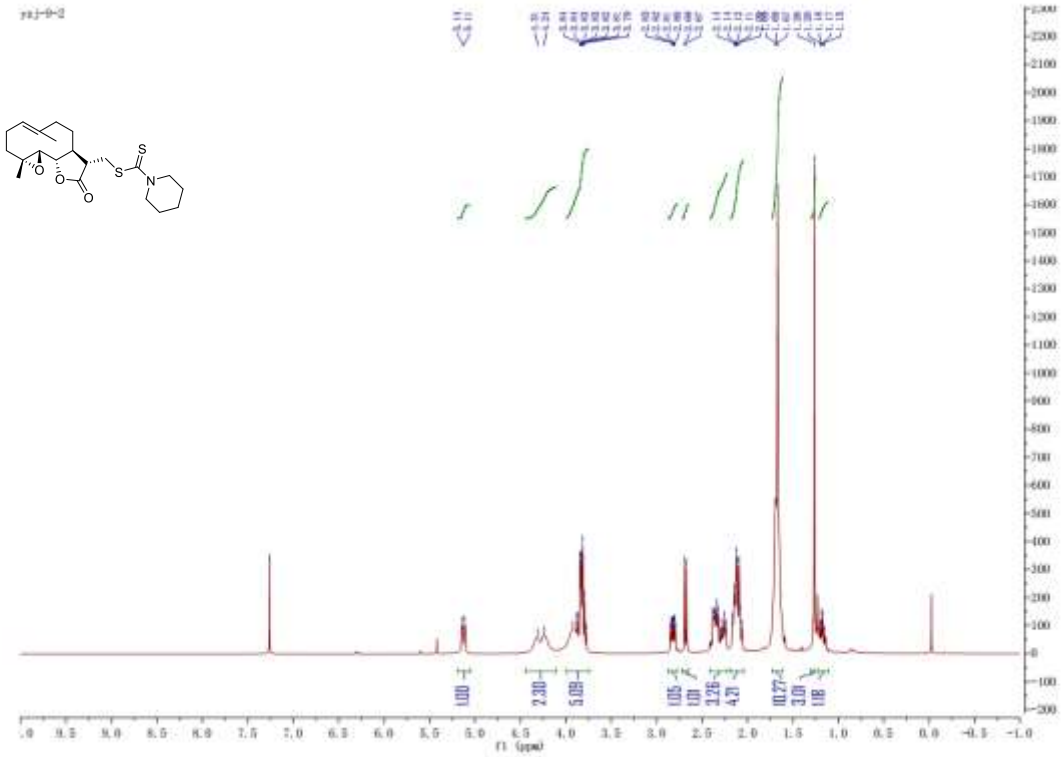


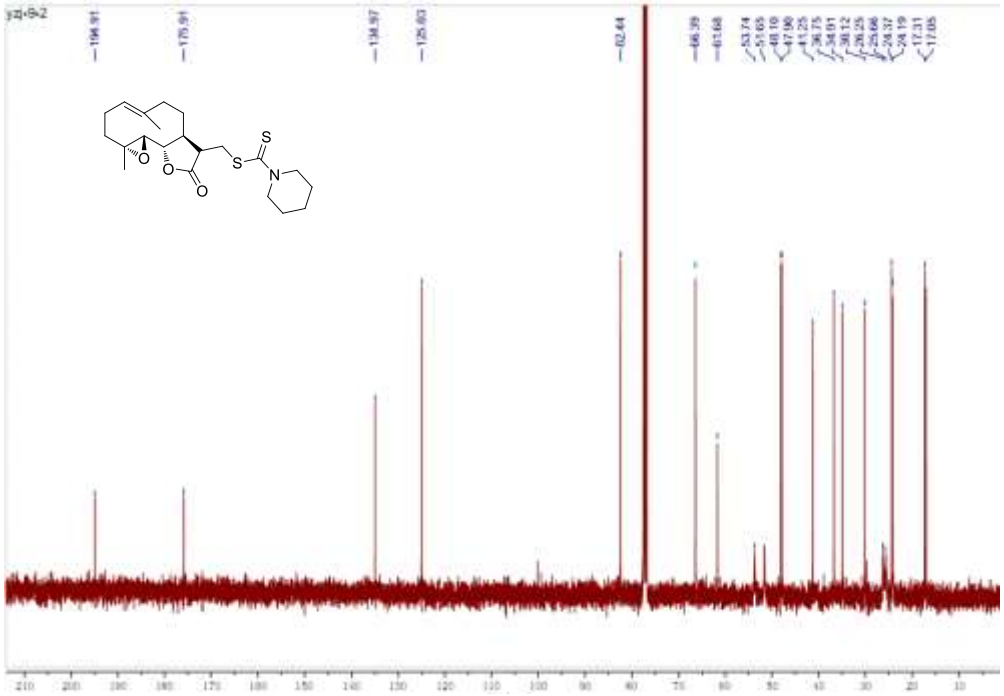
NMR spectra of **7h** in $CDCl_3$



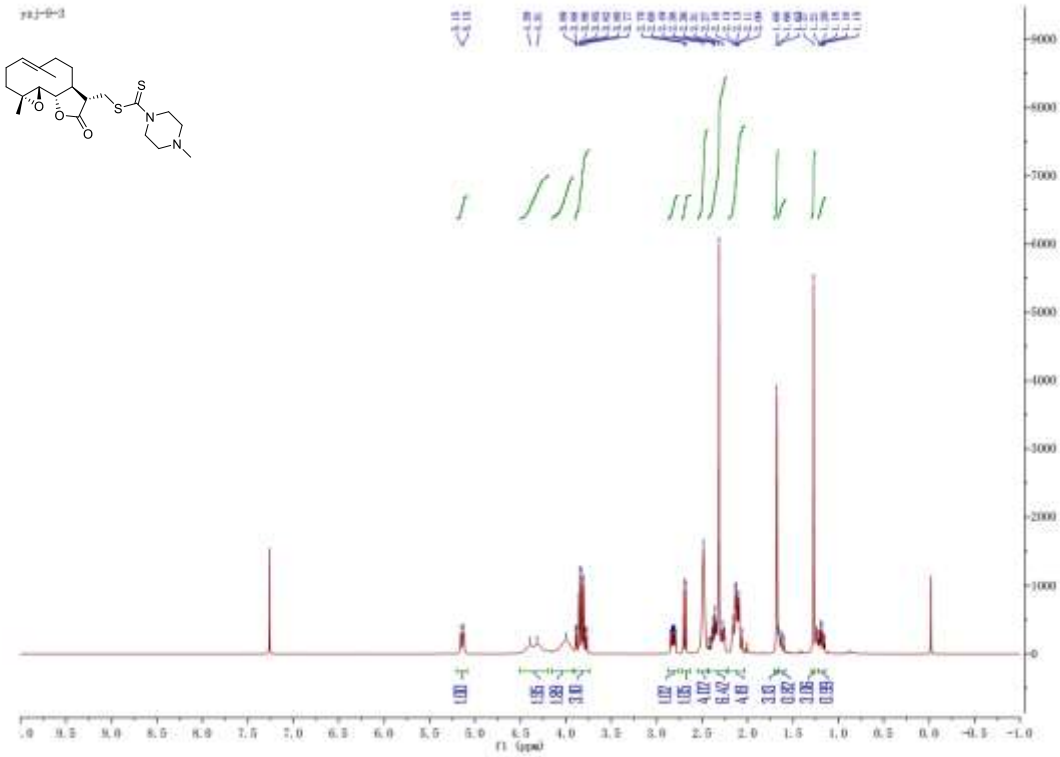


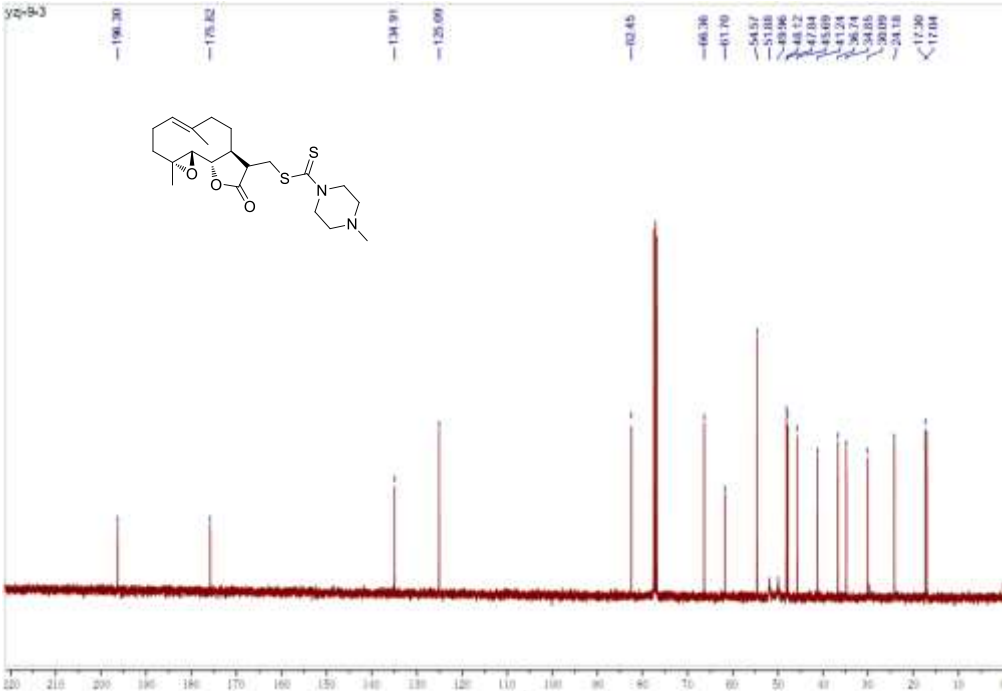
NMR spectra of **7i** in $CDCl_3$



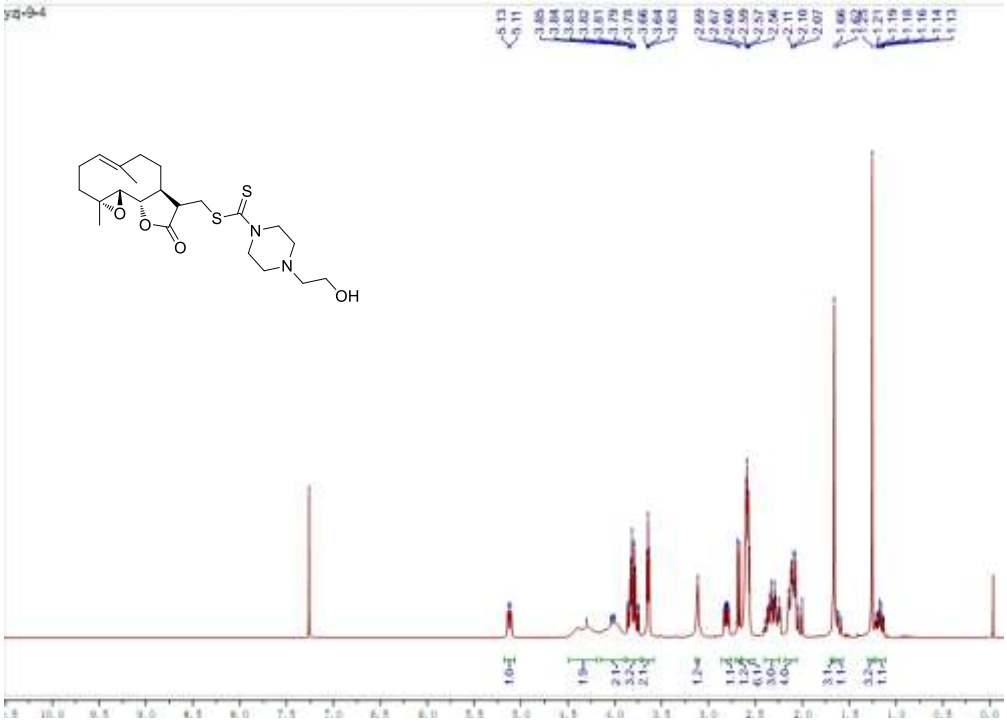


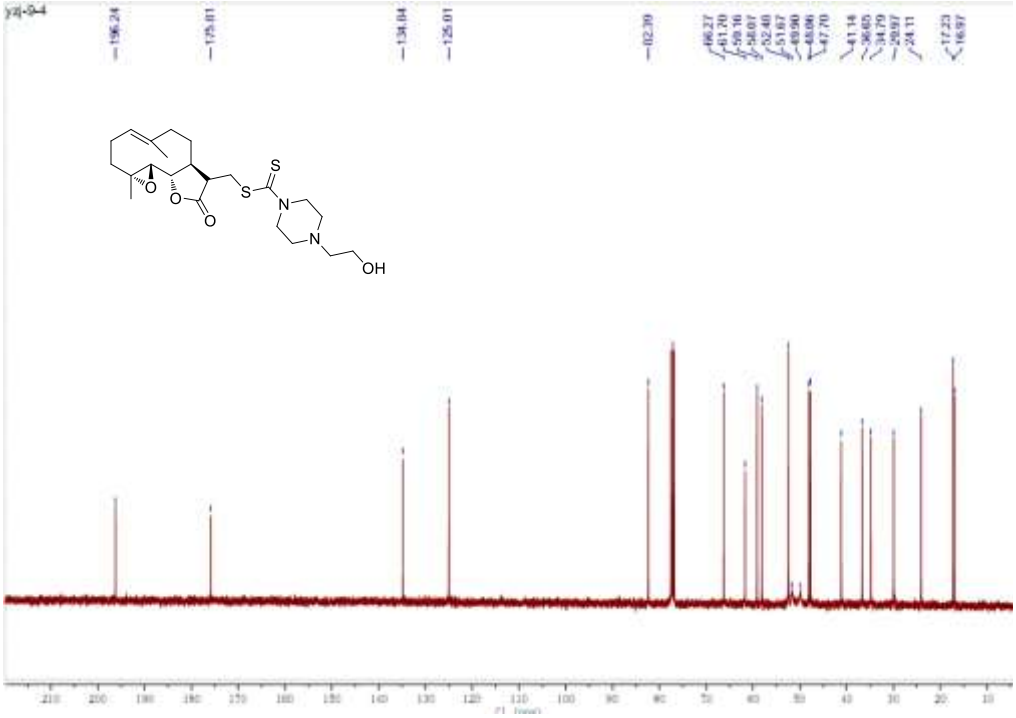
NMR spectra of **7j** in $CDCl_3$



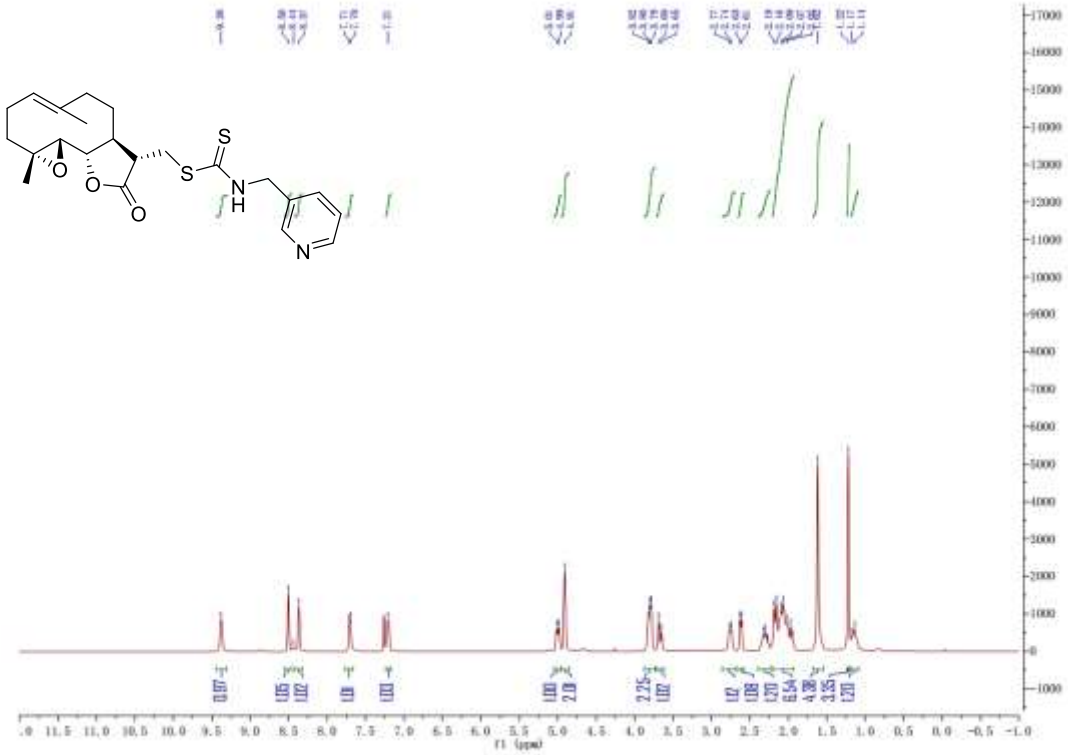


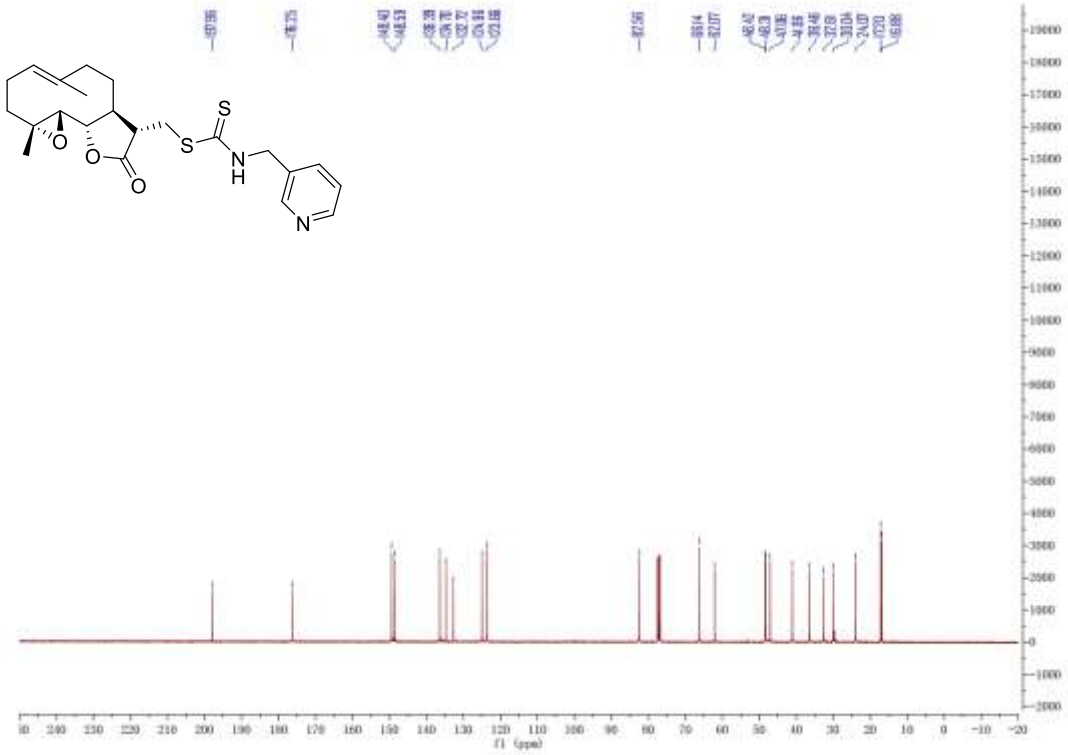
NMR spectra of **7k** in $CDCl_3$



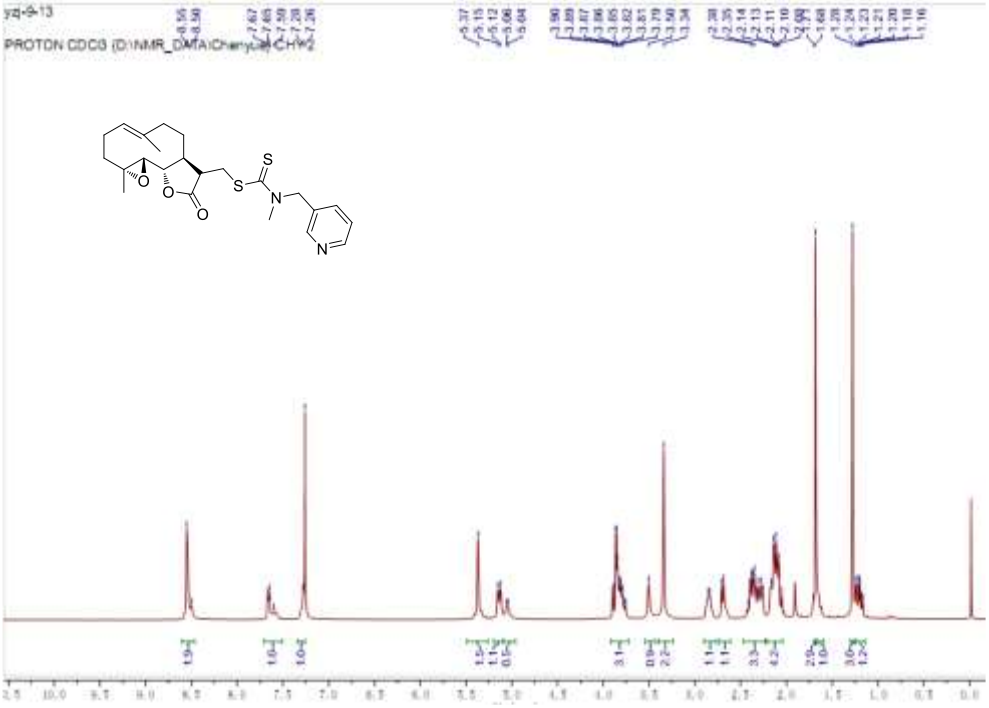


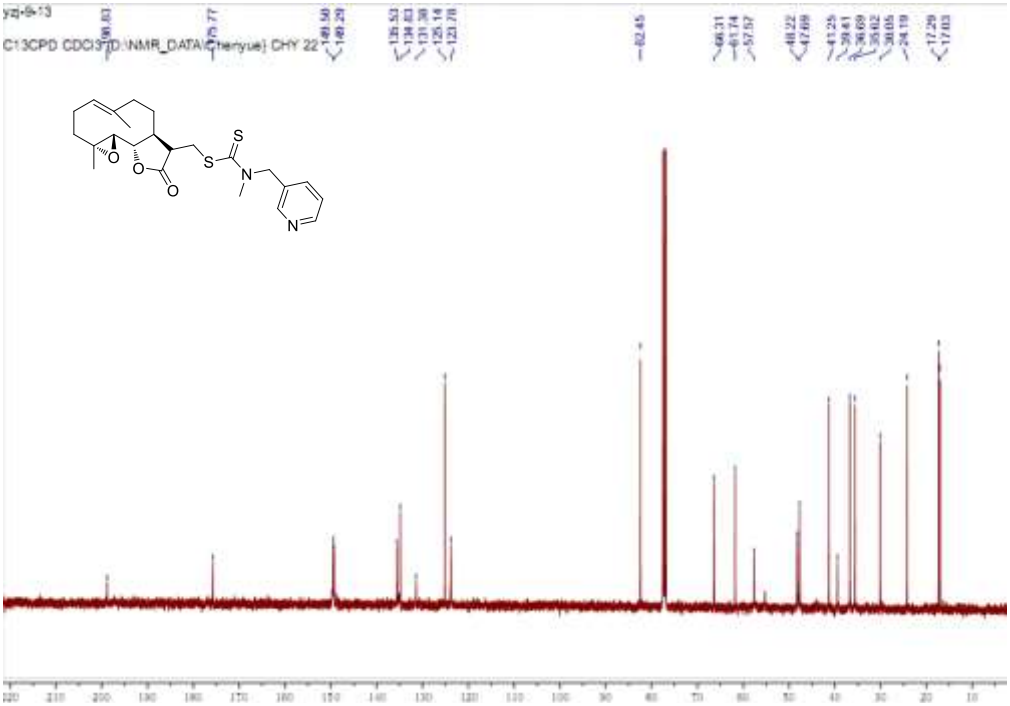
NMR spectra of **7l** in $CDCl_3$



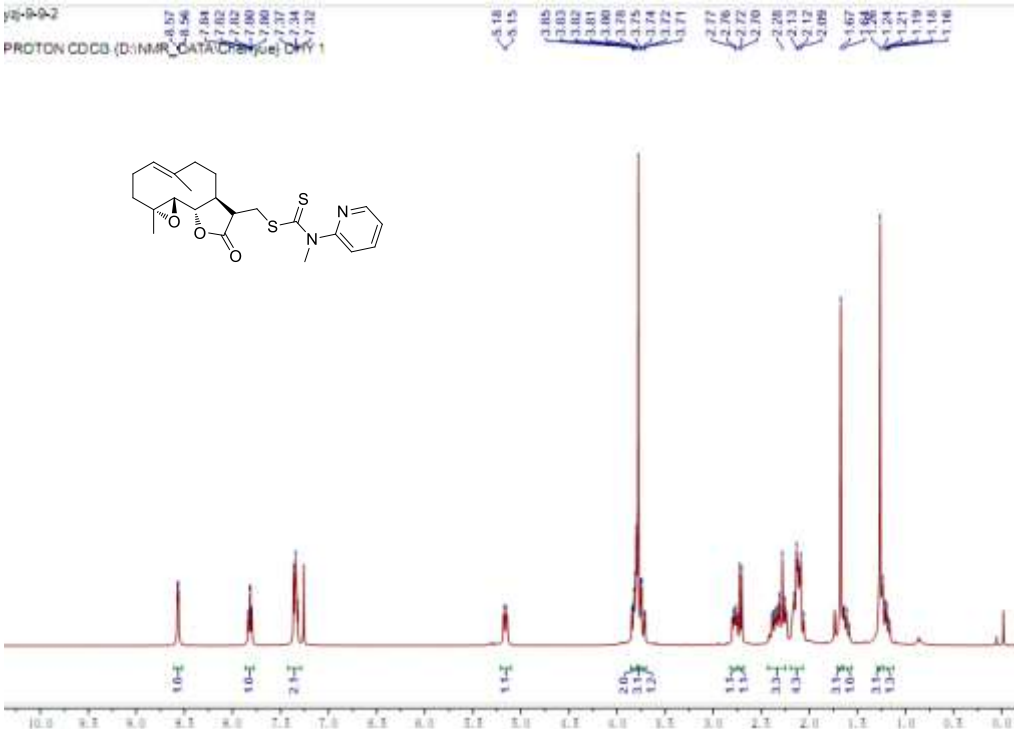


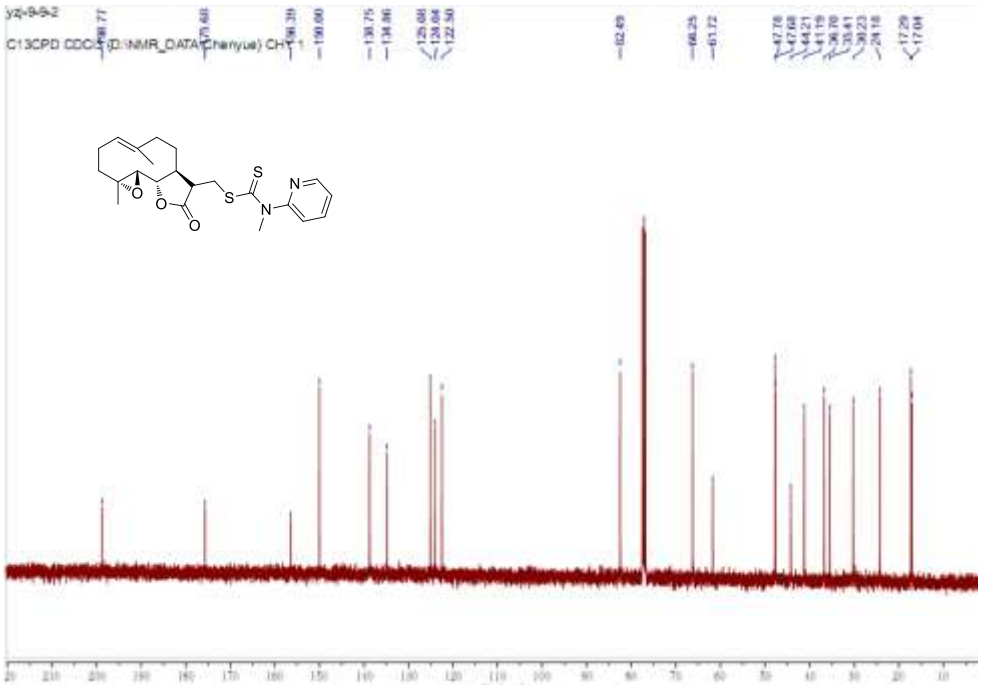
NMR spectra of **7m** in $CDCl_3$



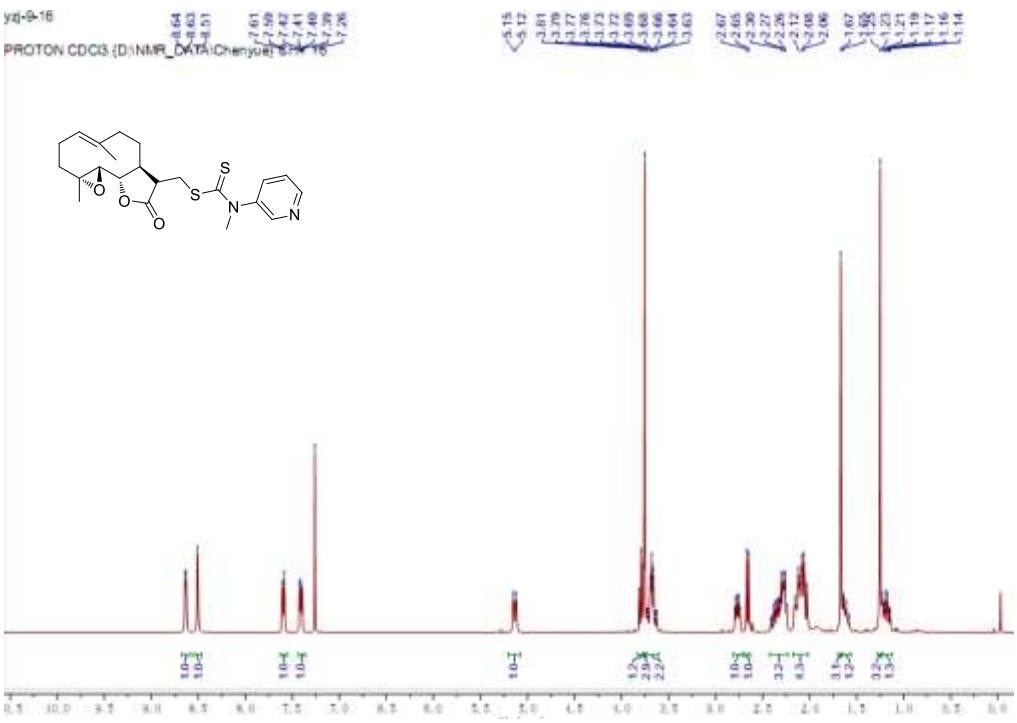


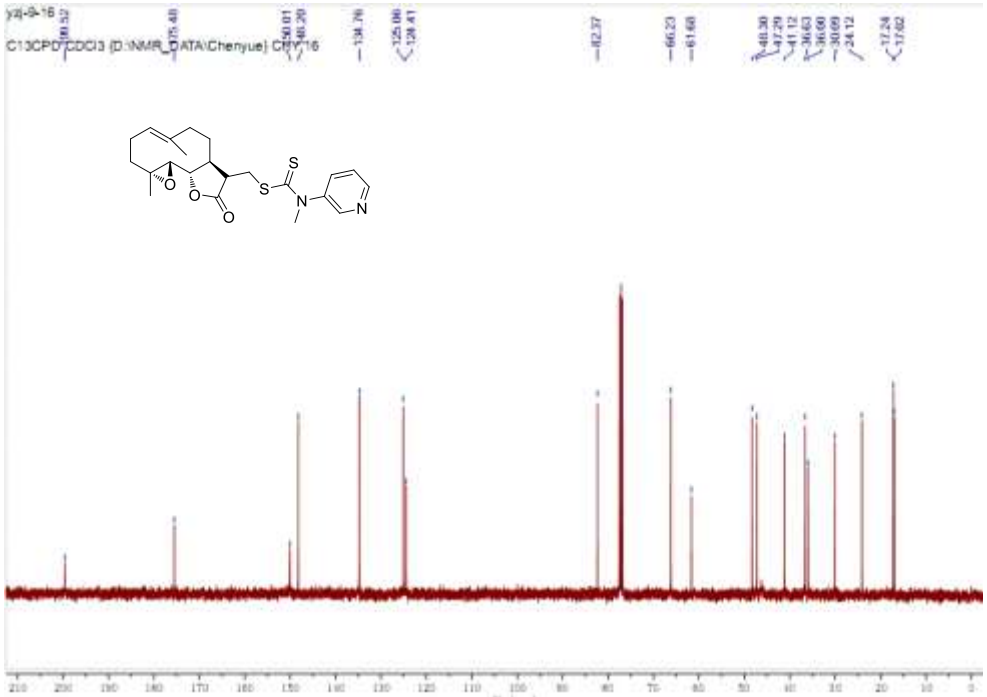
NMR spectra of **7n** in $CDCl_3$



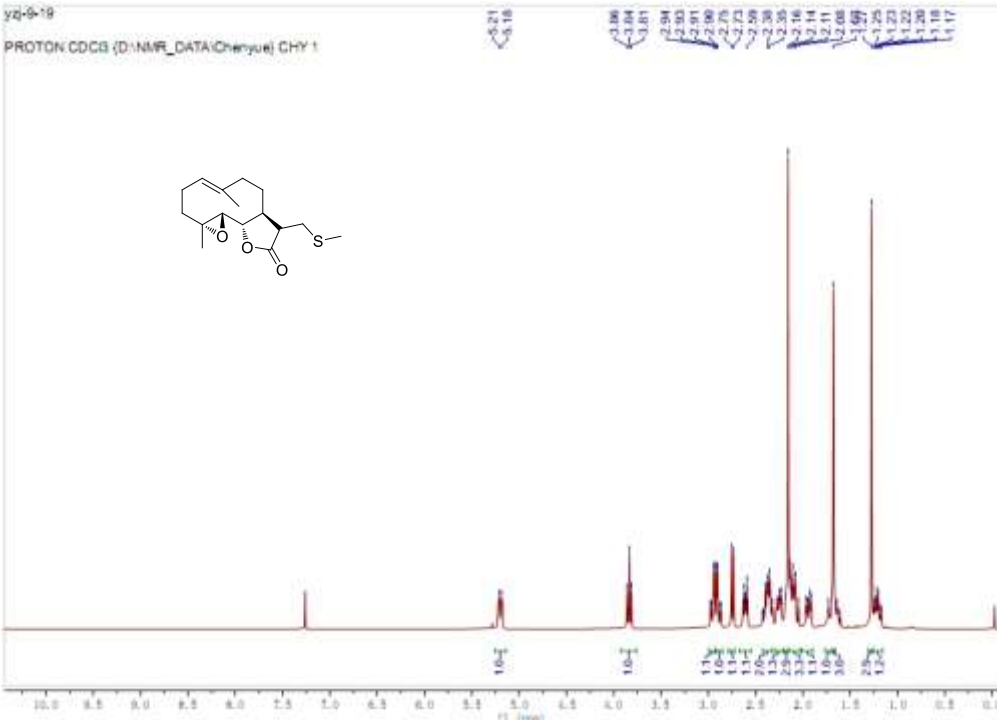


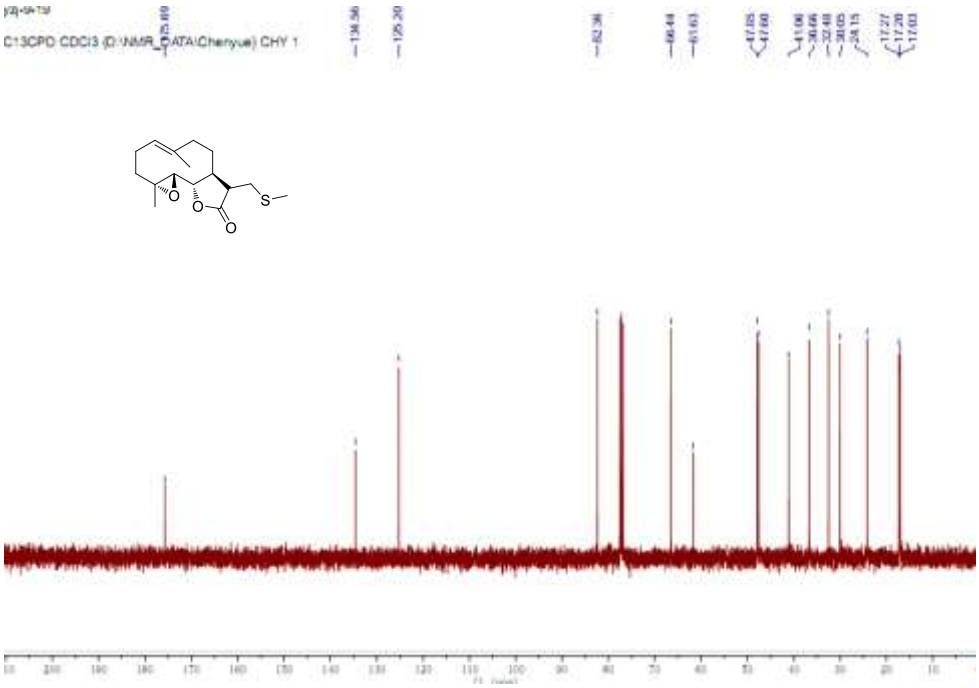
NMR spectra of **7o** in $CDCl_3$



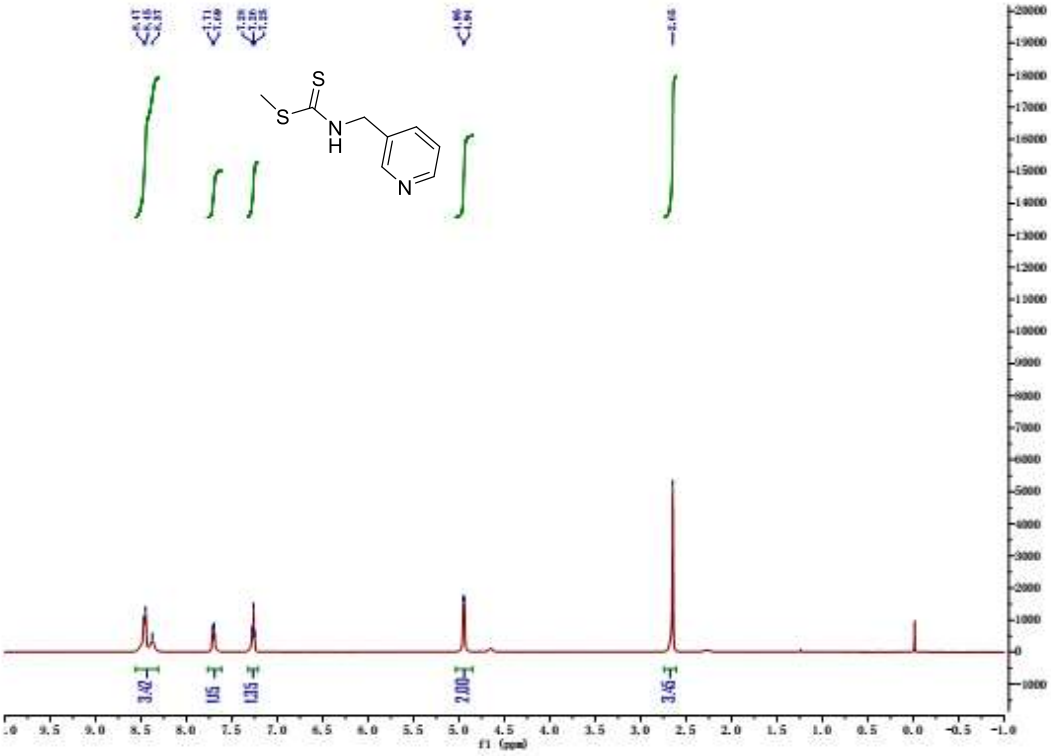


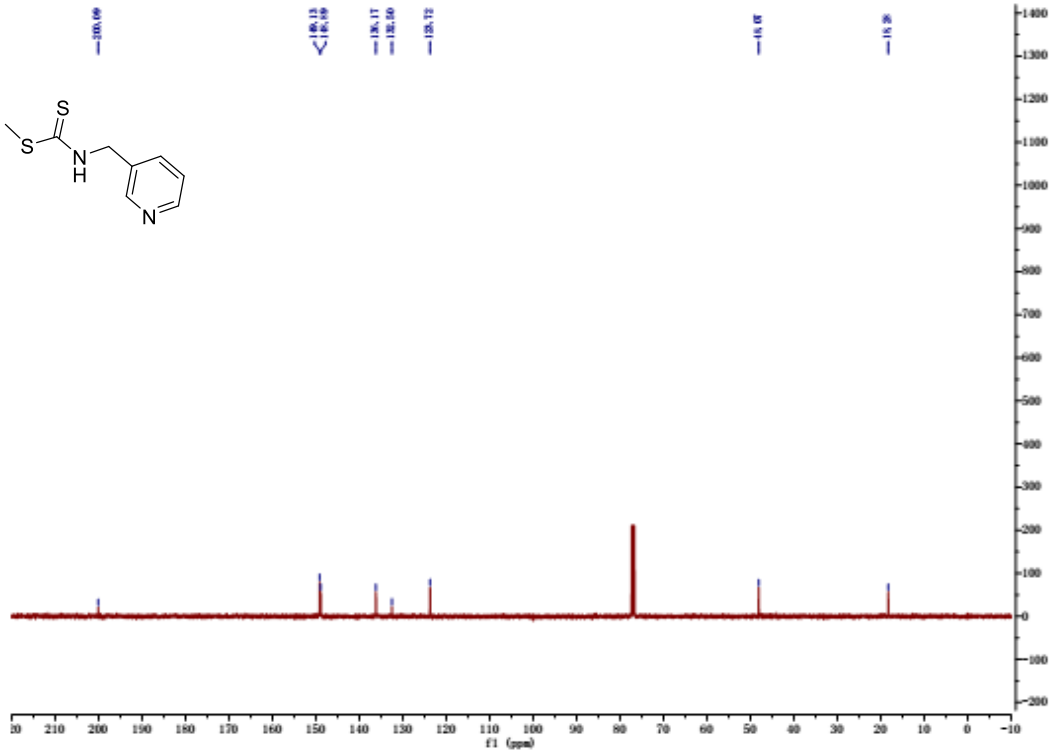
NMR spectra of **8** in $CDCl_3$



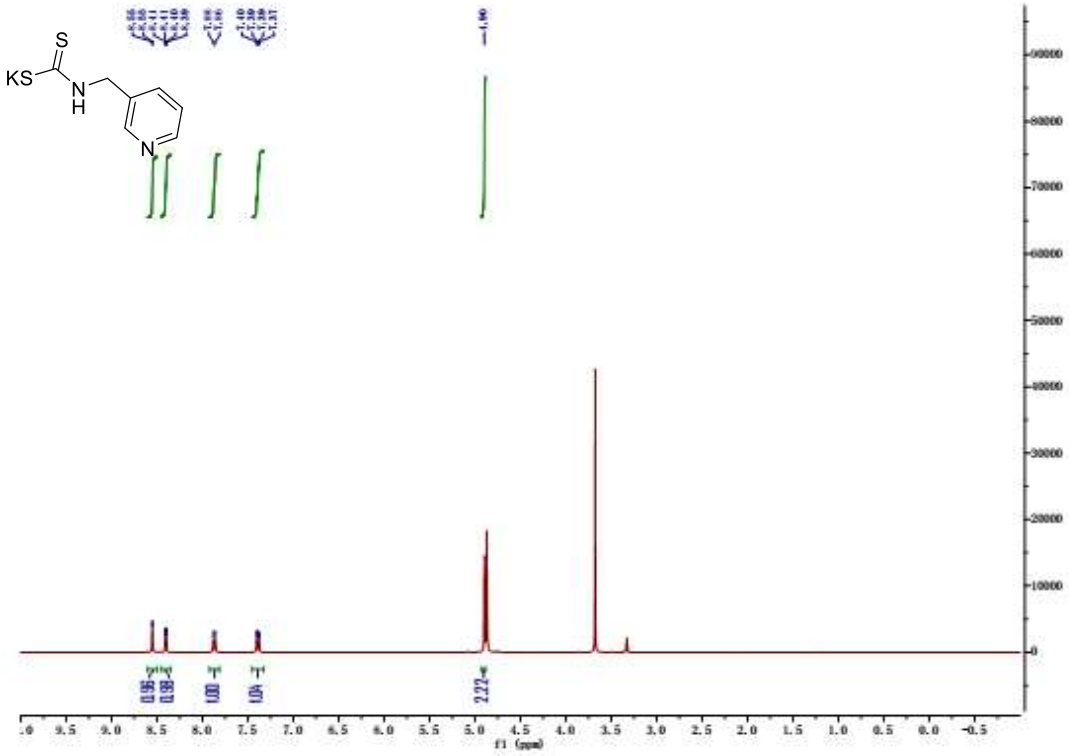


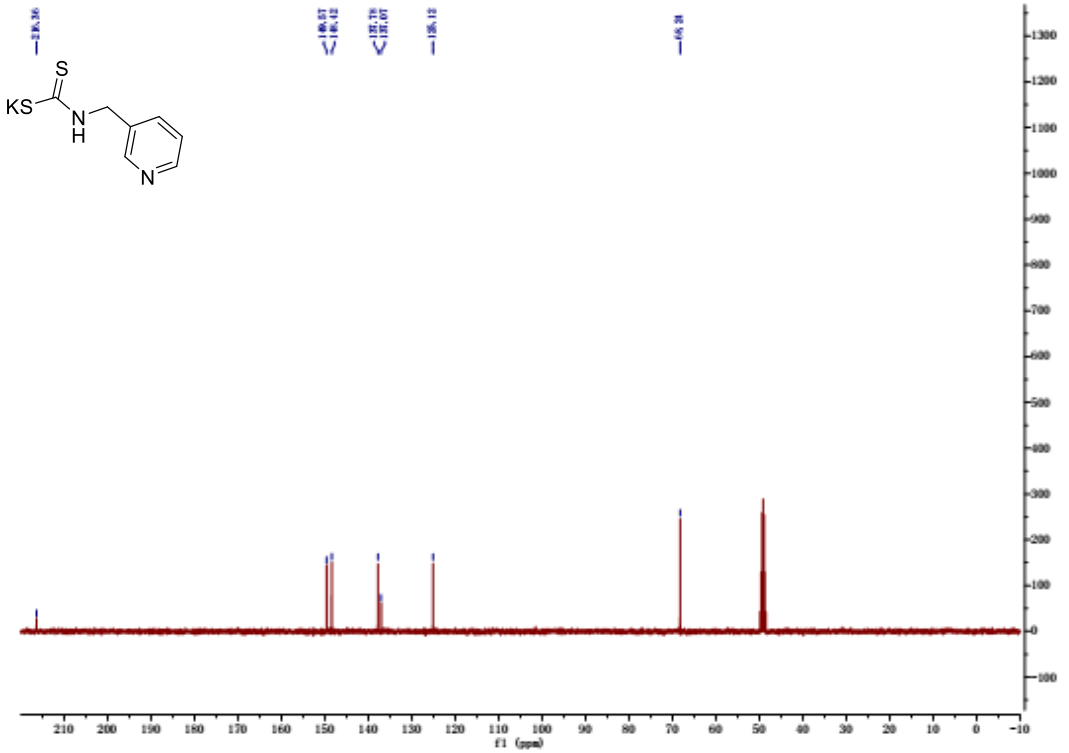
NMR spectra of **11** in $CDCl_3$

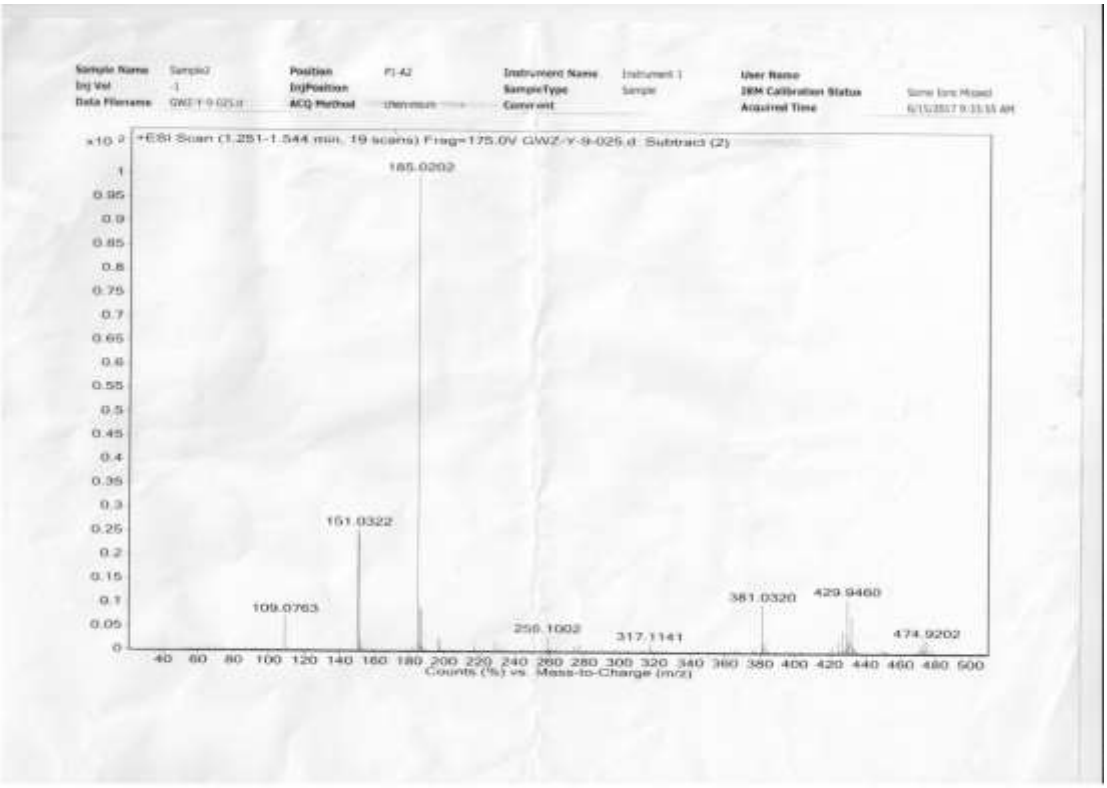




NMR spectra of **10** in CDOD

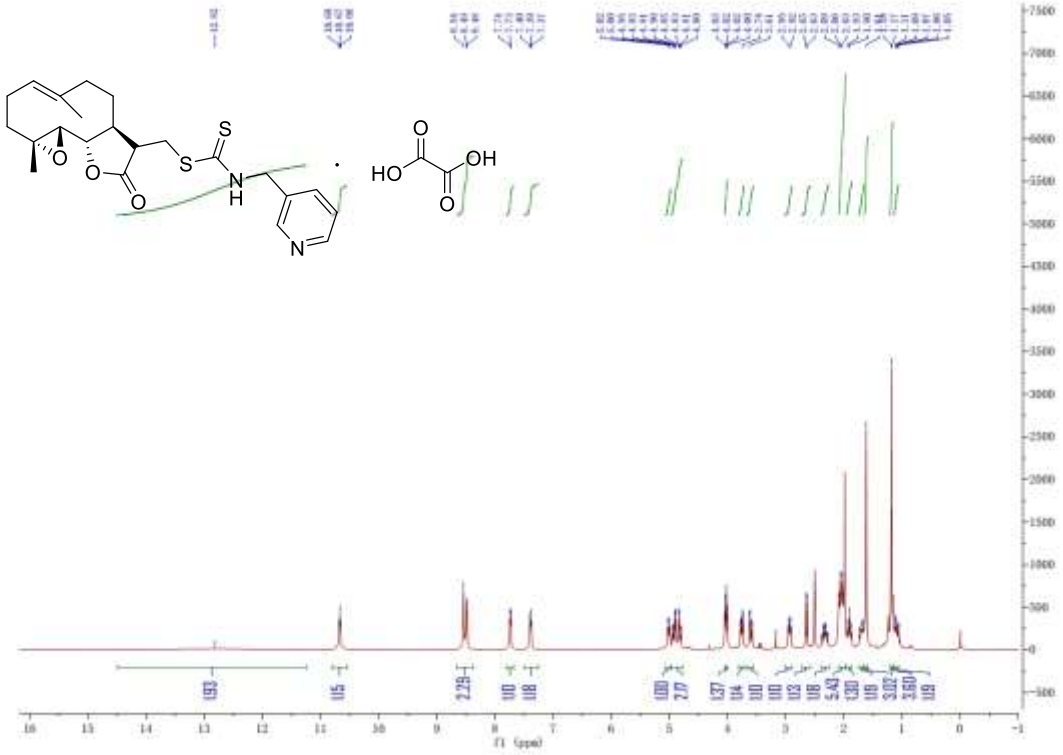

KS
S
N
H
N
f1 (ppm)

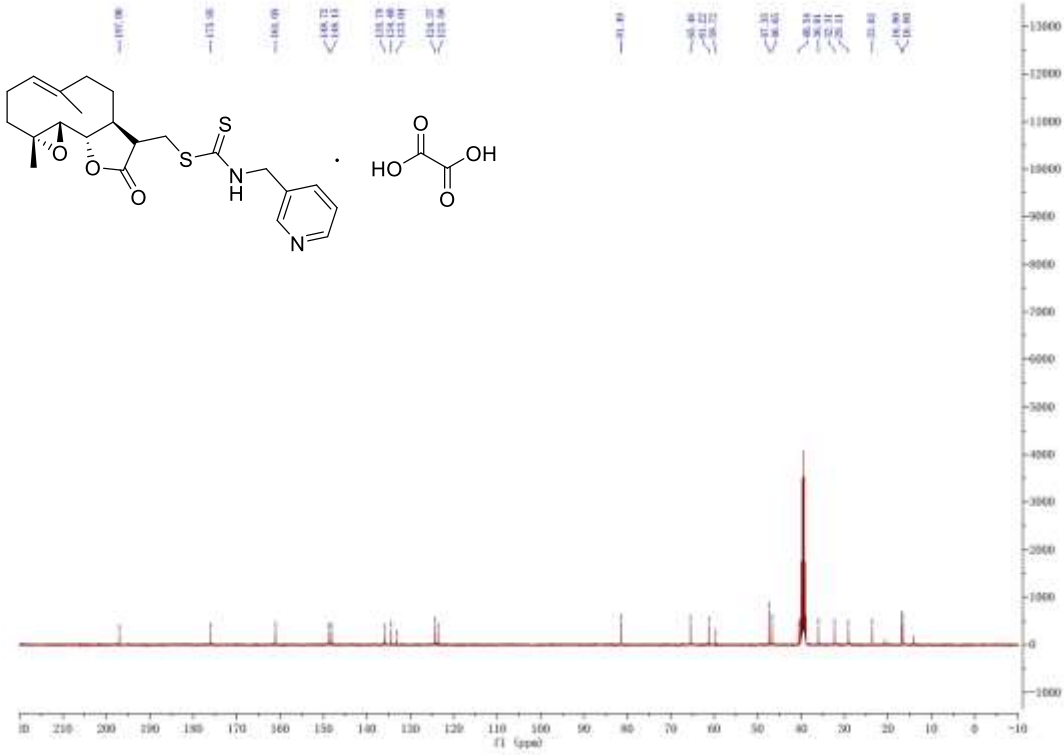

KS
S
N
H
N
f1 (ppm)



HRMS- ESI of **10**

NMR spectra of compound **12** in DMSO-*d*6

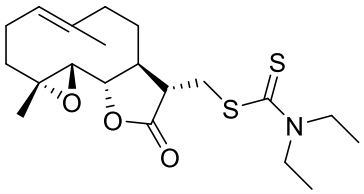




2. X-ray data of compound 7c

7c

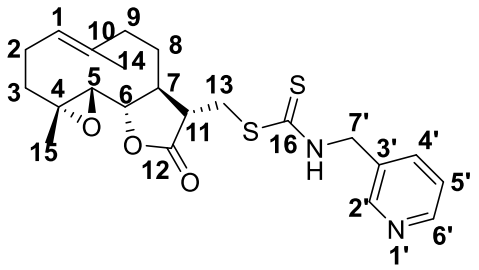
≡



7c

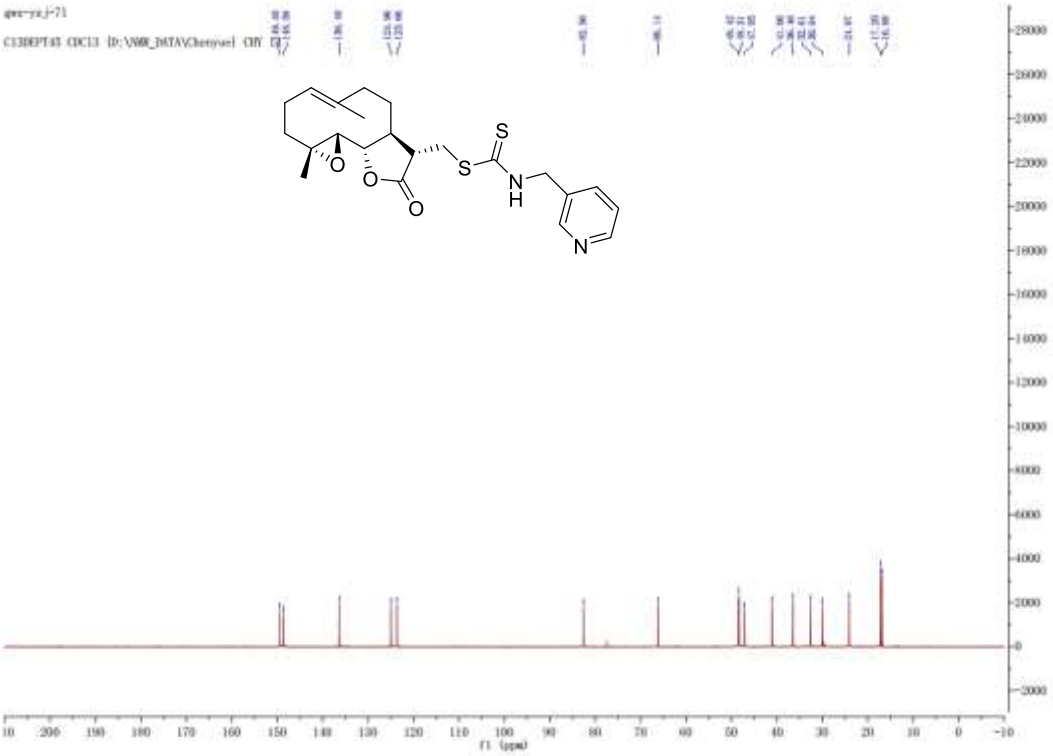
Empirical Formula	$C_{20}H_{31}NO_3S_2$
Formula Weight	397.59
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.300 X 0.240 X 0.160 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	a = 7.0896(18) Å b = 14.018(2) Å c = 21.583(3) Å V = 2145.0(7) Å^3
Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.231 g/cm^3
F_{000}	856.00
μ(CuKα)	23.948 cm^{-1}

3. 2D NMR spectra of 7l

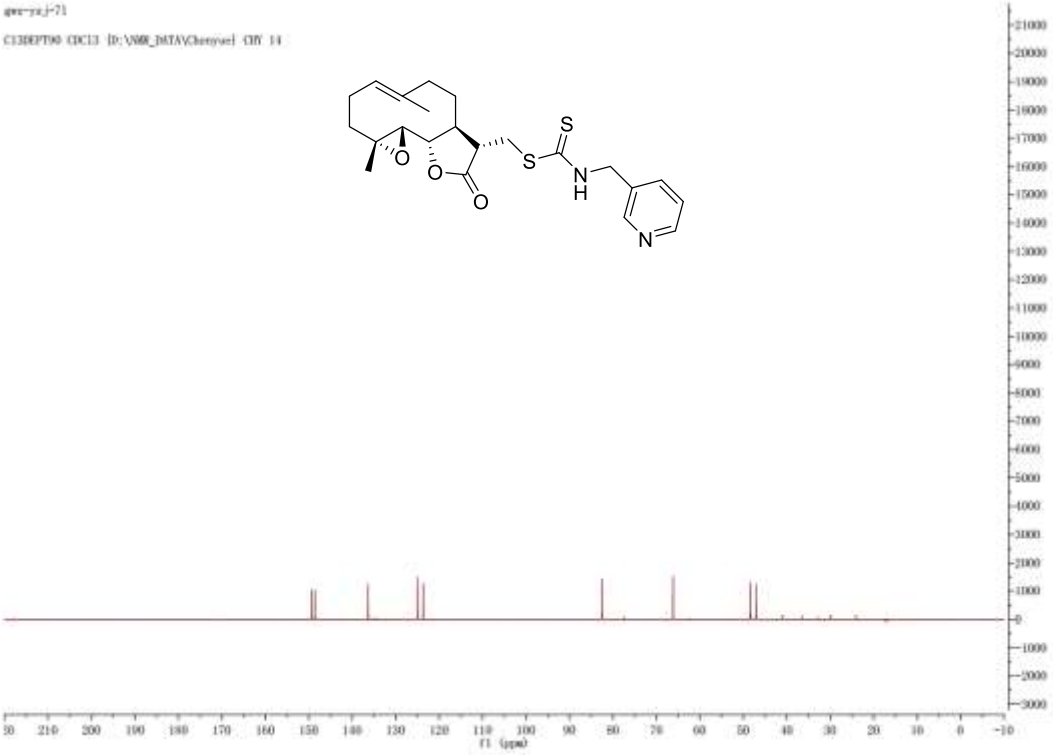


7l

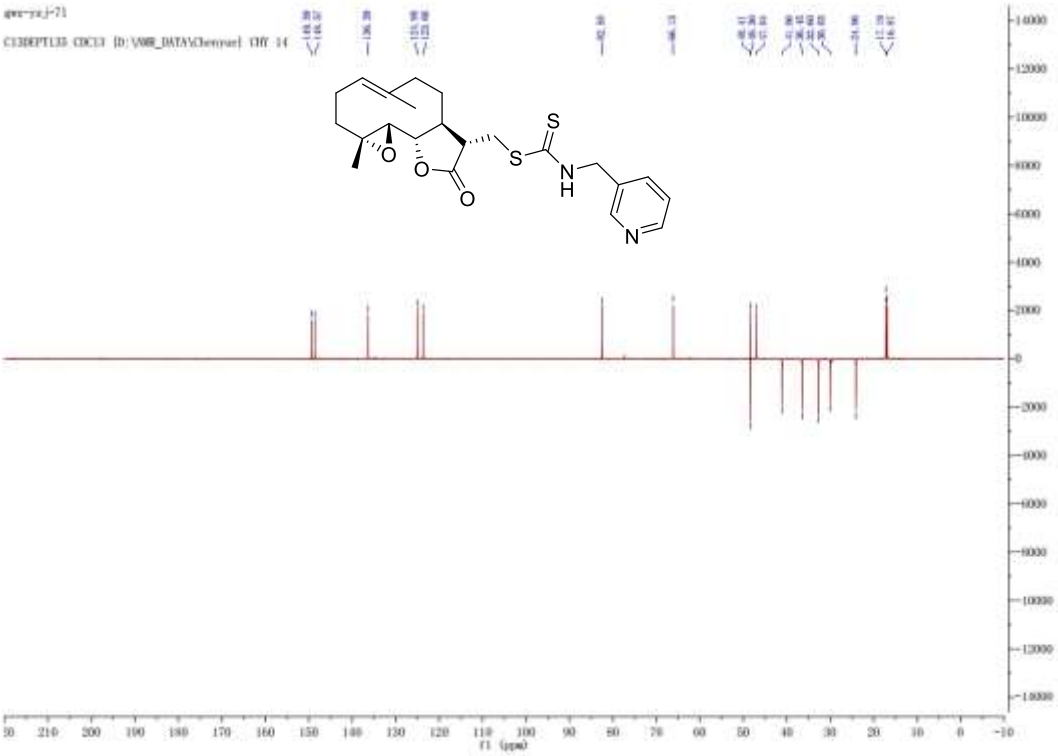
	^{13}C NMR	^{1}H NMR
1	125.0	5.00 (d, *J* = 11.3 Hz, 1H)
2	24.1	2.38 – 2.24 (m, 1H) 2.21 – 1.92 (m, 1H)
3	36.5	1.15 (d, *J* = 12.3 Hz, 1H) 2.21 – 1.92 (m, 1H)
4	62.1	
5	66.1	2.62 (d, *J* = 8.2 Hz, 1H)
6	82.6	3.87 – 3.73 (m, 1H)
7	47.1	2.21 – 1.92 (m, 1H)
8	30.0	1.62 (s, 1H) 2.21 – 1.92 (m, 1H)
9	41.1	2.21 – 1.92 (m, 2H)
10	134.7	
11	48.3	2.75 (d, *J* = 8.7 Hz, 1H)
12	176.3	
13	32.6	3.87 – 3.73 (m, 1H) 3.67 (d, *J* = 14.3 Hz, 1H)
14	17.2	1.62 (s, 3H)
15	16.9	1.22 (s, 3H),
16	198.0	
2’	149.4	8.50 (s, 1H)
3’	132.7	
4’	136.4	7.70 (d, *J* = 5.7 Hz, 1H)
5’	123.7	7.21 (s, 1H)
6’	148.6	8.37 (s, 1H)
7’	48.4	4.91 (s, 2H)
N-H		9.38 (s, 1H)



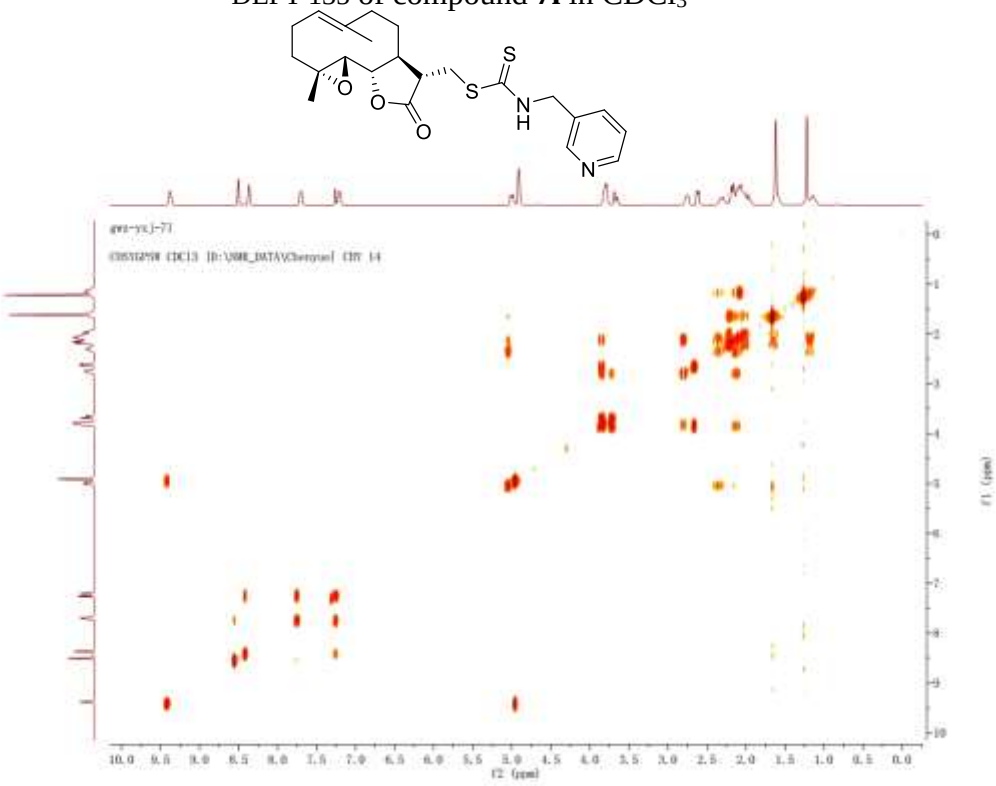
DEPT 45 of compound **7l** in $CDCl_3$



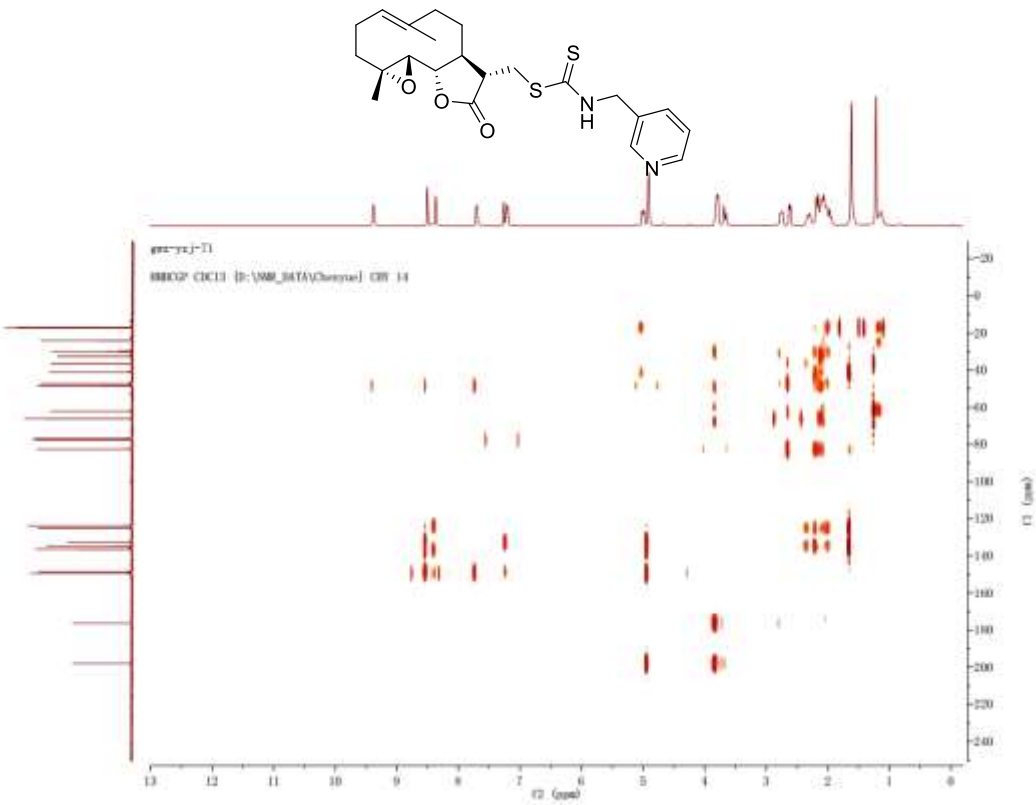
DEPT 90 of compound **7l** in $CDCl_3$



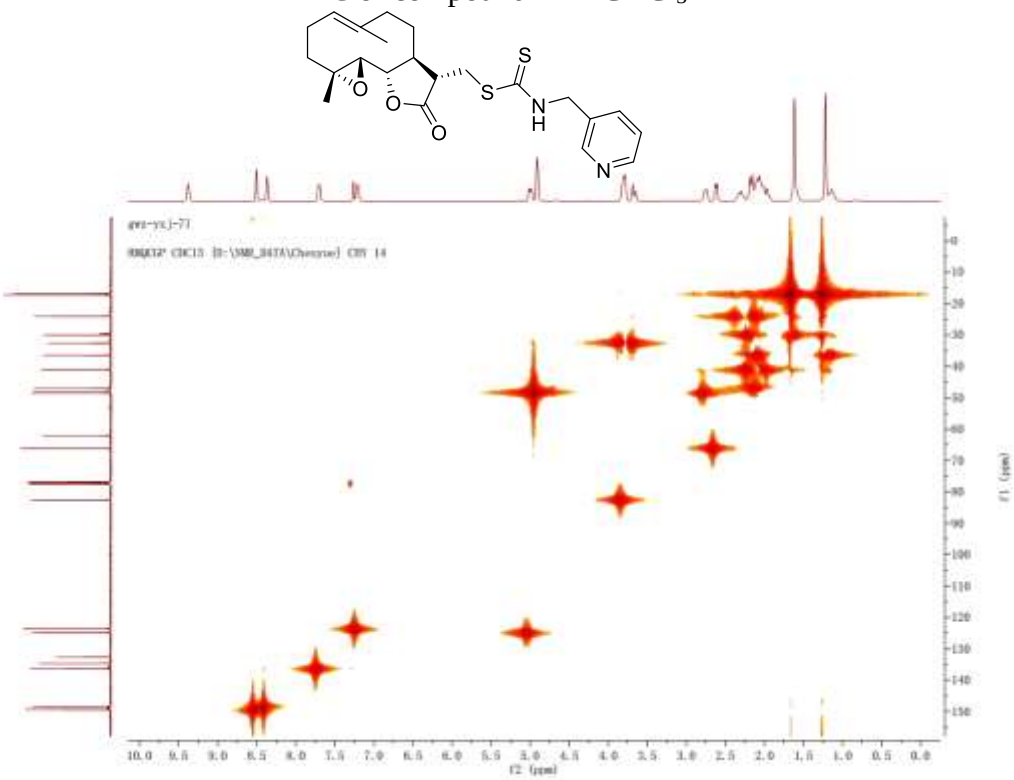
DEPT 135 of compound **7l** in $CDCl_3$



H-H COSY of compound **7l** in $CDCl_3$



HMBC of compound **7l** in $CDCl_3$



HMQC of compound **7l** in $CDCl_3$