

Supplementary Materials

Melatonin receptors agonistic activities of phenols from *Gastrodia elata*

Si-Yue Chen^{a,b}, Chang-An Geng^a, Yun-Bao Ma^a and Ji-Jun Chen^{a,b}*

^a State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Yunnan Key Laboratory of Natural Medicinal Chemistry, Kunming 650201, China

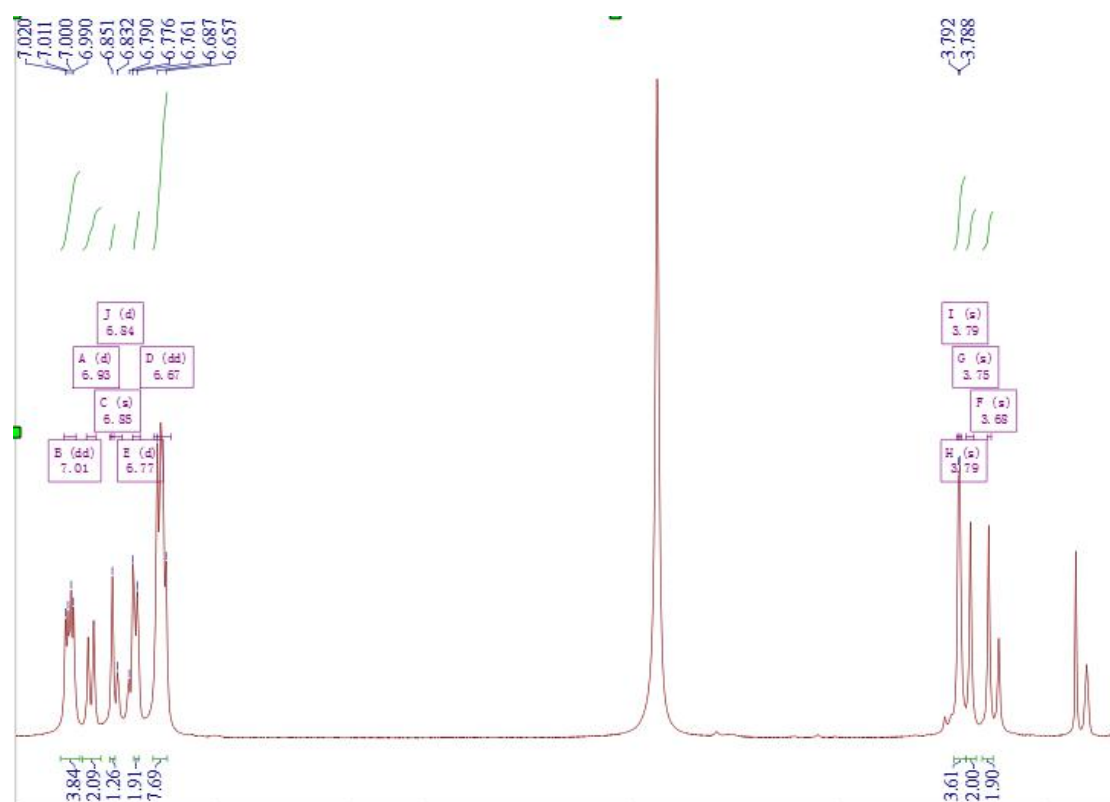
^b University of Chinese Academy of Sciences, Beijing 100049, China

*Corresponding author. Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, P. R. China. Tel.: +86 871 65223265; Fax: +86 871 65227197. *E-mail address*: chenjj@mail.kib.ac.cn (Ji -Jun Chen).

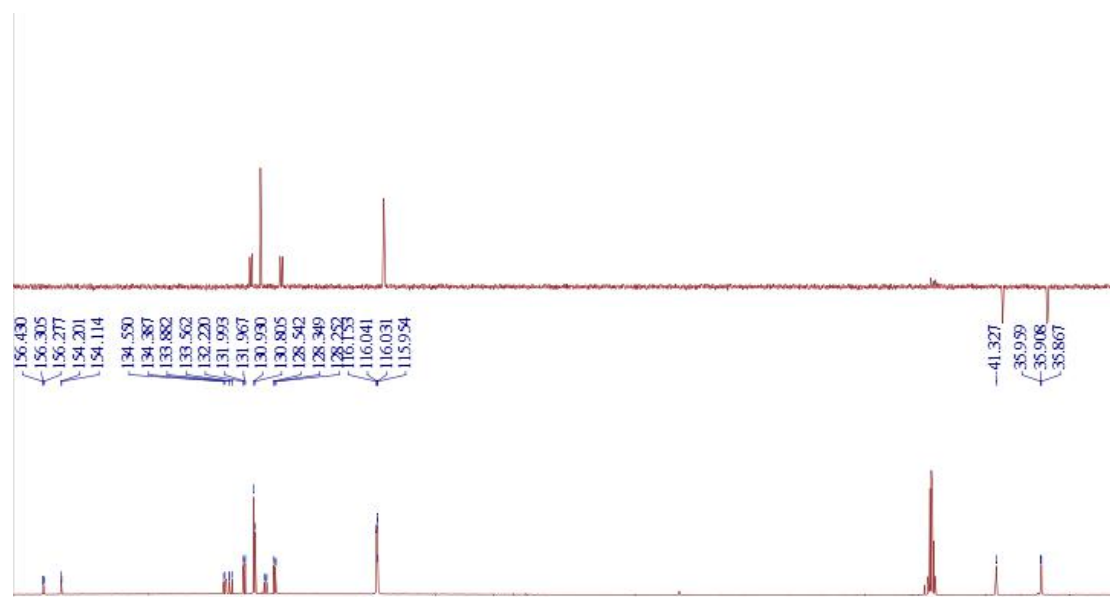
List of Supplementary material

1D NMR, 2D NMR ,HRESIMS , UV and IR Spectra of compound 1	S1—S8
1D NMR, 2D NMR ,HRESIMS , UV and IR Spectra of compound 2	S9—S16
1D NMR, HRESIMS , UV and IR Spectra of compound 3	S17—S21

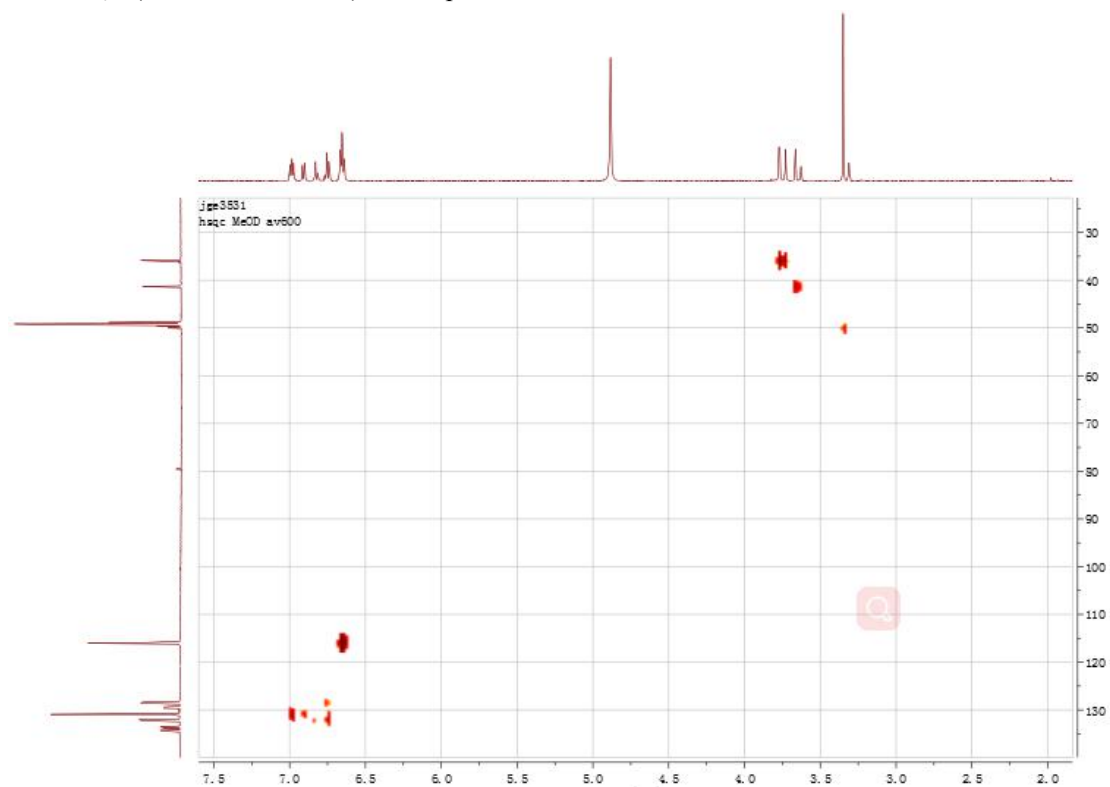
S1. ^1H -NMR (150 MHz, CD_3OD) of compound **1**



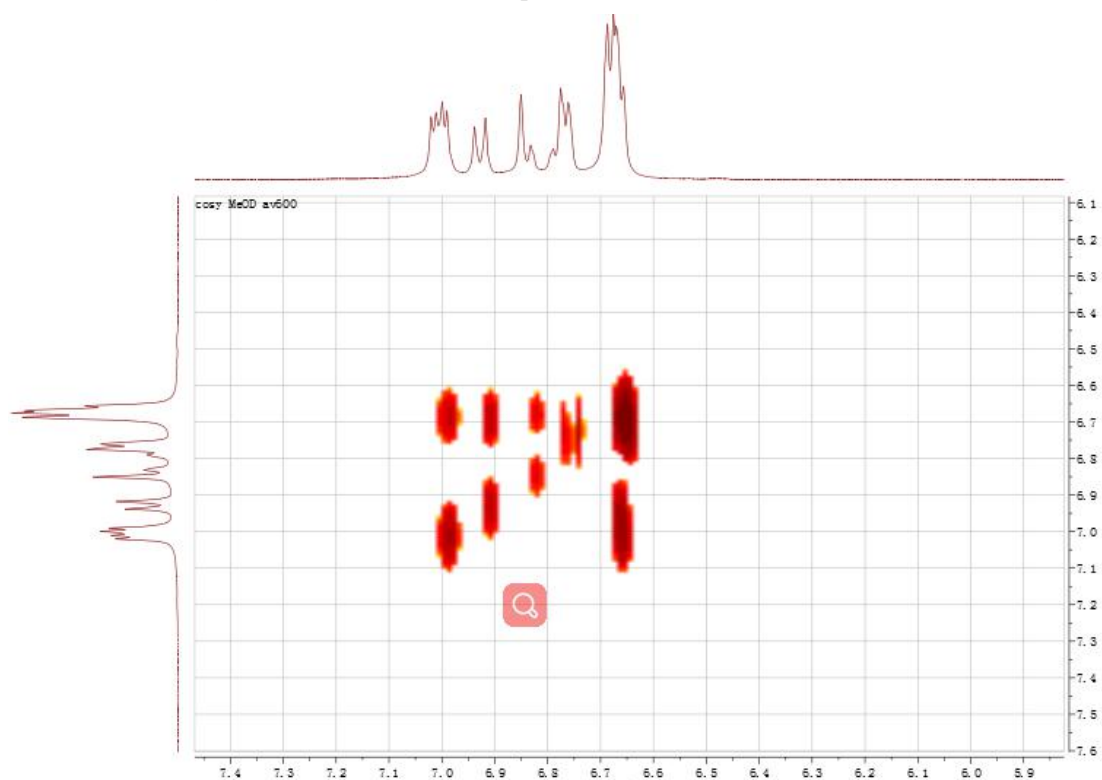
S2. ^{13}C -NMR (150 MHz, CD_3OD) of compound **1**



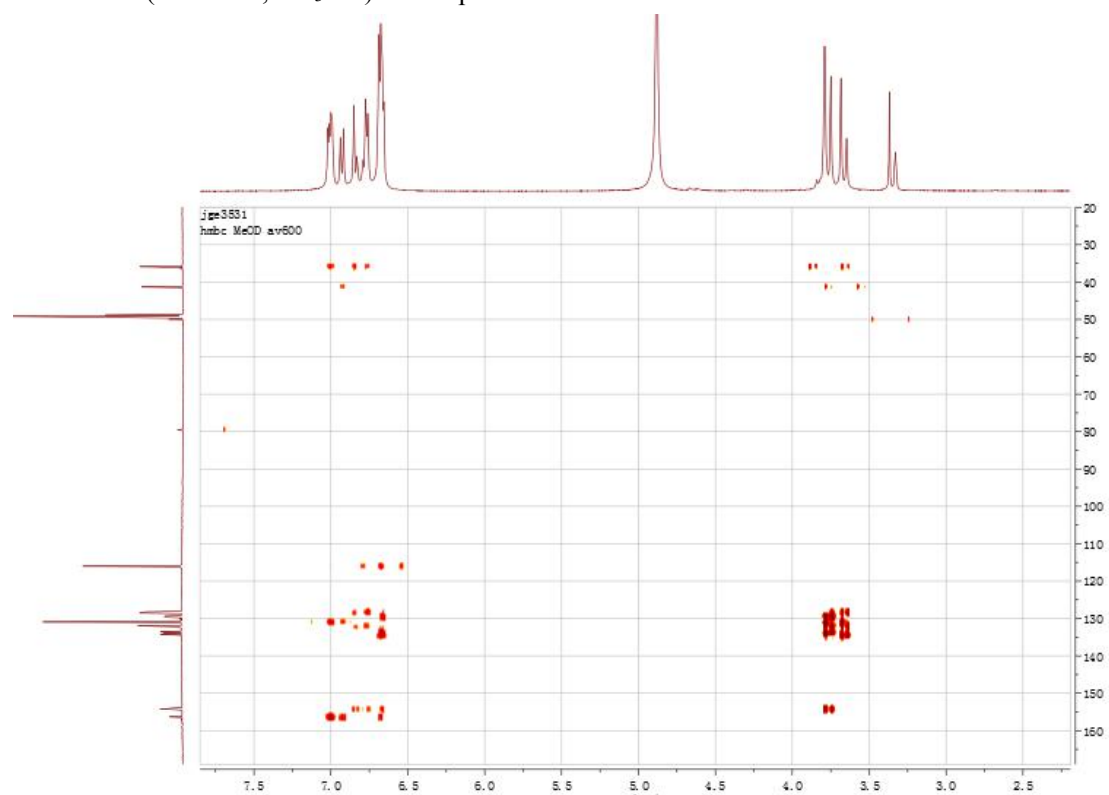
S3. HSQC (600 MHz, CD₃OD) of compound 1



S4. ¹H-¹H COSY (600 MHz, CD₃OD) of compound 1



S5. HMBC (600 MHz, CD₃OD) of compound **1**



S6. HRESIMS spectra of compound 1

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	300	S	2	0	0	H
C	4	0	100					HCOO
N	3	0	0					CH3COO
O	2	0	40					Cl

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: 0.0 - 20.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

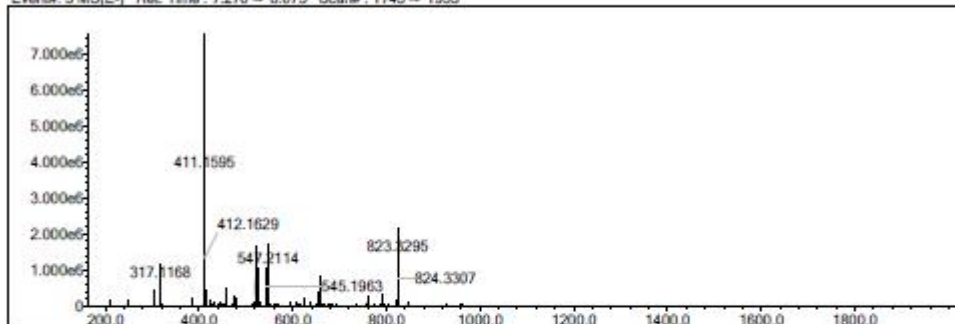
Electron Ions: both

Use MSn Info: no

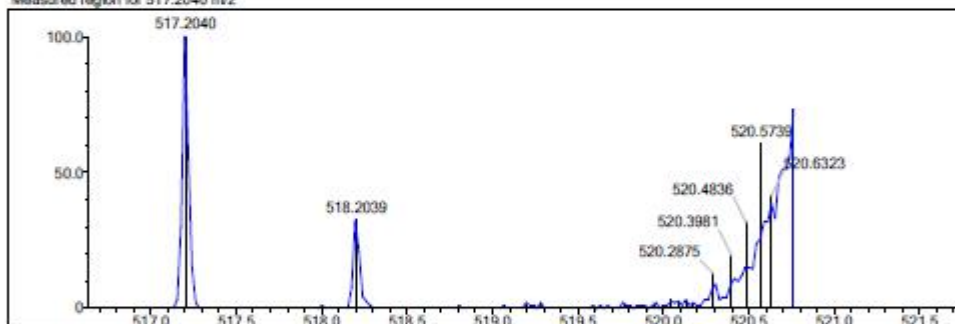
Isotope Res: 10000

Max Results: 500

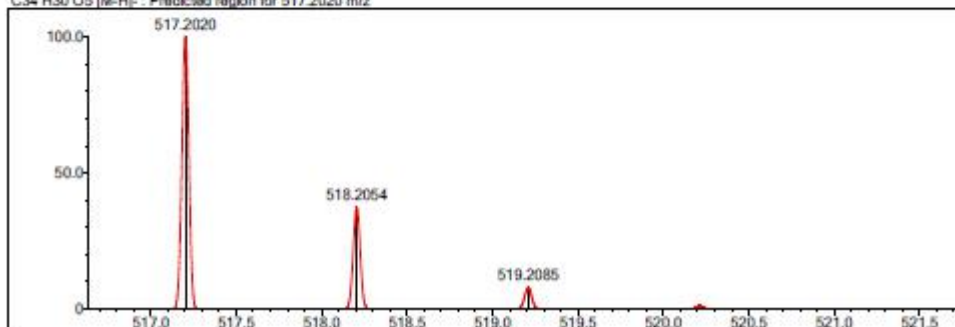
Event#: 3 MS(E-) Ret. Time : 7.270 -> 8.075 Scan#: 1743 -> 1935



Measured region for 517.2040 m/z

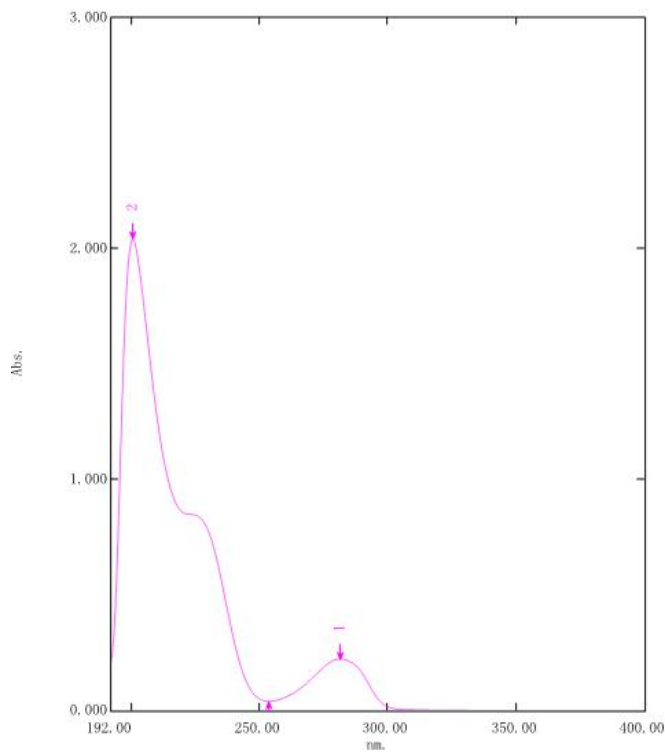


C34 H30 O5 (M-H)- : Predicted region for 517.2020 m/z



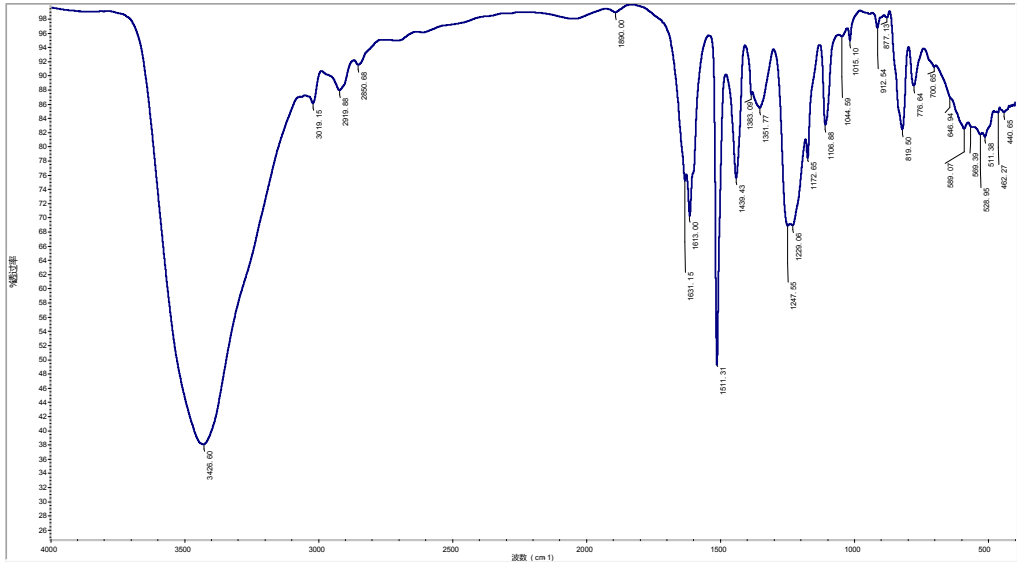
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	30.09	C34 H30 O5	[M-H]-	517.2040	517.2020	2.0	3.87	32.42	20.0

S7. UV spectra of compound 1



No.	P/V	波长(nm)	Abs.	描述
1		281.40	0.221	
2		200.60	2.039	
3		253.80	0.038	

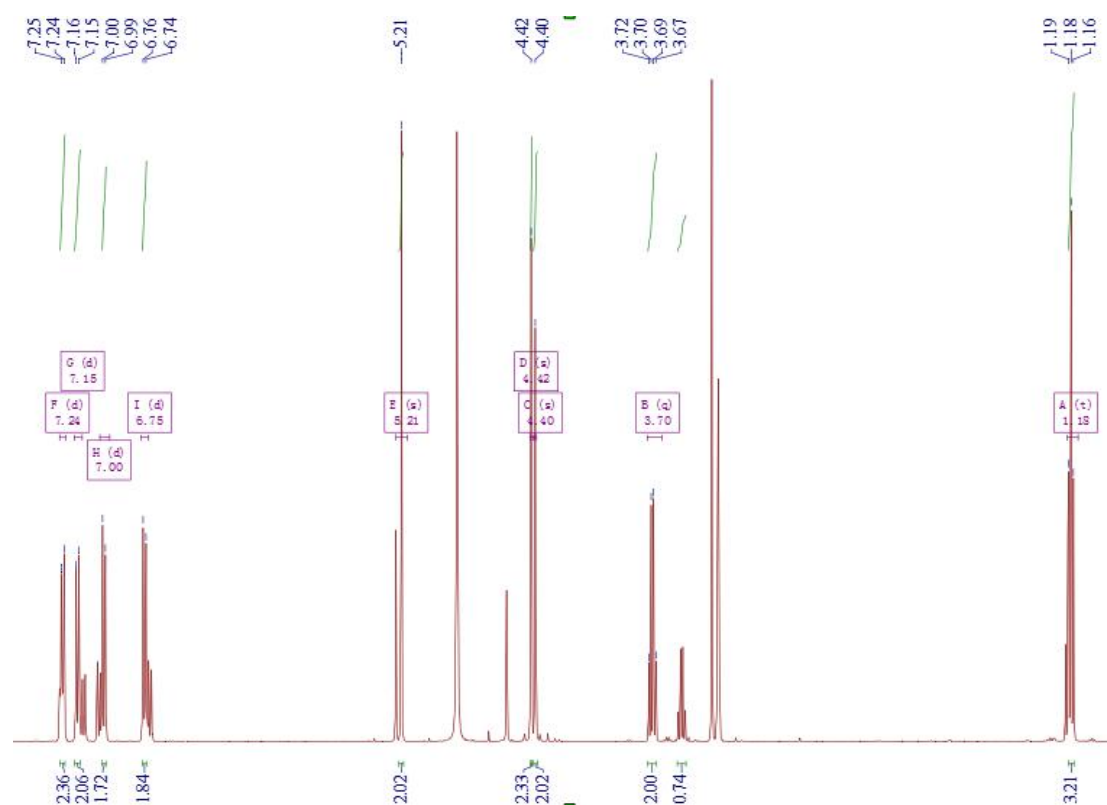
S8. UV spectra of compound 2



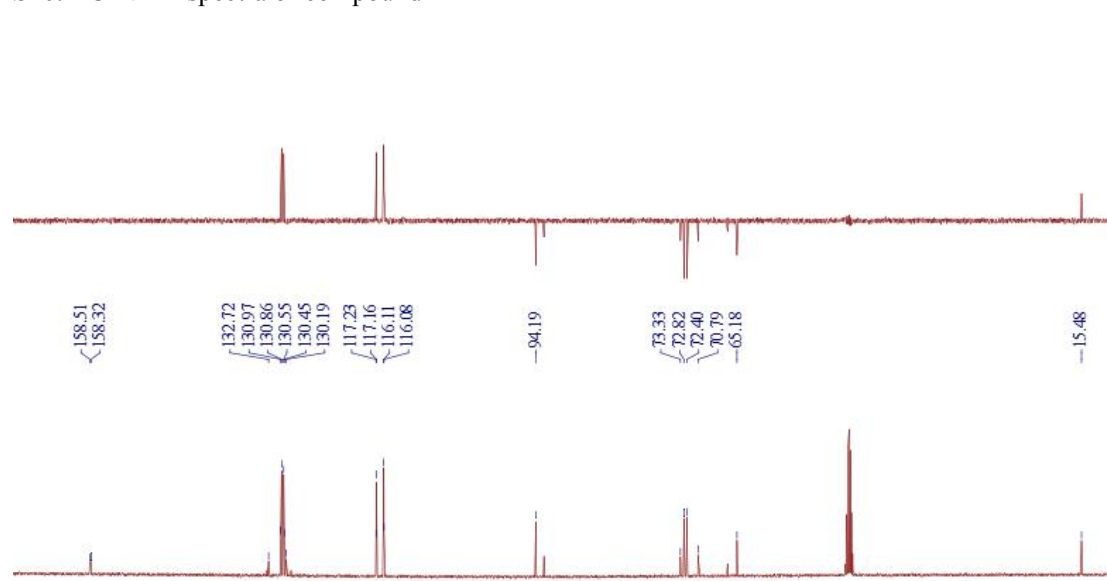
Sample Name: jge33531
KBr 压片
采集时间: 星期二 3月 26 13:55:09 2019 (GMT+08:00)
仪器型号: NI COLET iS10
Software version: OMNI C 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光圈: 80.00

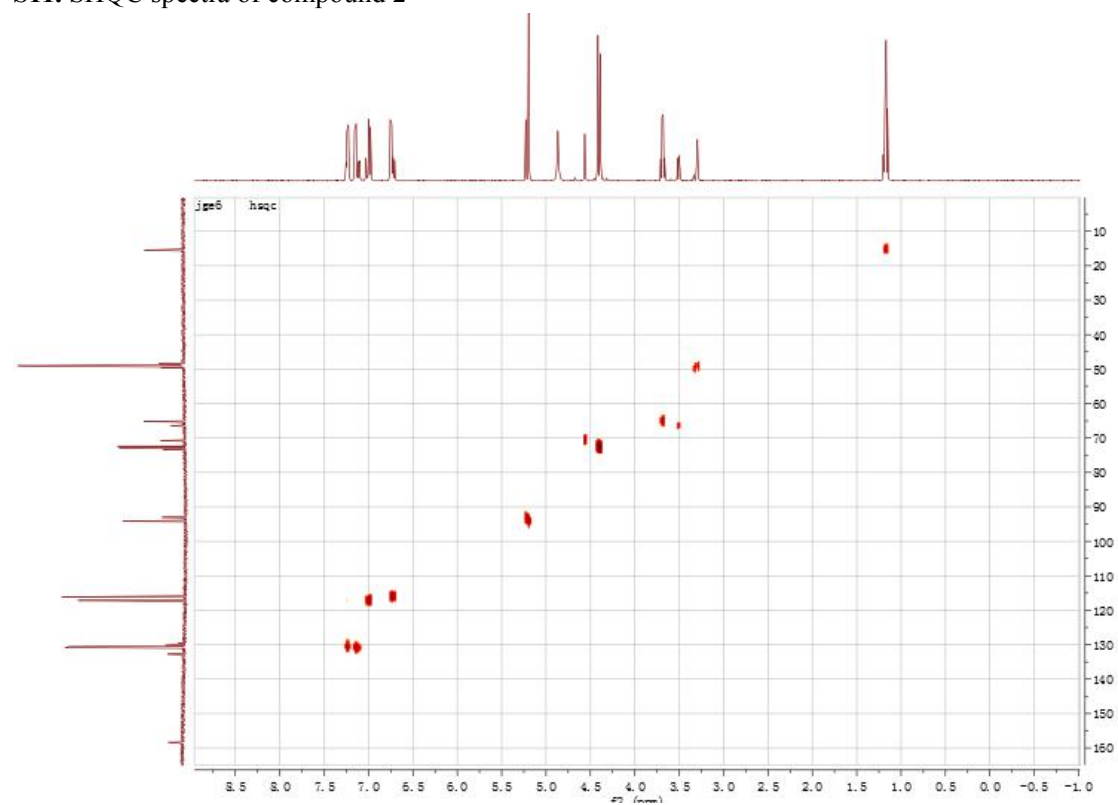
S9 ^1H -NMR spectra of compound **2**



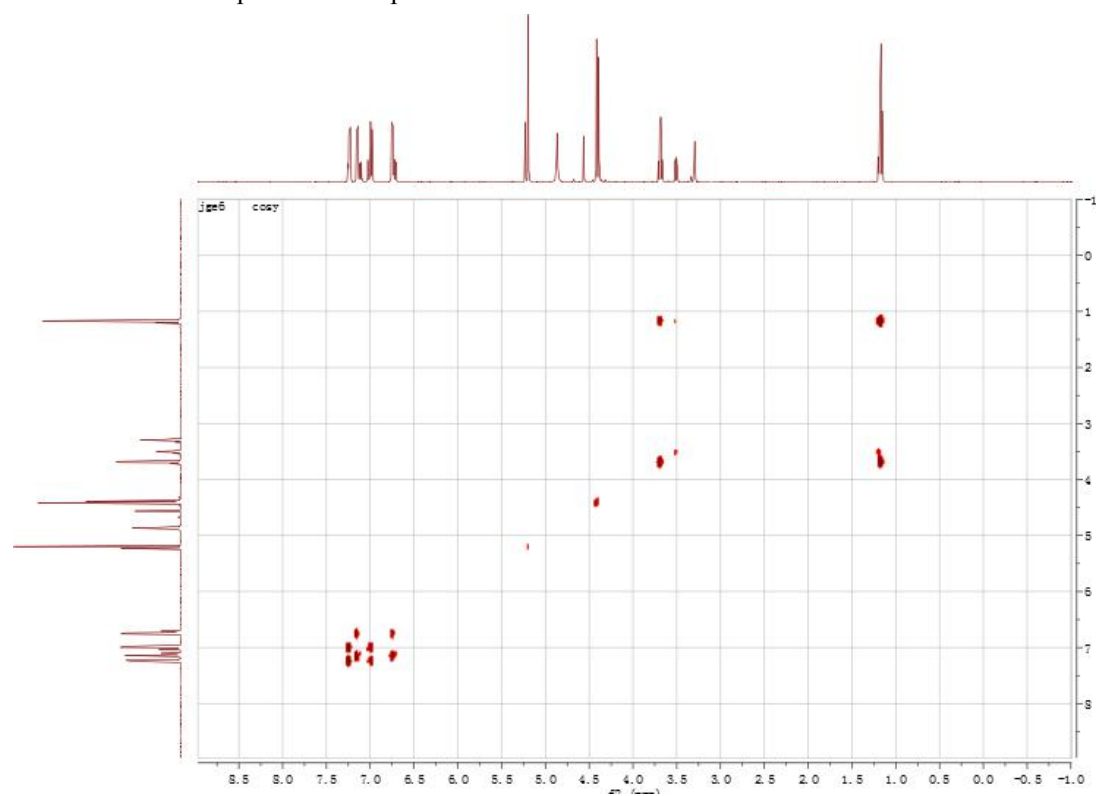
S10. ^{13}C -NMR spectra of compound **2**



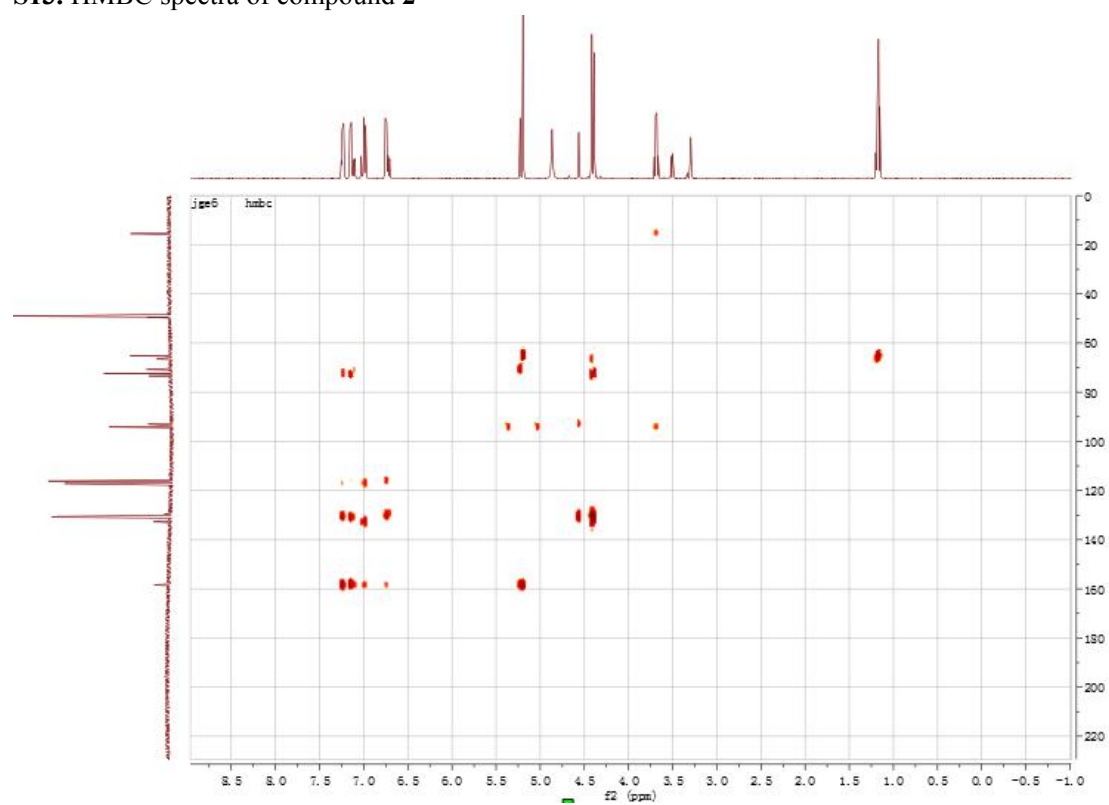
S11. SHQC spectra of compound **2**



S12. ^1H - ^1H COSY spectra of compound **2**



S13. HMBC spectra of compound 2



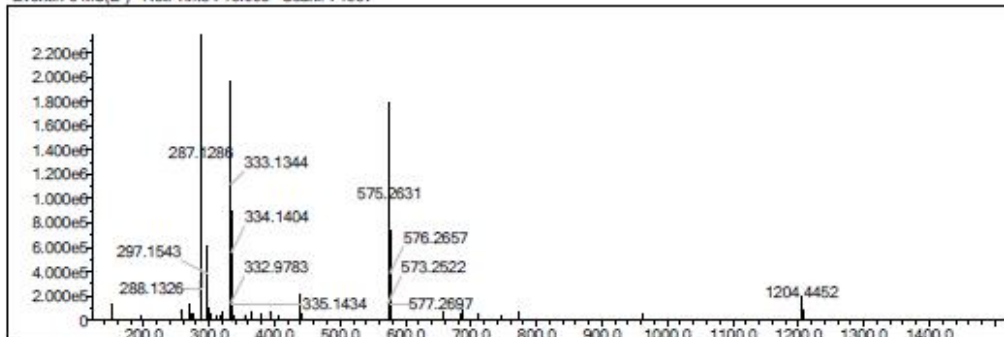
S14. HRESIMS spectra of compound 2

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

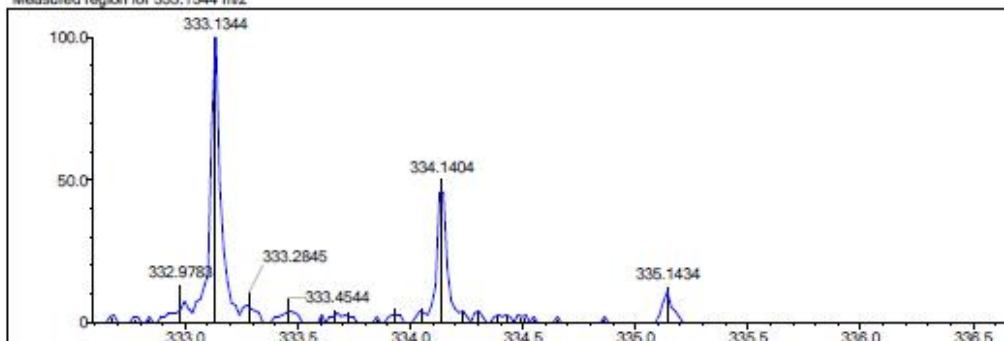
DBE Range: 0.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

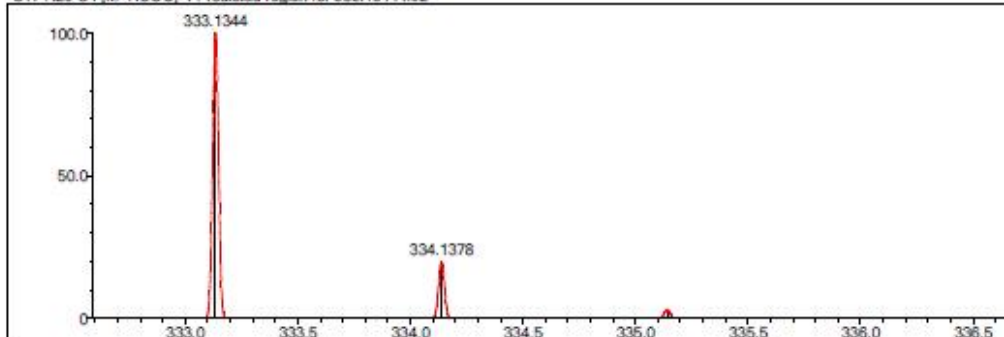
Event#: 3 MS(E-) Ret. Time : 10.003 Scan#: 1397



Measured region for 333.1344 m/z

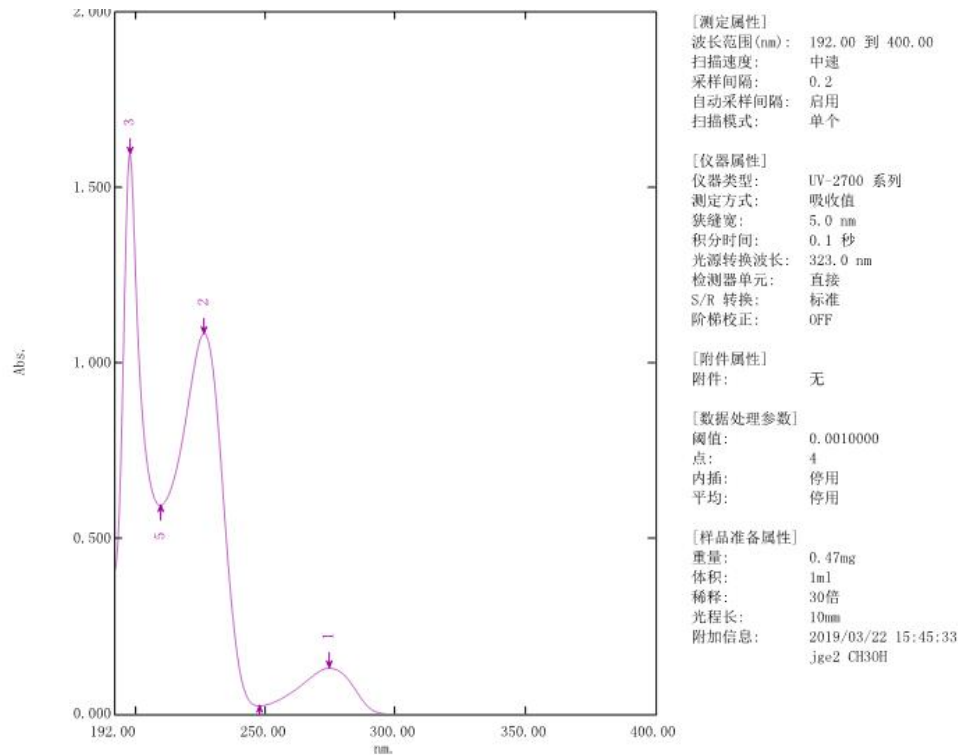


C17 H20 O4 [M+HCOO]- : Predicted region for 333.1344 m/z



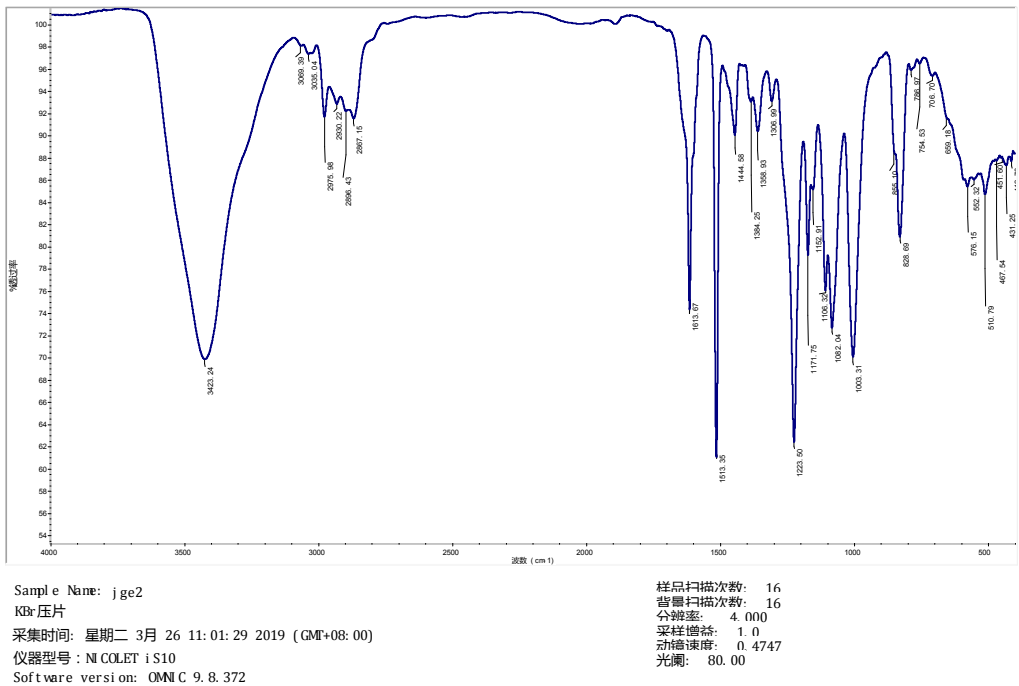
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	48.68	C17 H20 O4	[M+HCOO]-	333.1344	333.1344	0.0	0.00	48.68	8.0

S15. UV spectra of compound 2

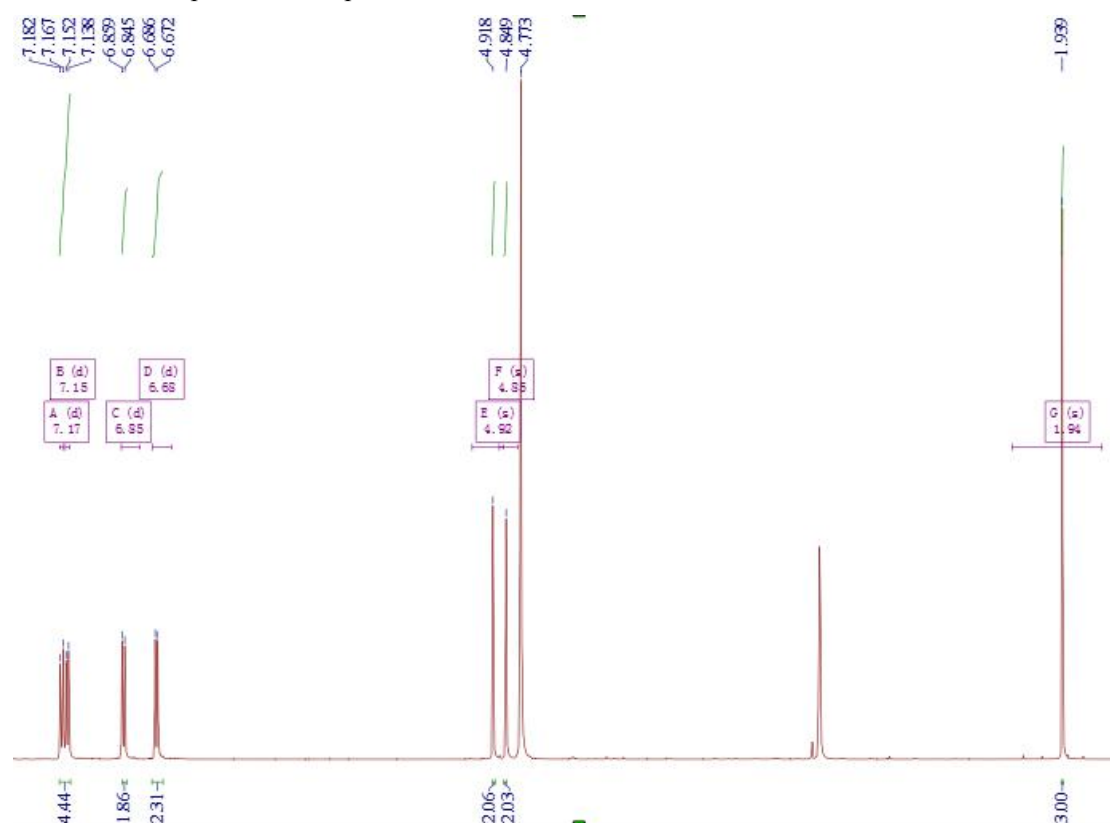


No.	P/V	波长 (nm)	Abs.	描述
1		274.60	0.130	
2		226.40	1.084	
3		197.80	1.596	
4		247.60	0.022	
5		209.60	0.594	

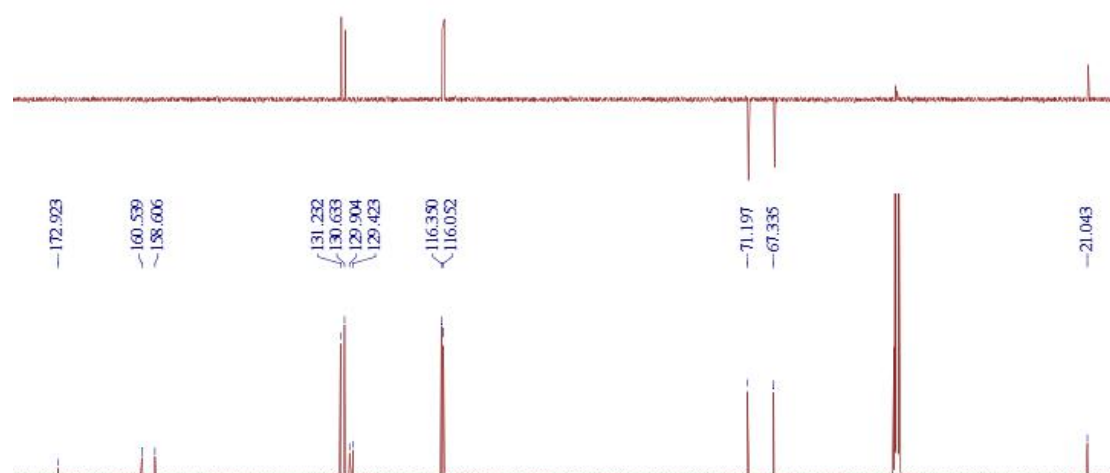
S16. IR spectra of compound 2



S17. ^1H -NMR spectra of compound **3**



S18. ^{13}C -NMR spectra of compound **3**



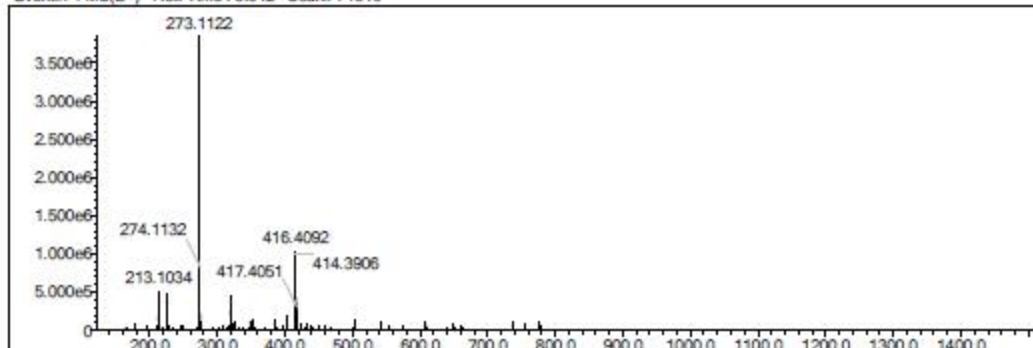
S19. HRESIMS spectra of compound 3

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

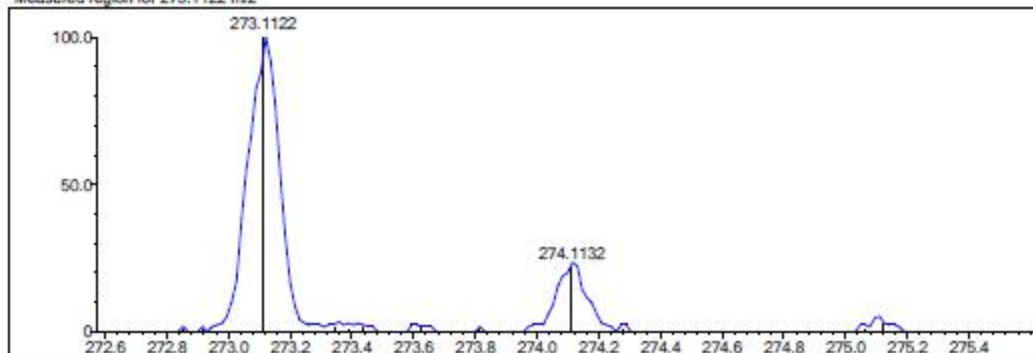
DBE Range: 0.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

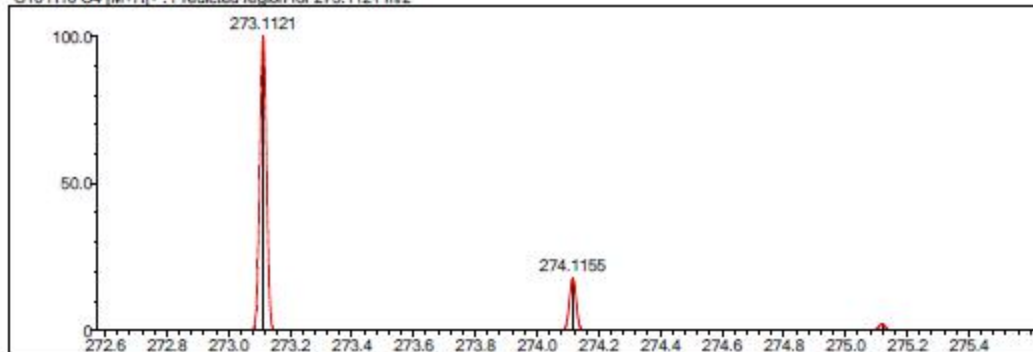
Event#: 1 MS(E+) Ret. Time : 9.542 Scan#: 1340



Measured region for 273.1122 m/z

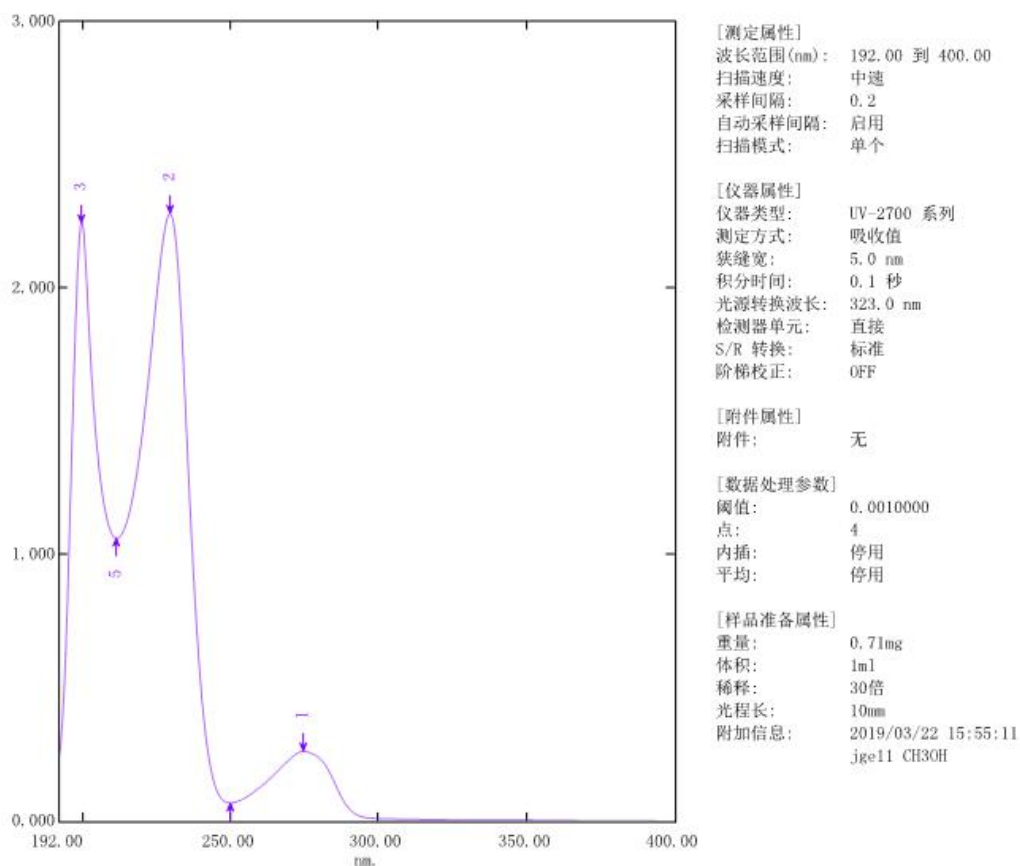


C16 H16 O4 [M+H]⁺ : Predicted region for 273.1121 m/z



Rank	Score	Formula (M)	Ion	Mess. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	42.21	C16 H16 O4	[M+H] ⁺	273.1122	273.1121	0.1	0.37	42.21	9.0

S20. UV spectra of compound 3



S21. IR spectra of compound 3

