

Supplementary Information

A New Ergosterol Analogue, a New Bis-Anthraquinone and Anti-obesity Activity of Anthraquinones from the Marine Sponge-Associated Fungus *Talaromyces stipitatus* KUFA 0207

Jidapa Noinart ¹, Suradet Buttachon ^{1,2}, Tida Dethoup ³, Luís Gales ^{1,4}, José A. Pereira ^{1,2}, Ralph Urbatzka ², Sara Freitas ², Michael Lee ⁵, Artur M.S. Silva ⁶, Madalena M. M. Pinto ^{2,7}, Vítor Vasconcelos ^{2,8}, Anake Kijjoa ^{1,2*}

¹ ICBAS-Instituto de Ciências Biomédicas Abel Salazar, Rua de Jorge Viterbo Ferreira, 228, 4050-313 Porto, Portugal. E-mail: jidainoart@gmail.com (JN), jpereira@icbas.up.pt (JAP).

² Interdisciplinary Centre of Marine and Environmental Research (CIIMAR), Terminal de Cruzeiros do Porto de Leixões, Av. General Norton de Matos s/n, 4450-208, Matosinhos, Portugal. E-mail: nokrari_209@hotmail.com (SB), ralph.urbatzka.ciimar@gmail.com (RU), freitas.srf.09@gmail.com (SF), vmvascon@fc.up.pt (VV).

³ Department of Plant Pathology, Faculty of Agriculture, Kasetsart University, Bangkok 10240, Thailand. E-mail: tdethoup@yahoo.com.

⁴ Instituto de Biologia Molecular e Celular (IBMC), Universidade do Porto, Rua de Jorge Viterbo Ferreira, 228, 4050-313 Porto, Portugal. E-mail: lgales@ibmc.up.pt.

⁵ Department of Chemistry, University of Leicester, University Road, Leicester LE 7 RH, UK. E-mail: ml34@leicester.ac.uk.

⁶ Departamento de Química & QOPNA, Universidade de Aveiro, 3810-193 Aveiro, Portugal. E-mail: artur.silva@ua.pt.

⁷ Laboratório de Química Orgânica, Departamento de Ciências Químicas, Faculdade de Farmácia, Universidade do Porto, Rua de Jorge Viterbo Ferreira, 228, 4050-313 Porto, Portugal. E-mail: madalena@ff.up.pt.

⁸ Departamento de Biologia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, s/n, 4169-007 Porto, Portugal

* To whom correspondence should be addressed, E-mail: ankijjoa@icbas.up.pt; Tel.: +351-220428331. Fax: +351-22-2062232.

Figure S1. ¹H NMR spectrum of compound **1** (CDCl₃, 300.13 MHz).

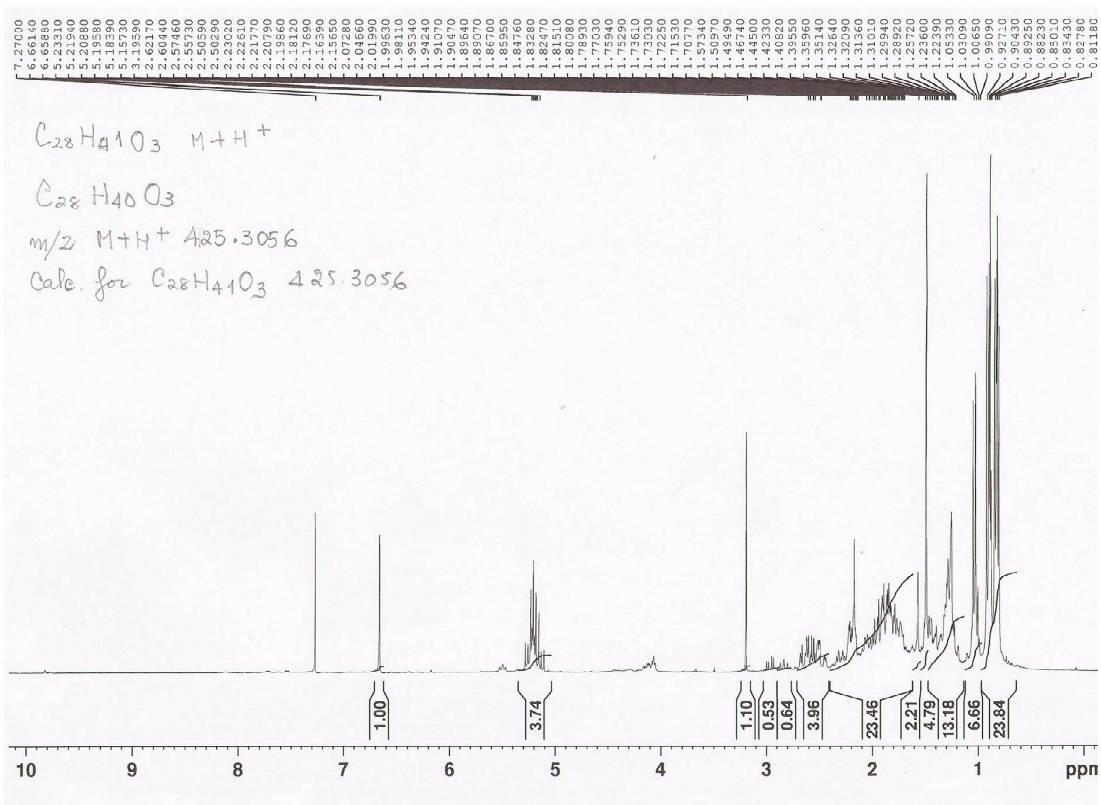


Figure S2. ^{13}C NMR spectrum of compound **1** ($CDCl_3$, 75.4 MHz).

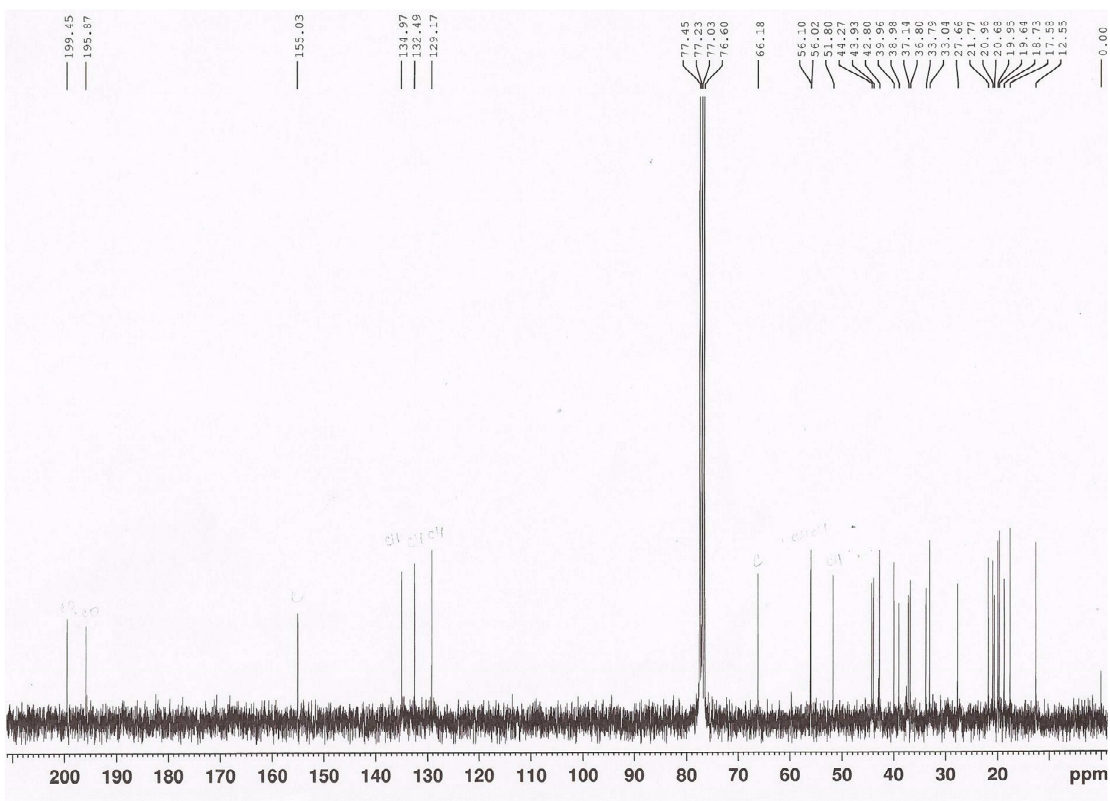


Figure S3. COSY spectrum of compound **1** ($CDCl_3$, 300.13 MHz).

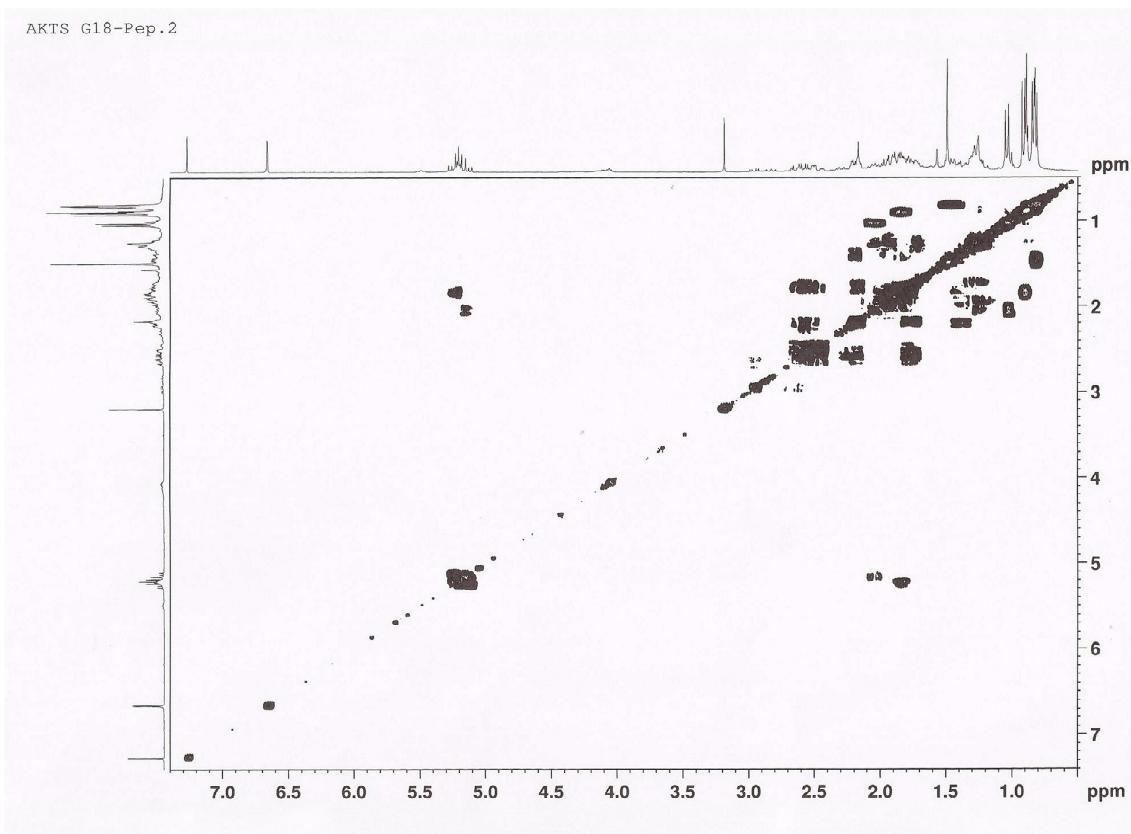


Figure S4. HSQC spectrum of compound **1** (CDCl₃, 300.13 MHz).

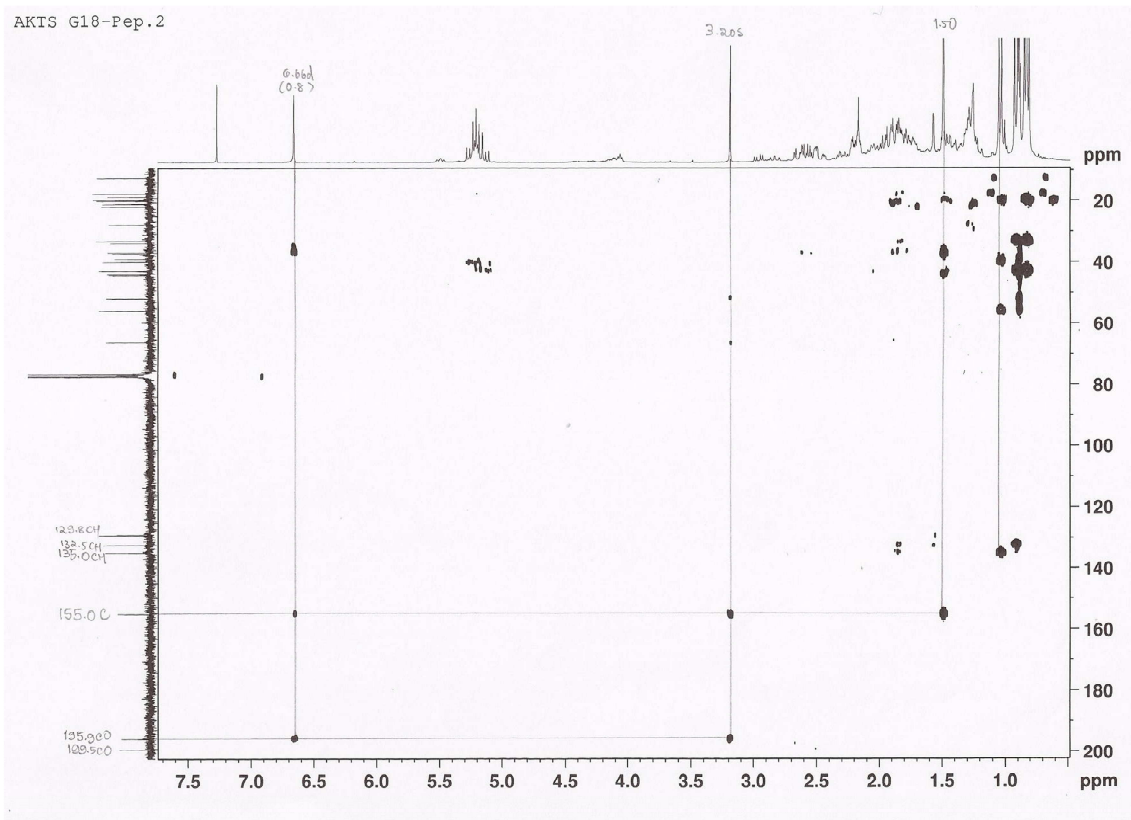


Figure S5. HMBC spectrum of compound **1** (CDCl₃, 300.13 MHz).

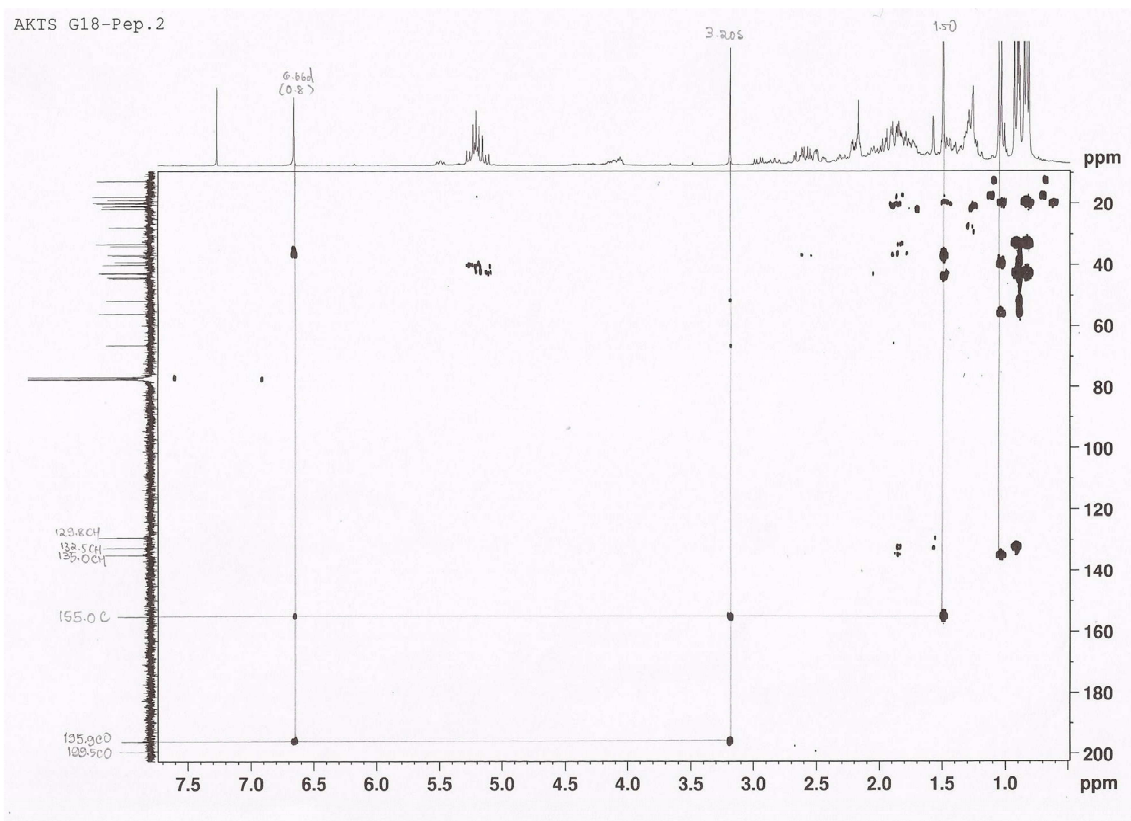


Figure S6. NOESY spectrum of compound **1** (CDCl_3 , 500.13 MHz).

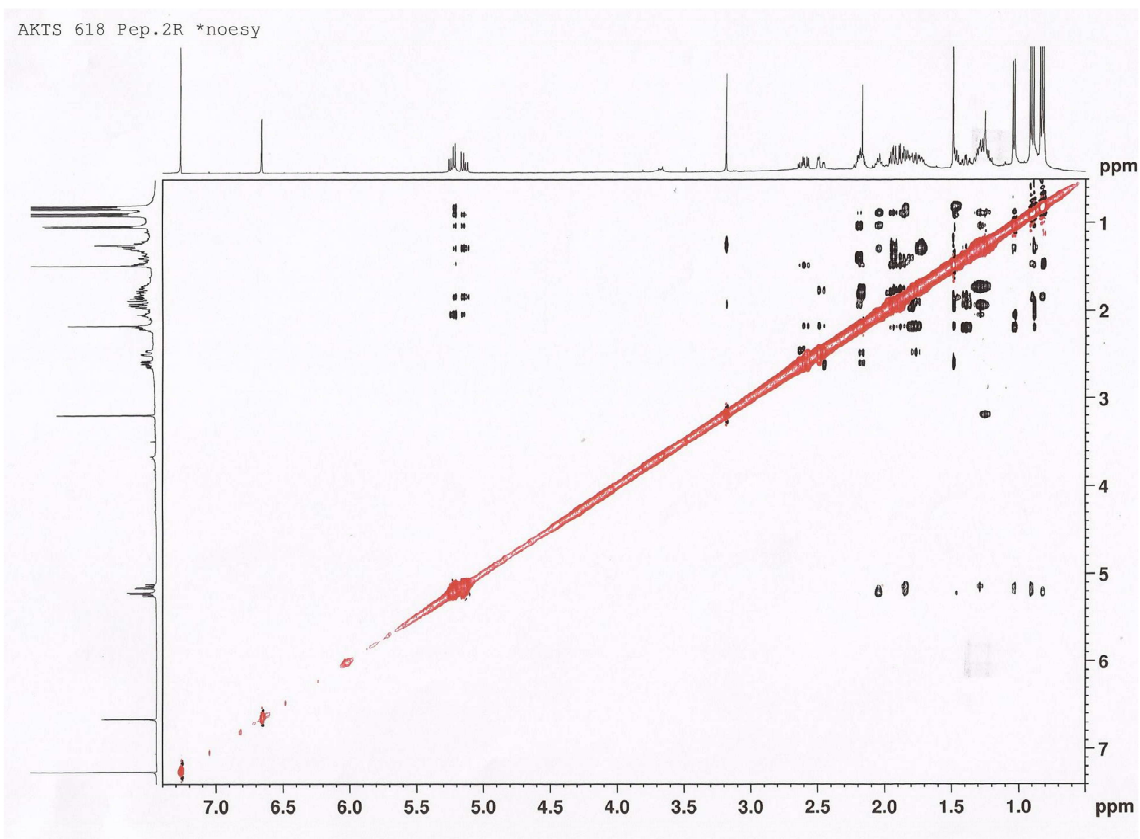


Figure S7. ROESY spectrum of compound **1** (CDCl₃, 500.13 MHz).

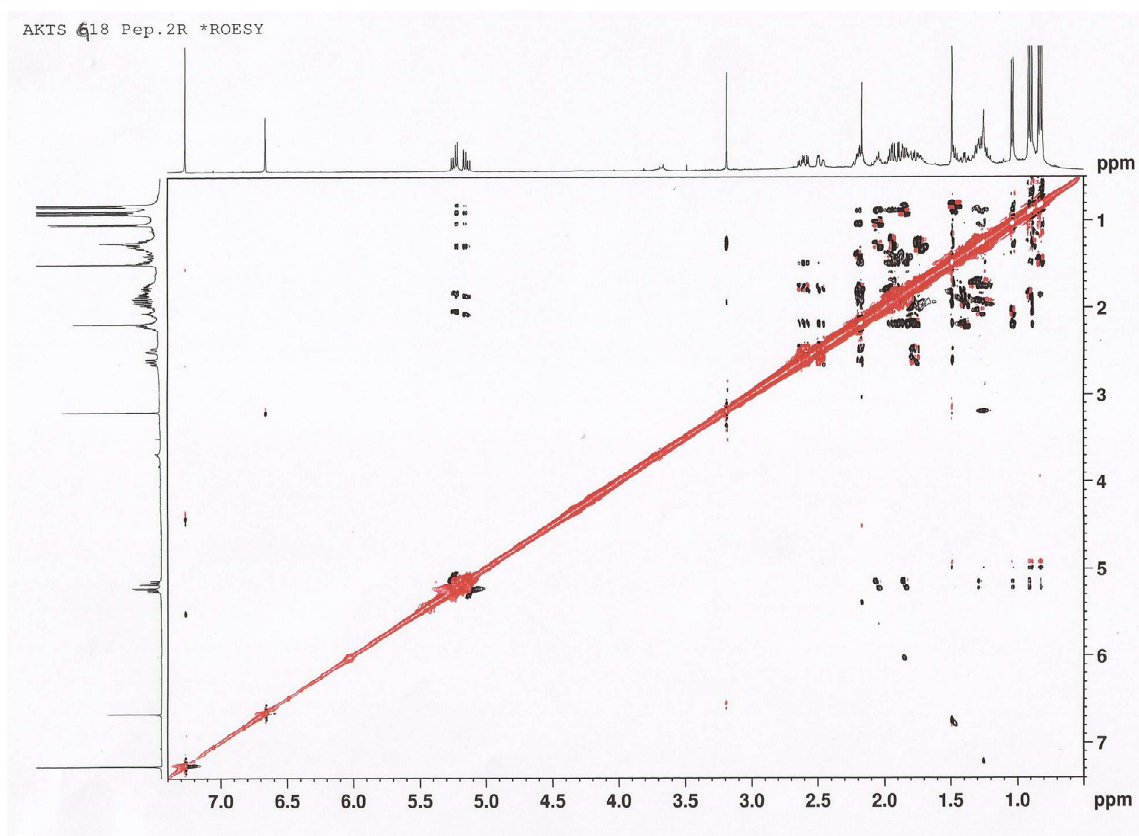


Figure S8. ¹H NMR spectrum of compound **2** (CDCl₃, 300.13 MHz).

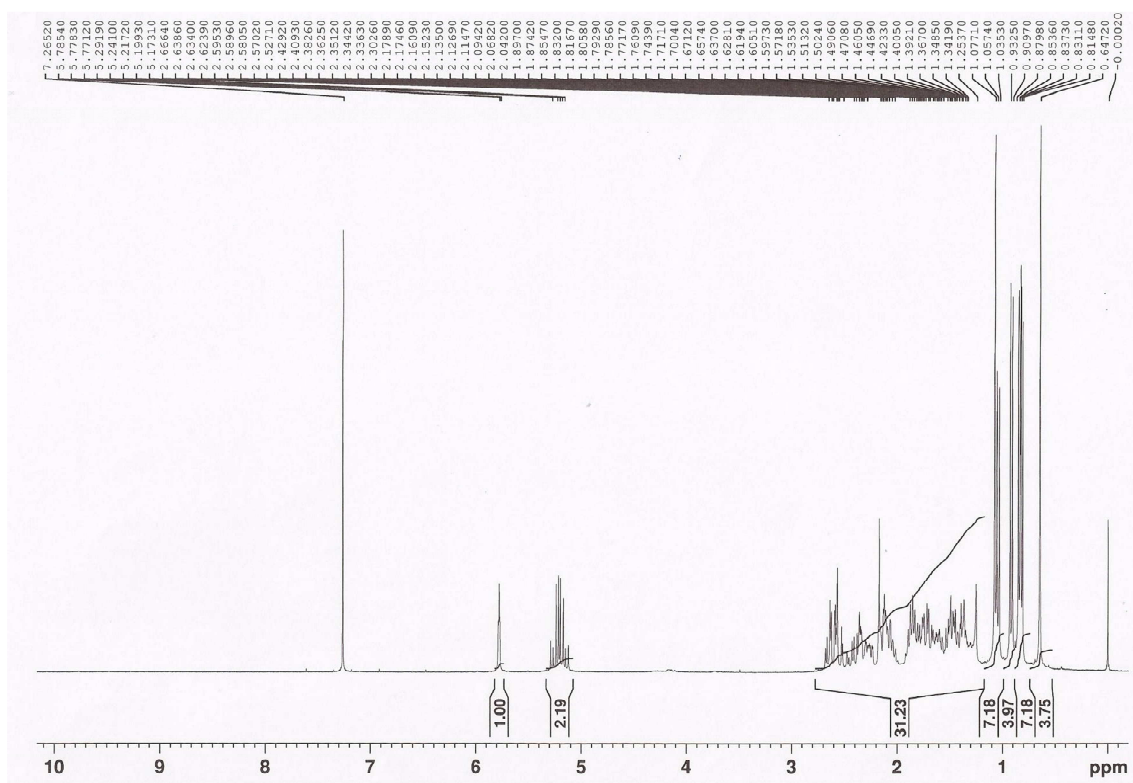


Figure S9. ^{13}C NMR spectrum of compound **2** (CDCl_3 , 75.4 MHz).

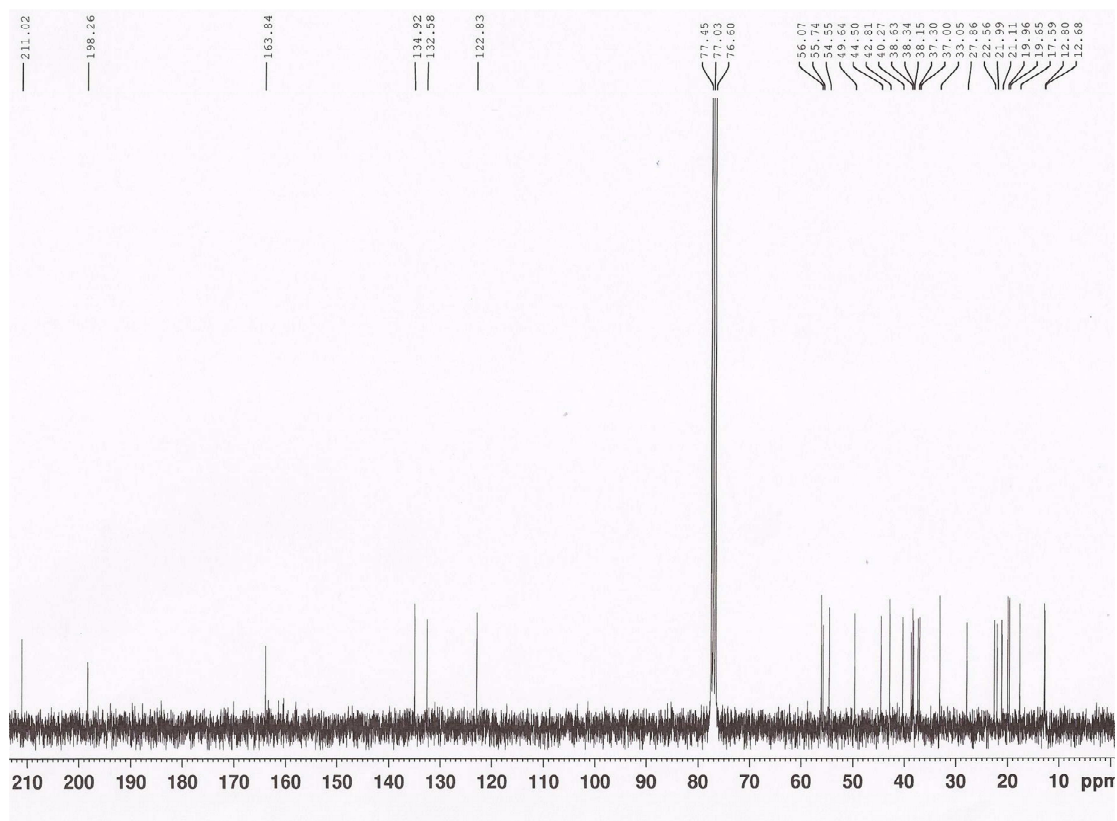


Figure S10. COSY spectrum of compound **2** (CDCl_3 , 300.13 MHz).

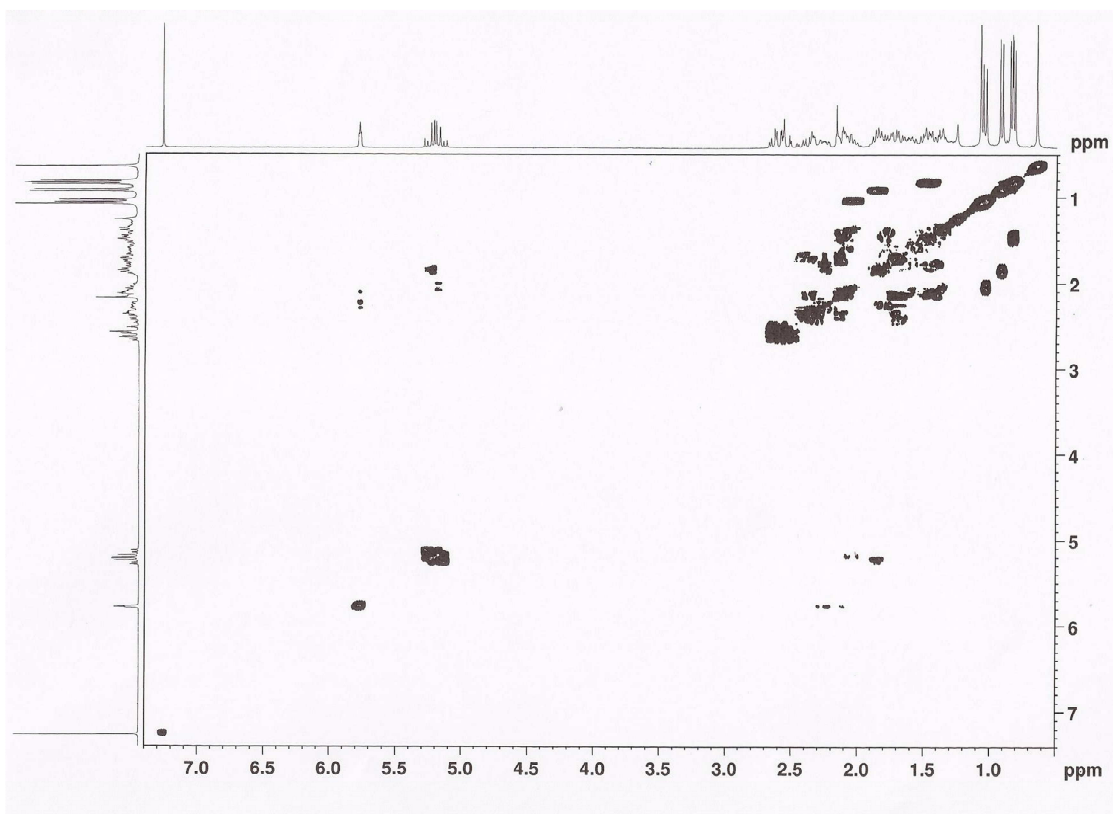


Figure S11. HSQC spectrum of compound **2** (CDCl₃, 300.13 MHz).

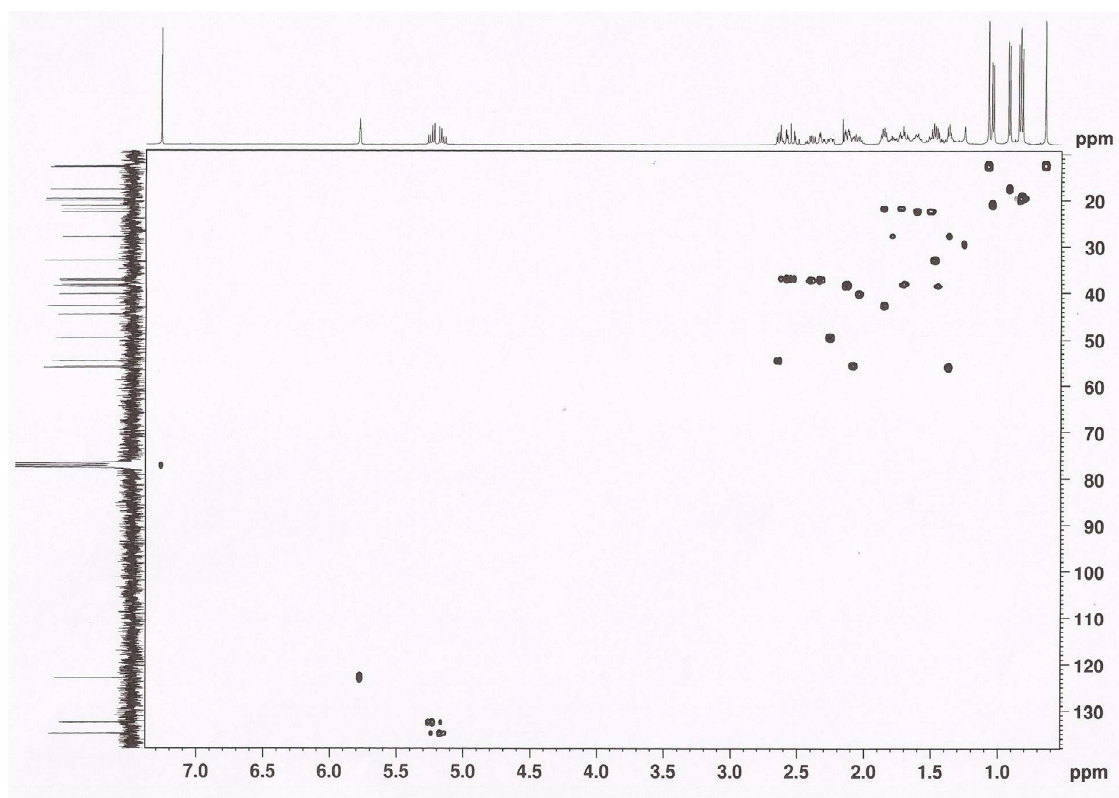


Figure S12. HMBC spectrum of compound **2** (CDCl₃, 300.13 MHz).

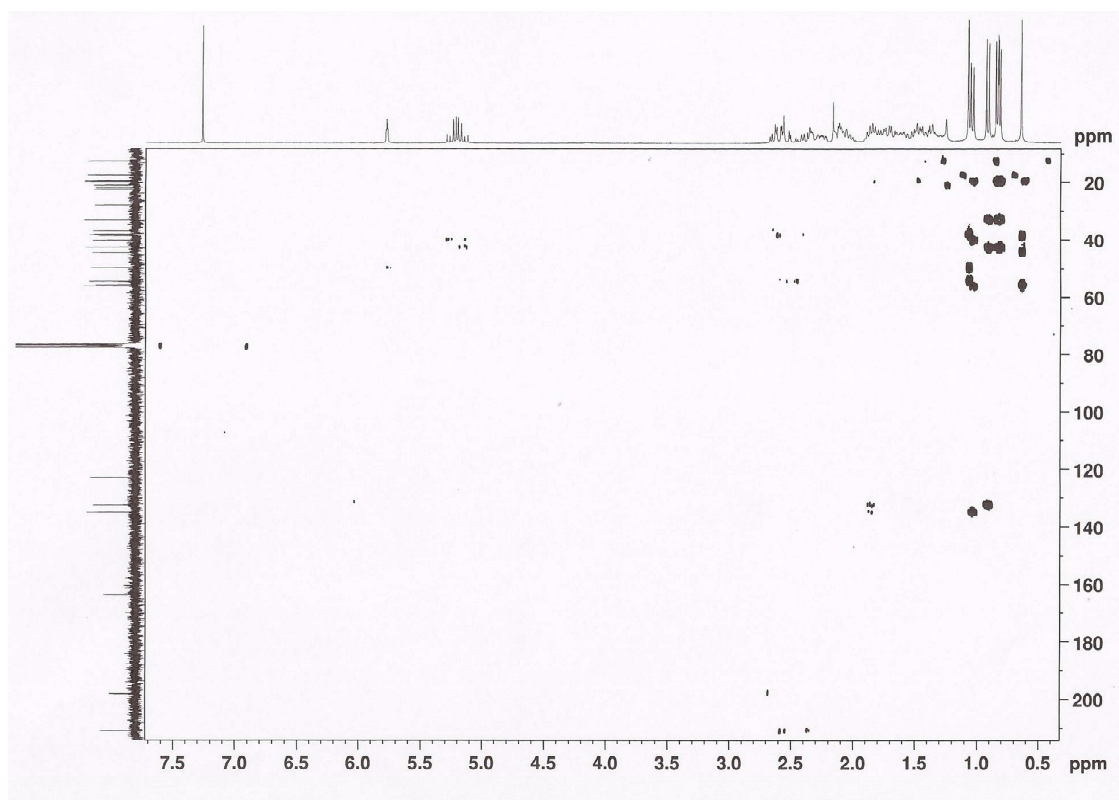


Figure S13. ^1H NMR spectrum of compound **3** (DMSO, 500.13 MHz).

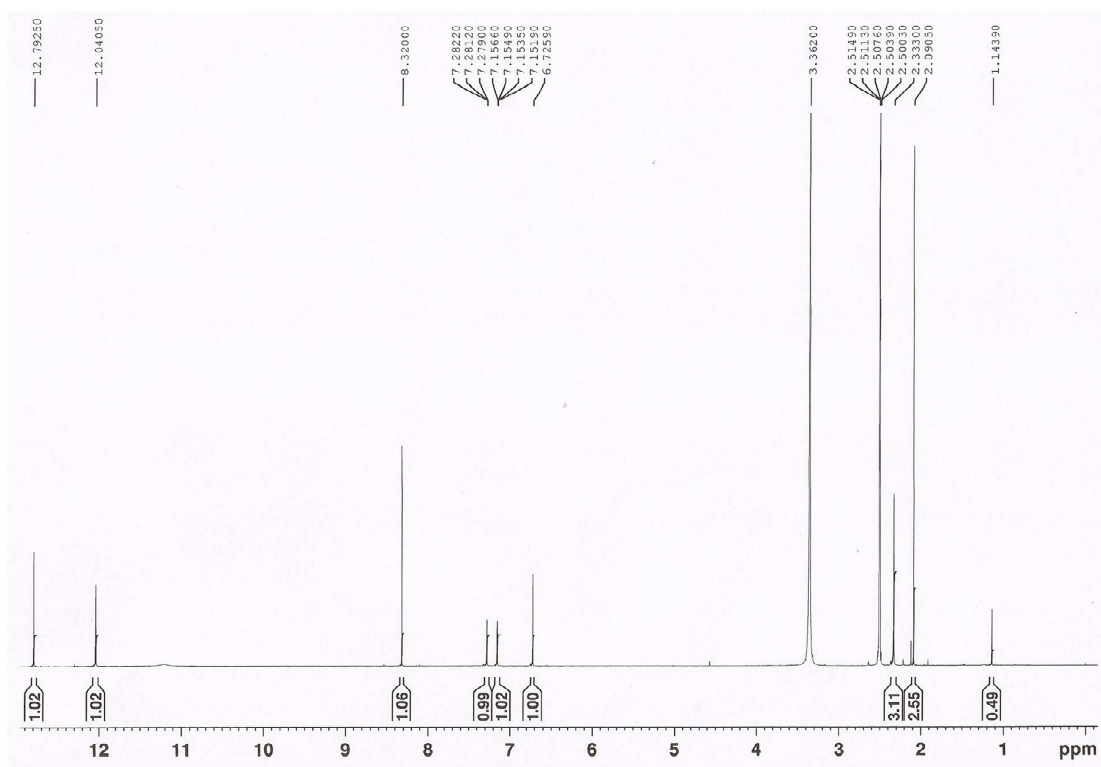


Figure S14. ^{13}C NMR spectrum of compound **3** (DMSO, 125.4 MHz).

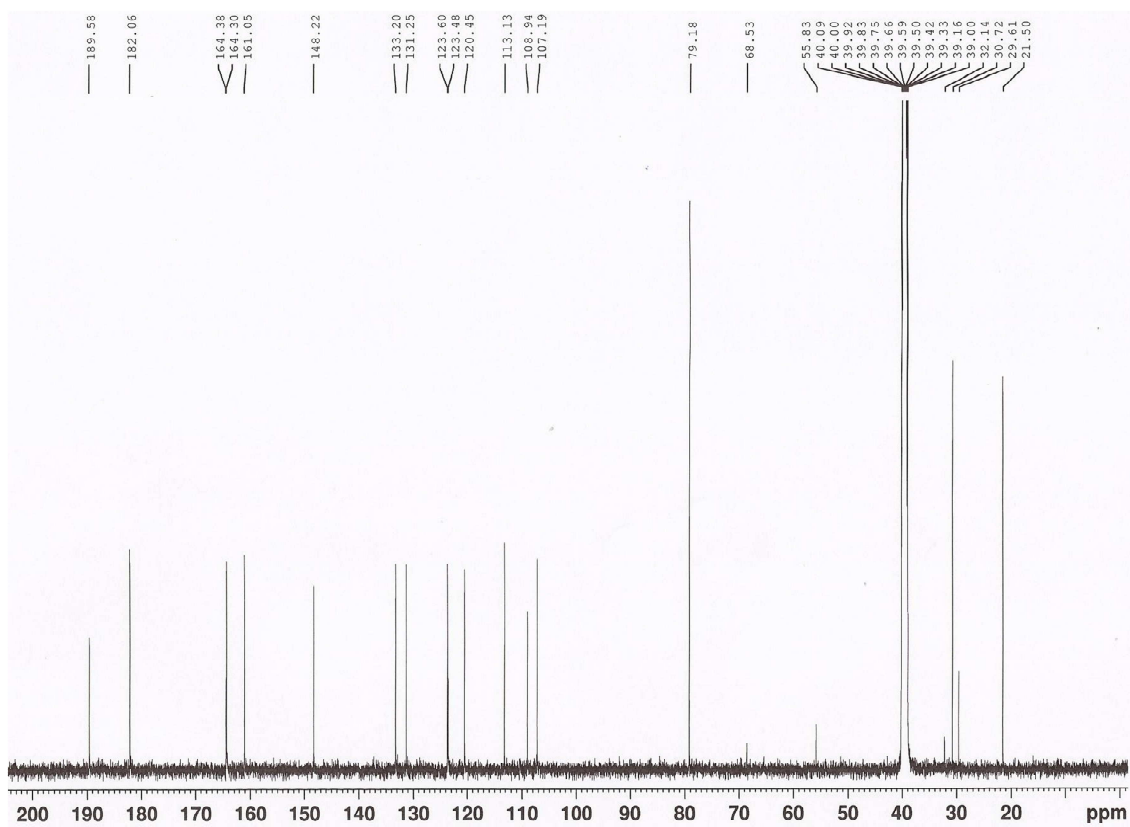


Figure S15. COSY spectrum of compound **3** (DMSO, 500.13 MHz).

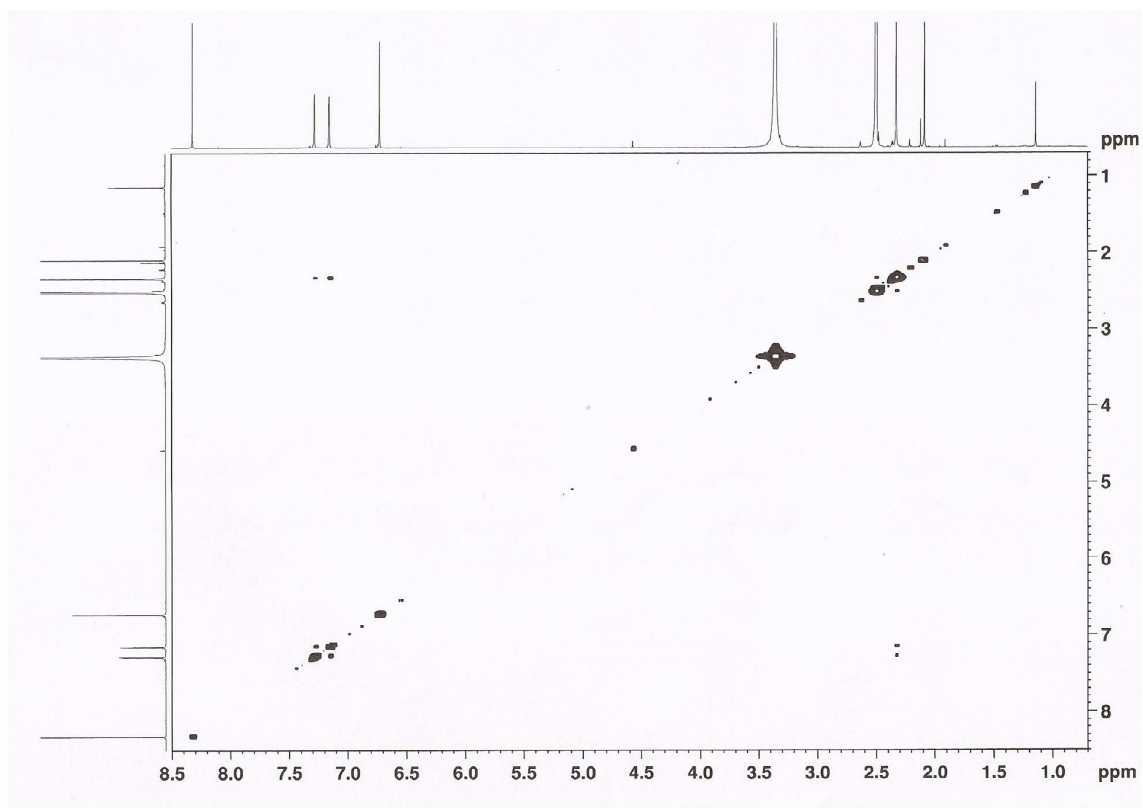


Figure S16. HSQC spectrum of compound **3** (DMSO, 500.13 MHz).

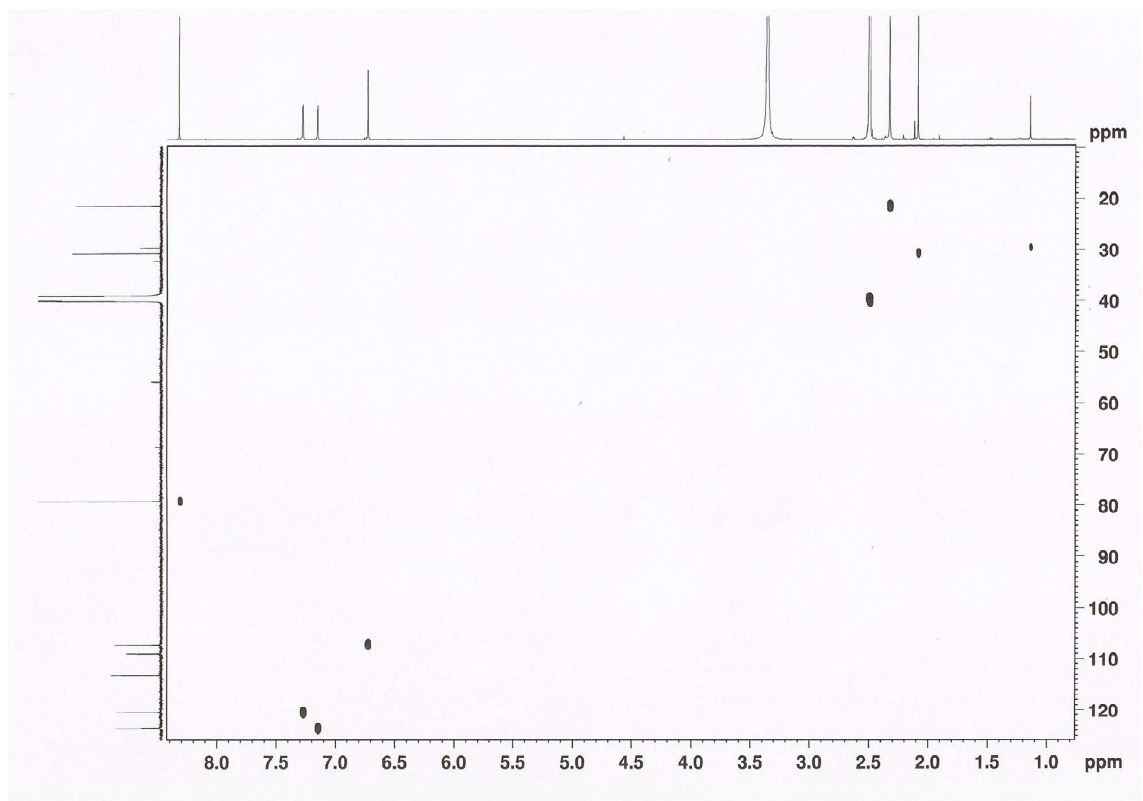
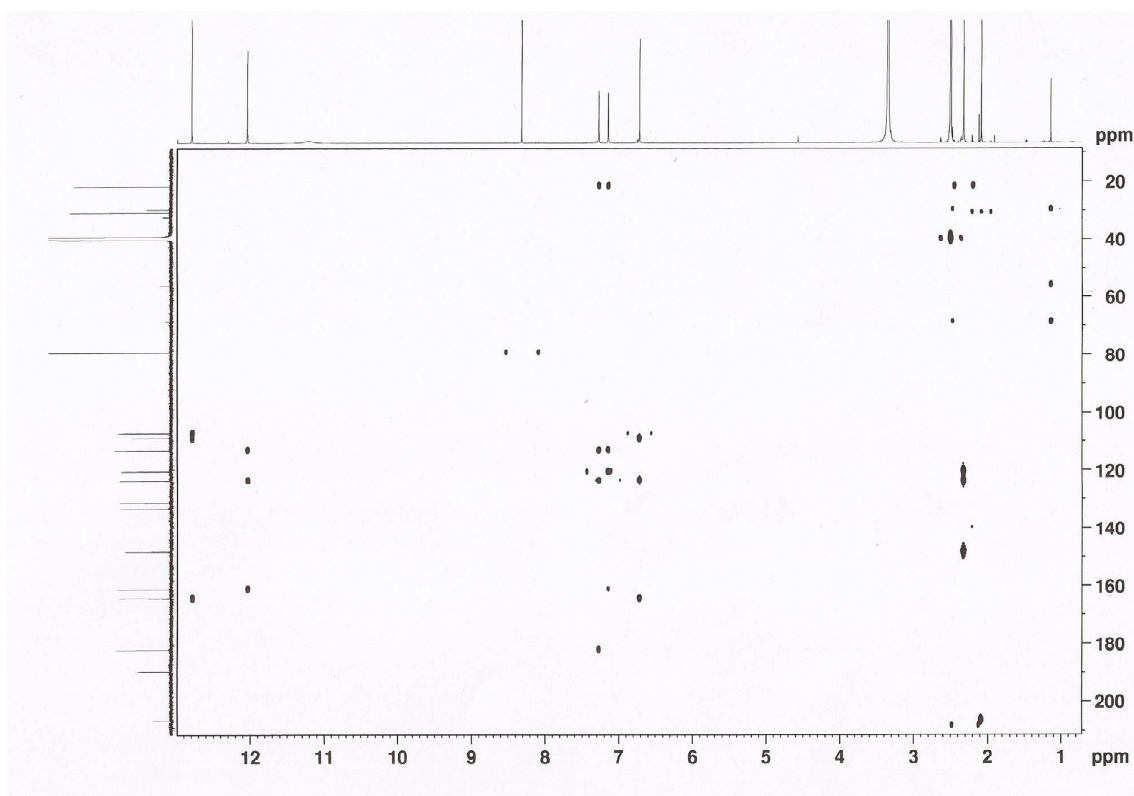


Figure S17. HMBC spectrum of compound **3** (DMSO, 500.13 MHz).



~

Table 1S¹H and ¹³C NMR (CDCl₃, 300.13 MHz and 75.4 MHz) and HMBC assignment for **2**.

Position	δ_C , type	δ_H , (<i>J</i> in Hz)	COSY	HMBC
1	38.2, CH ₂	1.70, m 2.14, m		
2	37.3, CH ₂	2.33, m 2.38, m		CO-3
3	211.0, CO	-		
4	37.0, CH ₂	2.59, m	H-5	CO-3
5	54.6, CH	2.64, dd (12.8, 4.5)	H-4	
6	198.3, CO	-		
7	122.8, CH	5.78, t (2.3)	H-9, 14	C-9
8	163.8, C	-		
9	49.6, CH	2.26, m	H-7, 11	
10	38.3, C	-		
11	22.0, CH ₂	1.72, m 1.85, m		
12	38.6, CH ₂	1.45, m 2.14, m		
13	44.5, C	-		
14	55.7, C	2.09, m	H-9, 15	
15	22.6, CH ₂	1.50, m 1.60, m		
16	27.9, CH ₂	1.37, m 1.79, m		
17	56.1, CH	1.36, m	H-16, 20	
18	12.7, CH ₃	0.65, s	-	
19	12.8, CH ₃	1.08, s	-	C-5, 9, 10
20	40.3, CH	2.04, m	H-21, 22	
21	21.1, CH ₃	1.05, d (6.6)	H-20	C-17, 20, 22
22	134.9, CH	5.16, dd (15.2, 7.9)	H-20, 23	C-20, 25
23	132.6, CH	5.25, dd (15.2, 7.2)	H-22, 24	C-20, 24
24	42.8, CH	1.85, m	H-22, 25, 26	C-22, 23
25	33.1, CH	1.48, m	H-24, 27, 28	C-23
26	17.6, CH ₃	0.92, d (6.8)	H-24	C-23, 24, 25
27	20.0, CH ₃	0.82, d (6.8)	H-25	C-24, 25, 26, 28
28	19.7, CH ₃	0.84, d (6.8)	H-25	C-24, 25, 26, 27