

Supplementary data

Structural characterization and assessment of anti-inflammatory activities of polyphenols and depsidone derivatives from *Melastoma malabathricum subsp. normale*

Rui-Jie He ¹, Ya-Feng Wang ¹, Bing-Yuan Yang ¹, Zhang-Bin Liu ¹, Dian-Peng Li ¹,
Bi-Qun Zou^{2,*}, Yong-Lin Huang ^{1,*}

*Correspondence: zoubiqun@163.com (B.-Q. Zou); hyl@gxib.cn(Y.-L.H.); Tel.: +86-773-355-0829; Fax: +86-773-355-0067

Figure S1. ¹H NMR (500 MHz, Acetone-*d*₆) spectrum of **1**

Figure S2. ¹³C NMR (125 MHz, Acetone-*d*₆) spectrum of **1**

Figure S3. HSQC spectrum of **1** in Acetone-*d*₆

Figure S4. HMBC spectrum of **1** in Acetone-*d*₆

Figure S5. ¹H-¹H COSY spectrum of **1** in Acetone-*d*₆

Figure S6. Roesy spectrum of **1** in Acetone-*d*₆

Figure S7. HR-ESI-MS spectrum of **1**

Figure S8. CD spectrum of **1**

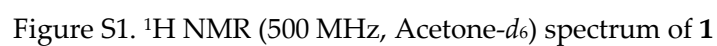
Figure S9. The ¹H NMR spectrum of **11** (500 MHz, DMSO-*d*₆)

Figure S10. The ¹³C NMR spectrum of **11** (125 MHz, DMSO-*d*₆)

Figure S11. The HSQC spectrum of **11** (500 MHz, DMSO-*d*₆)

Figure S12. The HMBC spectrum of **11** (500 MHz, DMSO-*d*₆)

Figure S13. The HR-ESI-MS spectrum of **11**



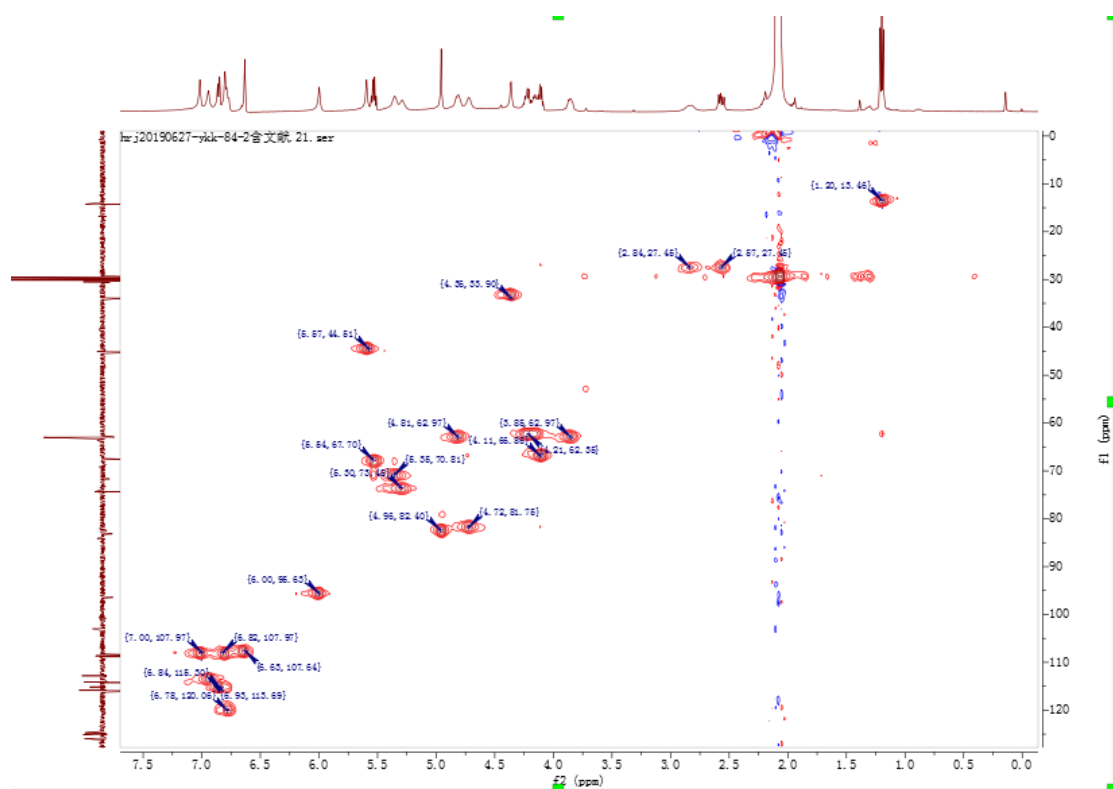


Figure S3. HSQC spectrum of **1** in Acetone- d_6

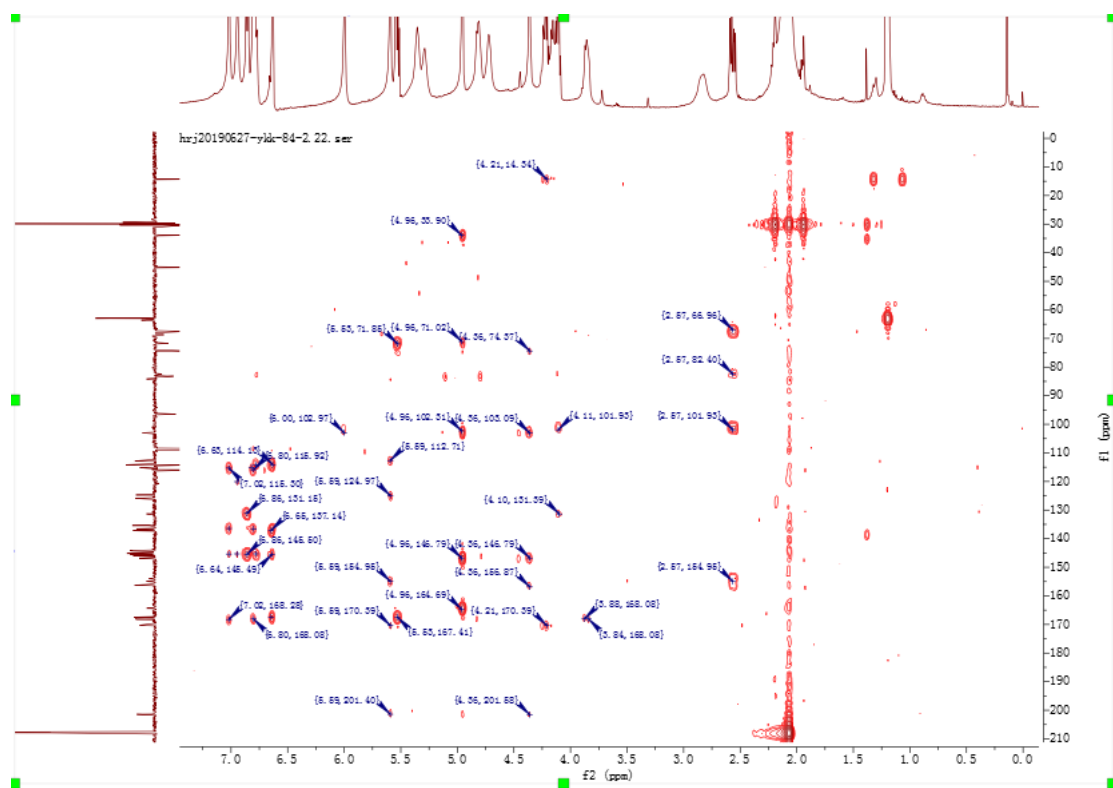


Figure S4. HMBC spectrum of **1** in Acetone- d_6

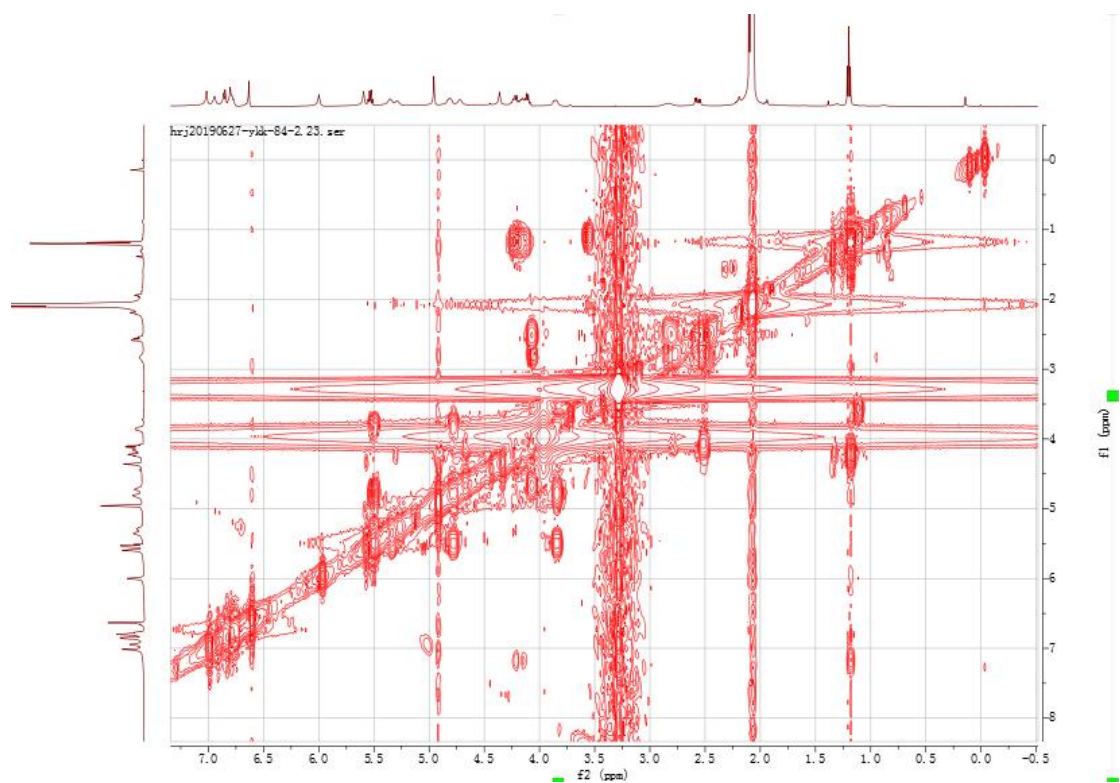


Figure S5. ^1H - ^1H COSY spectrum of **1** in Acetone- d_6

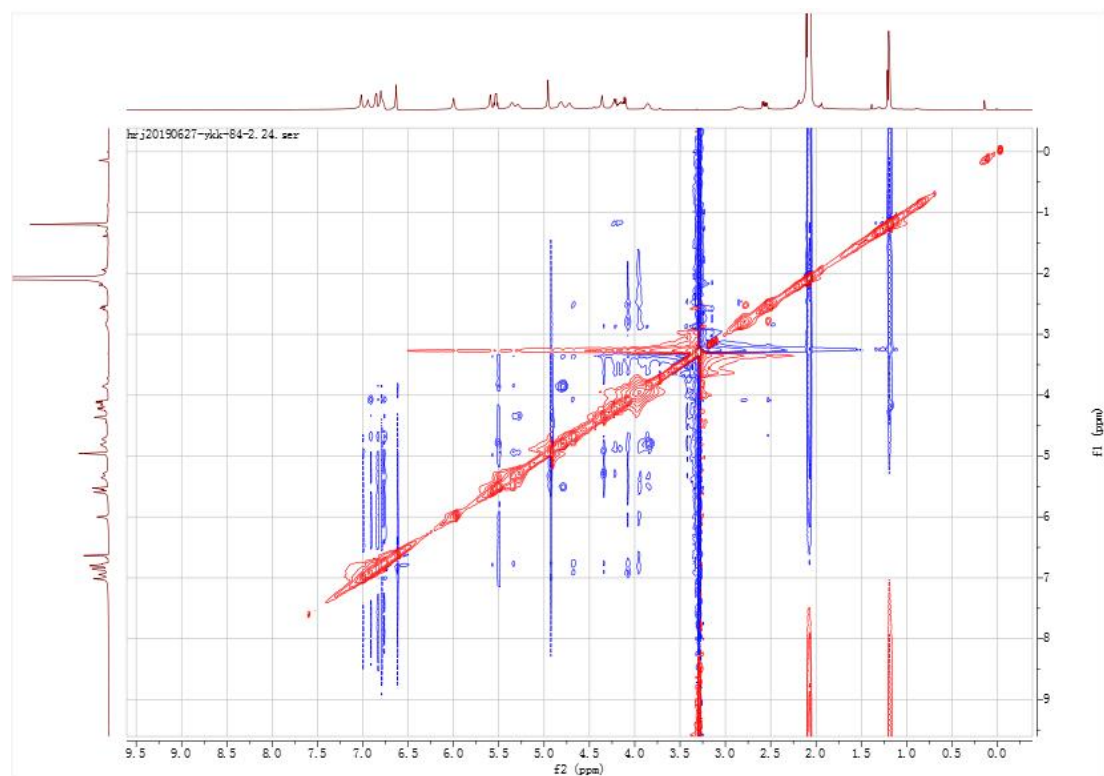


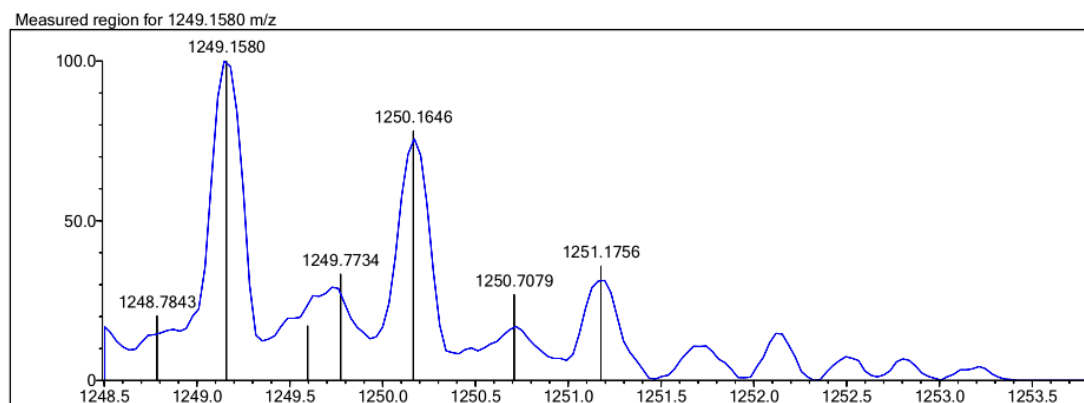
Figure S6. Roesy spectrum of **1** in Acetone- d_6

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	1	100	O	2	0	100	H
C	4	1	100					
N	3	0	0					

Error Margin (ppm): 10
 HC Ratio: 0.1 - 4.0
 Max Isotopes: all
 MSn Iso RI (%): 75.00

DBE Range: 1.0 - 50.0
 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



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	DBE	Df. (ppm)	Iso	Meas. (M)
2	42.26	C58 H42 O32	[M-H] ⁻	1249.1580	1249.1586	38.0	-0.48	42.26	1250.1653

Figure S7. HR-ESI-MS spectrum of **1**

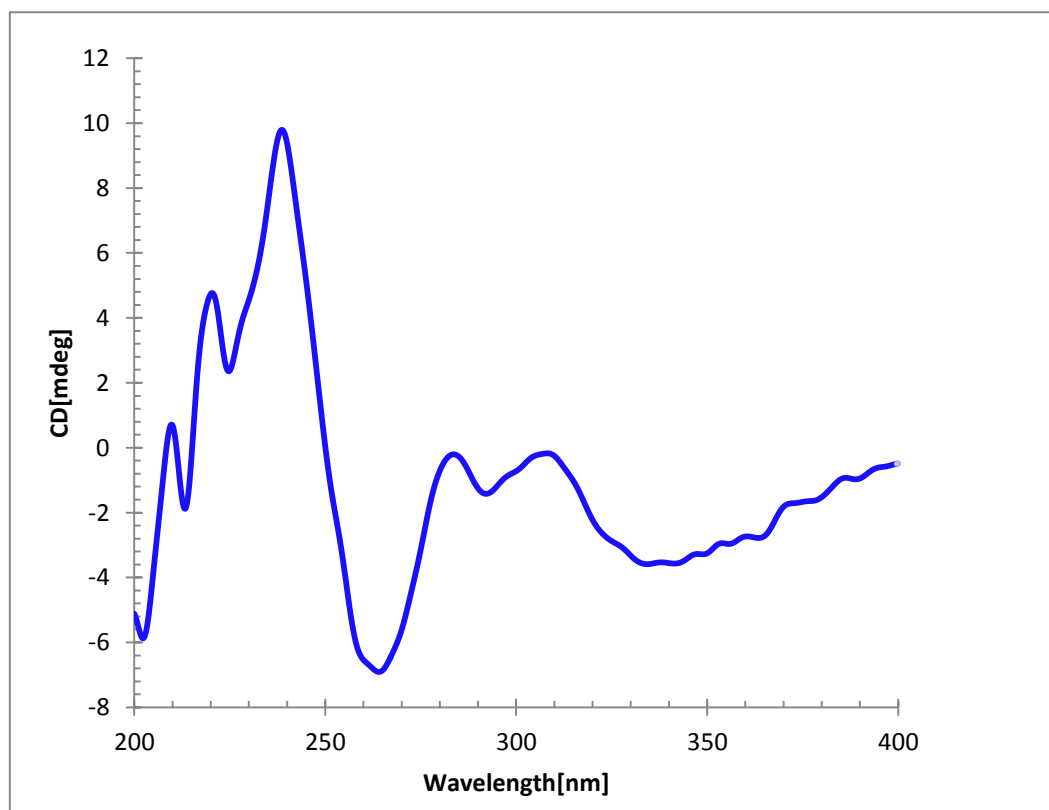


Figure S8. CD spectrum of **1**

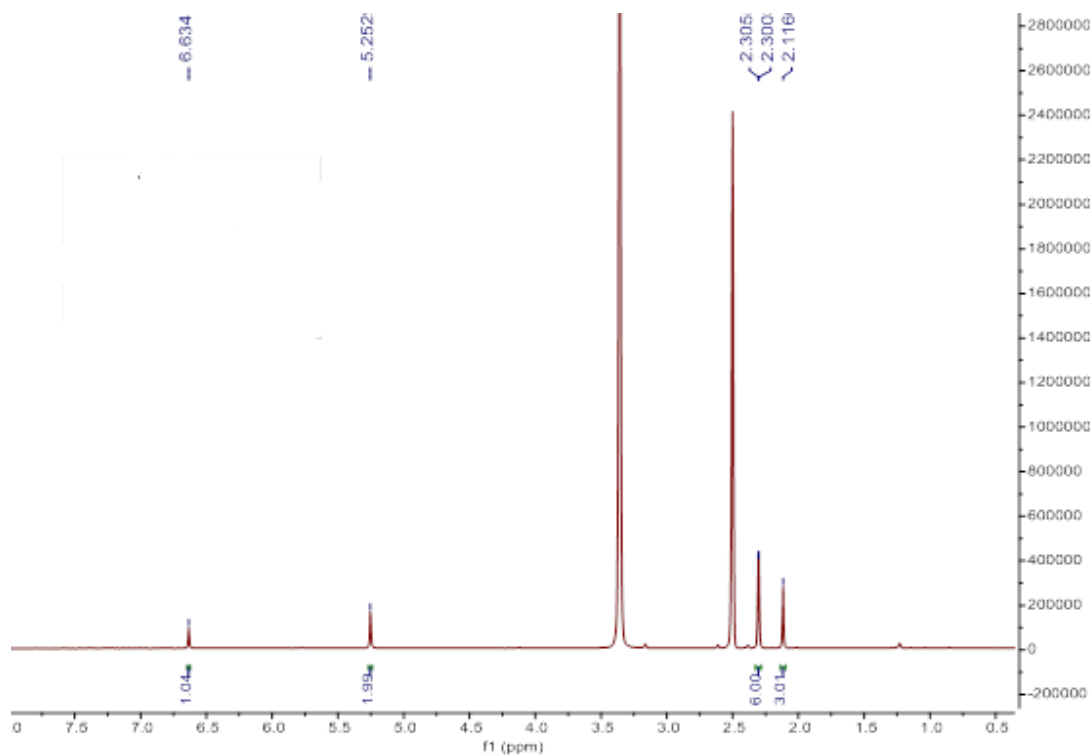


Figure S9 The ^1H NMR spectrum of **11** (500 MHz, $\text{DMSO-}d_6$)

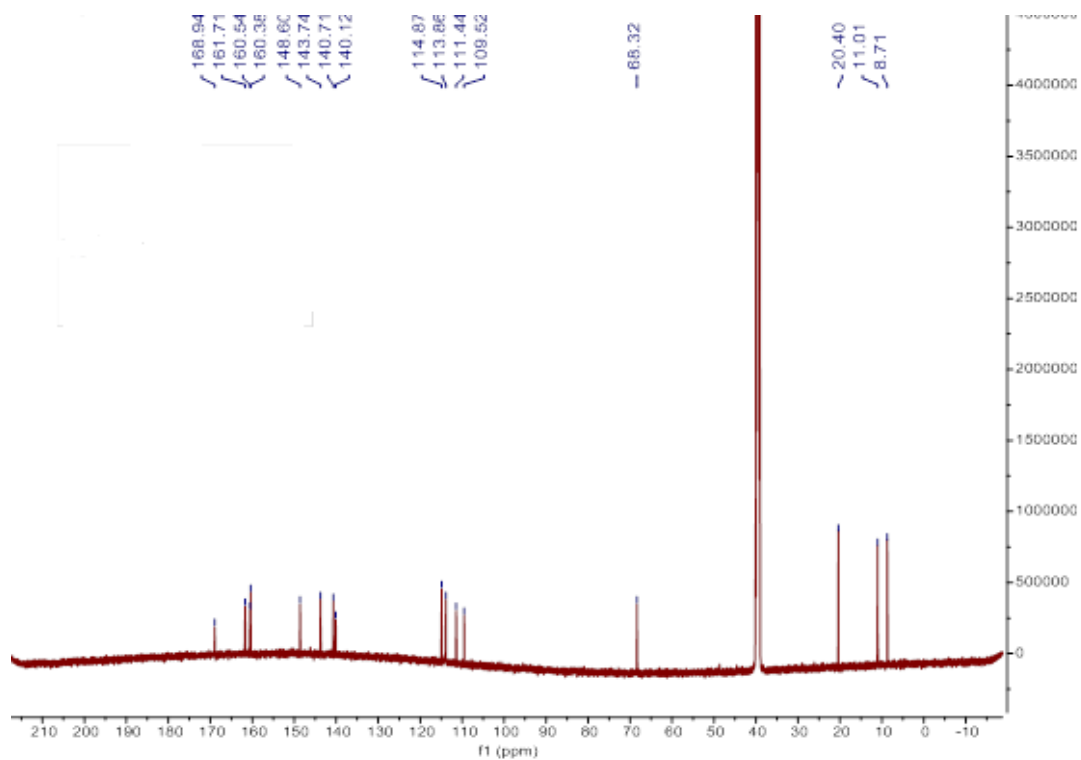


Figure S10 The ^{13}C NMR spectrum of **11** (125 MHz, $\text{DMSO-}d_6$)

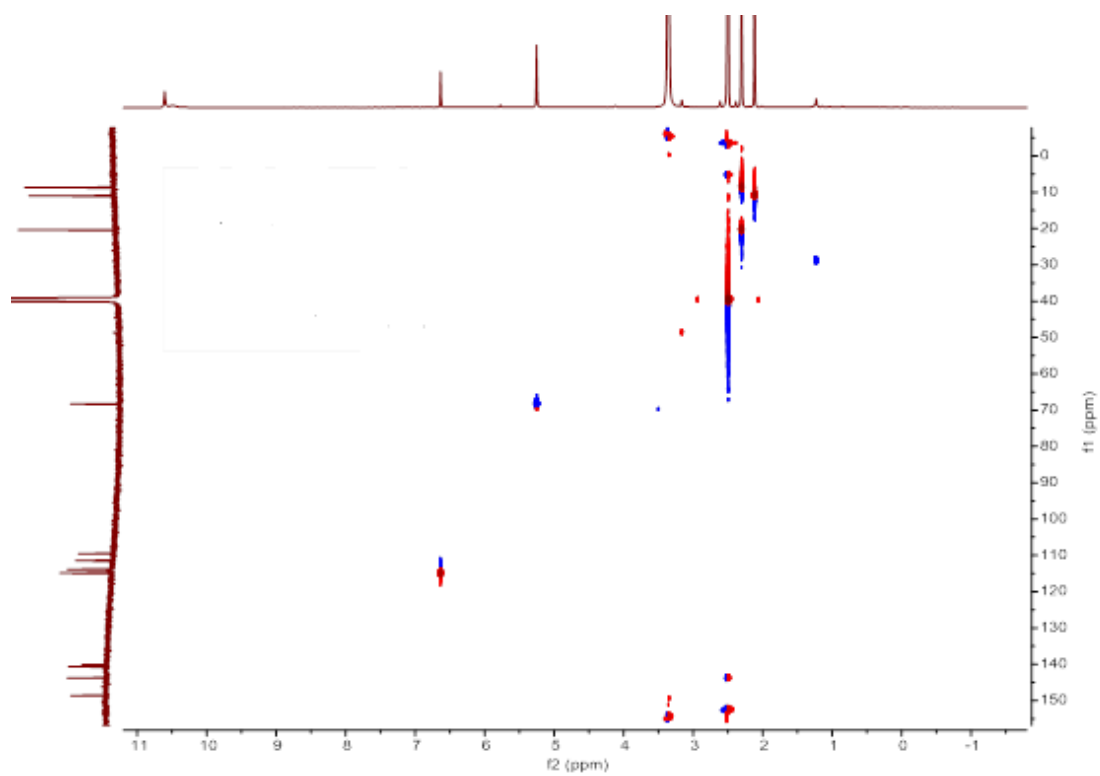


Figure S11 The HSQC spectrum of **11** (500 MHz, DMSO-*d*₆)

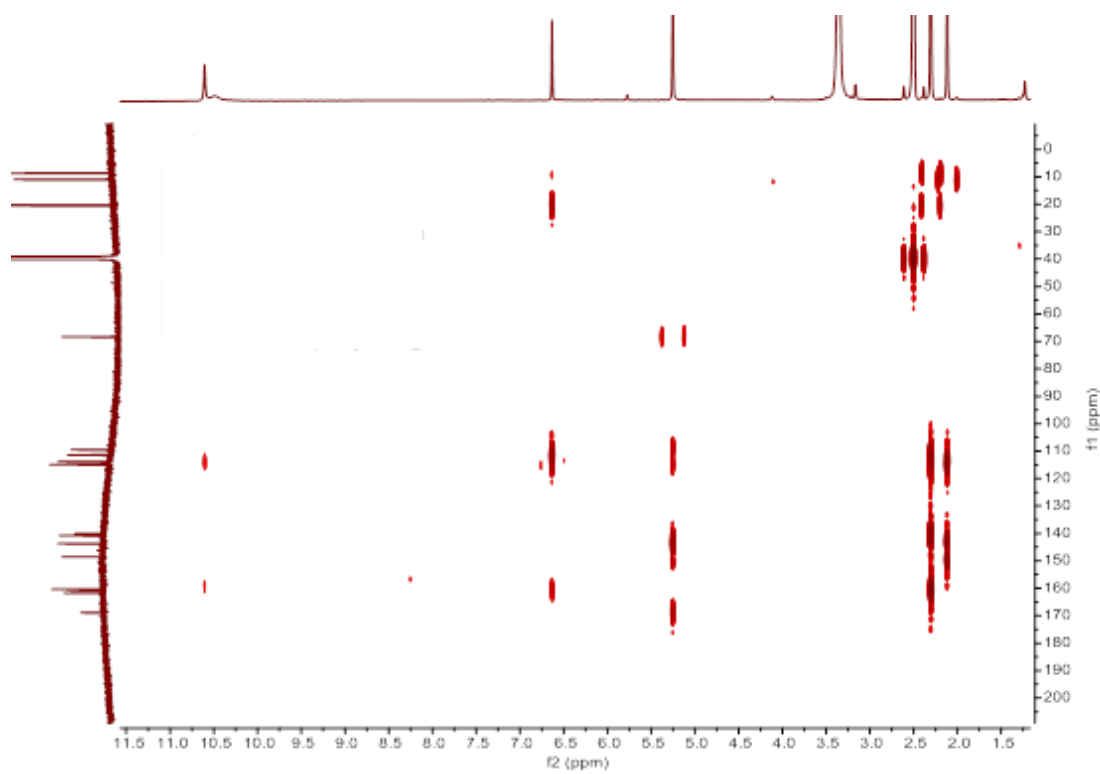


Figure S12 The HMBC spectrum of **11** (500 MHz, DMSO-*d*₆)

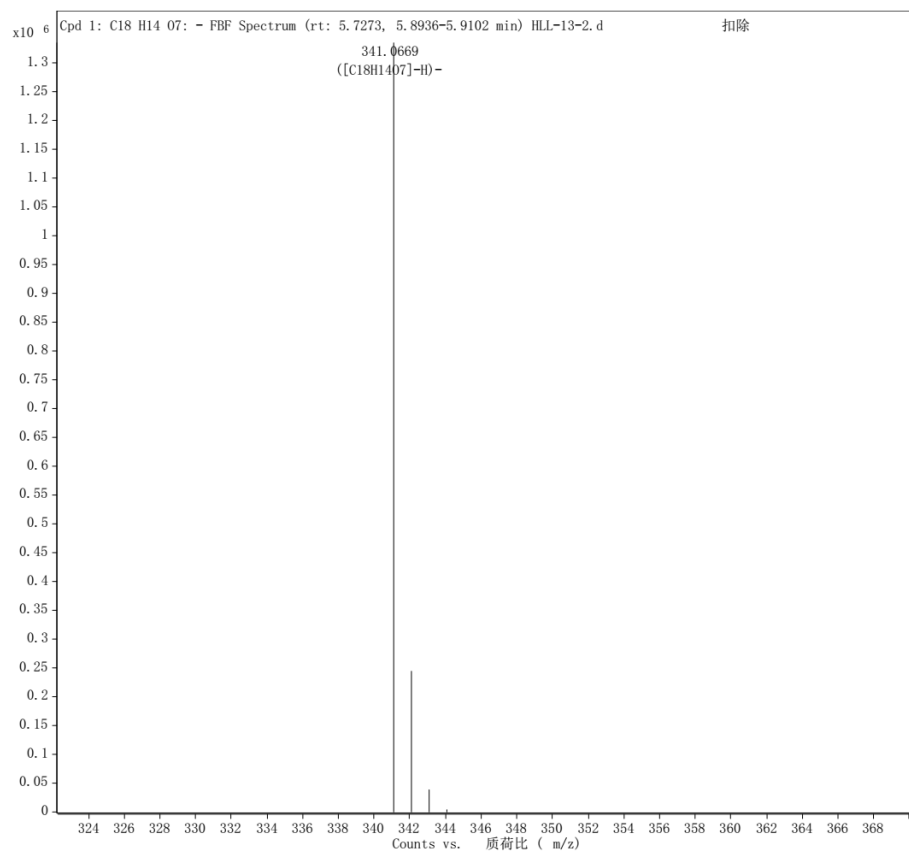


Figure S13 The HR-ESI-MS spectrum of **11**