

## SUPPORTING INFORMATION

# Quassinoids from Twigs of *Harrisonia Perforata* (Blanco) Merr and Their Anti-Parkinson's Disease Effect

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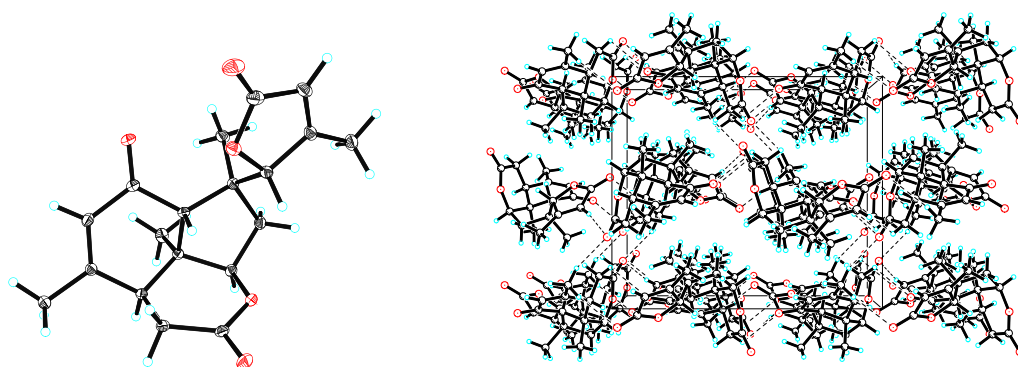
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## X-ray crystallographic data of Perforalactone **7**

Single-crystals of compound **7** was obtained from CH<sub>3</sub>OH/H<sub>2</sub>O (10:1) at room temperature.

Crystal data for compound **7**: C<sub>19</sub>H<sub>22</sub>O<sub>5</sub>, M = 330.36, a = 9.5789(4) Å, b = 12.0883(5) Å, c = 14.0568(6) Å,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ , V = 1627.67(12) Å<sup>3</sup>, T = 150.(2) K, space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, Z = 4,  $\mu(\text{Cu K}\alpha) = 0.797 \text{ mm}^{-1}$ , 13248 reflections measured, 3082 independent reflections (R<sub>int</sub> = 0.0639). The final R1 values were 0.0298 (I > 2 $\sigma$ (I)). The final wR(F2) values were 0.0751 (I > 2 $\sigma$ (I)). The final R1 values were 0.0322 (all data). The final wR(F2) values were 0.0763 (all data). The goodness of fit on F2 was 1.036. Flack parameter = 0.04(8).



Single-crystal X-ray structure of **7**

**Table S1. Crystal data and structure refinement for **7**.**

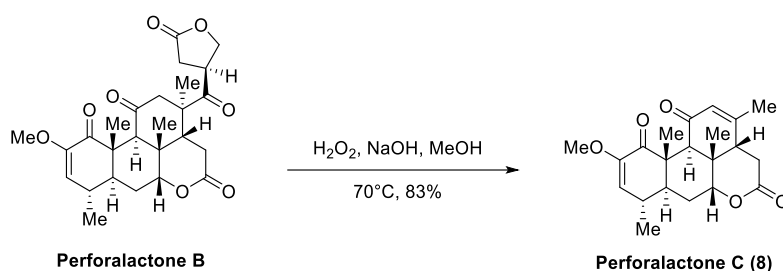
Identification code	global
Empirical formula	C <sub>19</sub> H <sub>22</sub> O <sub>5</sub>
Formula weight	330.36
Temperature	150(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>

Unit cell dimensions	a = 9.5789(4) Å b = 12.0883(5) Å c = 14.0568(6) Å	a = 90°. b = 90°. g = 90°.
Volume	1627.67(12) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.348 Mg/m <sup>3</sup>	
Absorption coefficient	0.797 mm <sup>-1</sup>	
F(000)	704	
Crystal size	0.630 x 0.400 x 0.020 mm <sup>3</sup>	
Theta range for data collection	4.83 to 70.22°.	
Index ranges	-11<=h<=11, -14<=k<=14, -17<=l<=15	
Reflections collected	13248	
Independent reflections	3082 [R(int) = 0.0639]	
Completeness to theta = 70.22°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.98 and 0.70	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3082 / 0 / 221	
Goodness-of-fit on F <sup>2</sup>	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0298, wR2 = 0.0751	
R indices (all data)	R1 = 0.0322, wR2 = 0.0763	
Absolute structure parameter	0.04(8)	
Largest diff. peak and hole	0.209 and -0.158 e.Å <sup>-3</sup>	

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### Chemical transformation.

Compound **8** was obtained by oxidative conversion of natural product Perforalactone B via Bayer-Weilig.

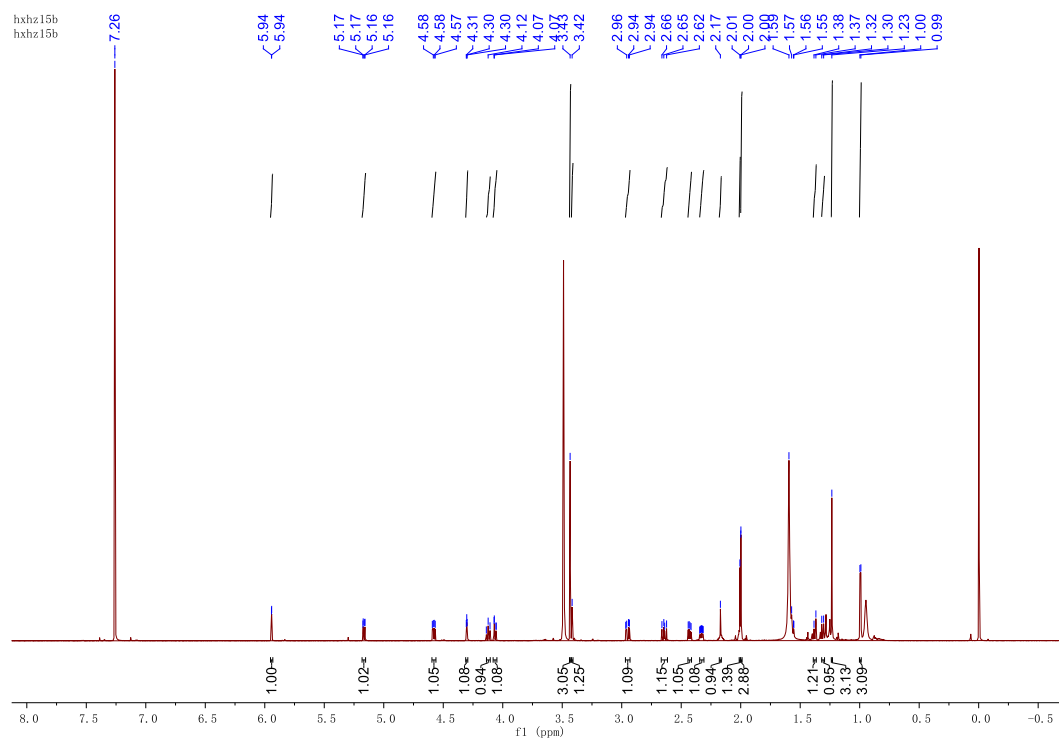


Yield 83%. To a solution of Perforalactone B (1) (20 mg, 42.32  $\mu\text{mol}$ ) in Chromatographic methanol was (20 ml) added  $\text{H}_2\text{O}_2$ (30%, 10 mml, 95.65  $\mu\text{mol}$ ) at that temperature, After being warmed to 60°C,  $\text{NaOH(aq)}$  (2.50 mol/L, 136  $\mu\text{ml}$ , 36.40  $\mu\text{mol}$ ) was added. After stirring for 30 min at 70 °C, the reaction mixture was quenched with sat.  $\text{Na}_2\text{S}_2\text{O}_4$ , and extracted with EtOAc. The organic phase was washed with brine, dried over  $\text{Na}_2\text{SO}_4$  filtered, and evaporated to dryness *in vacuo*. The crude product was purified by silica gel column chromatography to afford Compound **8**.

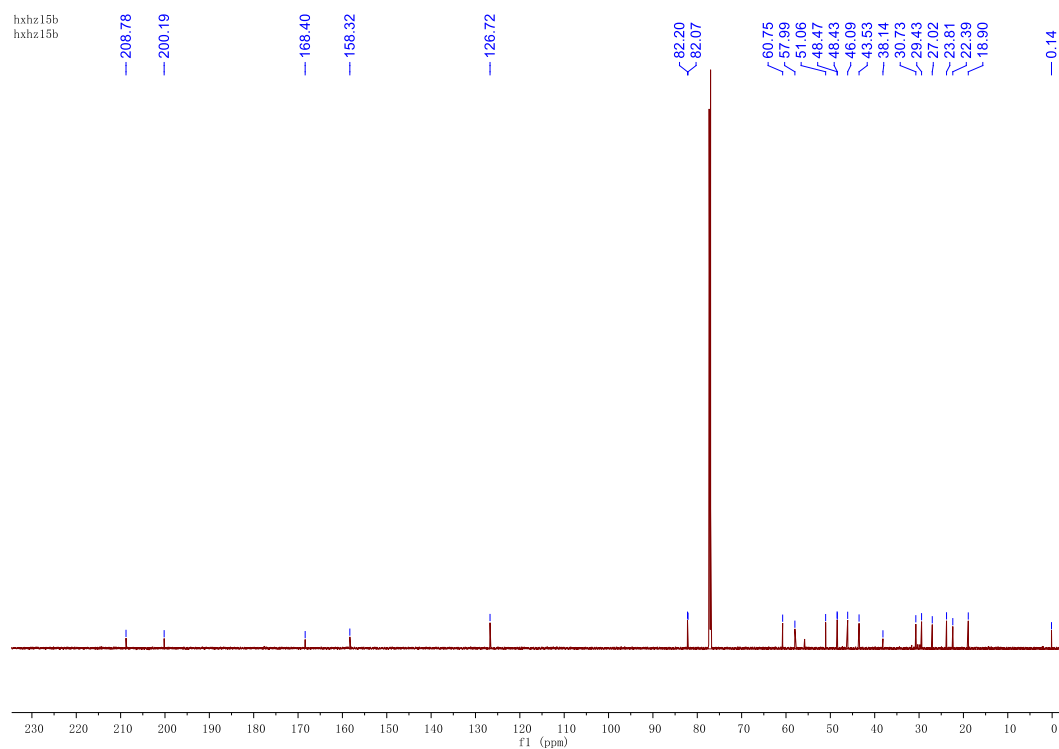
Of course, a number of reaction conditions were screened in order to successfully realize this chemical transformation.

**Table S2. reaction condition of Chemical transformation.**

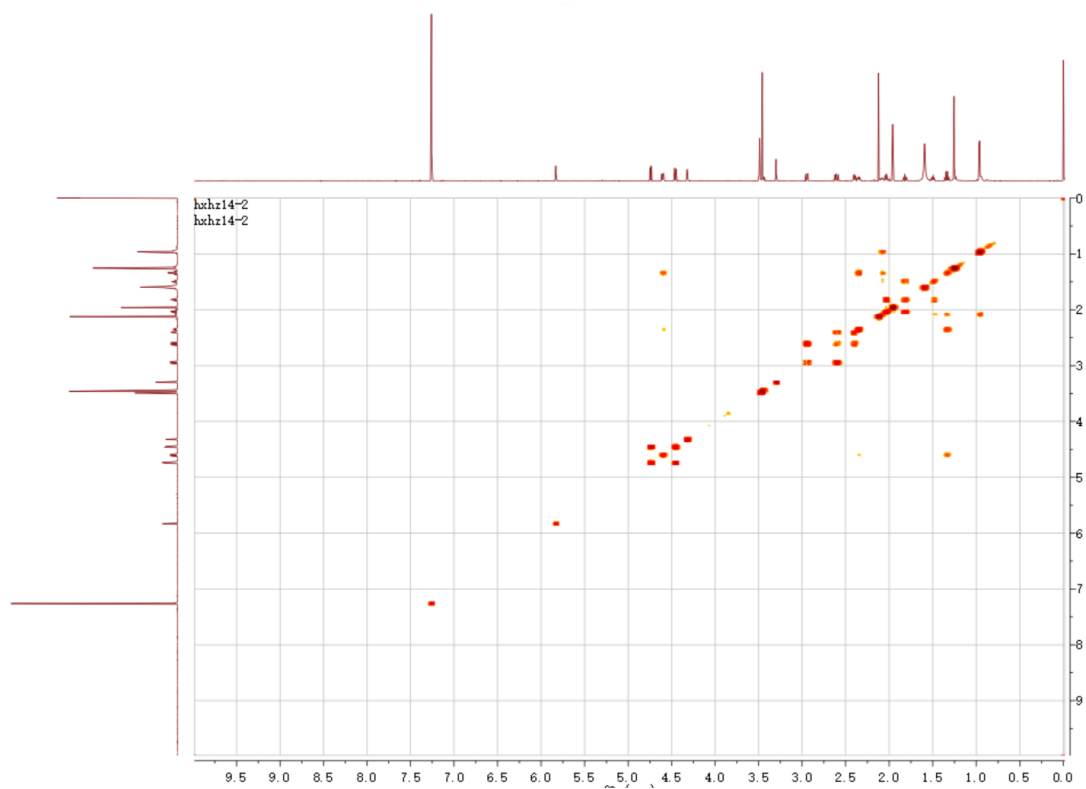
Entry	reagent/equiv	temp	yield
1	$\text{K}_2\text{CO}_3$ /1 equiv	r.t.	no rxn
2	$\text{K}_2\text{CO}_3$ /over equiv	r.t.	no rxn
3	$\text{K}_2\text{CO}_3$ /1 equiv	50°C	no rxn
4	$\text{K}_2\text{CO}_3$ , $\text{O}_2$ /1 equiv	r.t.	no rxn
5	$\text{NaOH}$ /1 equiv	r.t.	no rxn
6	$\text{K}_2\text{CO}_3$ /1 equiv+3-Chlorobenzoic acid/1equiv	r.t.	no rxn
7	$\text{NaOH}$ /0.86 equiv+ $\text{H}_2\text{O}_2$ /2.5	70 °C	no rxn



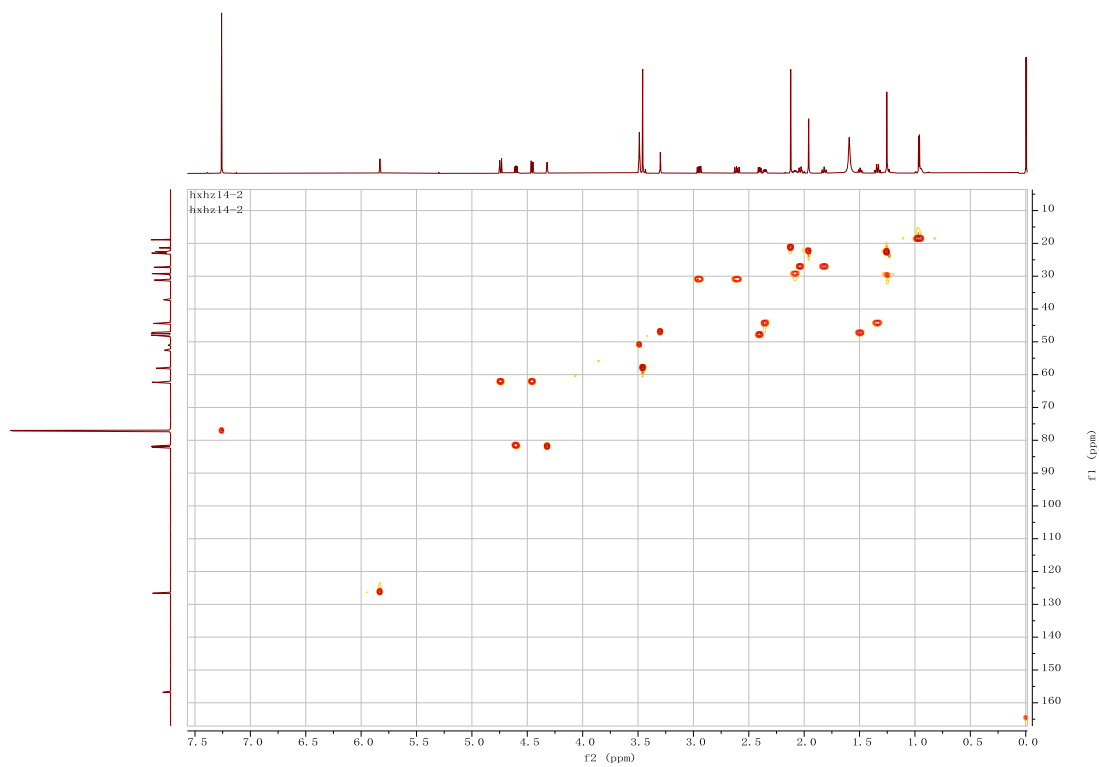
**Figure S1.  $^1\text{H}$  NMR spectrum of Perforalactone F (1) in  $\text{CDCl}_3$ .**



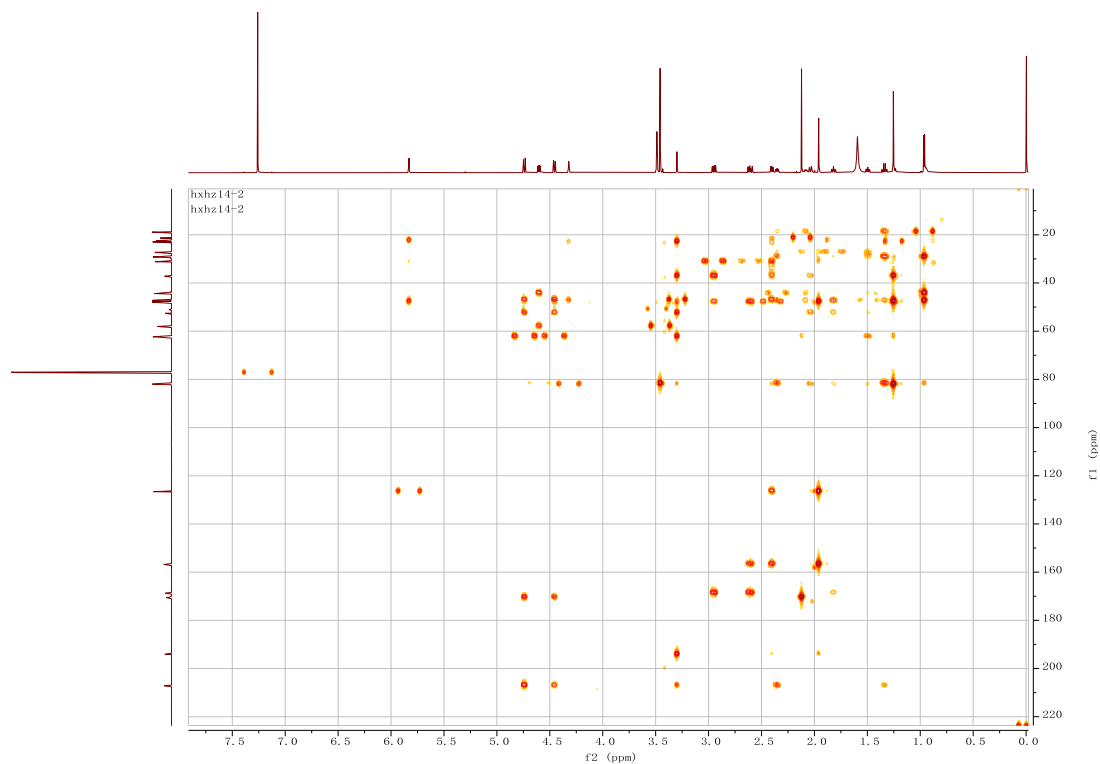
**Figure S2.  $^{13}\text{C}$  NMR spectrum of Perforalactone F (1) in  $\text{CDCl}_3$ .**



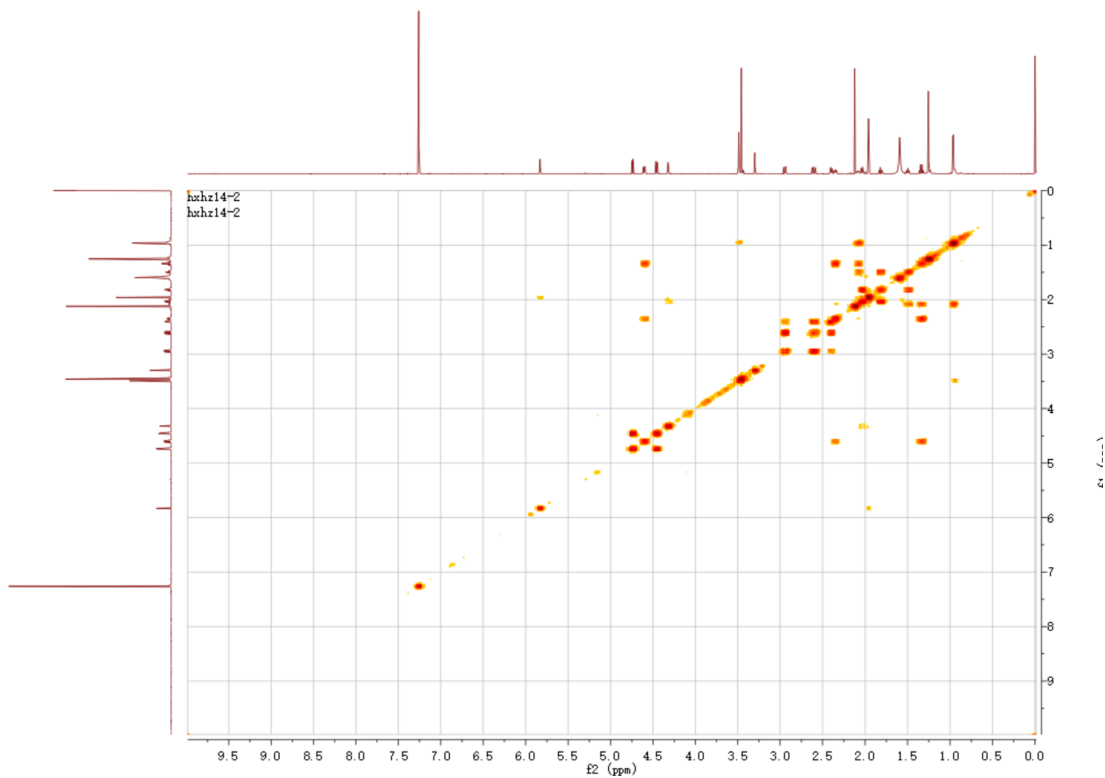
**Figure S3.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Perforalactone F (1) in  $\text{CDCl}_3$



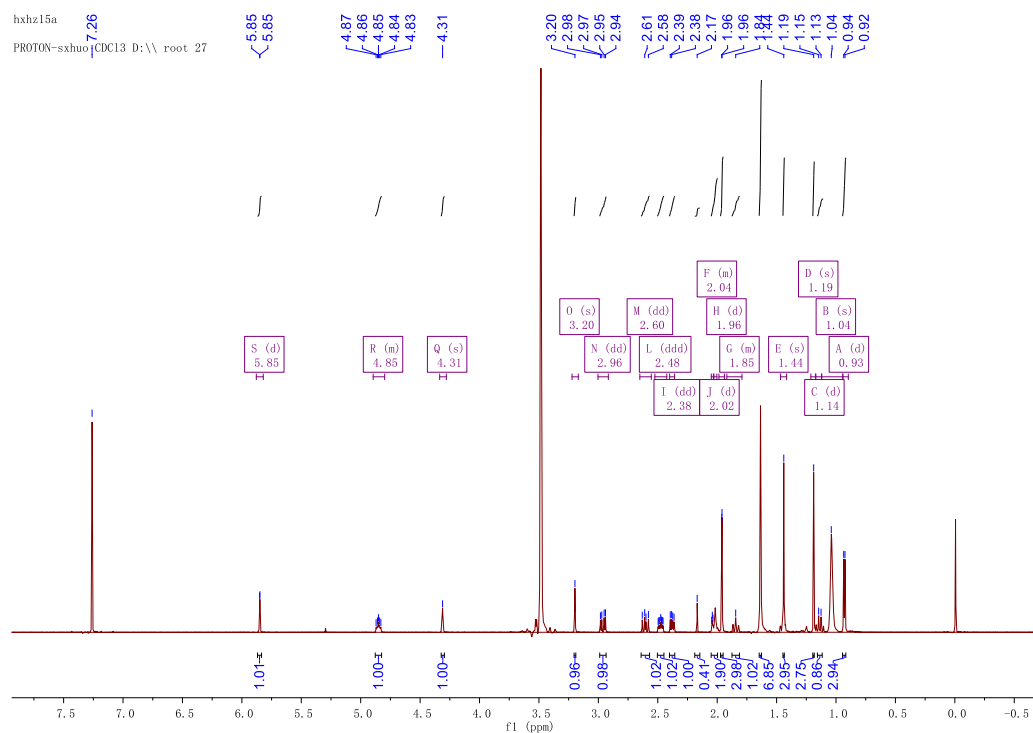
**Figure S4.** HSQC spectrum of Perforalactone F (1) in  $\text{CDCl}_3$ .



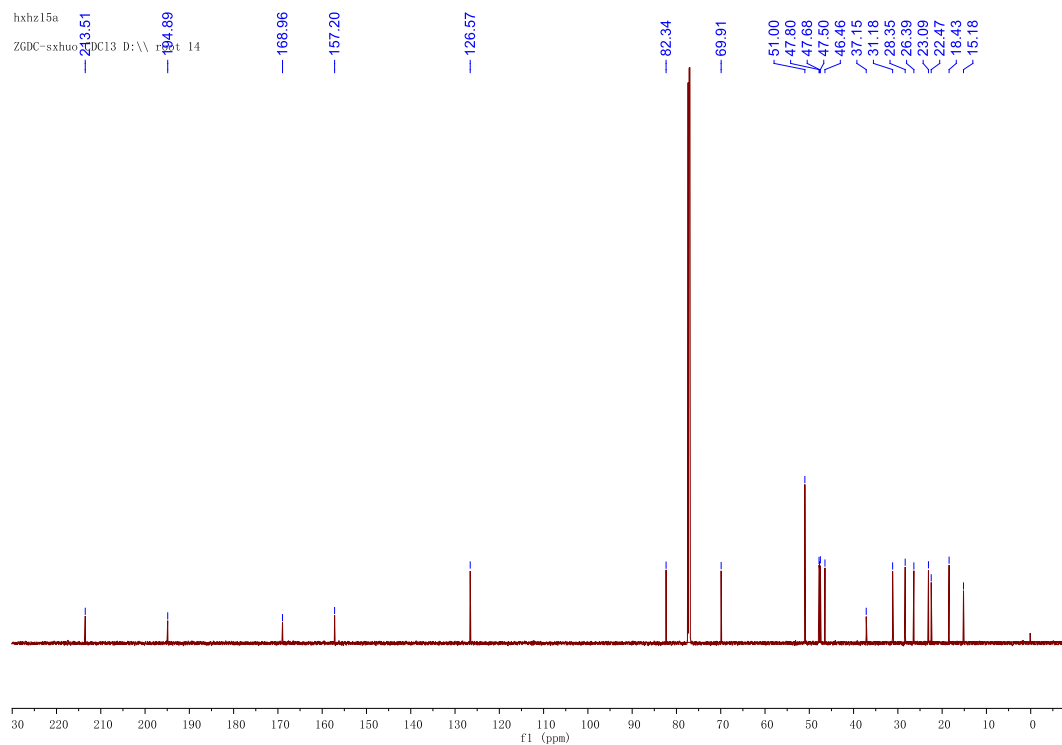
**Figure S5. HMBC spectrum of Perforalactone F (1) in CDCl<sub>3</sub>.**



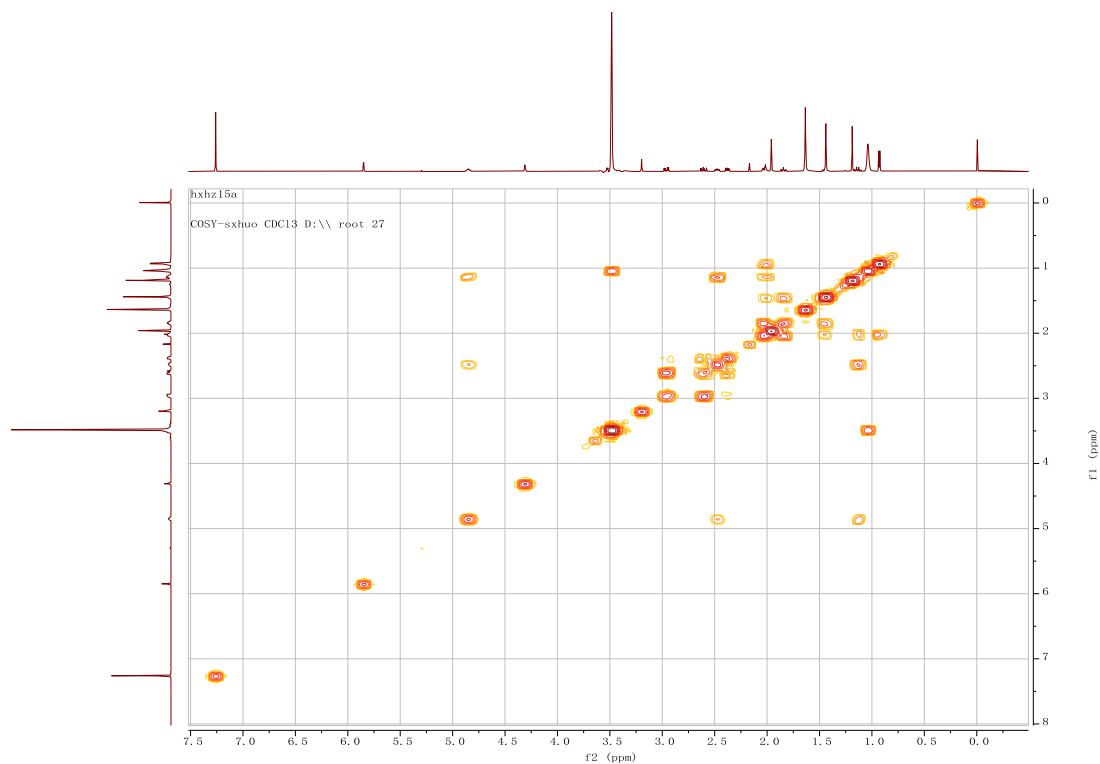
**Figure S6. ROESY spectrum of Perforalactone F (1) in CDCl<sub>3</sub>.**



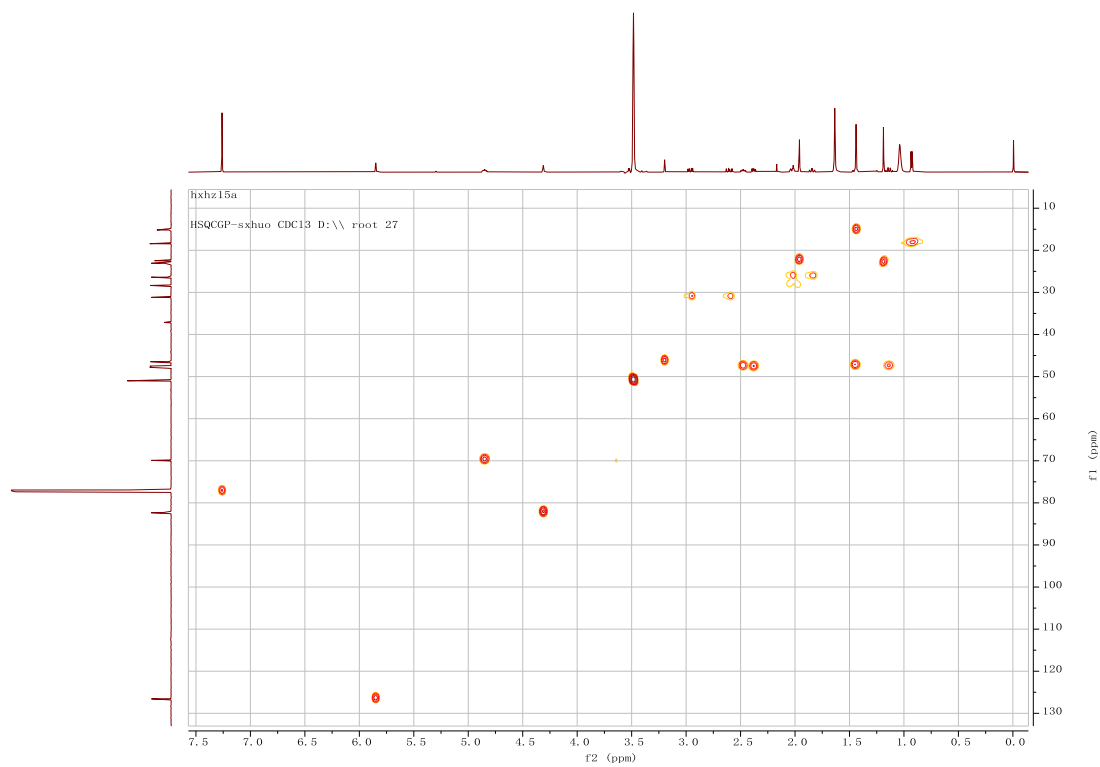
**Figure S7.  $^1\text{H}$  NMR spectrum of Perforalactone G (2) in  $\text{CDCl}_3$ .**



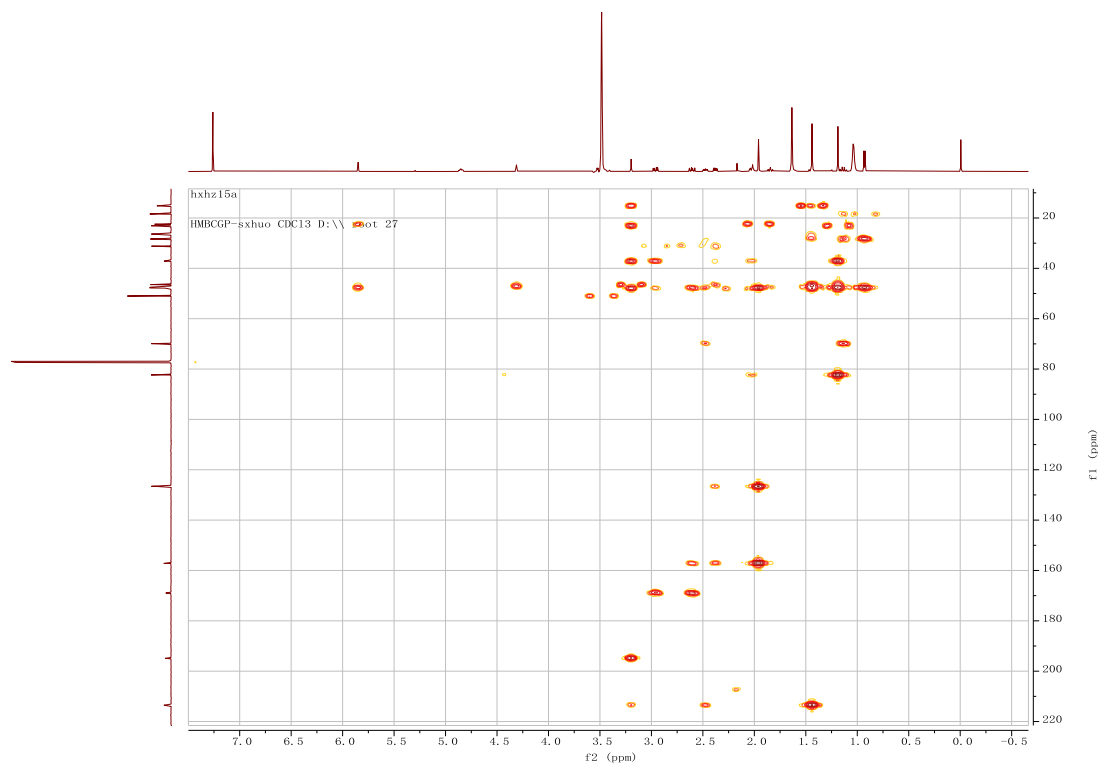
**Figure S8.  $^{13}\text{C}$  NMR spectrum of Perforalactone G (2) in  $\text{CDCl}_3$ .**



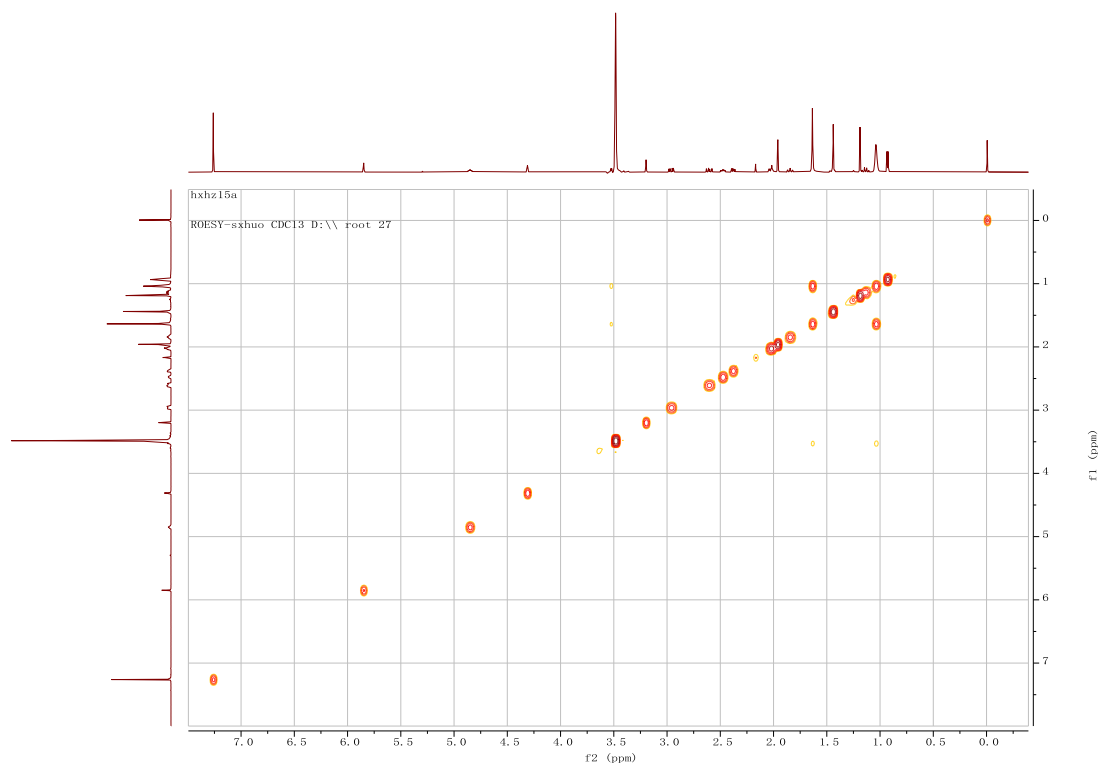
**Figure S9.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Perforalactone G (2) in  $\text{CDCl}_3$ .



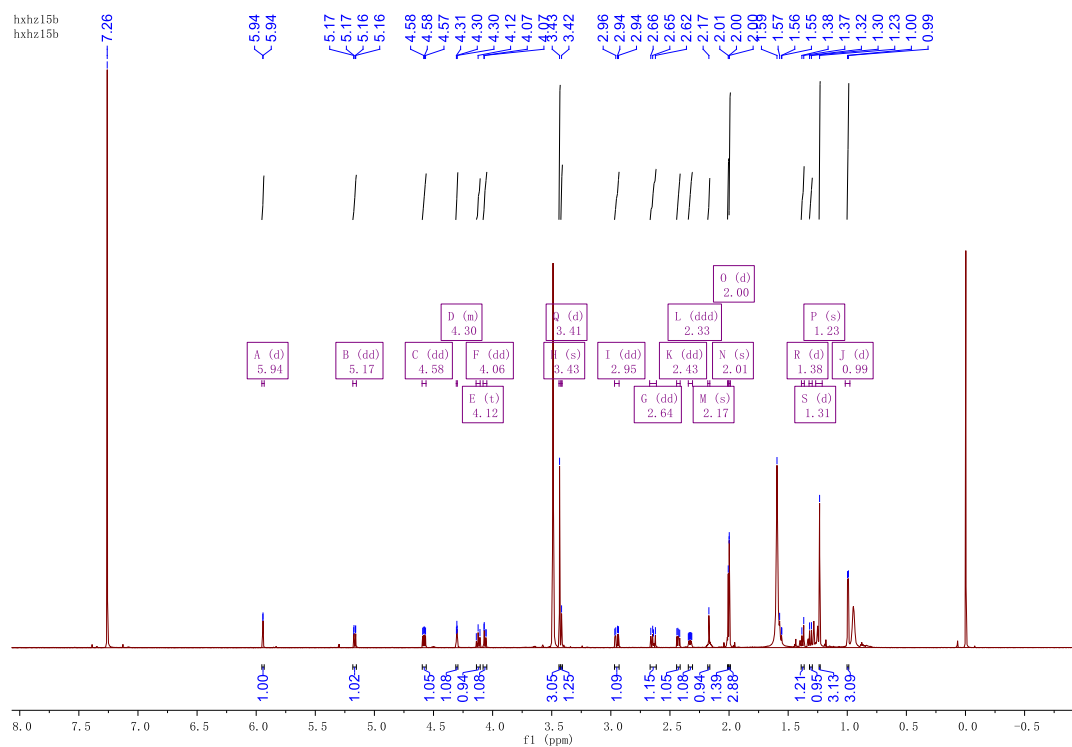
**Figure S10.** HSQC spectrum of Perforalactone G (2) in  $\text{CDCl}_3$ .



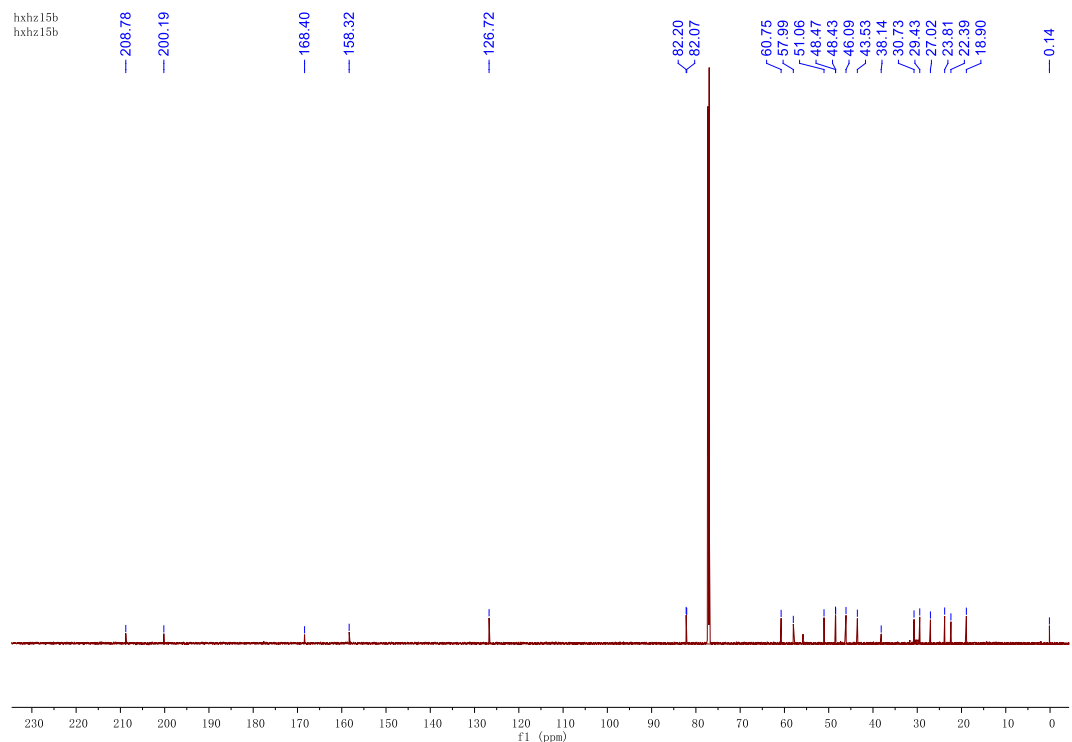
**Figure S11. HMBC spectrum of Perforalactone G (2) in CDCl<sub>3</sub>.**



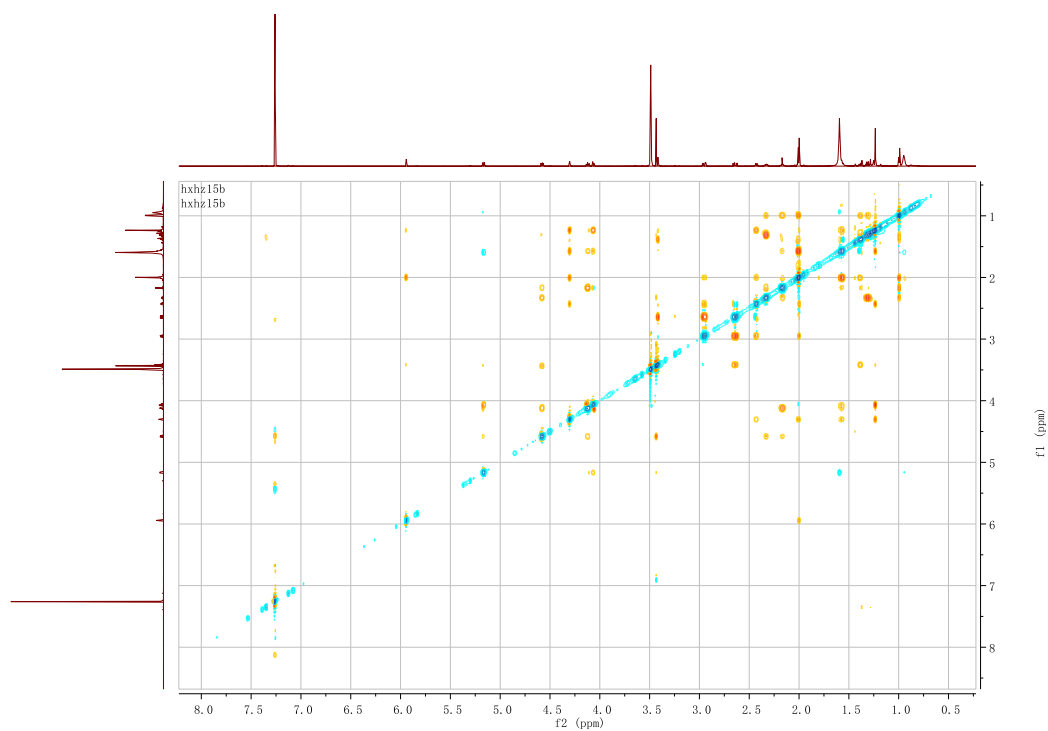
**Figure S12. ROESY spectrum of Perforalactone G (2) in CDCl<sub>3</sub>.**



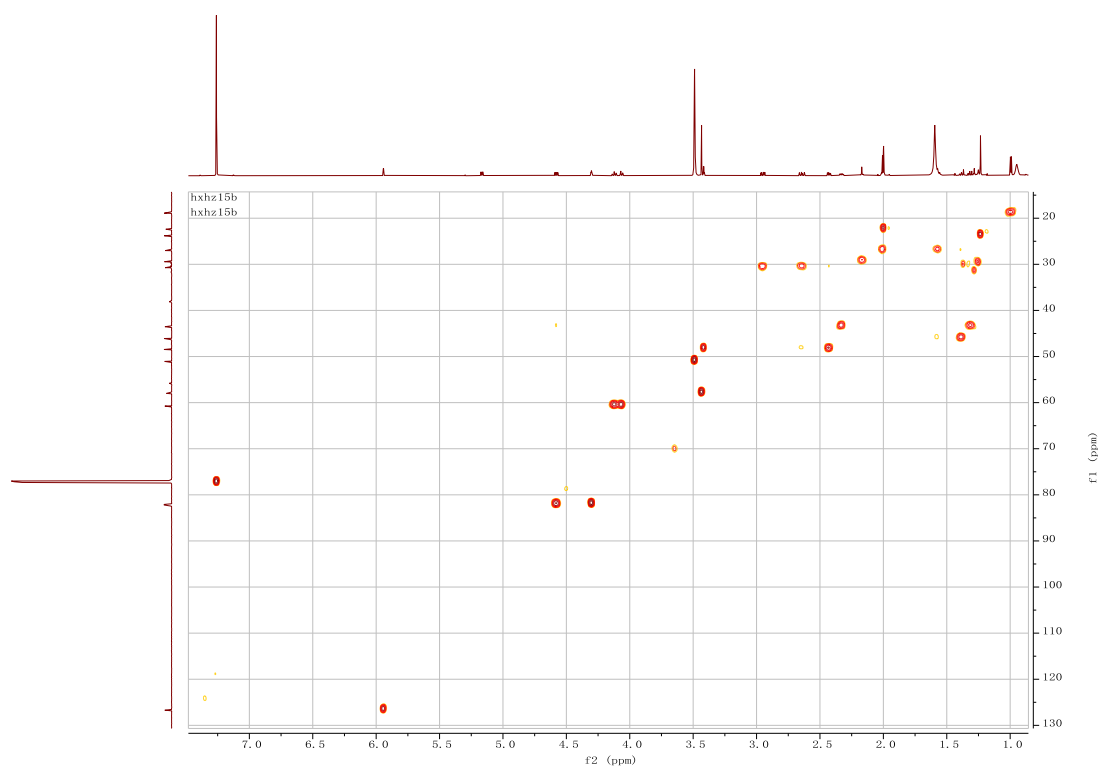
**Figure S13.  $^1\text{H}$  NMR spectrum of Perforalactone H (3) in  $\text{CDCl}_3$ .**



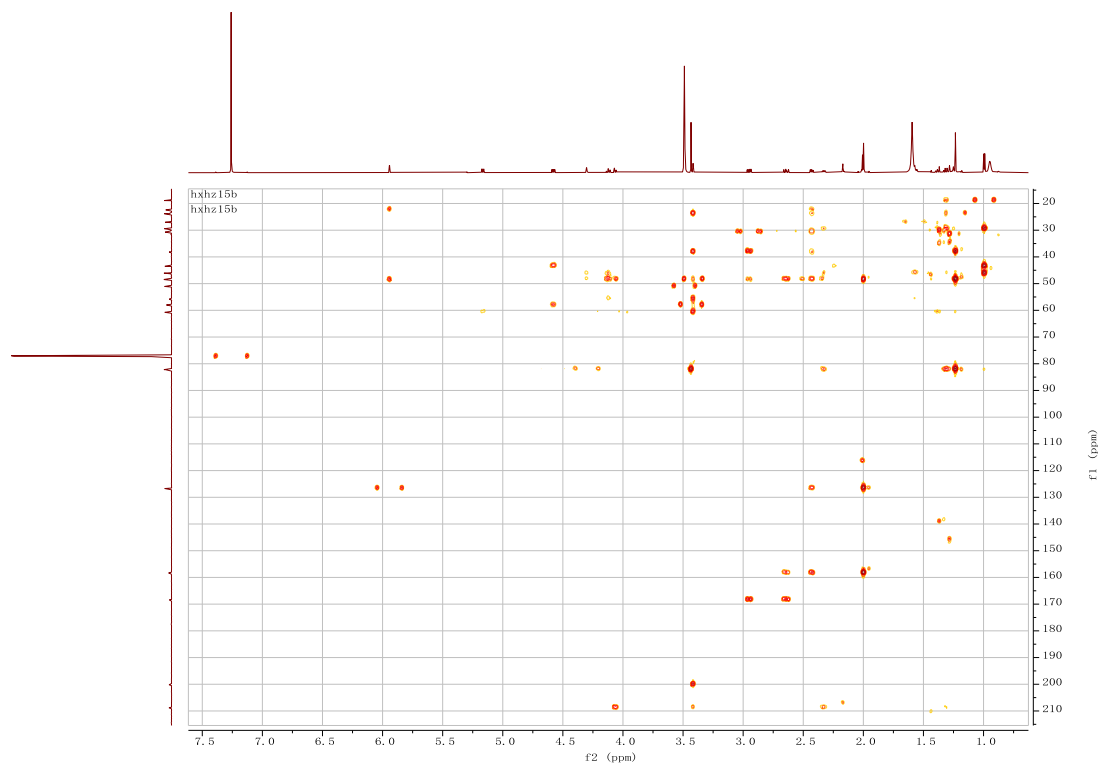
**Figure S14.  $^{13}\text{C}$  NMR spectrum of Perforalactone H (3) in  $\text{CDCl}_3$ .**



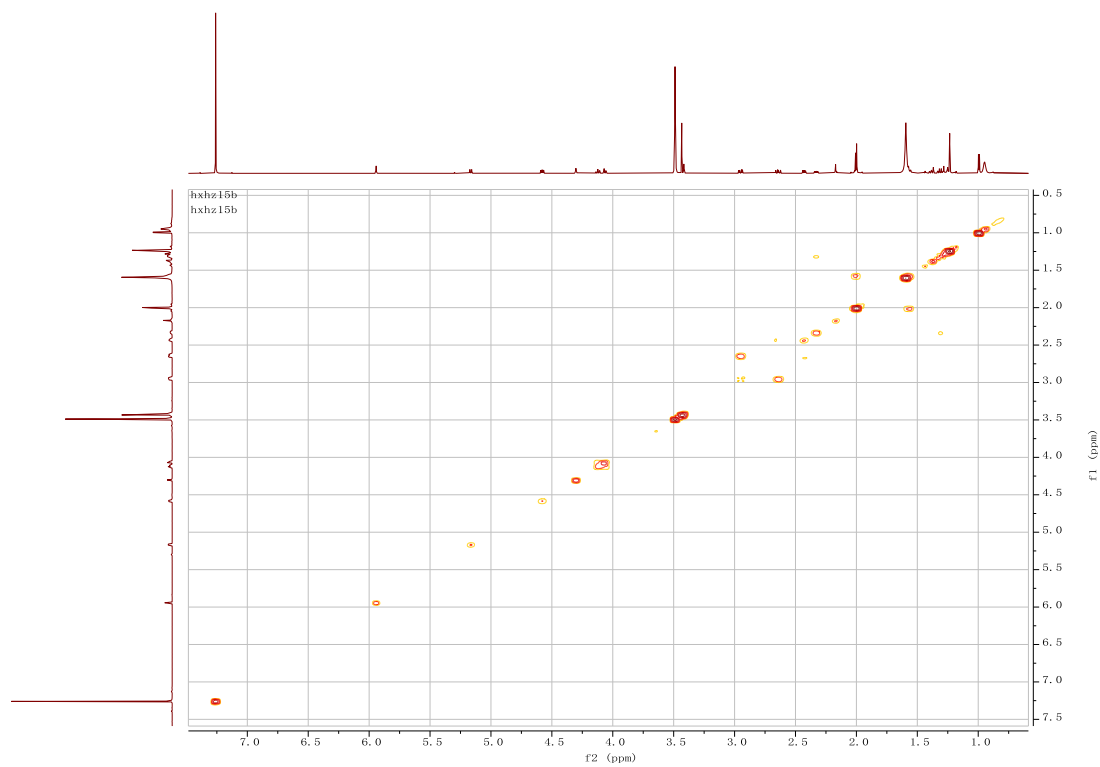
**Figure S15.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Perforalactone H (3) in  $\text{CDCl}_3$ .**



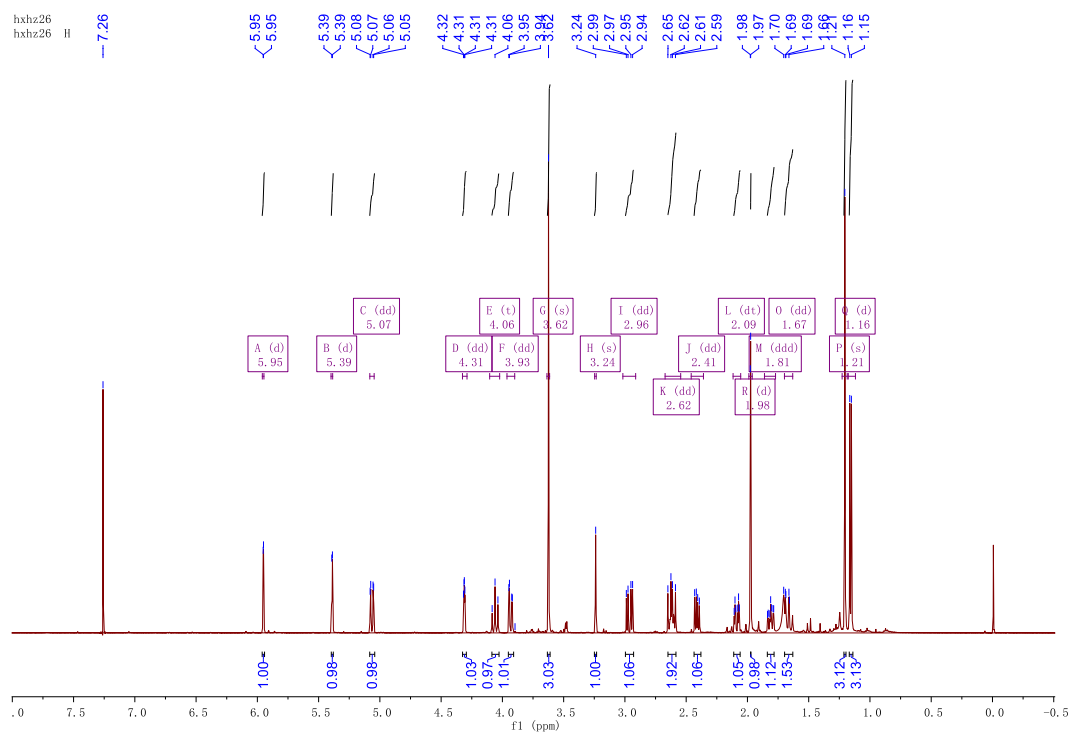
**Figure S16. HSQC spectrum of Perforalactone H (3) in  $\text{CDCl}_3$ .**



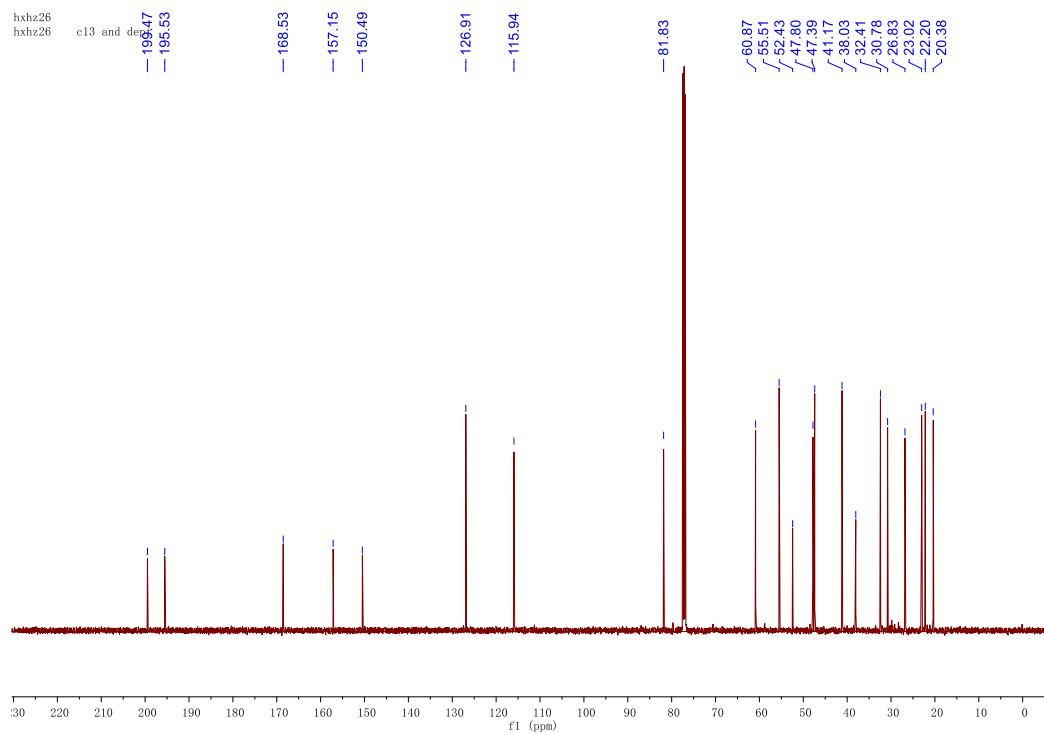
**Figure S17. HMBC spectrum of Perforalactone H (3) in CDCl<sub>3</sub>.**



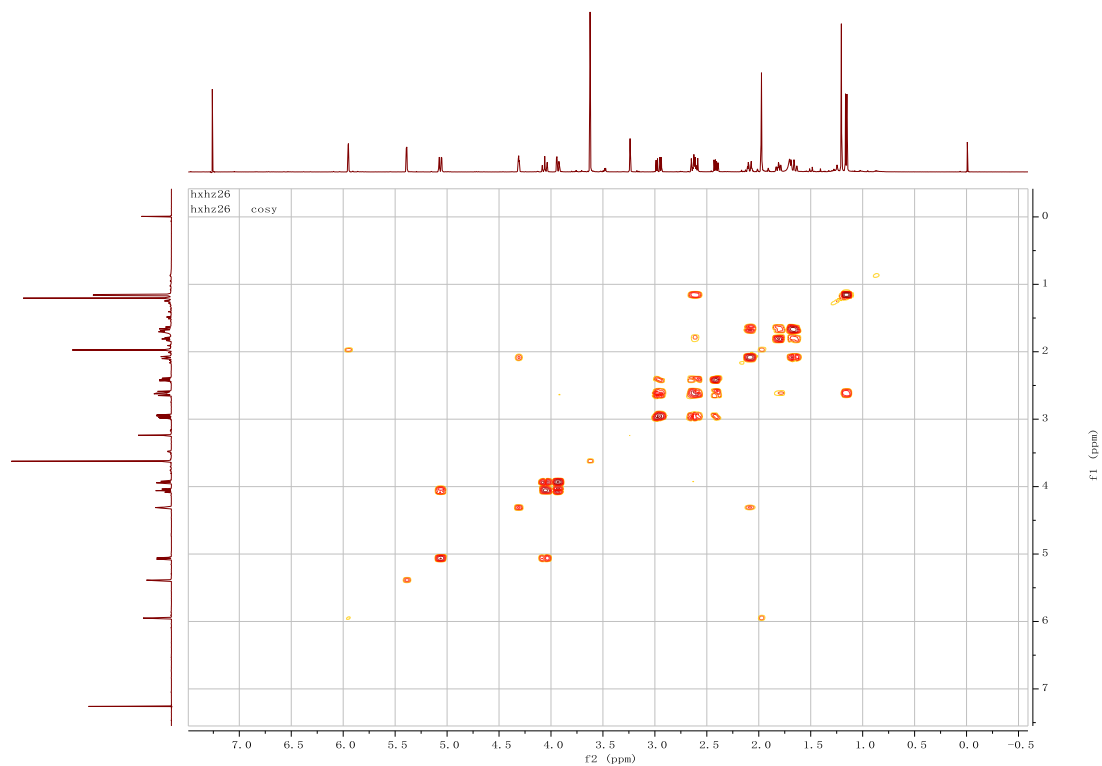
**Figure S18. ROESY spectrum of Perforalactone H (3) in CDCl<sub>3</sub>.**



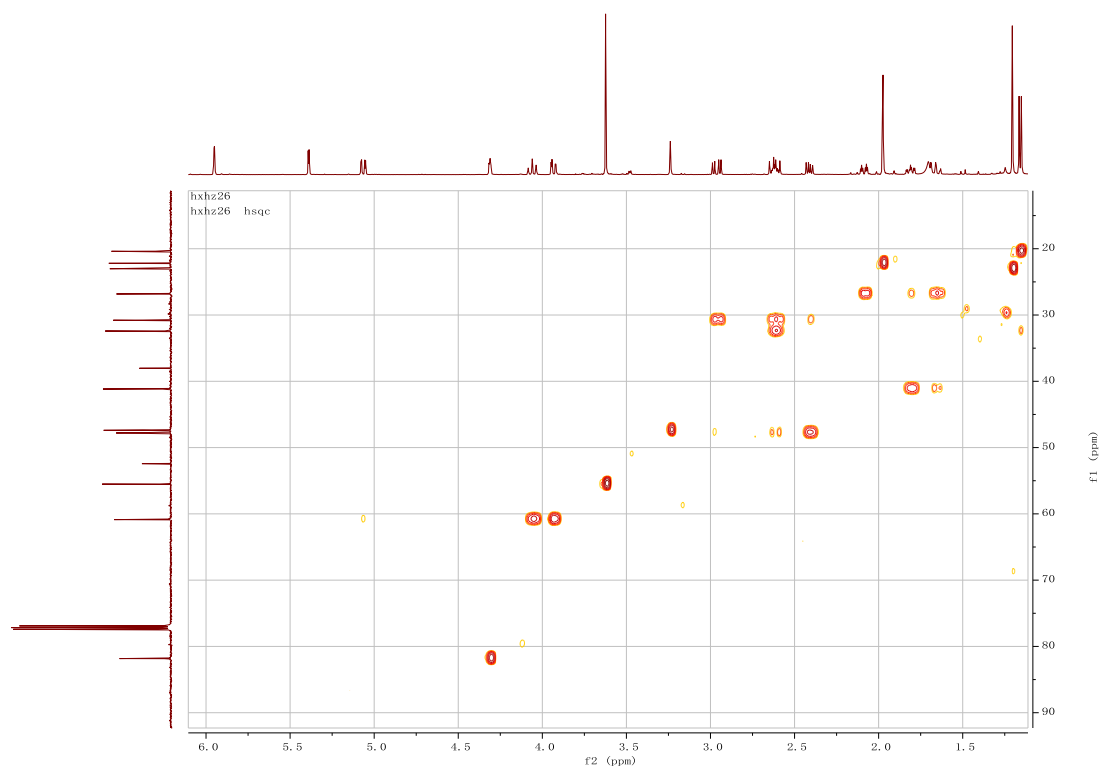
**Figure S19.  $^1\text{H}$  NMR spectrum of Perforalactone I (4) in  $\text{CDCl}_3$ .**



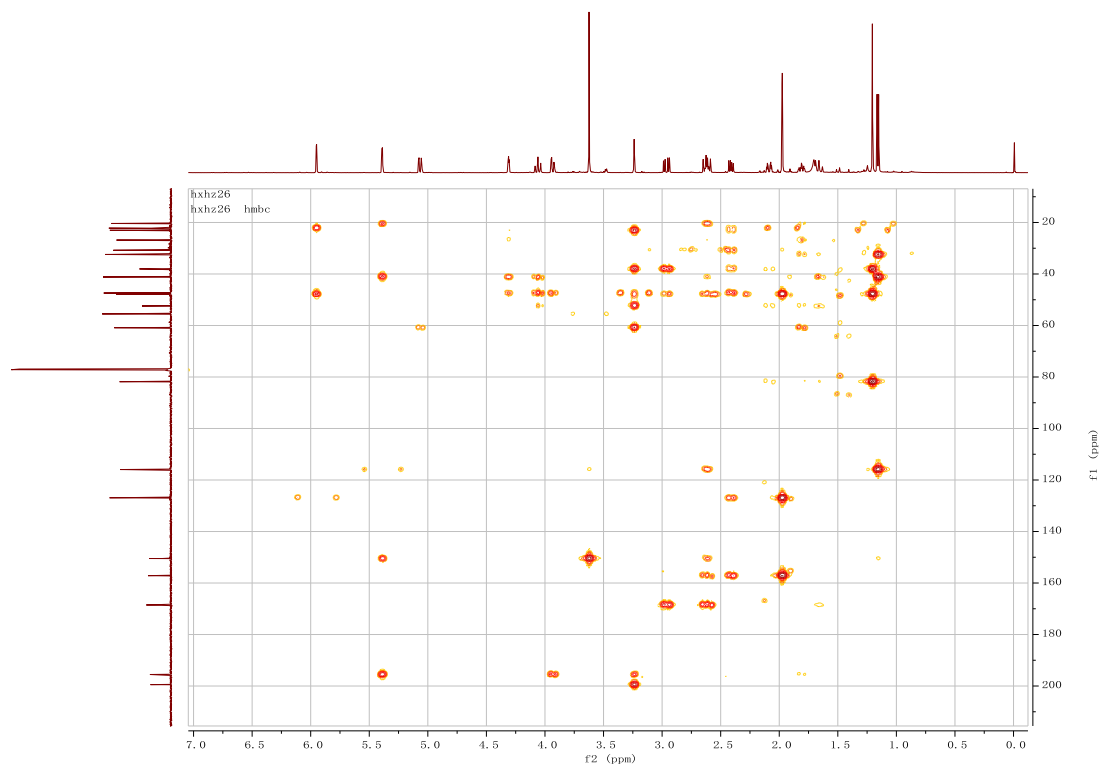
**Figure S20.  $^{13}\text{C}$  NMR spectrum of Perforalactone I (4) in  $\text{CDCl}_3$ .**



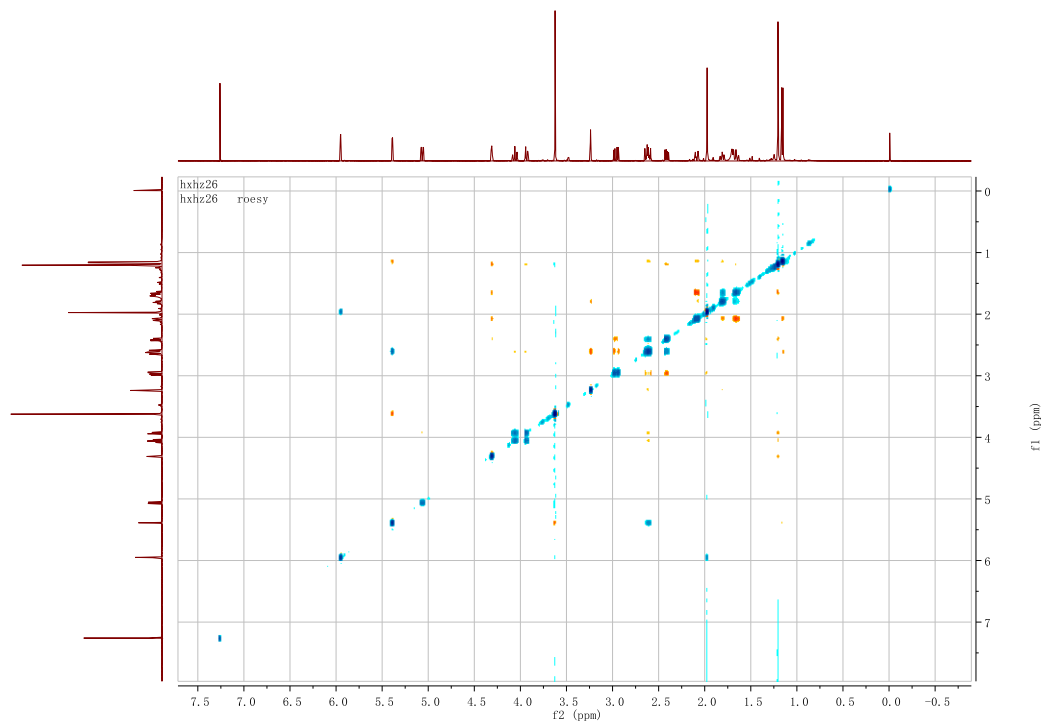
**Figure S21.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Perforalactone I (4) in  $\text{CDCl}_3$ .



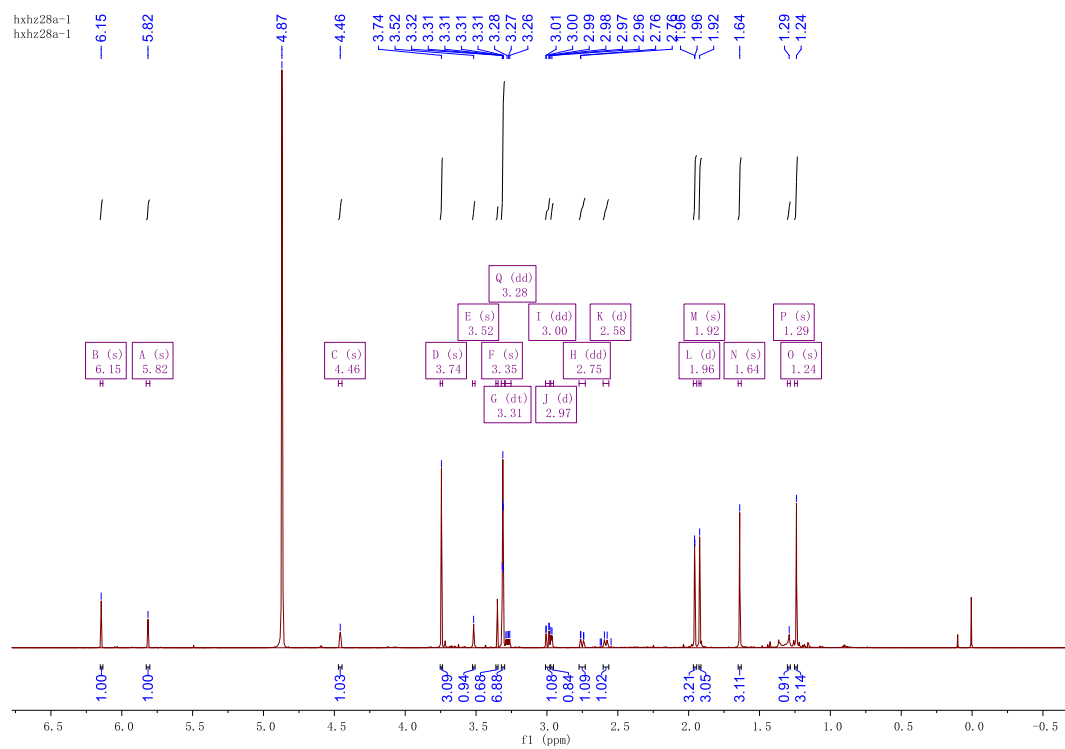
**Figure S22.** HSQC spectrum of Perforalactone I (4) in  $\text{CDCl}_3$ .



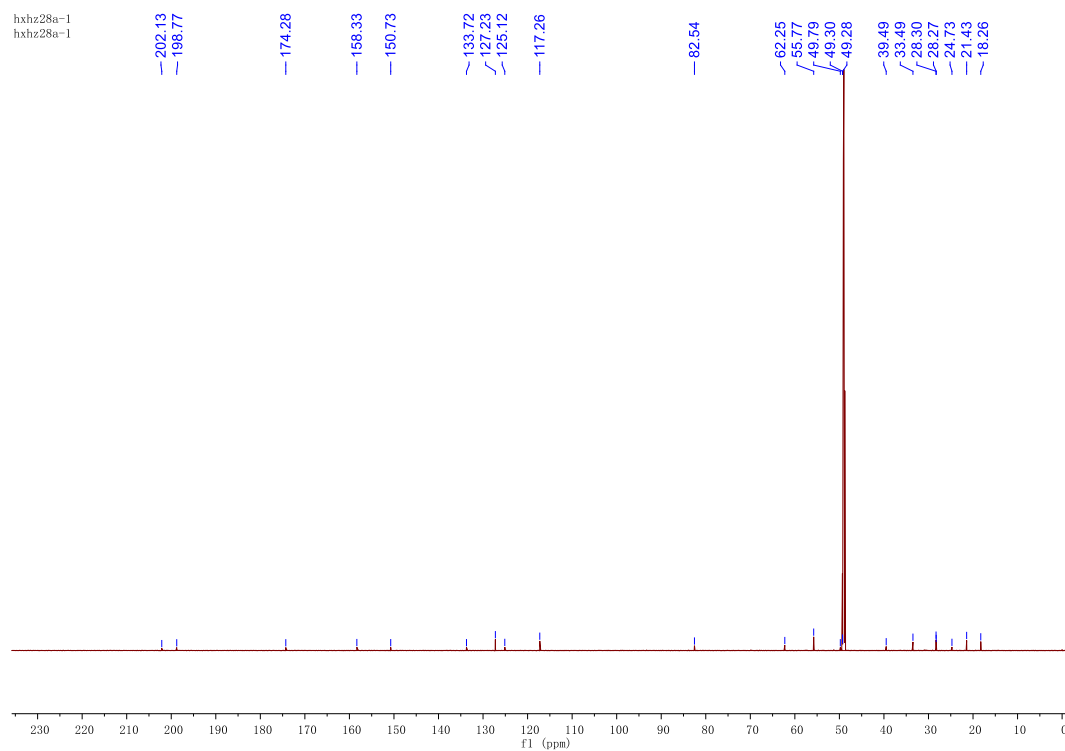
**Figure S23. HMBC spectrum of Perforalactone I (4) in CDCl<sub>3</sub>.**



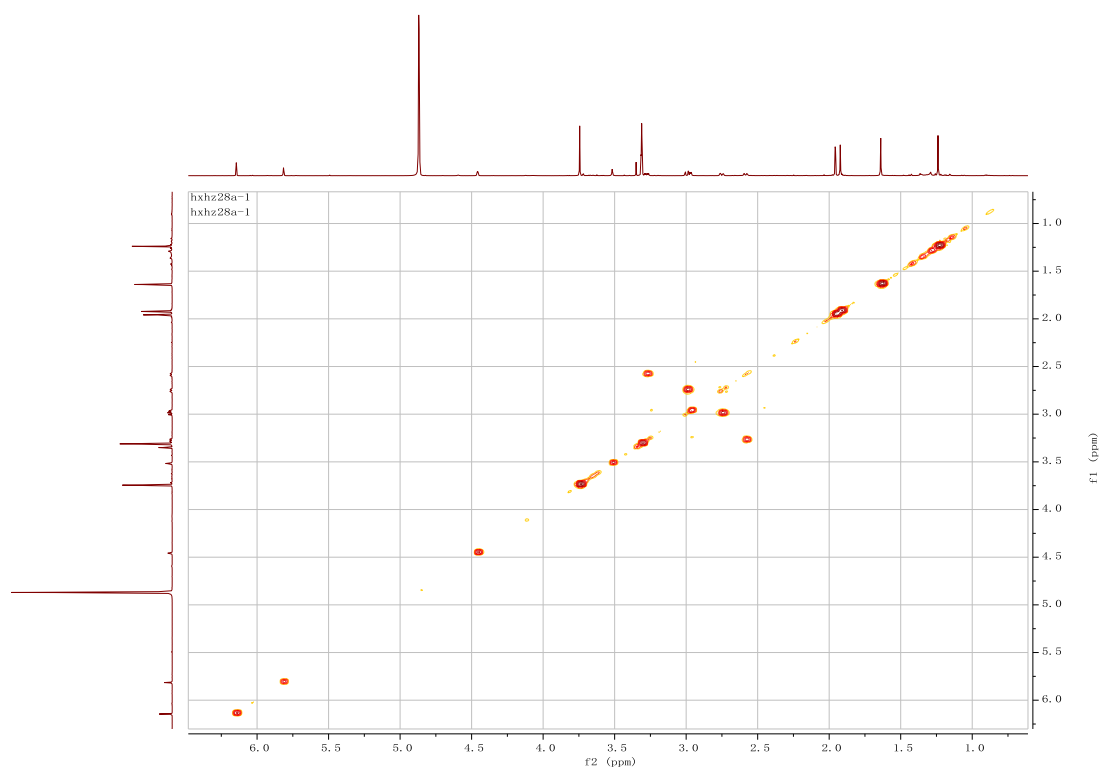
**Figure S24. ROESY spectrum of Perforalactone I (4) in CDCl<sub>3</sub>.**



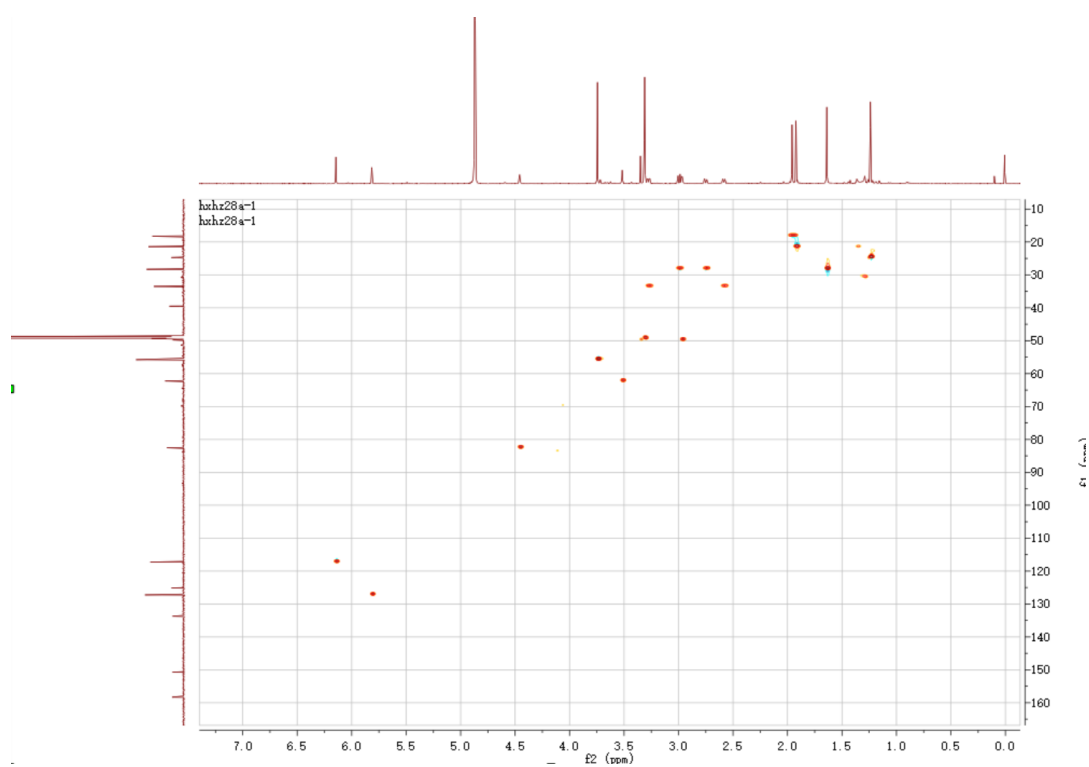
**Figure S25.  $^1\text{H}$  NMR spectrum of Perforalactone J (5) in  $\text{CD}_3\text{OD}$ .**



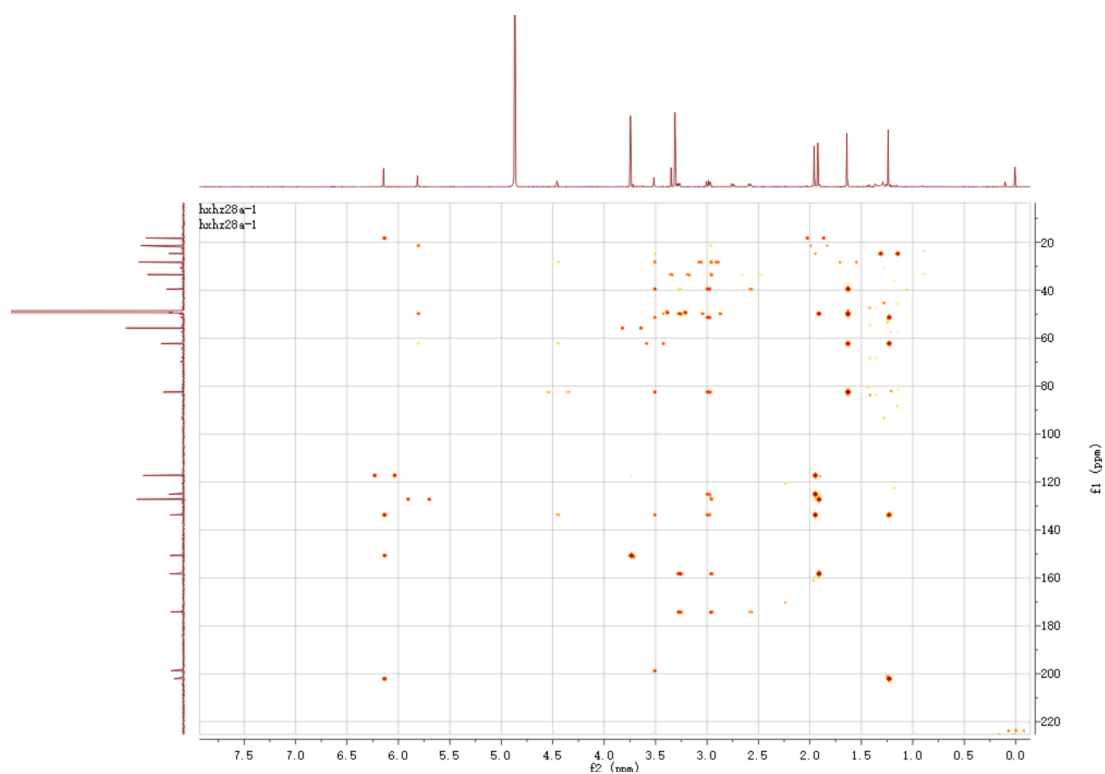
**Figure S26.  $^{13}\text{C}$  NMR spectrum of Perforalactone J (5) in  $\text{CD}_3\text{OD}$ .**



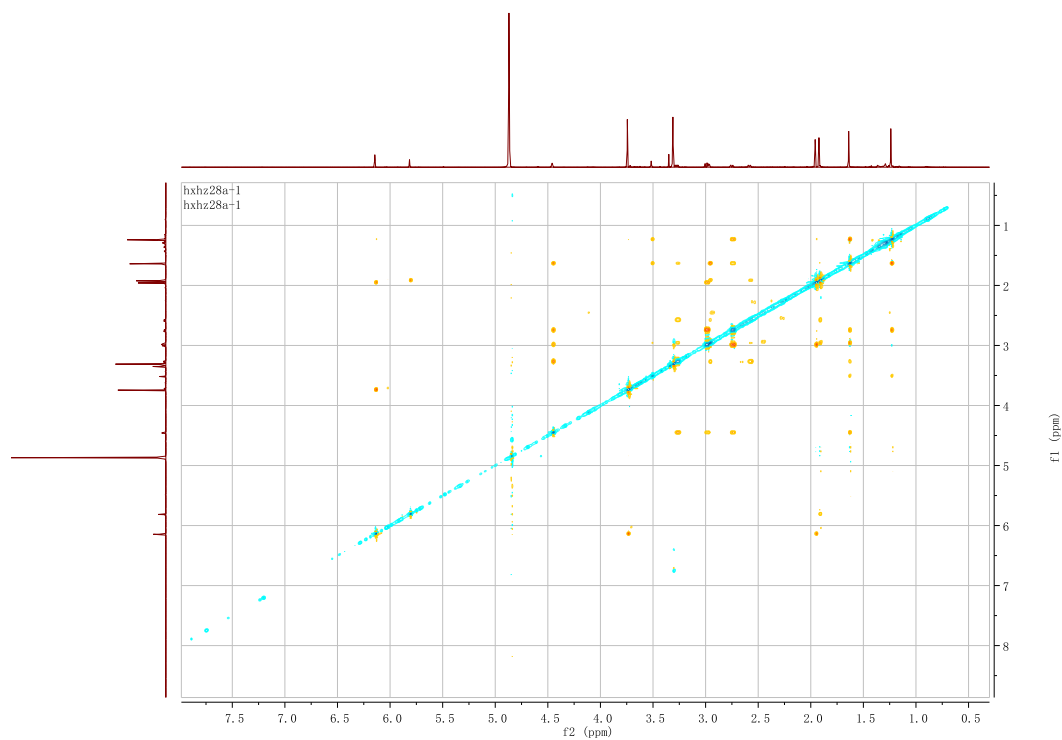
**Figure S27.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Perforalactone J (5) in  $\text{CD}_3\text{OD}$ .**



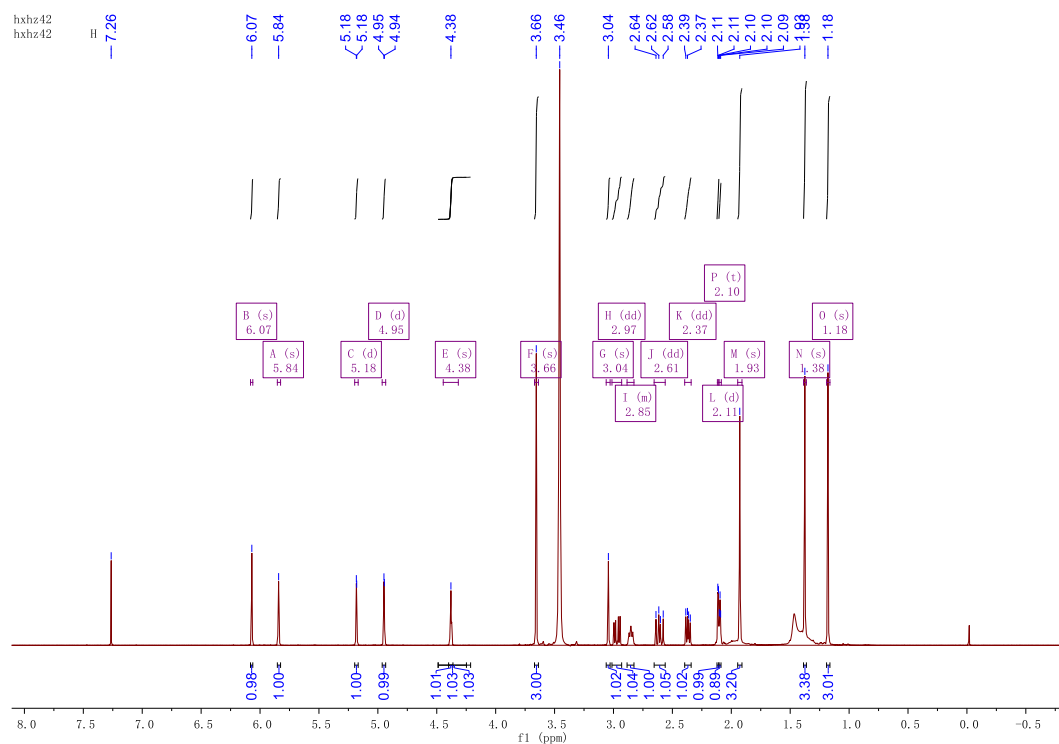
**Figure S28. HSQC spectrum of Perforalactone J (5) in  $\text{CD}_3\text{OD}$ .**



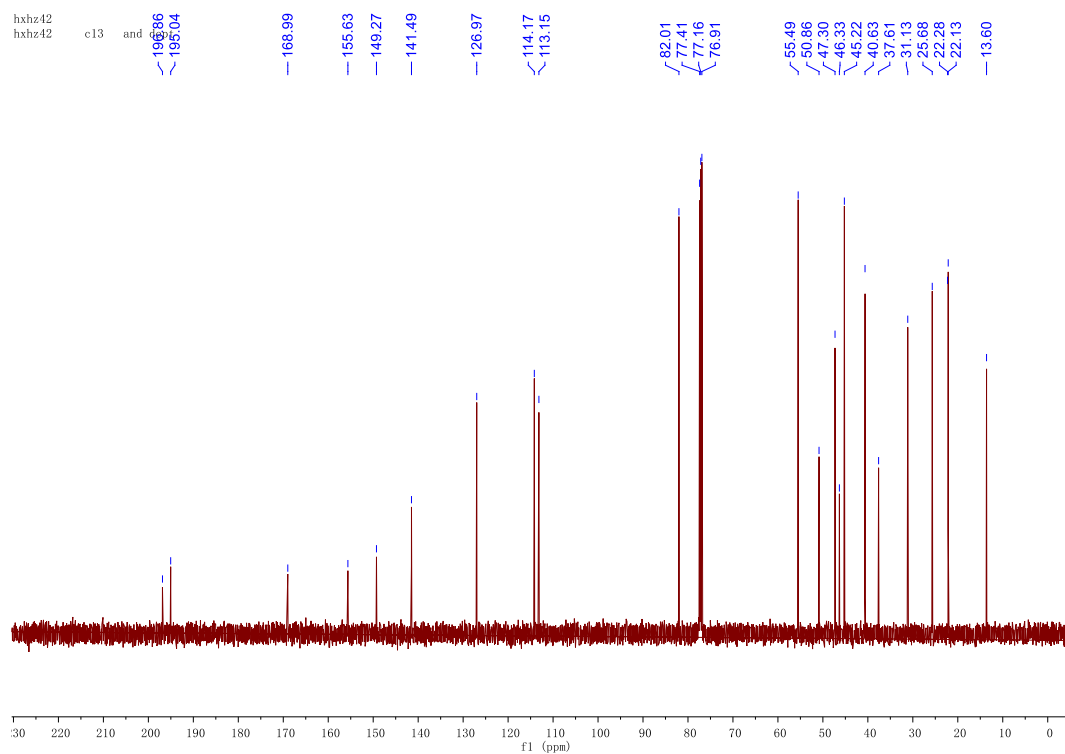
**Figure S29. HMBC spectrum of Perforalactone J (5) in CD<sub>3</sub>OD.**



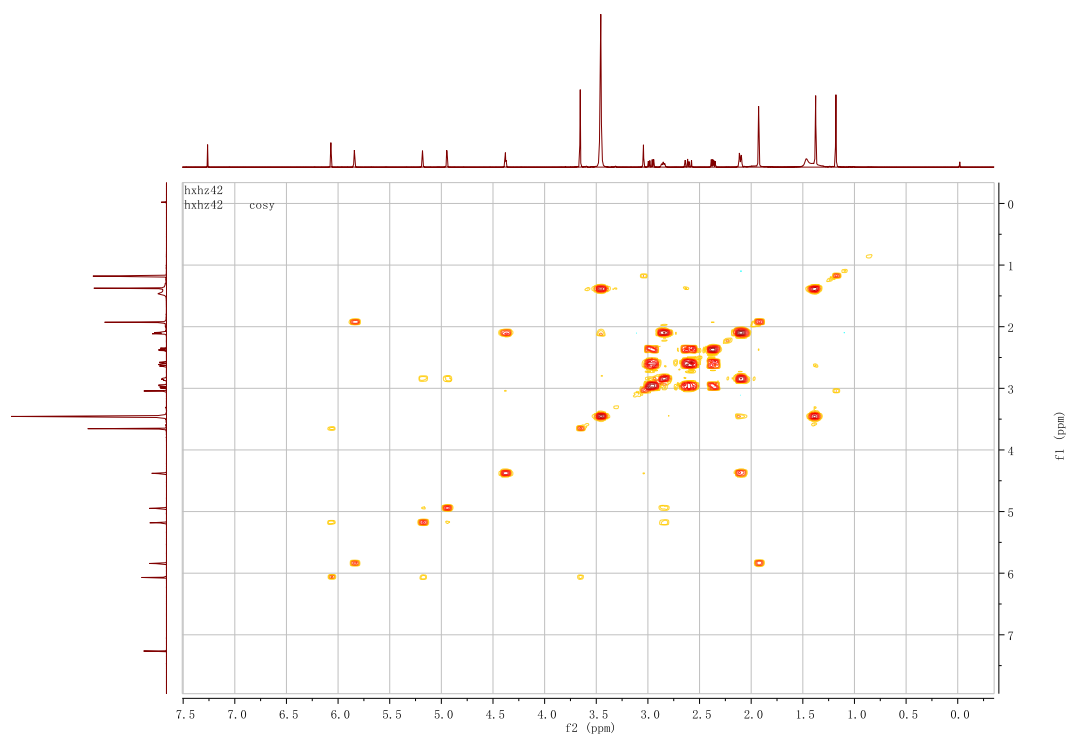
**Figure S30. ROESY spectrum of Perforalactone J (5) in CD<sub>3</sub>OD.**



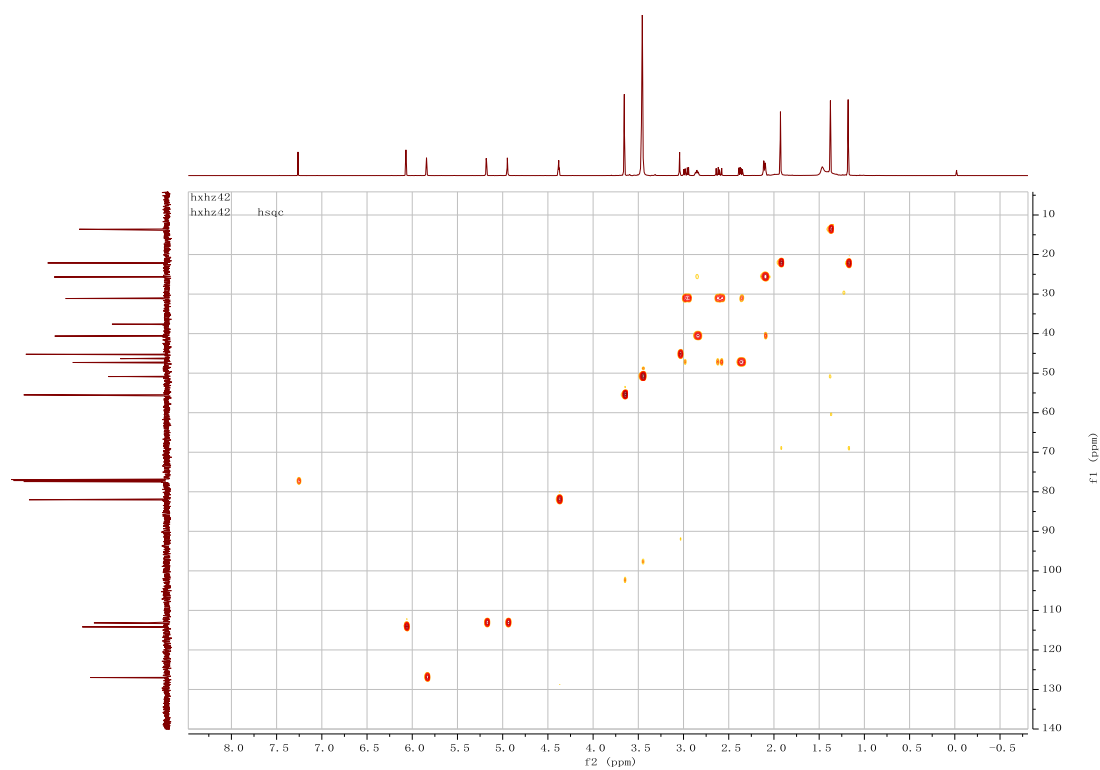
**Figure S31.  $^1\text{H}$  NMR spectrum of Perforalactone K (6) in  $\text{CDCl}_3$ .**



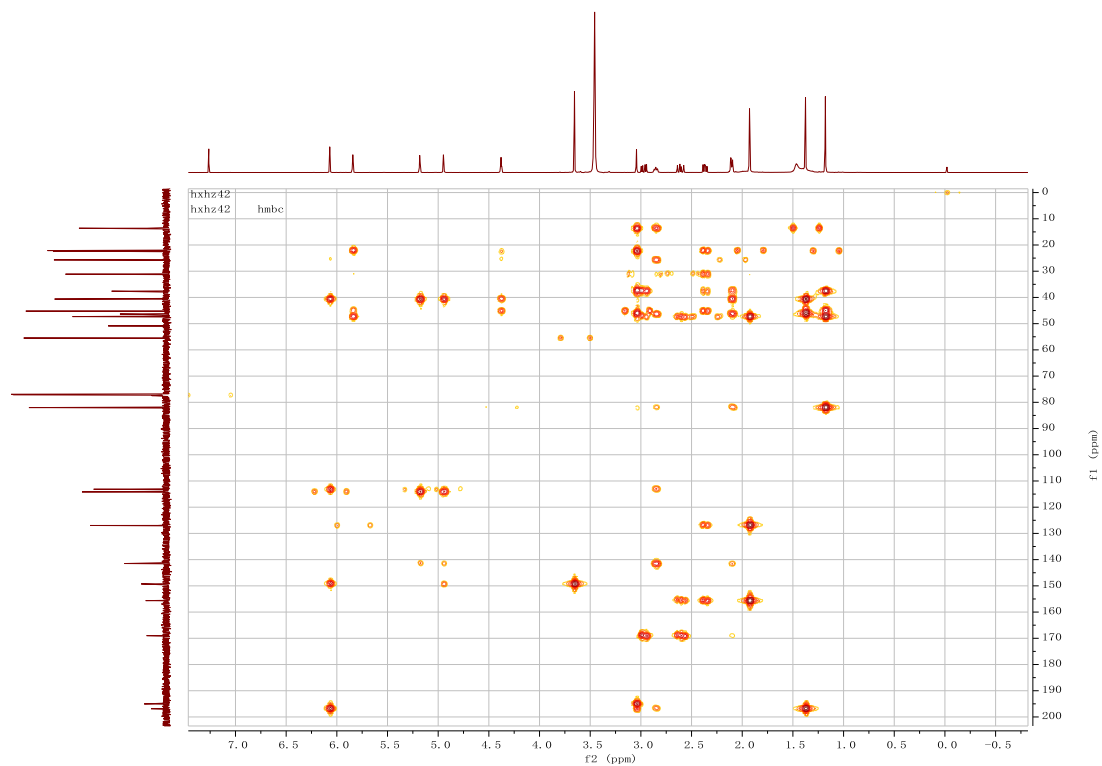
**Figure S32.  $^{13}\text{C}$  NMR spectrum of Perforalactone K (6) in  $\text{CDCl}_3$ .**



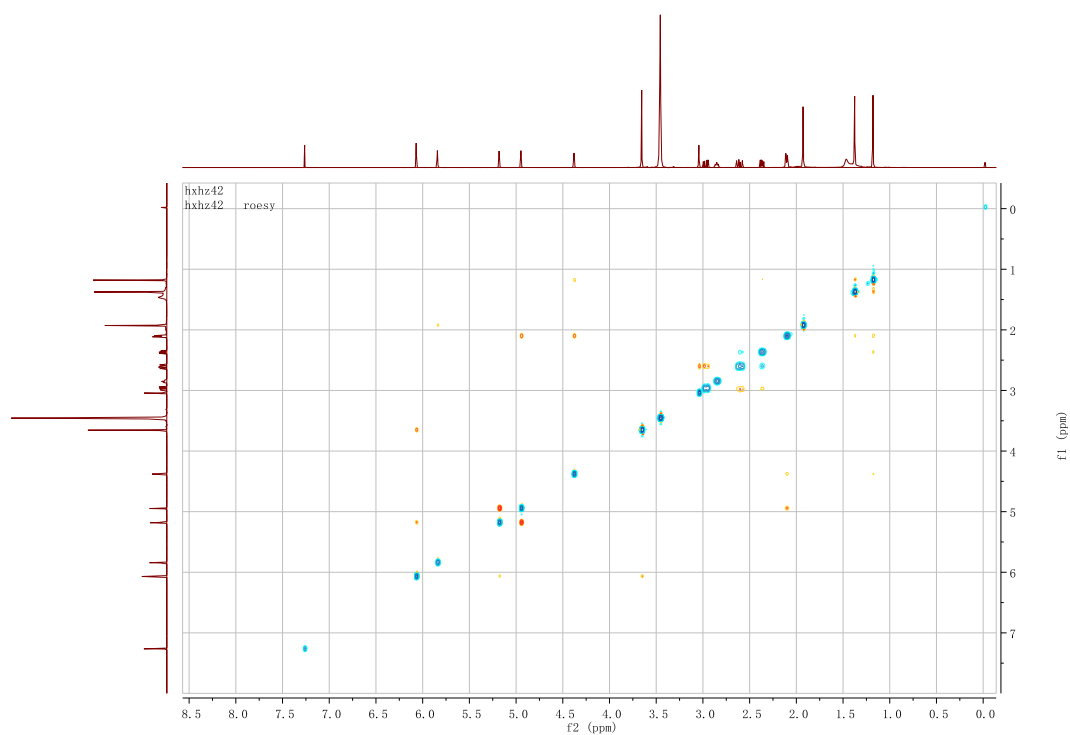
**Figure S33.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Perforalactone K (6) in  $\text{CDCl}_3$ .**



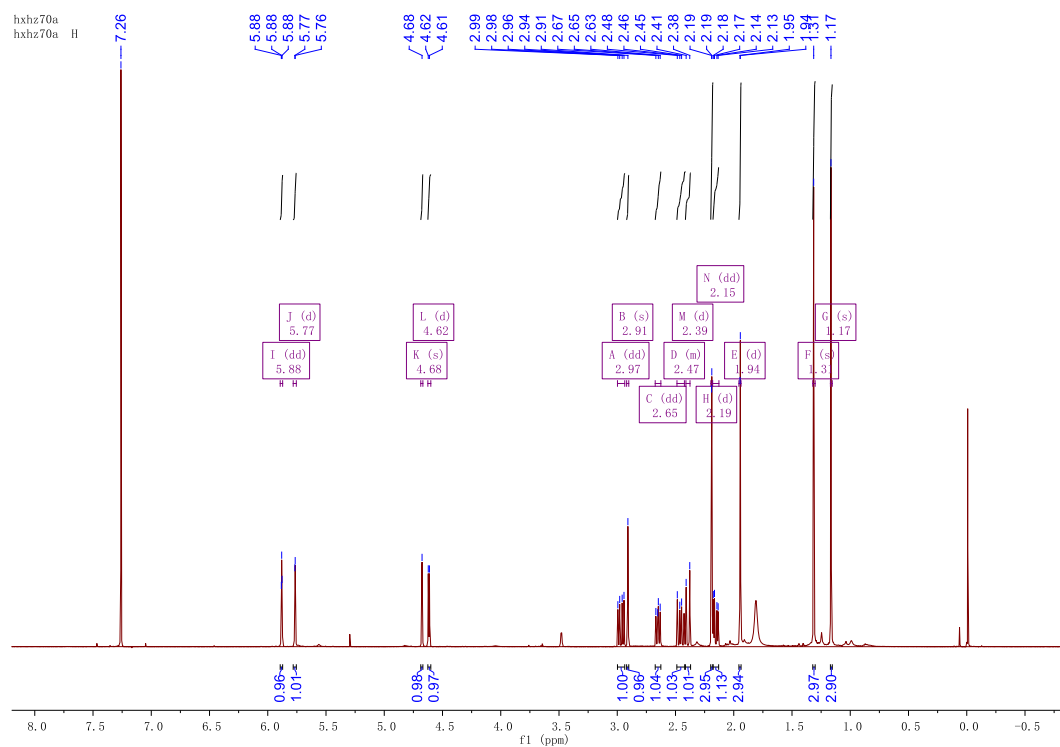
**Figure S34. HSQC spectrum of Perforalactone K (6) in  $\text{CDCl}_3$ .**



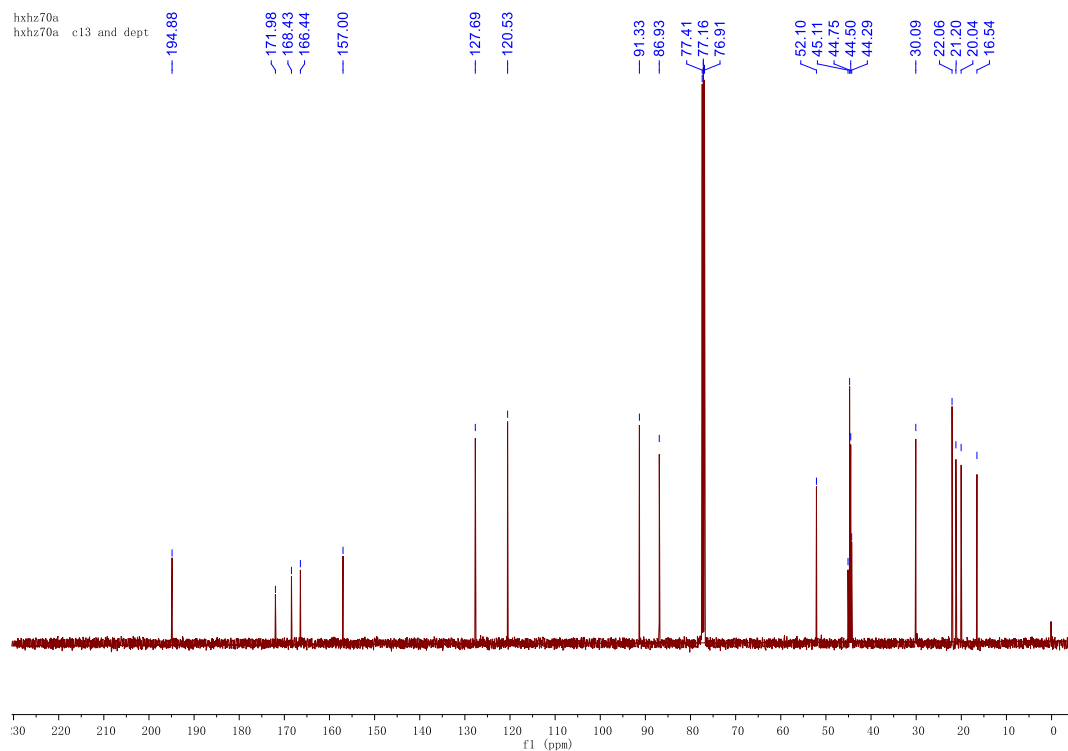
**Figure S35. HMBC spectrum of Perforalactone K (6) in CDCl<sub>3</sub>.**



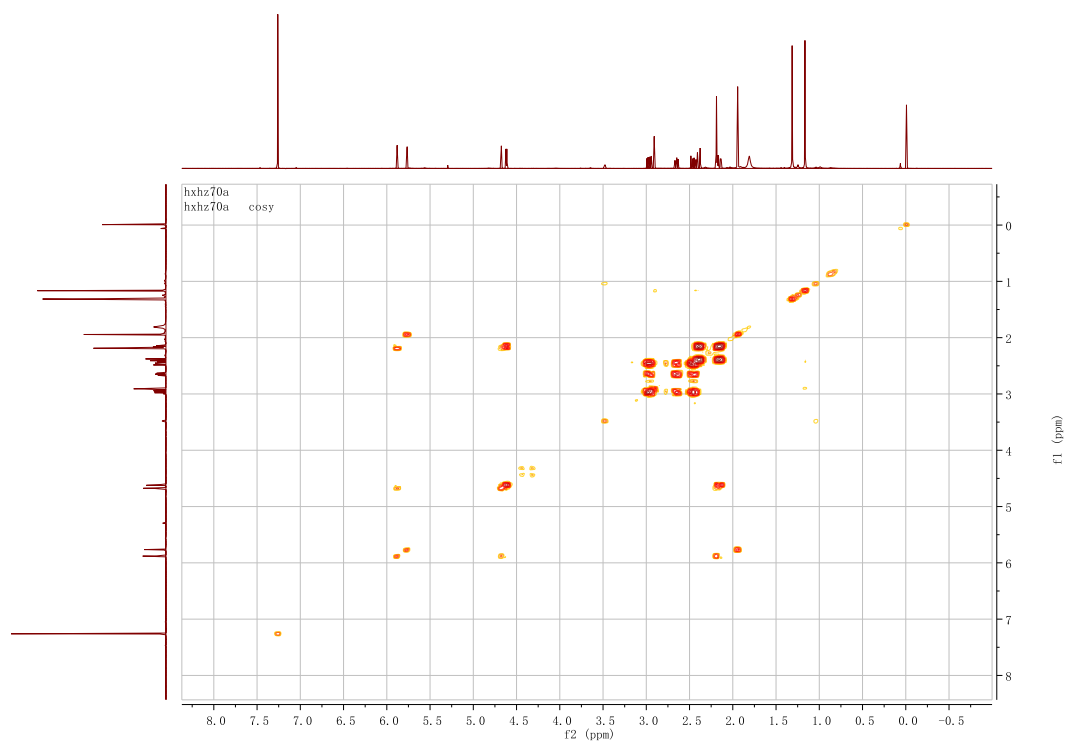
**Figure S36. ROESY spectrum of Perforalactone K (6) in CDCl<sub>3</sub>.**



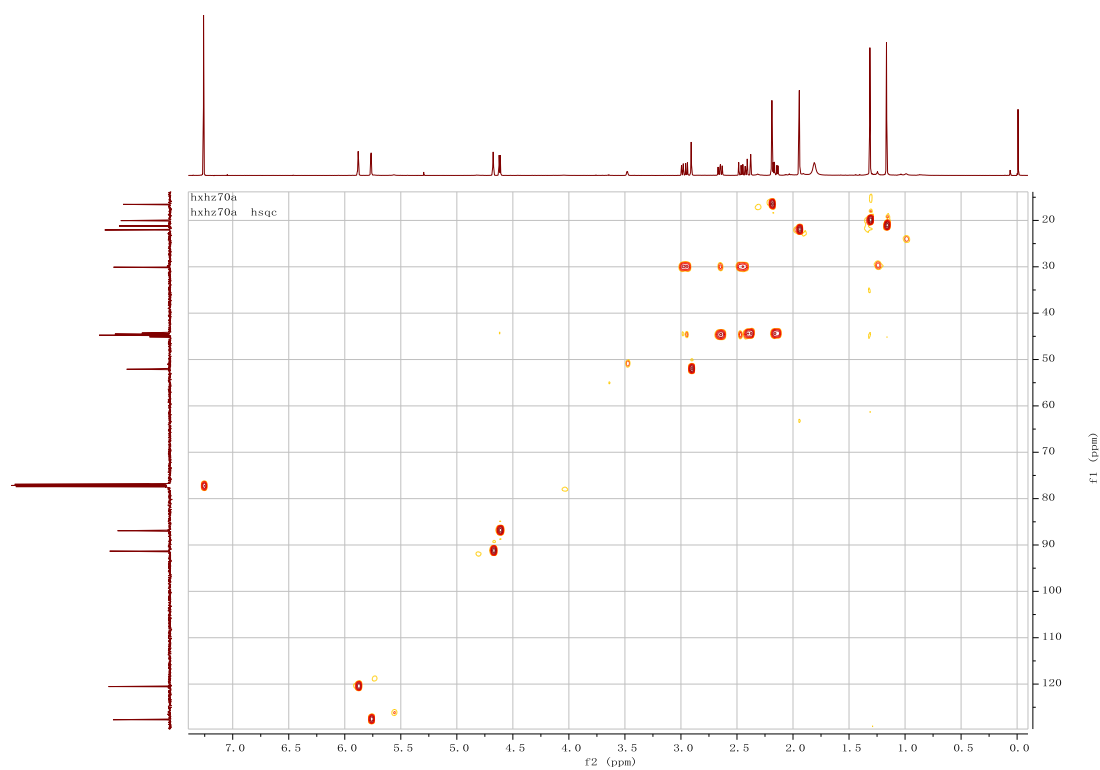
**Figure S37.  $^1\text{H}$  NMR spectrum of Perforalactone L (7) in  $\text{CDCl}_3$ .**



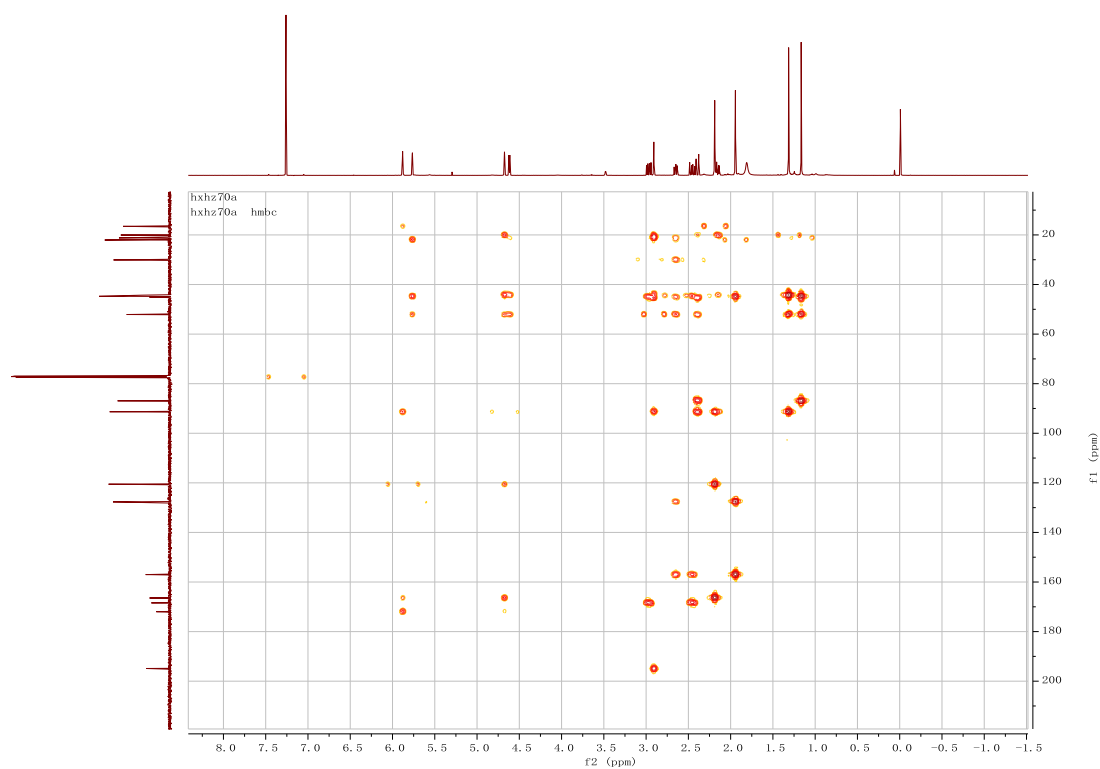
**Figure S38.  $^{13}\text{C}$  NMR spectrum of Perforalactone L (7) in  $\text{CDCl}_3$ .**



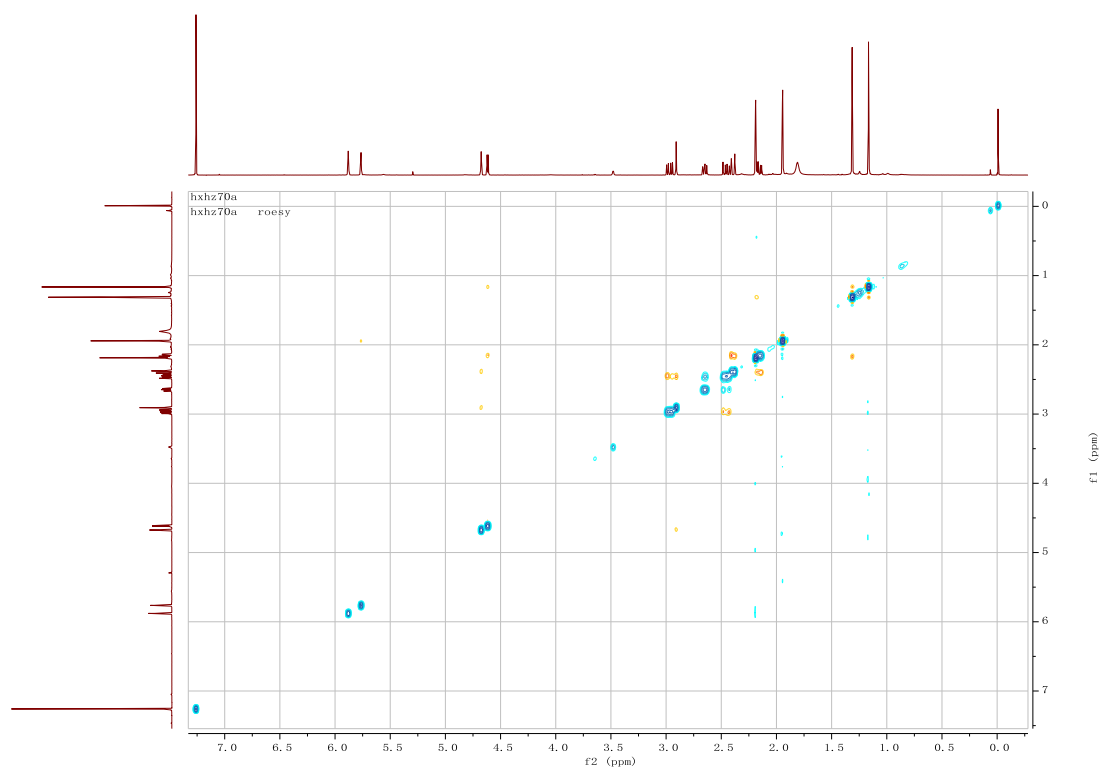
**Figure S39.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Perforalactone L (7) in  $\text{CDCl}_3$ .**



**Figure S40. HSQC spectrum of Perforalactone L (7) in  $\text{CDCl}_3$ .**



**Figure S41. HMBC spectrum of Perforalactone L (7) in CDCl<sub>3</sub>.**



**Figure S42. ROESY spectrum of Perforalactone L (7) in CDCl<sub>3</sub>.**