SUPPLEMENTARY MATERIAL

Secondary metabolites from the fermented rice of the fungus *Monascus purpureus* and their bioactivities

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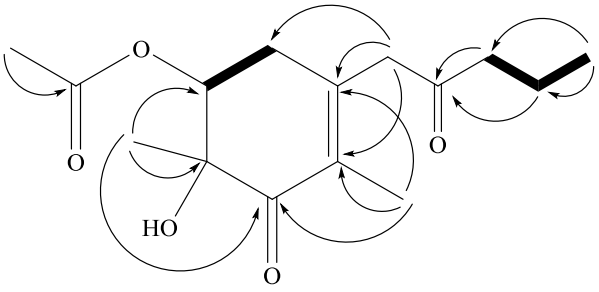
Phytochemical investigation of the EtOAc-soluble fraction of the ethanolic extract of a yellow mutant of the fungus *Monascus purpureus* BCRC 38110 (Eurotiaceae) grown on rice resulted in the isolation of one new azaphilone derivative, monapurpureusone (**1**), one acetophenone metabolite isolated for the first time from natural source, monapurpureusin (**2**), along with four known compounds, TW94a (**3**), ergosterol (**4**), monascin (**5**), and ankaflavin (**6**). The structures and relative configurations of these compounds were elucidated by spectroscopic analyses, including 1D- and 2D-NMR spectroscopy and mass spectrometry, and by the comparison of their NMR data with those of related compounds. Some phytochemicals were evaluated for both anti-inflammatory activity through the measurement of nitric oxide (NO) production levels in lipopolysaccharide (LPS)-stimulated murine-derived macrophages RAW264.7 cell lines and antioxidant activities.

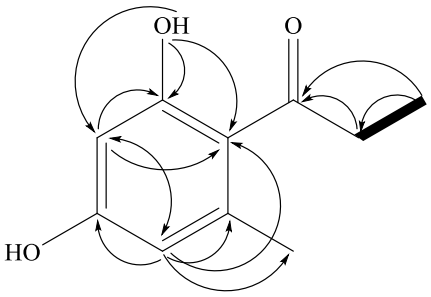
Contents

Table S1. ^{1}H- and ^{13}C-NMR Data ($CDCl_3$, 600 and 150 MHz, resp.) of compounds **1** and **2**. δ in ppm, J in Hz.

	1			**2**	
	δ_C	δ_H		δ_C	δ_H
1	11.7	1.76 (*q*, *J* = 1.2)		166.3	
2				101.8	6.26 (*dd*, *J* = 2.7, 0.6)
3	205.6			160.5	
4	48.8	3.33 (*d*, *J* = 16.8), 3.50 (*d*, *J* = 16.8)		111.8	6.23 (*dq*, *J* = 2.7, 1.2)
4a	146.2				
5	37.9	2.49 (*ddd*, *J* = 18.0, 10.5, 1.2, H_{ax}), 2.53 (*ddd*, *J* = 18.0, 6.2, 1.2, H_{eq})		142.2	
6	67.9	4.84 (*dd*, *J* = 10.5, 6.2)		115.6	11.49 (*s*)
7	85.1			207.4	
8	195.1			37.3	2.92 (*q*, *J* = 7.2)
8a	132.1				
9	45.0	2.45 (*t*, *J* = 7.8)		8.9	1.21 (*t*, *J* = 7.2)
10	17.2	1.61 (*sextet*, *J* = 7.8)		25.1	2.56 (*s*)
11	13.6	0.92 (*t*, *J* = 7.8)			
Me-12	15.8	1.39 (*s*)			
14	170.2				
15	21.5	2.10 (*s*)			
OH-1					13.2 (br *s*)
OH-3					5.60 (br *s*)
OH-7		2.50 (br *s*)			

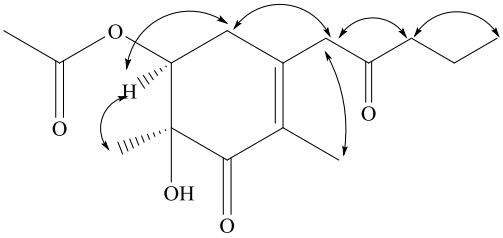


1

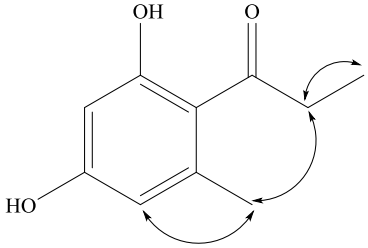


2

Figure S1. COSY (▬) and HMBC (→) correlations of **1** and **2**.



1



2

Figure S2. NOESY correlations of **1** and **2**.

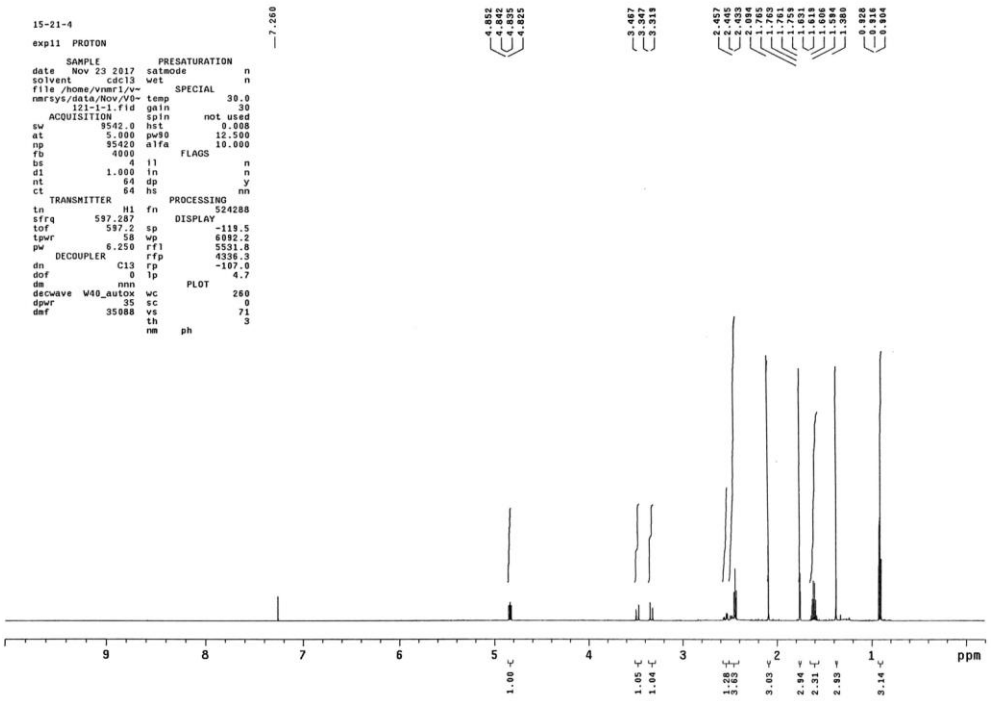


Figure S3. ^{1}H NMR spectrum of **1** (600 MHz in $CDCl_3$)

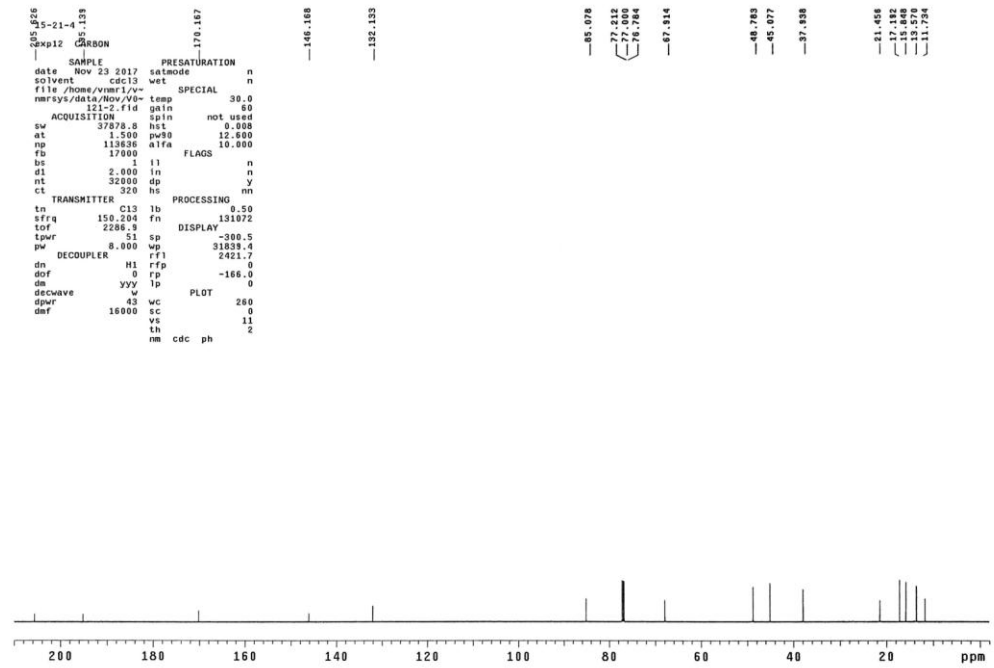


Figure S4. ^{13}C NMR spectrum of **1** (150 MHz in $CDCl_3$)

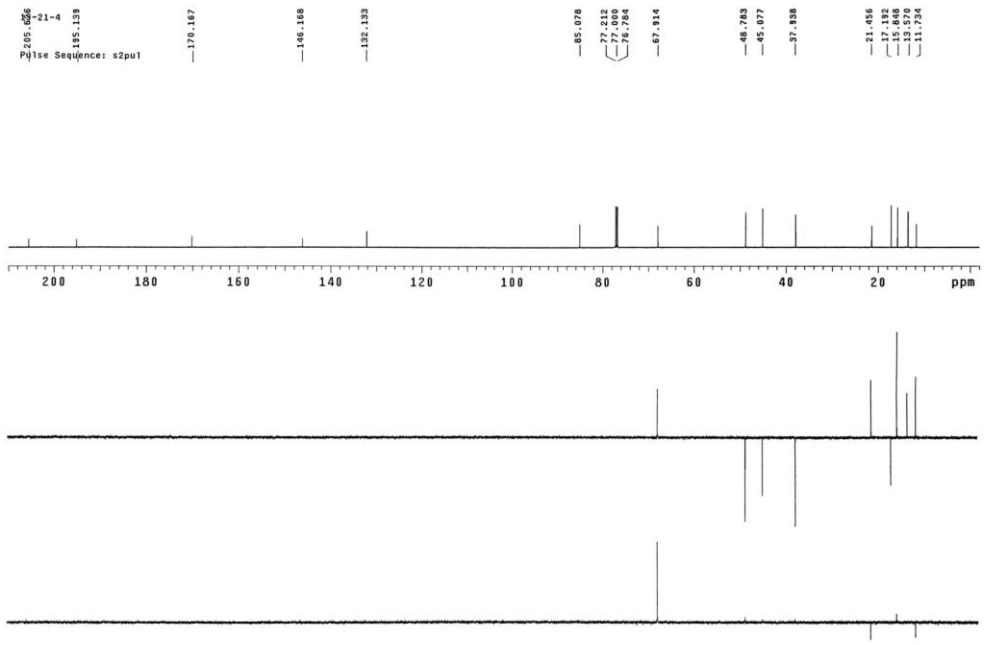


Figure S5. DEPT spectrum of **1** (150 MHz in $CDCl_3$)

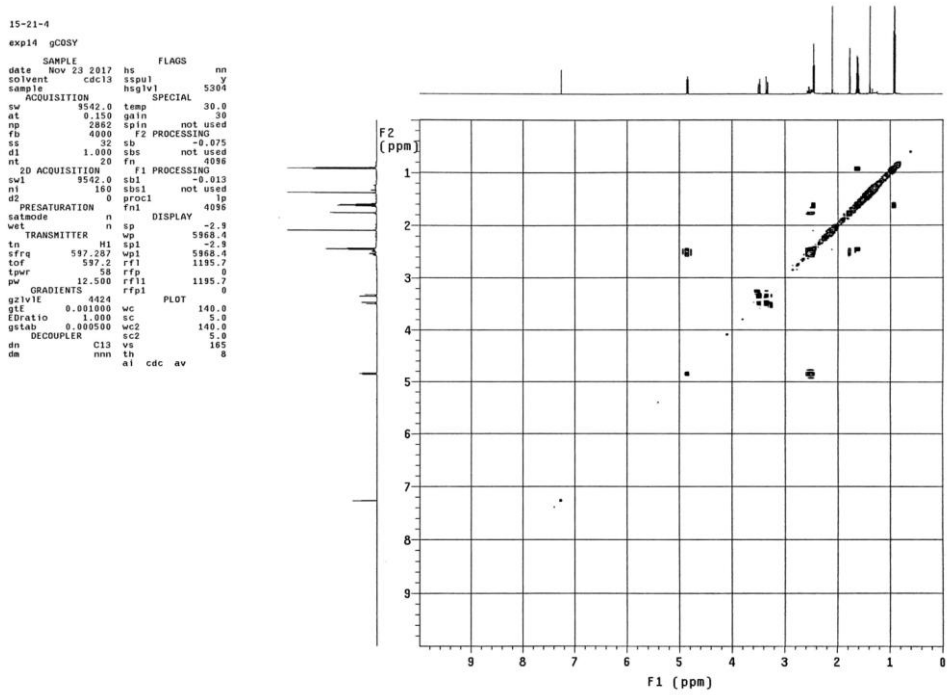


Figure S6. ^{1}H-^{1}H COSY spectrum of **1**

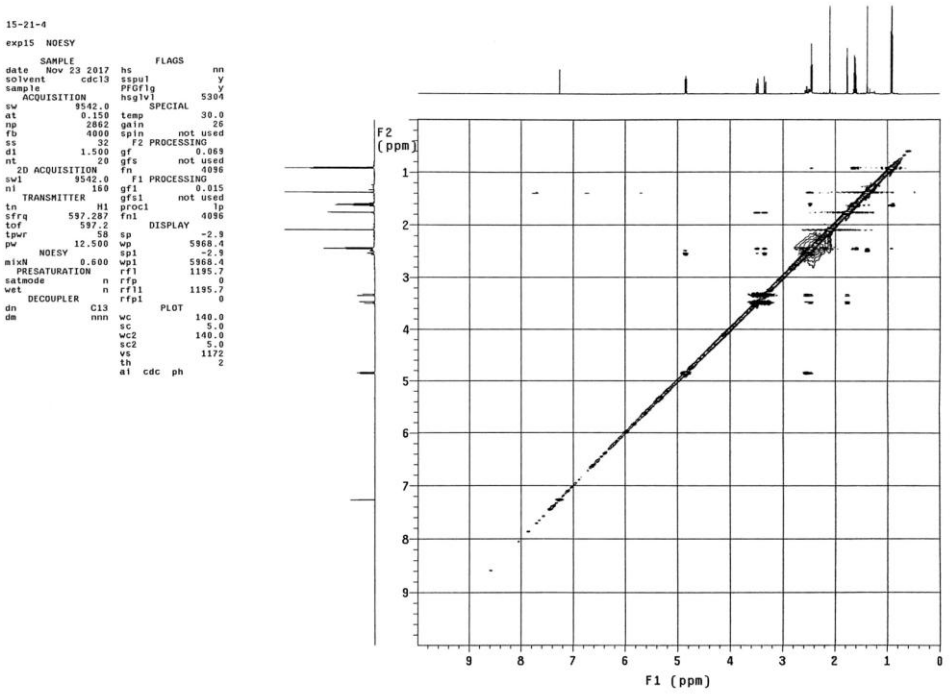


Figure S7. NOESY spectrum of **1**

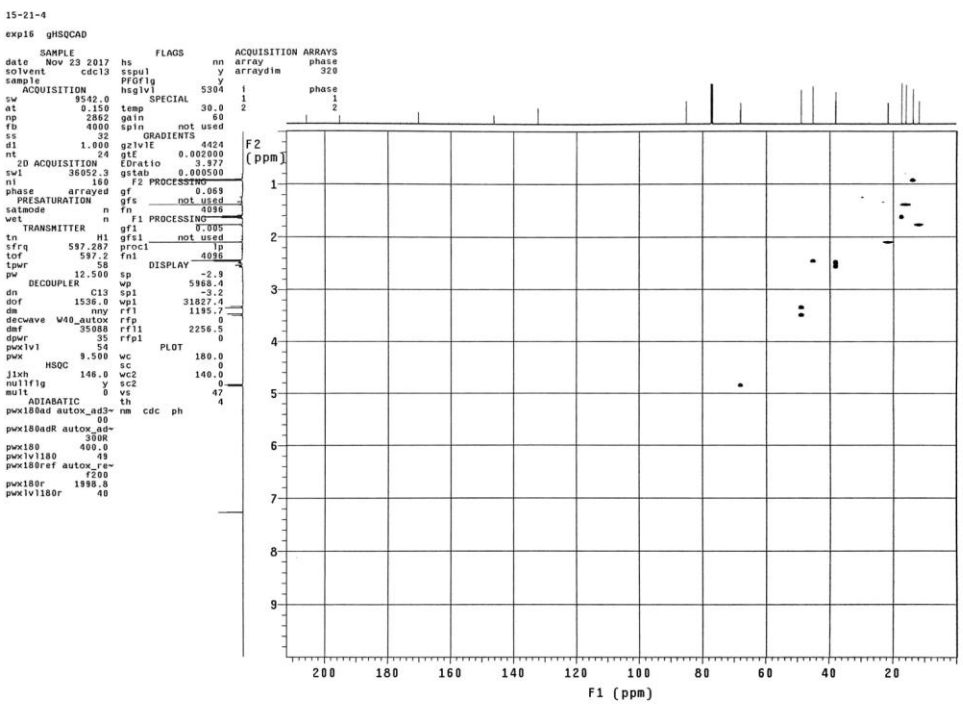


Figure S8. HSQC spectrum of **1**

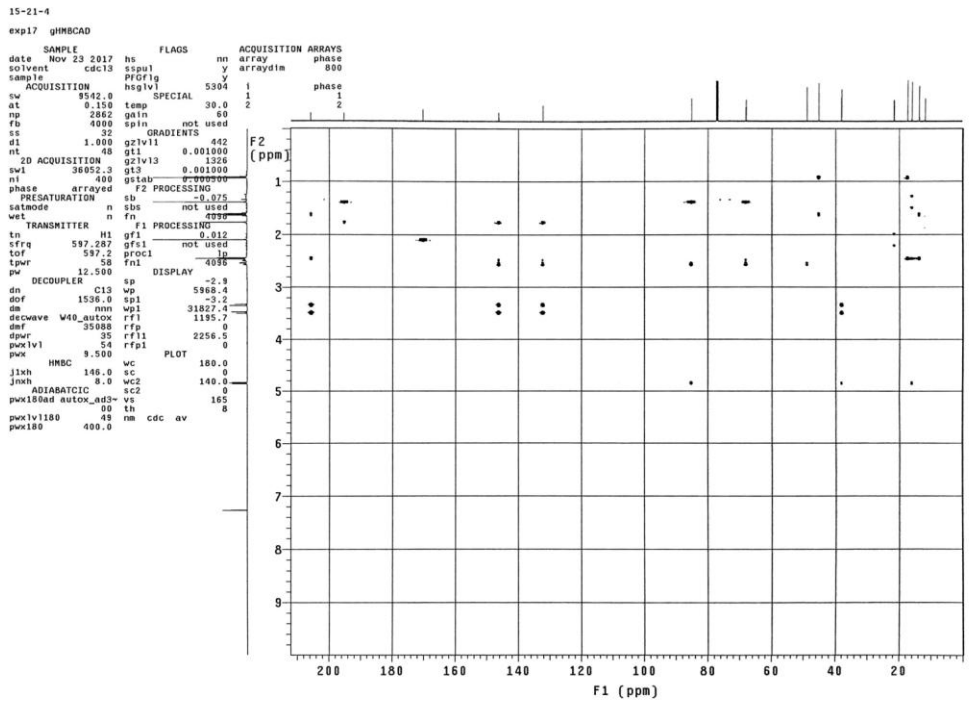


Figure S9. HMBC spectrum of **1**

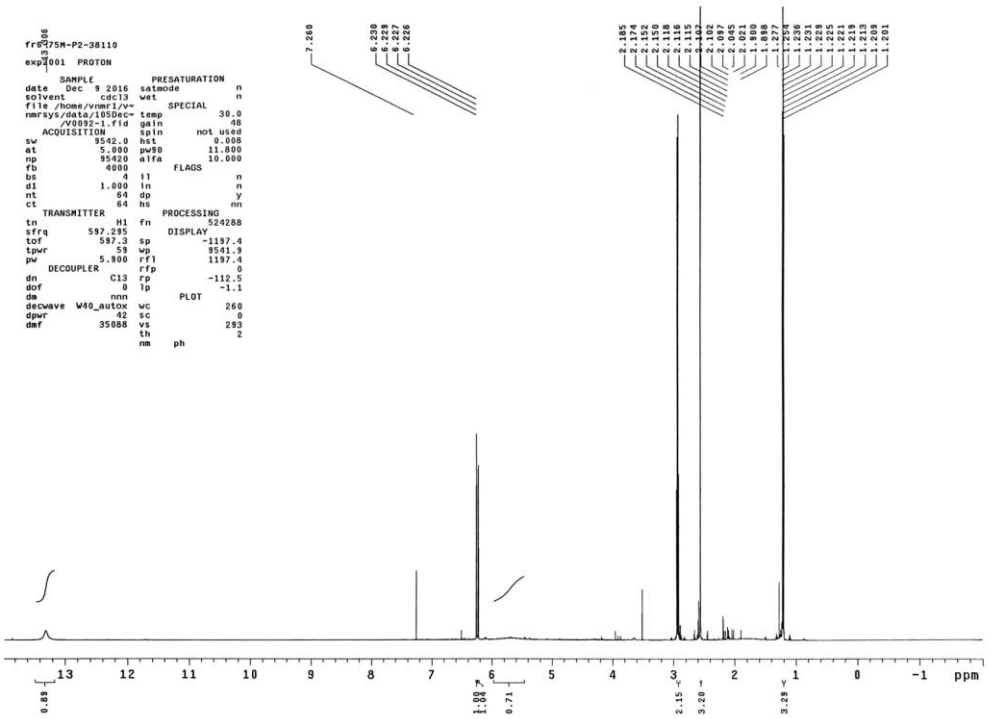


Figure S10. ^{1}H NMR spectrum of **2** (600 MHz in $CDCl_3$)

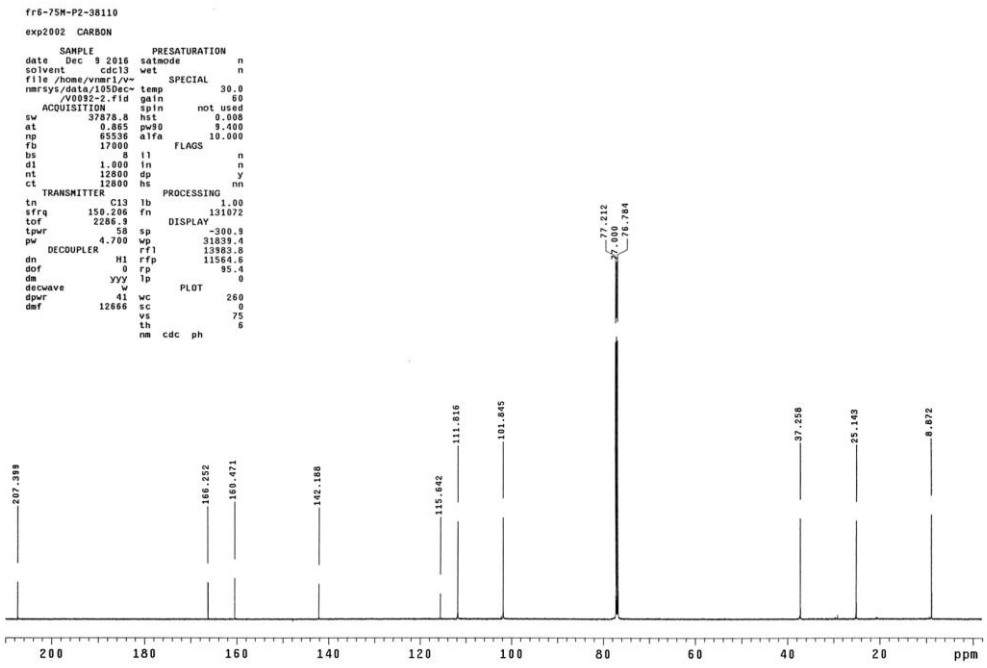


Figure S11. ^{13}C NMR spectrum of **2** (150 MHz in $CDCl_3$)

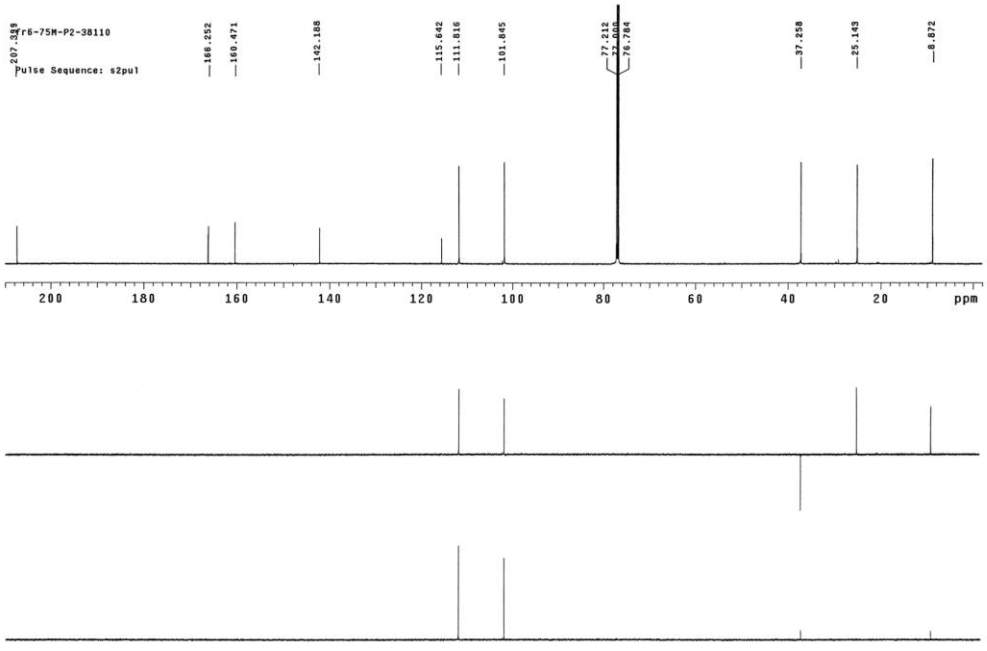


Figure S12. DEPT spectrum of **2** (150 MHz in $CDCl_3$)

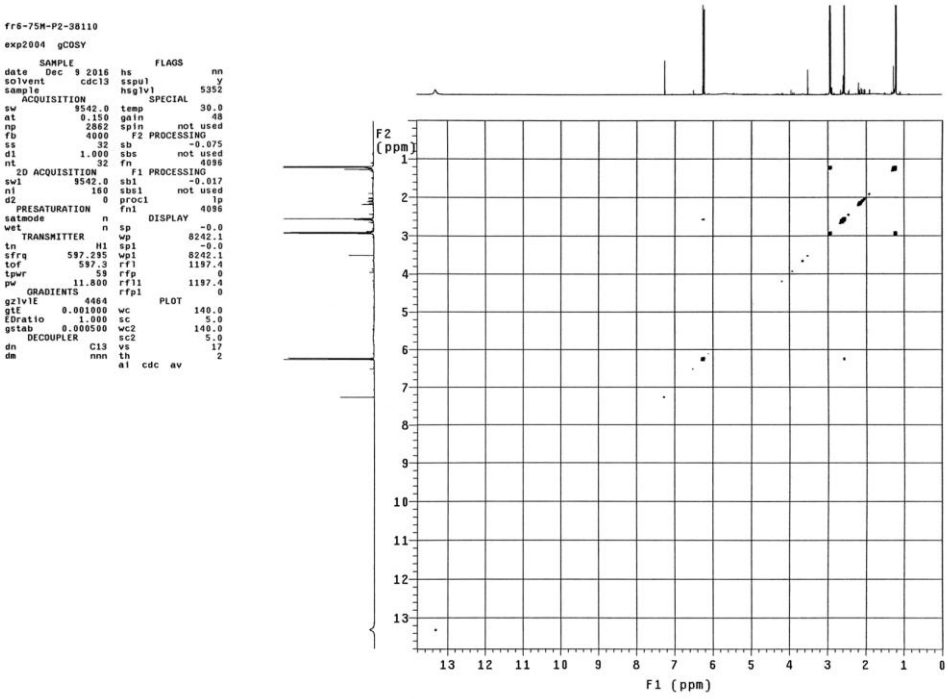


Figure S13. ^{1}H-^{1}H COSY spectrum of **2**

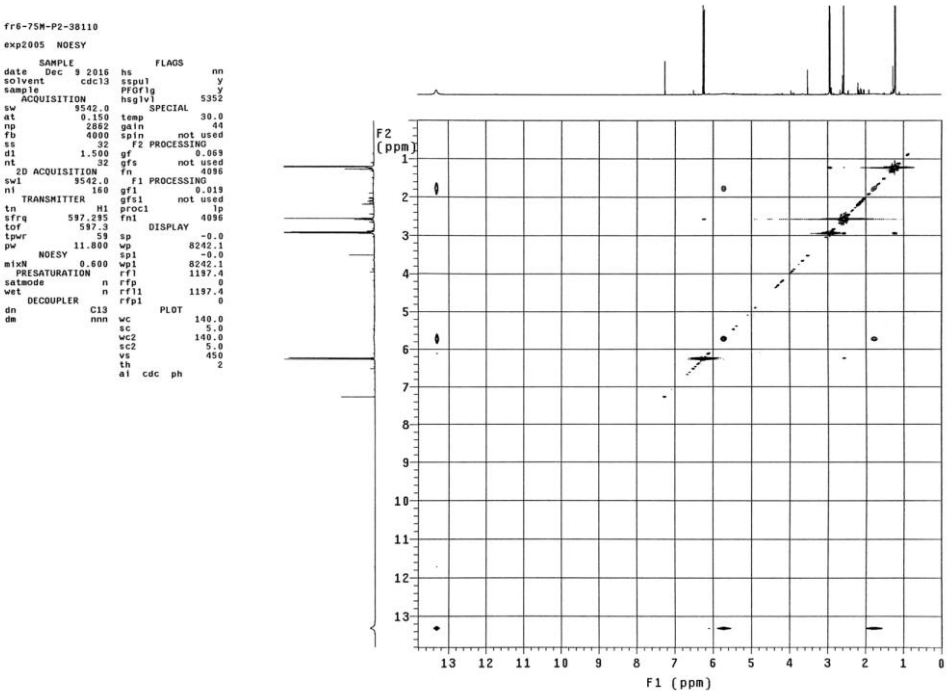


Figure S14. NOESY spectrum of **2**

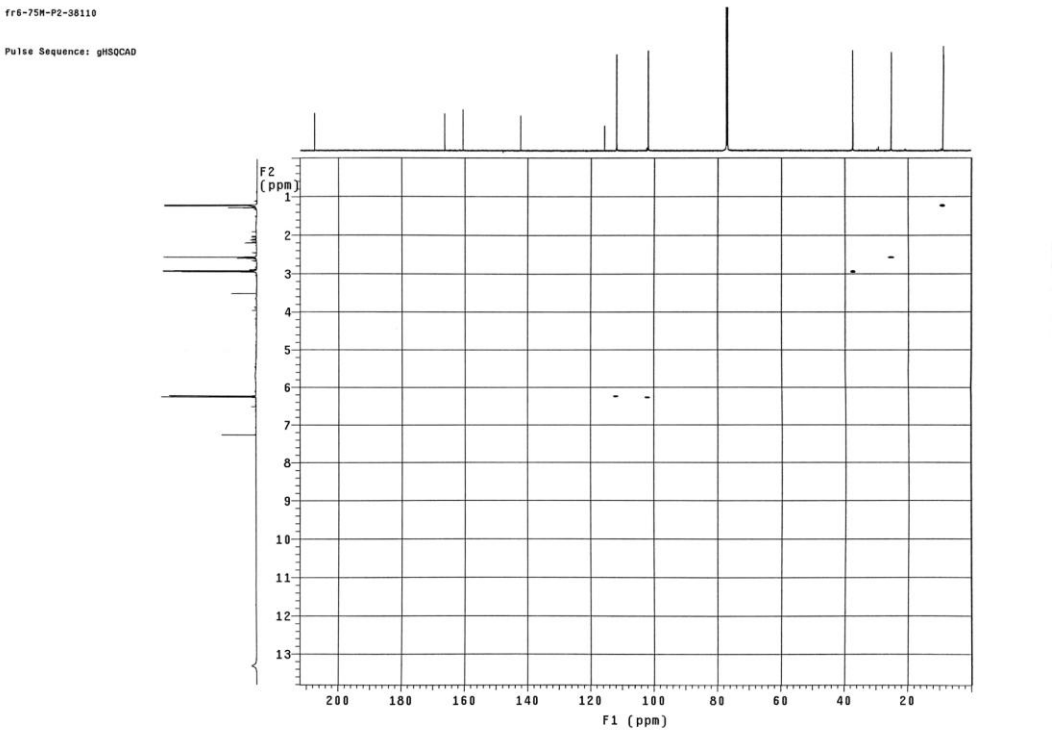


Figure S15. HSQC spectrum of **2**

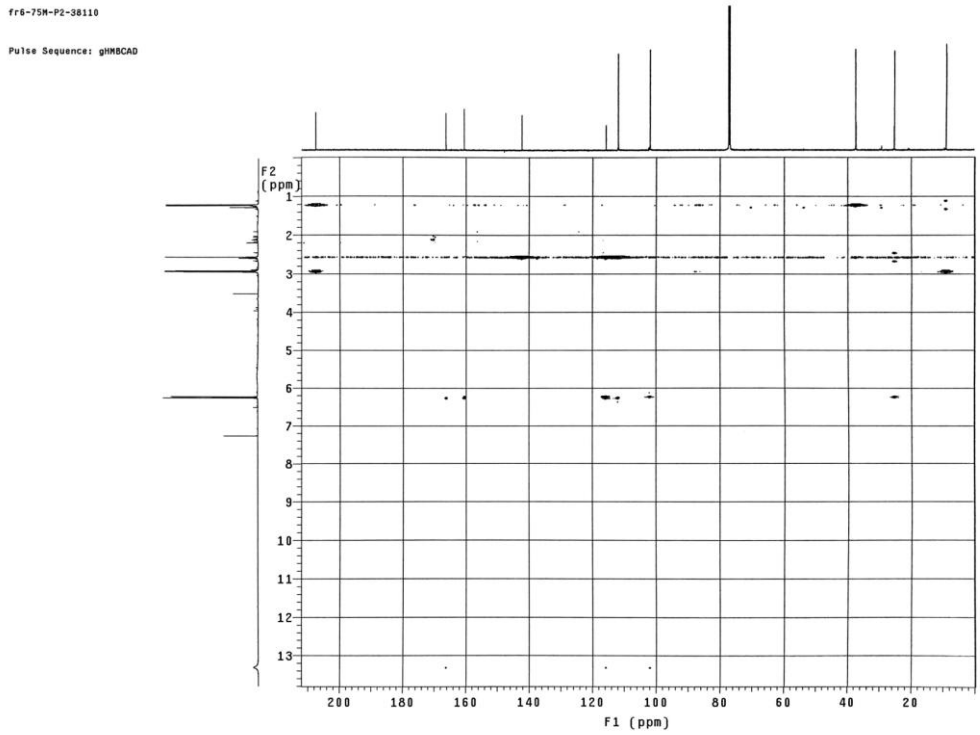


Figure S16. HMBC spectrum of **2**