

SUPPLEMENTARY MATERIAL

A new 12-membered lactone from the stems of *Ficus auriculata*

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Abstract:

A new lactone ficusine D (**1**), together with six known compounds (**2-7**) were isolated from the stems of the *Ficus auriculata*. The new compound **1** was a rare 12-membered lactone containing a quinone ring skeleton. The structure of the **1** was elucidated by comprehensive spectroscopic data. The relative and absolute configuration of **1** were elucidated by the ROESY analyses and biogenesis pathway. All compounds were evaluated for their antibacterial activities against six pathogenic bacteria *in vitro*. Compounds **6** and **7** exhibited antibacterial activities against *Bacillus cereus* with the MIC values of 2.5 and 5 μ M, respectively.

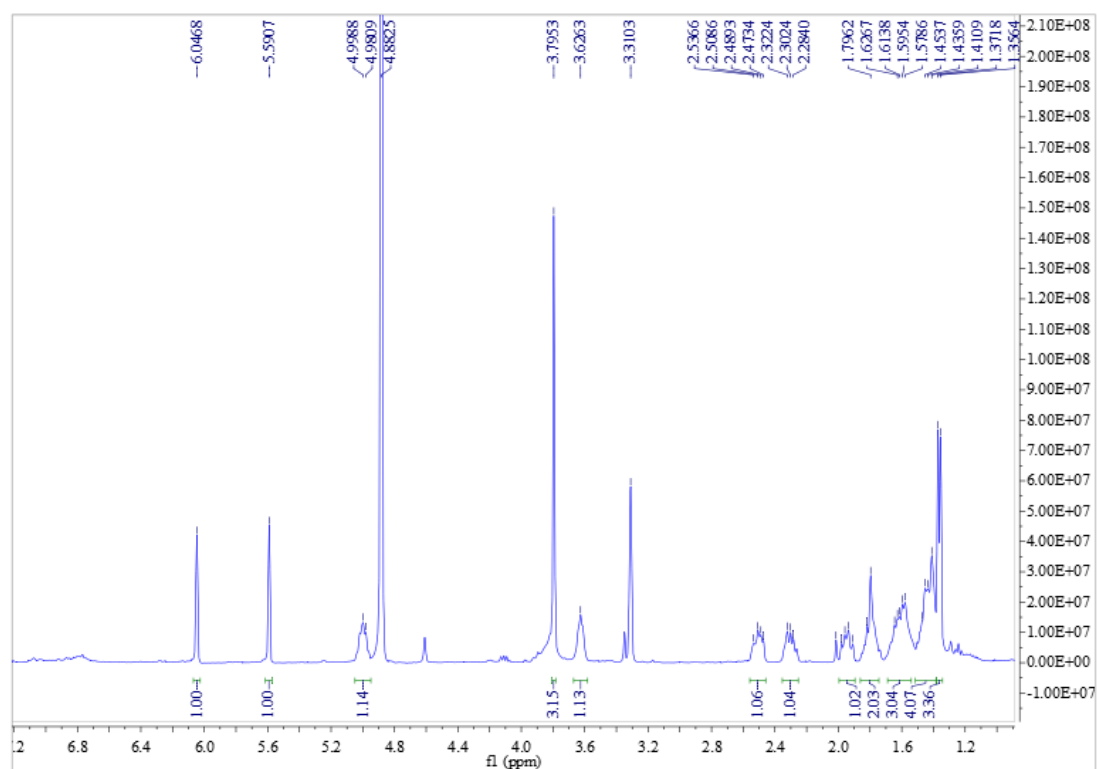
Keywords: *Ficus auriculata*; Lactone; antibacterial activity

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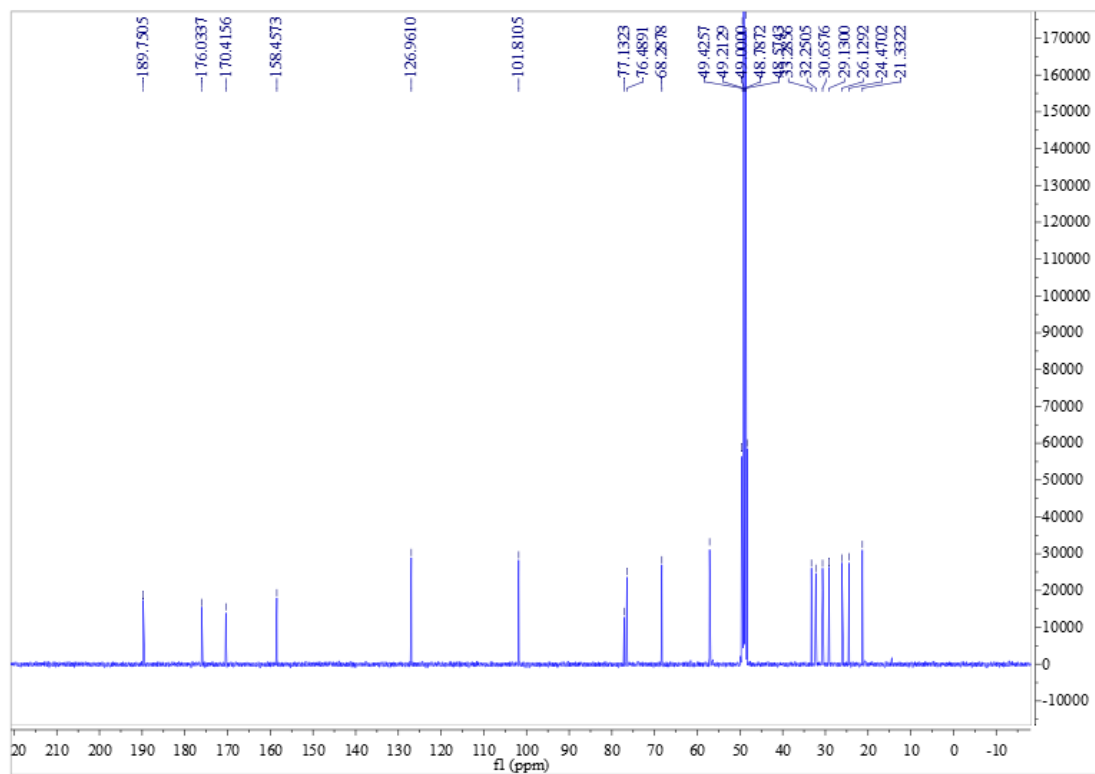
E-mail address: sxp628@126.com, hchr116@126.com

List of Supplementary Material

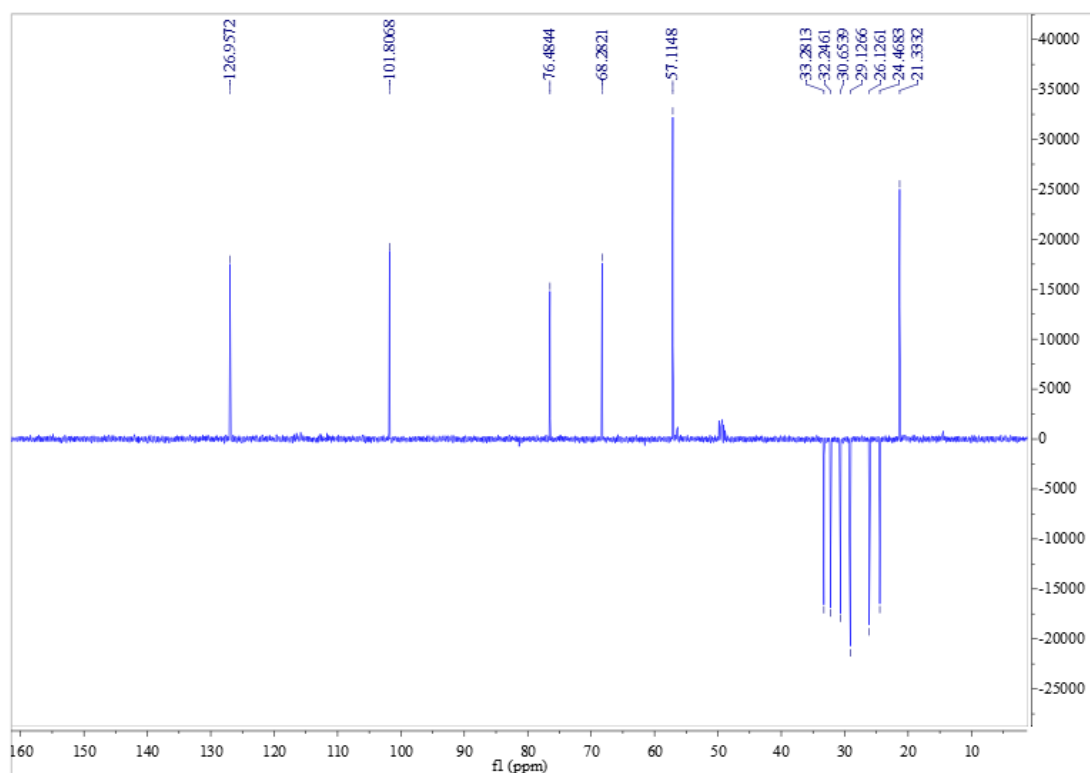
FigureS1. ^1H NMR (400 MHz, CD_3OD) spectrum of 1	3
FigureS2. ^{13}C NMR (100 MHz, CD_3OD) spectrum of 1	3
FigureS3. DEPT (100 MHz, CD_3OD) spectrum of 1	4
Figure S4. HSQC (CD_3OD) spectrum of 1	4
Figure S5. HMBC (CD_3OD) spectrum of 1	5
Figure S6. ^1H - ^1H COSY (CD_3OD) spectrum of 1	5
Figure S7. ROESY (CD_3OD) spectrum of 1	6
Figure S8. Key HMBC, ^1H - ^1H COSY and ROESY correlations of 1	6
Figure S9. HRESIMS spectrum of 1	7
Figure S10. IR spectrum of 1	7



FigureS1. ¹H NMR (400 MHz, CD₃OD) spectrum of **1**



FigureS2. ¹³C NMR (100 MHz, CD₃OD) spectrum of **1**



FigureS3. DEPT (100 MHz, CD₃OD) spectrum of **1**

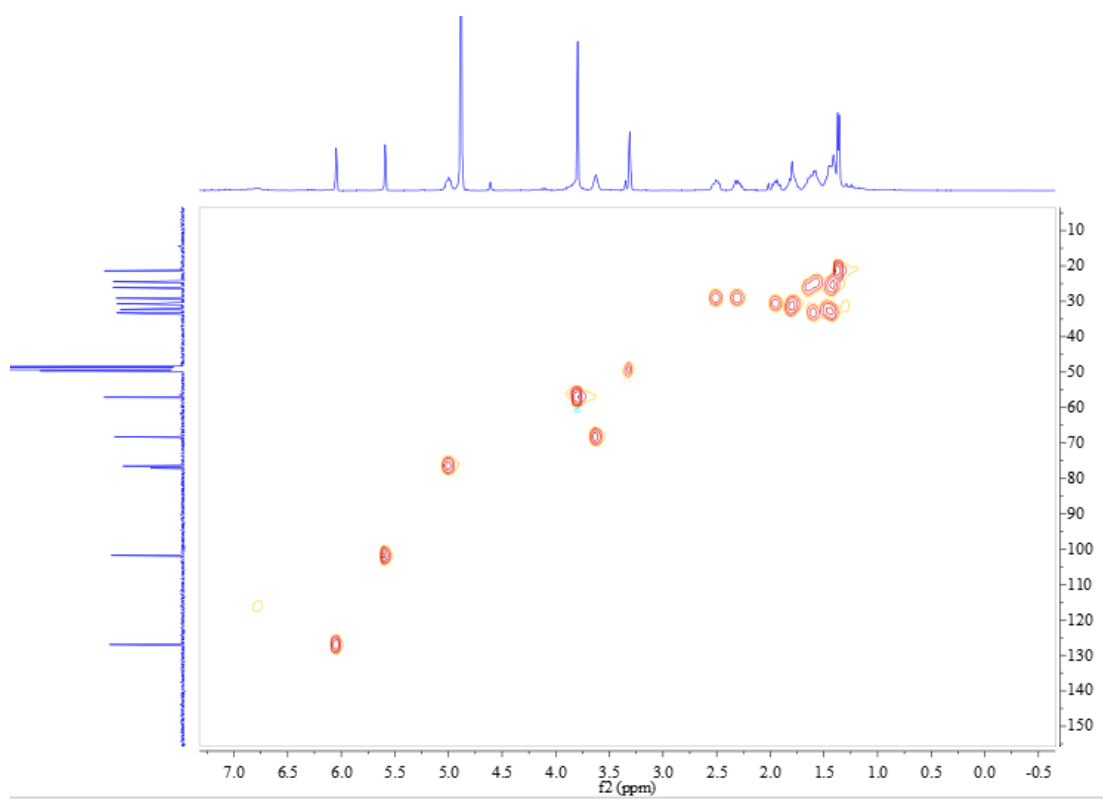


Figure S4. HSQC (CD₃OD) spectrum of **1**

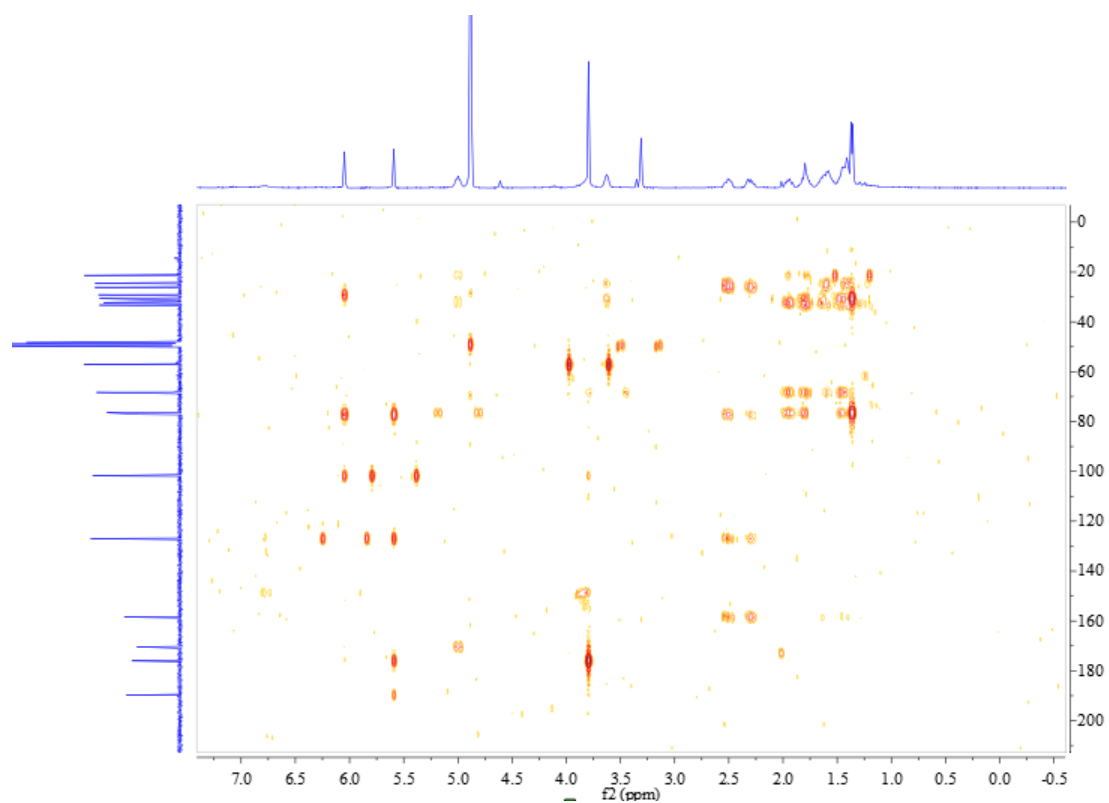


Figure S5. HMBC (CD₃OD) spectrum of **1**

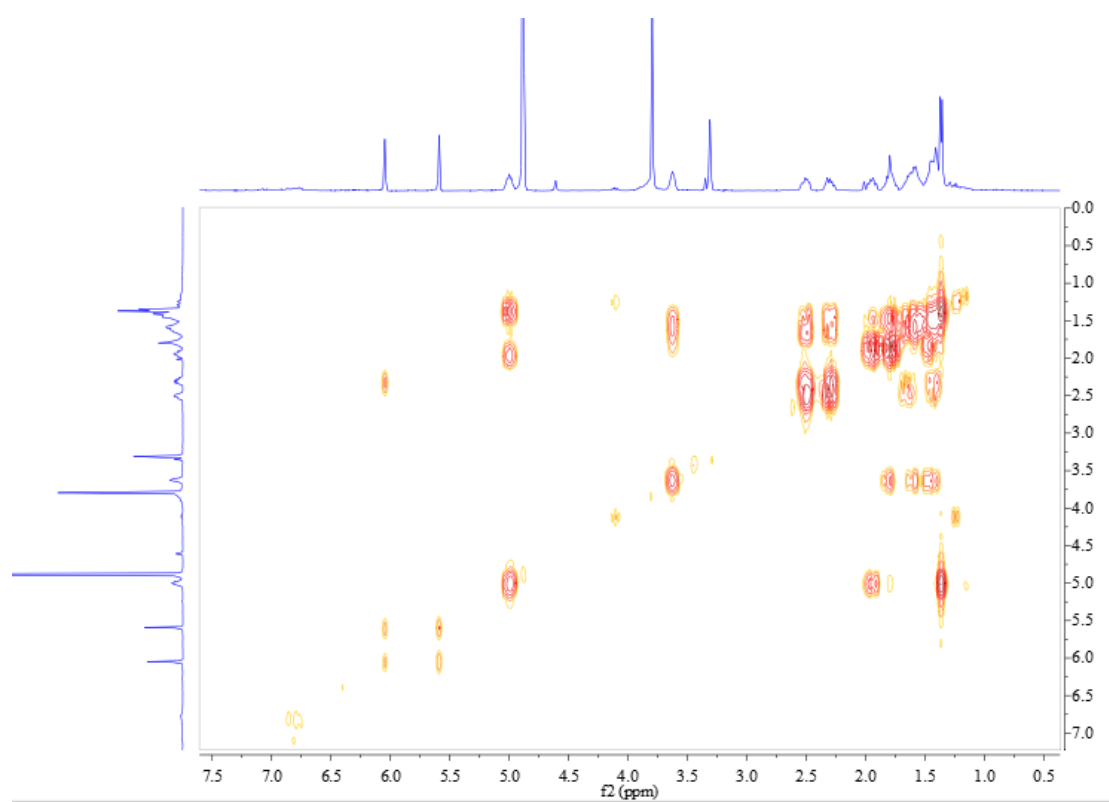


Figure S6. ¹H-¹H COSY (CD₃OD) spectrum of **1**

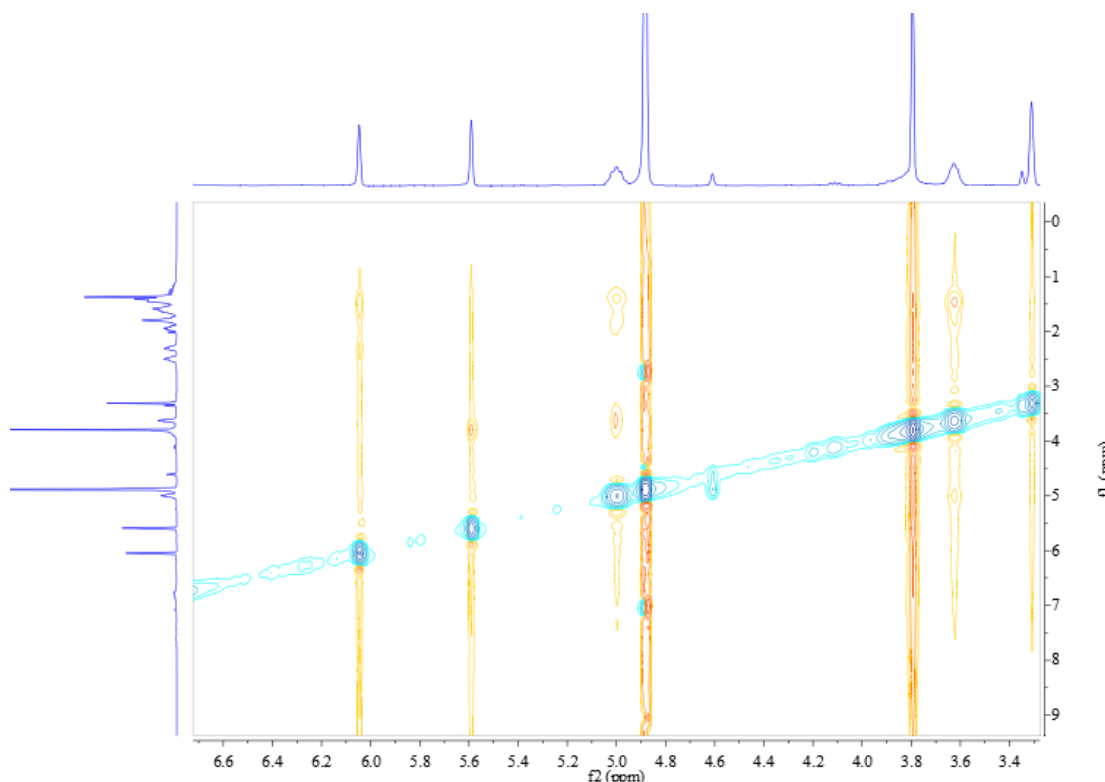


Figure S7. ROESY (CD₃OD) spectrum of **1**

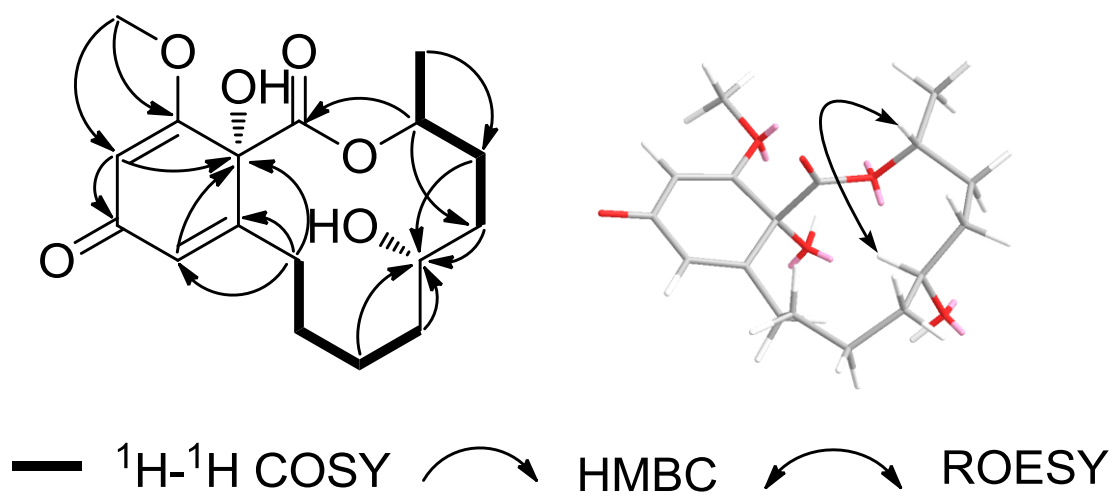


Figure S8. Key HMBC, ^1H - ^1H COSY and ROESY correlations of **1**

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\20170113\DGR-7-2_000002.d
 Method runing-20161228
 Sample Name
 Comment

Acquisition Date 2017/1/13 13:34:48

Operator ChuanqiZhou@163.com
 Instrument apex-Ultra

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1000.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 μ m
Acquisition Mode	Single MS	Skimmer 1	20.0 V	Calibration Date	Thu Jan 9 03:14:48 2017
Pulse Program	basic	Drying Gas Temperature	180.0 $^{\circ}$ C	Data Acquisition Size	131072
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				

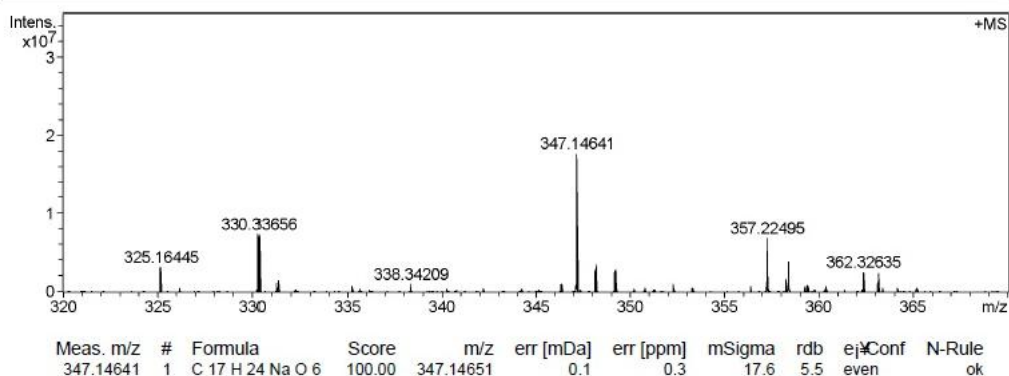


Figure S9. HRESIMS spectrum of 1

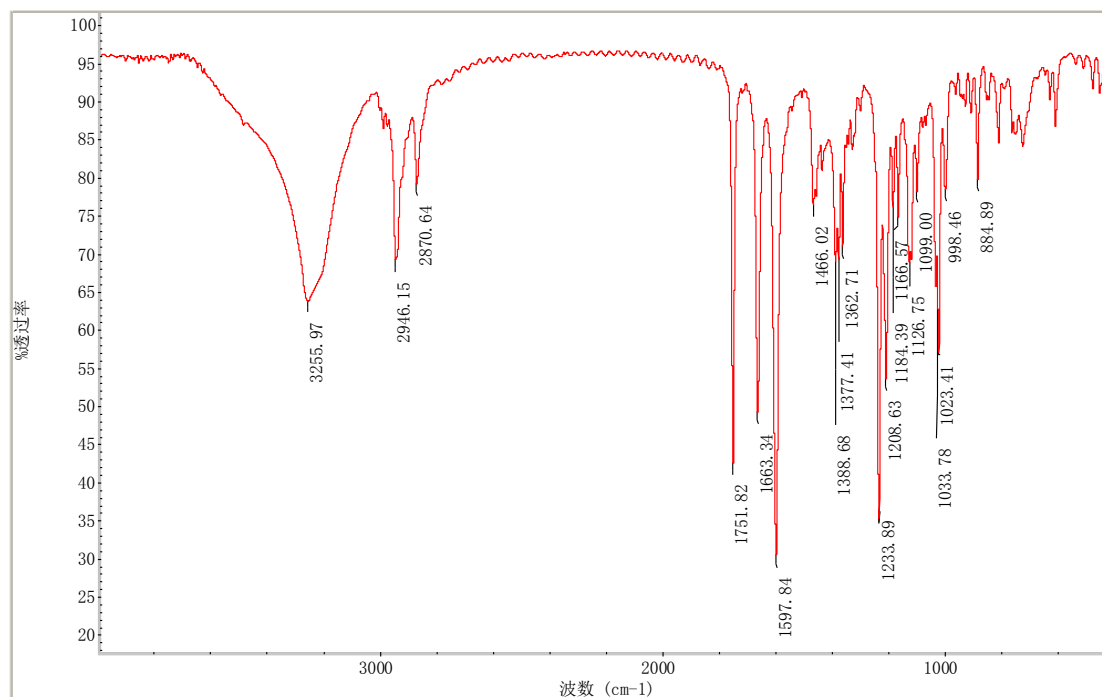


Figure S10. IR spectrum of 1