

补充数据

舟叶橐吾中具有植物毒活性的佛术烷类倍半萜

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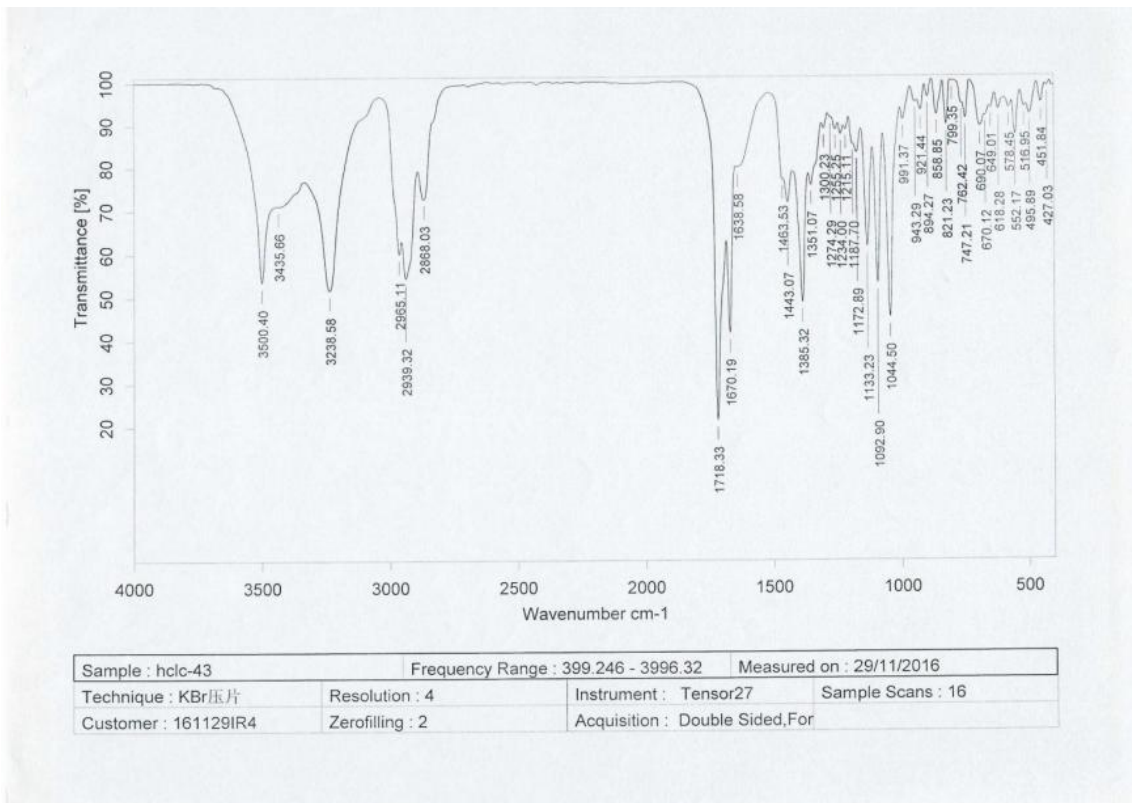


图1 化合物1的红外光谱图

Optical rotation measurement

Model: P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp. Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	16 (1/3)	Sp.Rot	133.0000	0.0133 0.0000	22.4 10.00 Cell	Wed Nov 16 18:51:55 2016 0.00100g/mL MeOH HCLC-43	Na 589nm	2 sec 10 sec
No.2	16 (2/3)	Sp.Rot	133.0000	0.0133 0.0000	22.4 10.00 Cell	Wed Nov 16 18:52:09 2016 0.00100g/mL MeOH HCLC-43	Na 589nm	2 sec 10 sec
No.3	16 (3/3)	Sp.Rot	132.0000	0.0132 0.0000	22.4 10.00 Cell	Wed Nov 16 18:52:22 2016 0.00100g/mL MeOH HCLC-43	Na 589nm	2 sec 10 sec

+133.0000

1/16

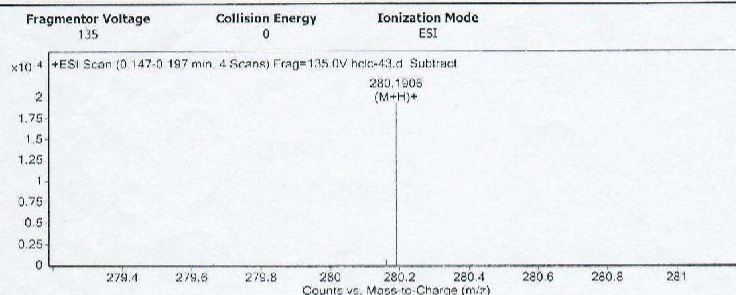
图3 化合物1的旋光光谱谱

Qualitative Analysis Report

Data Filename	hdc-43.d	Sample Name	hdc-43
Sample Type	Sample	Position	P1-D5
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	7/26/2016 11:13:35 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (RS125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
230.154	1	14627.32		
274.2741	1	33759.96		
280.1906	1	19299.21	C16 H25 N O3	(M+H)+
302.1728	1	26227.28		
318.3005	1	18816.92		
437.1934	1	12574.13		
453.1672	1	13467.26		
581.356	1	17622.28		

Formula Calculator Element Limits

Element	Min	Max
C	2	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C16 H25 N O3	279.1834	280.1907	280.1906	0.3	0.9	5.0000

--- End Of Report ---

图4 化合物1的HR-EI-MS图谱

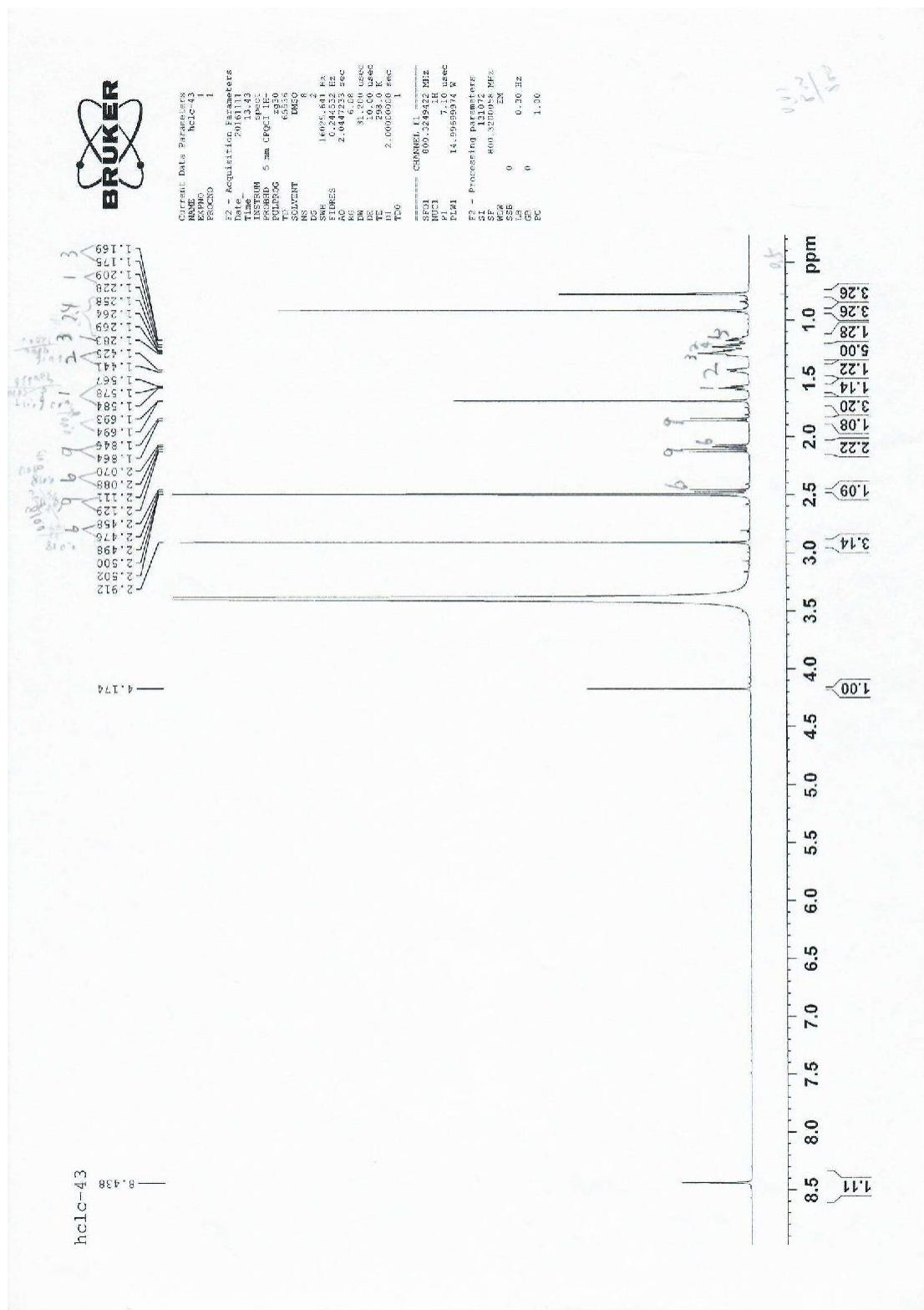


图5 化合物1的¹H NMR图谱 (800 MHz, DMSO-d₆)

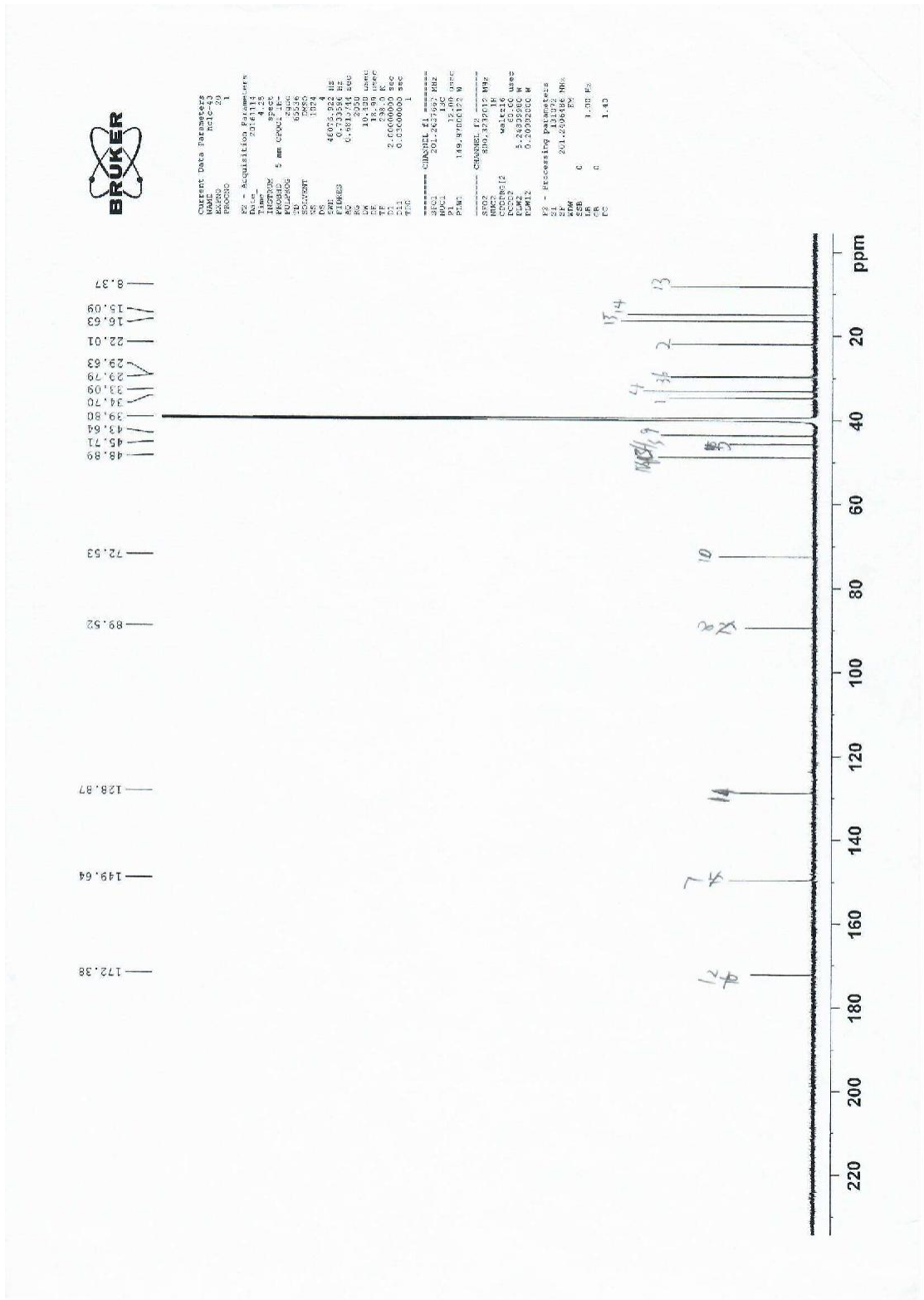


图6 化合物1的¹³C NMR图谱 (200 MHz, DMSO-d₆)

hclc-43 bc



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NAME hclc-43
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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PROBHD 5 mm QNP1H
PULPROG zgpg30
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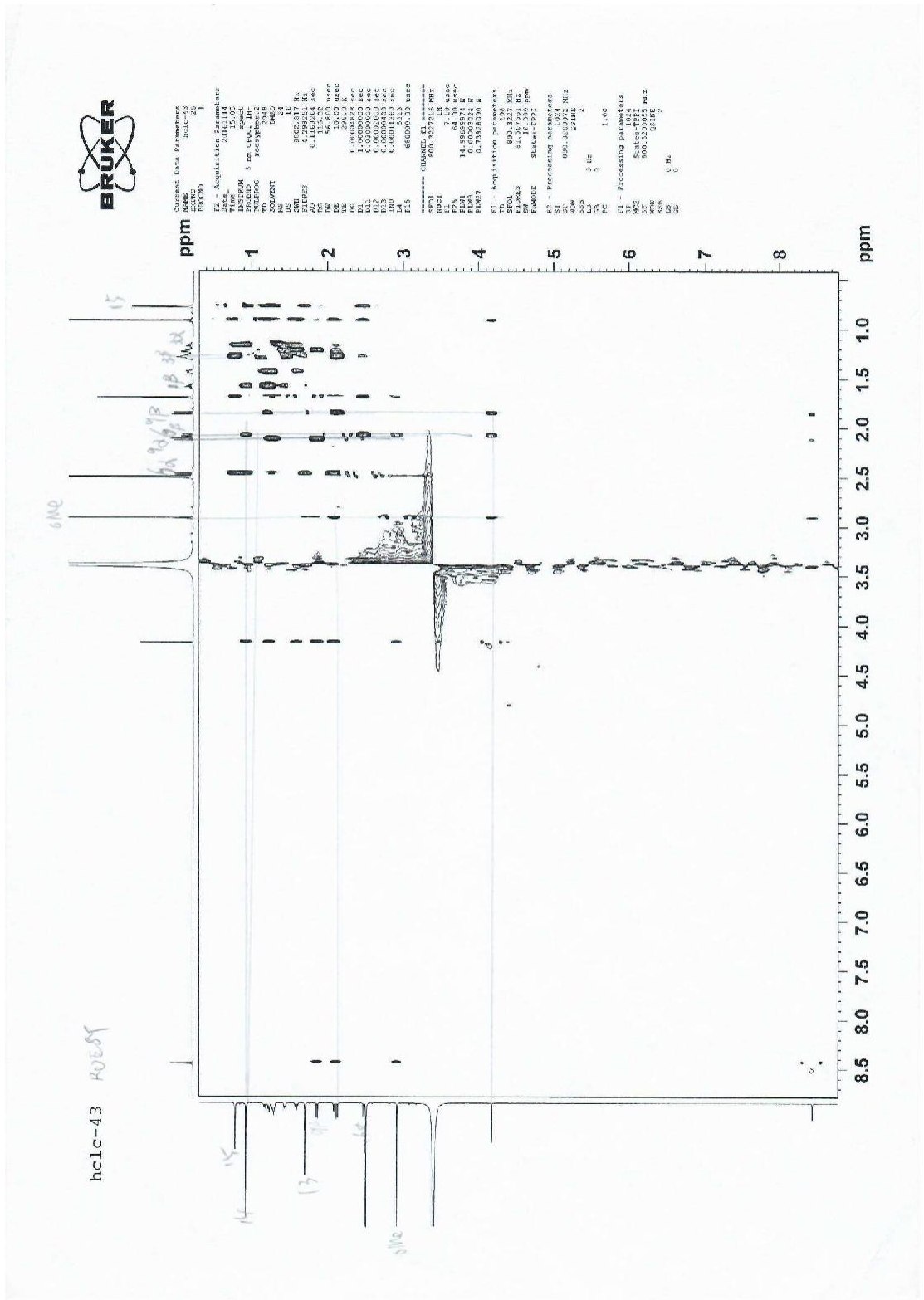


图11 化合物1的ROESY图谱