

Supporting Information

Rec. Nat. Prod. 17:3 (2023) 446-452

Anti-inflammatory Compounds from the Heartwood of *Dalbergia melanoxylon*

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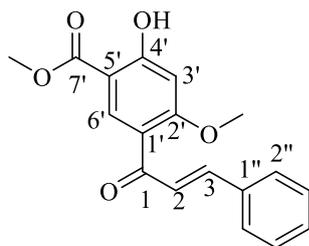
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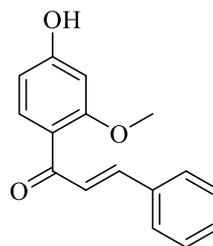
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compound 1



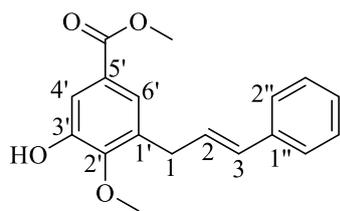
2'-methoxy-4'-hydroxychalcone

Table S1 : The most similar compound data to compound 1

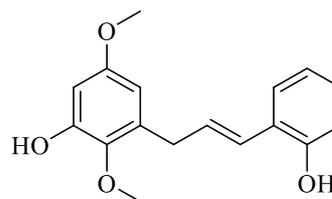
Position	1 ^a		2'-methoxy-4'-hydroxychalcone ^b	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	-	188.5		191.2
2	7.59 (1H, d, J = 15.8 Hz)	126.7	7.52 (1H, d, J = 15.6)	127.1
3	7.66 (1H, d, J = 15.8 Hz)	141.8	7.68 (1H, d, J = 15.6)	142.7
1'	-	130.2	-	121.5
2'	-	164.5	-	161.6
3'	6.69 (1H, s)	99.8		99.4
5'	-	105.5	6.52~6.49 (2H, d, J = 8.0)	108.1
4'	-	166.1	-	161
6'	8.23 (1H, s)	133.5	7.70 (1H, d, J = 8.0)	133.1
7'	-	170.0	-	-
1''	-	135.3	-	135.4
2'', 6''	7.75 (2H, dd, J = 7.2, 1.8 Hz)	128.4		128.9
4''		126.8	7.40~7.37 (3H, m)	130.1
3'', 5''	7.46 (3H, d, J = 5.9 Hz)	128.9		128.4
2'-OCH ₃	4.05 (3H, s)	56.0	3.85 (3H, s)	55.7
7'-OCH ₃	3.98 (3H, s)	52.0	-	-
4'-OH	11.27 (1H, s)	-	-	-

^a Measured in Acetone-*d*₆.

^b Measured in CDCl₃.



compound **2**



candenatenin H

Table S2 : The most similar compound data to compound **2**

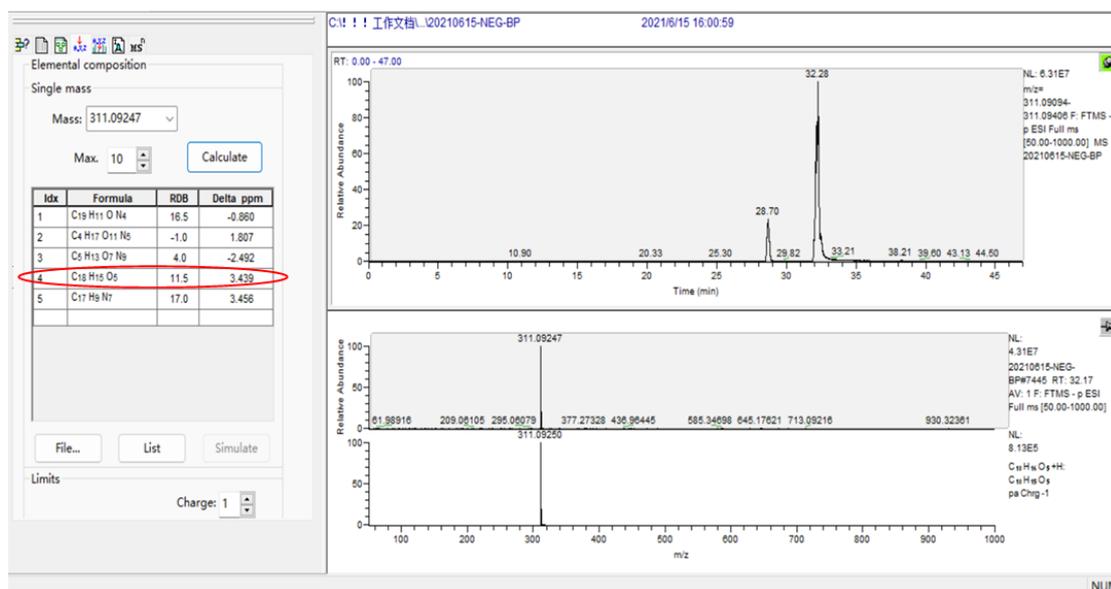
Position	2 ^a		candenatenin H ^b	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	3.46 (2H, d, J = 6.5 Hz)	30.7	3.25 (dd, 7.8, 1.5)	29.8
2	7.22 (1H, t, J = 7.3 Hz)	128.5	5.93 (dt, 15.4, 7.8)	135.4
3	6.35 (1H, m)	137.6	6.34 (br d, 15.4)	123.3
1'	-	130.8	-	119.0
2'	-	163.4	-	151.8
3'	-	162.7	-	144.7
4'	6.48 (1H, s)	127.0	6.47 (s)	99.4
5'	-	120.5	-	140.2
6'	7.62 (1H, s)	98.1	6.52 (s)	113.2
7'	-	170.5	-	-
1''	-	130.4	-	123.7
2''	-	128.4	-	152.7
6''	-	-	7.06 (br d, 7.5)	129.8
3''	7.33 (5H, m)	126.1	6.85 (br d, 7.5)	115.4
5''	-	-	6.83 (br t, 7.5)	120.2
4''	-	127.0	7.12 (td, 7.5, 1.5)	128.7
2'-OCH ₃	3.89 (3H, s)	51.9	3.67 (s)	56.0
5'-OCH ₃	-	-	3.73 (s)	56.7
7'-OCH ₃	3.92 (3H, s)	55.7	-	-
3'-OH	10.95 (1H, s)	-	5.49 (s)	-

^a Measured in Acetone-*d*₆.

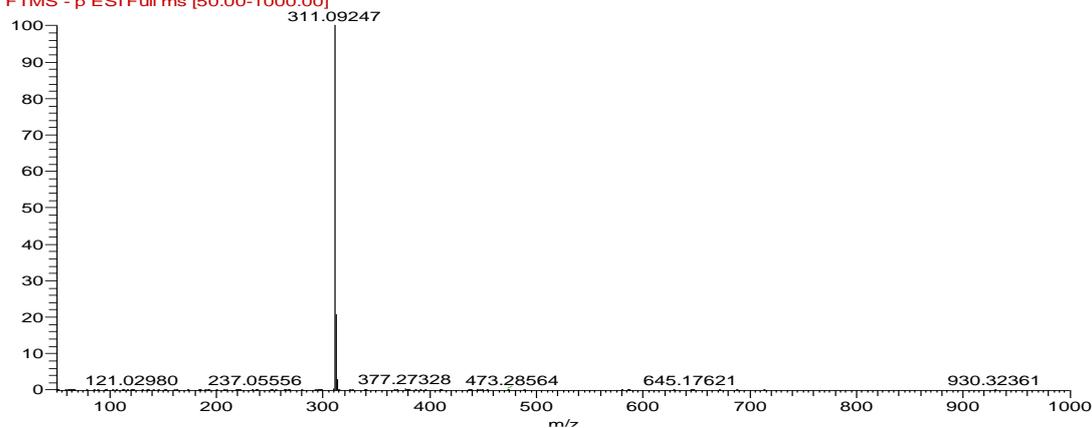
^b Measured in CDCl₃.

Table S3 :Mass information of compound 1-2 in HR-ESI-MS spectrum

Compounds	Ionic mode	Formula	Measured value (m/z)	Calculated value (m/z)	Error (ppm)
1	[M-H] ⁻	C ₁₈ H ₁₅ O ₅	311.09247	311.09250	3.439
2	[M-H] ⁻	C ₁₈ H ₁₇ O ₄	297.11346	297.11323	4.458



20210615-NEG-BP #7445 RT: 32.17 AV: 1 NL: 4.31E7
 F: FTMS - p ESI Full ms [50.00-1000.00]



20210615-NEG-BP #7350 RT: 31.84 AV: 1 NL: 6.69E3
 F: FTMS - c ESI d Full ms2 311.09@cid35.00 [7]

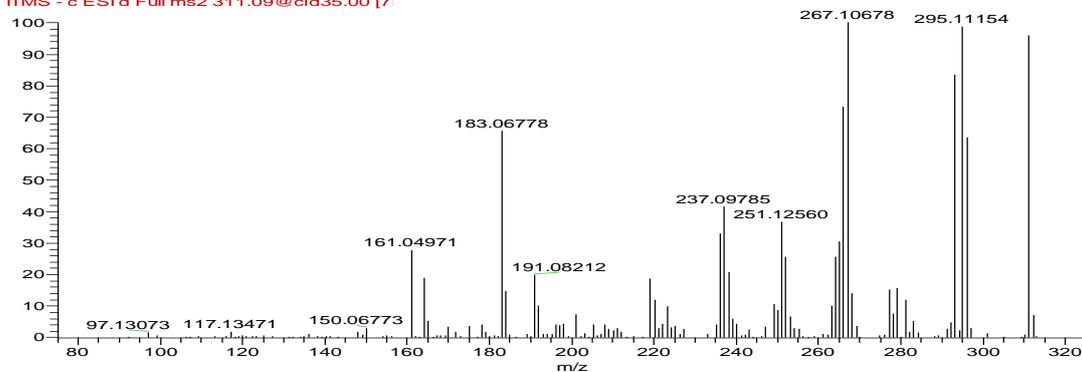


Figure S1: HR-ESI-MS spectrum of compound 1

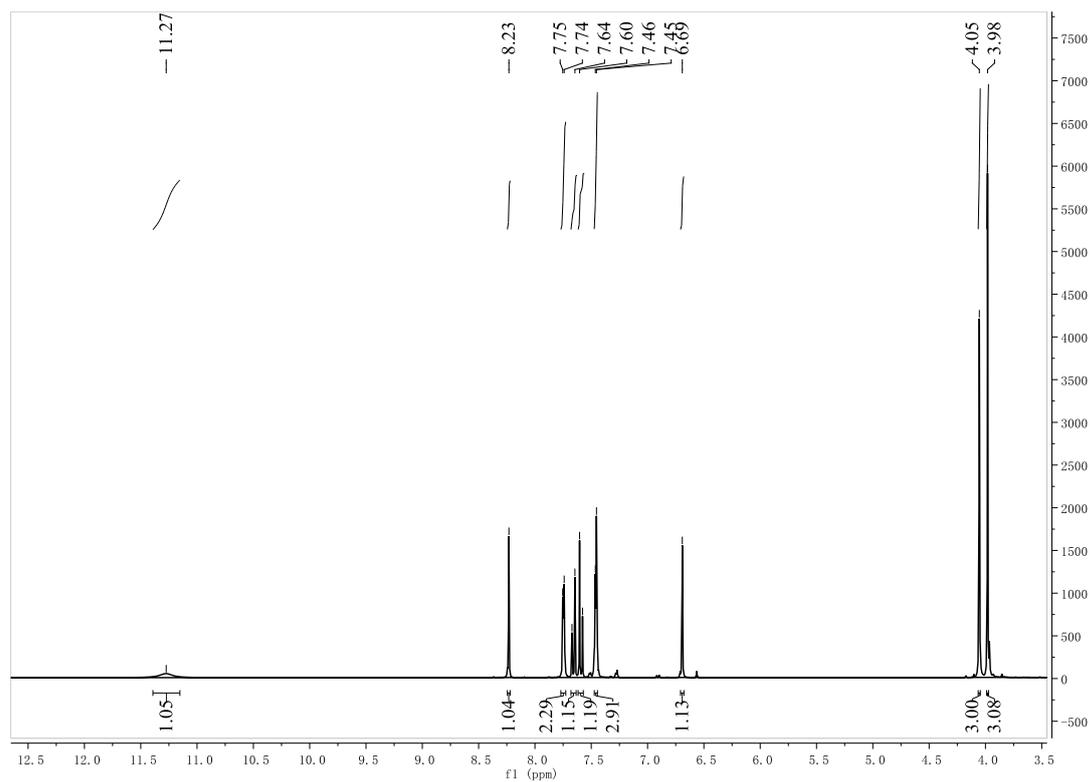


Figure S2: $^1\text{H-NMR}$ (600 MHz, Acetone- d_6) spectrum of **1**

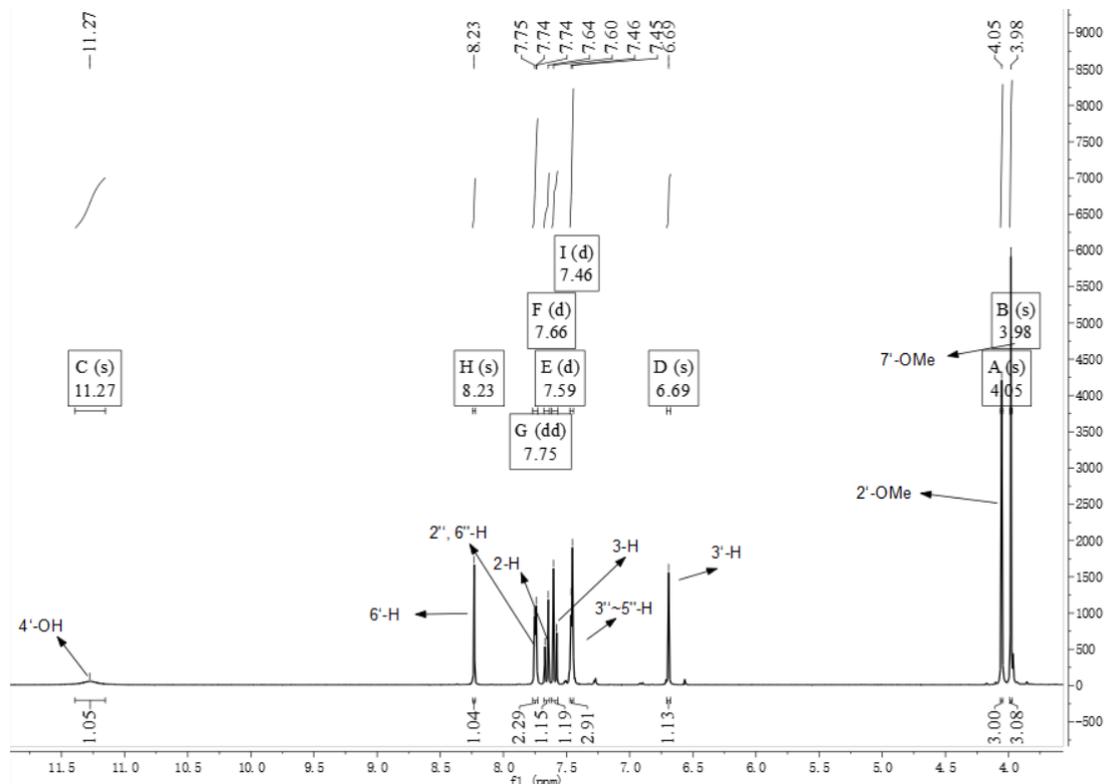


Figure S3: The labeled $^1\text{H-NMR}$ spectrum of compound **1**

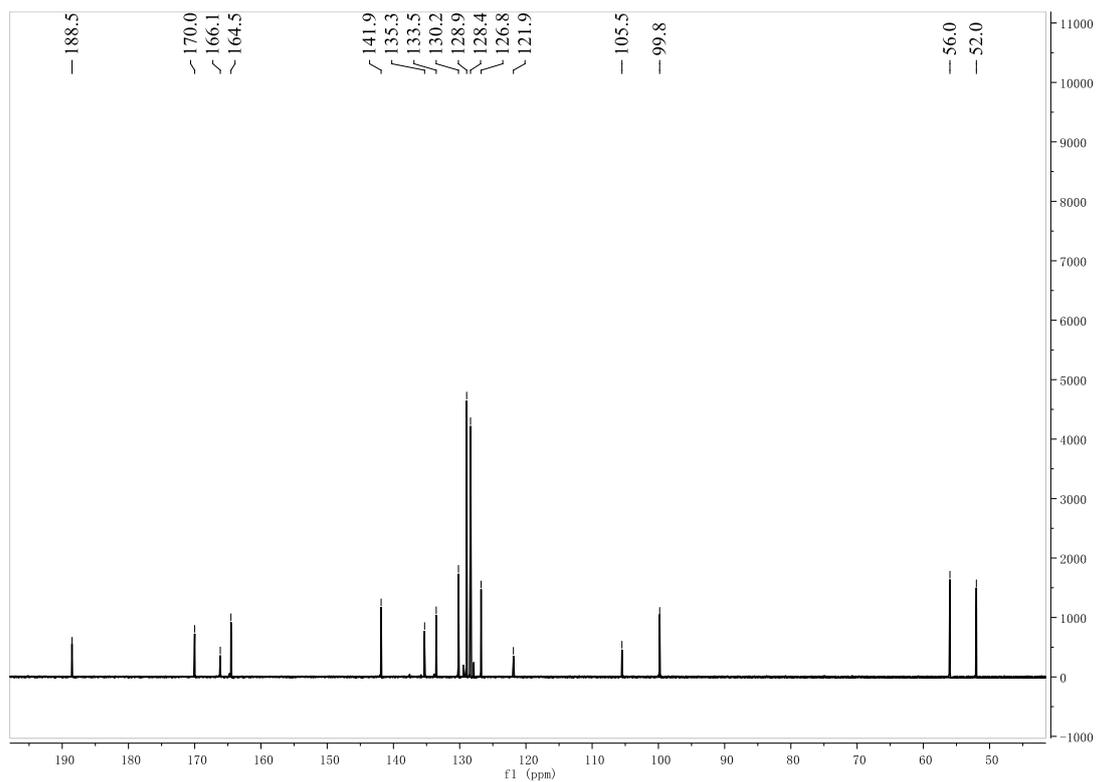


Figure S4: ^{13}C -NMR (151 MHz, $\text{Acetone-}d_6$) spectrum of compound **1**

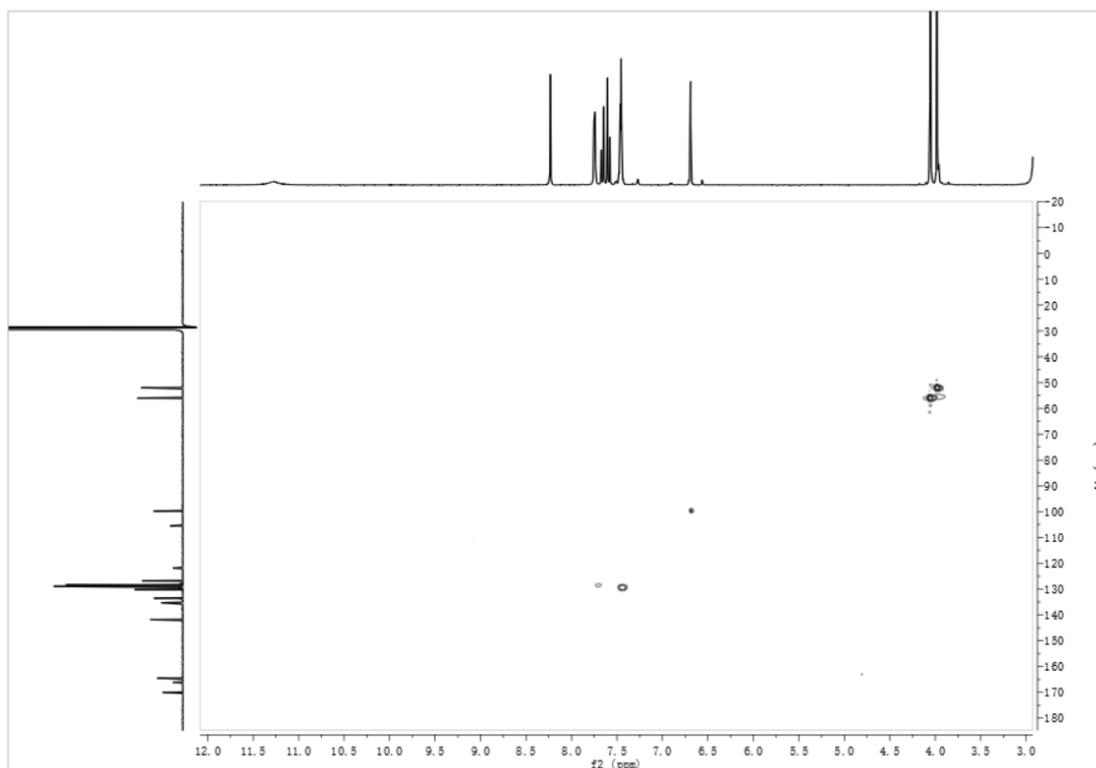


Figure S5: HSQC spectrum of compound **1**

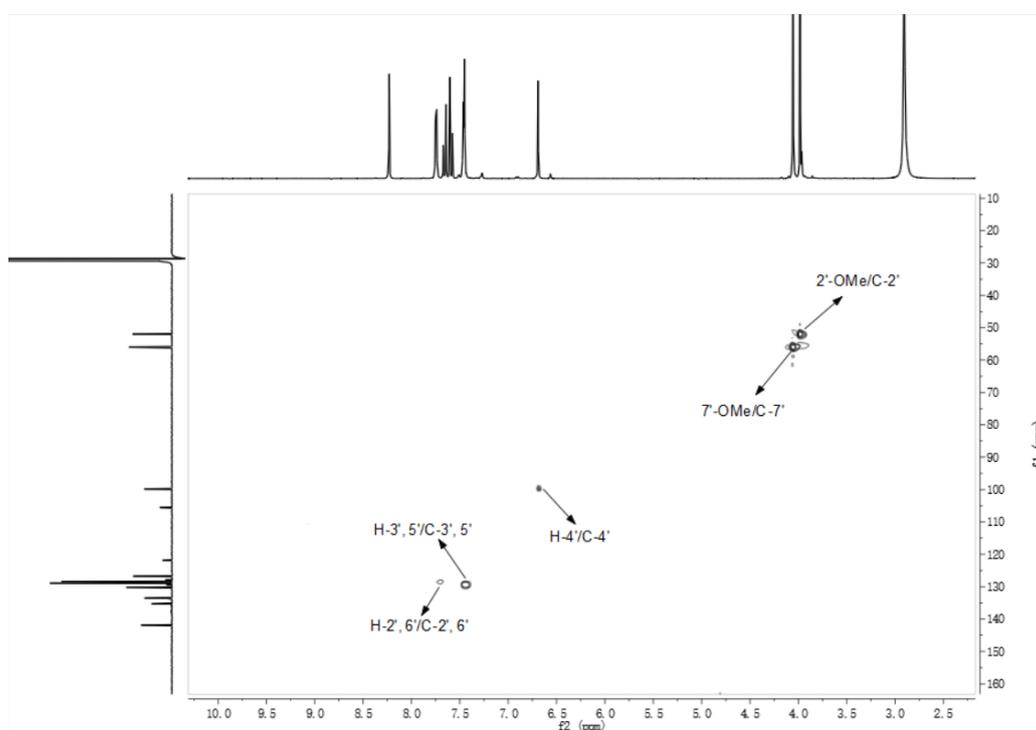


Figure S6: The labeled HSQC spectrum of compound **1**

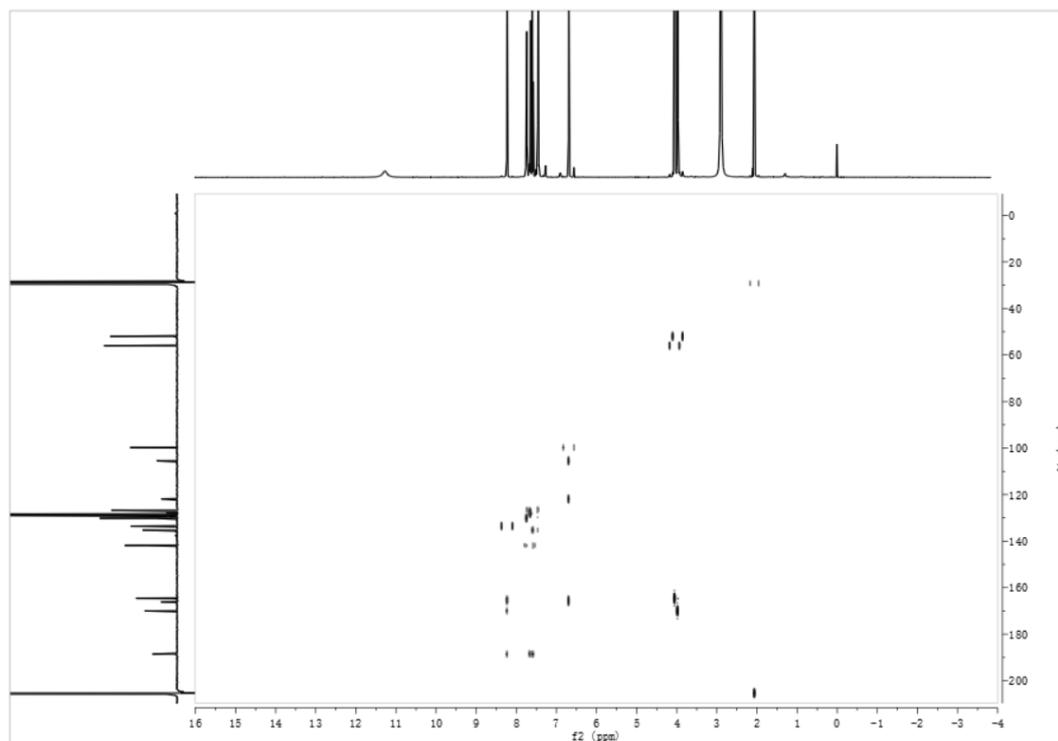


Figure S7: HMBC spectrum of compound **1**

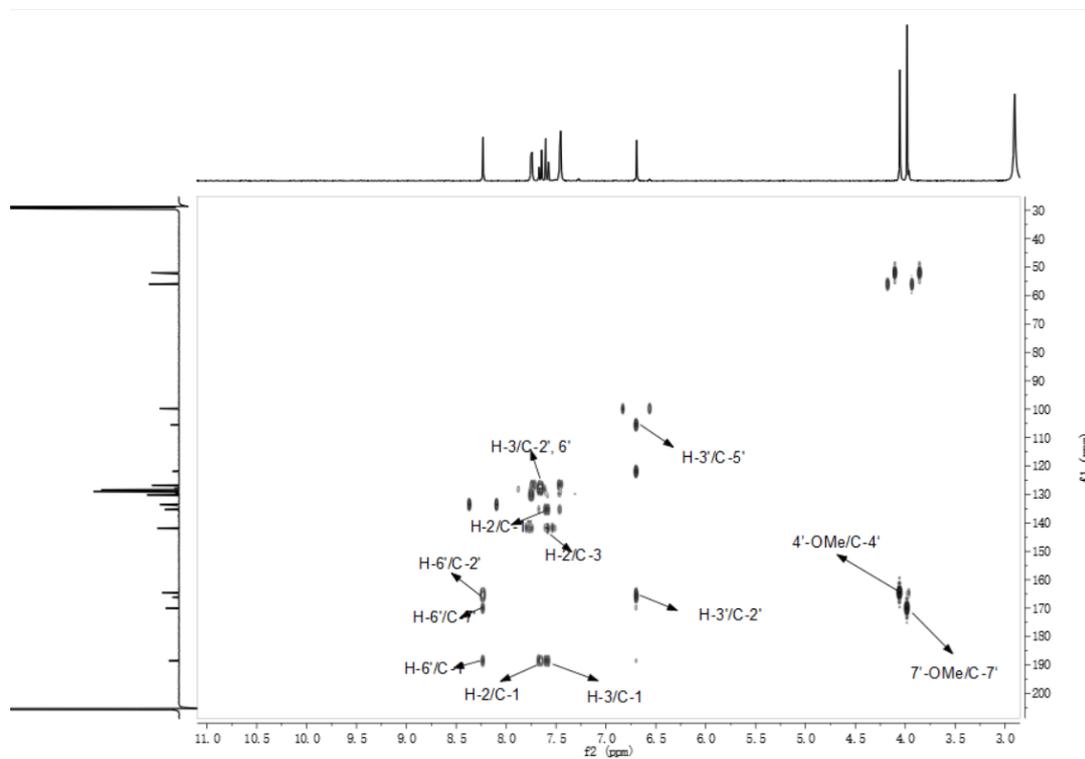


Figure S8: The labeled HMBC spectrum of compound **1**

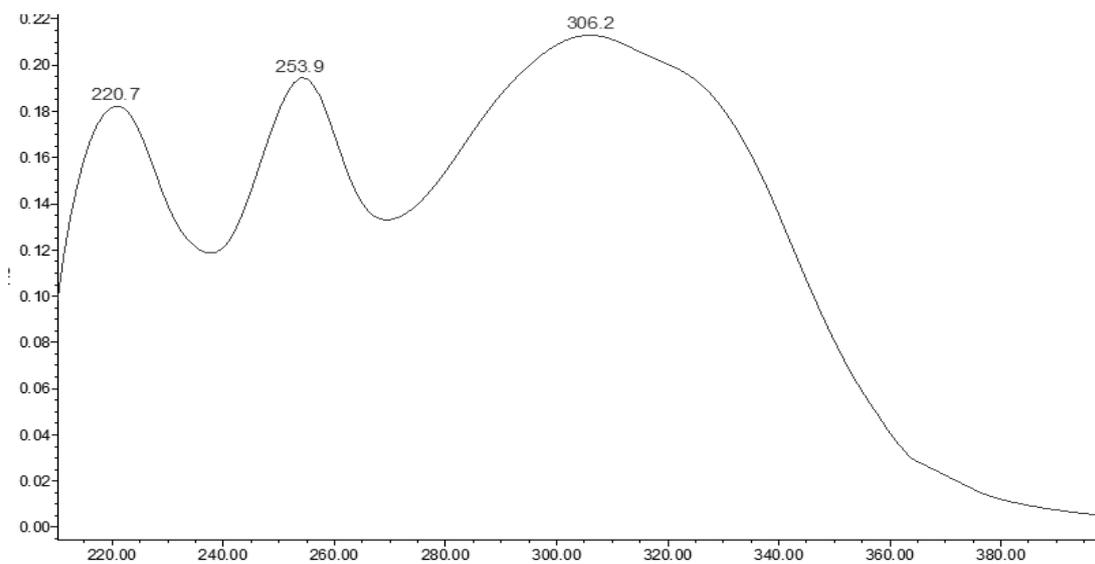


Figure S9: UV spectra of compound **1**

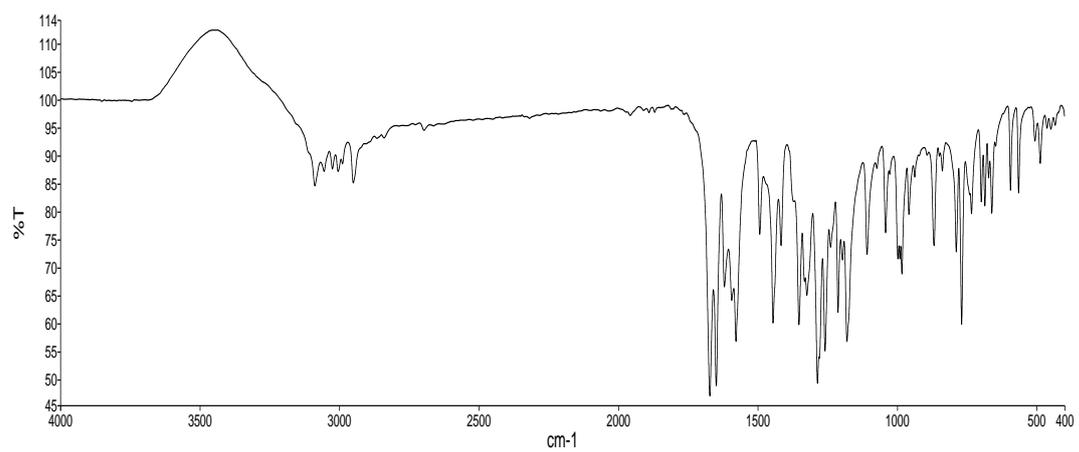


Figure S10: IR spectra of compound **1**

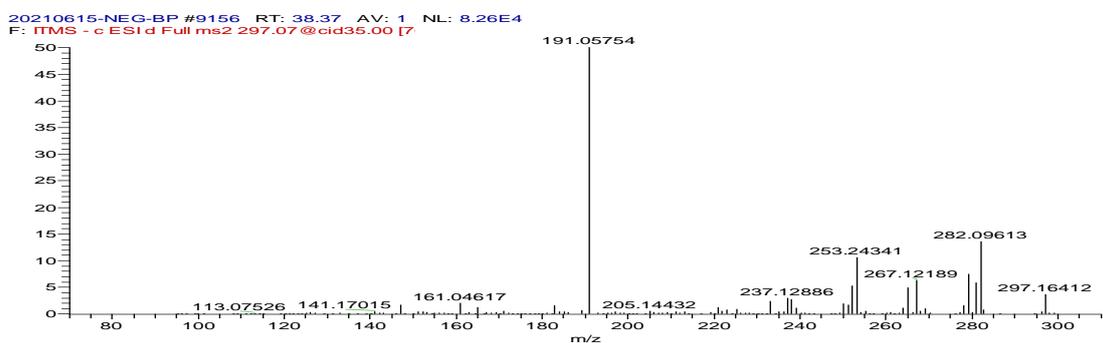
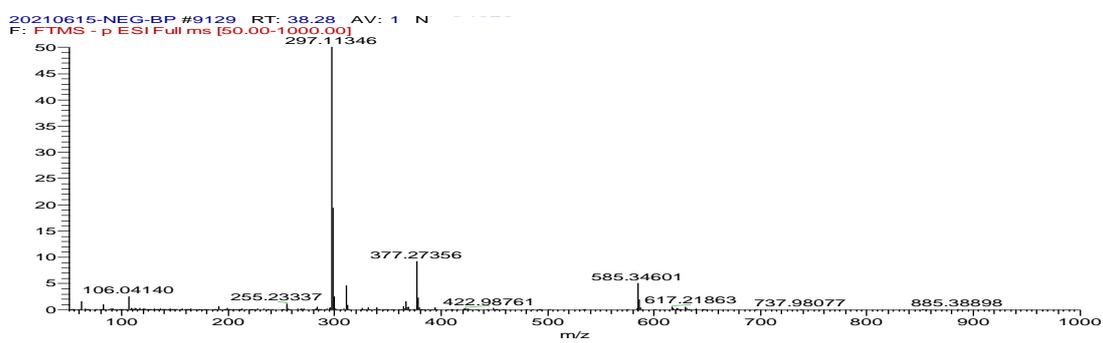
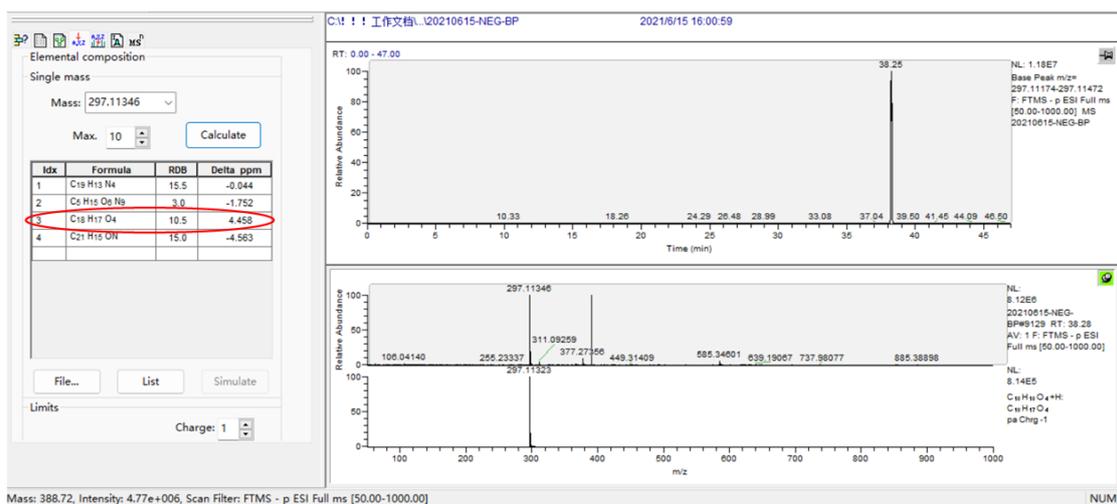


Figure S11: HR-ESI-MS spectrum of compound 2

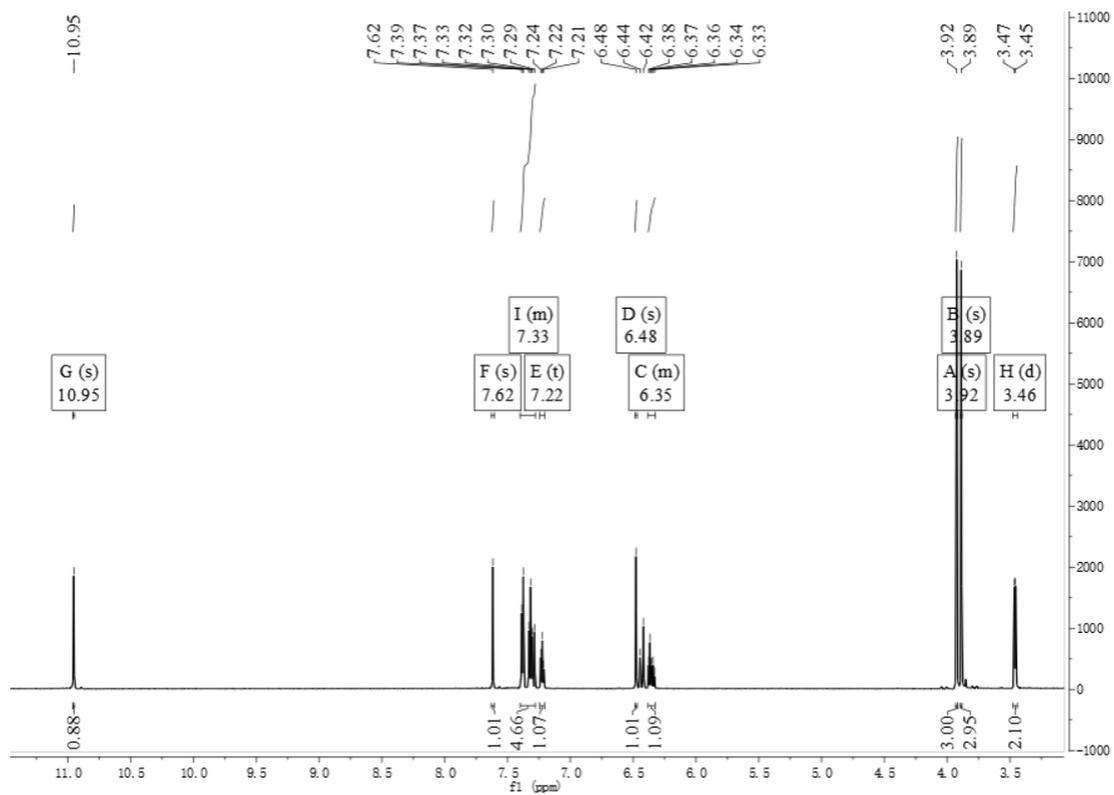


Figure S12: $^1\text{H-NMR}$ (600 MHz, CDCl_3-d_6) spectrum of compound 2

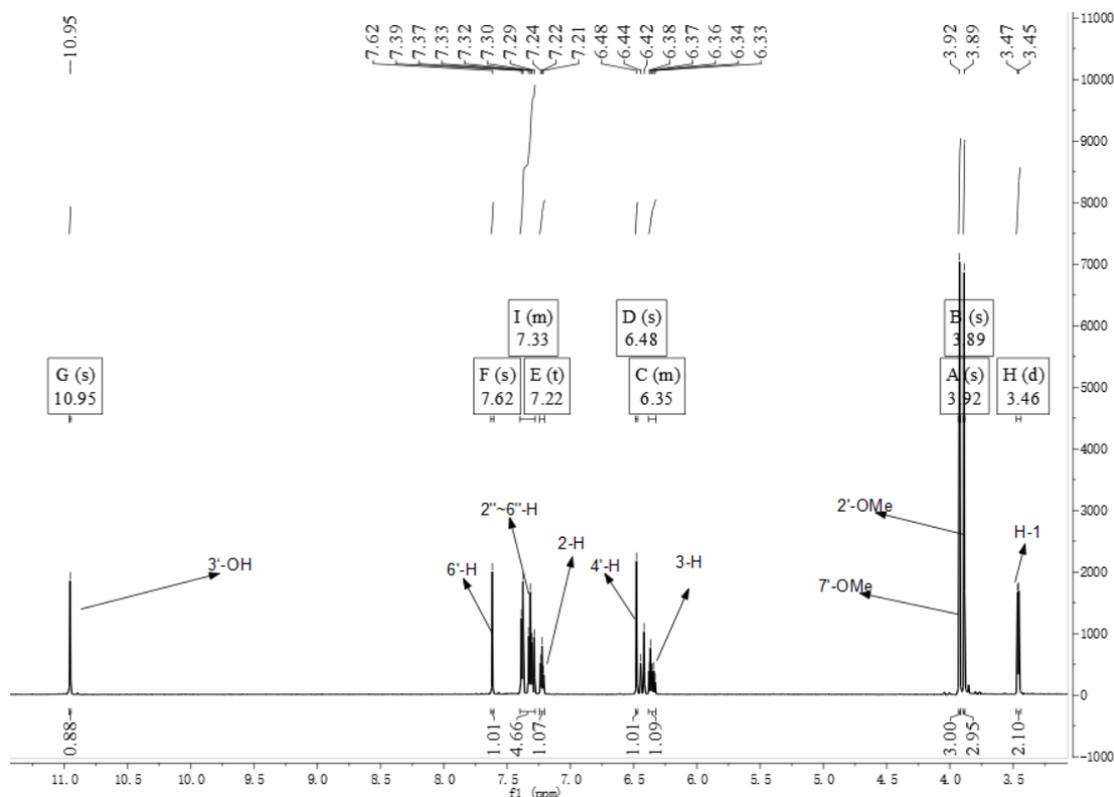


Figure S13: The labeled ^1H -NMR spectrum of compound **2**

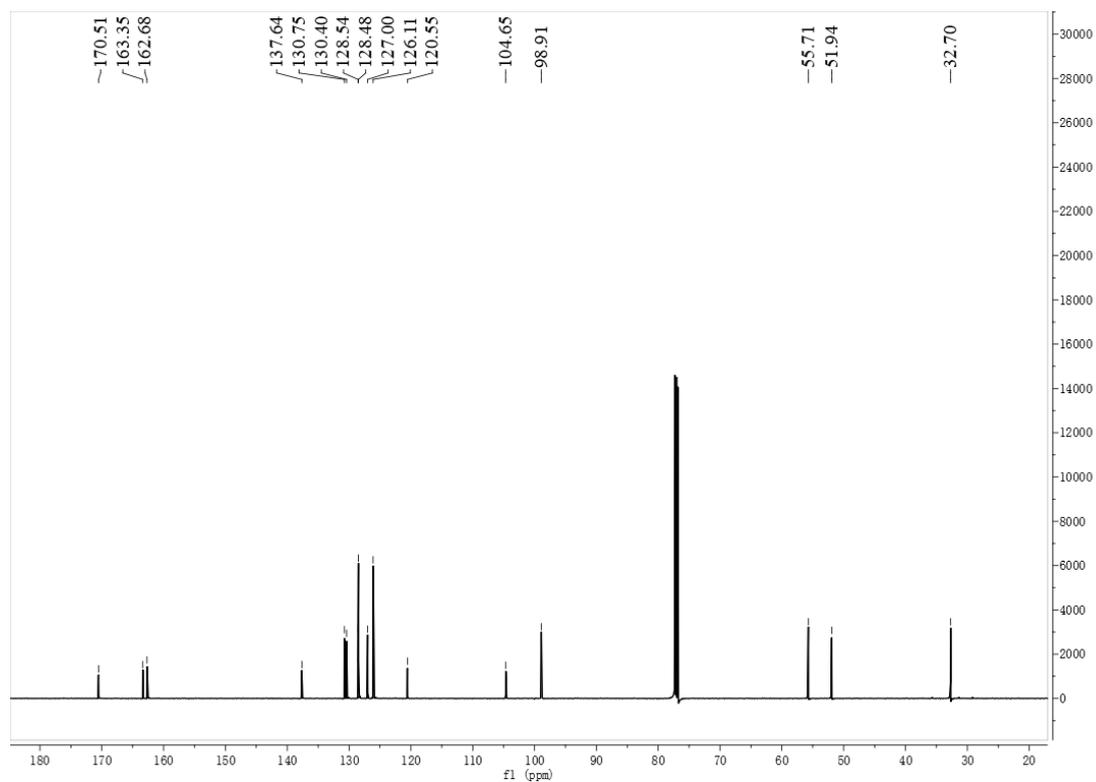


Figure S14: ^{13}C -NMR (151 MHz, CDCl_3 - d_6) spectrum of compound **2**

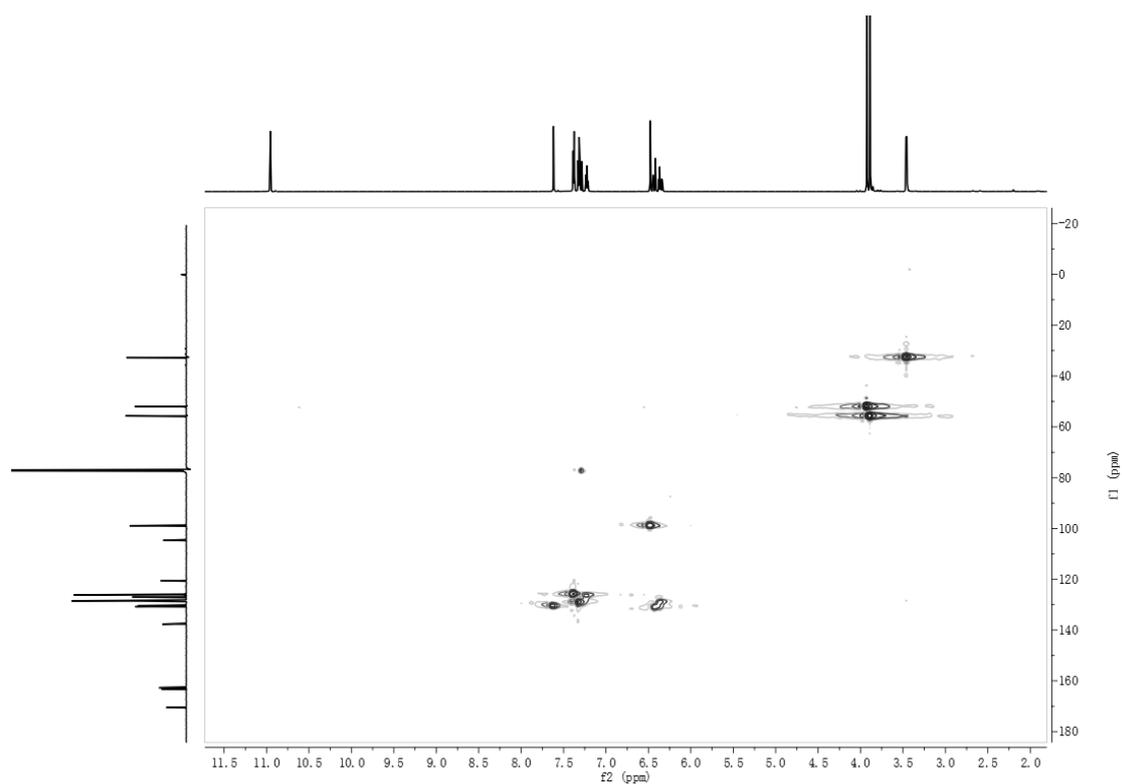


Figure S15: HSQC spectrum of compound 2

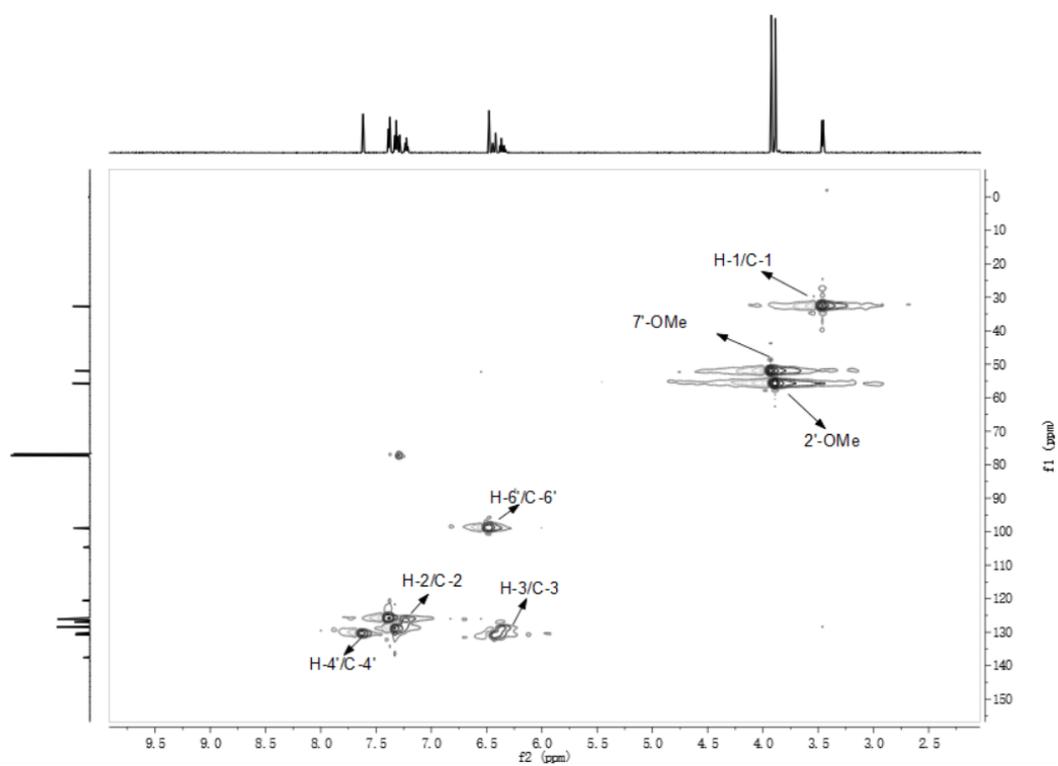


Figure S16: The labeled HSQC spectrum of compound **2**

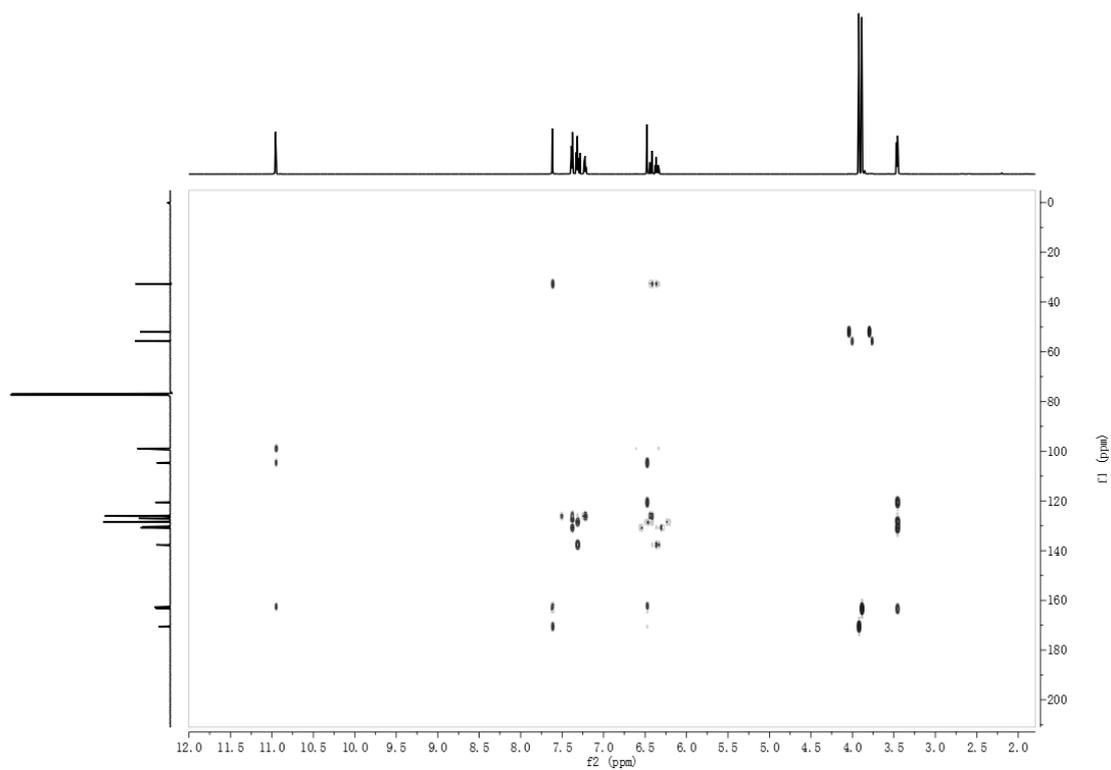


Figure S17: HMBC spectrum of compound **2**

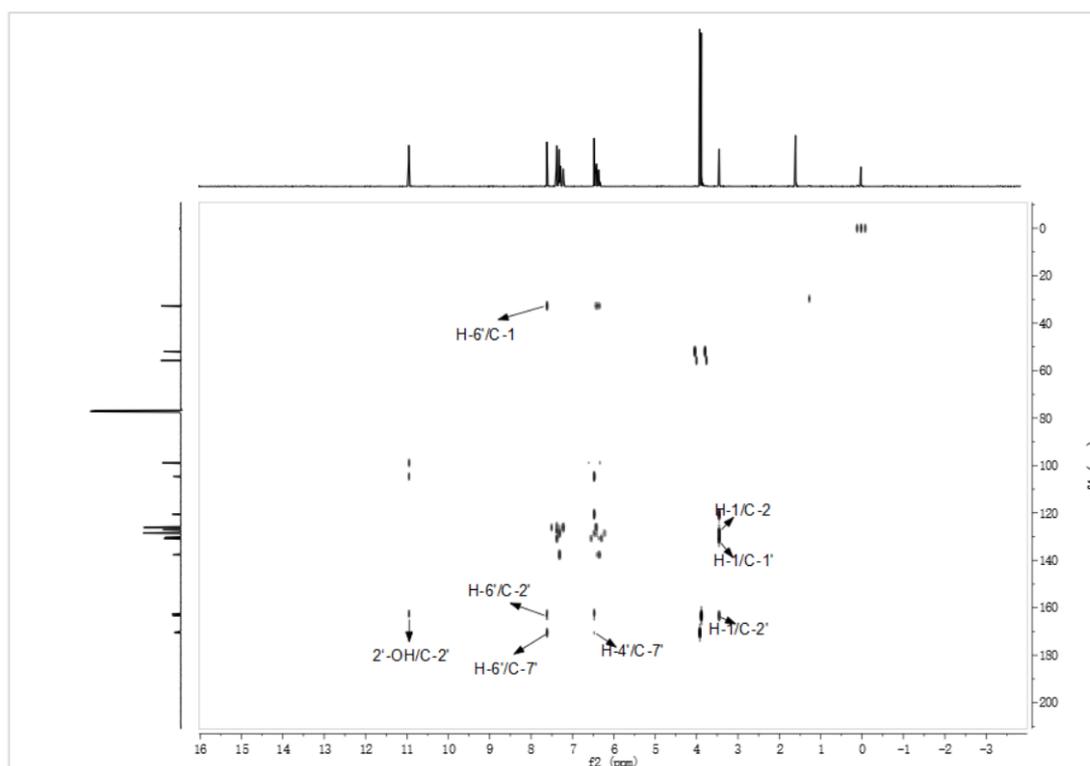


Figure S18: The labeled HMBC spectrum of compound **2**

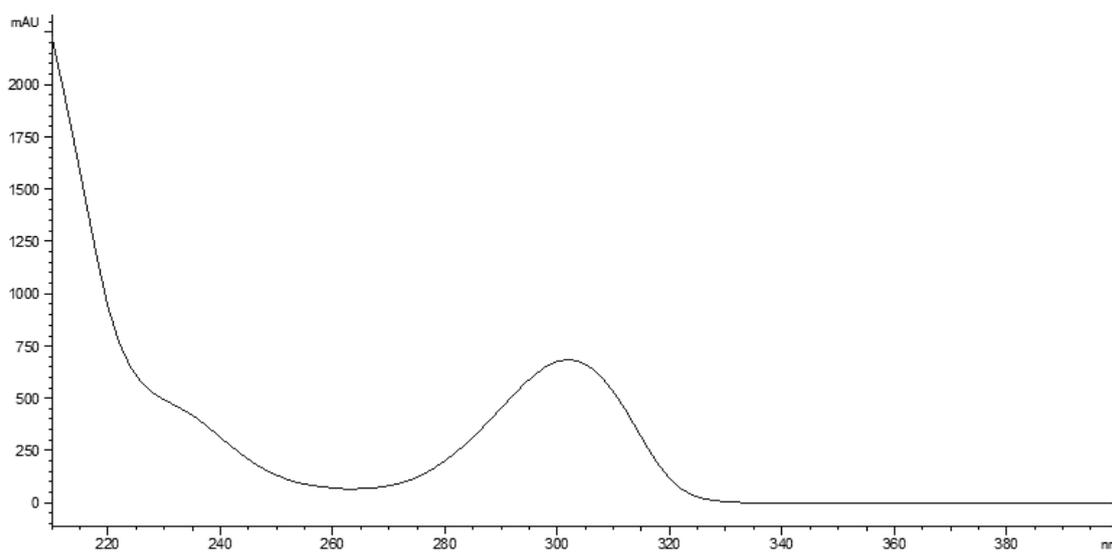


Figure S19: UV spectrum of compound **2**

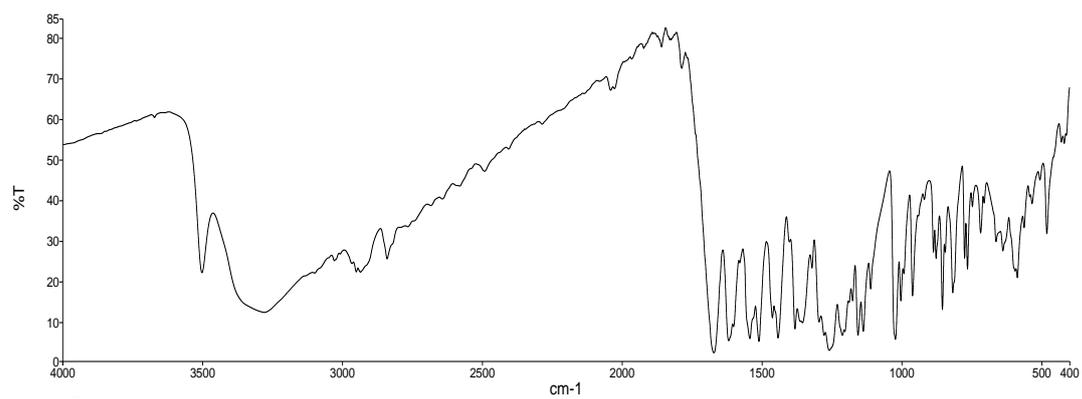


Figure S20: IR spectrum of compound **2**

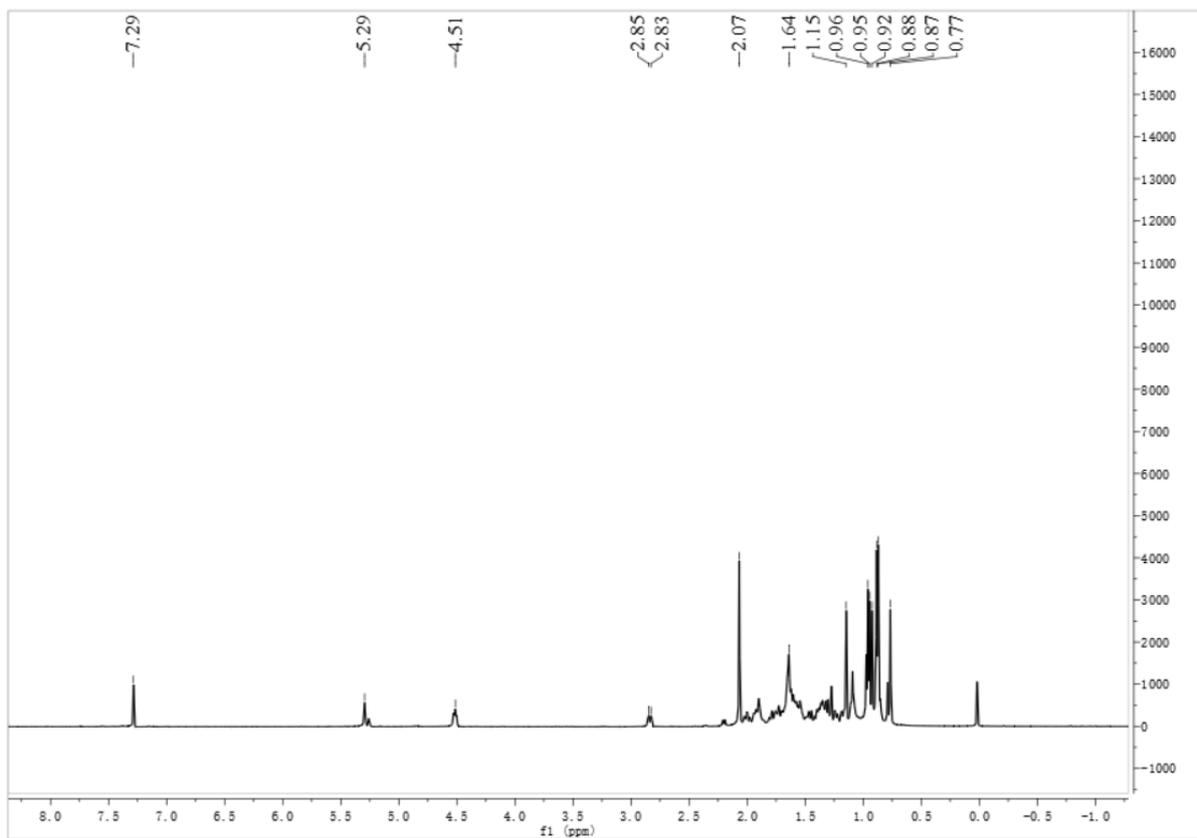


Figure S21: ¹H-NMR spectrum of compound **3** (600 MHz, Acetone-*d*₆)

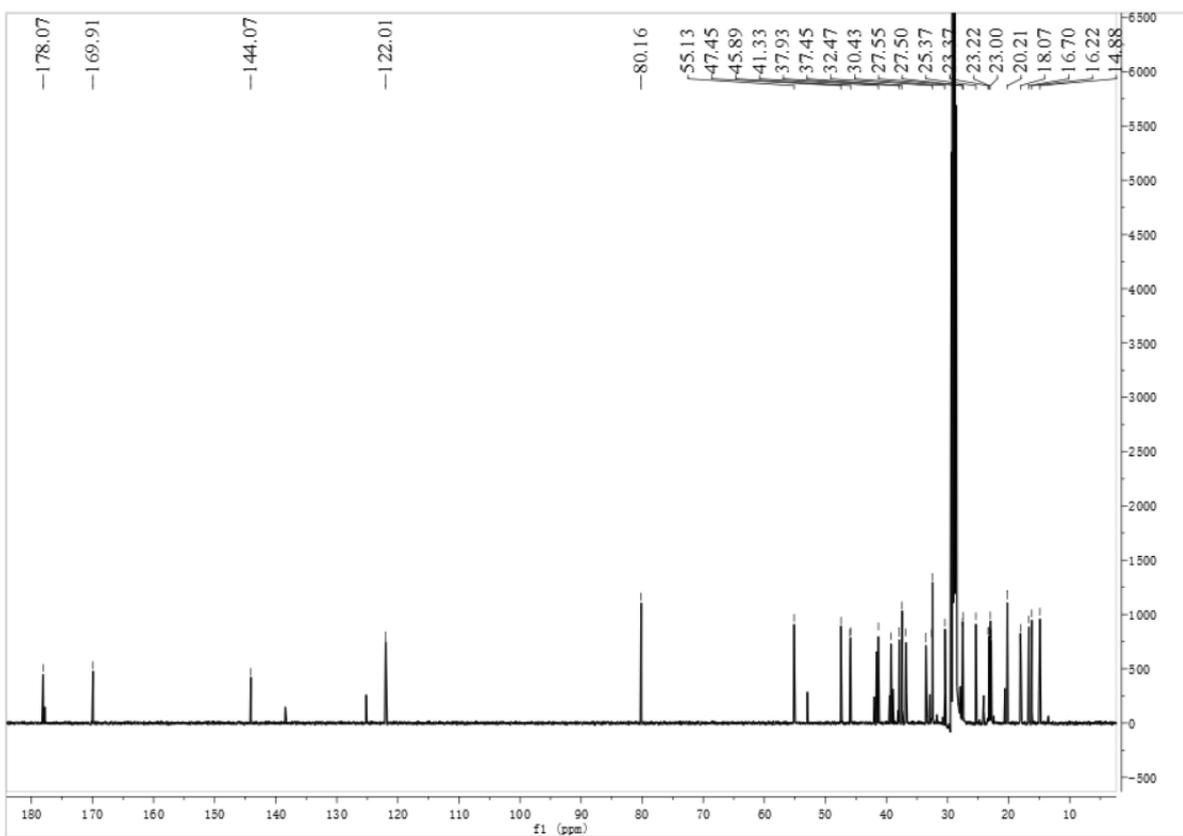


Figure S22 : ^{13}C -NMR spectra of compound compound **3** (151 MHz, Acetone- d_6)

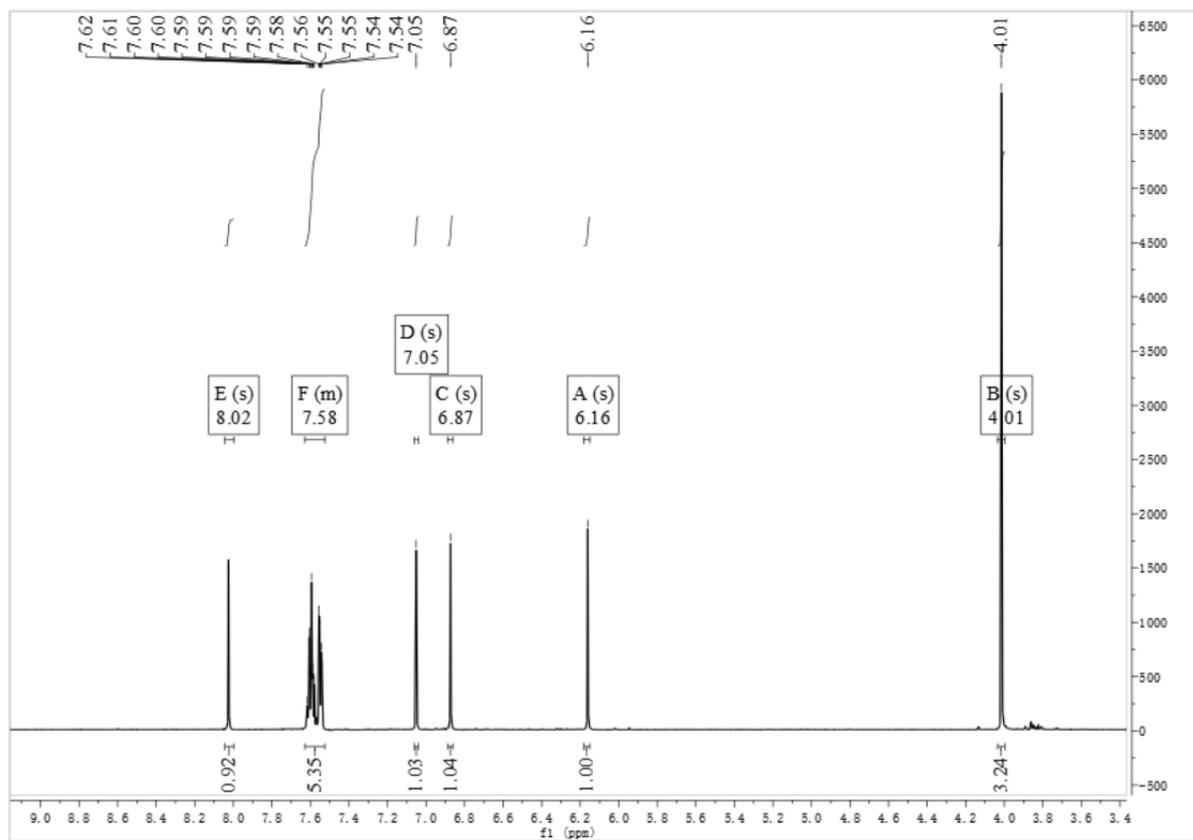


Figure S23 : $^1\text{H-NMR}$ spectra of compound **4** (600 MHz, Acetone- d_6)

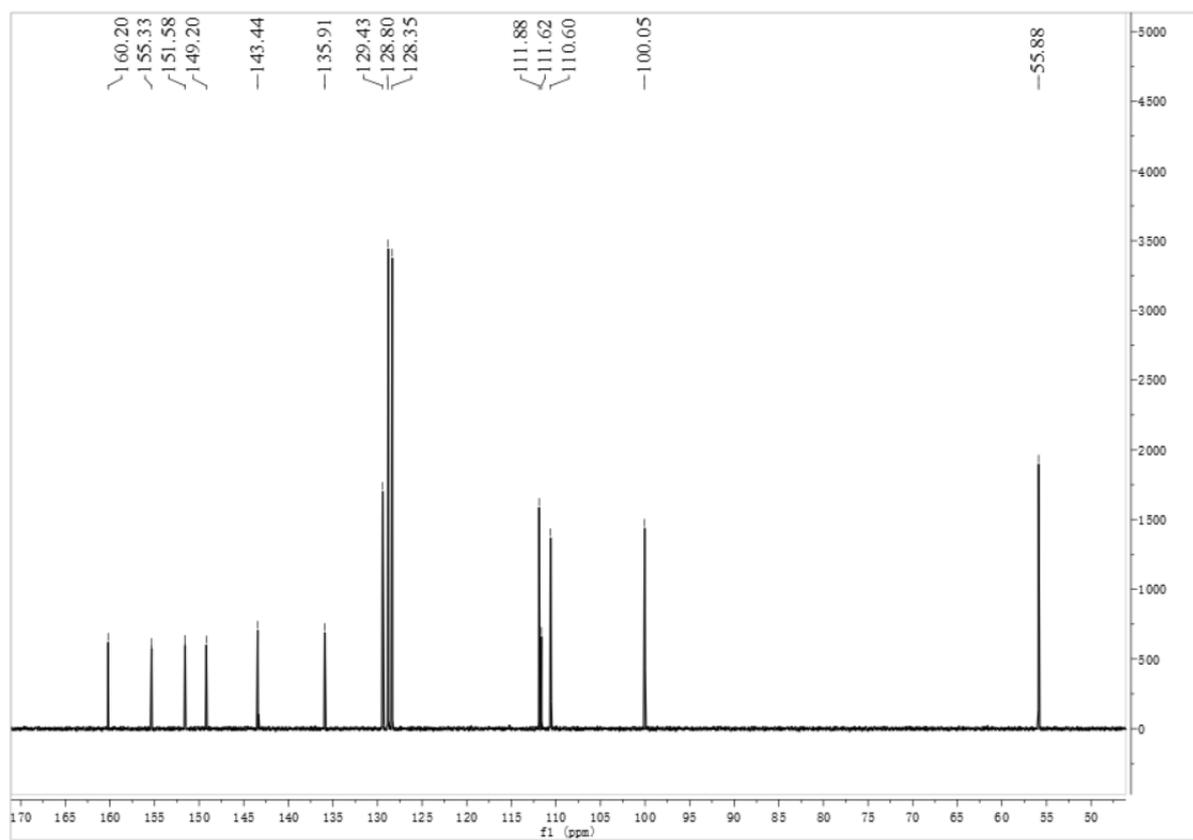


Figure S24 : ^{13}C -NMR spectra of compound **4** (600 MHz, $\text{Acetone-}d_6$)

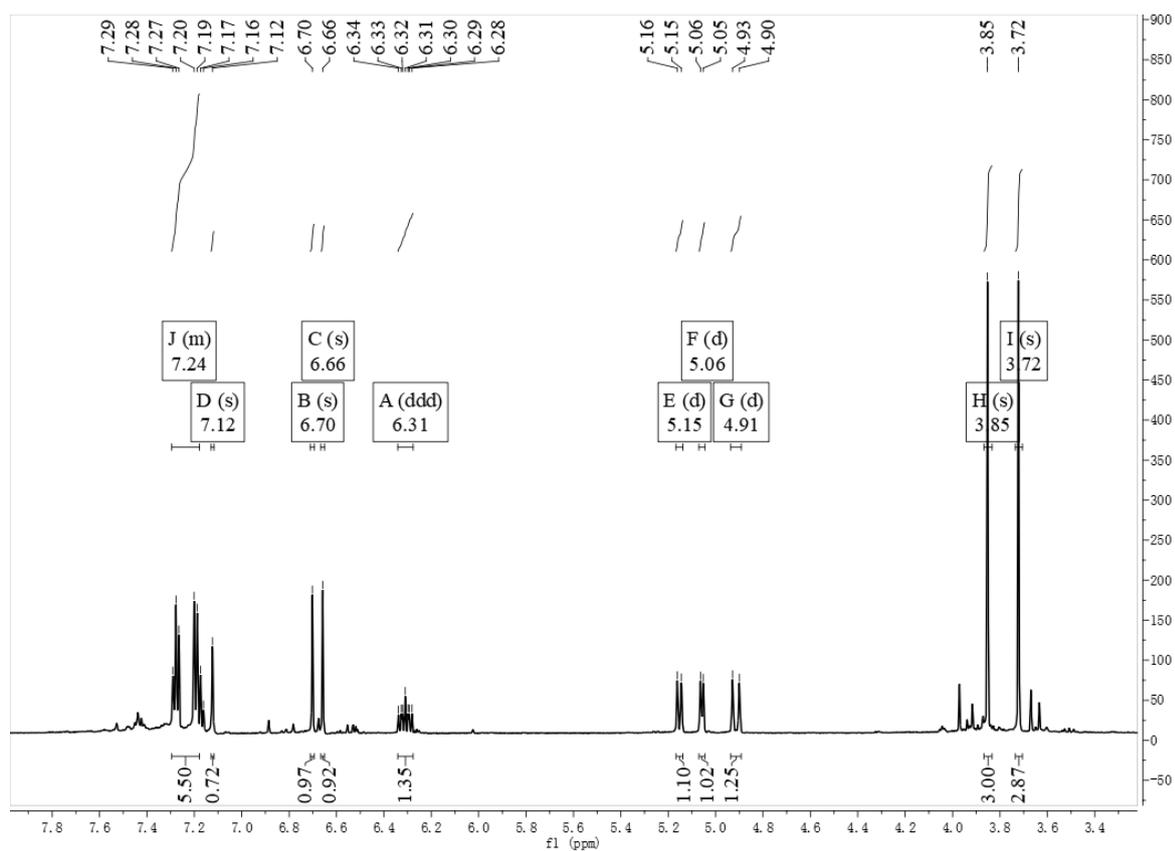


Figure S25 : ^1H -NMR spectra of compound **5** (600 MHz, Acetone- d_6)

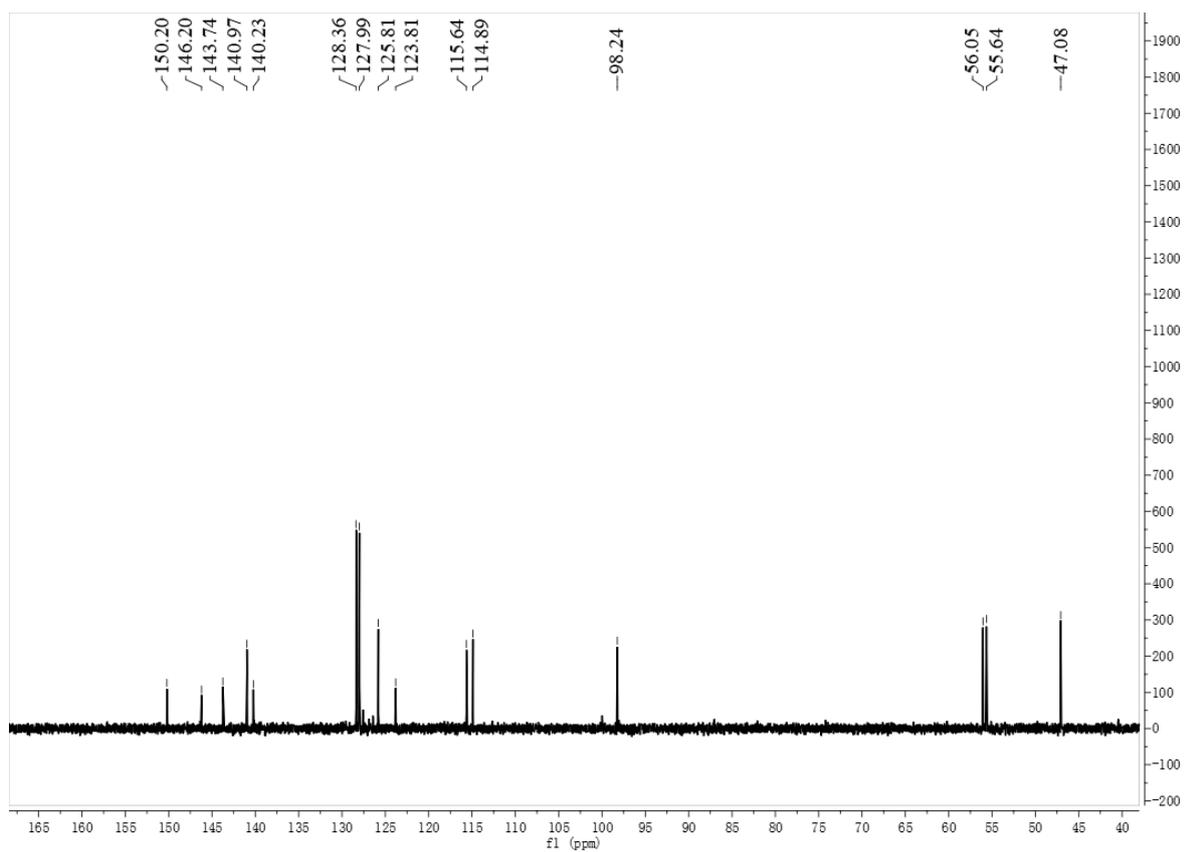


Figure S26 : ^{13}C -NMR spectra of compound 5 (151 MHz, Acetone- d_6)

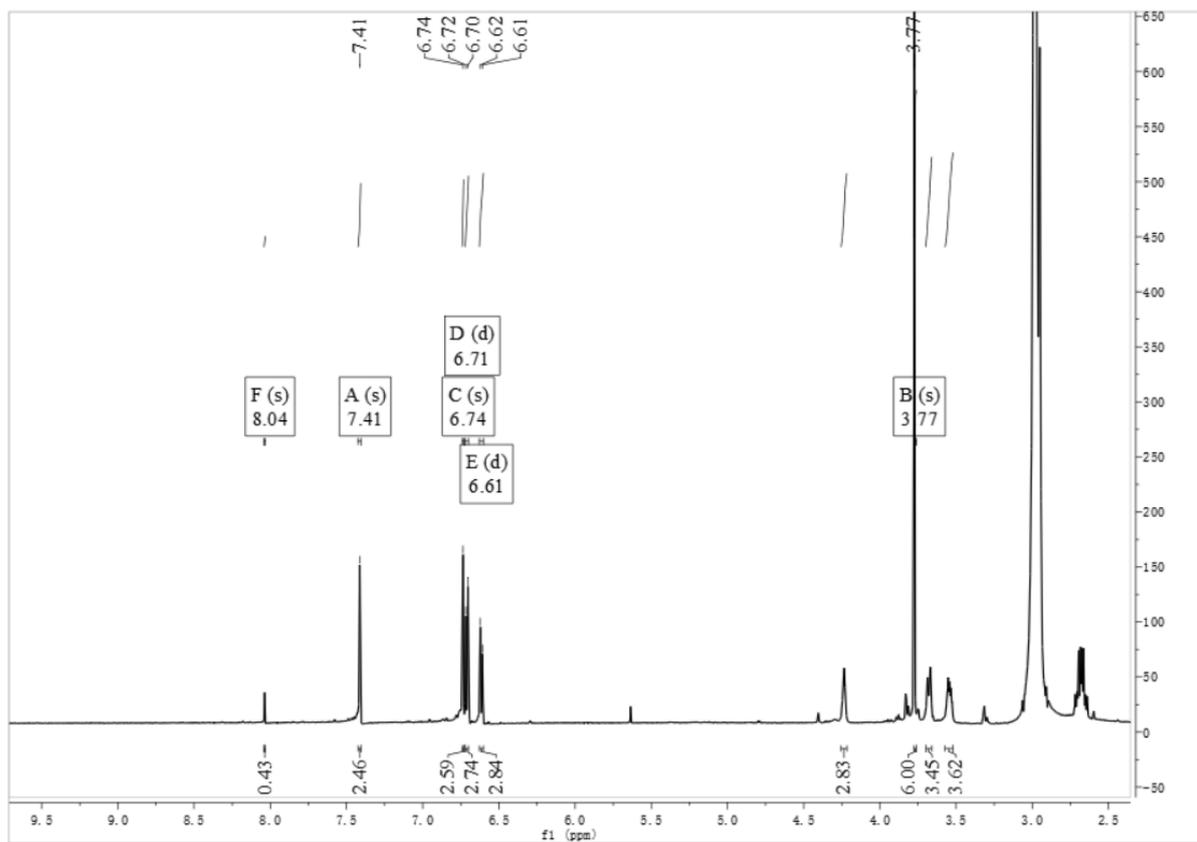


Figure S27: $^1\text{H-NMR}$ spectra of compound **6** (600 MHz, Acetone- d_6)

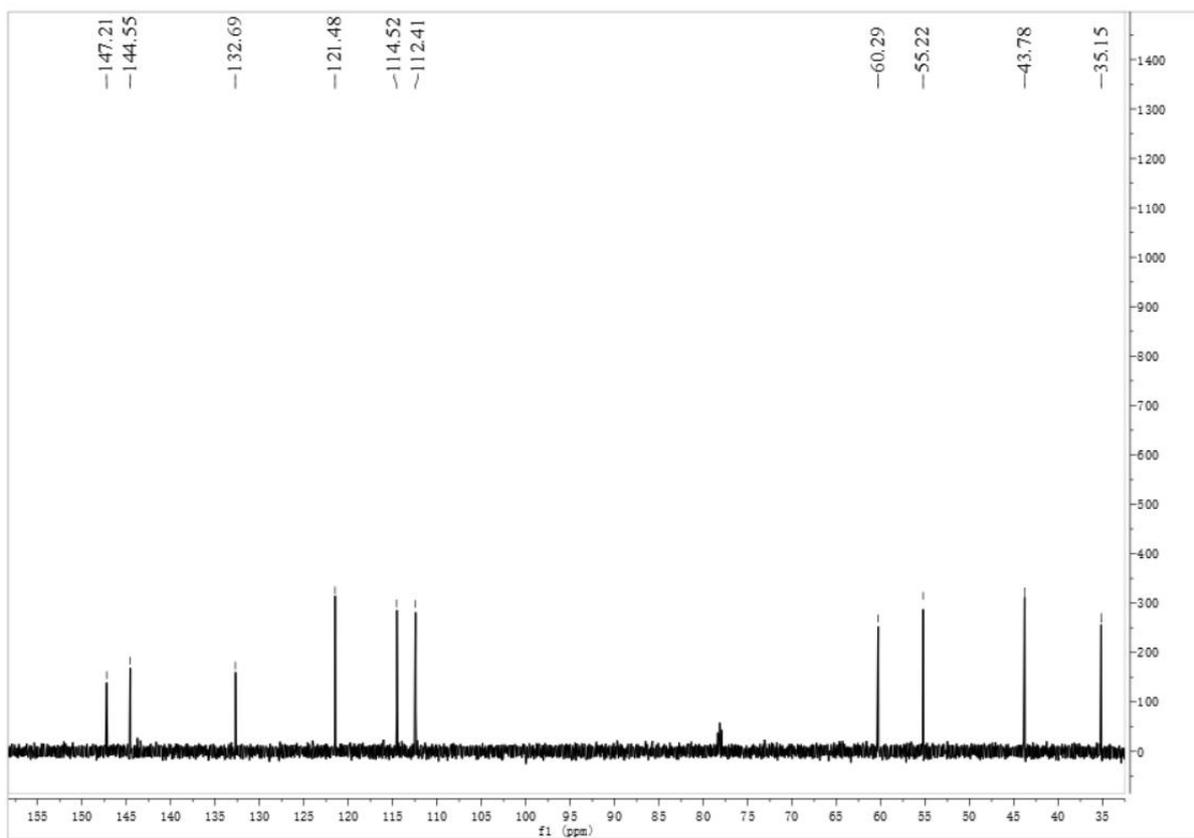


Figure S28: ^{13}C -NMR spectra of compound **6** (151 MHz, $\text{Acetone-}d_6$)