SUPPLEMENTARY MATERIAL

Novel ferulic acid and benzophenone derivatives from the flower buds of *Syzygium aromaticum*

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ABSTRACT

Phytochemical investigation of clove resulted in the isolation of two new natural compounds, a ferulic acid derivative, sabrinic acid (**1**) and a benzophenone derivative (**2**) together with two known compounds kaempferol-3,5-dimethyl ether (**3**) and 4-methyl benzoic acid (**4**). Compounds **3** and **4** were isolated for the first time from the genus *Syzygium.*The structures of compounds were elucidated through modern spectroscopic techniques including 1D and 2D NMR spectroscopy.

CONTENT

Table 1S. ^{1}H and ^{13}C NMR spectral data of 1 (500 MHz for ^{1}H and 125 MHz for ^{13}C in $CDCl_3$)

No.	δ_H (m, *J* in Hz)	^{13}C	HMBC (H→C)
1		188.7	
2	7.35 (d, 15.5)	119.5	1, 4
3	7.72 (d, 15.5)	144.5	1, 2,
4		127.7	
5	7.10 (d, 2.0)	110.0	2
6		146.8	
7		141.7	
8	6.93 (d, 8.5)	114.8	4, 6
9	7.19 (dd, 8.5, 2.0)	123.1	2
1’		159.6	
2’		131.7	
3’	7.97 (d, 8.5)	131.0	1′
4’	6.90 (d, 8.5)	115.3	1′, 2′
5’		148.1	
6’	6.90 (d, 8.5)	115.3	1′, 2′
7’	7.97 (d, 8.5)	131.0	1′
6-OCH3	3.95 (s)	56.0	6

Table 2S. ^{1}H and ^{13}C NMR spectral data of compound 2 (500 MHz for ^{1}H and 125 MHz for ^{13}C in $CDCl_3$)

No.	δ_H (m, *J* in Hz)	^{13}C	HMBC (H→C)
1, 1′		129.0	
2, 2′	7.82 (d, 8.5)	130.8	1, C=O
3, 3′	6.80 (d, 8.5)	115.1	1, 2
4, 4′		Not observed	
5, 5′	6.80 (d, 8.5)	115.1	1, 6
6, 6′	7.82 (d, 8.5)	130.8	1, C=O
C=O		197.8	
2 × ester C=O		161.9	
2 × Me	2.49 (s)	25.0	ester C=O

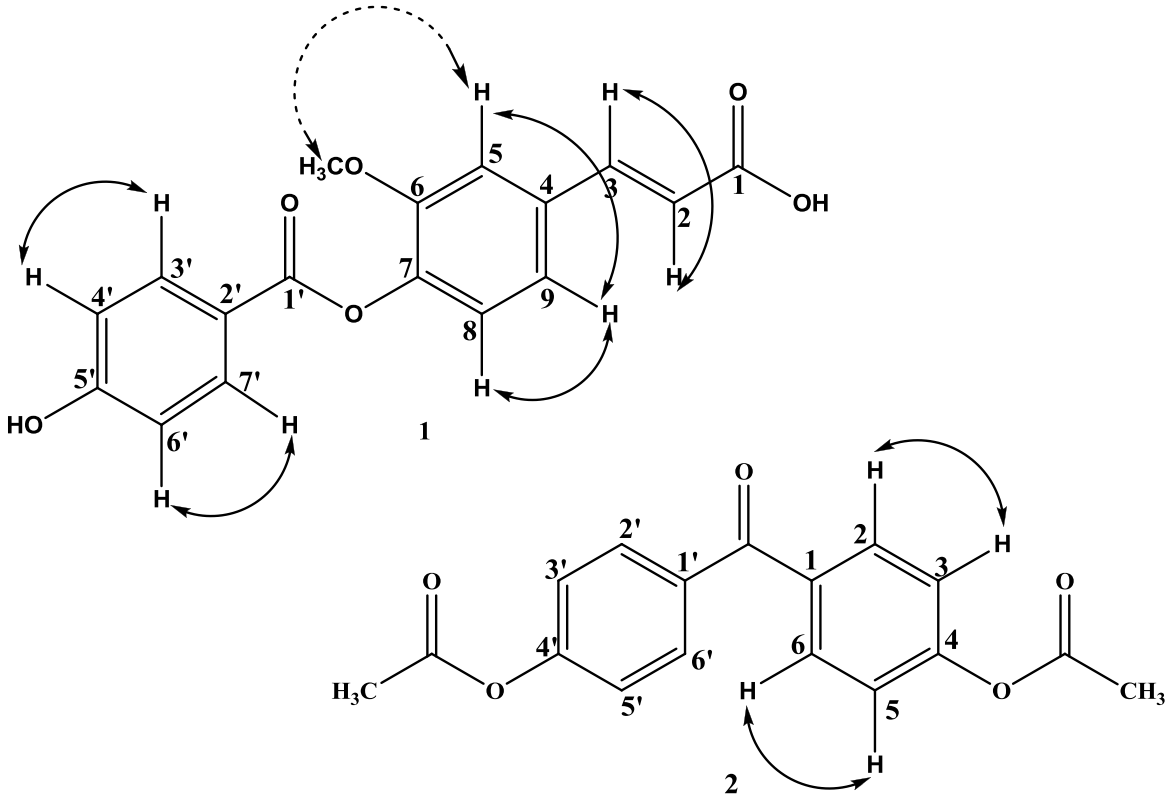

Figure 1S. ^{1}H-^{1}H COSY (⟷) and NOESY (⇠⇢) correlations of compounds 1 and 2.

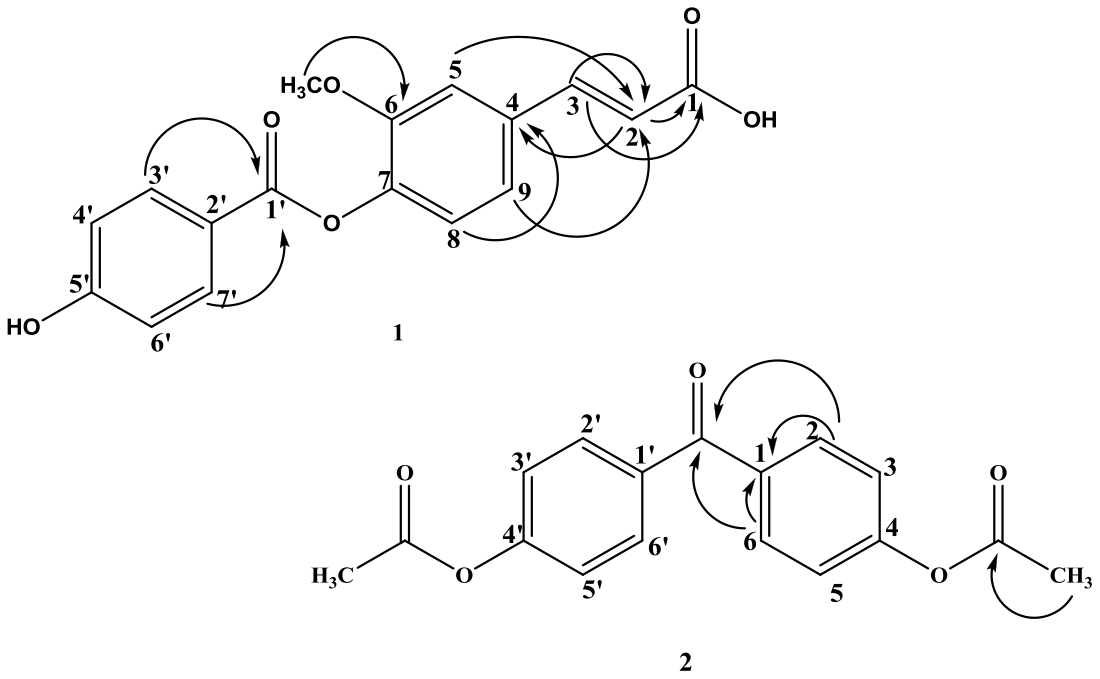

Figure 2S. HMBC correlation (H→C) of compounds 1 and 2.

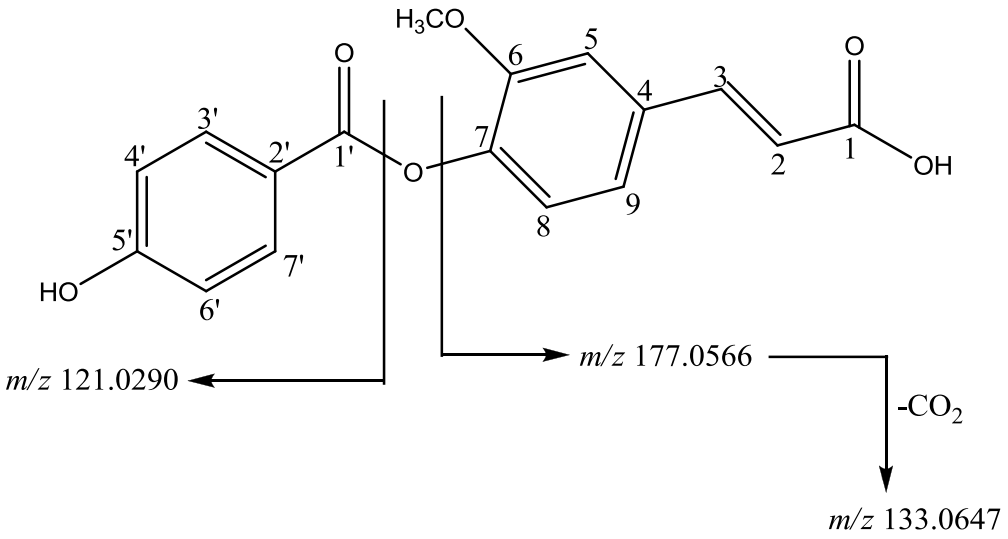

Figure 3S. Significant mass fragmentation of compound 1.

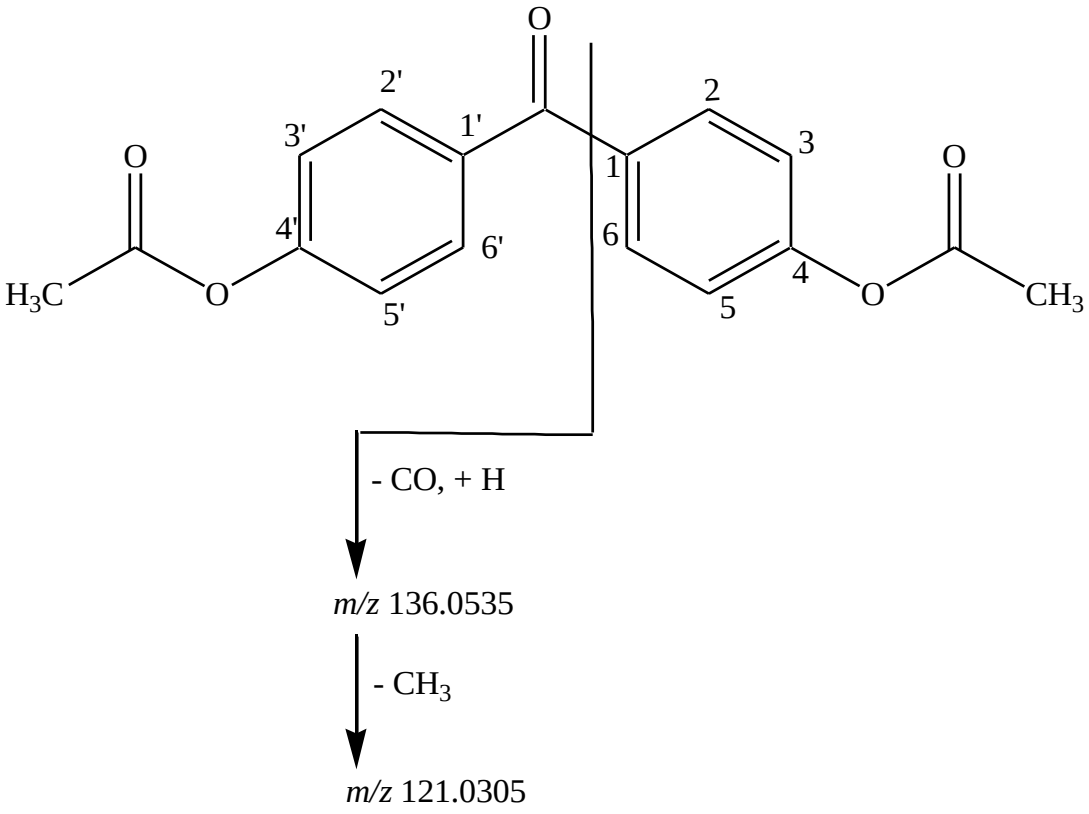

Figure 4S. Significant mass fragmentation of compound 2.

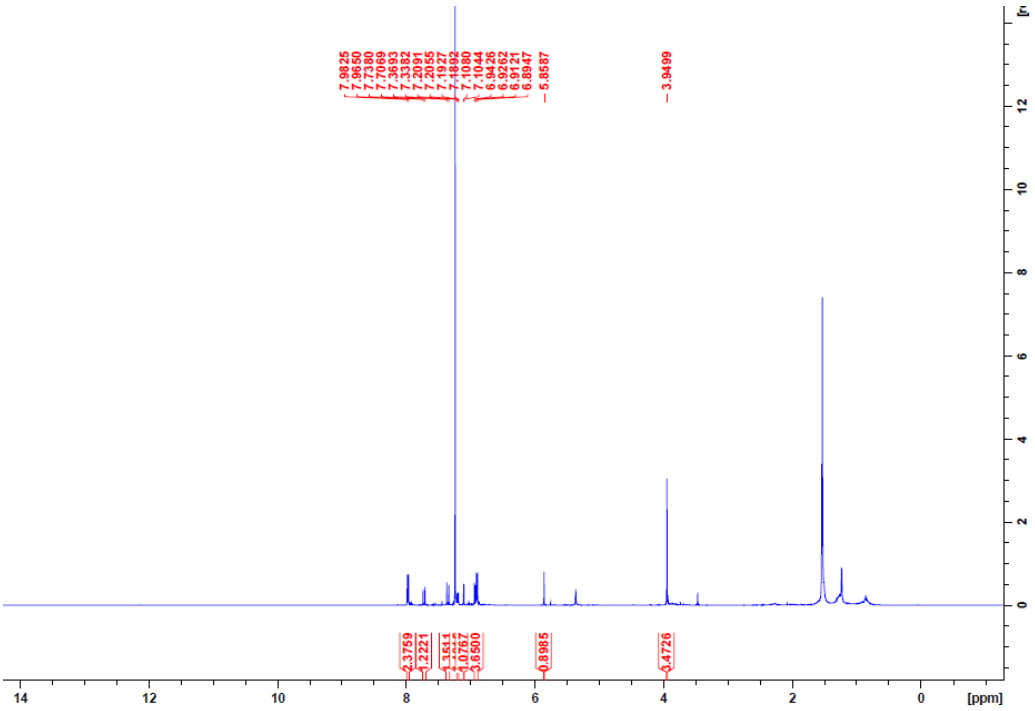

Figure 5S. The ^{1}H NMR (500 MHz, $CDCl_3$) data of 1.

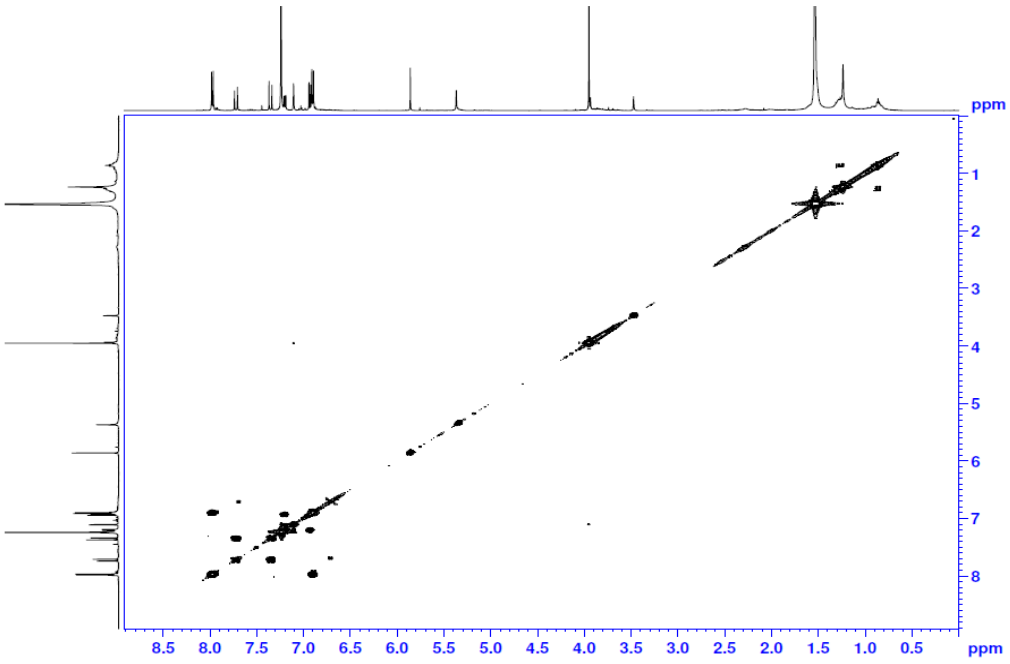

Figure 6S. $^{1}H^{1}H$ COSY data of 1.

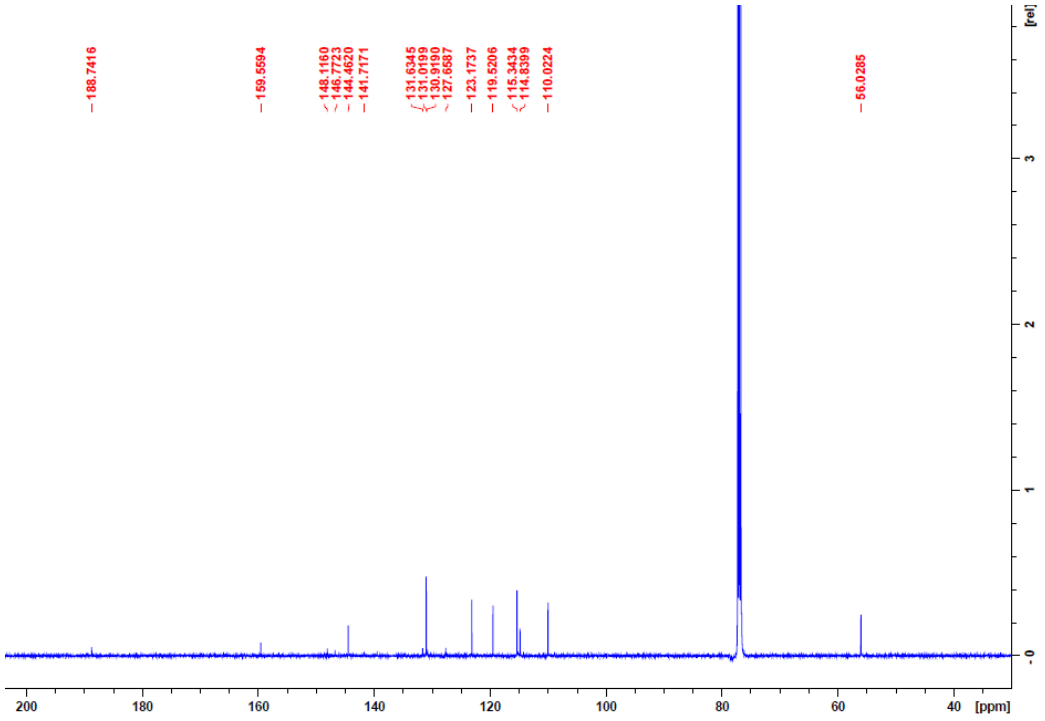

Figure 7S. The ^{13}C NMR (125 MHz, $CDCl_3$) data of 1.

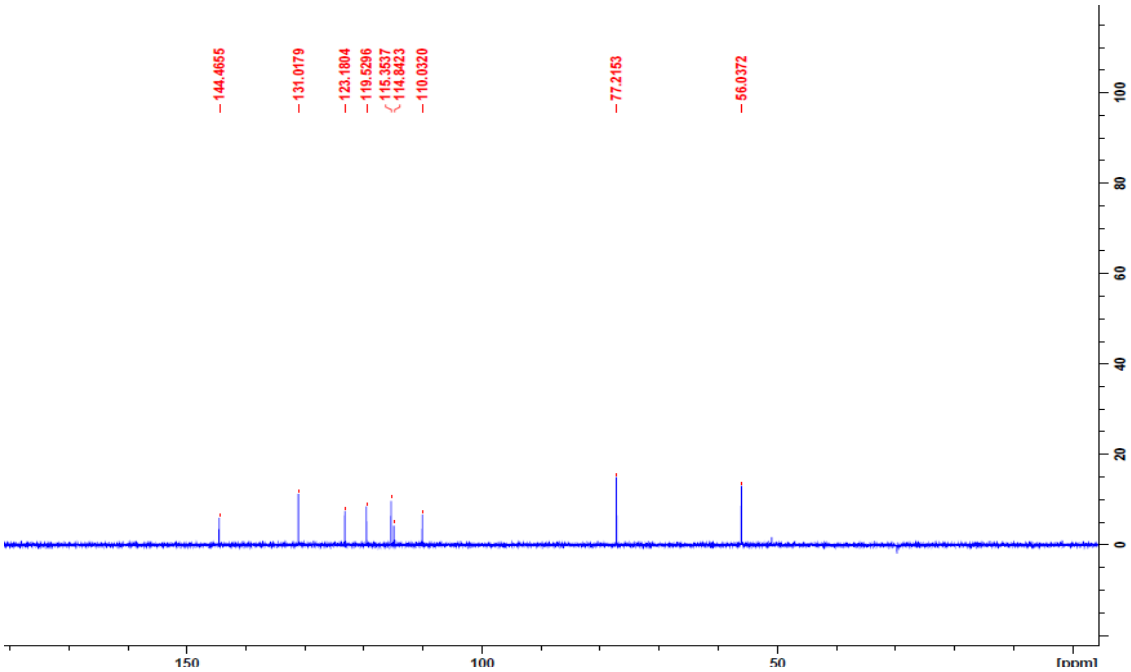

Figure 8S. The ^{13}C NMR (DEPT 135) data of 1.

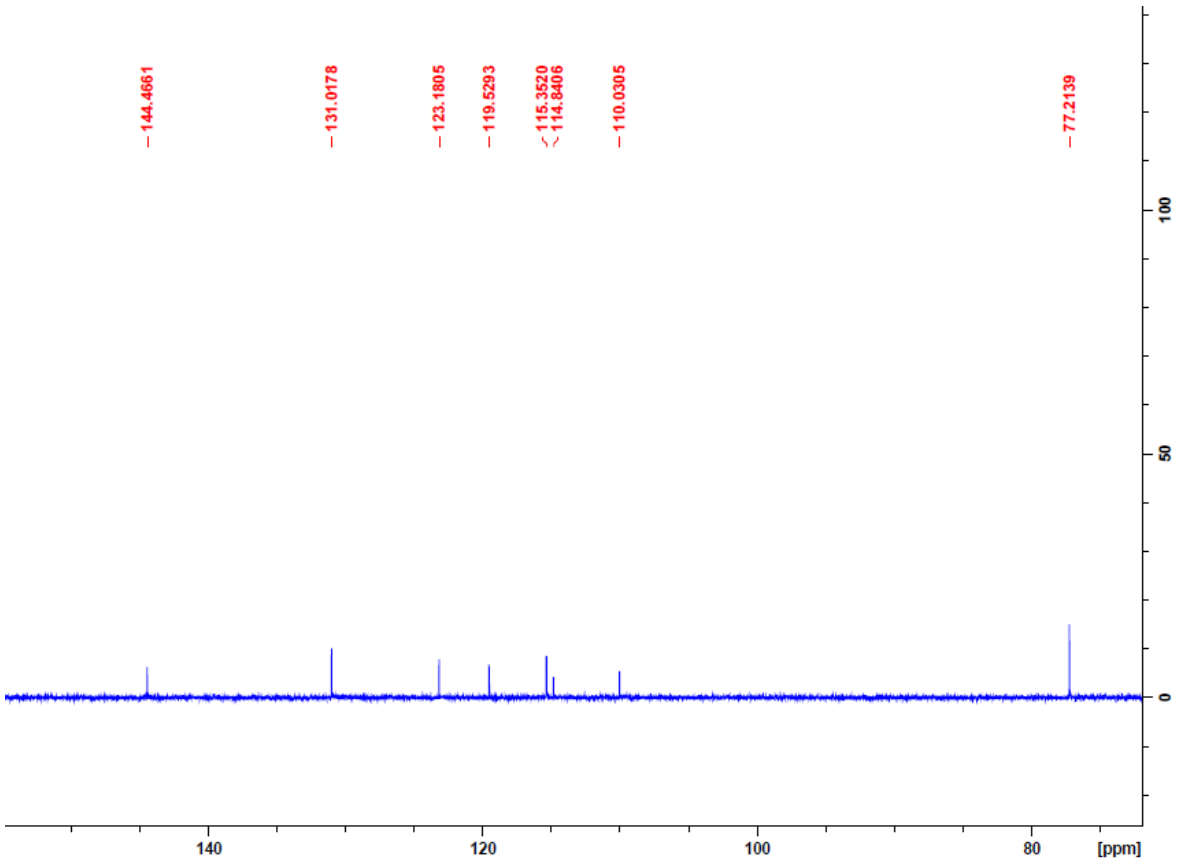

Figure 9S. The ^{13}C NMR (DEPT 90) data of 1.

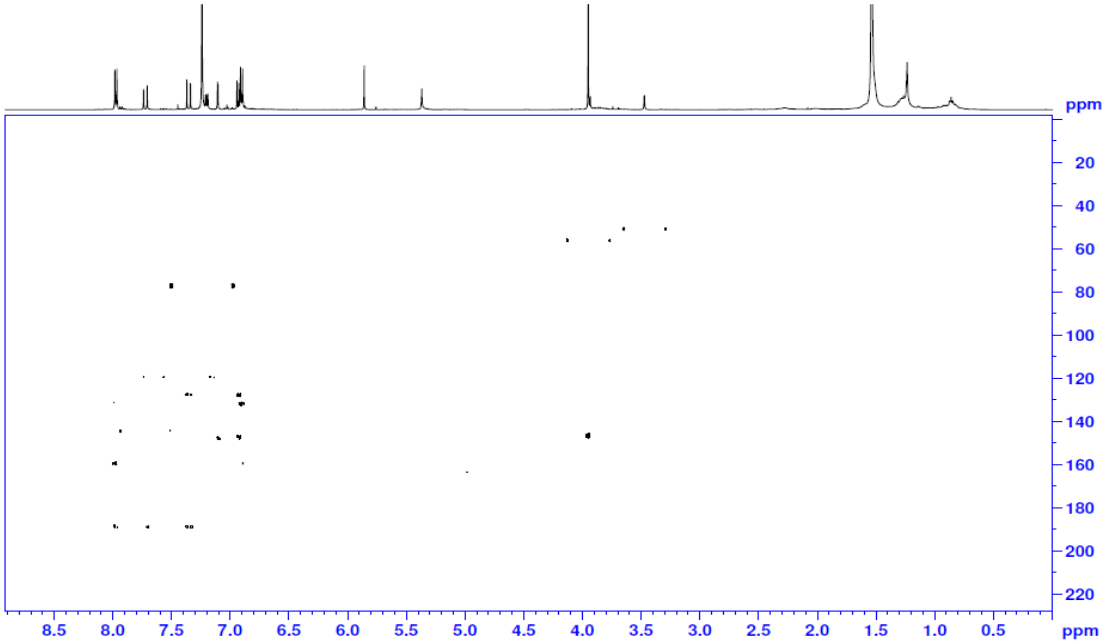

Figure 10S. HMBC data of 1.

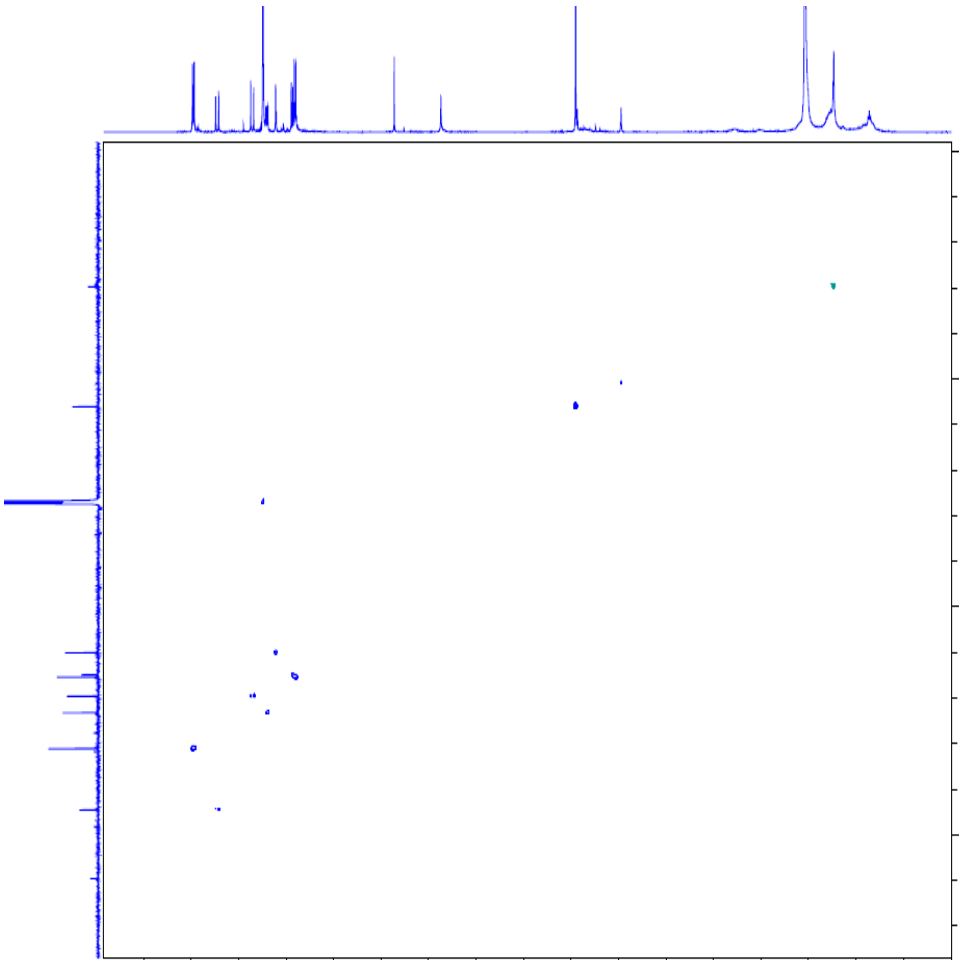

Figure 11S. HMQC data of 1.

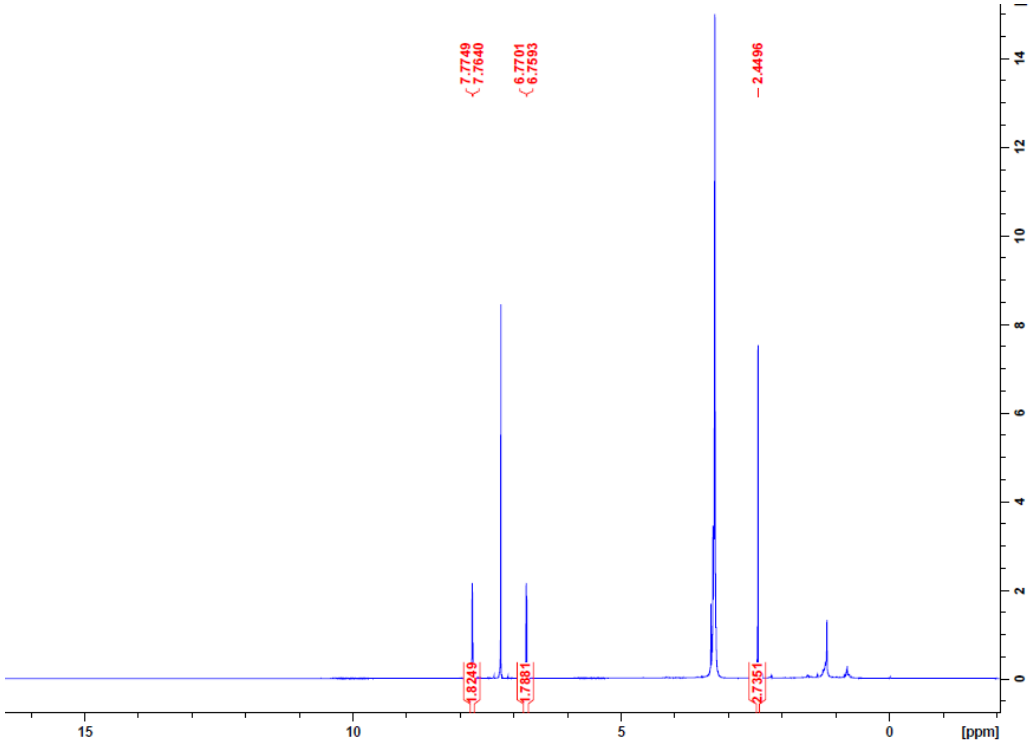

Figure 12S. The ^{1}H NMR (500 MHz, CDCl3) data of 2.

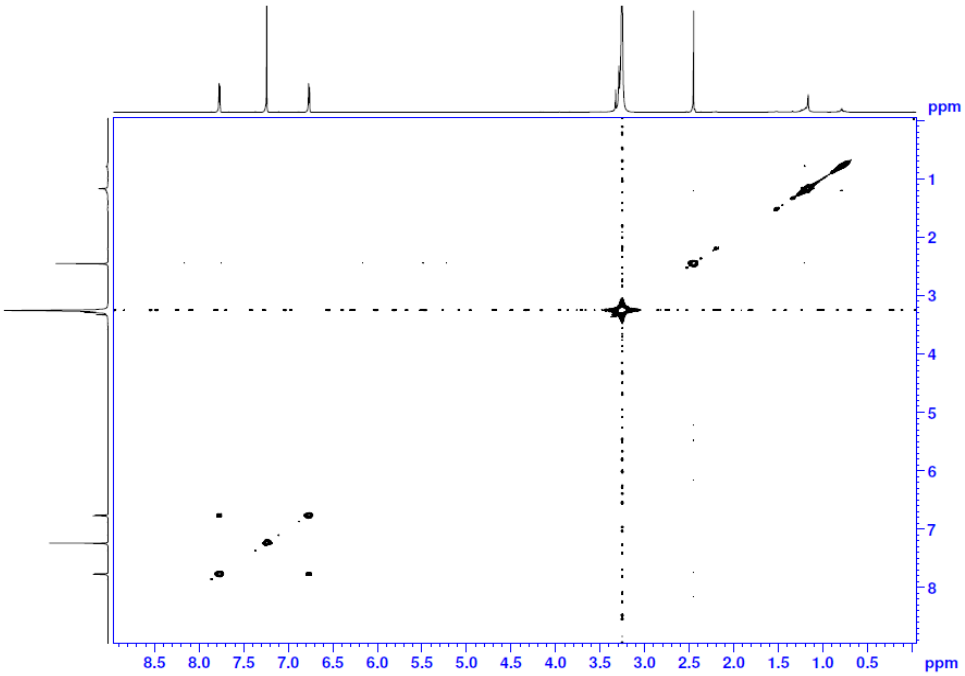

Figure 13S. $^{1}H^{1}H$ COSY data of 2.

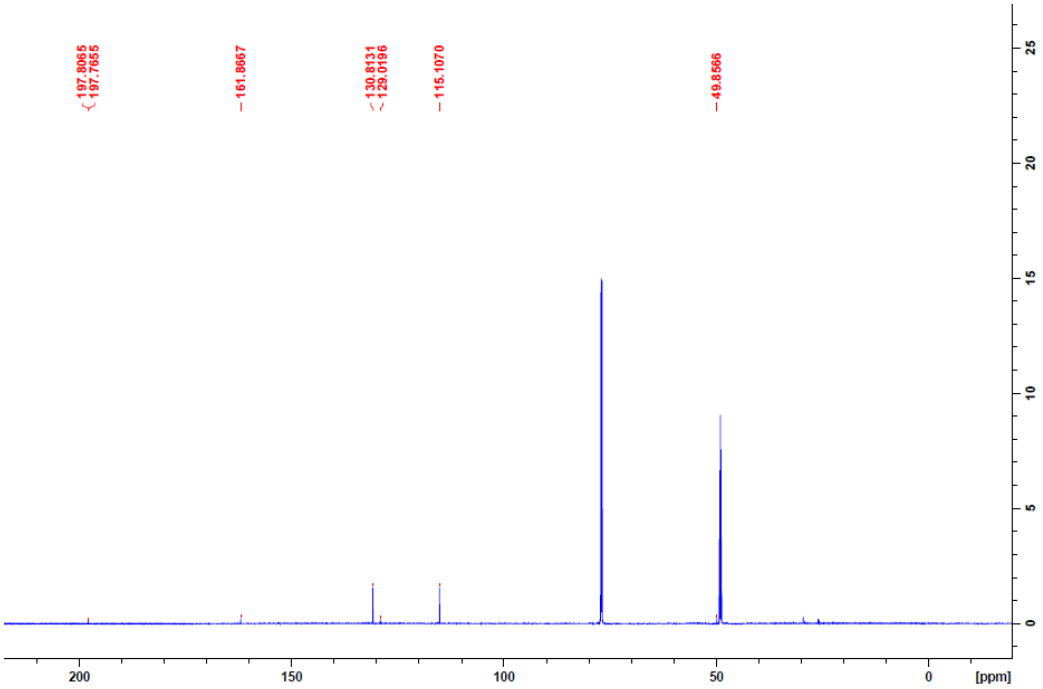

Figure 14S. The ^{13}C NMR (125 MHz, CDCl3) data of 2.

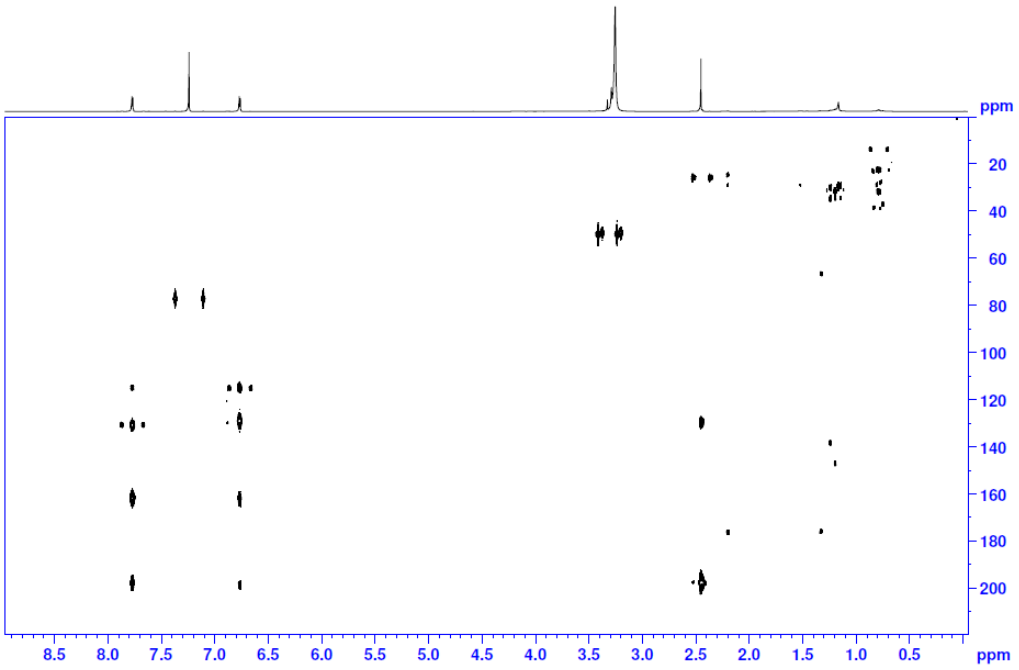

Figure 15S. HMBC data of 2.

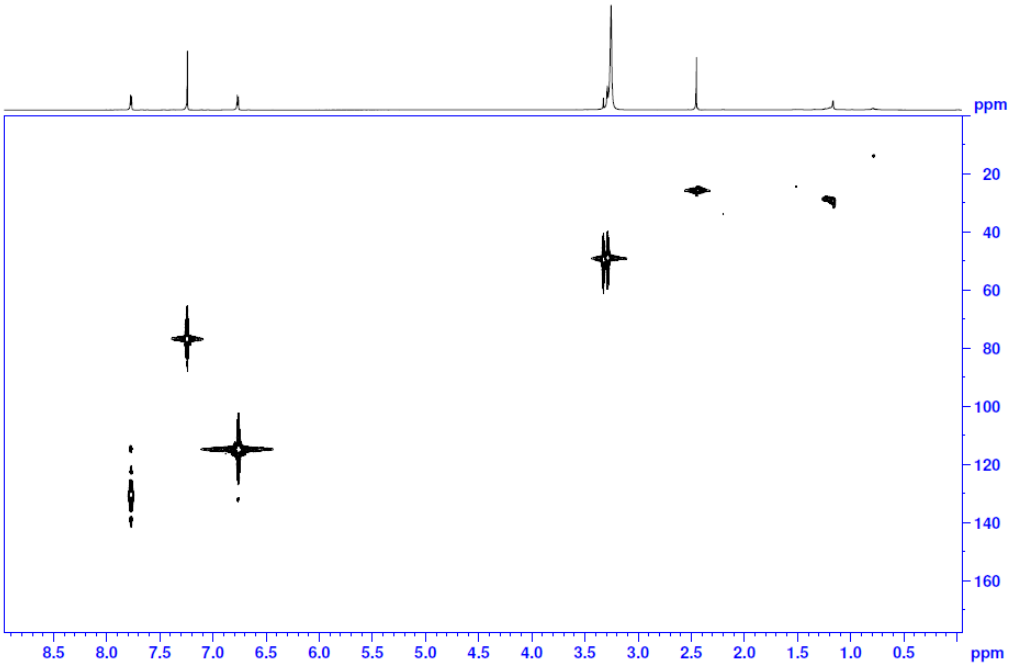

Figure 16S. HMQC data of 2.