

SUPPLEMENTARY MATERIAL

Isolation and Identification of new Prenylated Acetophenone

Derivatives from *Acronychia oligophlebia*

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Three new prenylated acetophenone derivatives, acronyculatin P (**1**), acronyculatin Q (**2**), and acronyculatin R (**3**) were isolated from the leaves of *Acronychia oligophlebia*. Their structures were identified by extensive analyses of spectroscopic data (IR, UV, ESI-HRMS, 1D and 2D NMR) and comparison with the literatures. In addition, the cytotoxic activity against MCF-7 cells of the isolates were evaluated by the MTT assay and the IC₅₀ values were 56.8, 40.4 and 69.1 μ M, respectively.

Keywords: *Acronychia oligophlebia*; prenylated acetophenone derivatives; cytotoxic activity.

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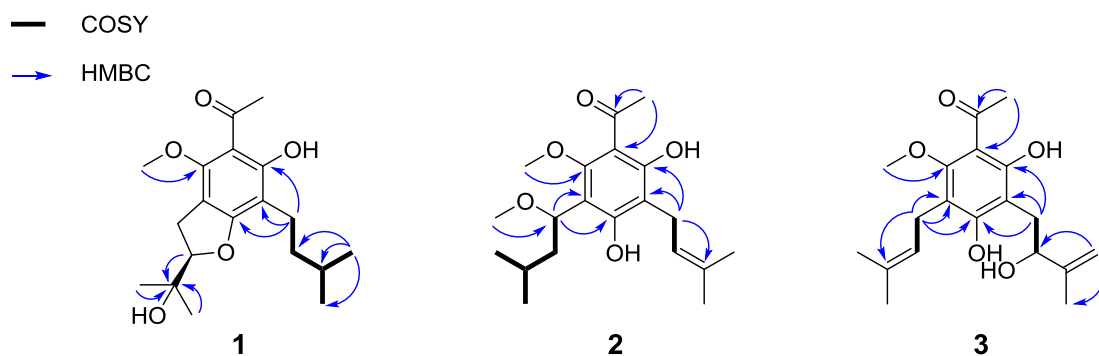


Fig. S1. Key ^1H - ^1H COSY and HMBC correlations of **1-3**

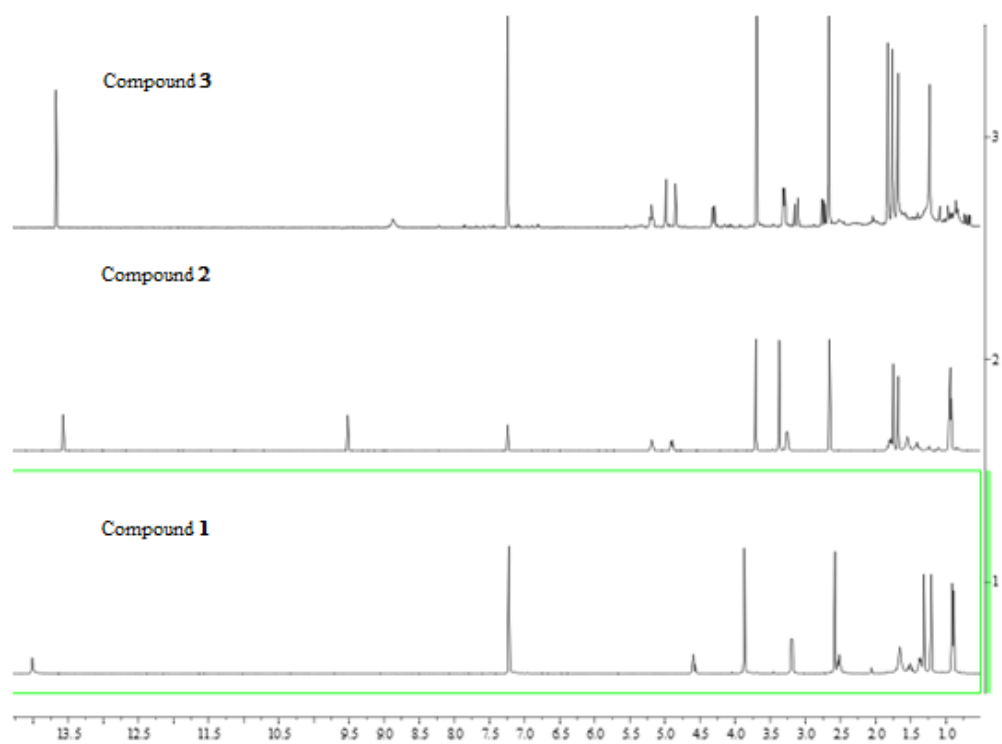


Fig. S2. ^1H NMR superimposed spectrum of **1-3**

Table 1. ^1H and ^{13}C NMR spectral data of compounds **1–3** in CDCl_3 (δ in ppm, J in Hz).

Position	1	2		3		
	$\delta_{\text{H}}^{\text{a,c}}$	$\delta_{\text{C}}^{\text{b}}$	$\delta_{\text{H}}^{\text{a,c}}$	$\delta_{\text{C}}^{\text{b}}$	$\delta_{\text{H}}^{\text{a,c}}$	$\delta_{\text{C}}^{\text{b}}$
1	-	203.2	-	203.7	-	203.7
2	2.62 (s)	32.3	2.68 (s)	31.1	2.69 (s)	31.2
1'	-	108.3	-	108.5	-	108.9
2'	-	164.8	-	161.3	-	162.1
3'	-	107.9	-	114.9	-	109.5
4'	-	165.1	-	162.2	-	162.4
5'	-	107.1	-	108.9	-	115.0
6'	-	156.7	-	160.8	-	160.1
1''	3.23 (d, 8.6)	29.0	4.92 (dd, 12.0 4.0)	78.2	3.33 (d, 6.0)	23.1
2''	4.63 (t, 8.6)	91.4	1.81 (m); 1.43 (m)	44.3	5.21 (t, 6.0)	123.3
3''	-	72.2	1.83 (m)	24.9	-	132.2
4''	1.36 (s)	26.0	0.95 (d, 5.4)	21.9	1.70 (s)	25.9
5''	1.24 (s)	24.6	0.96 (d, 5.4)	23.5	1.78 (s)	18.1
1'''	2.55 (m)	21.0	3.28 (d, 8.0)	22.5	2.75 (m)	29.0
					3.15 (dd, 14.9, 1.9)	
2'''	1.42 (m)	38.1	5.21 (t, 8.0)	123.4	4.33 (d, 8.3)	77.8
3'''	1.55 (m)	27.6	-	131.6	-	147.2
4'''	0.93 (d, 6.5)	22.7	1.70 (s)	25.8	5.01 (m); 4.87 (m)	110.5
5'''	0.93 (d, 6.5)	22.7	1.77 (s)	18.0	1.85 (s)	18.6
1''-OMe	-	-	3.39 (s)	57.8	-	-
6'-OMe	3.90 (s)	59.3	3.73 (s)	62.8	3.72 (s)	62.8
2'-OH	14.05 (s)	-	13.59 (s)	-	13.69 (s)	-
4'-OH	-	-	9.54 (s)	-	8.91(s)	-

^a ^1H NMR spectra were measured at 400 MHz^b ^{13}C NMR spectra were measured at 100 MHz^c Overlapped signals were reported without designating multiplicity

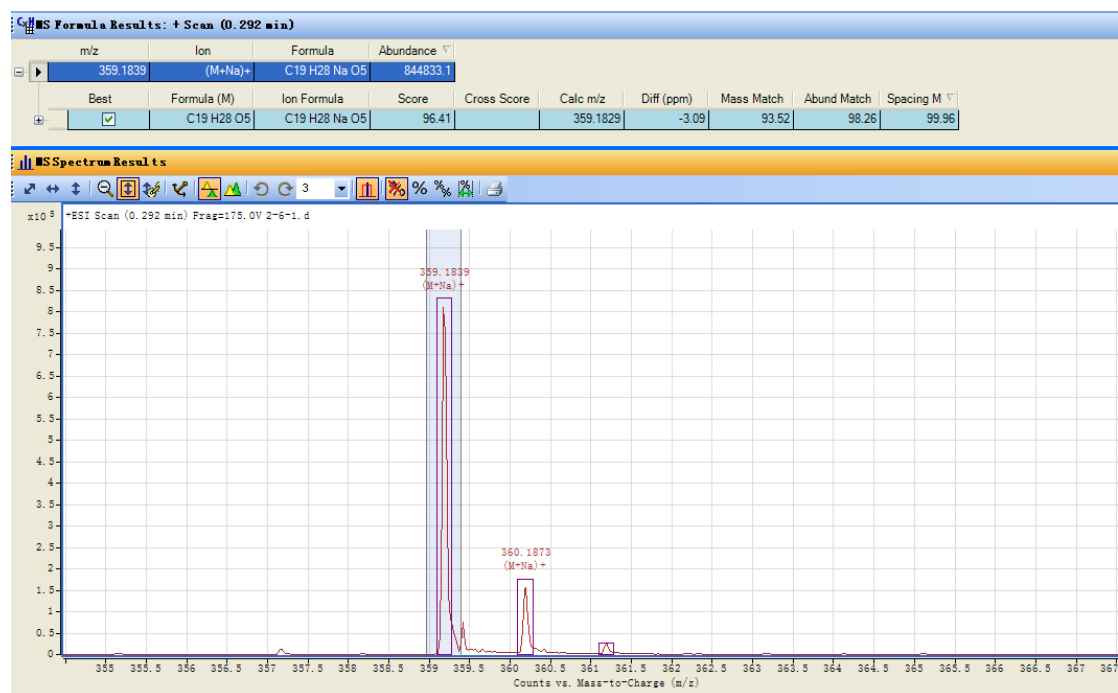


Fig. S3. ESI-HRMS of **1**

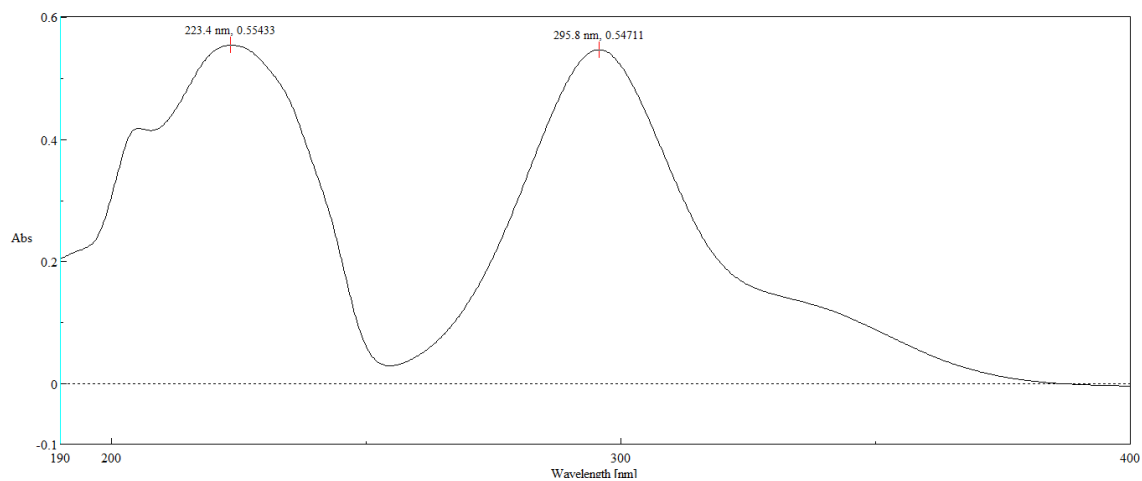


Fig. S4. UV spectrum of **1** (CH₃OH)

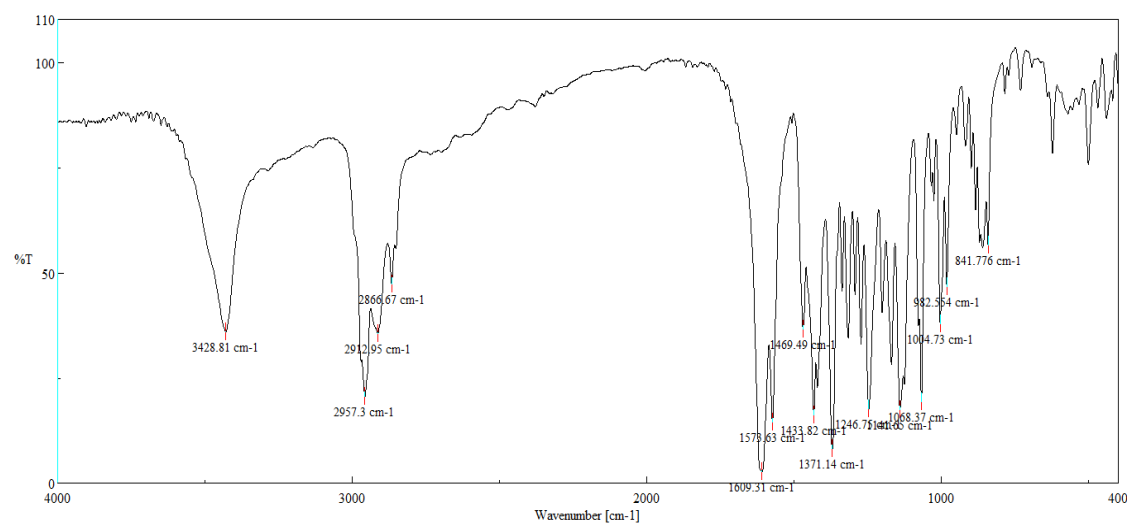


Fig. S5. IR spectrum of **1** (KBr disc)

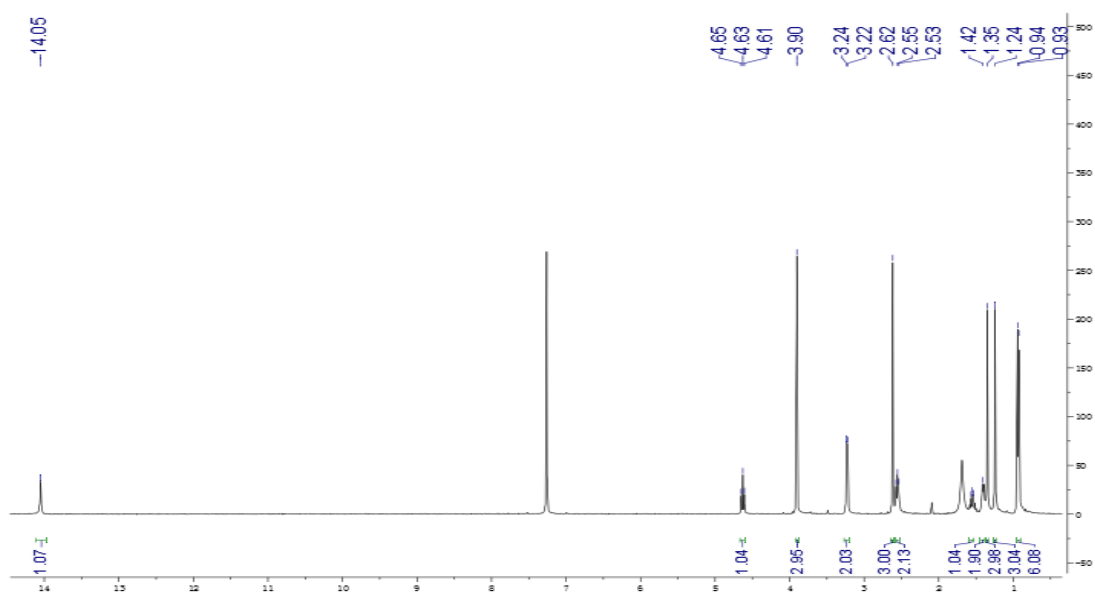


Fig. S6. ¹H NMR spectrum of **1** in CDCl₃

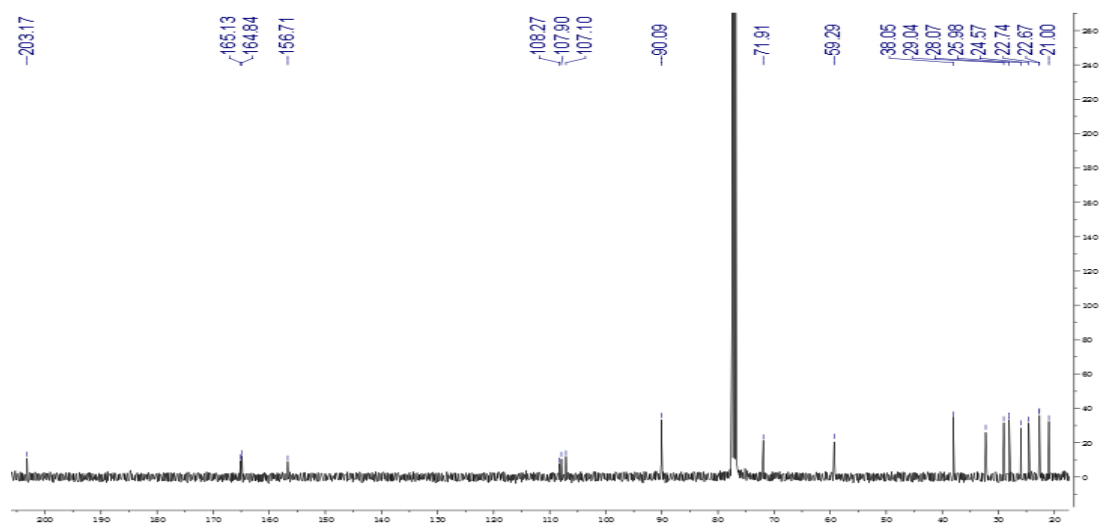


Fig. S7. ^{13}C NMR spectrum of **1** in CDCl_3

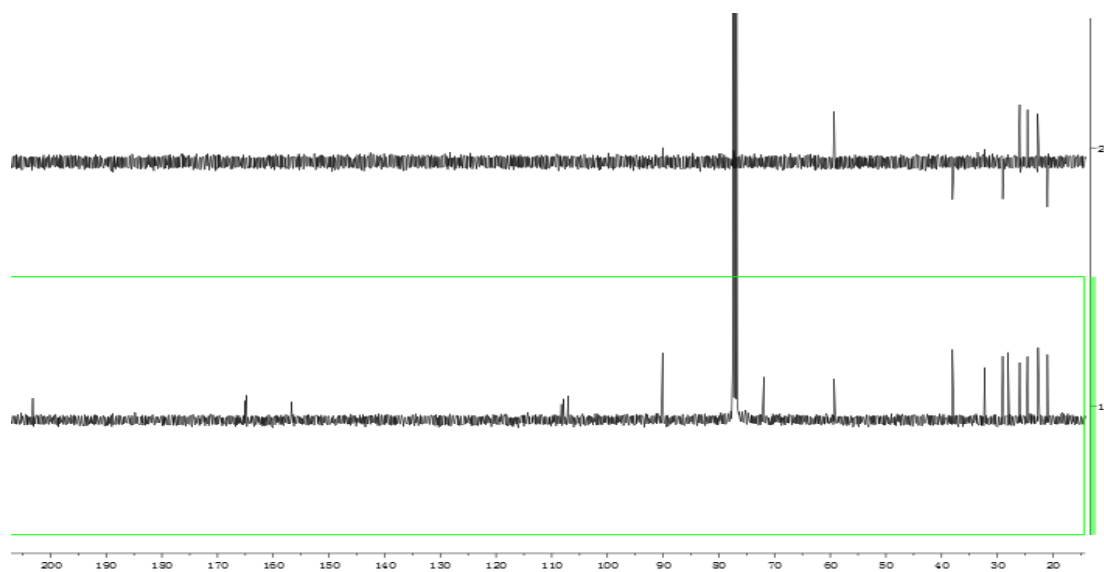


Fig. S8. DEPT-135 spectrum of **1** in CDCl_3

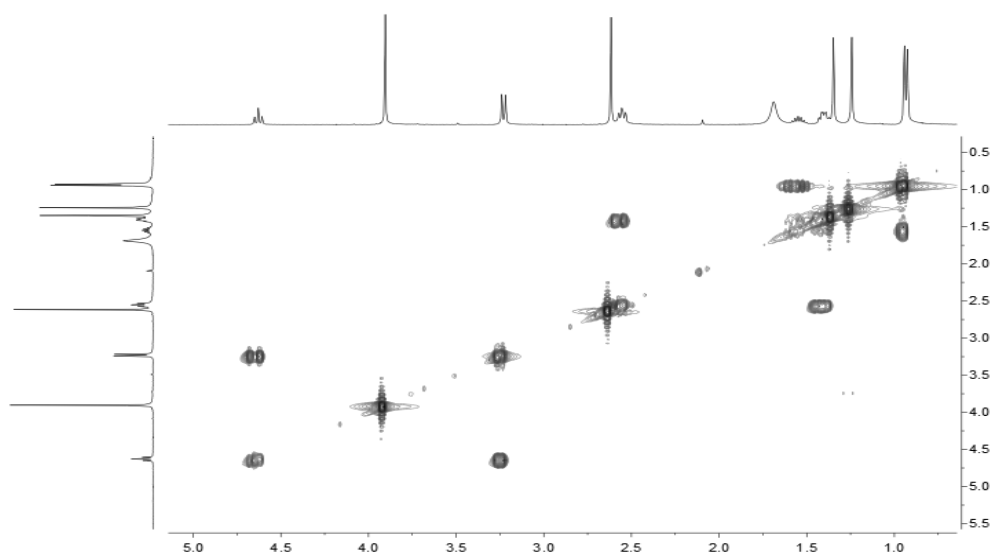


Fig. S9. ^1H - ^1H COSY spectrum of **1** in CDCl_3

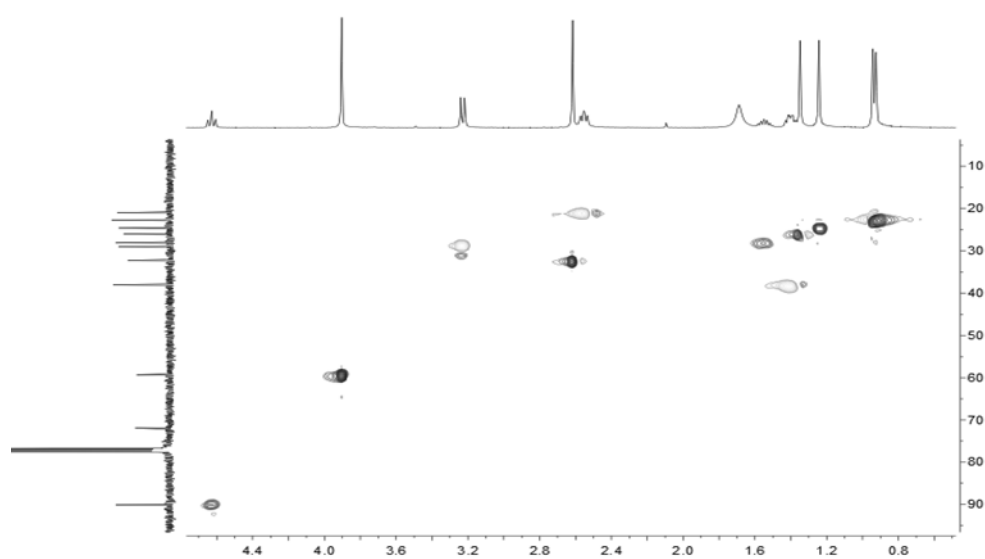


Fig. S10. HSQC spectrum of **1** in CDCl_3

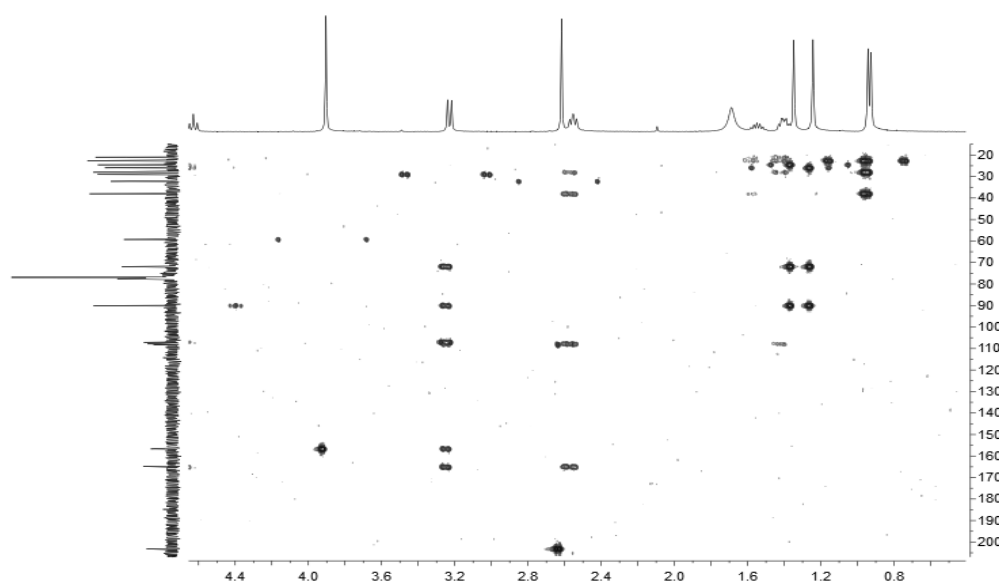


Fig. S11. HMBC spectrum of **1** in CDCl₃

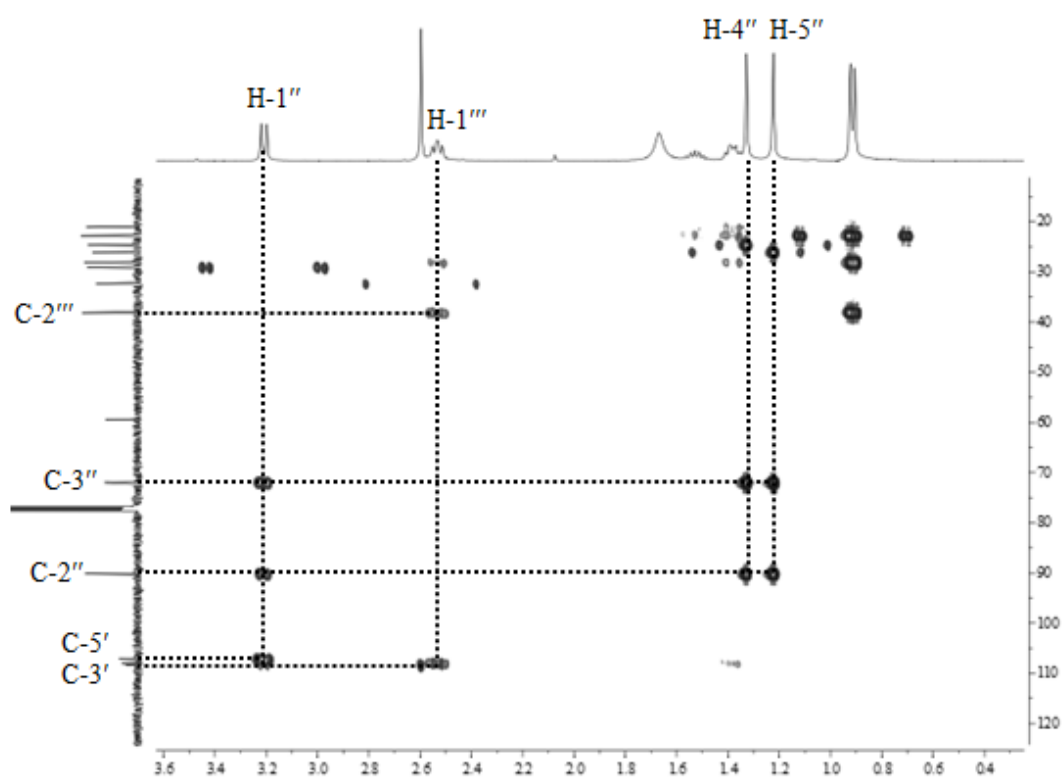


Fig. S12. HMBC spectrum zoom region of **1** in CDCl₃

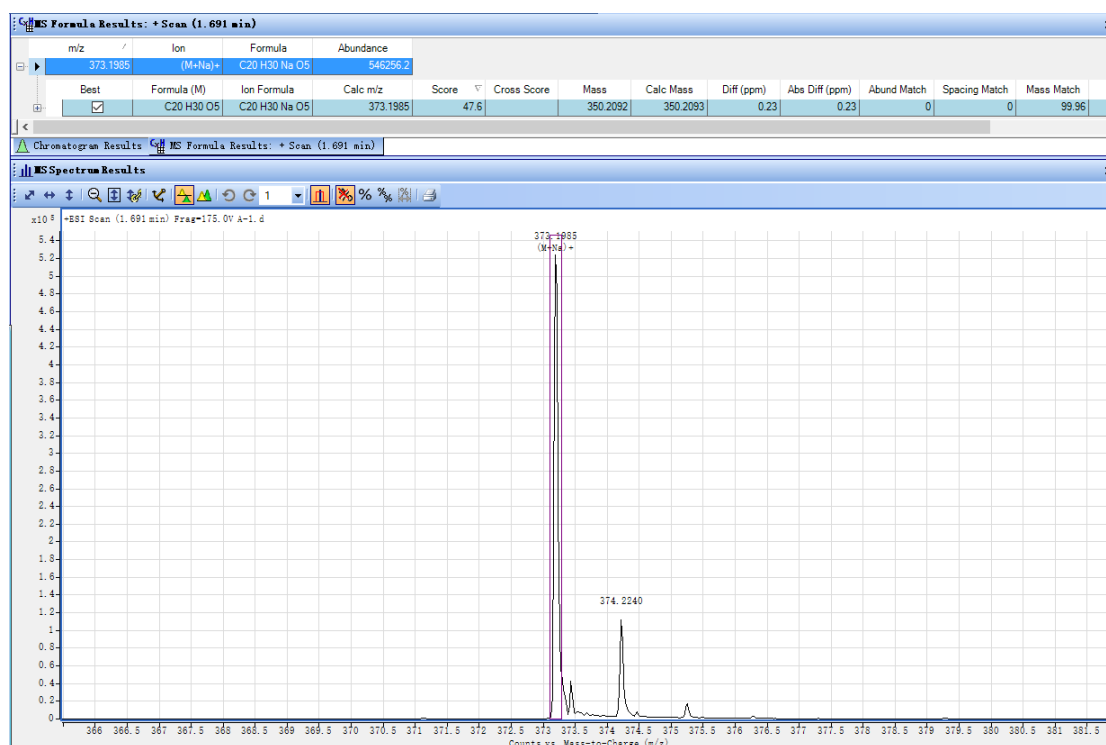


Fig. S13. ESI-HRMS of **2**

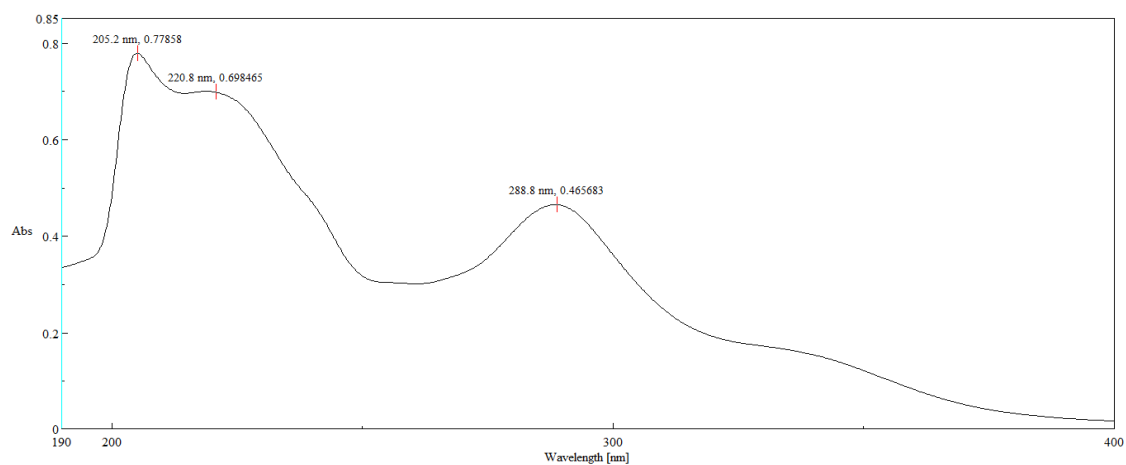


Fig. S14. UV spectrum of **2** (CH₃OH)

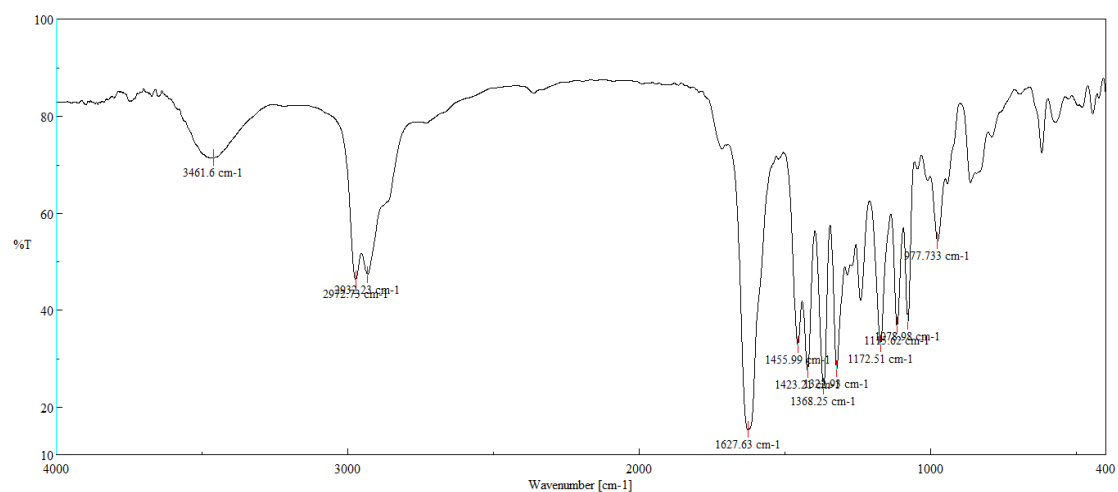


Fig. S15. IR spectrum of 2 (KBr disc)

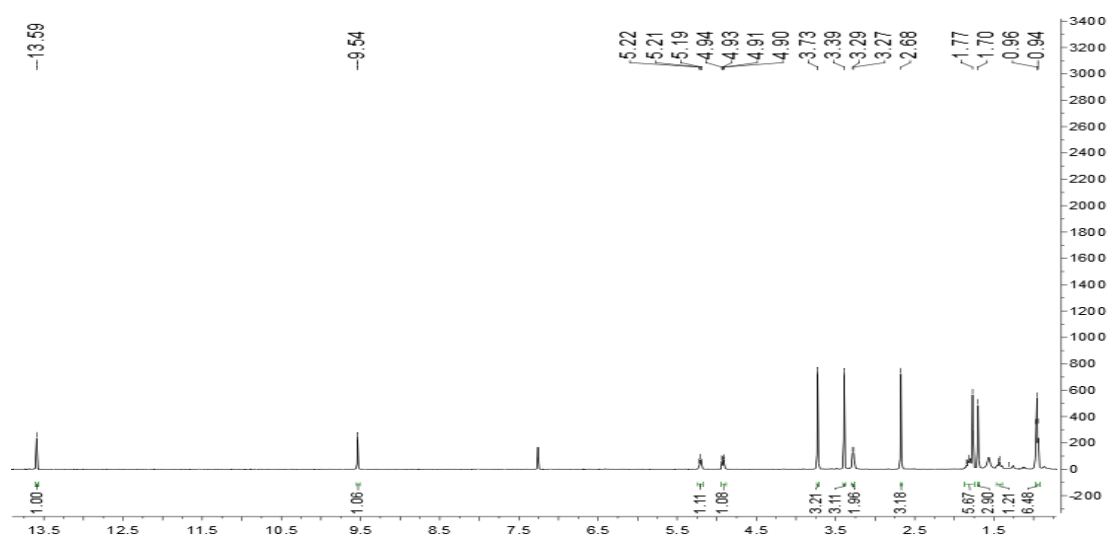


Fig. S16. ¹H NMR spectrum of 2 in CDCl₃

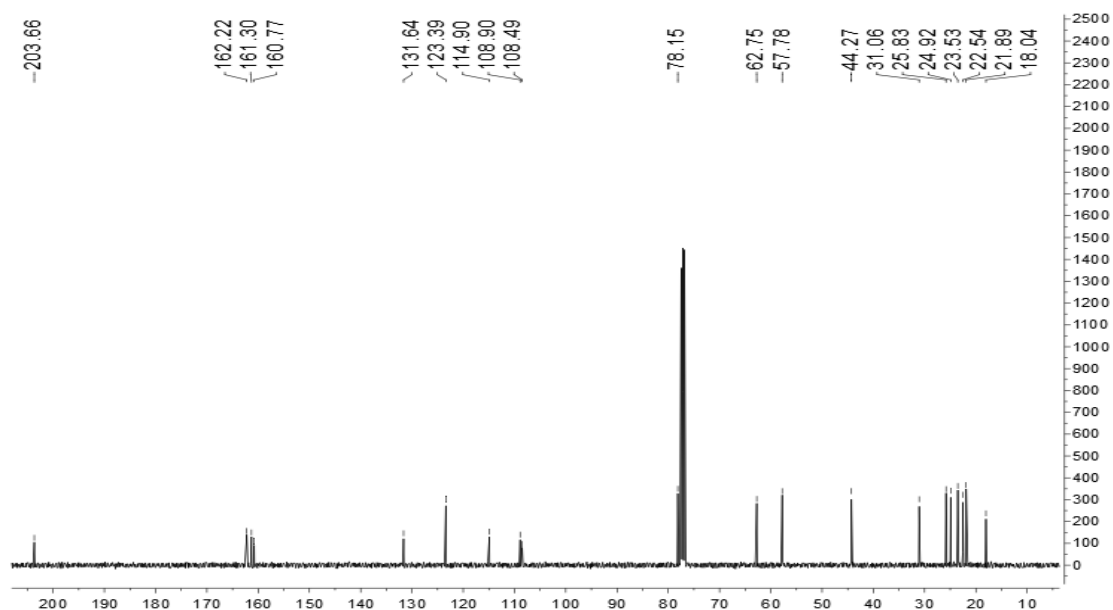


Fig. S17. ^{13}C NMR spectrum of **2** in CDCl_3

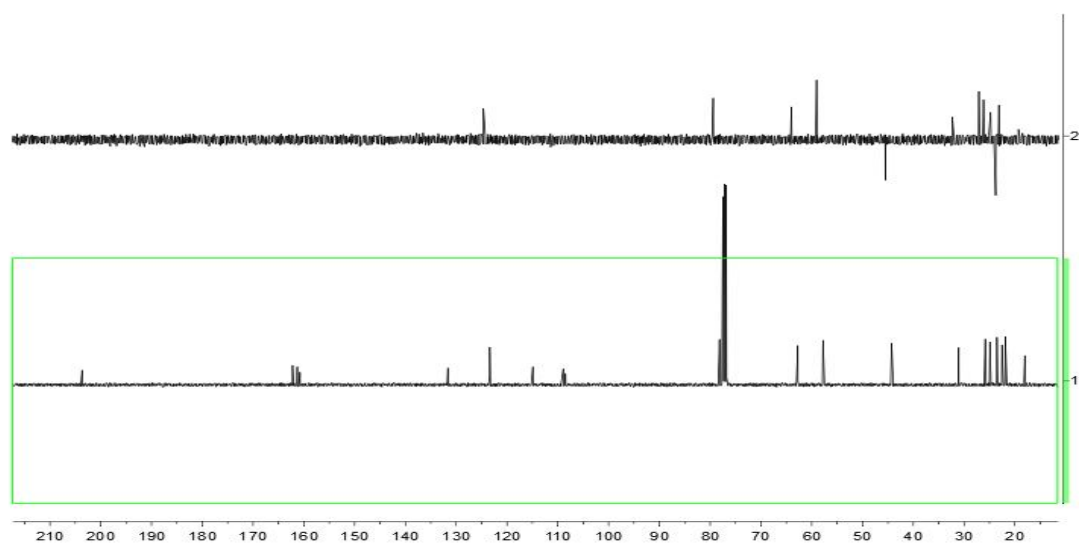


Fig. S18. DEPT-135 spectrum of **2** in CDCl_3

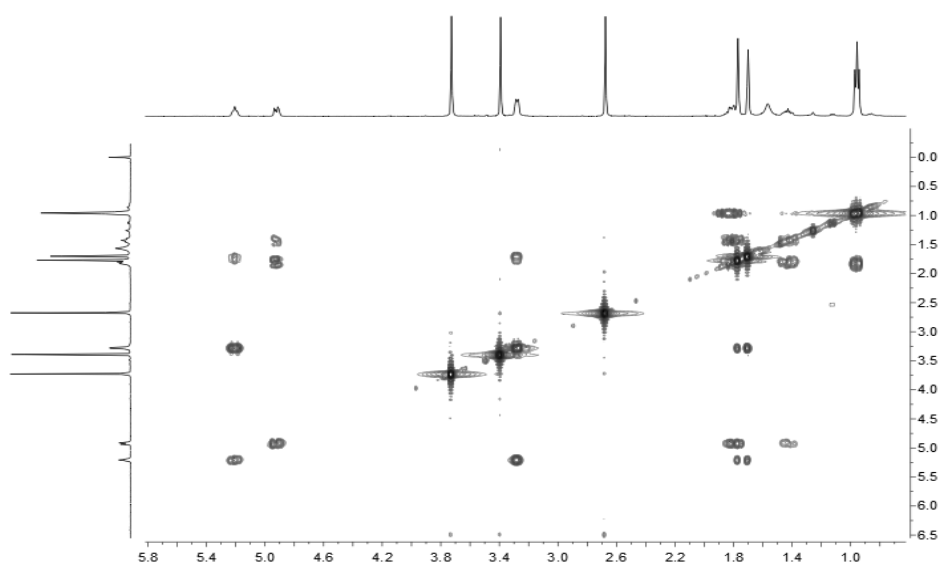


Fig. S19. ^1H - ^1H COSY spectrum of **2** in CDCl_3

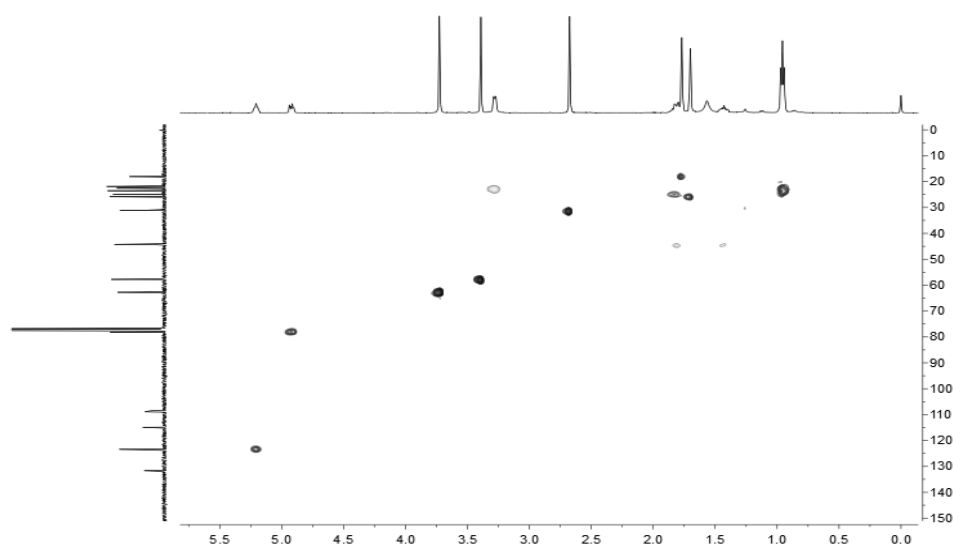


Fig. S20. HSQC spectrum of **2** in CDCl_3

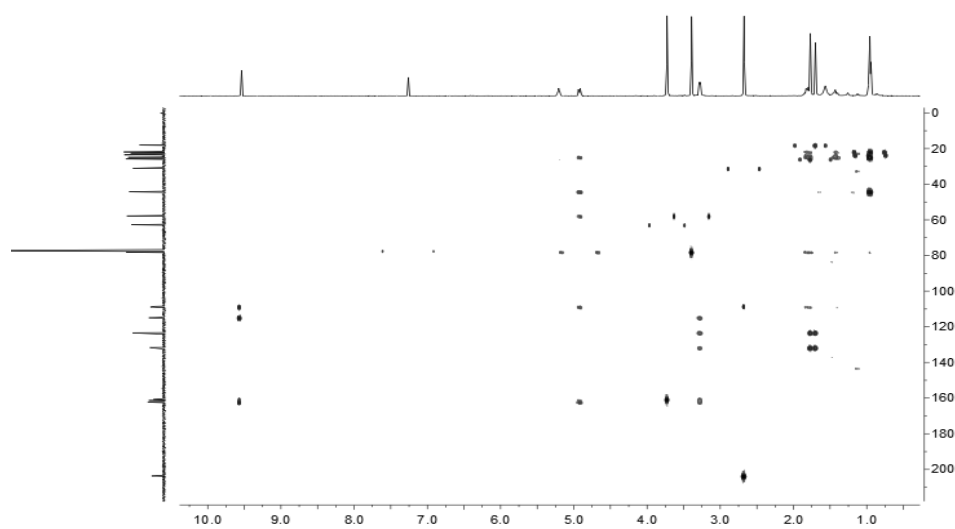


Fig. S21. HMBC spectrum of **2** in CDCl₃

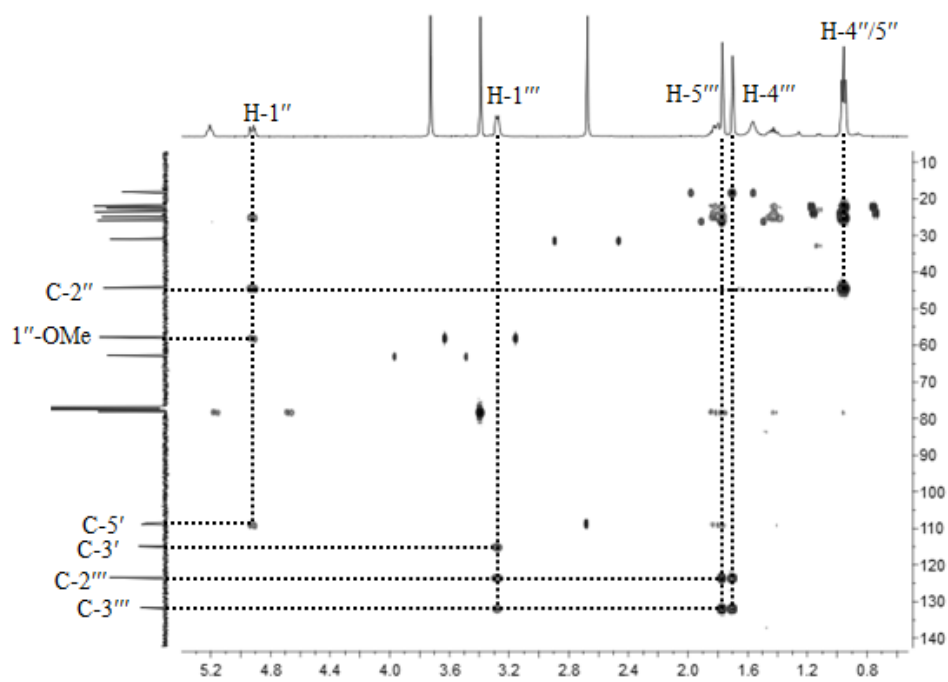


Fig. S22. HMBC spectrum zoom region of **2** in CDCl₃

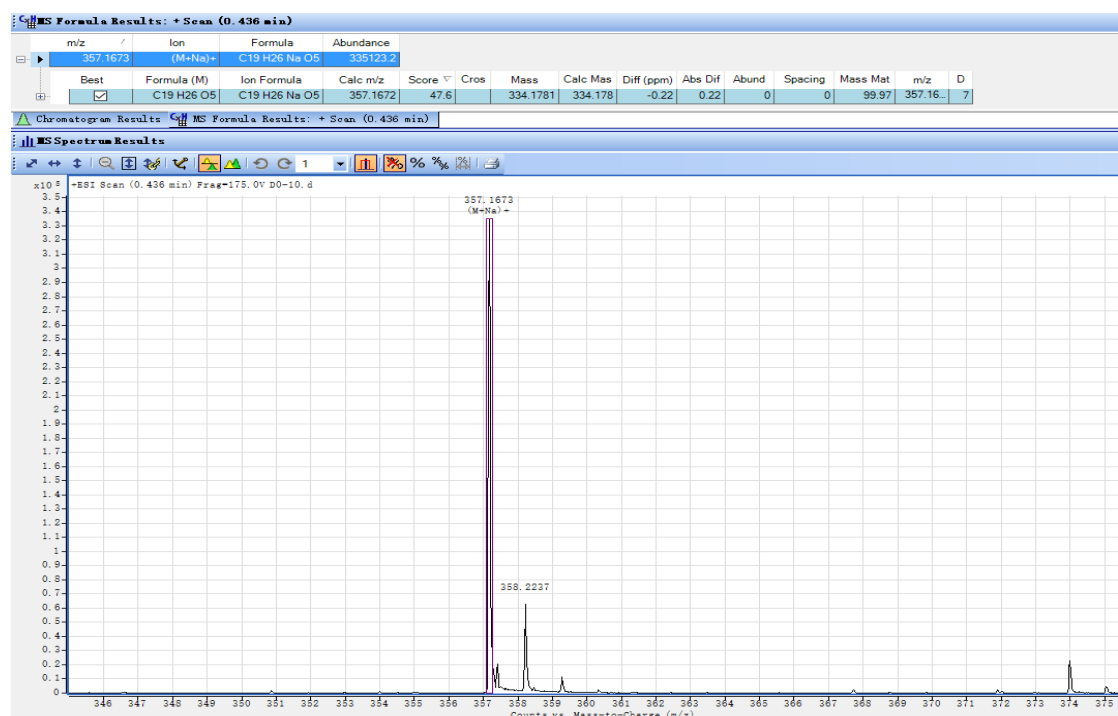


Fig. S23. ESI-HRMS of **3**

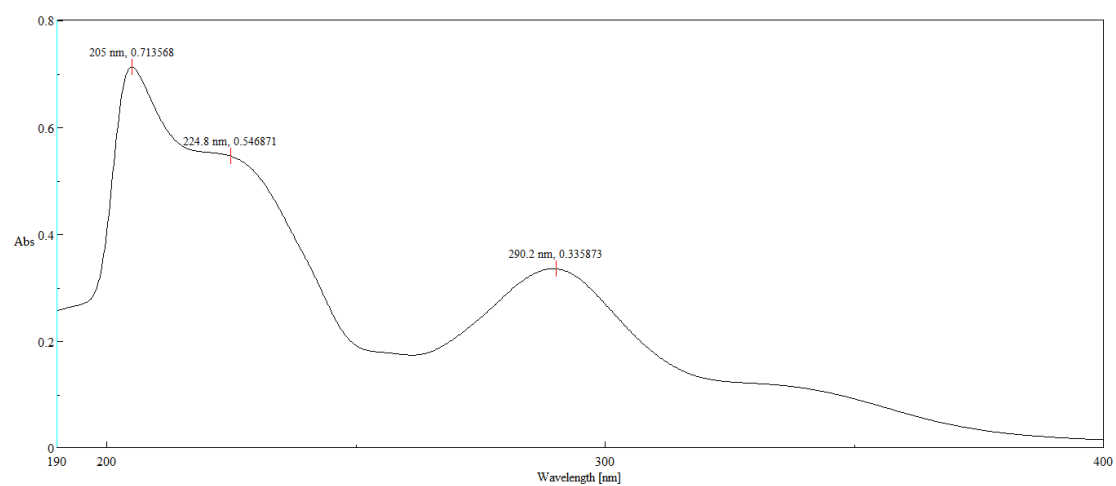


Fig. S24. UV spectrum of **3** (CH₃OH)

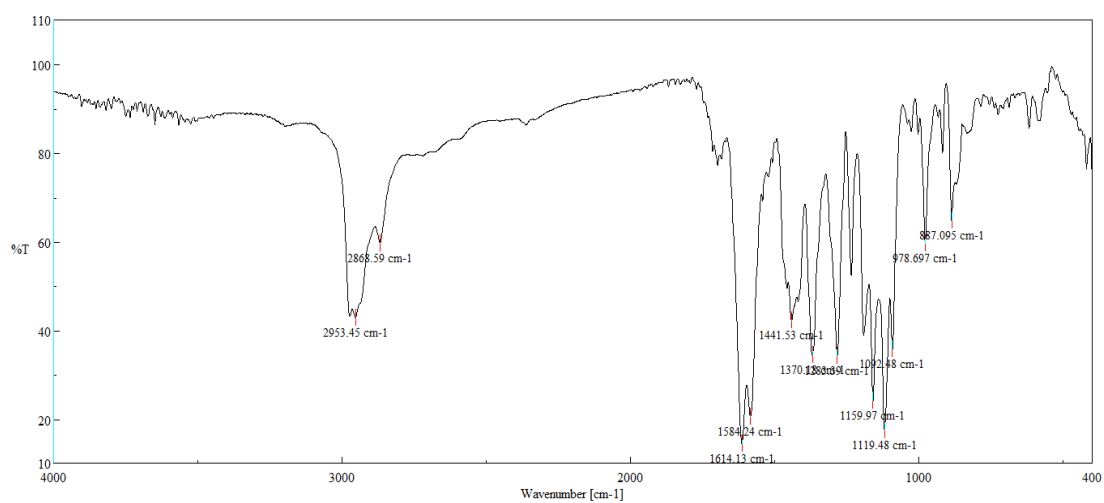


Fig. S25. IR spectrum of **3** (KBr disc)

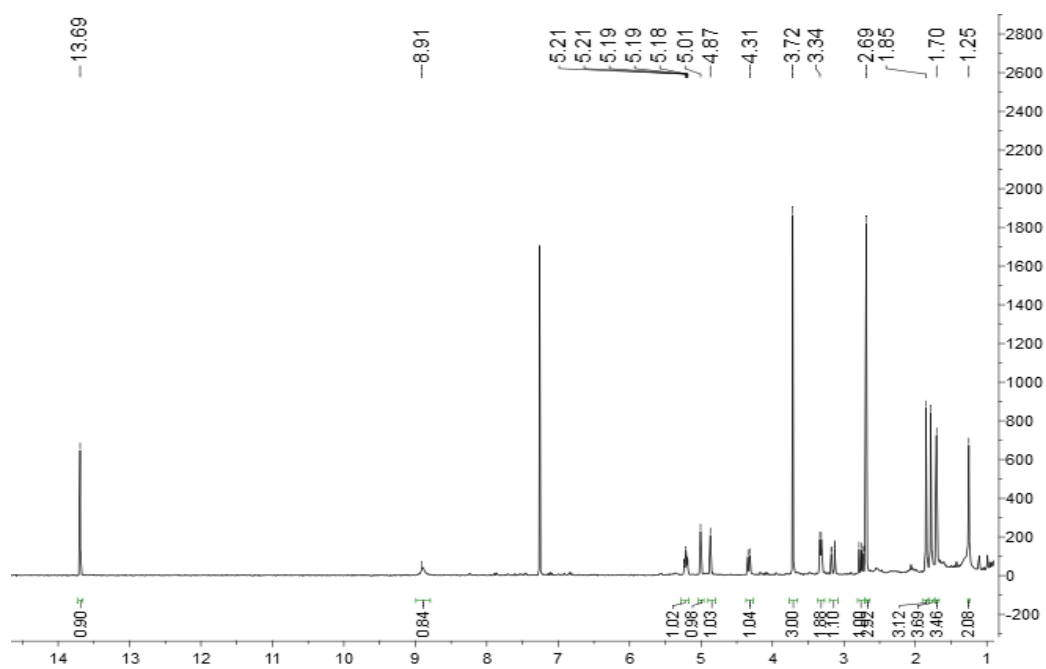


Fig. S26. ¹H NMR spectrum of **3** in CDCl₃

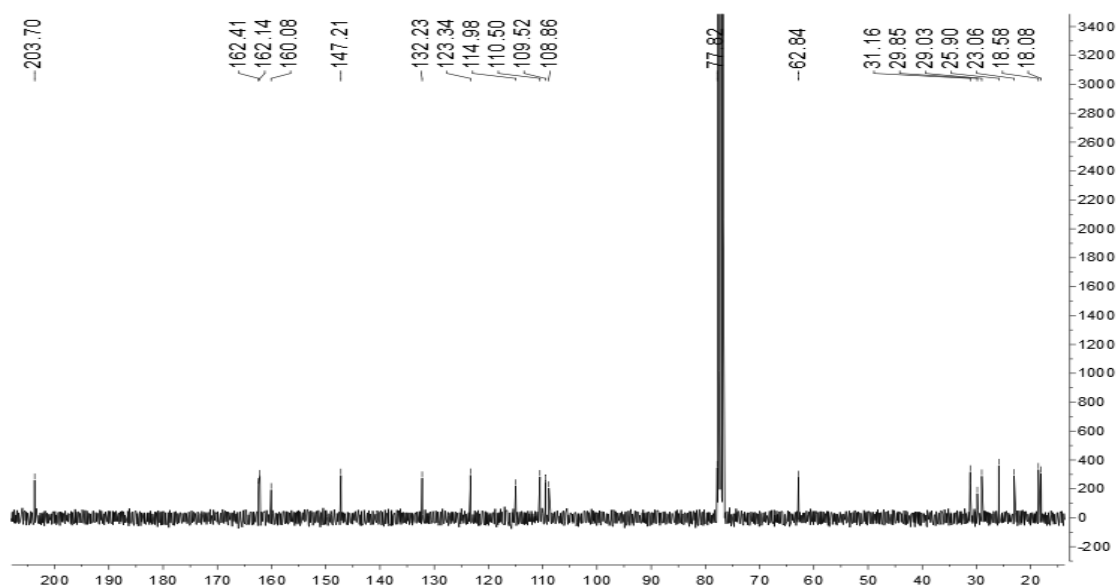


Fig. S27. ^{13}C NMR spectrum of **3** in CDCl_3

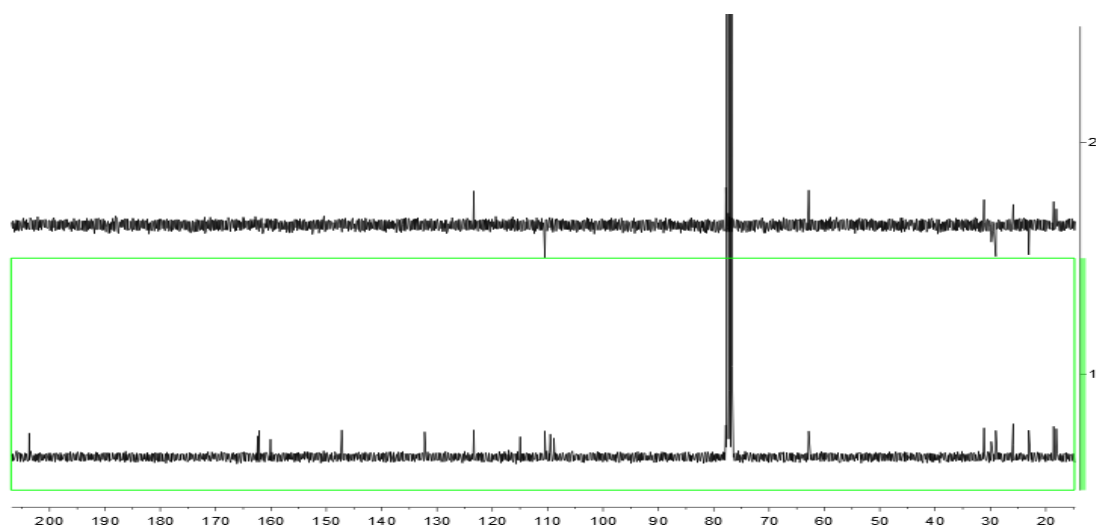


Fig. S28. DEPT-135 spectrum of **3** in CDCl_3

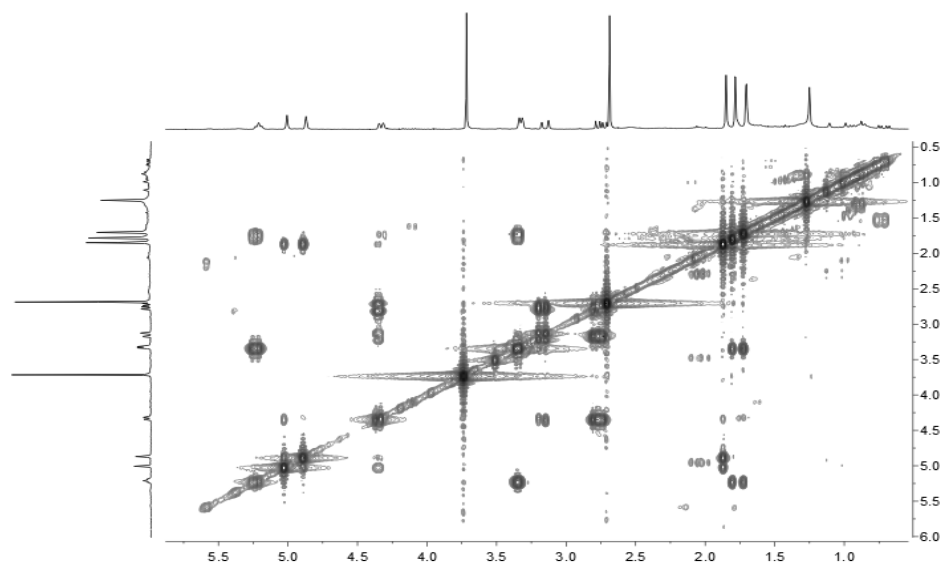


Fig. S29. ^1H - ^1H COSY spectrum of **3** in CDCl_3

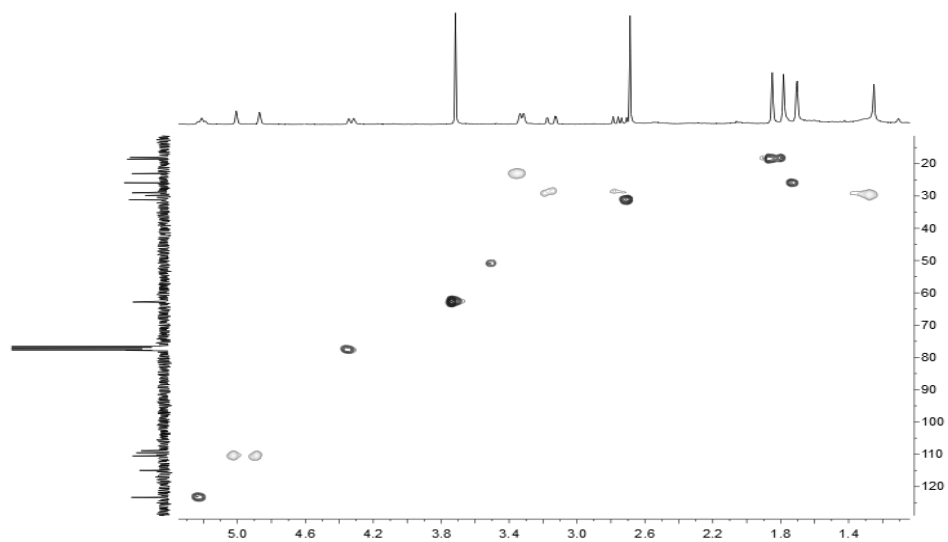


Fig. S30. HSQC spectrum of **3** in CDCl_3

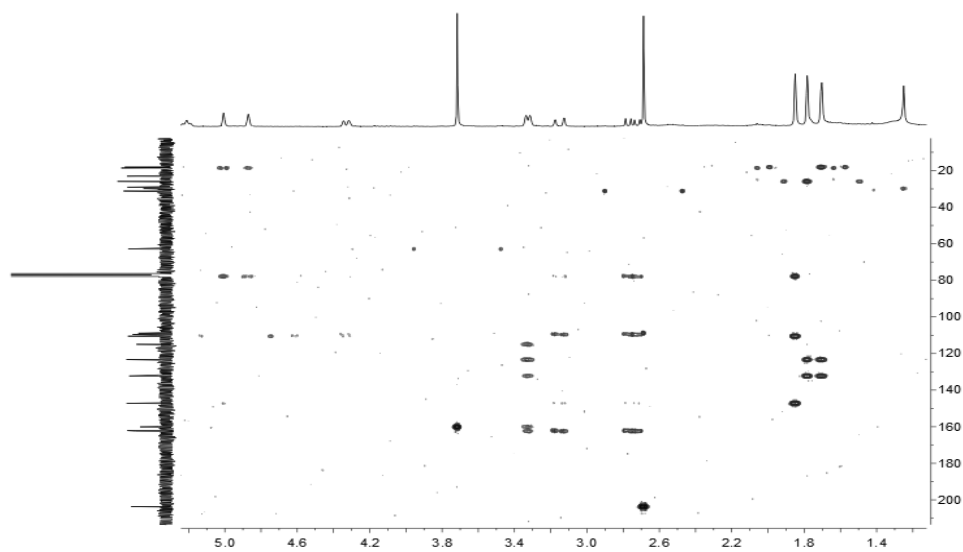


Fig. S31. HMBC spectrum of **3** in CDCl_3

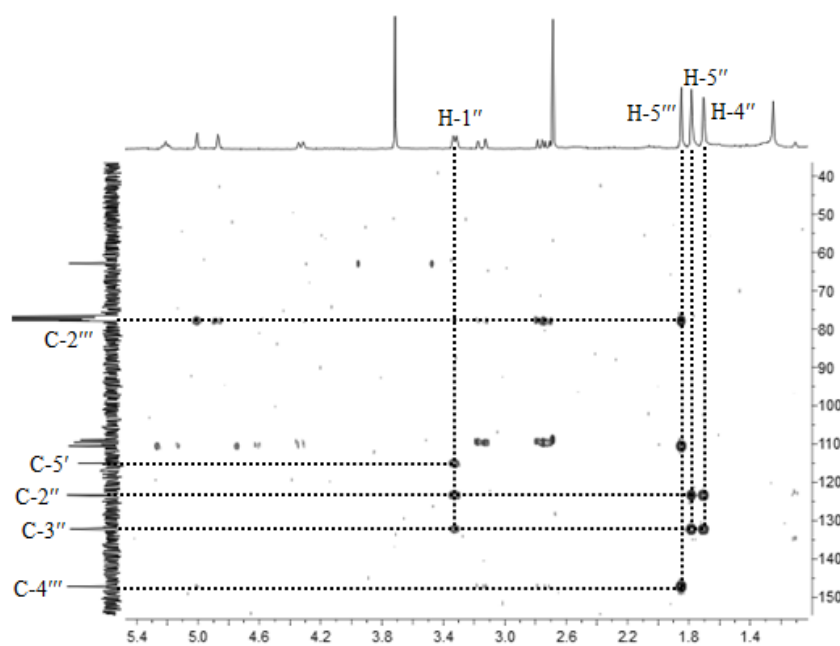


Fig. S32. HMBC spectrum zoom region of **3** in CDCl_3