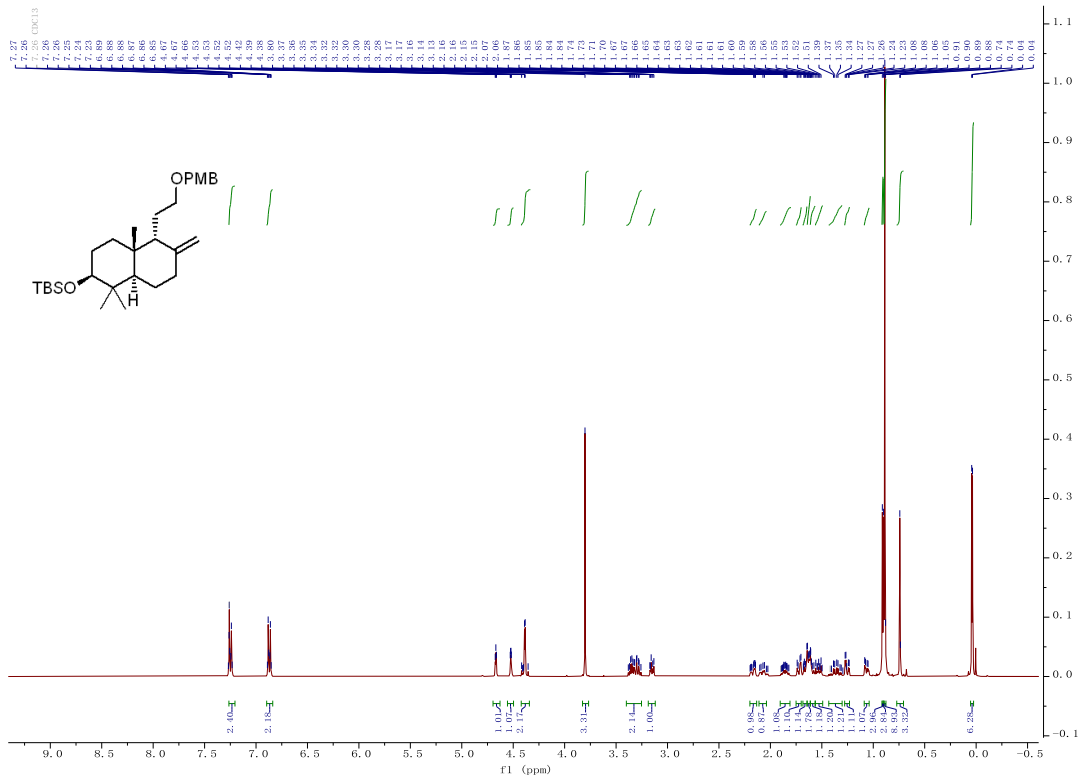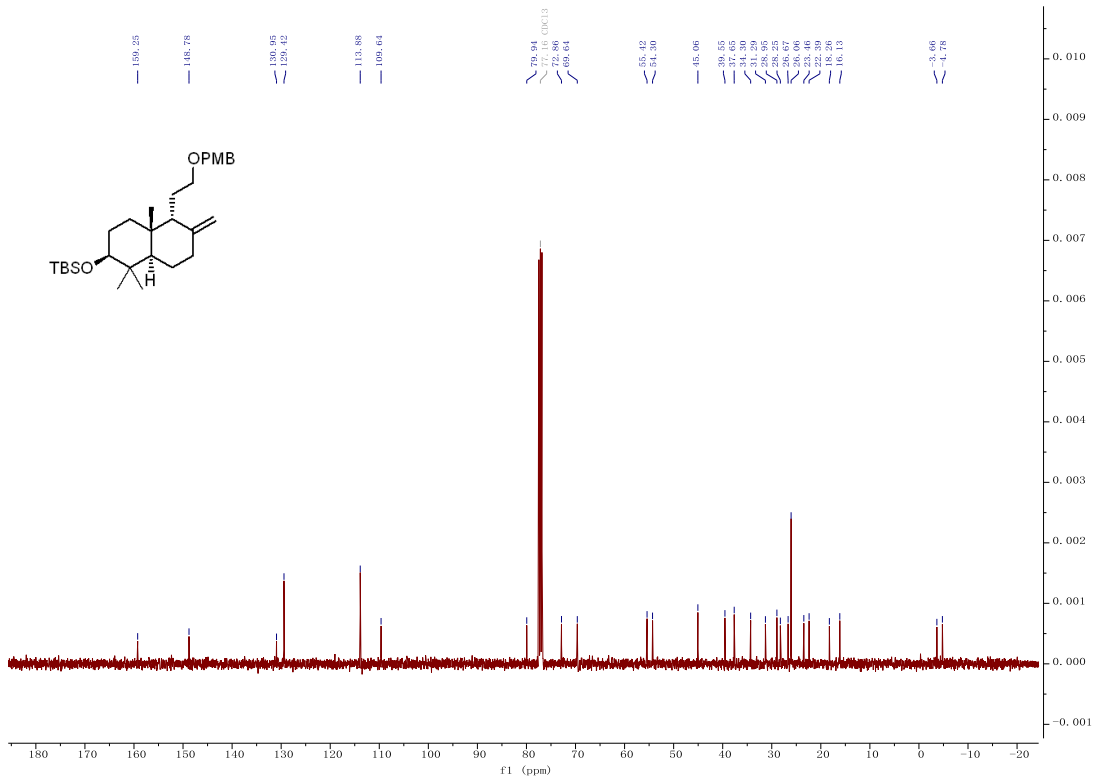**Supporting Information**

**Synthesis of Isoxazoline Analogs of Stellettins**

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Fax: +86 10 63017757; Tel: +86 10 63165242

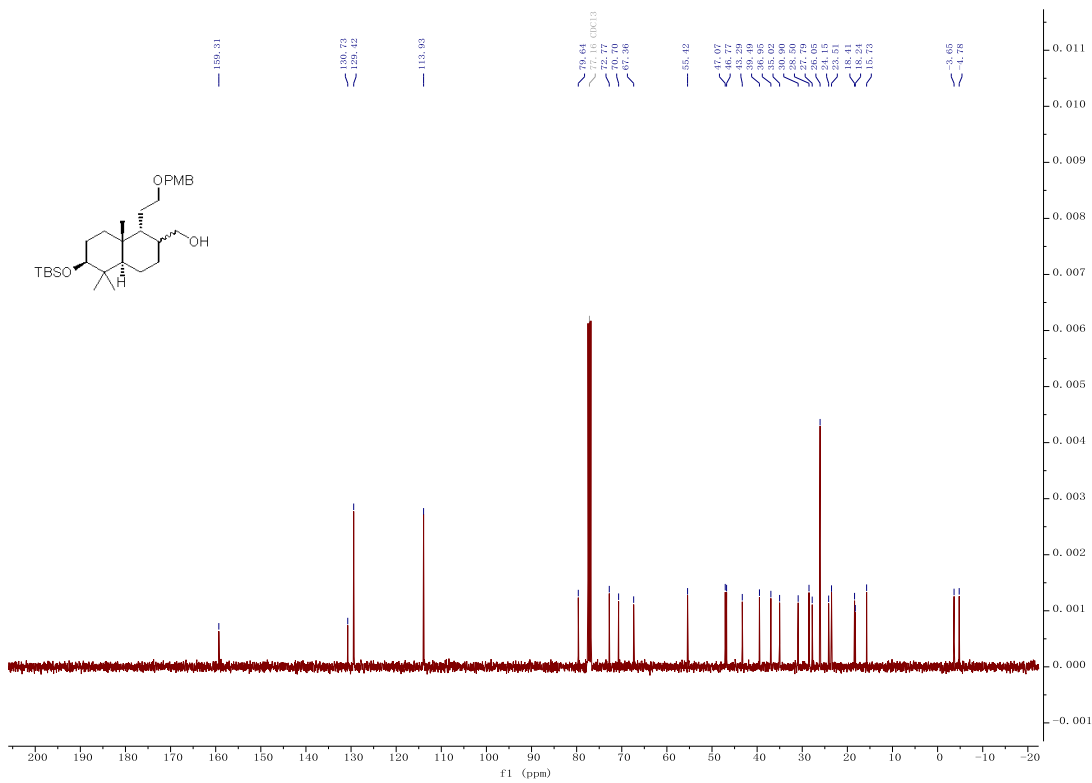*Email: lxya@imm.ac.cn; jiaoxz@imm.ac.cn*

Contents

^{1}H NMR of compound (±)6 (400 MHz, CDCl$_3$)

^{13}C NMR of compound (±)6 (100 MHz, CDCl$_3$)

2

^{1}H NMR of compound (±)**7** (400 MHz, CDCl$_3$)
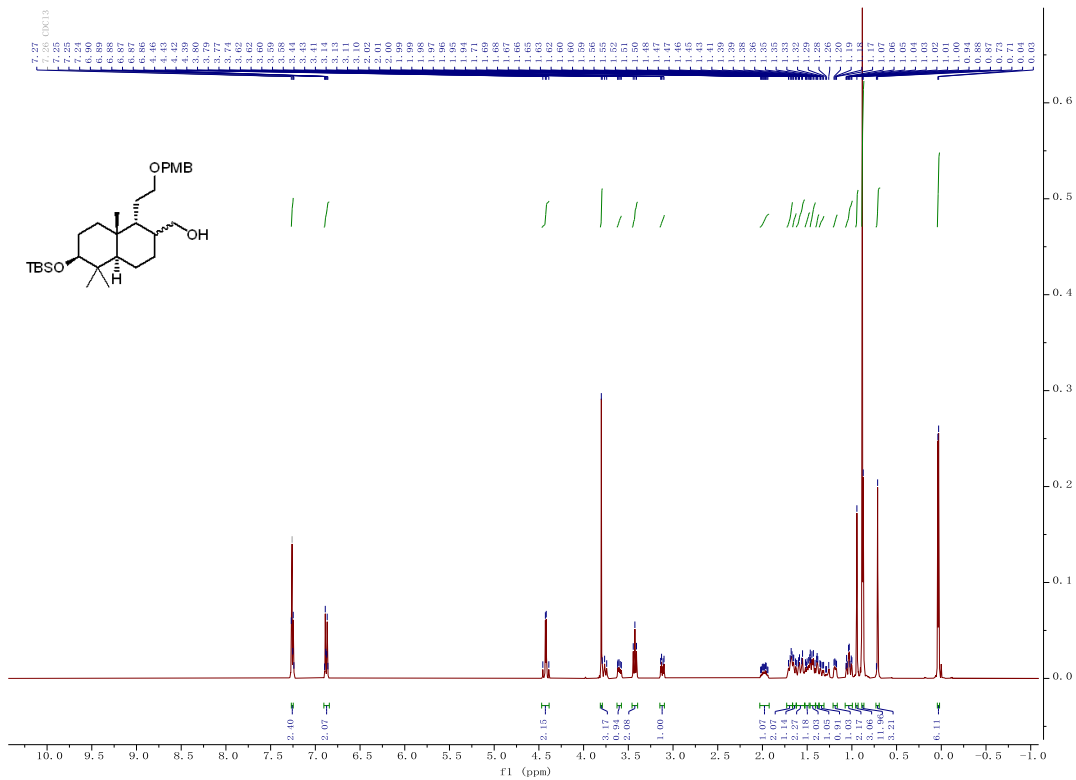
^{13}C NMR of compound (±)**7** (100 MHz, CDCl$_3$)

3

^{1}H NMR of compound (±)**8** (400 MHz, CDCl$_3$)
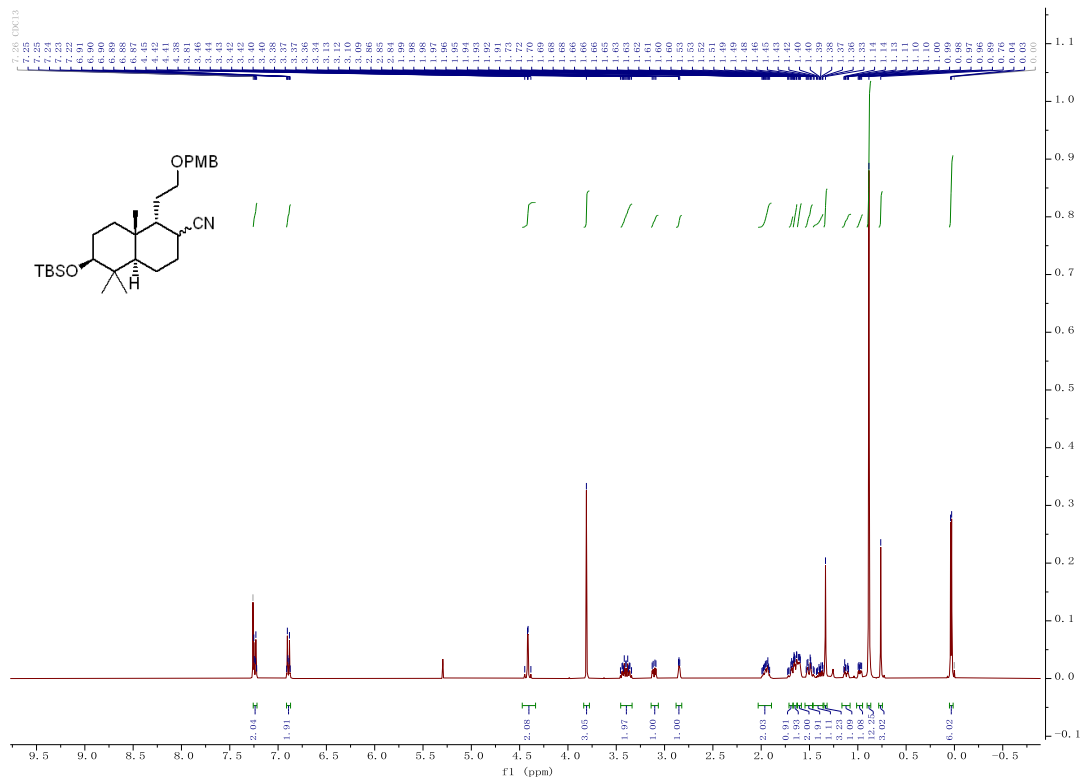
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4
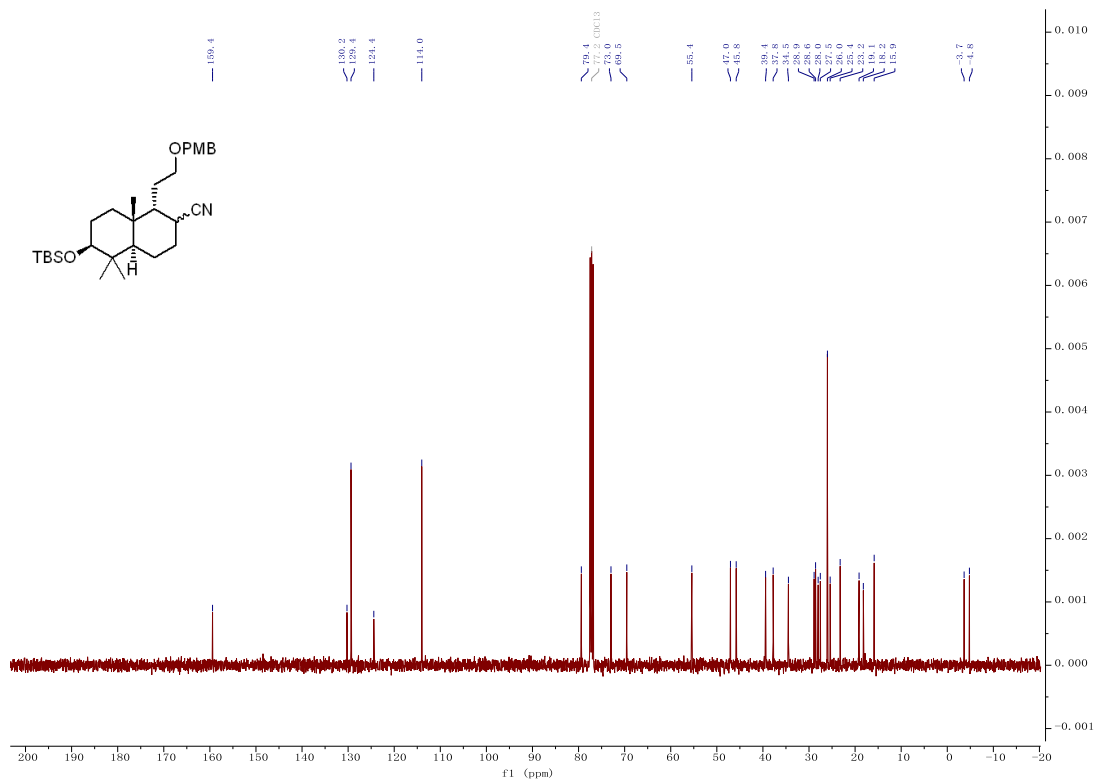
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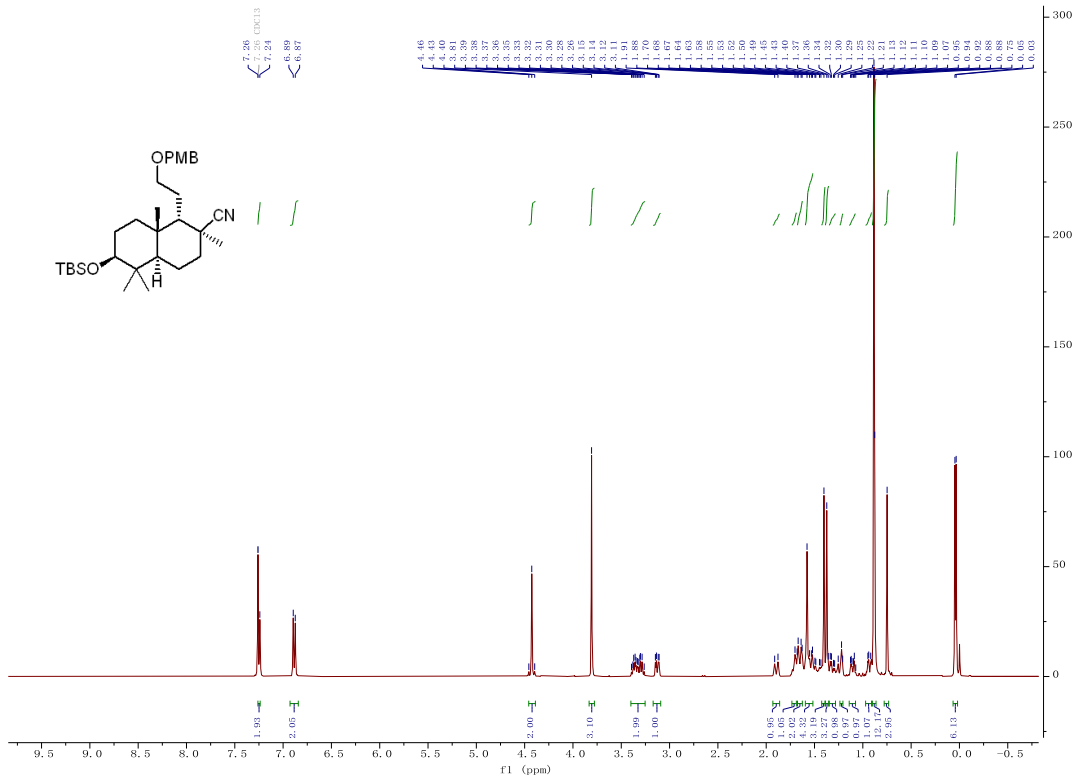
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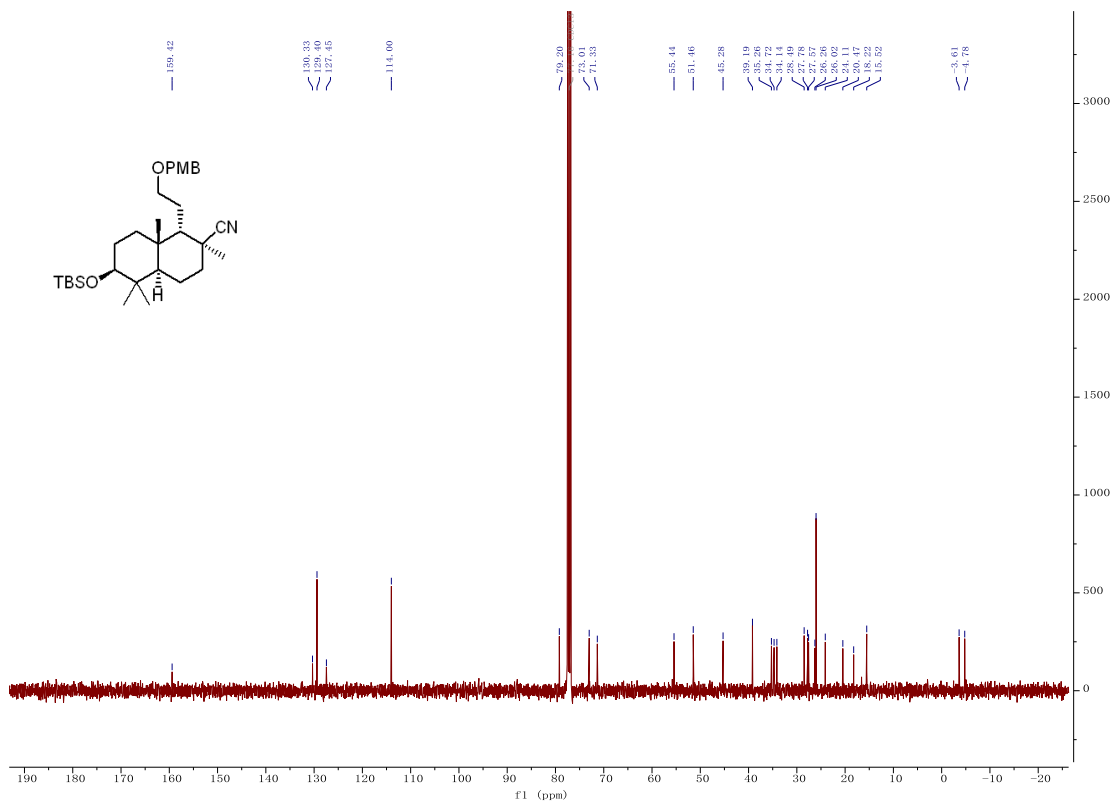
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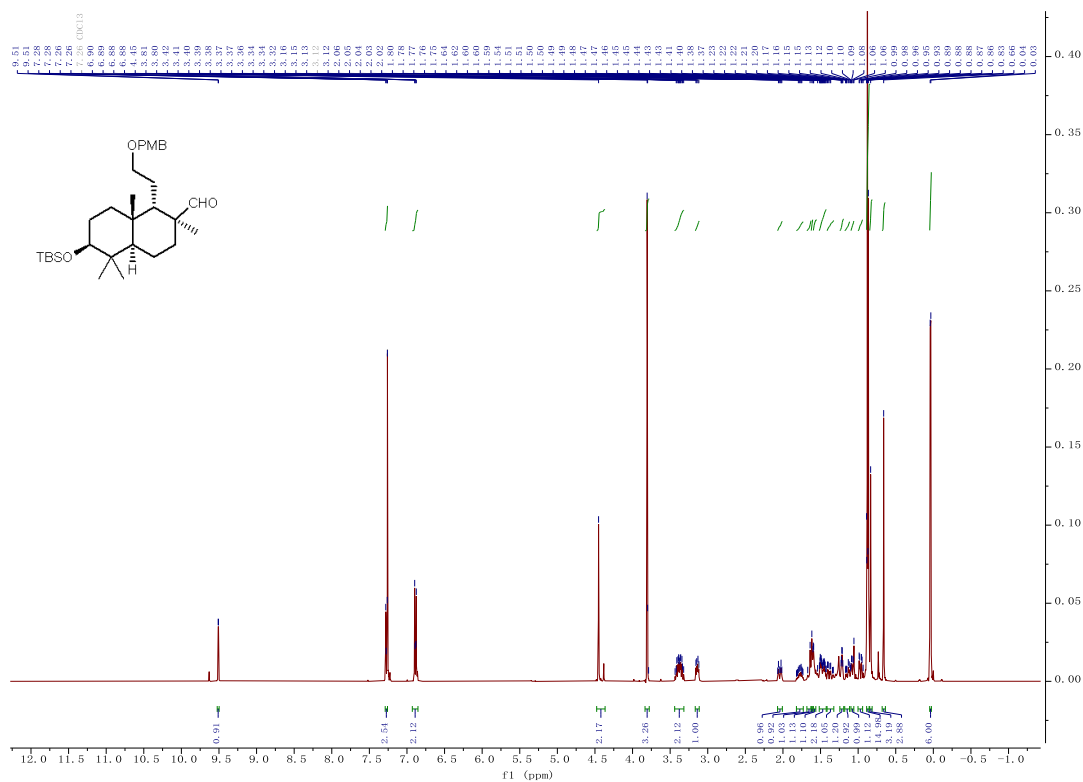
^{13}C NMR of compound (±)**10** (100 MHz, CDCl$_3$)

^{1}H NMR of compound (±)**11** (400 MHz, CDCl$_3$)
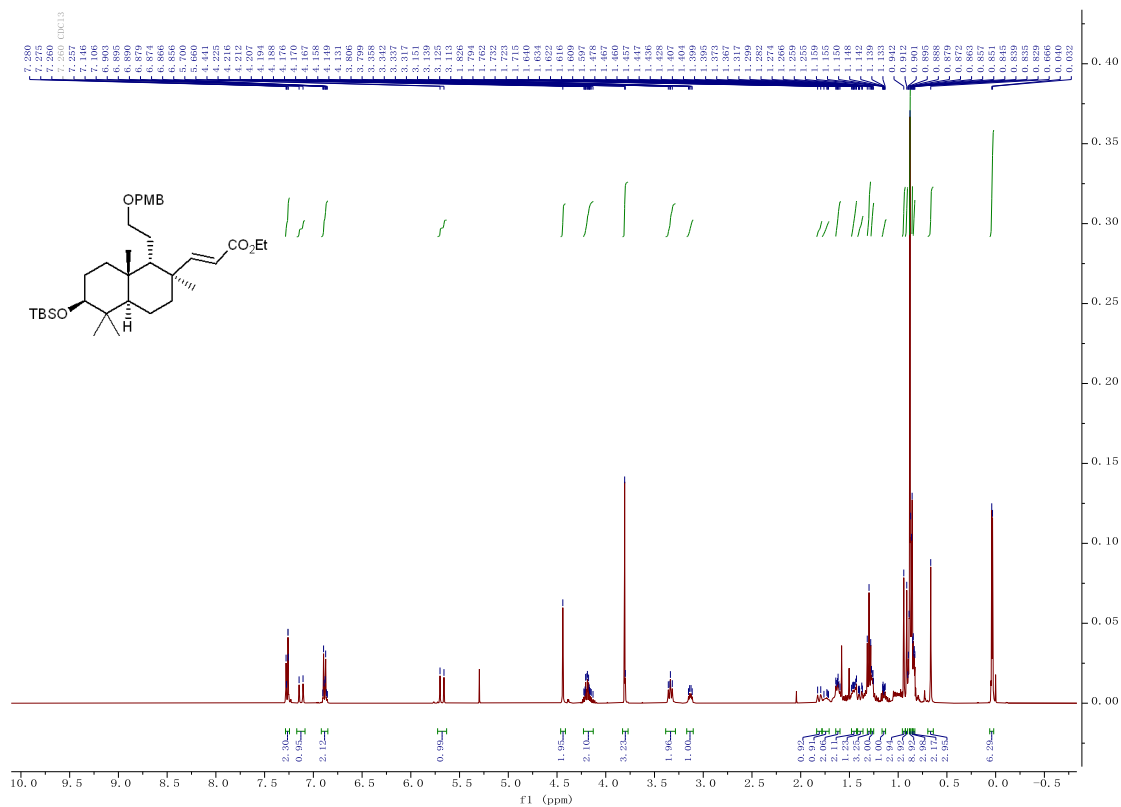
^{13}C NMR of compound (±)**11** (100 MHz, CDCl$_3$)

^{1}H NMR of compound (±)**12** (400 MHz, CDCl$_3$)

^{13}C NMR of compound (±)**12** (100 MHz, CDCl$_3$)

^{1}H NMR of compound ($\pm$)**13** (400 MHz, CDCl$_3$)

^{13}C NMR of compound ($\pm$)**13** (100 MHz, CDCl$_3$)

^{1}H NMR of compound (±)**14** (500 MHz, CDCl$_3$)

^{13}C NMR of compound (±)**14** (125 MHz, CDCl$_3$)

10

^{1}H NMR of compound (±)**15** (400 MHz, CDCl$_3$)

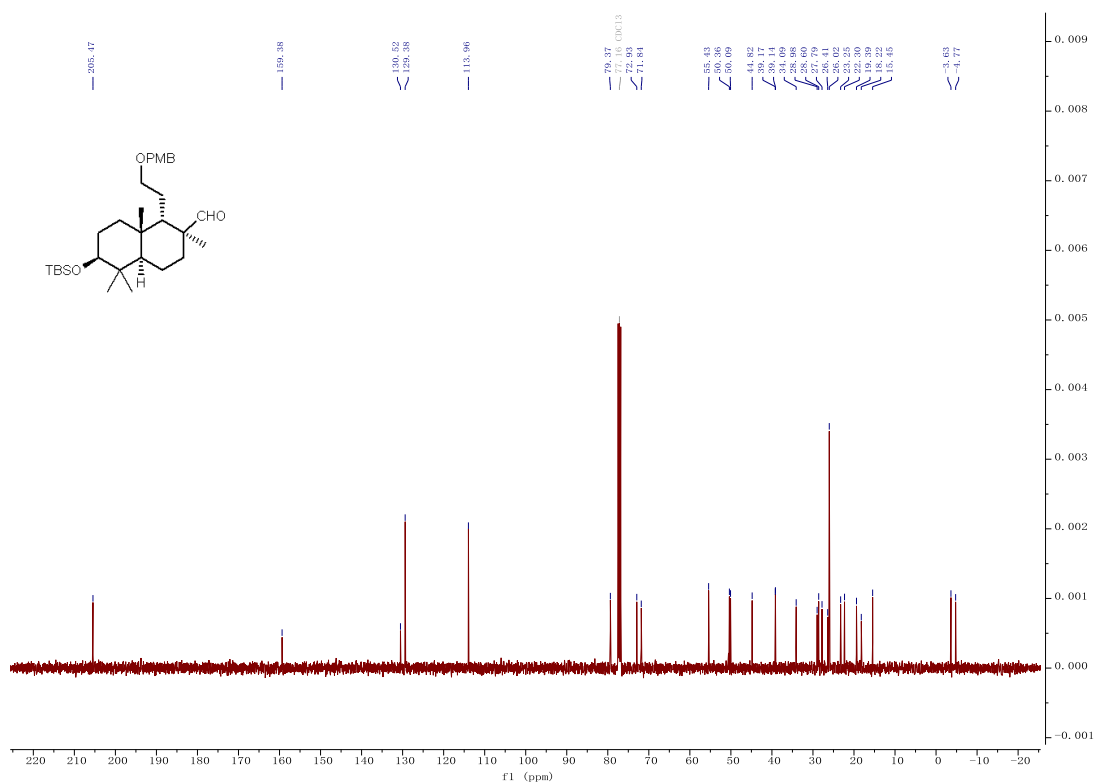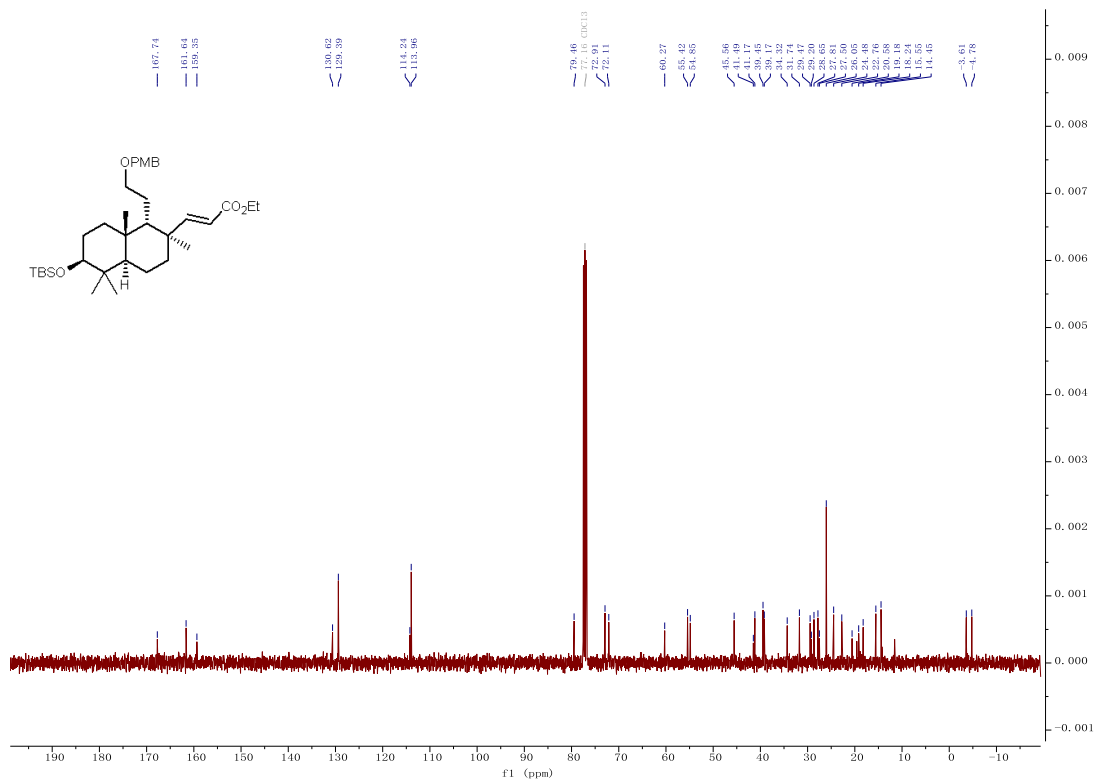# ^{13}C NMR of compound (±)**15** (100 MHz, CDCl$_3$)

11
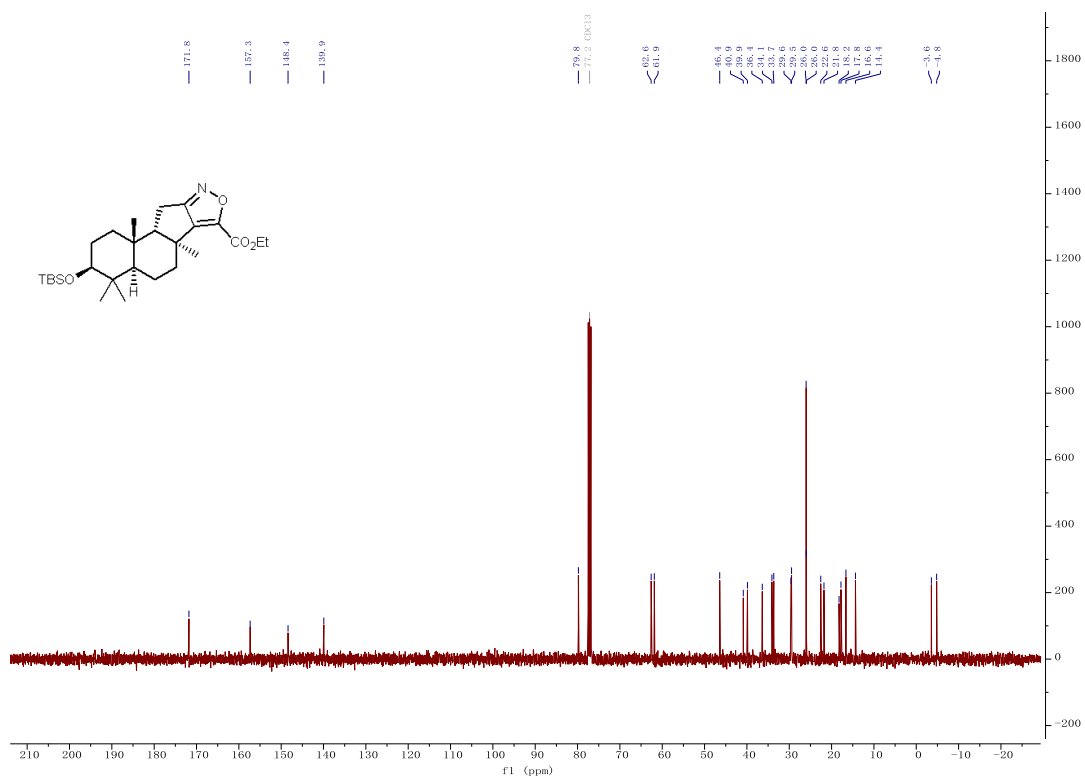
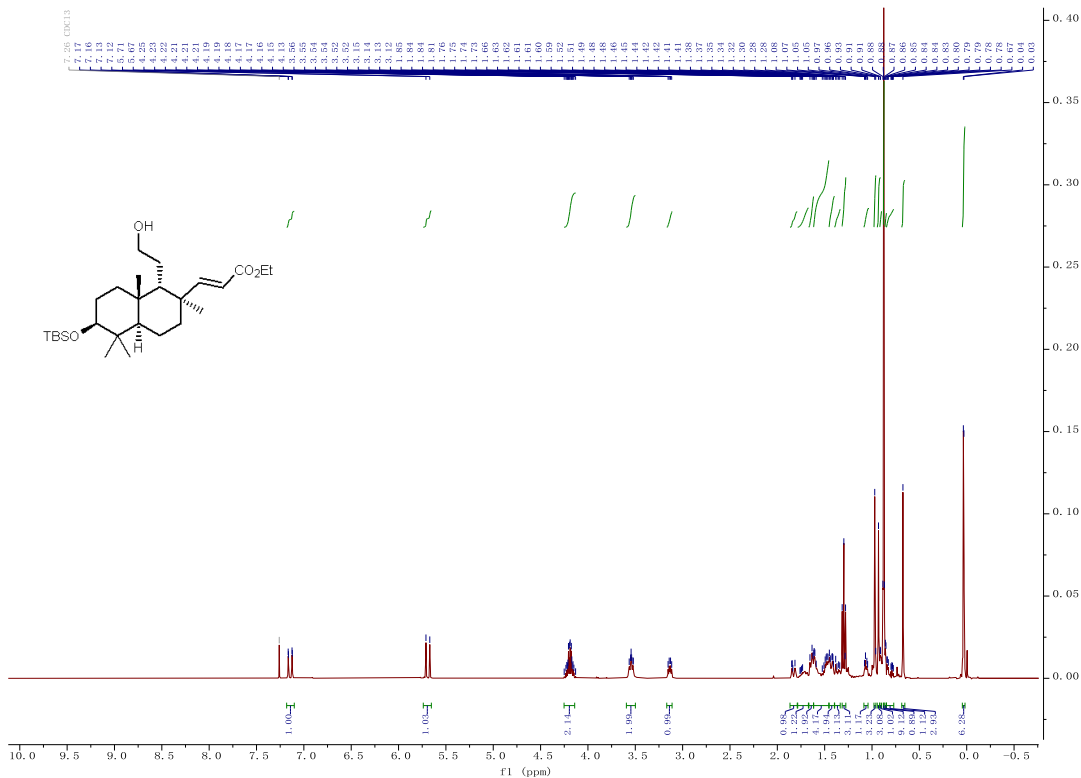# ^{1}H NMR of compound (±)**16** (400 MHz, CDCl$_3$)
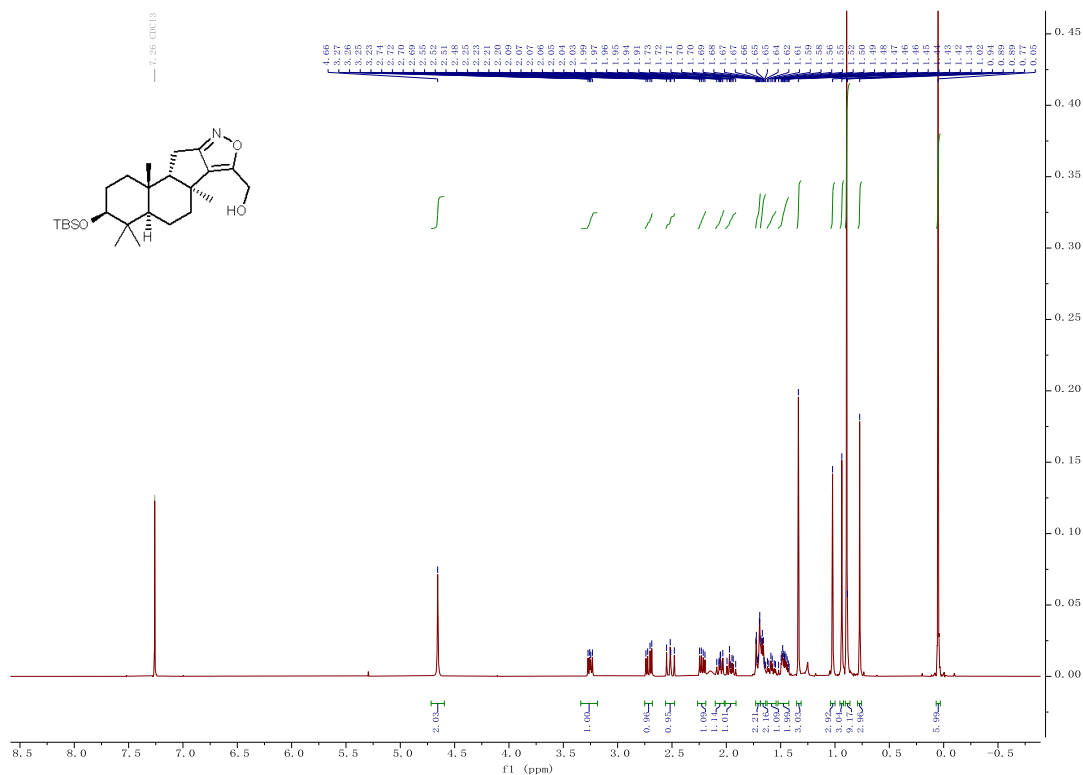
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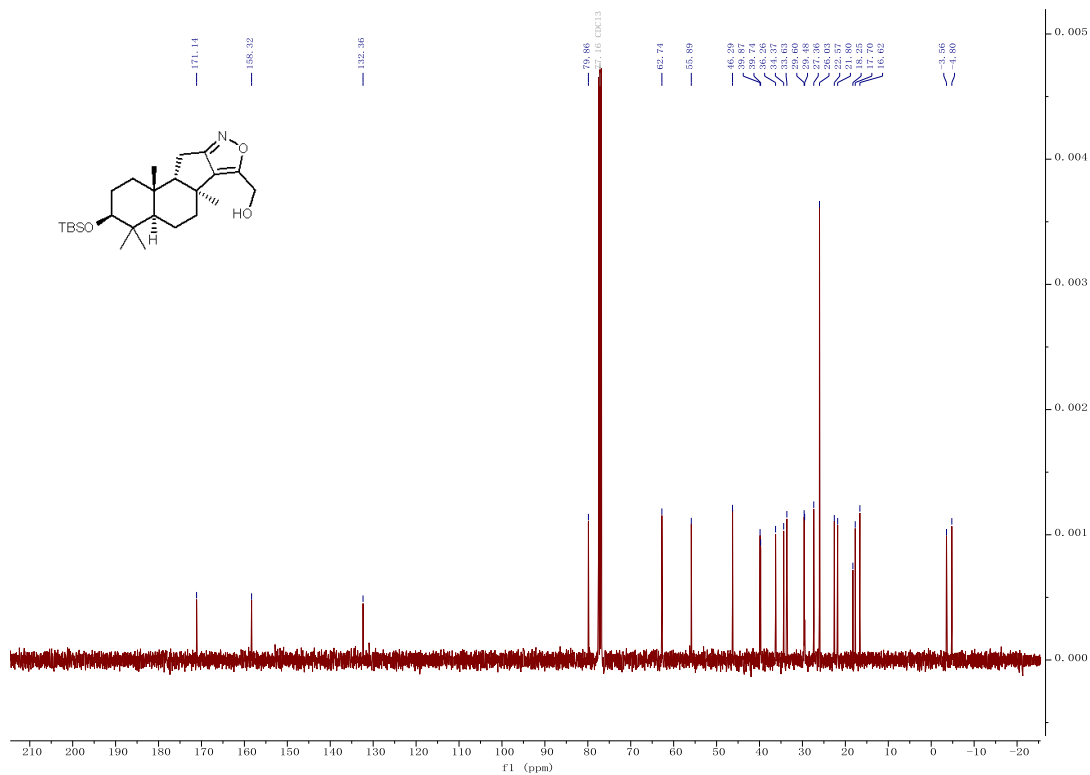
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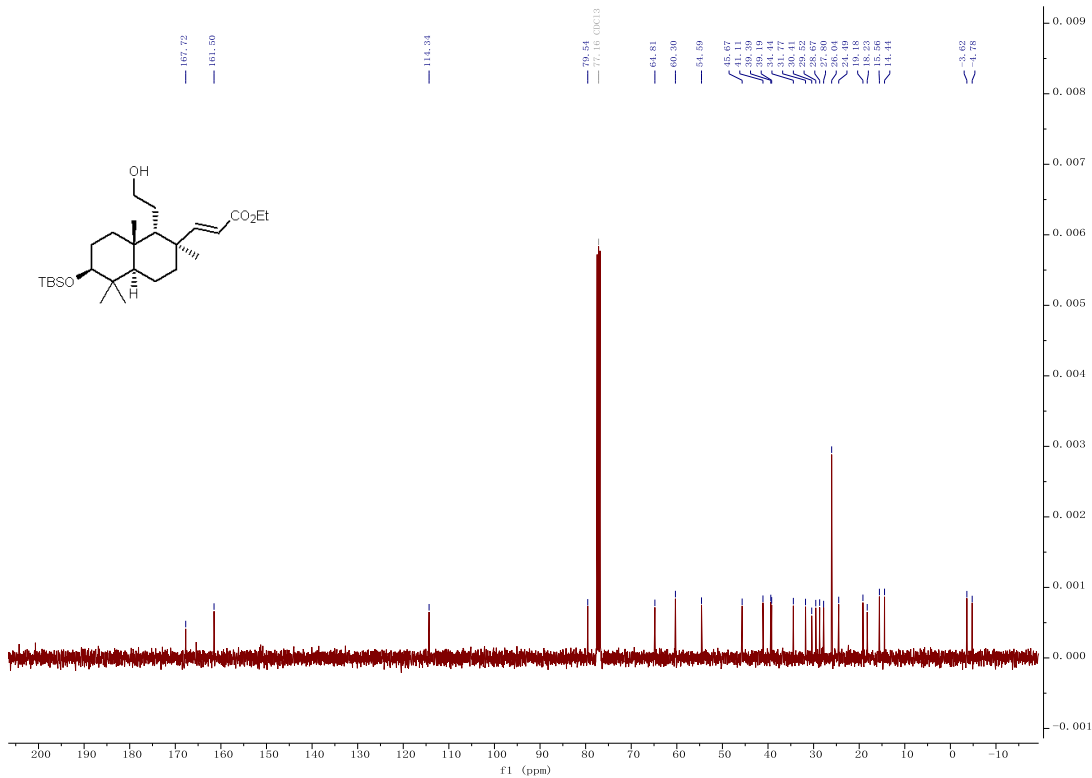

^{13}C NMR of compound (±)**17** (100 MHz, CDCl$_3$)

13

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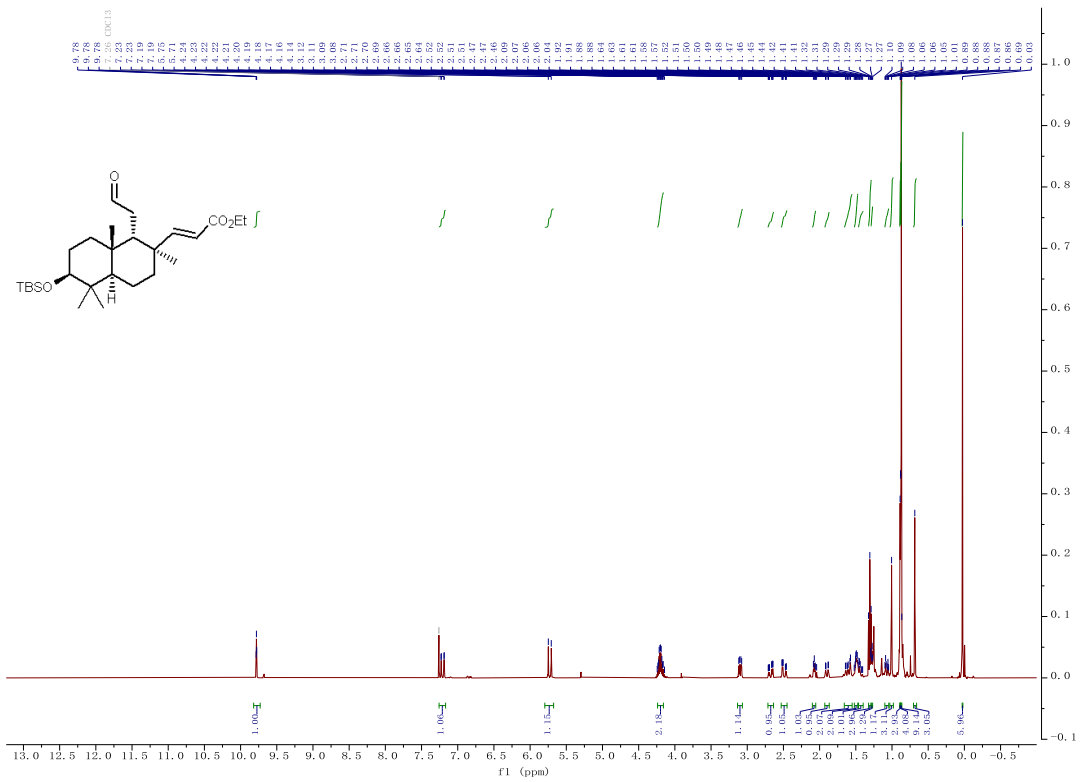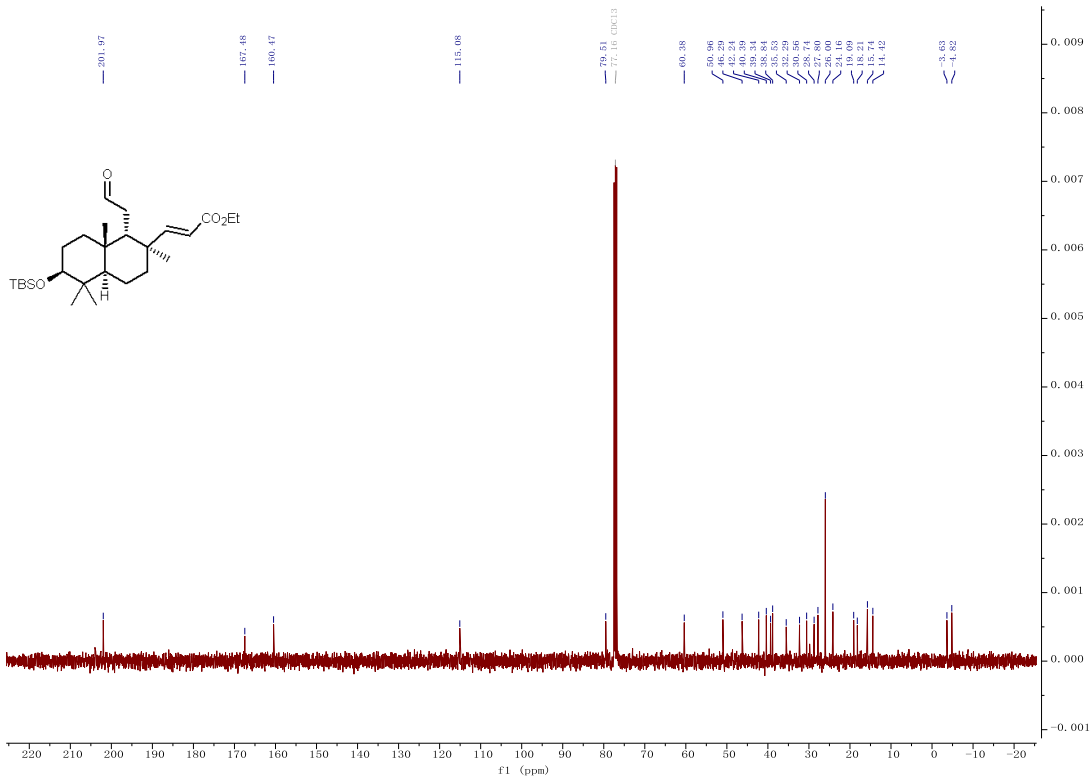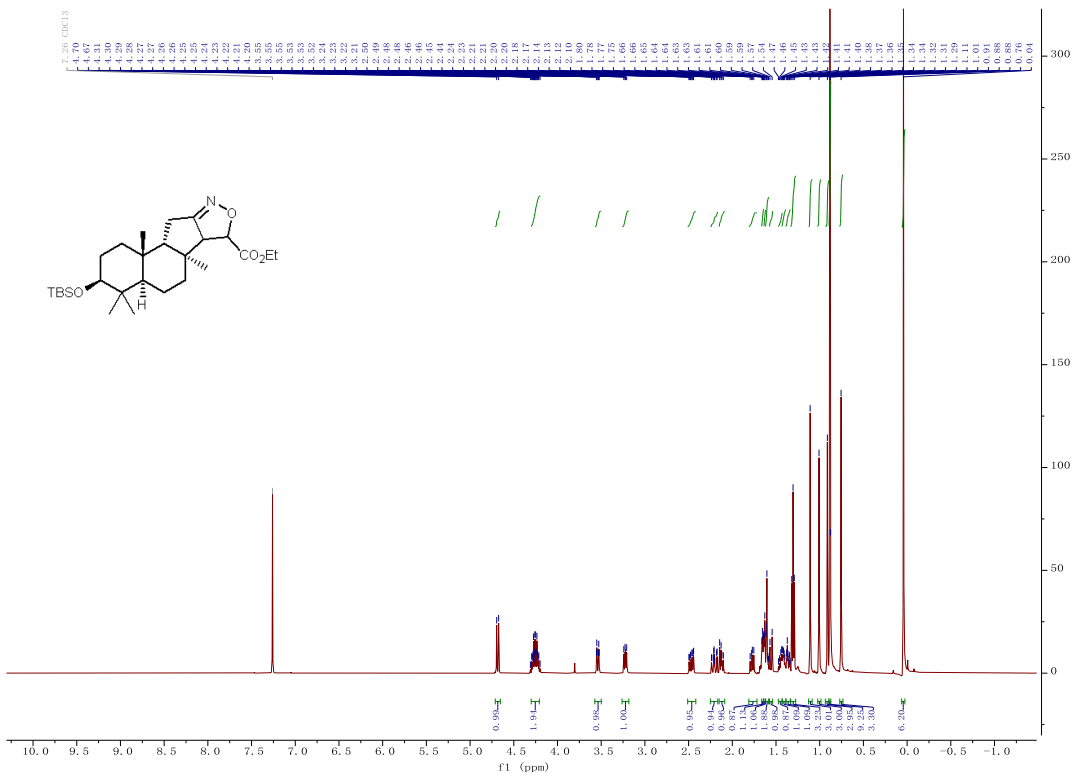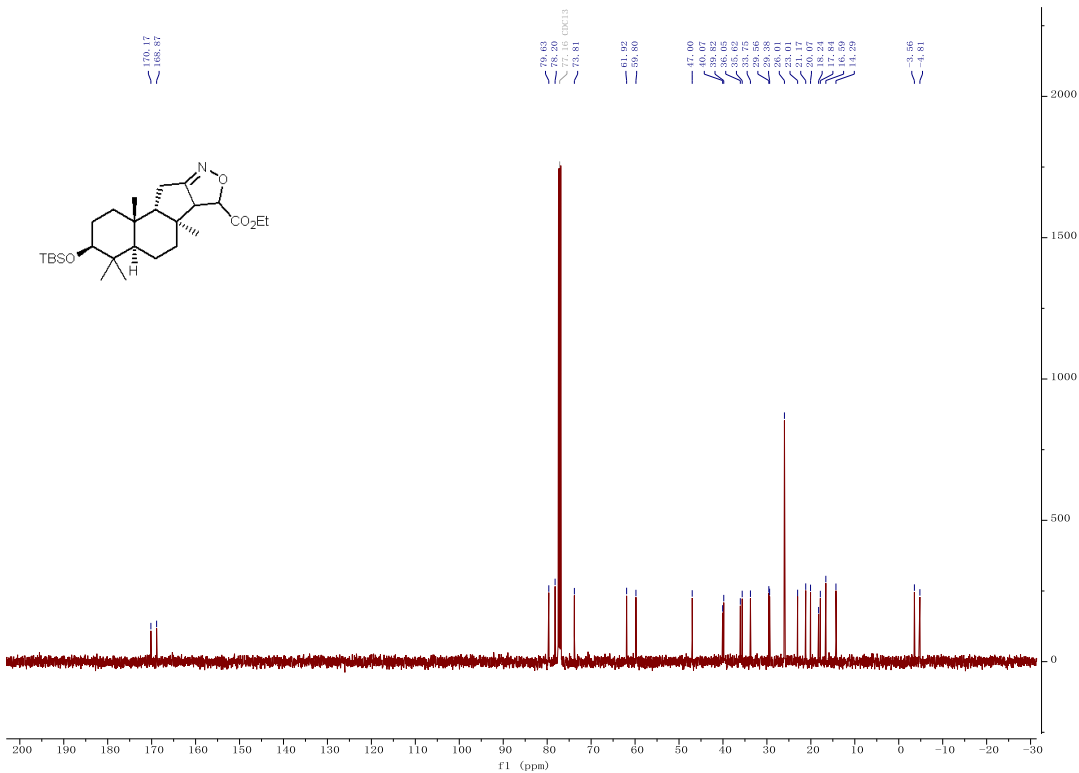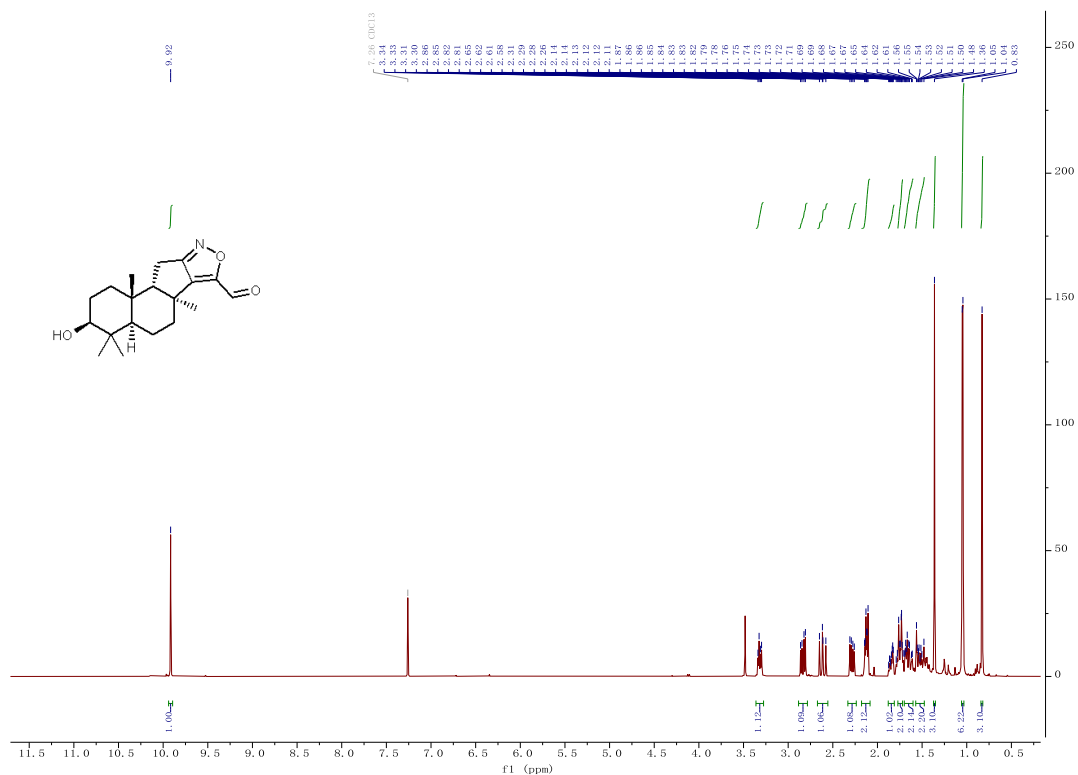

^{13}C NMR of compound (±)**1** (100 MHz, CDCl$_3$)
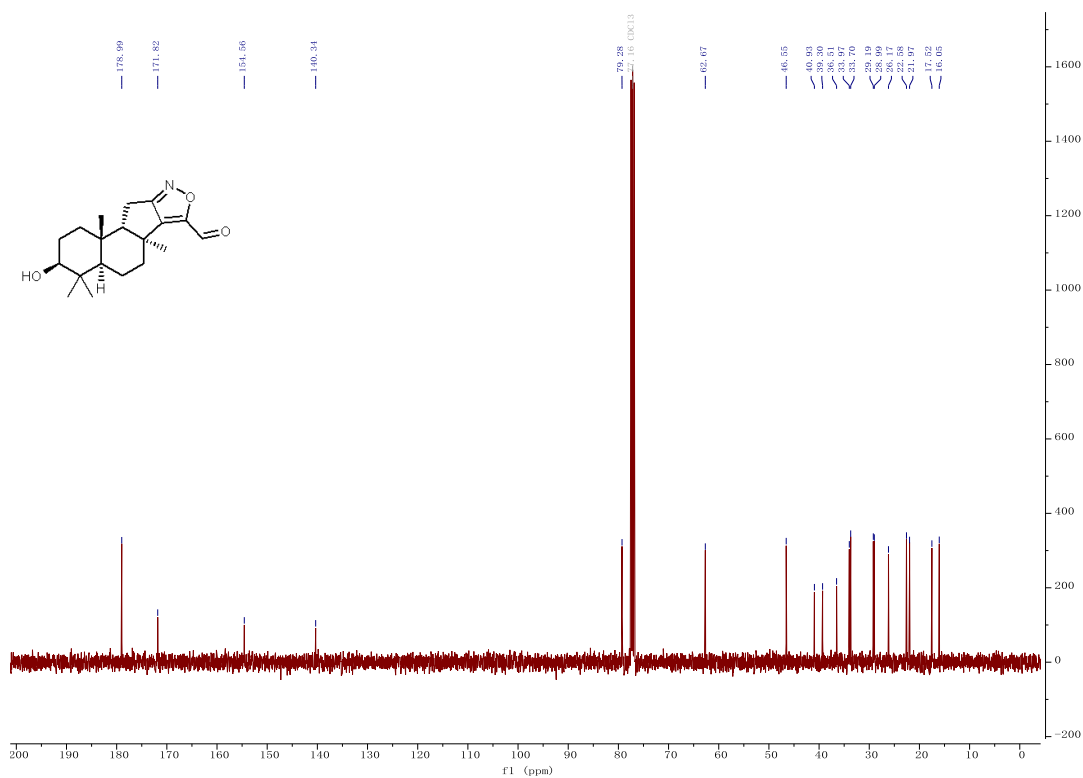
^{1}H NMR of compound **19** (400 MHz, CDCl$_3$)
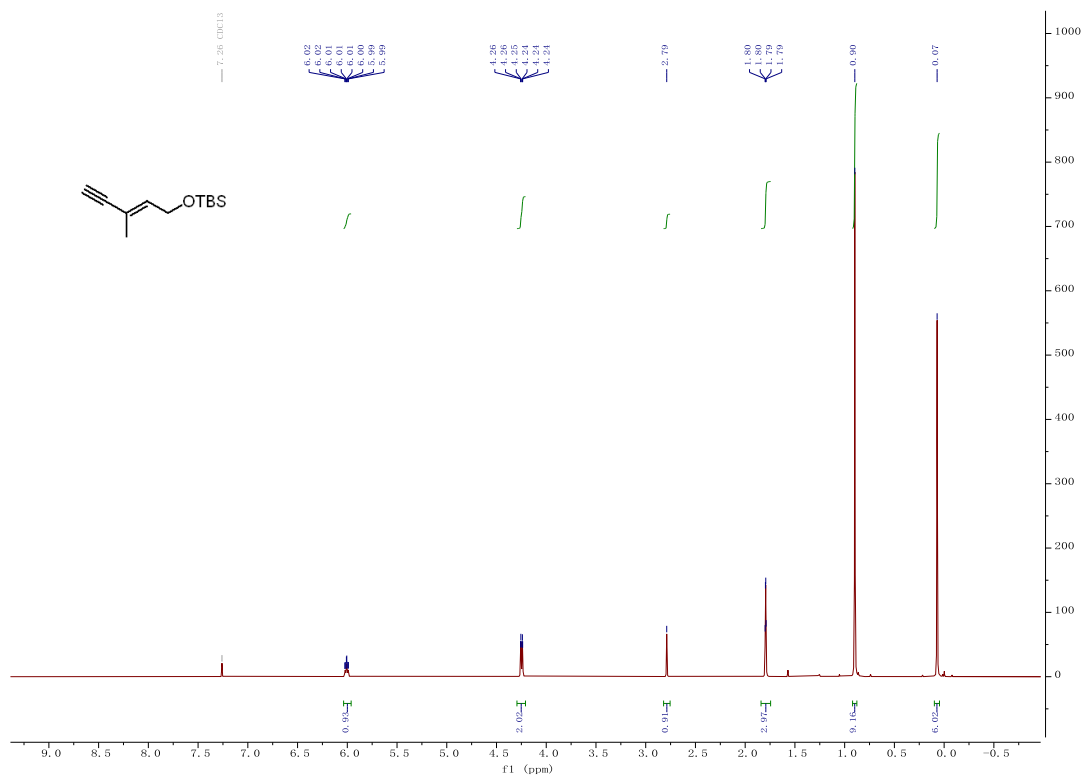
^{13}C NMR of compound **19** (100 MHz, CDCl$_3$)

^{1}H NMR of compound **21** (400 MHz, CDCl$_3$)
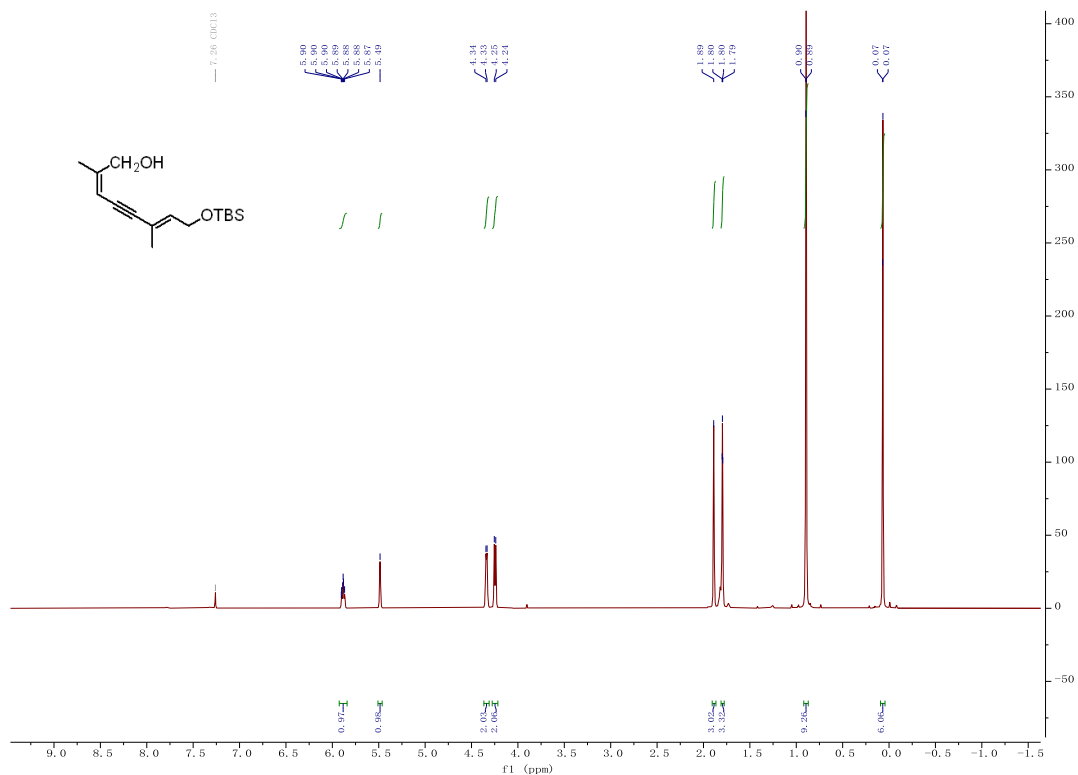
^{13}C NMR of compound **21** (100 MHz, CDCl$_3$)

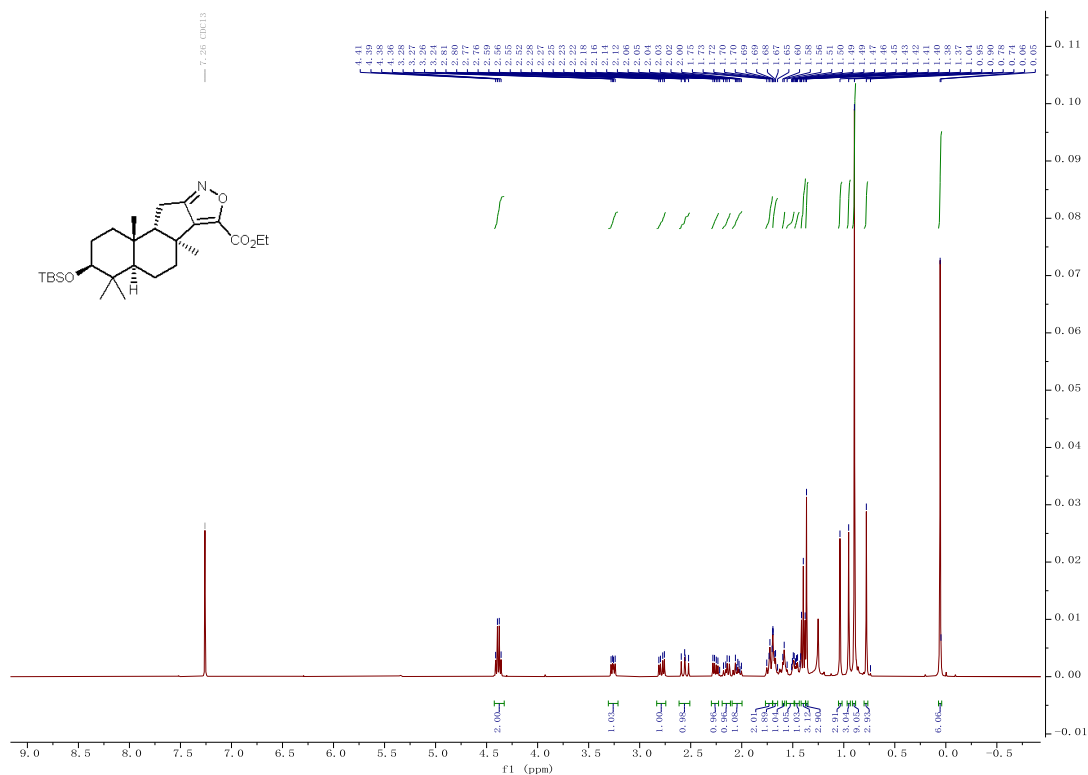# ^{1}H NMR of compound **22** (400 MHz, CDCl$_3$)
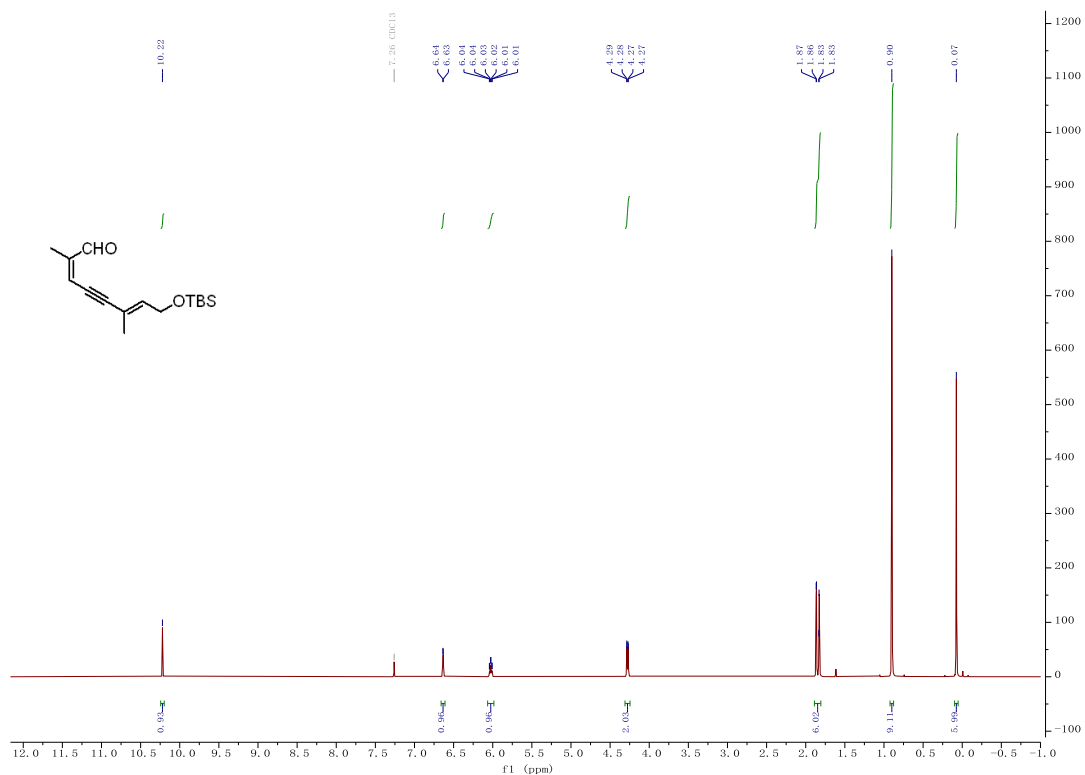
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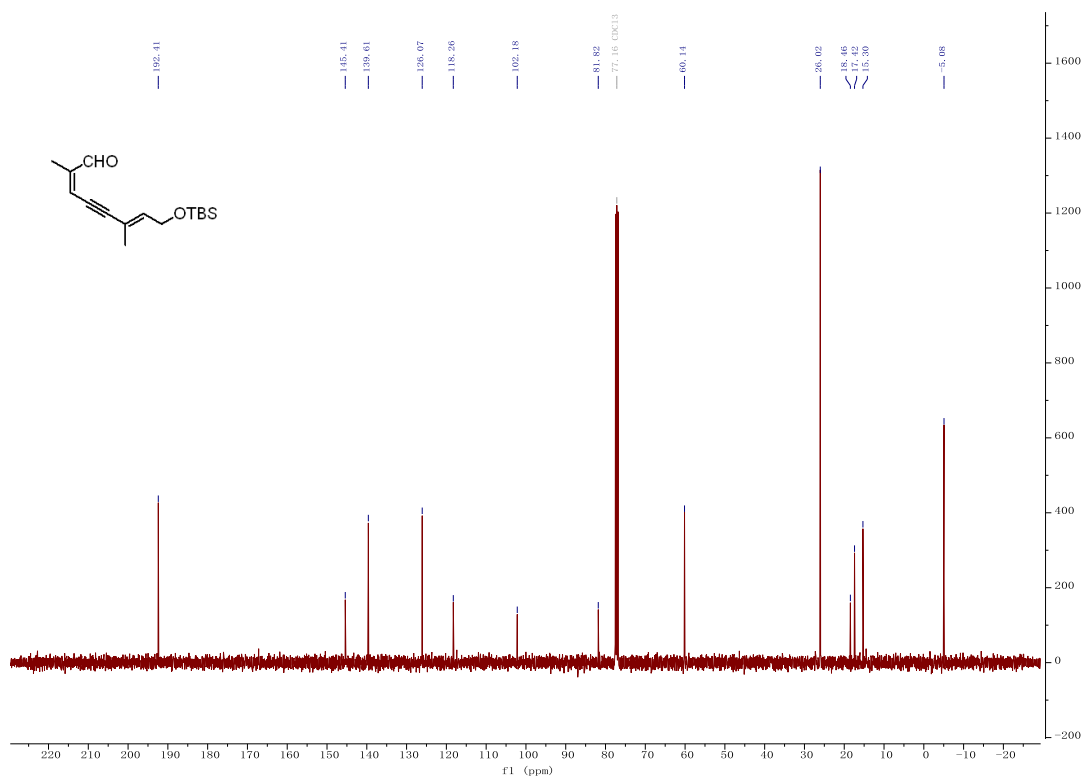
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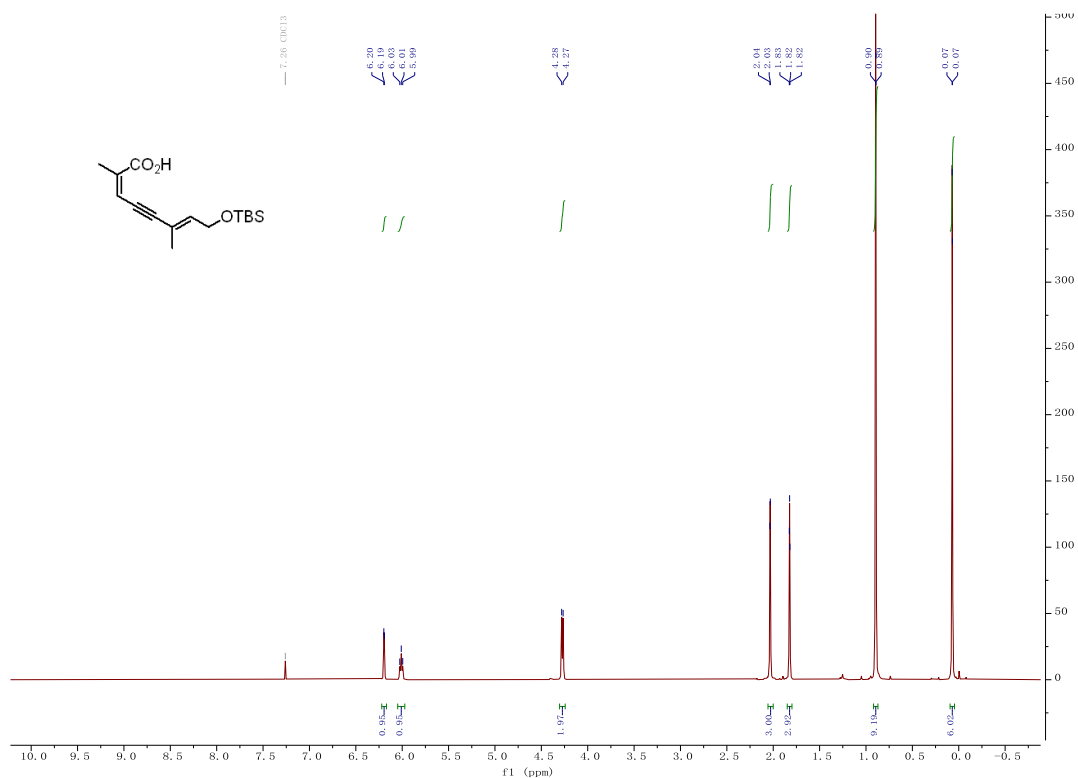
^{13}C NMR of compound **23** (100 MHz, CDCl$_3$)
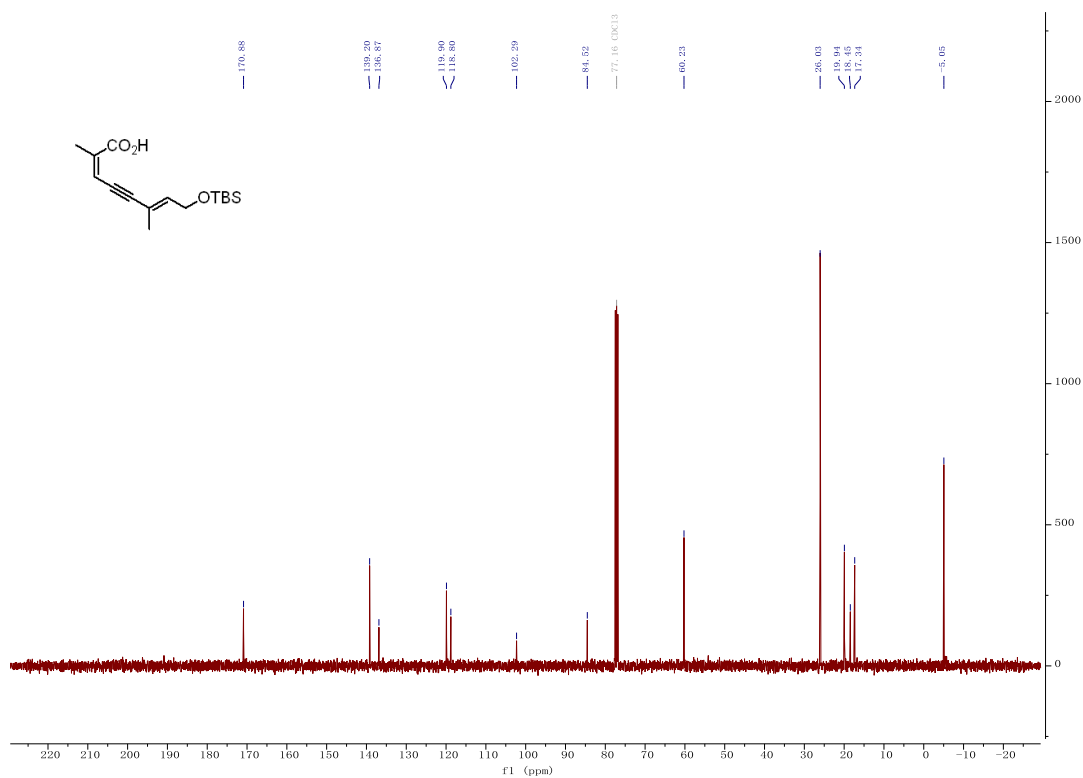
^{1}H NMR of compound **24** (400 MHz, CDCl$_3$)
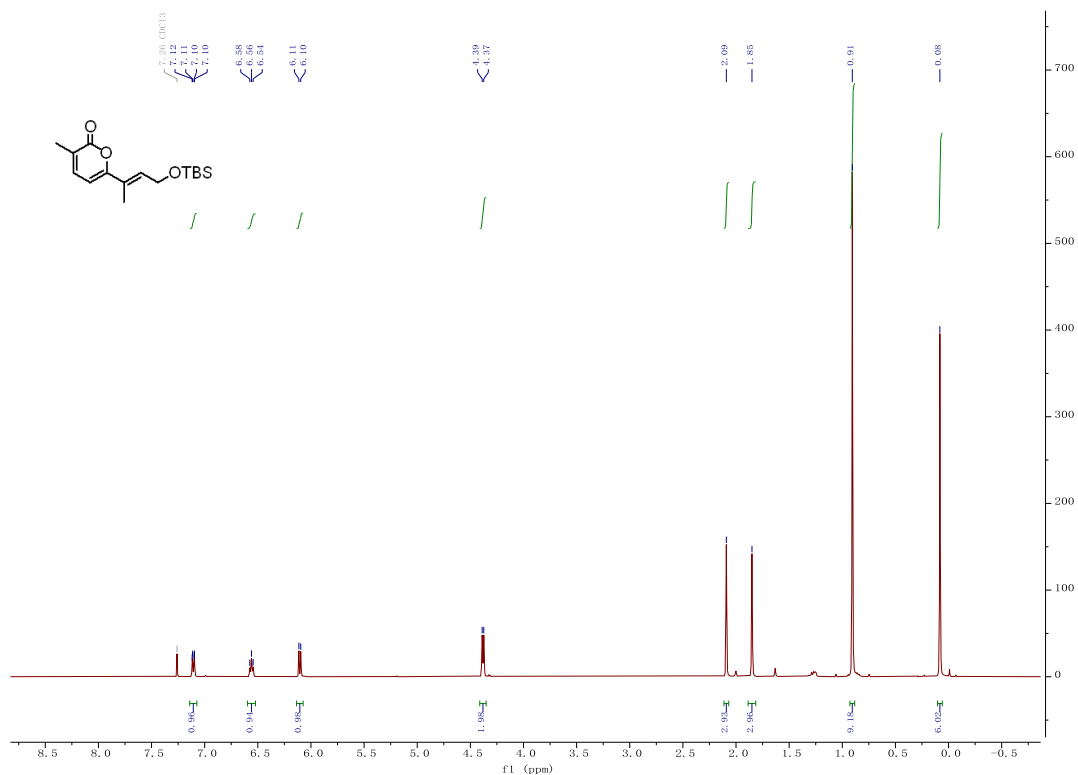
^{13}C NMR of compound **24** (100 MHz, CDCl$_3$)
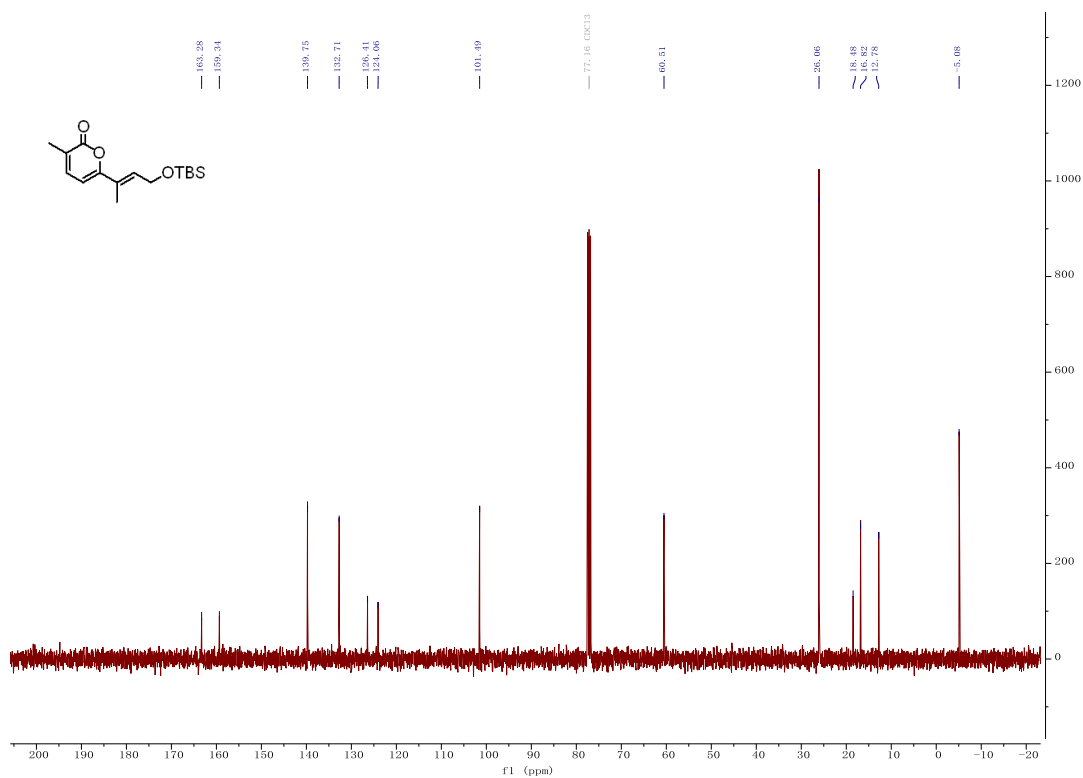
^{1}H NMR of compound **25** (400 MHz, CDCl$_3$)
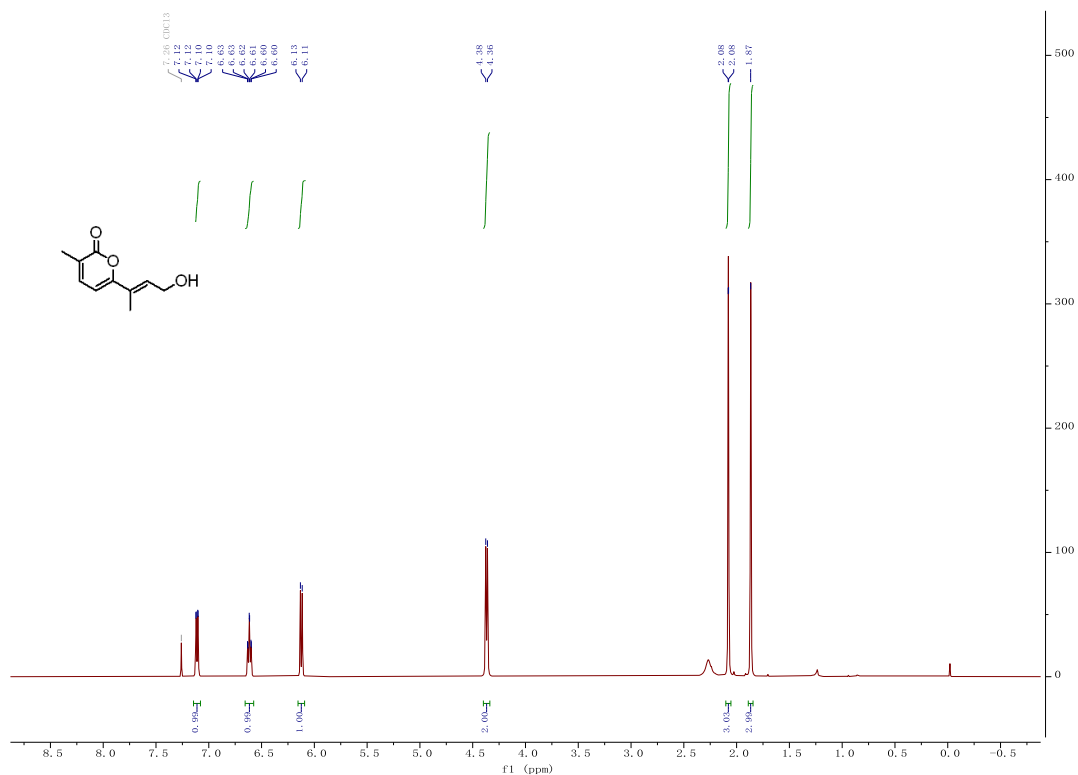
^{13}C NMR of compound **25** (100 MHz, CDCl$_3$)
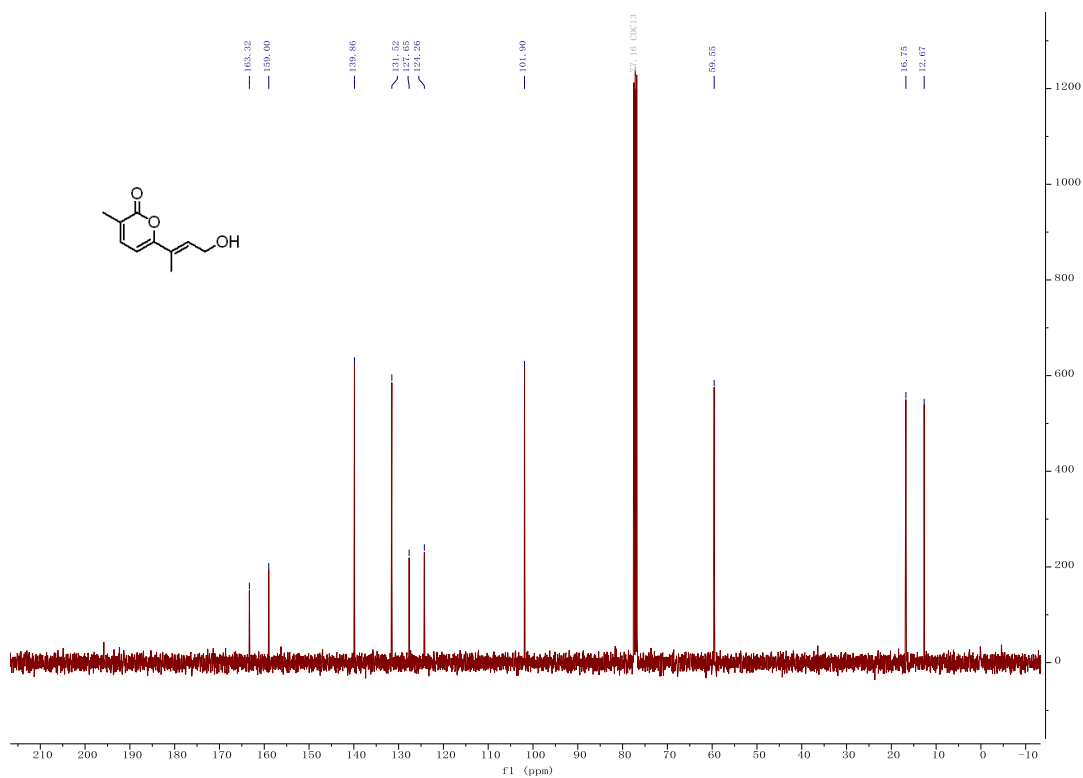
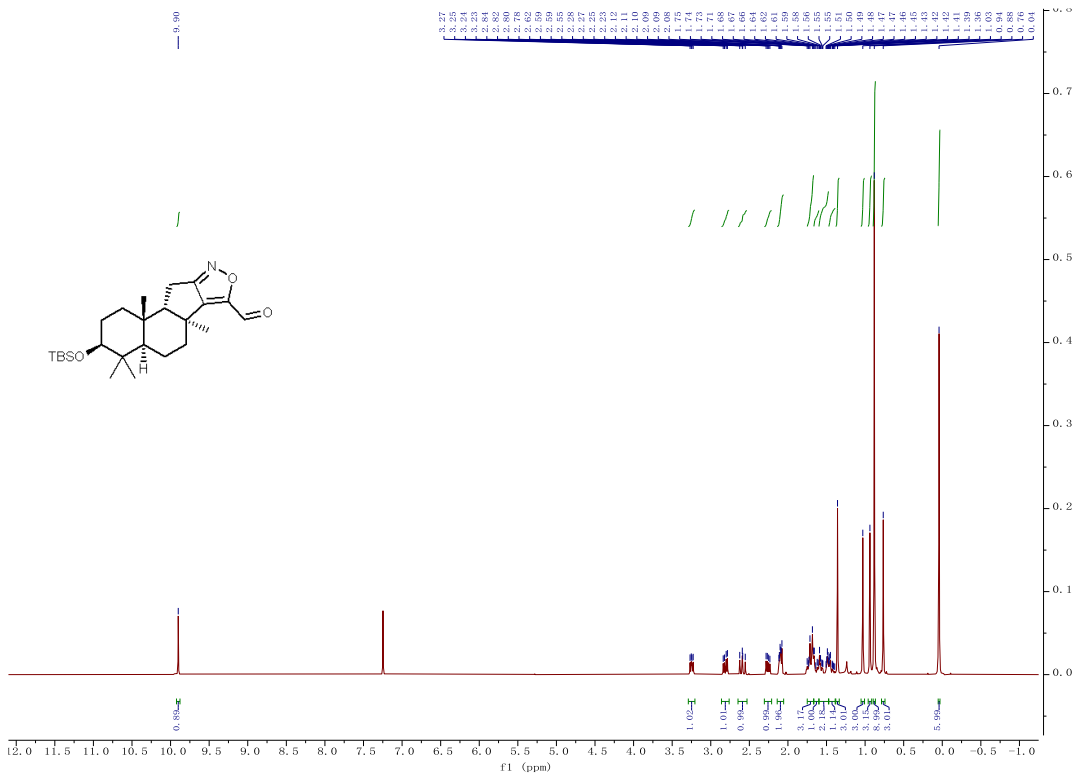¹H NMR of compound **2** (400 MHz, CDCl₃)
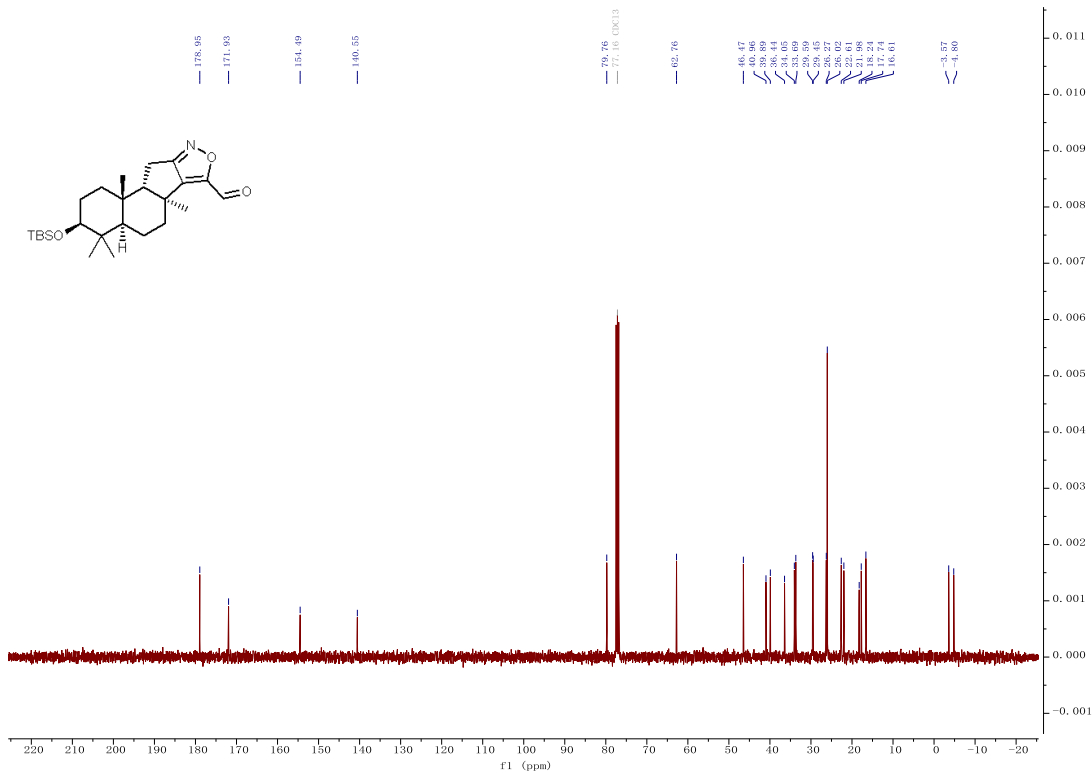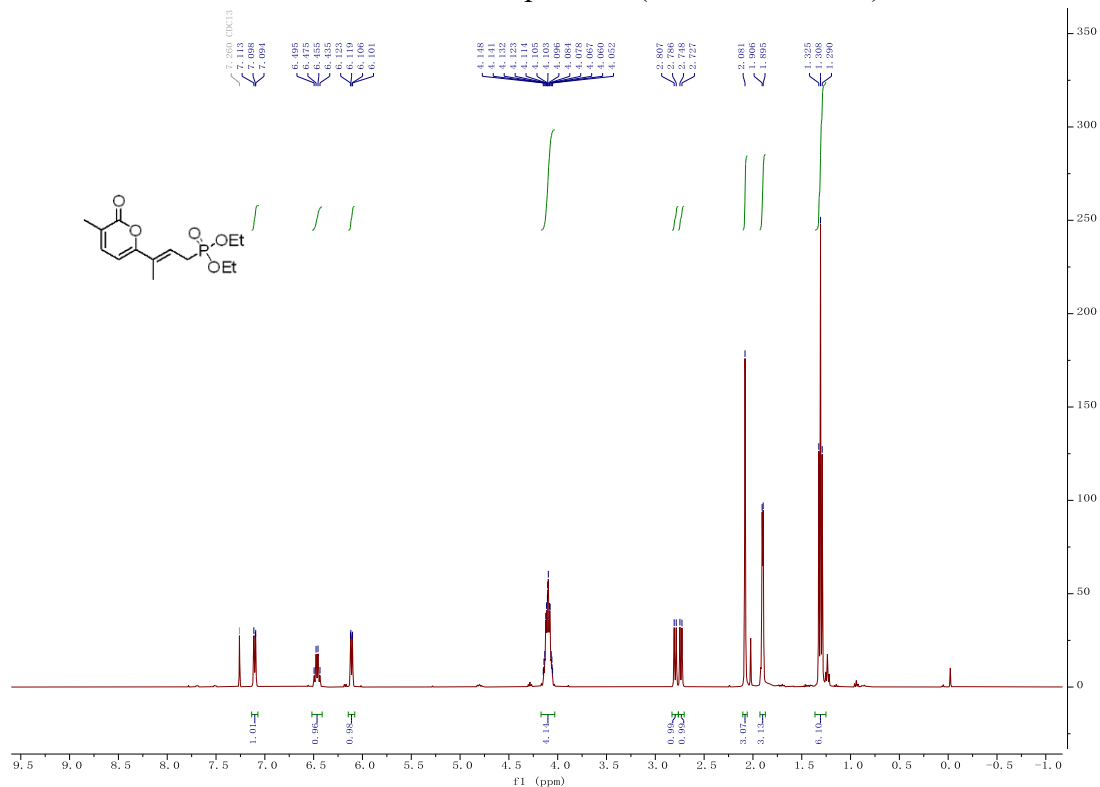

¹³C NMR of compound **2** (100 MHz, CDCl₃)

21

^{1}H NMR of compound **27** (400 MHz, CDCl$_3$)
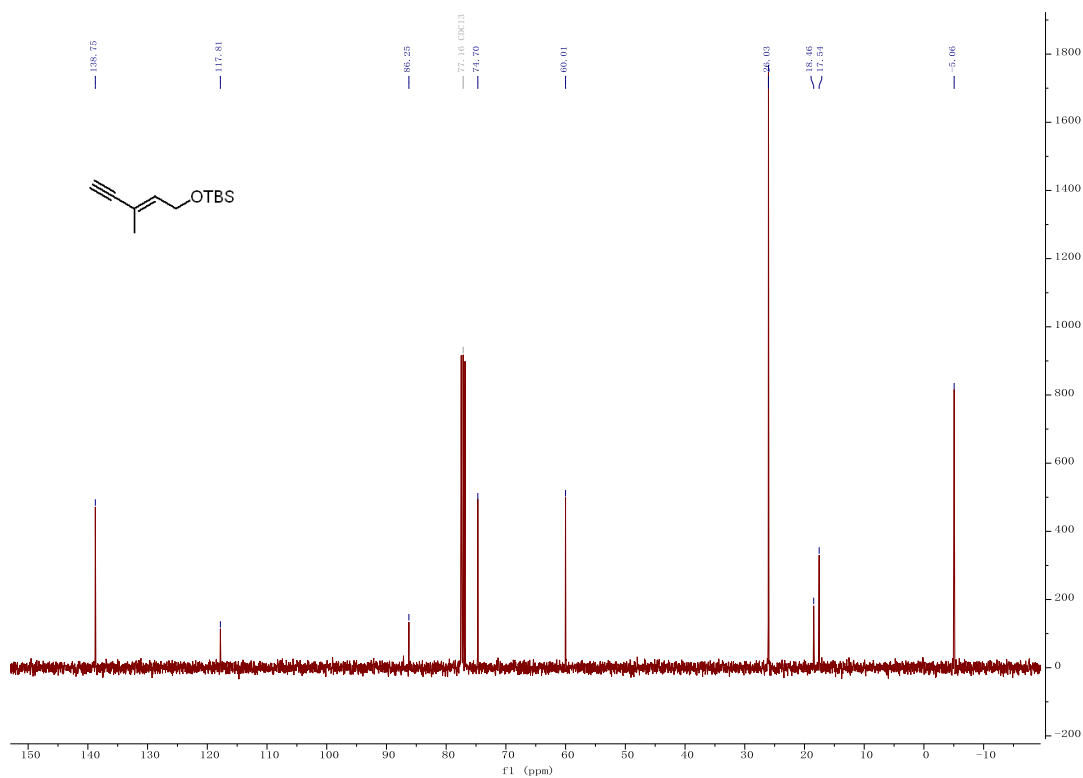

^{13}C NMR of compound **27** (100 MHz, CDCl$_3$)

^{1}H NMR of compound **29** (400 MHz, CDCl$_3$)

^{13}C NMR of compound **29** (100 MHz, CDCl$_3$)

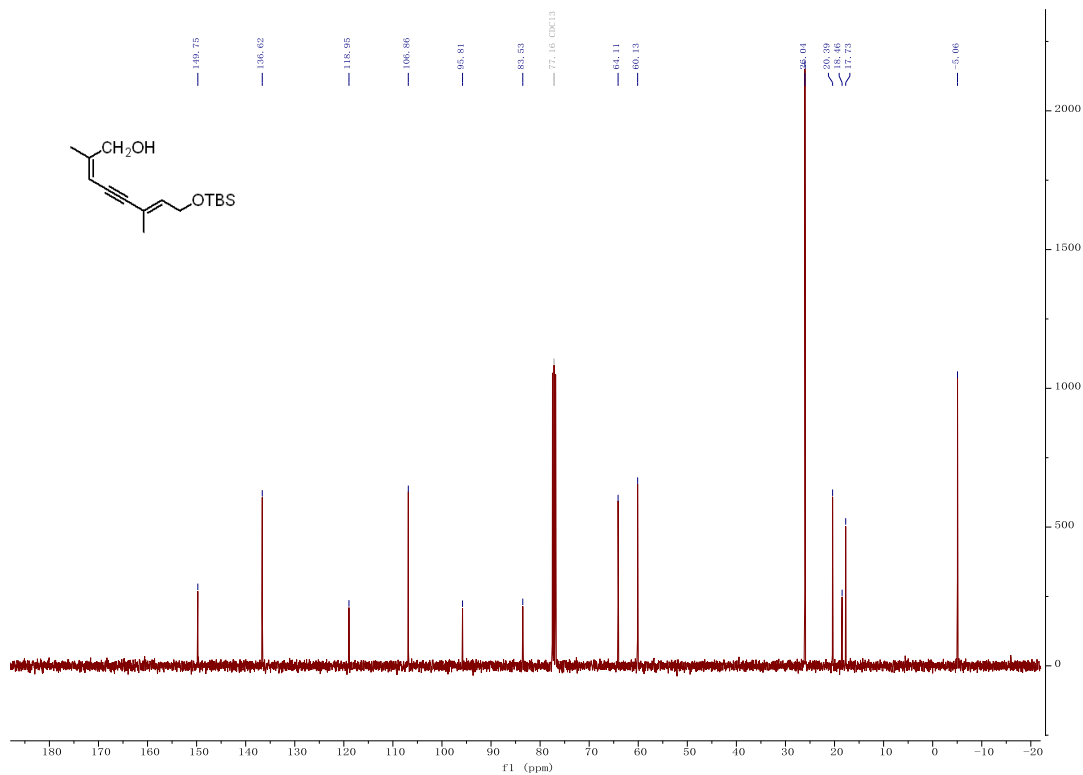# ¹H NMR of compound 30 (400 MHz, CDCl₃)
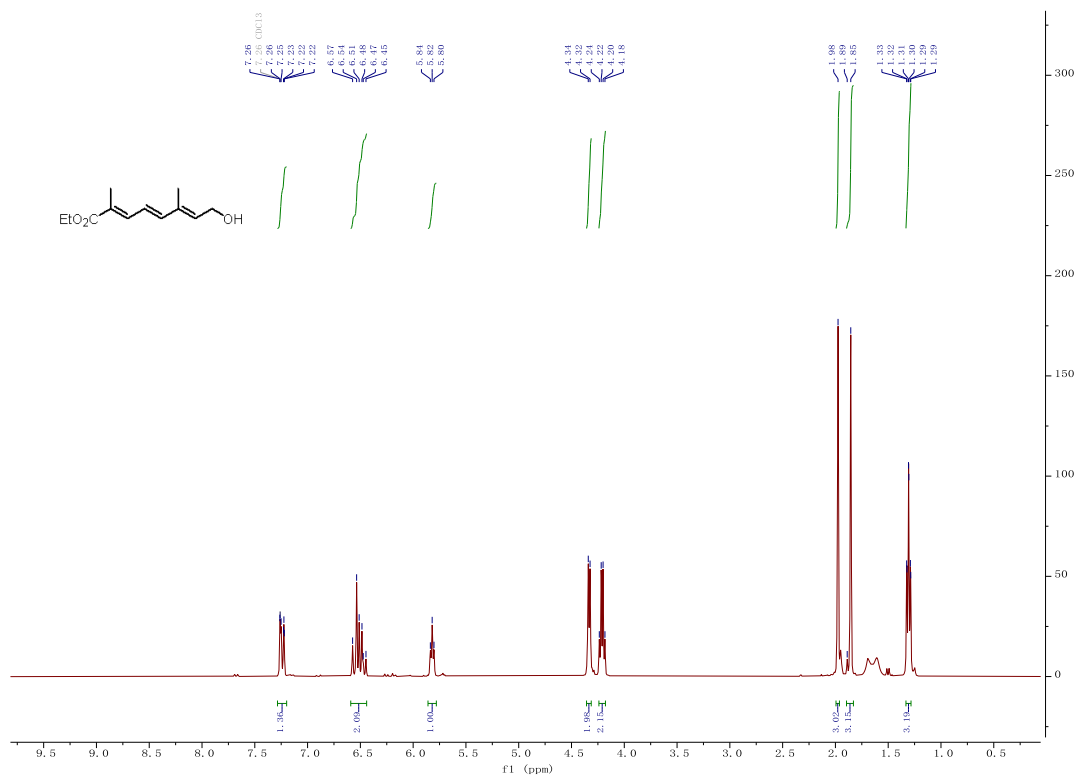
¹³C NMR of compound 30 (100 MHz, CDCl₃)
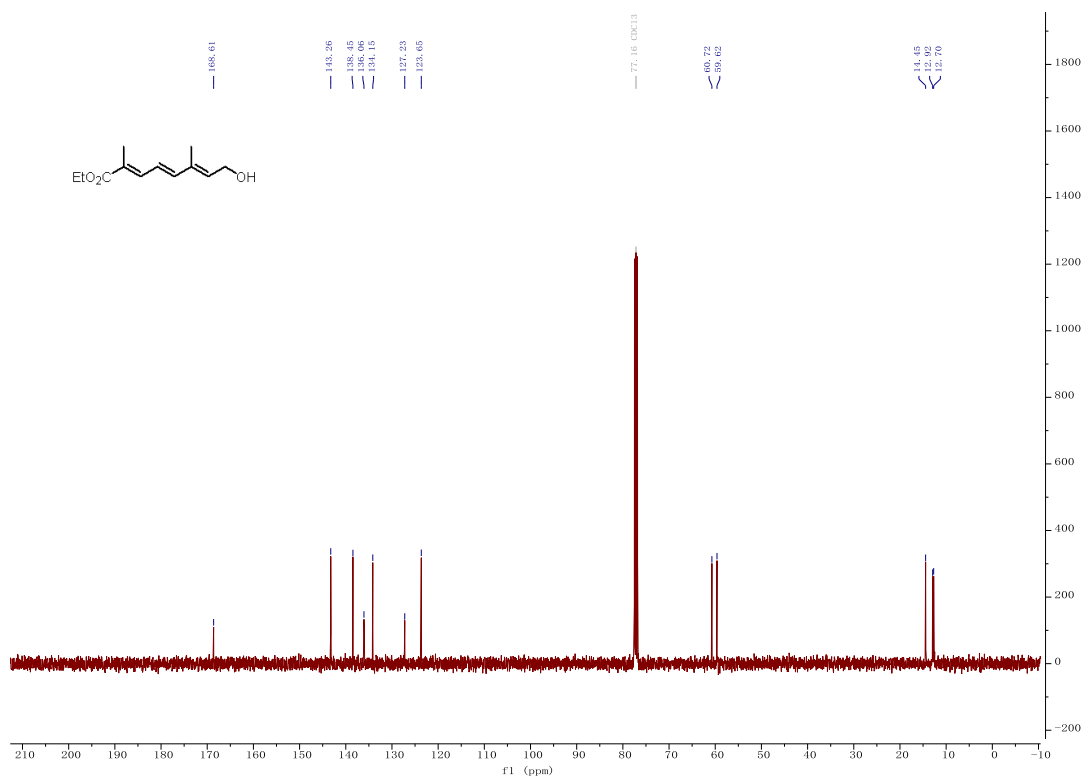
^{1}H NMR of compound **3** (400 MHz, CDCl$_3$)
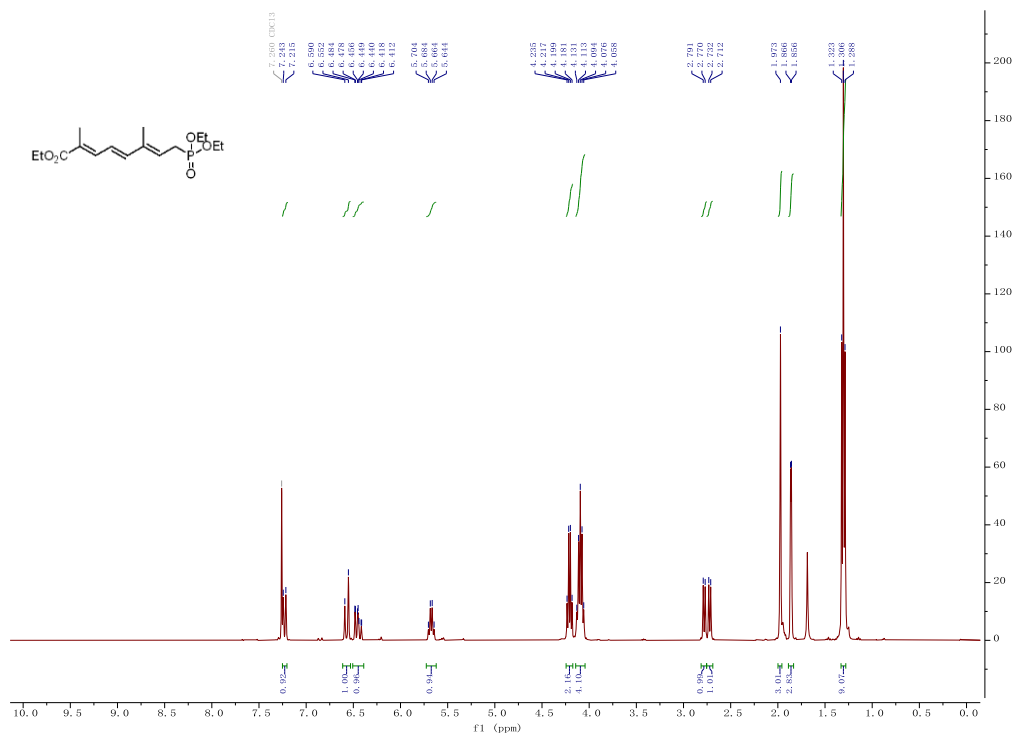
^{13}C NMR of compound **3** (100 MHz, CDCl$_3$)
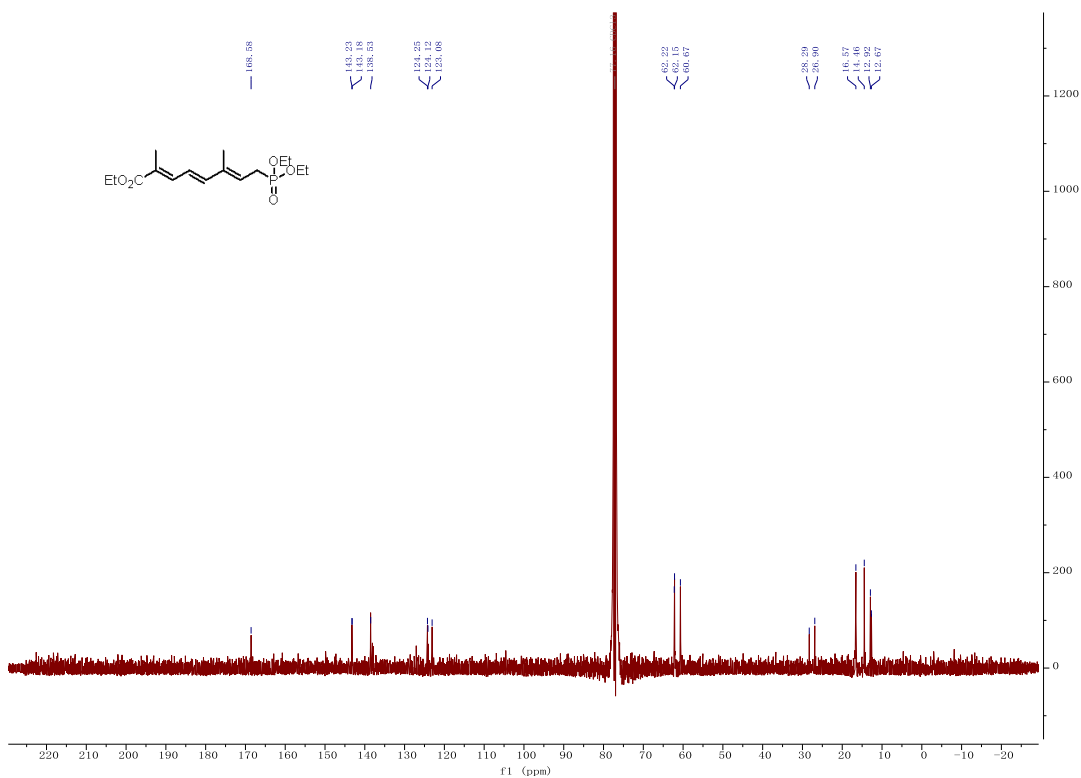
^{1}H NMR of compound (±)**1a** (400 MHz, CDCl$_3$)

^{13}C NMR of compound (±)**1a** (100 MHz, CDCl$_3$)

26
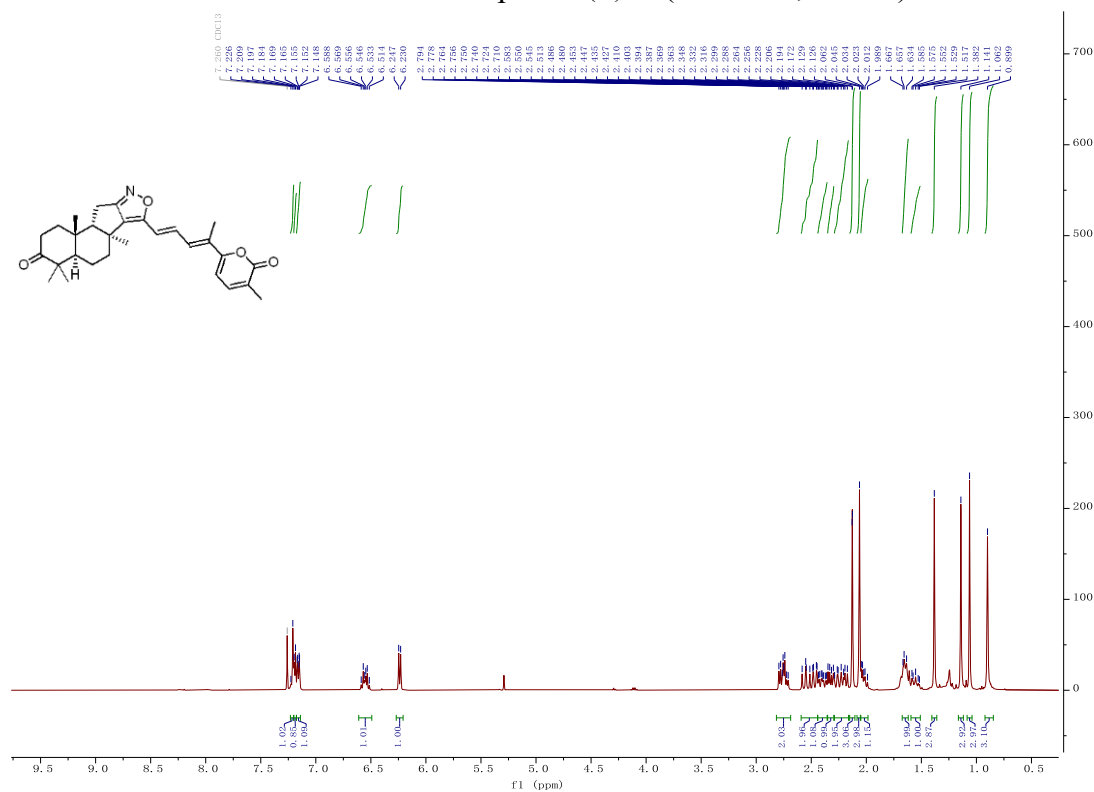
^{1}H NMR of compound (±)**1b** (400 MHz, CDCl$_3$)
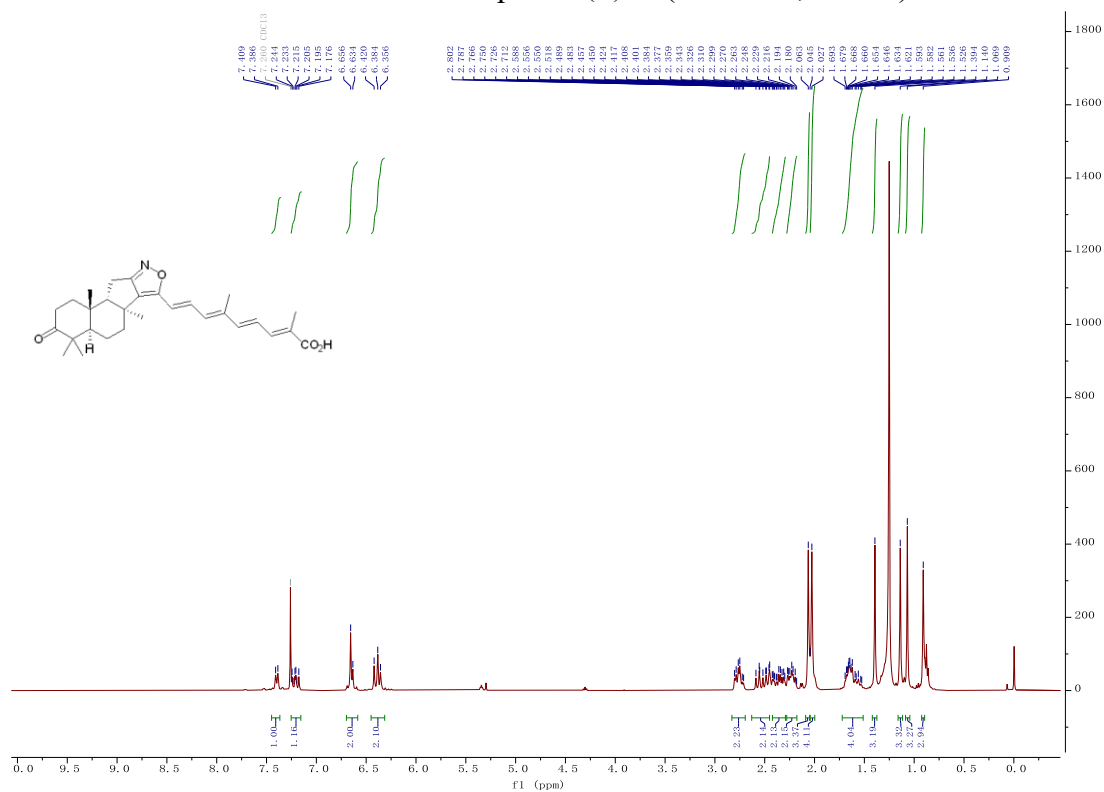
^{13}C NMR of compound (±)**1b** (100 MHz, CDCl$_3$)
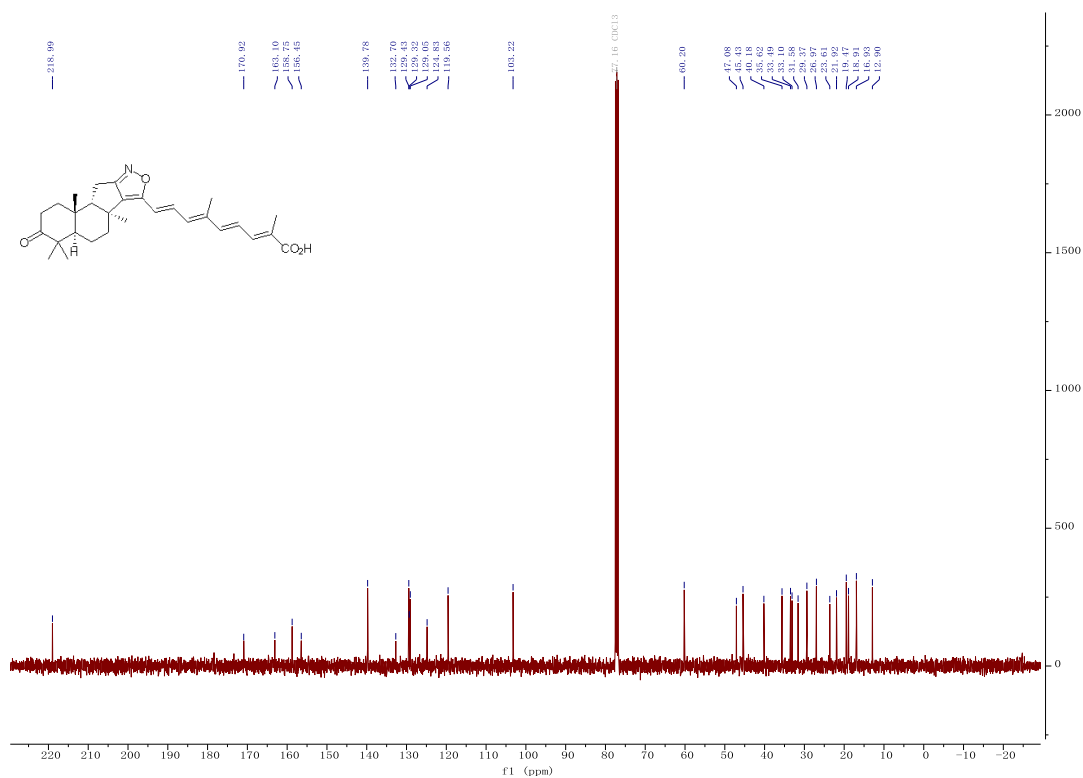
X-ray diffraction data of compound (±)**16** (CCDC 2473073)
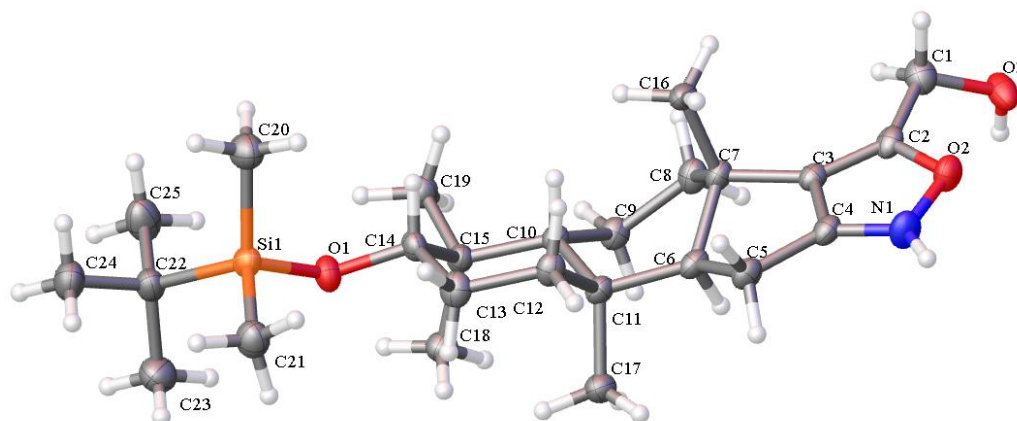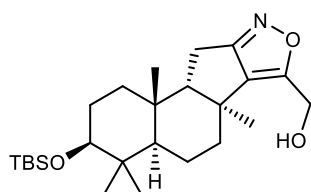
Crystal data and structure refinement compound (±)16

Identification code	WY1507
Empirical formula	$C_{25}H_{43}NO_3Si$
Formula weight	433.69
Temperature / K	118.2(3)
Crystal system	monoclinic
Space group	$P2_1/c$
a / Å, b / Å, c / Å	24.8728(12), 8.1363(4), 12.3226(6)
α/°, β/°, γ/°	90.00, 91.630(5), 90.00
Volume / Å^3	2492.8(2)
Z	4
ρ_{calc} / mg mm^{-3}	1.156
μ / mm^{-1}	0.119
F(000)	952
Crystal size / mm^3	0.42 × 0.39 × 0.02
2Θ range for data collection	5.98 to 52°
Index ranges	-30 ≤ h ≤ 30, -10 ≤ k ≤ 10, -15 ≤ l ≤ 14
Reflections collected	22043
Independent reflections	4840[R(int) = 0.0861 (inf-0.9Å)]
Data/restraints/parameters	4840/0/281

Goodness-of-fit on F^2		1.044
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]		$R_1 = 0.0568$, $wR_2 = 0.1195$
Final R indexes [all data]		$R_1 = 0.0870$, $wR_2 = 0.1364$
Largest diff. peak/hole / e Å^{-3}		0.302/-0.334
Flack Parameters		N
Completeness		0.9975

Table S1 The comparison of ^{13}C NMR data of 25 and reported natural Gibepyrone B[1]
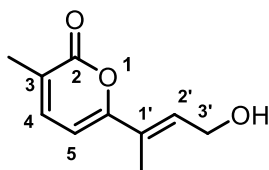
25 (Gibepyrone B)

	Gibepyrone B[1] ^{13}C NMR(δppm)	25 ^{13}C NMR(δppm)
C-2	163.2	163.3
C-3	128.3	127.7
C-4	139.7	139.9
C-5	101.9	101.9
C-6	160.0	159.0
C-1'	124.5	124.3
C-2'	131.1	131.5
C-3'	59.6	59.6
3-CH$_3$	16.8	16.8
1'-CH$_3$	12.7	12.7

Reference:

1. A. F. Barrero, J. E. Oltra, M. M. Herrador, E. Cabrera, J. F. Sanchez, J. F. Quílez, F. J. Rojas and J. F. Reyes, *Tetrahedron*, 1993, **49**, 141-150.

**The biological activity evaluation for (±)1a and (±)1b**

HL-60 human leukemia cell line was obtained from China Infrastructure of Cell Line Resources (Beijing, China). The cells were cultured in RPMI1640 medium supplemented with 10% FBS, 100 U/mL penicillin, and 100 mg/mL streptomycin at 37 °C in an atmosphere of 5% CO_2. The cells were then treated with a range of concentrations of compounds, along with a vehicle control (DMSO), in triplicate. After 72 hours of incubation, 30 μL of CellTiter-Glo reagent was added to each well. The plate was mixed on an orbital shaker for 2 minutes to induce cell lysis and subsequently incubated at room temperature for 10 minutes. Luminescence was recorded using a BioTek Synergy H1 plate reader. The half-maximal inhibitory concentration (IC_{50}) values were calculated using GraphPad Prism software (version 8.1, GraphPad Software, San Diego, CA, USA).
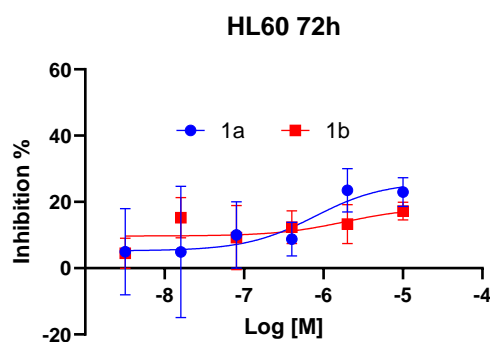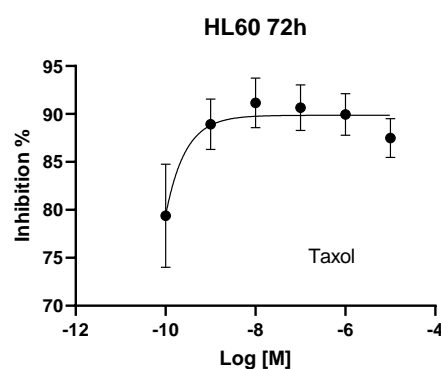
(A) (B)

Figure S1 (A) Antiproliferative activity of the model compounds in HL60 cell. (B) Antiproliferative activity of Taxol in HL60 cell.

TableS2 Antiproliferative activity of 1a and 1b in HL60 cell line

HL60	
Compound	IC_{50} (μM)
1a	>10
1b	>10
Taxol	<0.0001