Supporting Information

for

Aspergiloid I, an unprecedented spirolactone norditerpenoid from the plant-derived endophytic fungus *Aspergillus* sp. YXf3

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*Corresponding author

1D, 2D NMR spectra, HRMS–ESI, and the X-ray crystallographic structure of **1**

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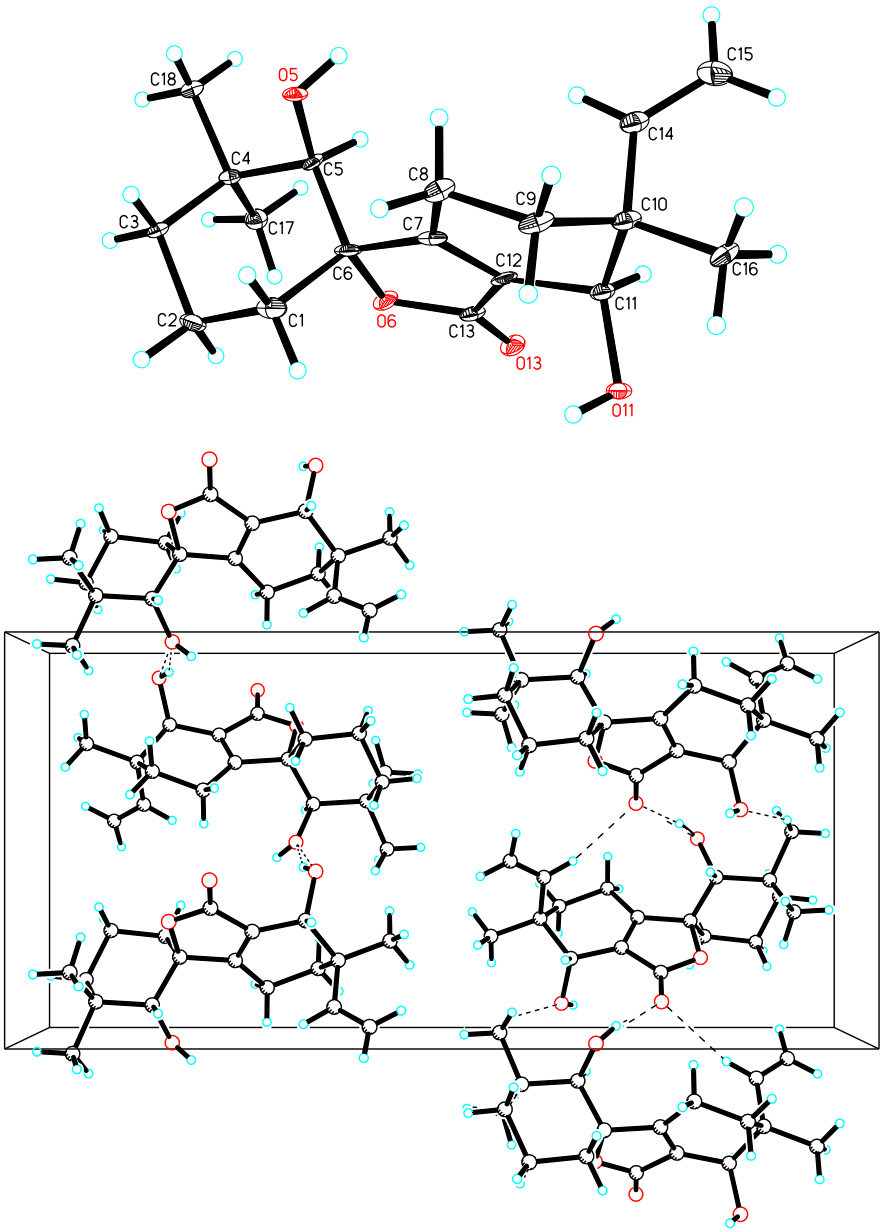
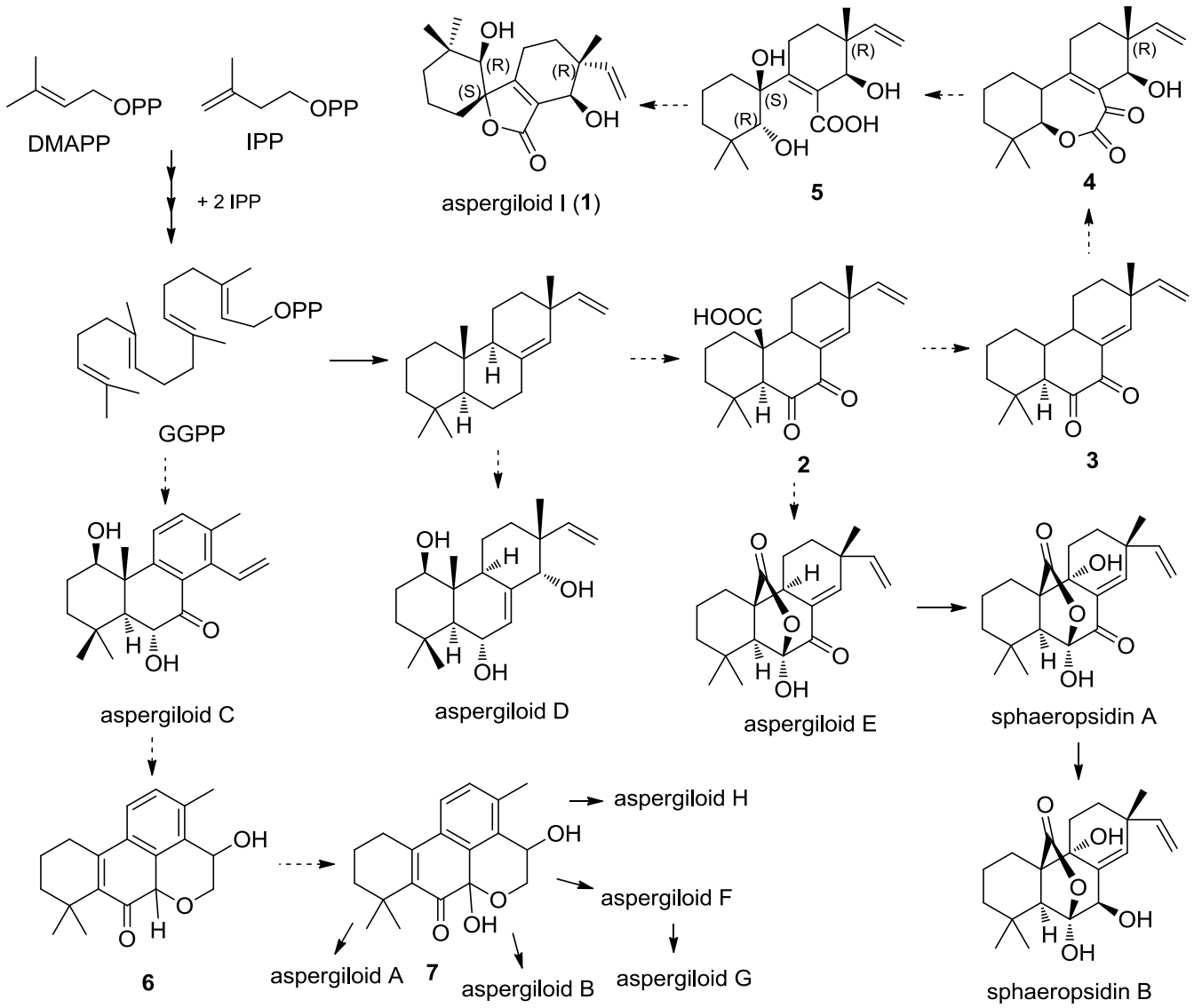
S1. The X-ray crystallographic structure of **1**



Scheme S1. Plausible biosynthetic pathway of apergiloid **A-I** and sphaeropsidin **A-F**



References:

1 Guo, Z. K.; Yan, T.; Guo, Y.; Song, Y. C.; Jiao, R. H.; Tan, R. X.; Ge, H. M. *J. Nat. Prod.* **2012**, *75*, 15–21.

2 Yan, T.; Guo, Z. K.; Jiang, R.; Wei, W.; Wang, T.; Guo, Y.; Song, Y. C.; Jiao, R. H.; Tan, R. X.; Ge, H. M. *Planta Med*. **2013**, *79*, 348–352.

3 Guo, Z. K.; Liu, S. B.; Ma S. Nat. Prod. Res. Dev. **2013**, *25*, 778–781.

4 Ellestad, G. A. ; Kunstmann, M. P. ; Mirando, P.; Morton, G. O. *J. Am. Chem. Soc.* **1972**, *94*, 6206–6208.

5 Evidente, A.; Sparapano, L.; Fierro, O.; Bruno, G.; Giordano, F.; Motta, A. *Phytochemistry*, **1997**, *45*, 705–713.

6 Evidente, A.; Sparapano, L.; Bruno, G.; Motta, A. *Phytochemistry*, **2002**, *59*, 817–823.

7 Dewick, P. M. *Nat. Prod. Rep.* **2002**, *19*, 181–122.

Figure S1. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **1**

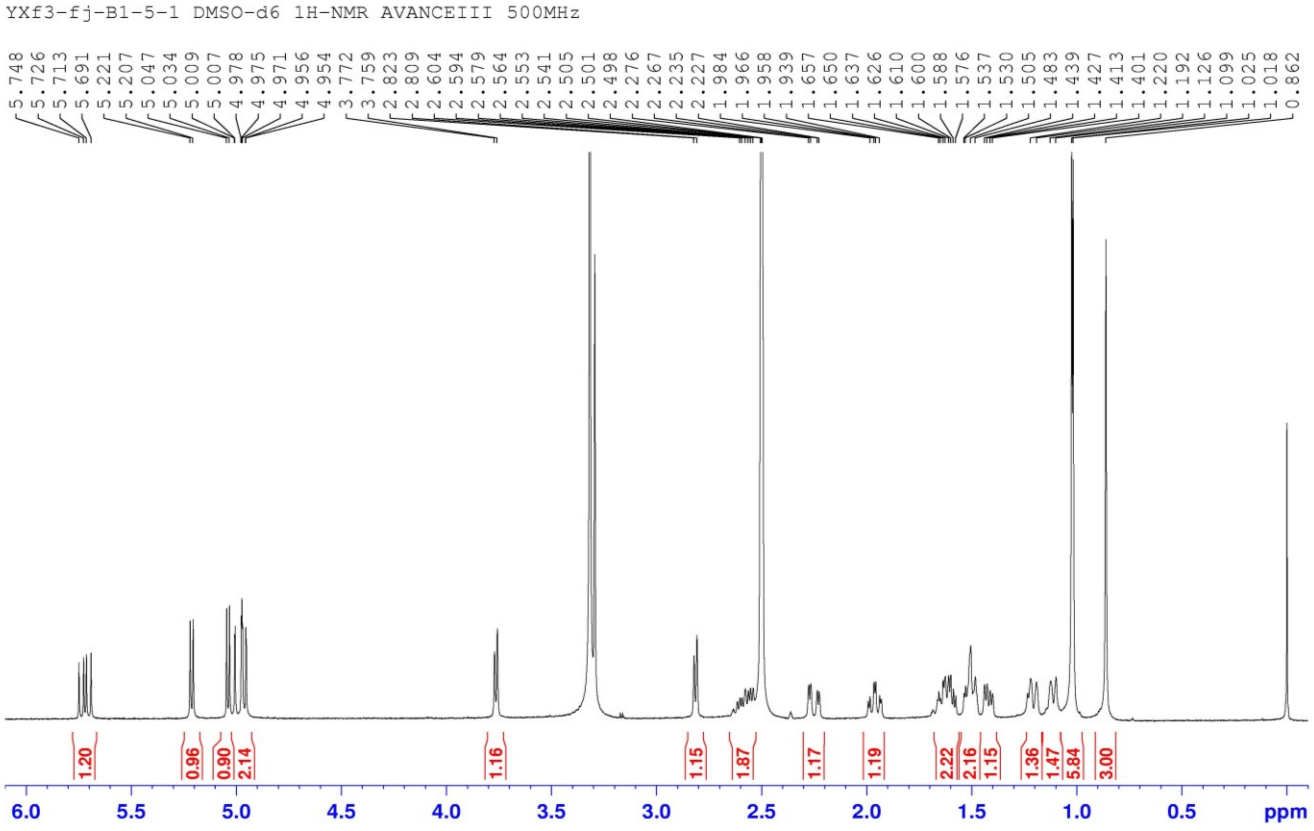


Figure S2. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **1**

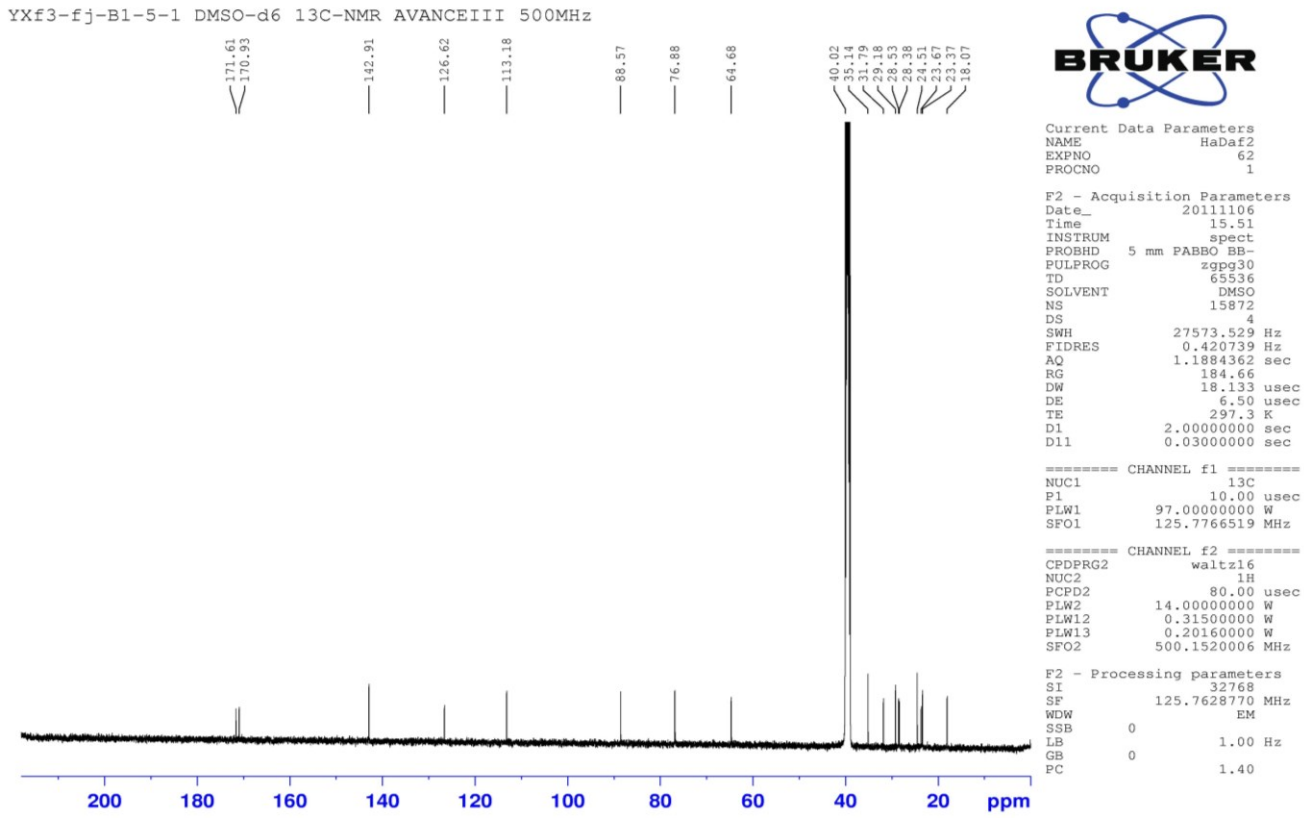


Figure S3. DEPT spectra of compound **1** in DMSO-d_6

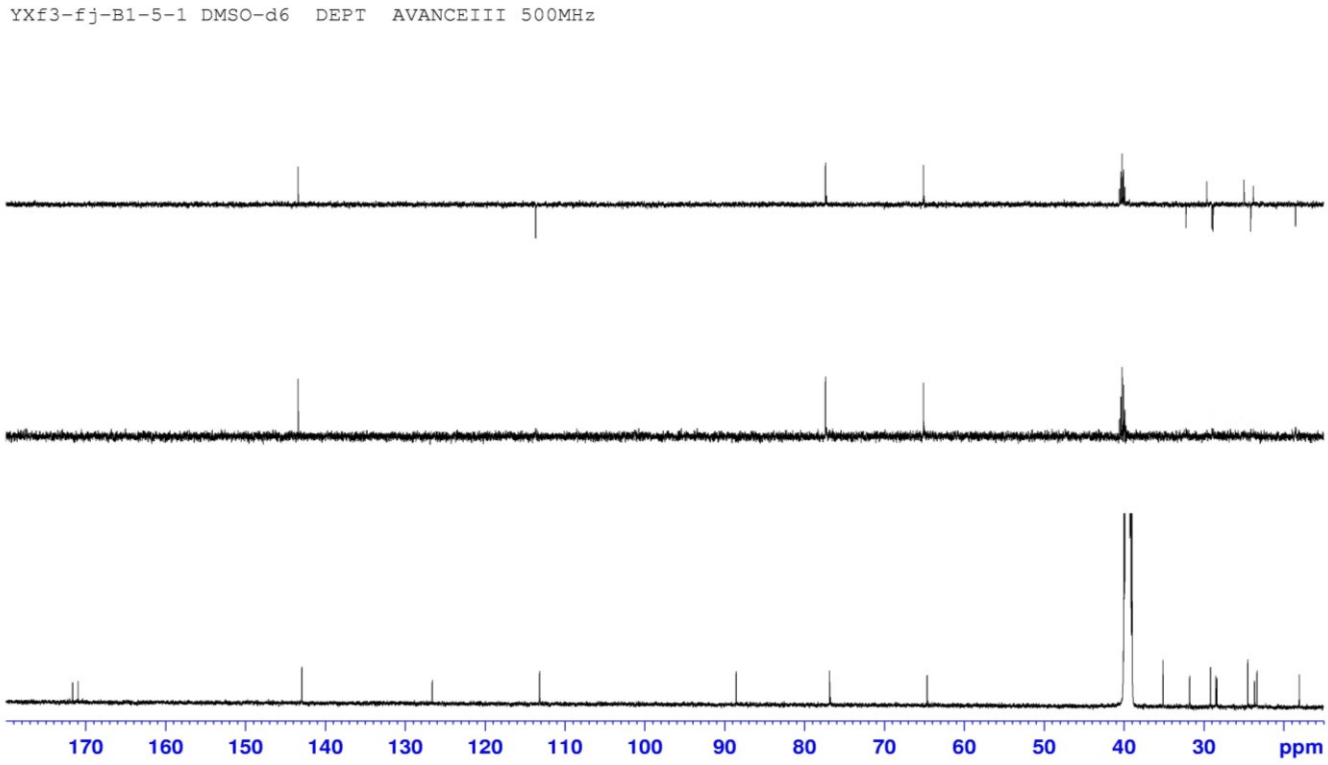


Figure S4. HSQC spectrum of compound **1** in DMSO-d_6

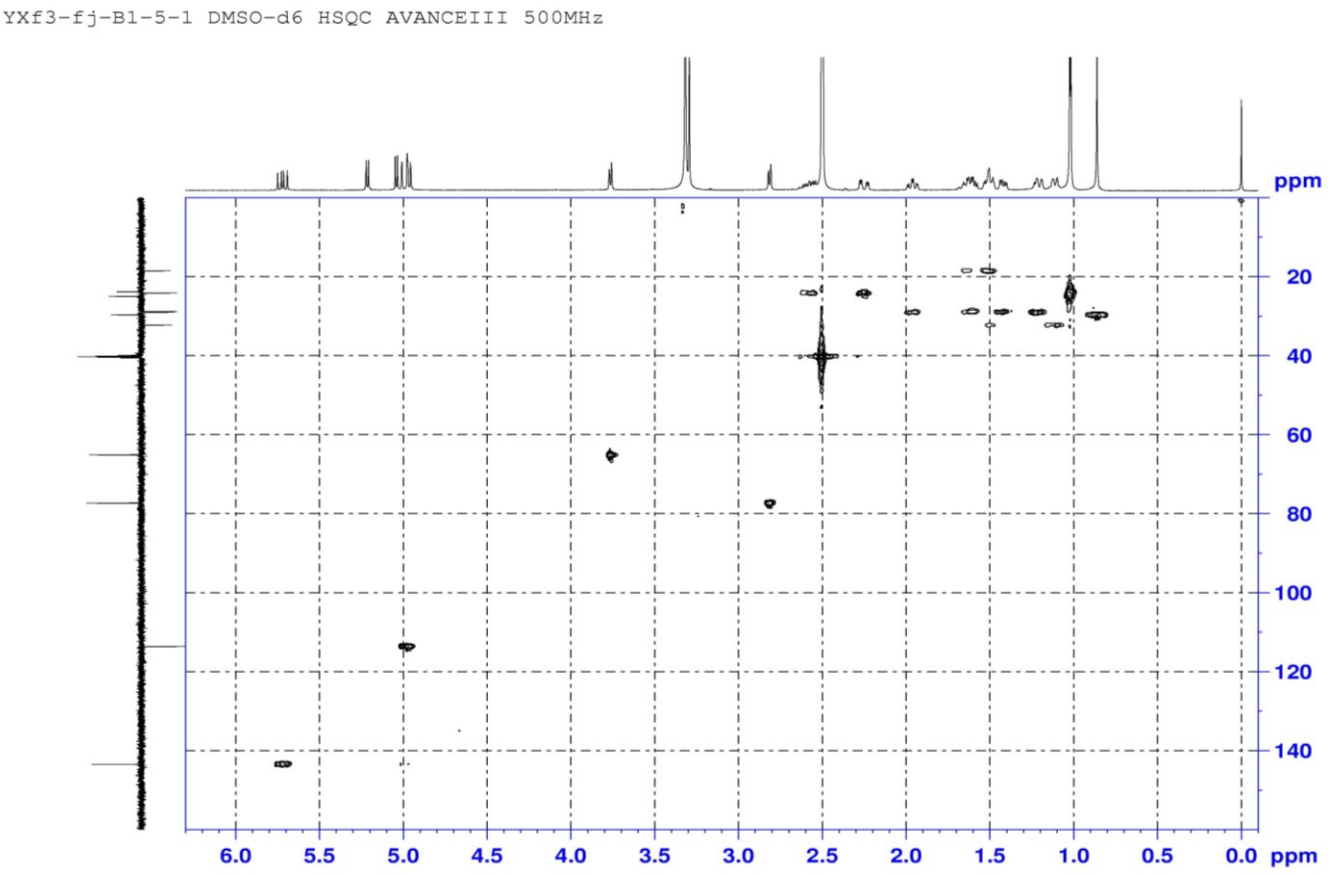


Figure S5. ^{1}H-^{1}H COSY spectrum of compound **1** in DMSO-d_6

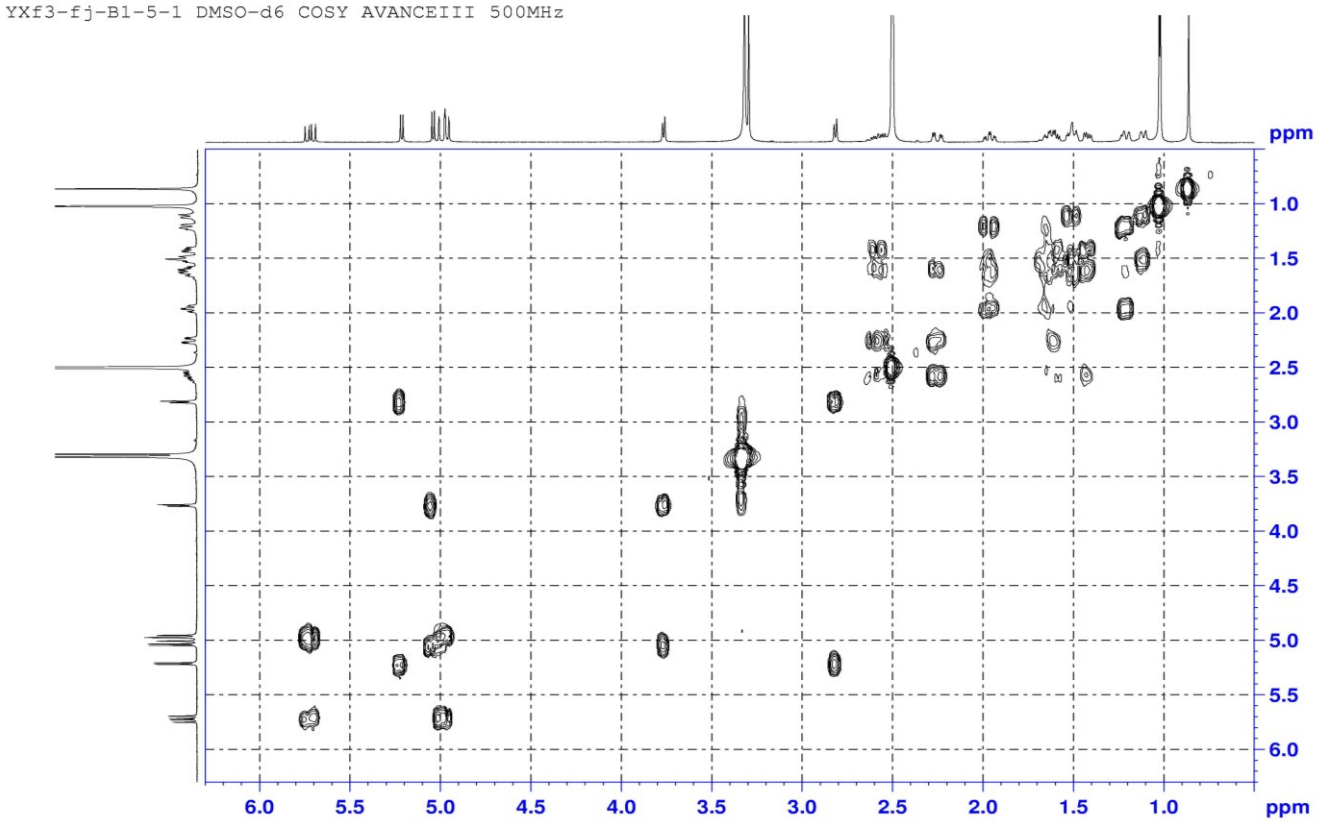


Figure S6. HMBC spectrum of compound **1** in DMSO-d_6

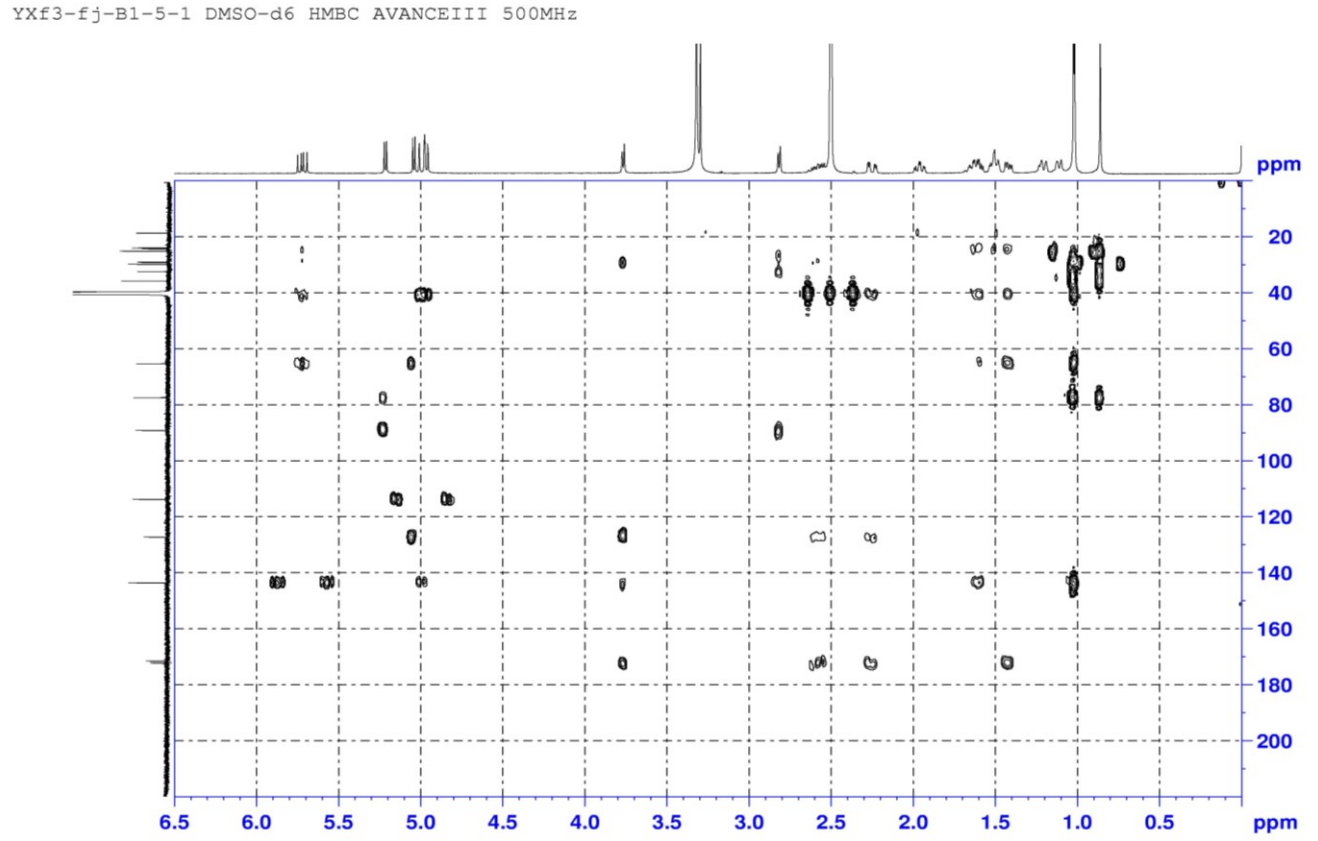


Figure S7. Enlarged HMBC spectrum (δ_C 180-160 ppm, δ_H 6.1-0.6 ppm) of compound **1** in DMSO-d_6

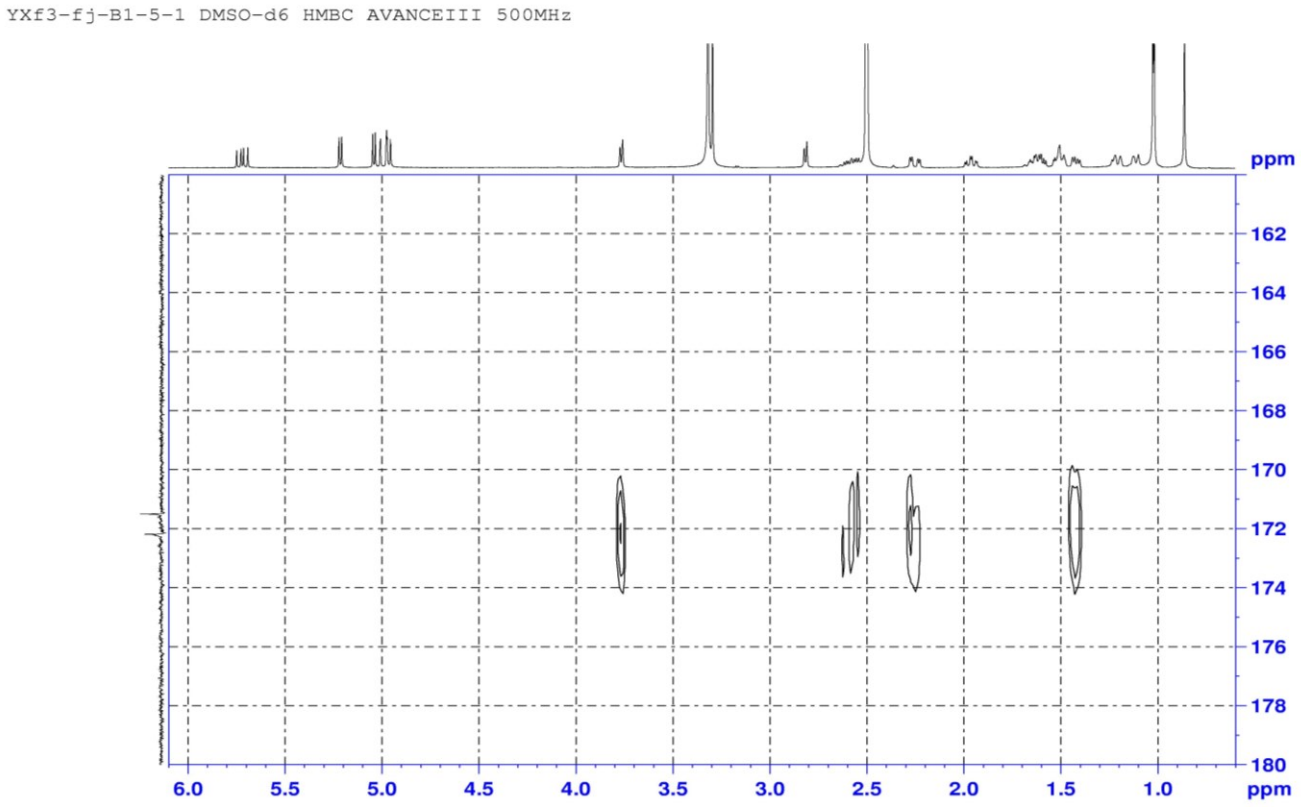


Figure S8. NOESY spectrum of compound **1** in DMSO-d_6

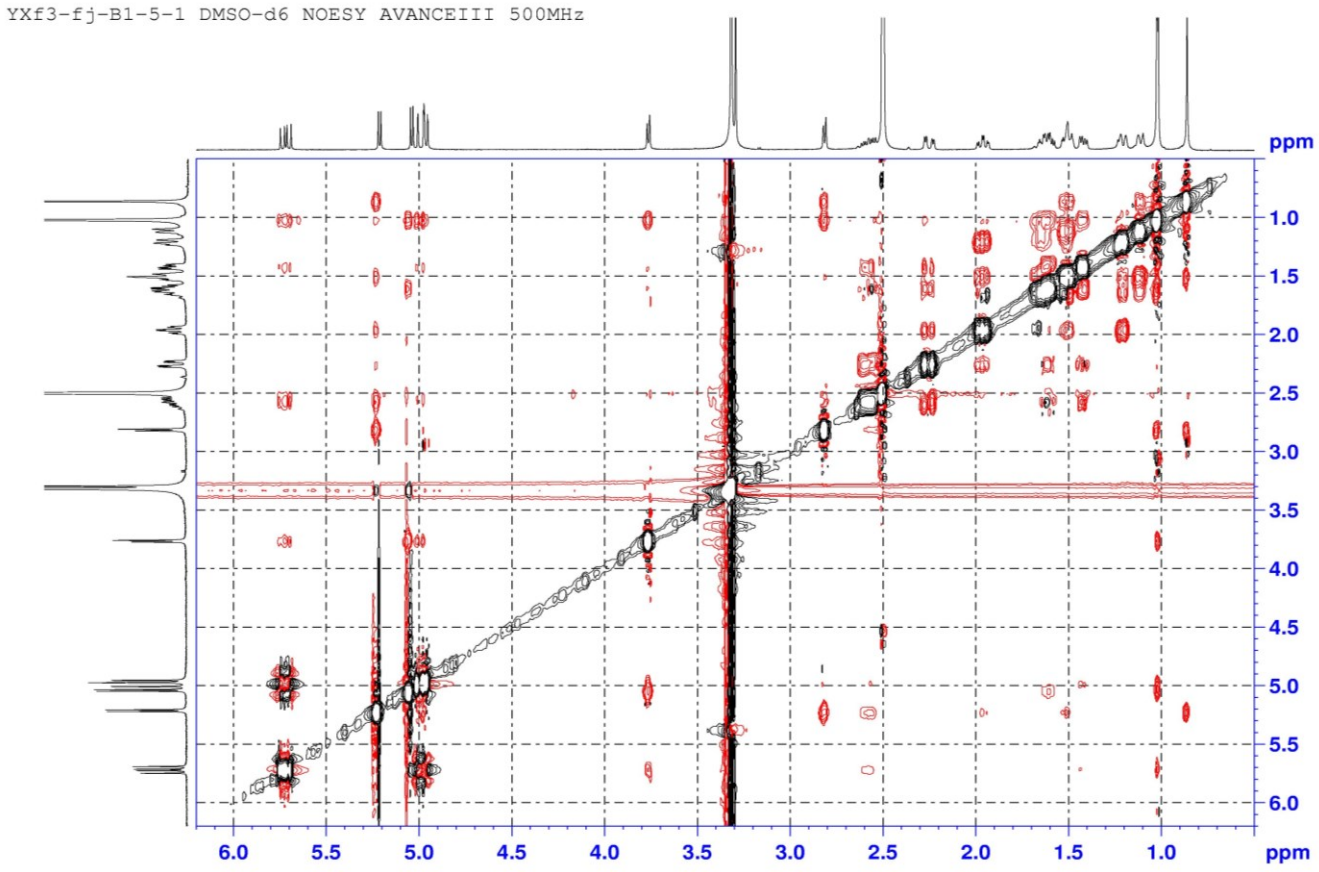


Figure S9. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **1**

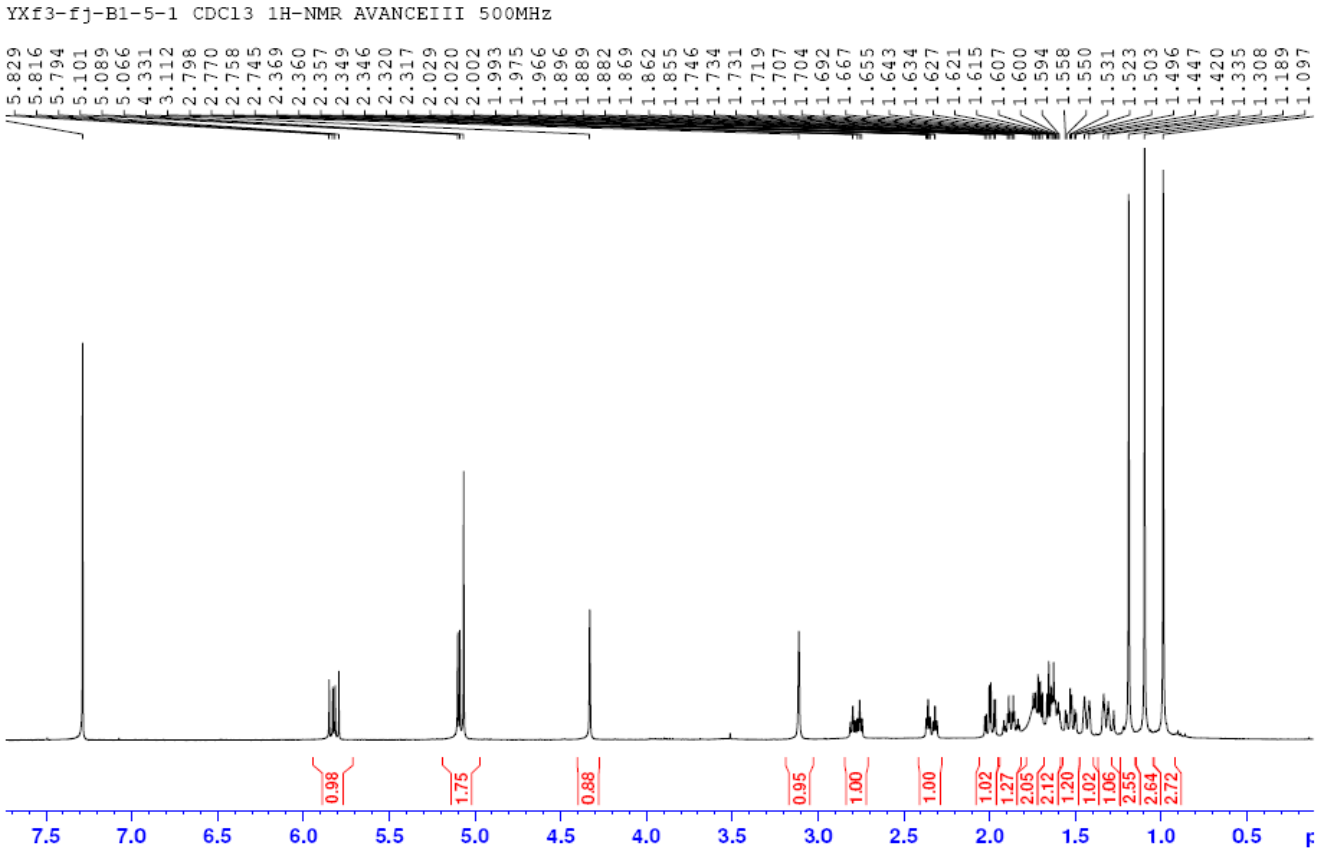


Figure S10. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **1**

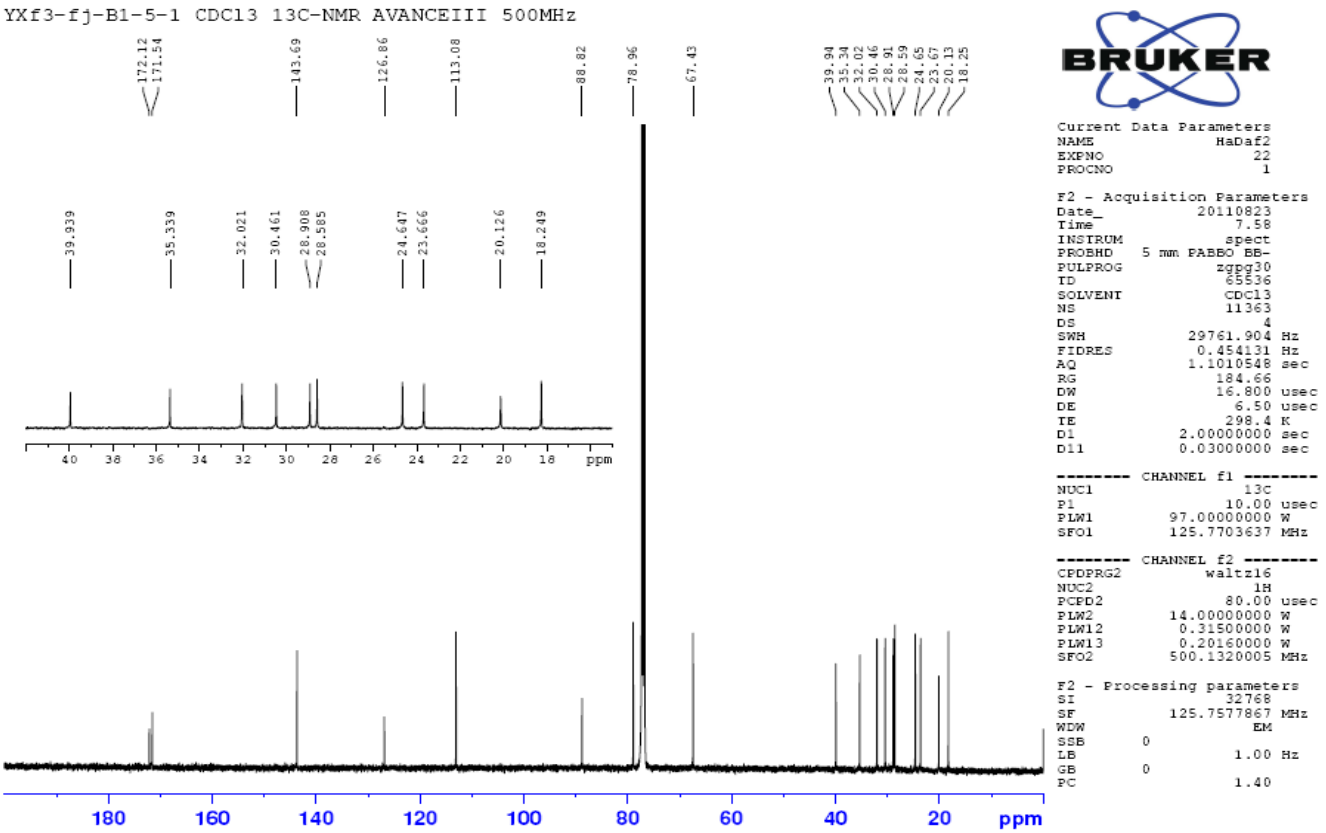


Figure S11. HMQC spectrum of compound **1** in $CDCl_3$

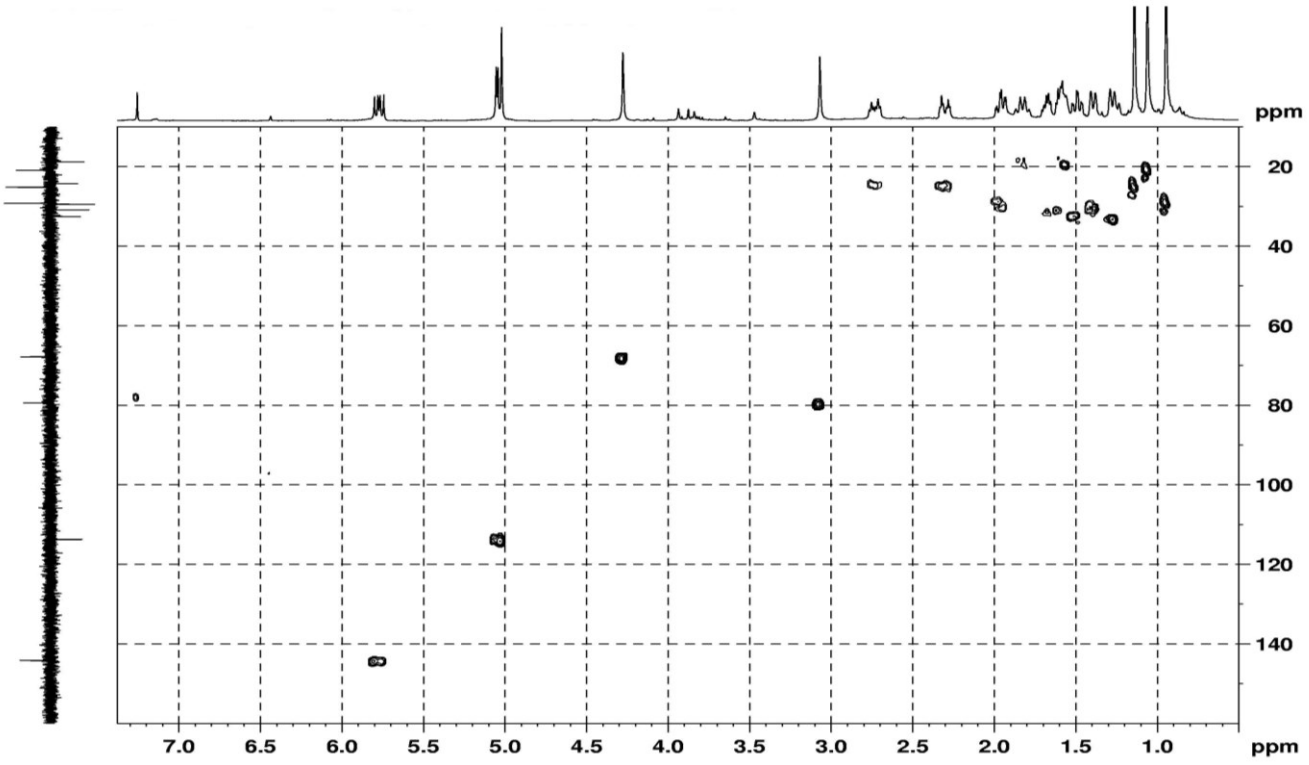


Figure S12. ^{1}H-^{1}H COSY spectrum of compound **1** in $CDCl_3$

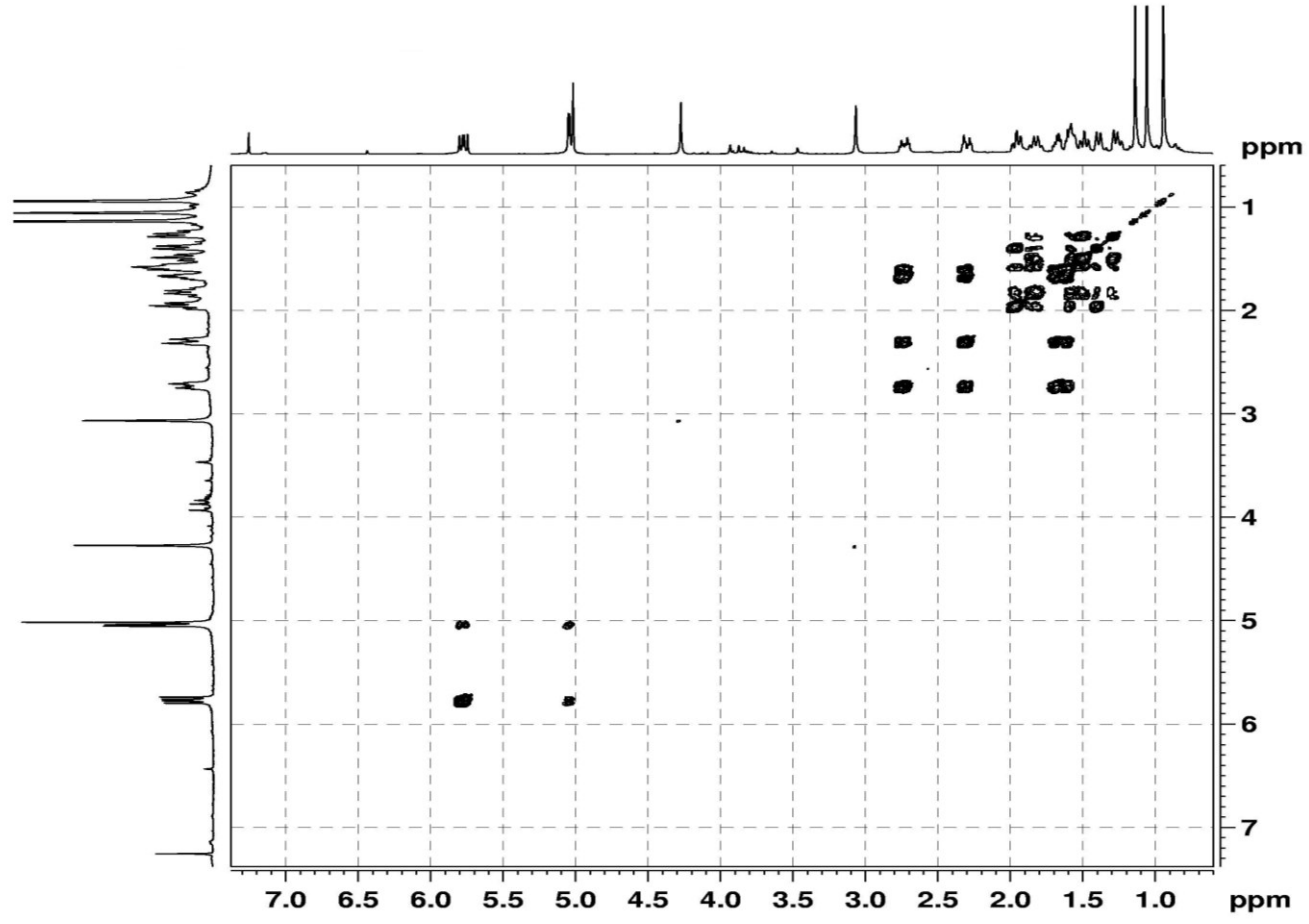


Figure S13. HMBC spectrum of compound **1** in $CDCl_3$

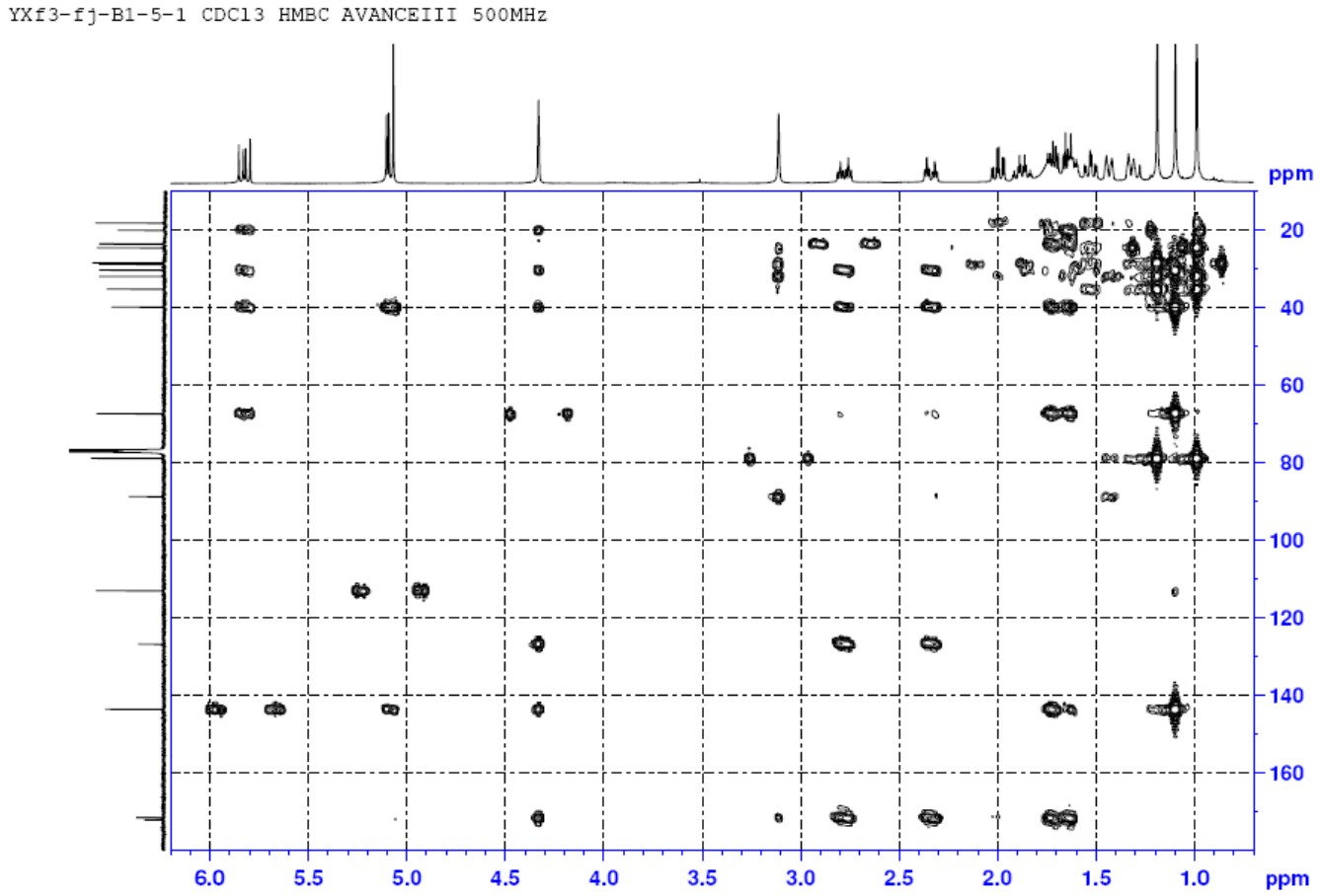


Figure S14. Enlarged HMBC spectrum (δ_C 177-167 ppm, δ_H 5.0-0.9 ppm) of compound **1** in $CDCl_3$

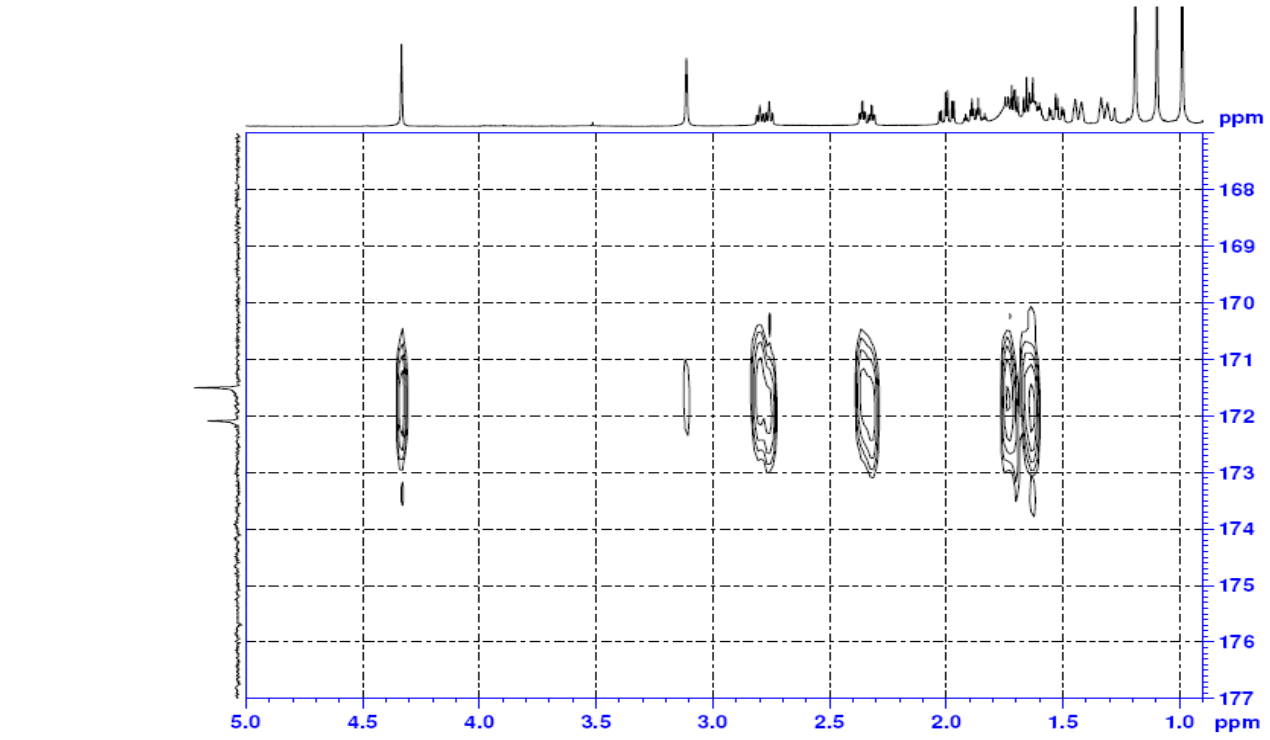


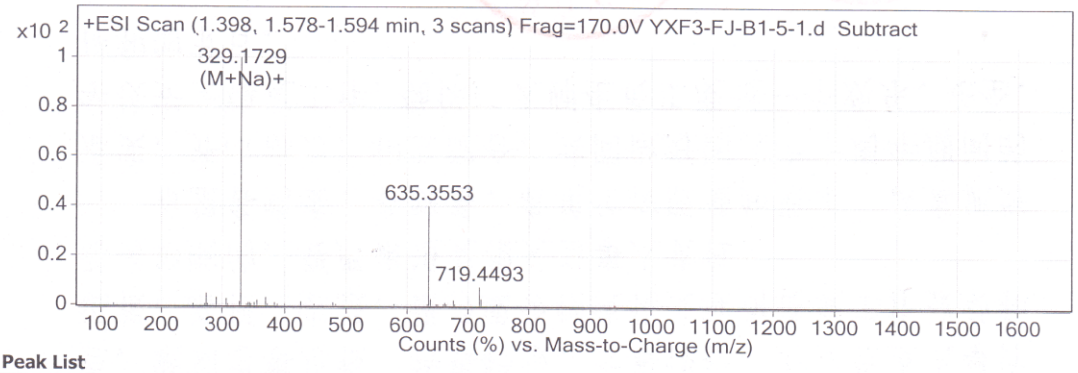
Figure S15. HRESI-MS spectrum of compound **1** in MeOH

Qualitative Analysis Report

Data Filename	YXF3-FJ-B1-5-1.d	**Sample Name**	YXF3-FJ-B1-5-1
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEMP2.m	**Acquired Time**	11/26/2010 3:40:55 PM
IRM Calibration Status	Some Ions Missed	**DA Method**	Default.m
Comment			

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+ TIC Scan"	170	0	Esi



Peak List

m/z	z	Abund	Formula	Ion
329.1729	1	778087	C18 H26 Na O4	(M+Na)+
329.399		51889		
330.1758	1	137615	C18 H26 Na O4	(M+Na)+
635.3553	1	309541		
636.3587	1	109646		
719.4493		57309		

--- End Of Report ---

Calc. (M+H)+ 307.1904

(M+Na)+ 329.1723

Figure S16. ^{1}H NMR (500 MHz, acetone-d_6) of compound **6**

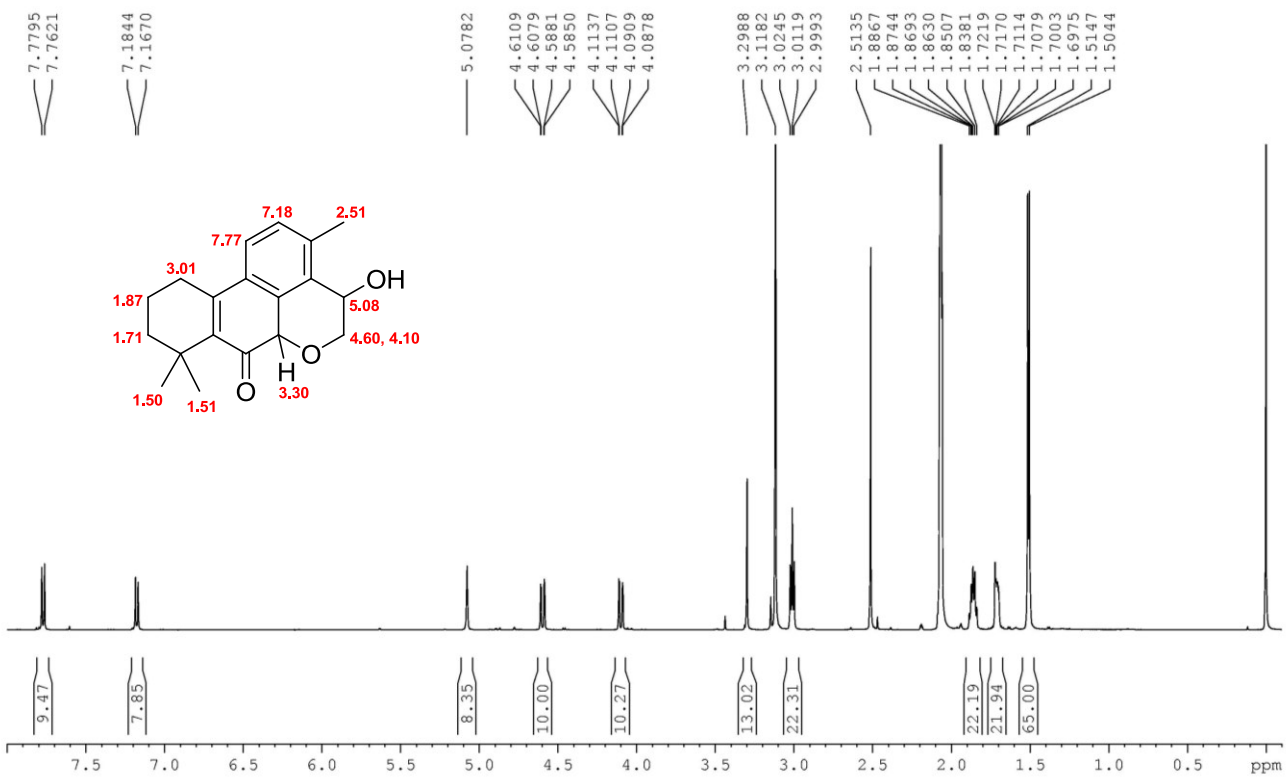


Figure S17. HRESIMS spectrum of compound **6**

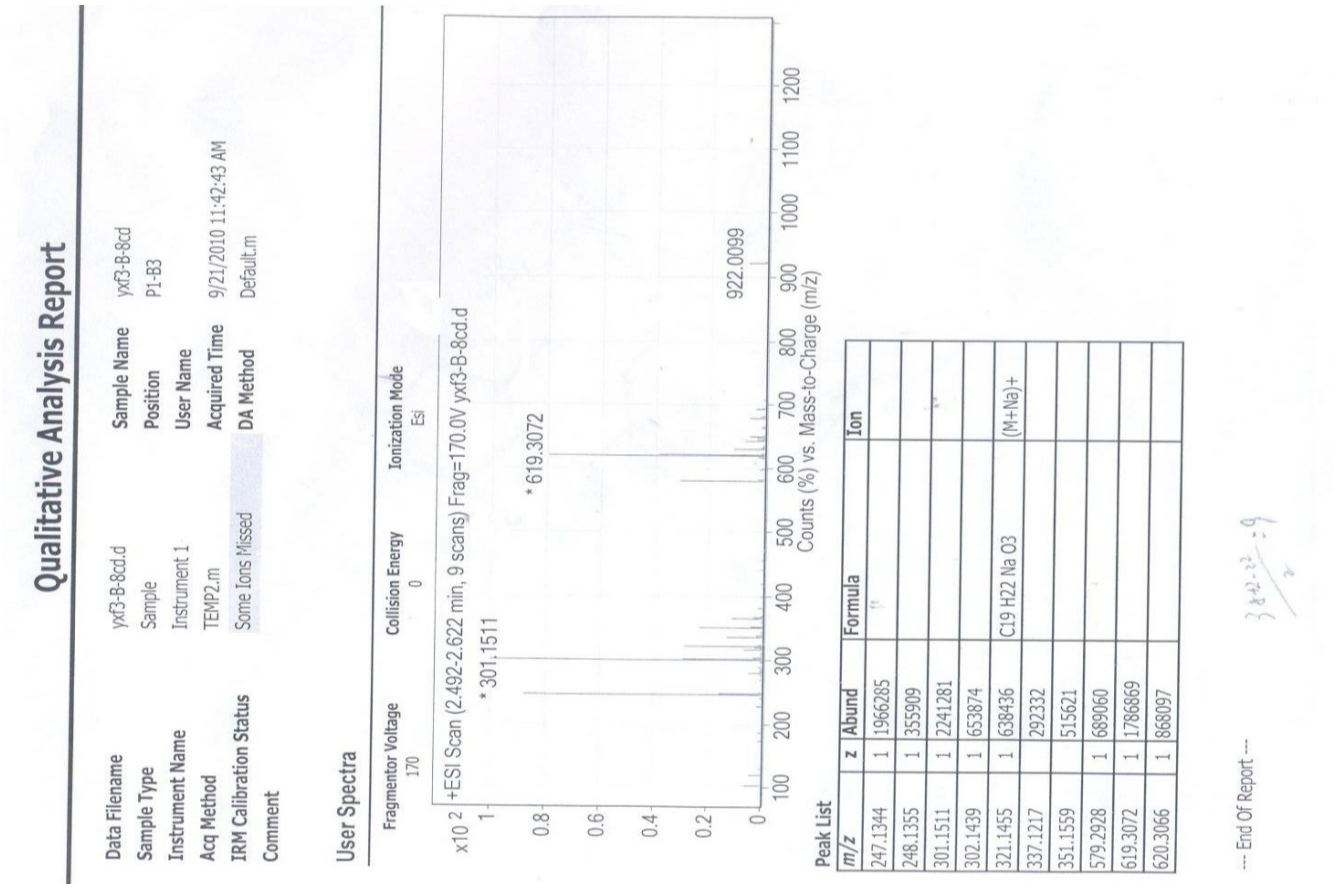


Figure S18. ^{1}H NMR (500 MHz, acetone-d_6) of compound **7**

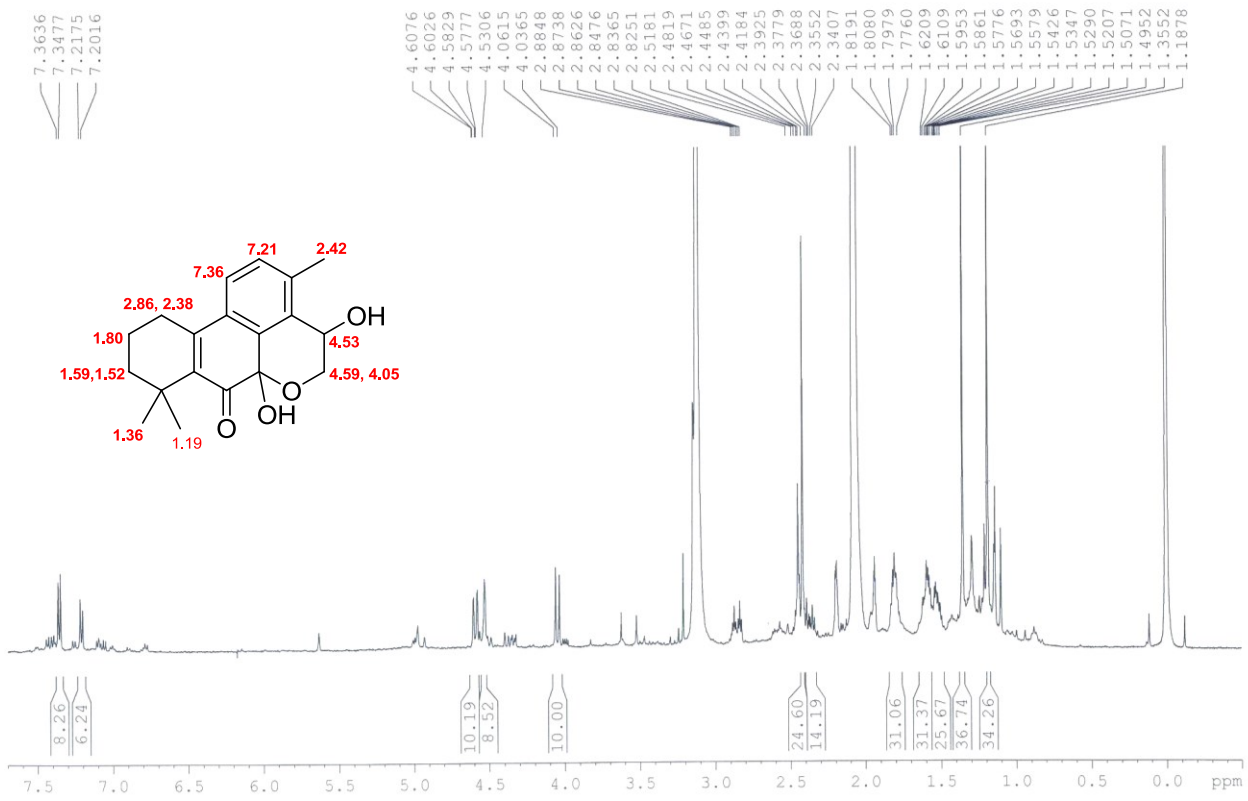


Figure S19. HRESIMS spectrum of compound **7**