Electronic supplementary information

Phomretones A-F, C_{12} polyketides from the co-cultivation of *Phoma* sp. YUD17001 and *Armillaria* sp.

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Contents

Table S1 ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data for phomretone A (**1**) and verbenanone [1] (δ in ppm)

	phomretone A (**1**)[a]		verbenanone[a 1]	
no.	δ_H (J in Hz)	$\delta_{C,}$ type	δ_H (J in Hz)	$\delta_{C,}$ type
1		208.4, C		212.4, C
2	4.16, dd (12.4, 6.8)	75.7, CH	4.24, dd (12.0, 6.7)	76.5, CH
3	2.22, m	30.8, CH_2	1.90, m	32.8, CH_2
	1.47, overlap		2.14, m	
4	2.13, m	29.7, CH_2	2.03, m	29.2, CH_2
	1.79, m			
5	3.79, dt (10.8, 4.0)	74.7, CH	3.97, d (2.6)	79.4, CH
6	2.48, d (10.8)	57.5, CH	3.15, br s	55.2, CH
7	4.35, br s	66.9, CH	3.49, dd (9.3, 5.0)	75.6, CH
8	3.14, dd (9.6, 2.4)	73.2, CH	3.63, dd (9.3, 9.3)	72.7, CH
9	3.54, m	76.4, CH	3.08, ddd (11.7, 9.3, 2.6)	81.9, CH
10	1.79, overlap	35.2, CH_2	1.38, m	35.3, CH_2
	1.37, overlap		1.78, m	
11	1.57, overlap	19.6, CH_2	1.35, m	19.7, CH_2
	1.36, overlap		1.49, m	
12	0.93, t (7.2)	14.5, CH_3	0.92, t (7.2)	14.6, CH_3

[a]Measured in methanol-d_4.

Bioactivities test of compounds 1-6

Phomretones A-F (**1-6**) were subjected to cytotoxicity bioassays utilizing the MTS way method. None of them showed notable inhibitory activity at the concentration of 40 μM in the tested cytotoxicity assays against human promyelocytic leukemia (HL-60), hepatoma (SMMC-7721), non-small-cell lung cancer (A-549), breast cancer (MCF-7), and colorectal carcinoma (SW480) cell lines (Fig. S1). These compounds were also evaluated by their acetylcholinesterase inhibitory activity, however, they were found to be inactive (Table S2). Furthermore, when tested protein tyrosine phosphatase 1B (PTP1B) inhibitory activity was tested, **1−6** were not determined to be active (Table S3).

Table S2 Inhibition of **1−6** on AChE

compound	Inhibition (%)[a]
Tacrineb[b]	58.85 ±0.03
1	23.16 ±1.20
2	20.43 ±0.49
3	21.14 ±0.36
4	20.69 ±1.44
5	22.39 ±0.77
6	21.86 ±0.62

[a]Tested at 50 μM; [b]Positive control.

Table S3 Inhibitory effects of **1−6** on PTP1B enzyme activity

compound	Inhibition (%)[a]
Suramin[b]	77.05 ±1.03
1	7.10 ±1.51
2	19.20 ±3.51
3	9.11 ±0.03
4	0.95 ±0.72
5	4.81 ±3.73
6	10.23 ±1.64

[a]Tested at 50 μM; [b]Positive control.

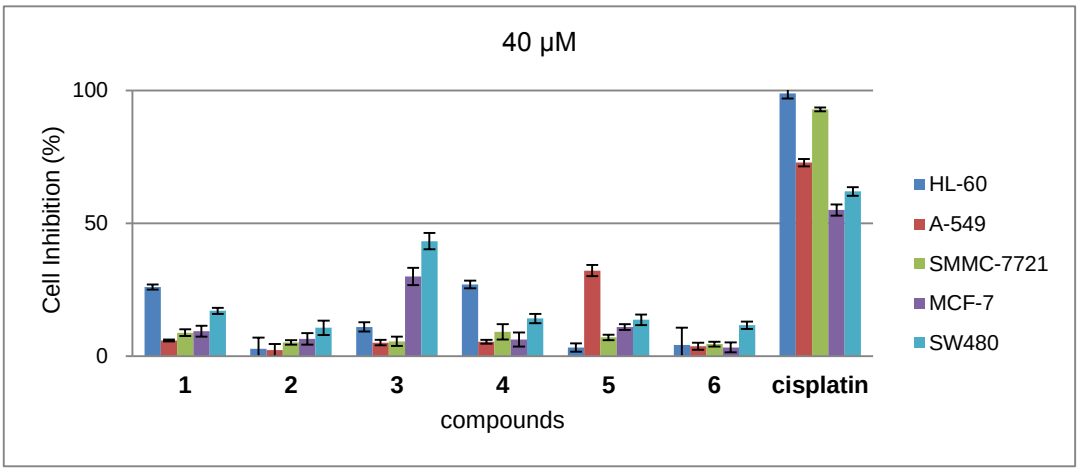

Fig. S1 Inhibition (%) of compounds **1-6** was tested at 40 μM against five human cancer cell lines (HL-60, A-549, SMMC-7721, MCF-7, and SW480).

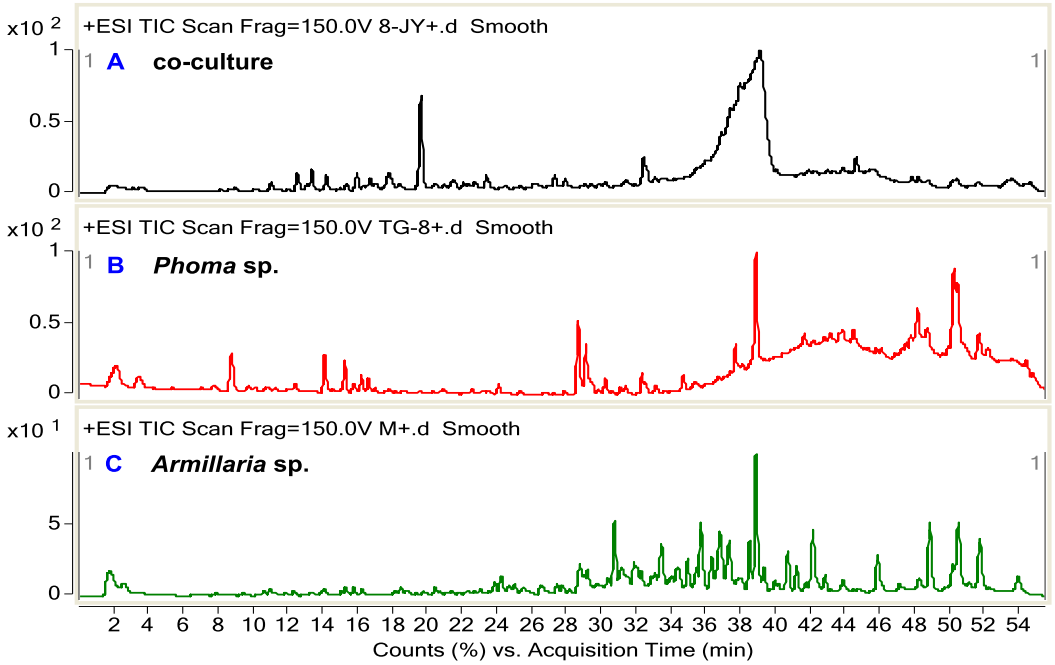

Fig. S2 Total ion chromatograms (TIC) of ethyl acetate extracts from the co-culture of *Phoma* sp. and *Armillaria* sp. (A); TIC of ethyl acetate extracts from *Phoma* sp. YUD17001 (B); TIC of ethyl acetate extracts from *Armillaria* sp. (C).

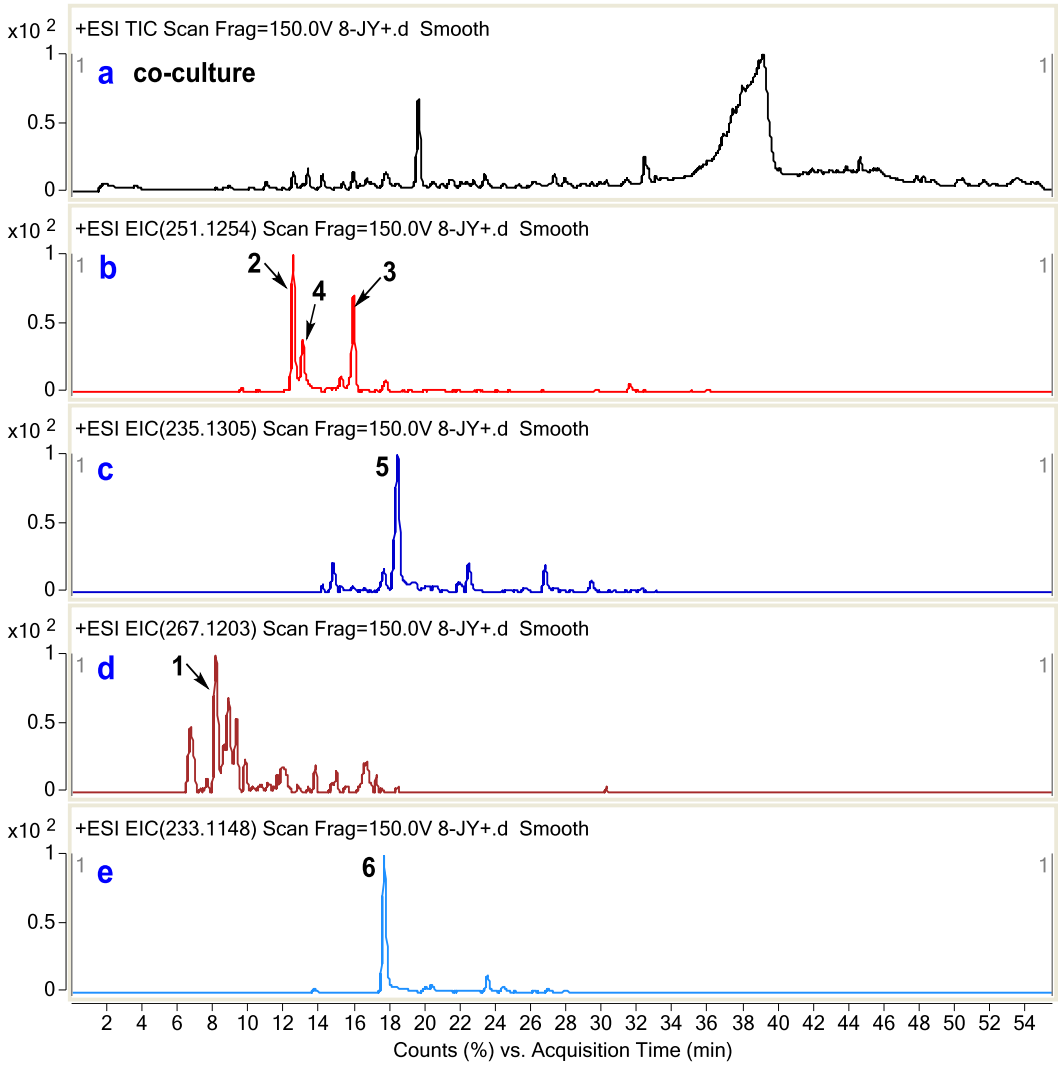

Fig. S3 Total ion chromatograms (TIC) of extracts from co-culture and high-resolution extracted ion chromatogram (EIC) of four selected masses. (TIC (positive) of the extracts from co-culture (a); EIC of compounds **2-4** at *m/z* 251.1254 $[M + Na]^+$ in the extracts of co-culture (b); EIC of compound **5** at *m/z* 235.1305 $[M + Na]^+$ in the extracts of co-culture (c); EIC of compound **1** at *m/z* 267.1203 $[M + Na]^+$ in the extracts of co-culture (d); EIC of compound **6** at *m/z* 233.1148 $[M + Na]^+$ in the extracts of co-culture (e)).

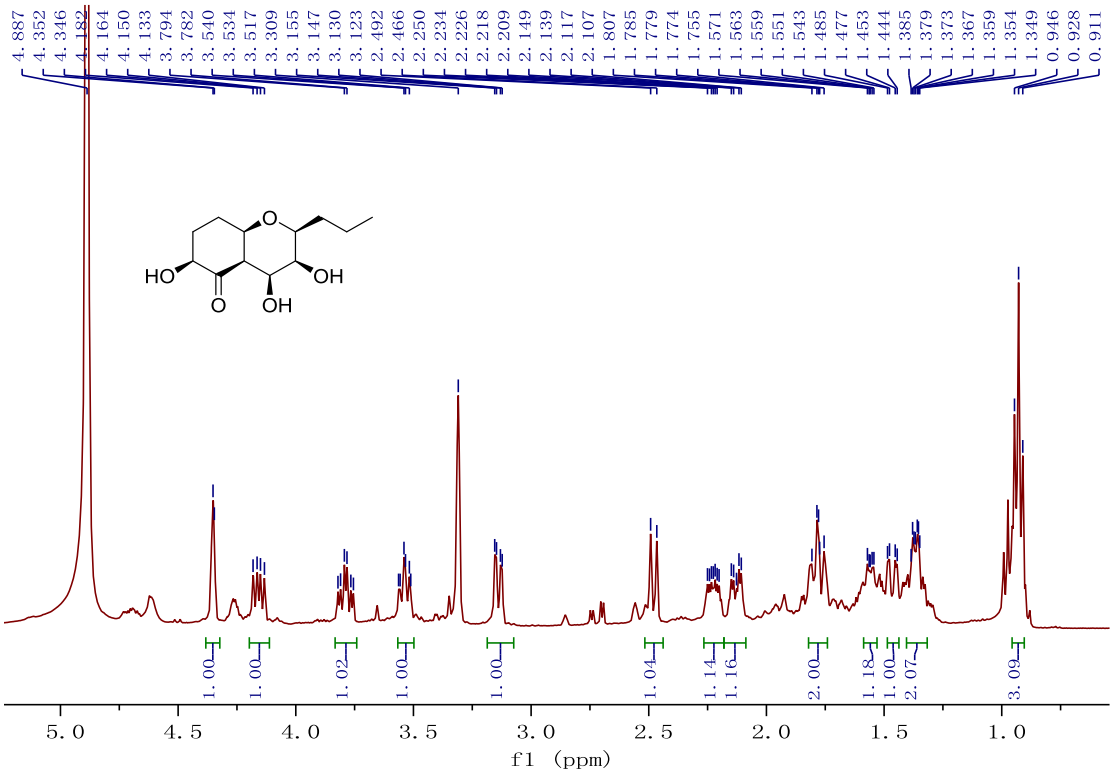

Fig. S4 ^{1}H NMR spectrum of phomretone A (**1**) in methanol-d_4 (400 MHz).

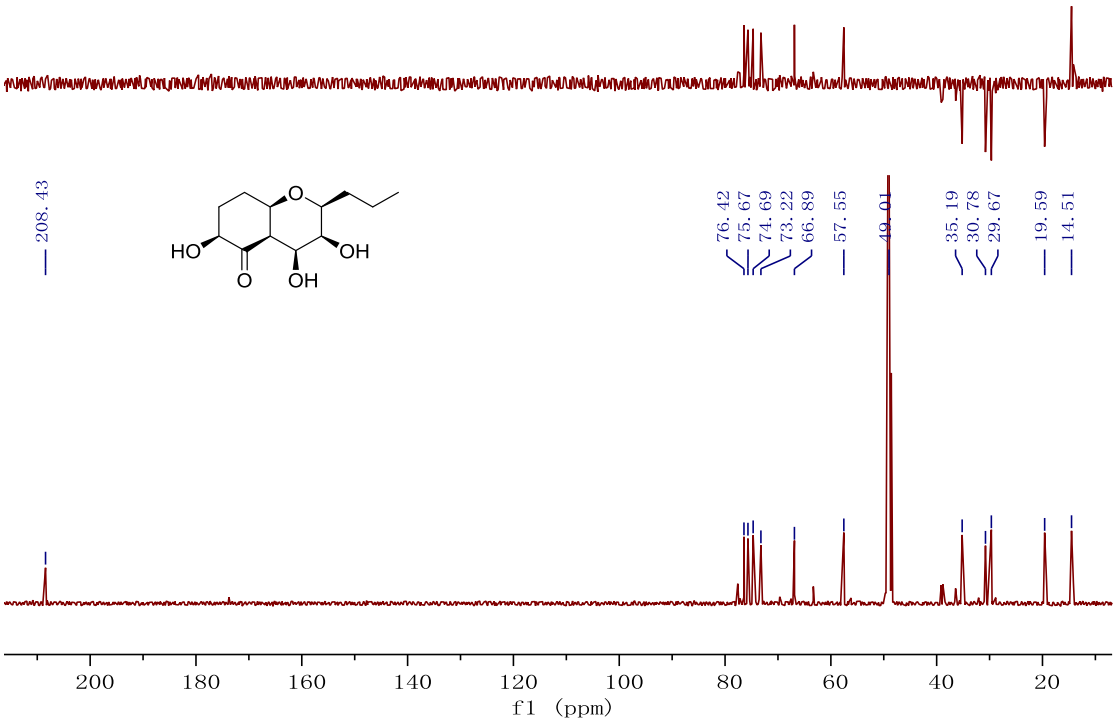

Fig. S5 ^{13}C NMR and DEPT spectrum of phomretone A (**1**) in methanol-d_4 (100 MHz).

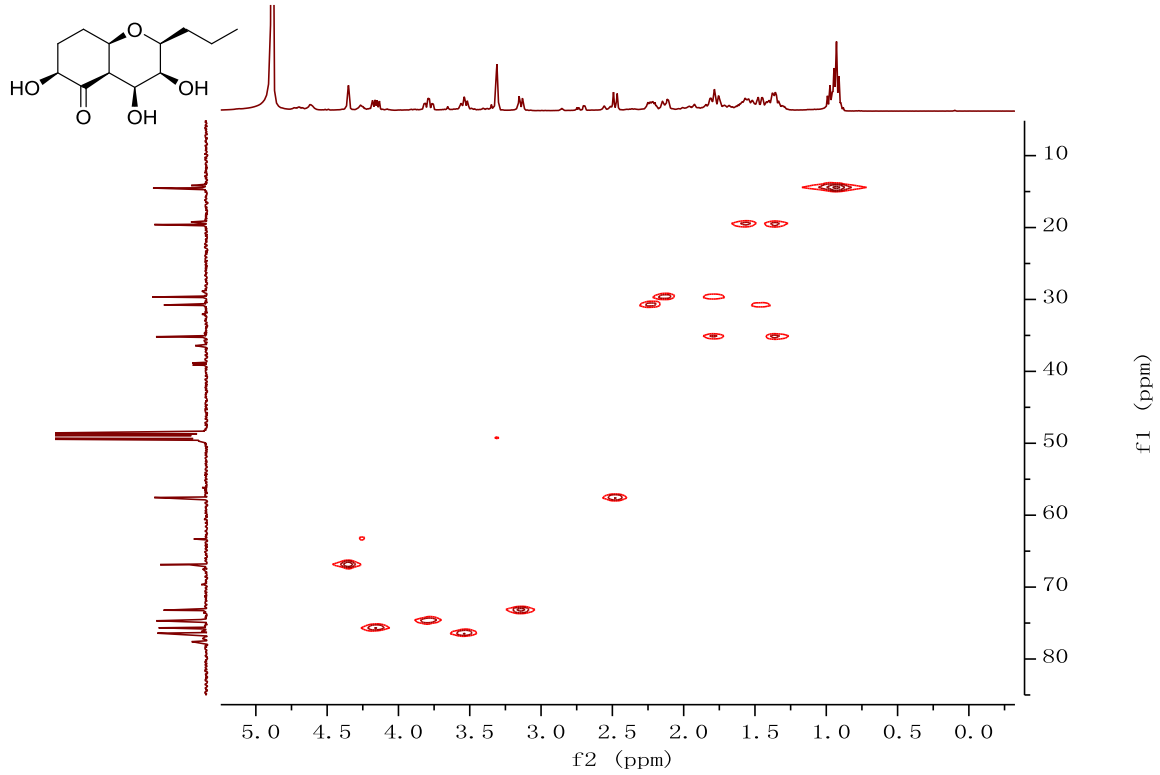

Fig. S6. HSQC spectrum of phomretone A (**1**) in methanol-d_4 (^{1}H-400 MHz).

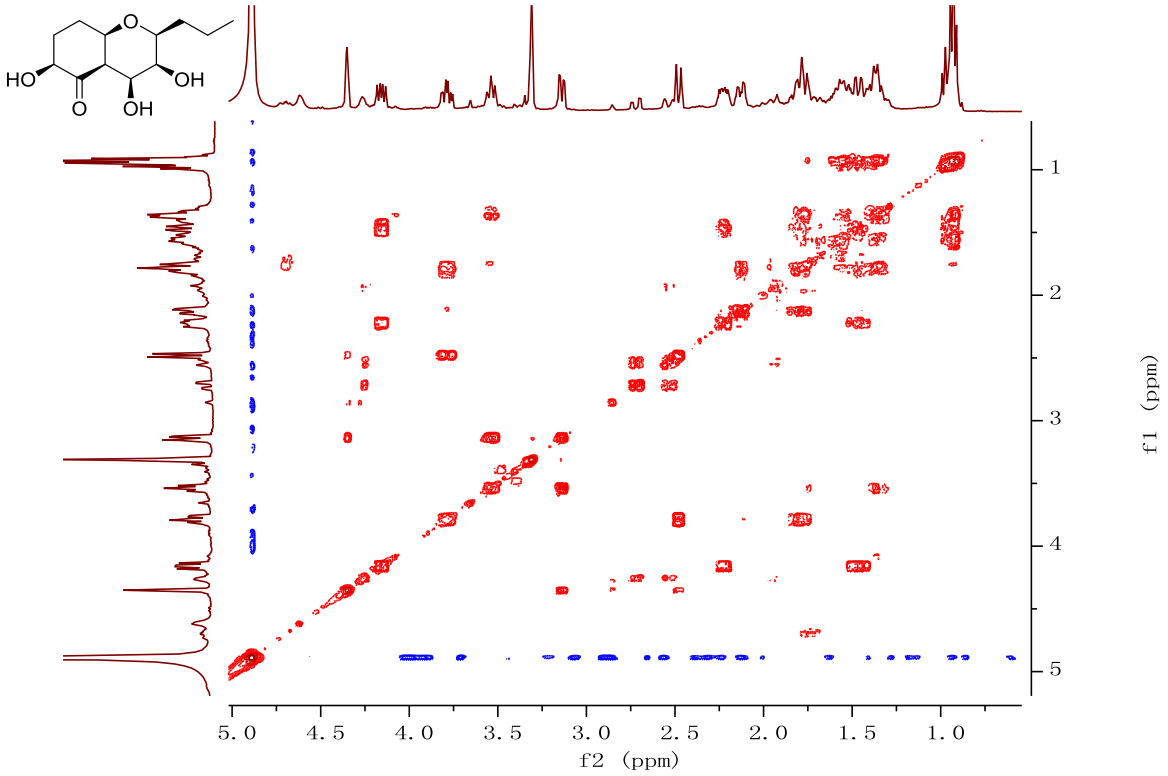

Fig. S7. ^{1}H-^{1}H COSY spectrum of phomretone A (**1**) in methanol-d_4 (400 MHz).

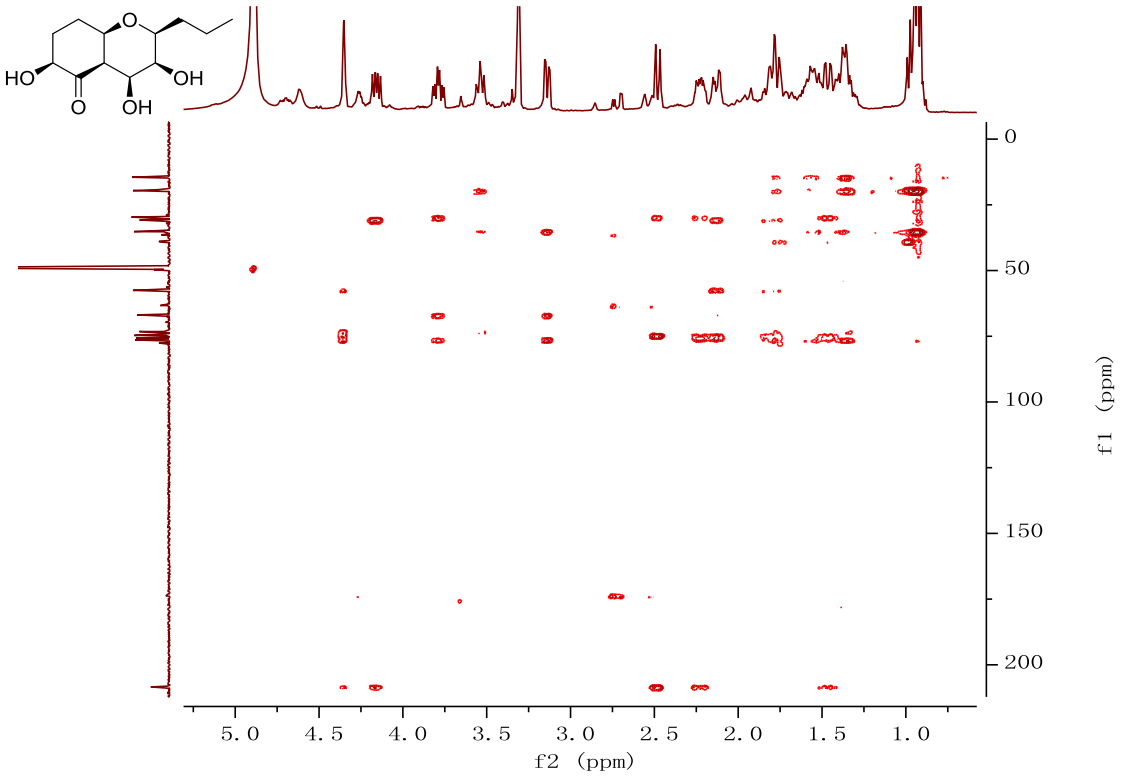

Fig. S8. HMBC spectrum of phomretone A (**1**) in methanol-d_4 (^{1}H-400 MHz).

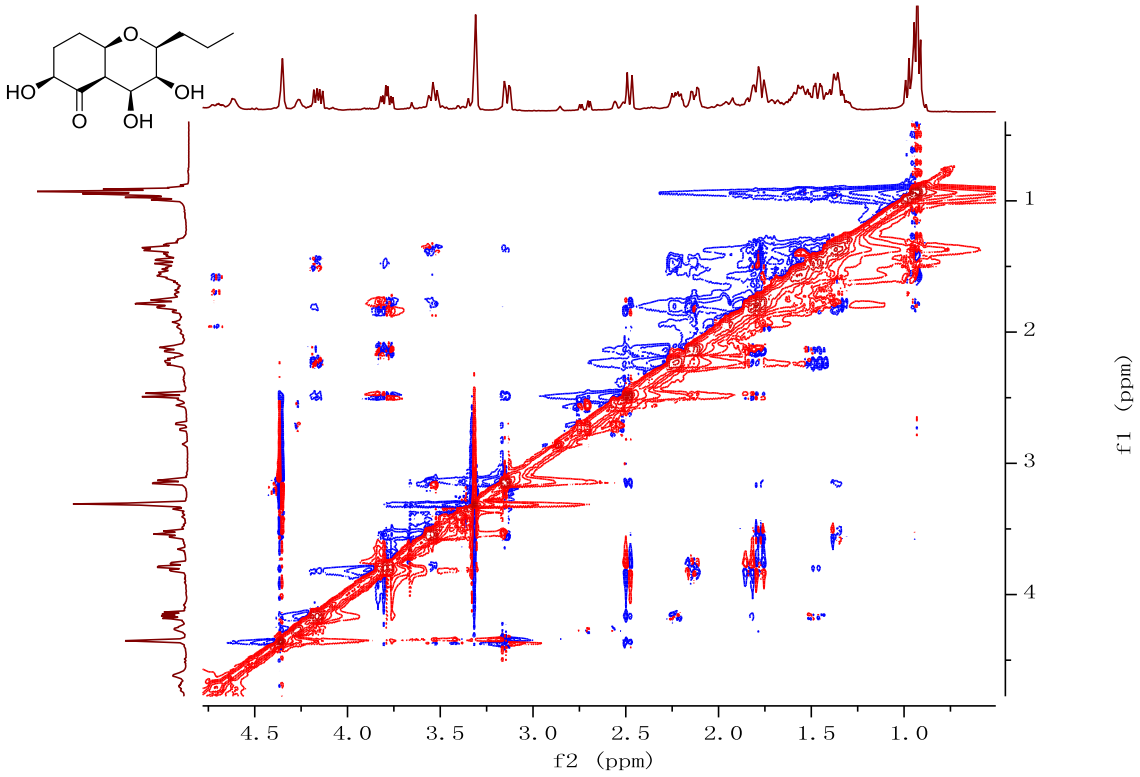

Fig. S9. ROESY spectrum of phomretone A (**1**) in methanol-d_4 (400 MHz).

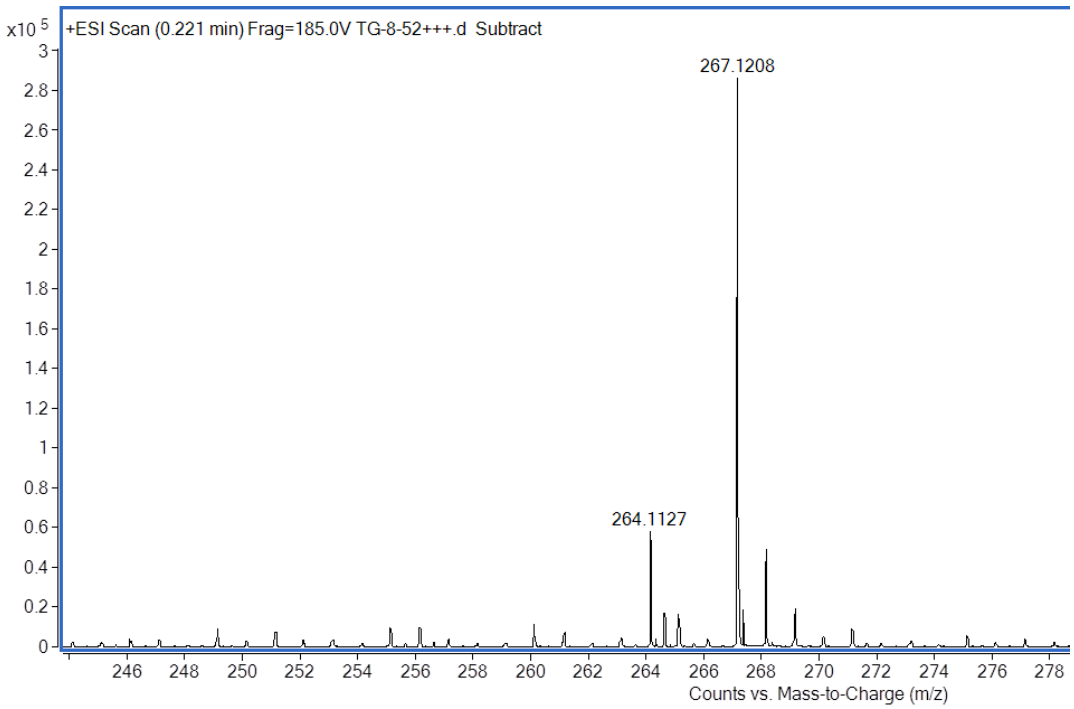

Fig. S10. (+)-HRESIMS data of phomretone A (**1**).

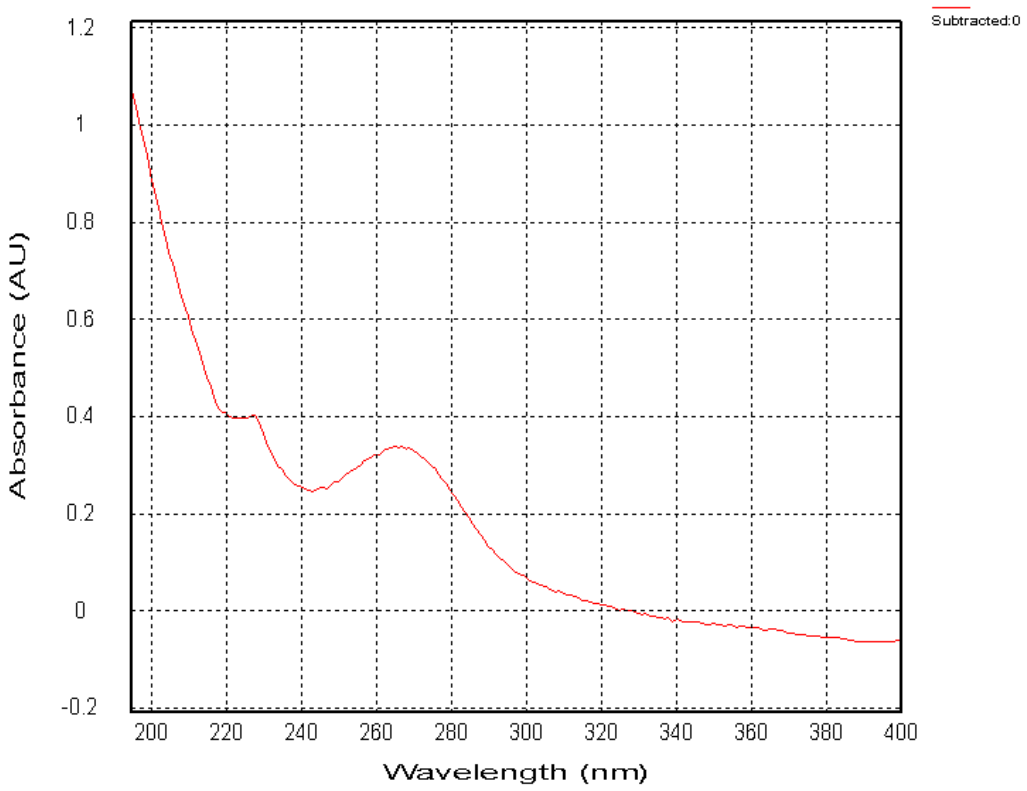

Fig. S11. Ultraviolet (UV) Spectrum of phomretone A (**1**) in MeOH.

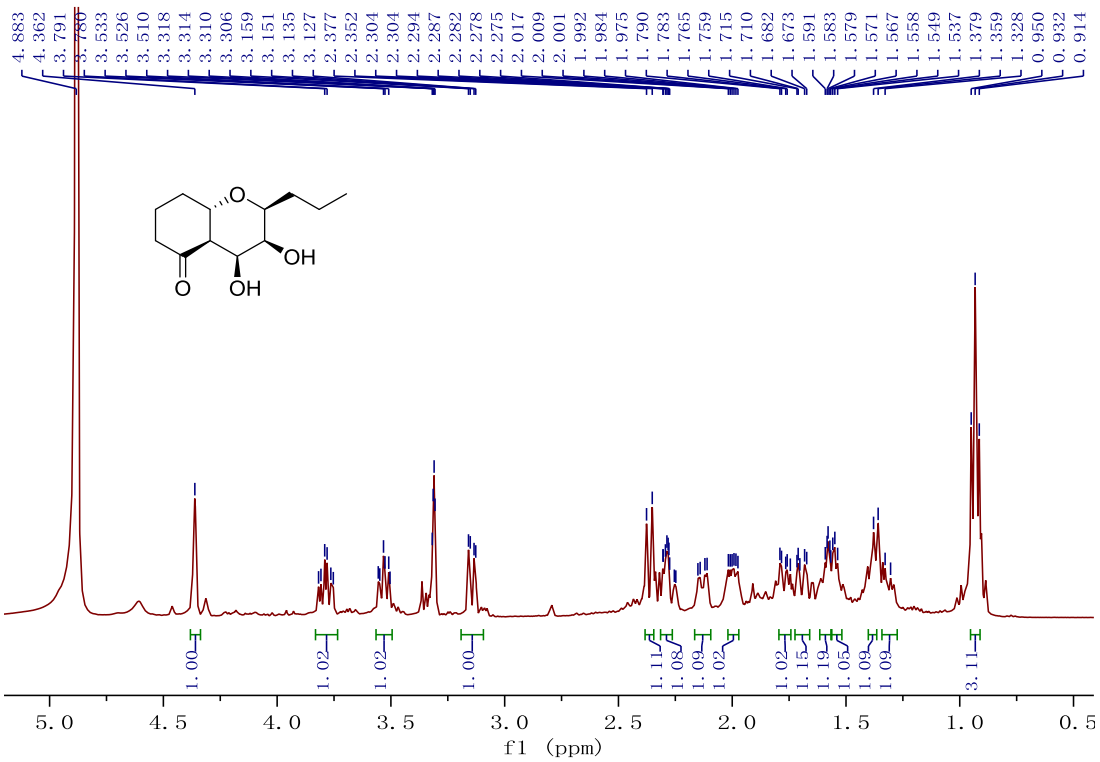

Fig. S12. ^{1}H NMR spectrum of phomretone B (**2**) in methanol-d_4 (400 MHz).

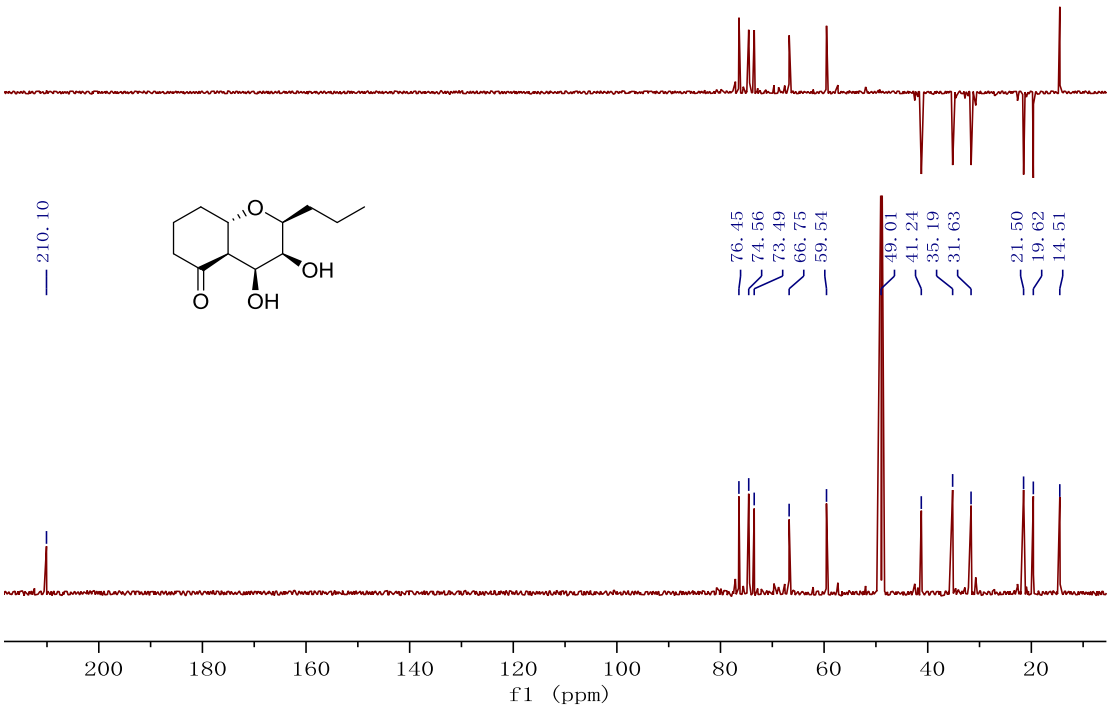

Fig. S13. ^{13}C NMR and DEPT spectrum of phomretone B (**2**) in methanol-d_4 (100 MHz).

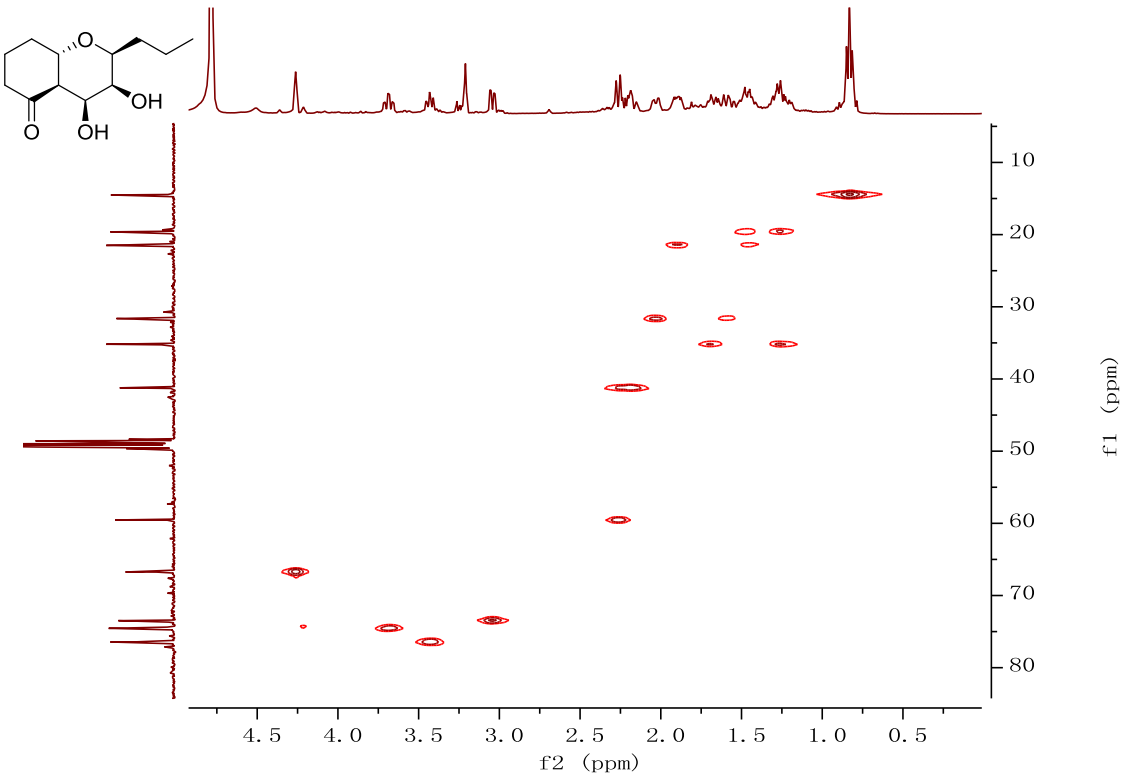

Fig. S14. HSQC spectrum of phomretone B (**2**) in methanol-d_4 (^{1}H-400 MHz).

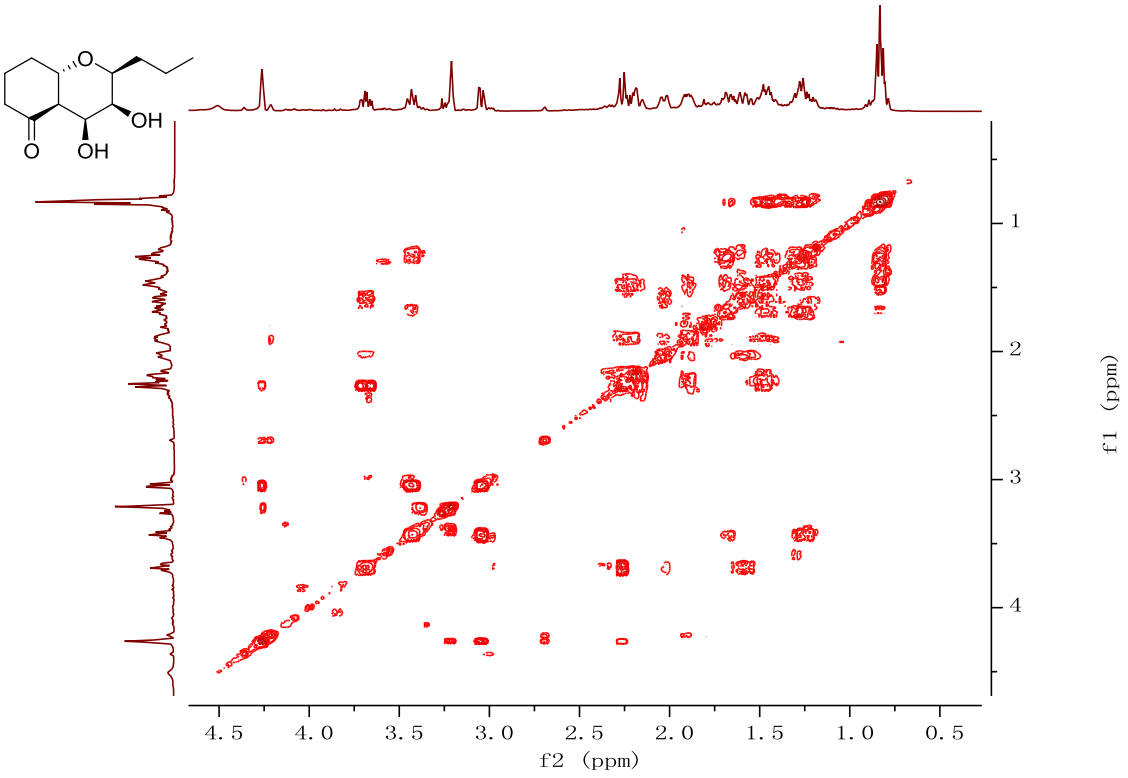

Fig. S15. ^{1}H-^{1}H COSY spectrum of phomretone B (**2**) in methanol-d_4 (400 MHz).

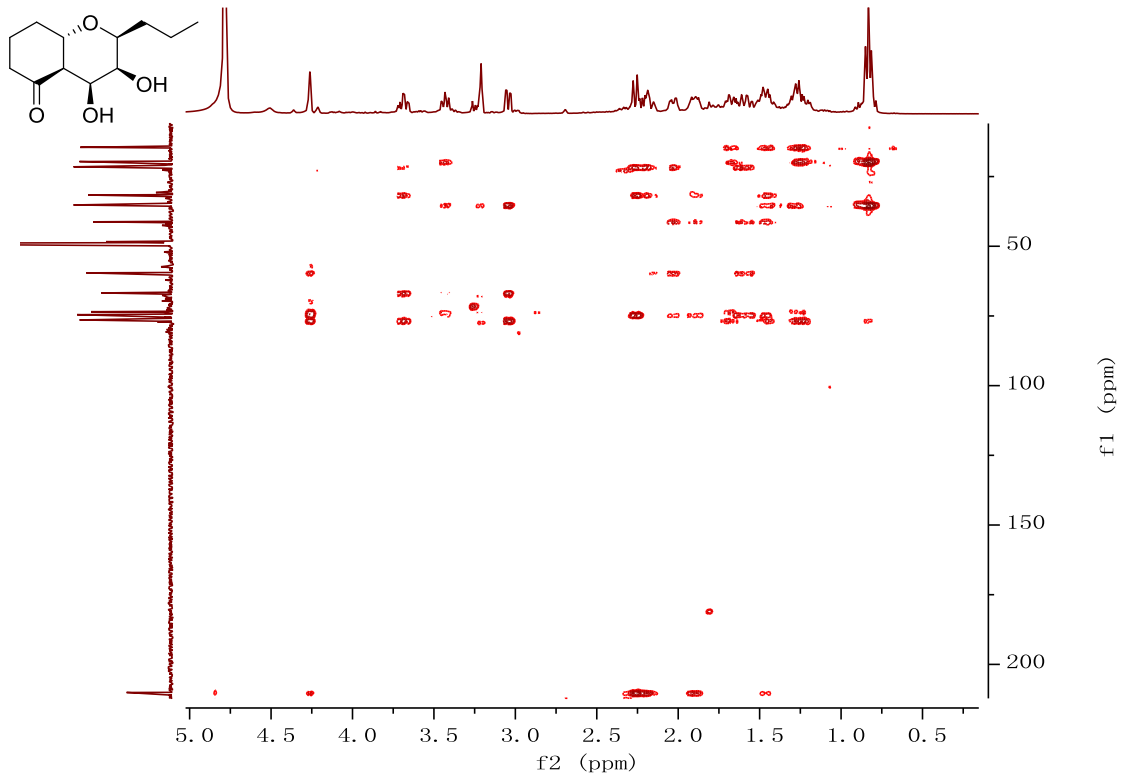

Fig. S16. HMBC spectrum of phomretone B (**2**) in methanol-d_4 (^{1}H-400 MHz).

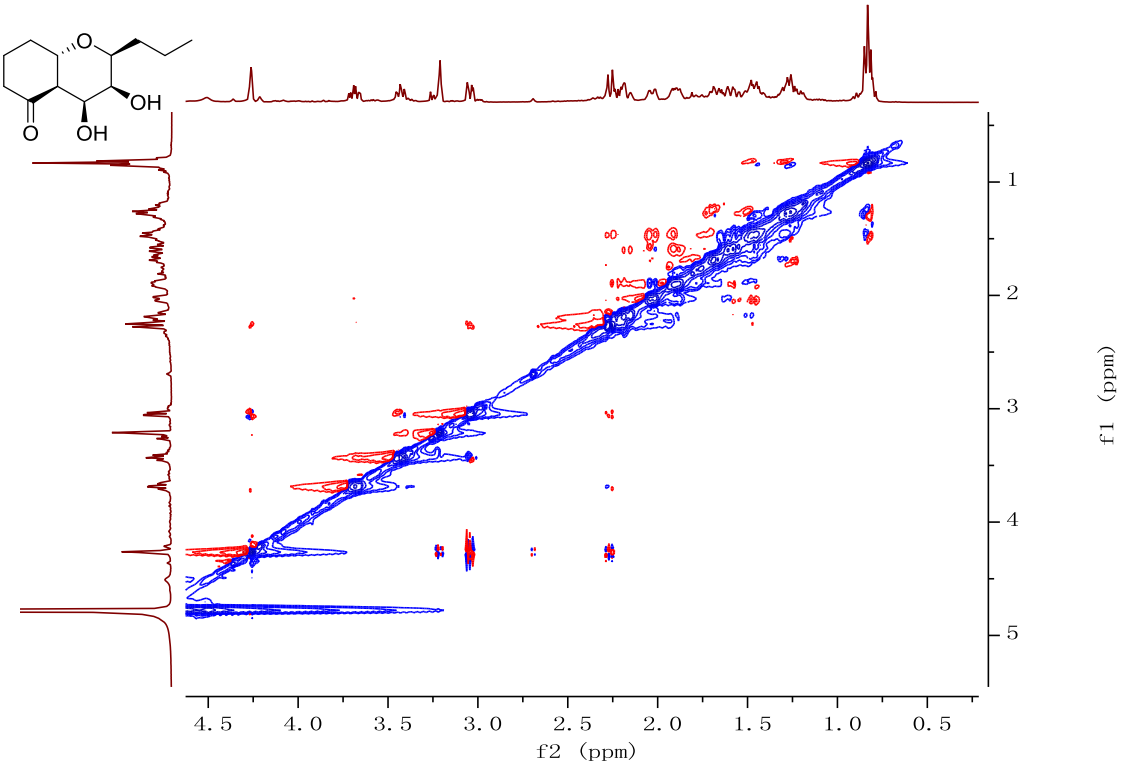

Fig. S17. ROESY spectrum of phomretone B (**2**) in methanol-d_4 (400 MHz).

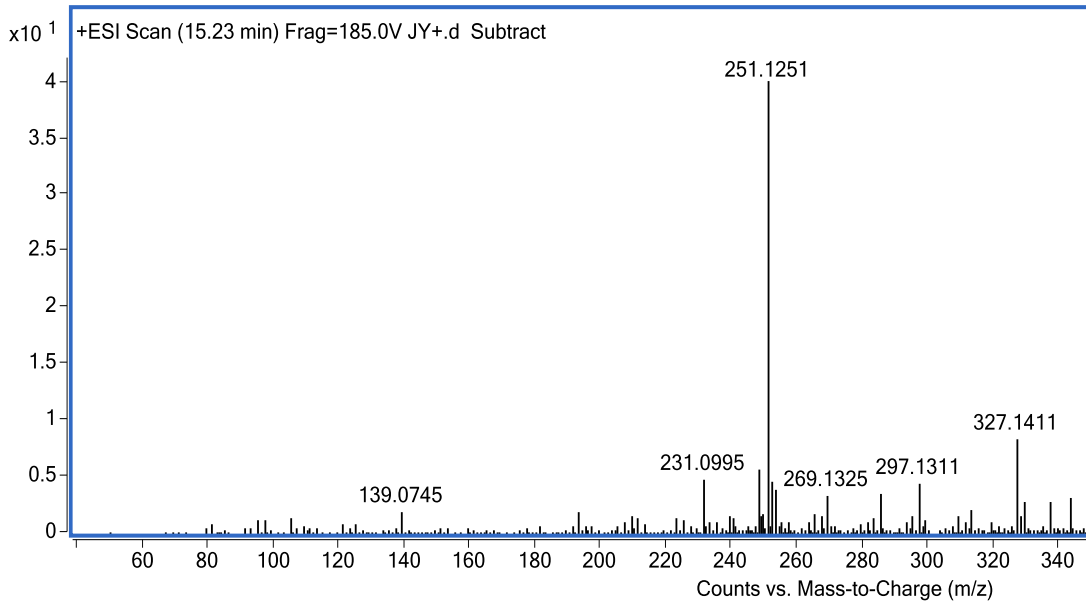

Fig. S18. (+)-HRESIMS data of phomretone B (**2**).

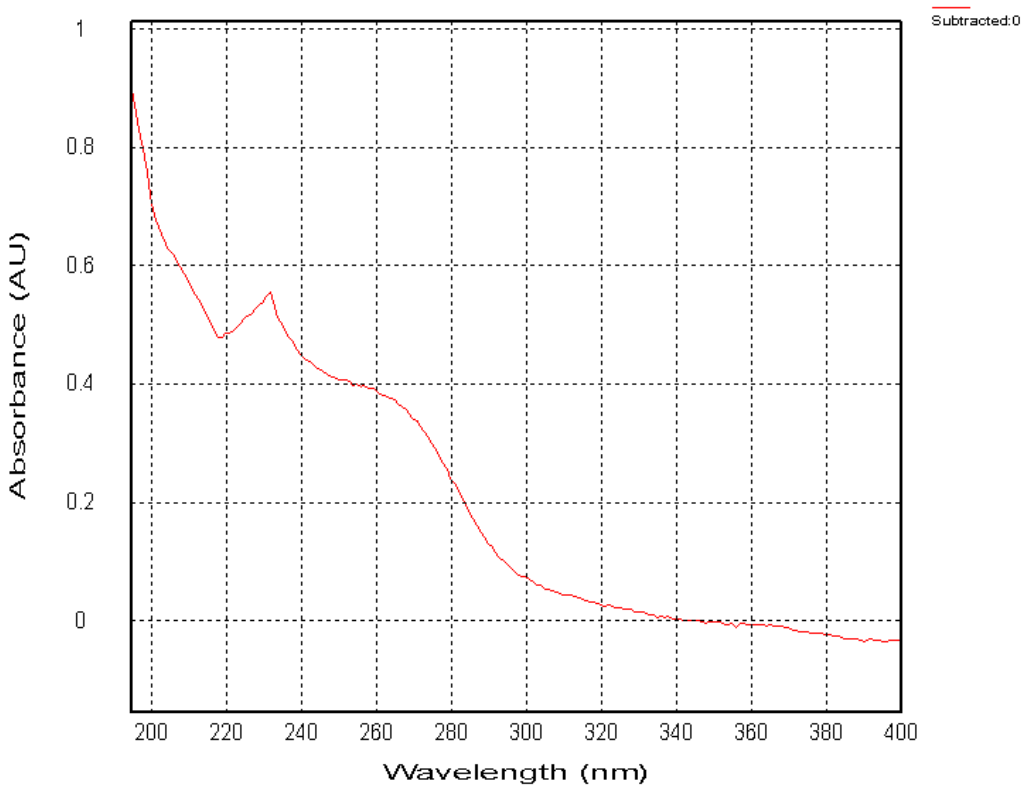

Fig. S19. UV absorption spectrum of phomretone B (**2**) in MeOH.

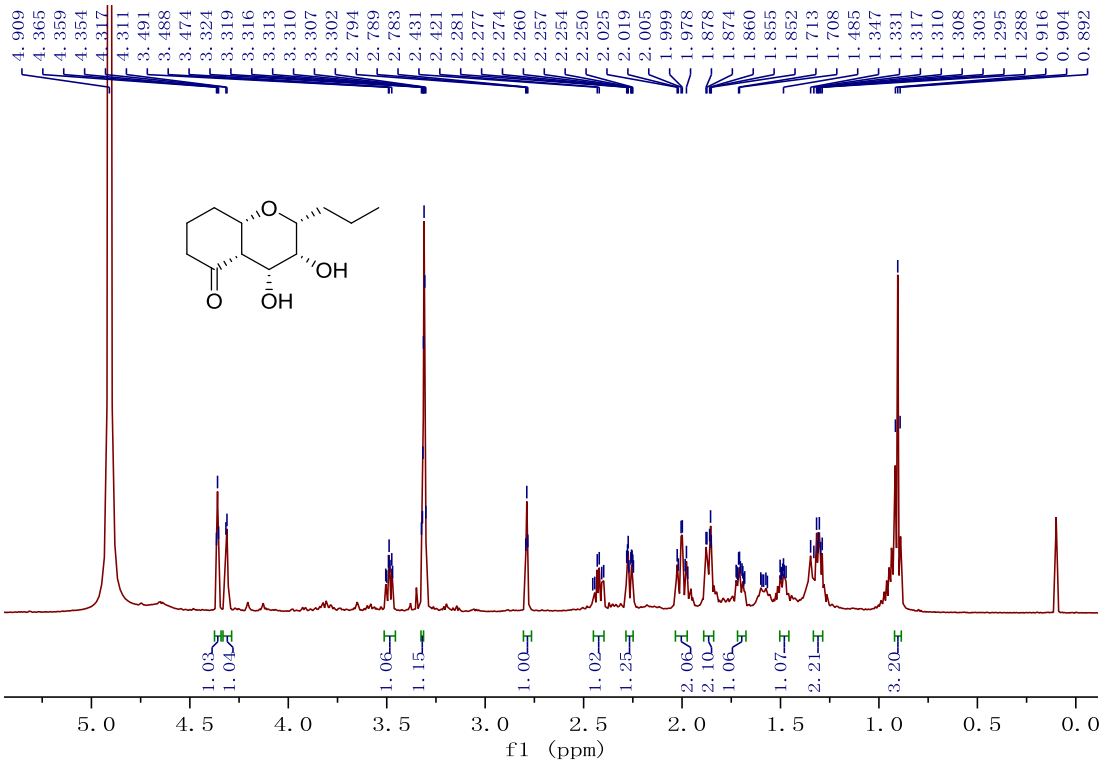

Fig. S20. ^{1}H NMR spectrum of phomretone C (**3**) in methanol-d_4 (400 MHz).

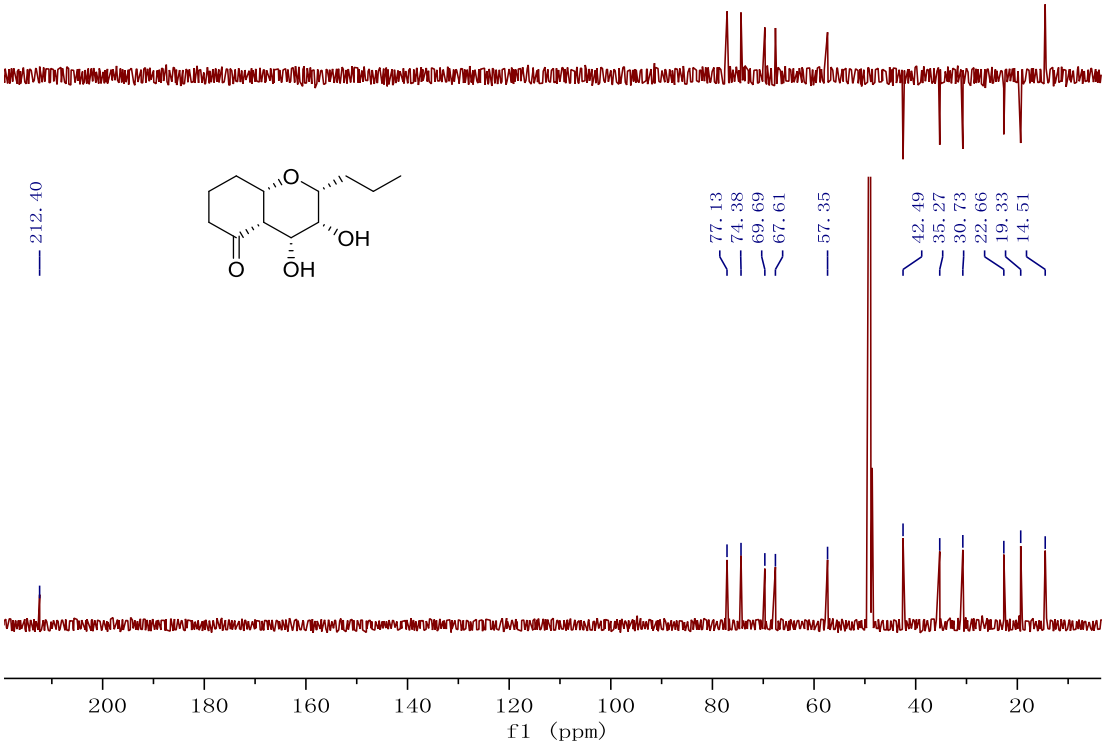

Fig. S21. ^{13}C NMR and DEPT spectrum of phomretone C (**3**) in methanol-d_4 (100 MHz).

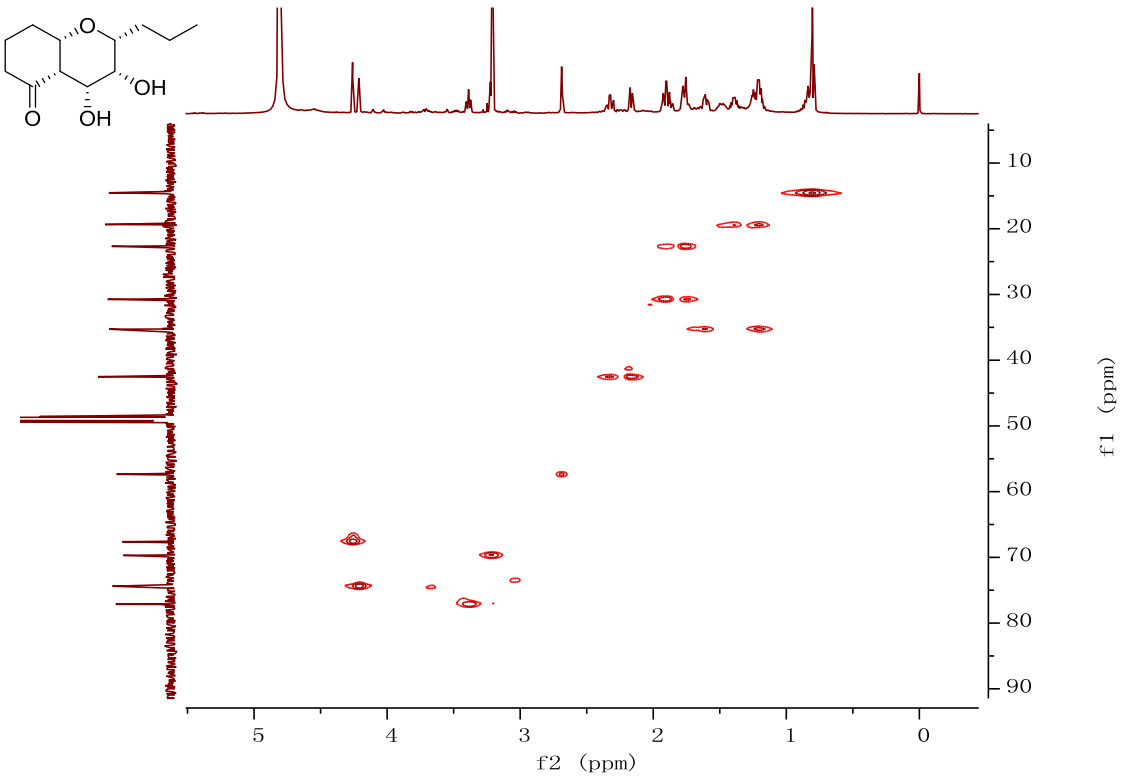

Fig. S22. HSQC spectrum of phomretone C (**3**) in methanol-d_4 (^{1}H-400 MHz).

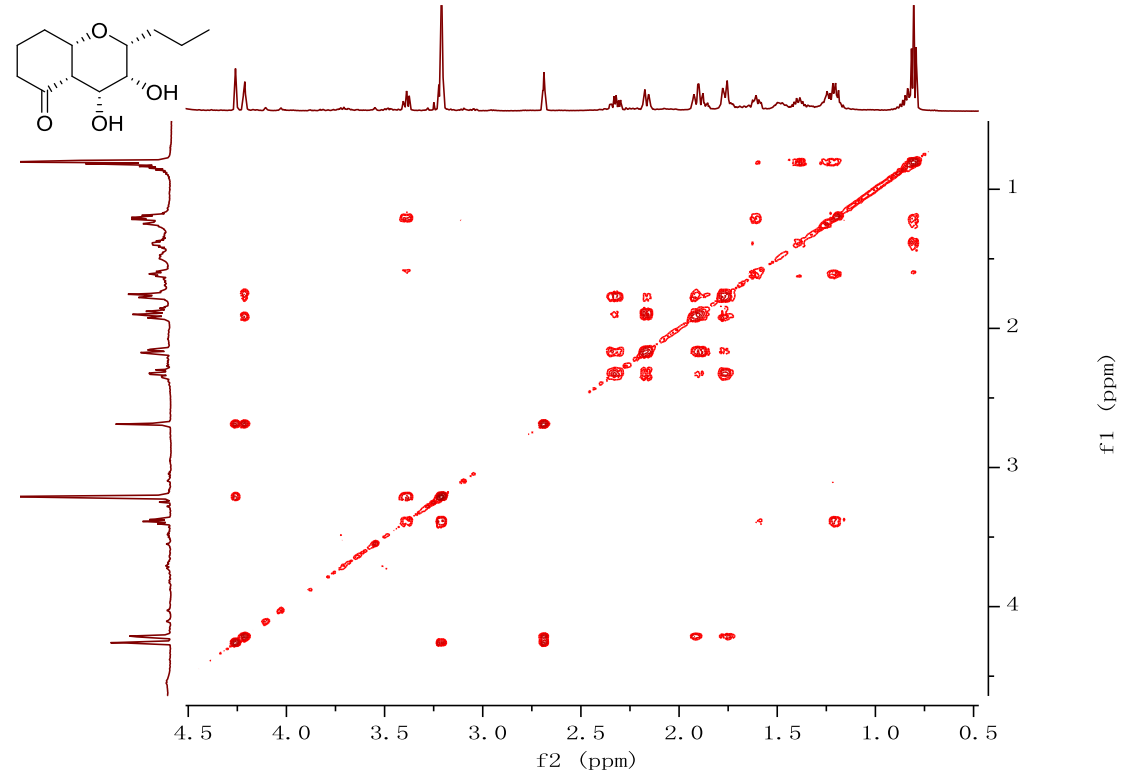

Fig. S23. ^{1}H-^{1}H COSY spectrum of phomretone C (**3**) in methanol-d_4 (400 MHz).

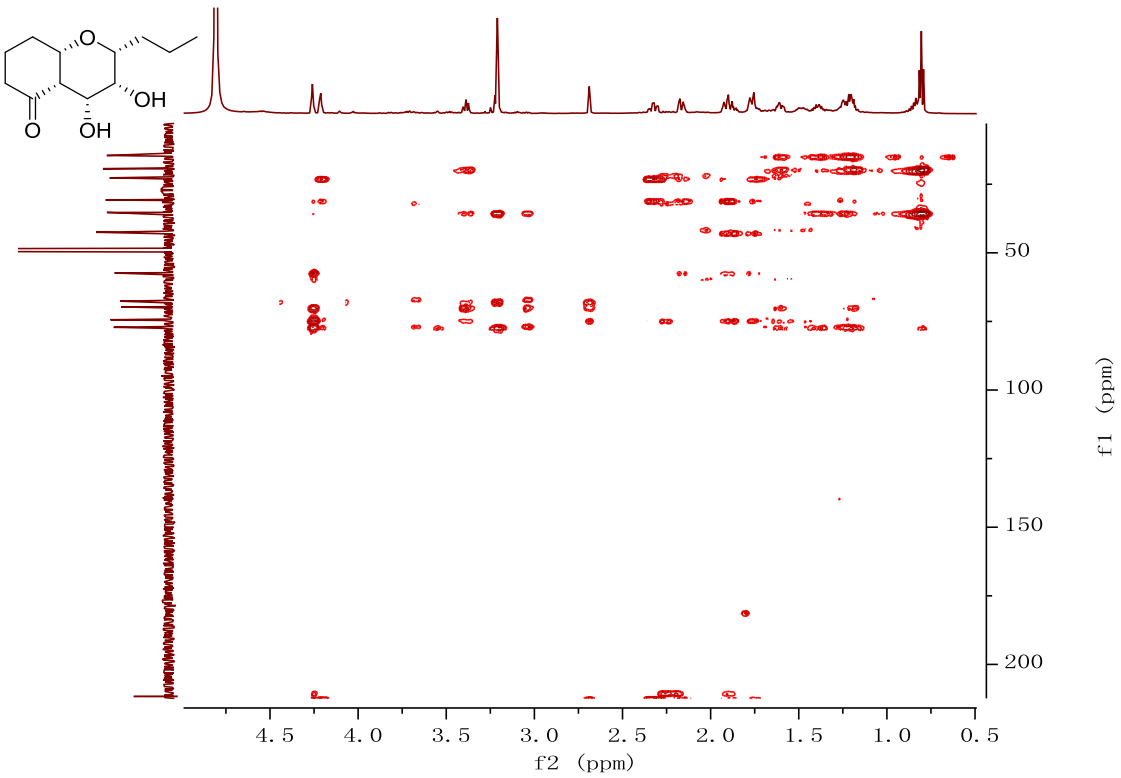

Fig. S24. HMBC spectrum of phomretone C (**3**) in methanol-d_4 (^{1}H-400 MHz).

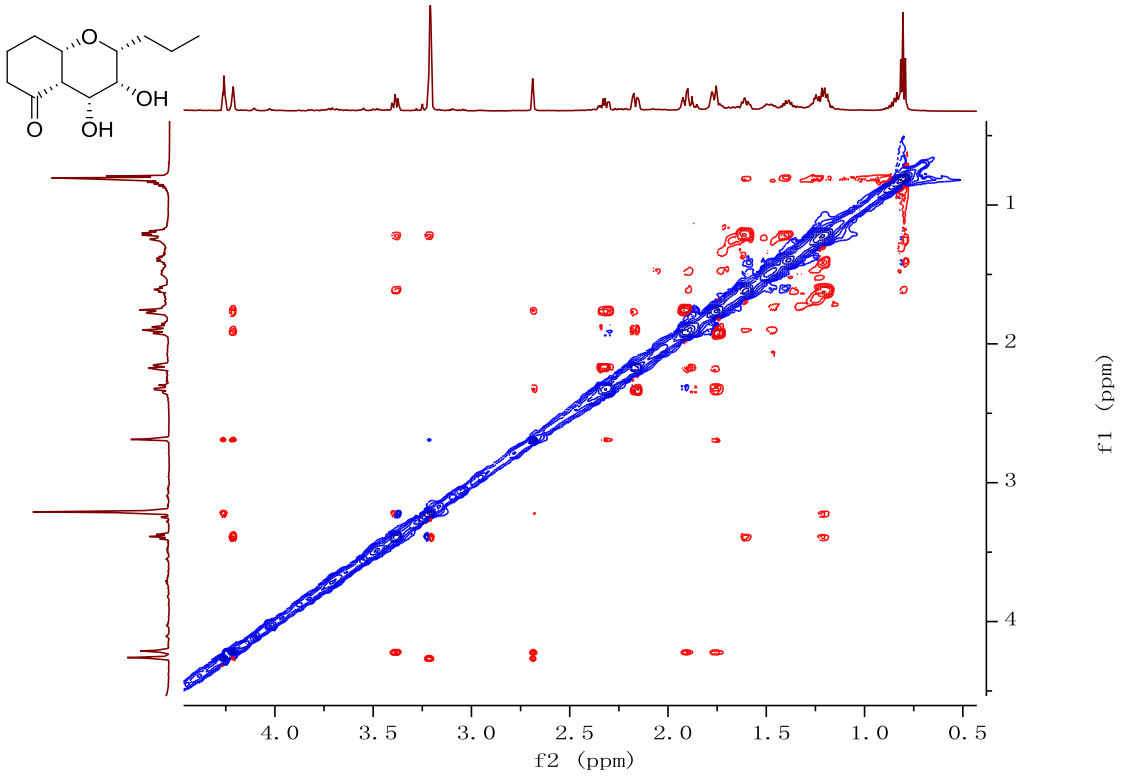

Fig. S25. ROESY spectrum of phomretone C (**3**) in methanol-d_4 (400 MHz).

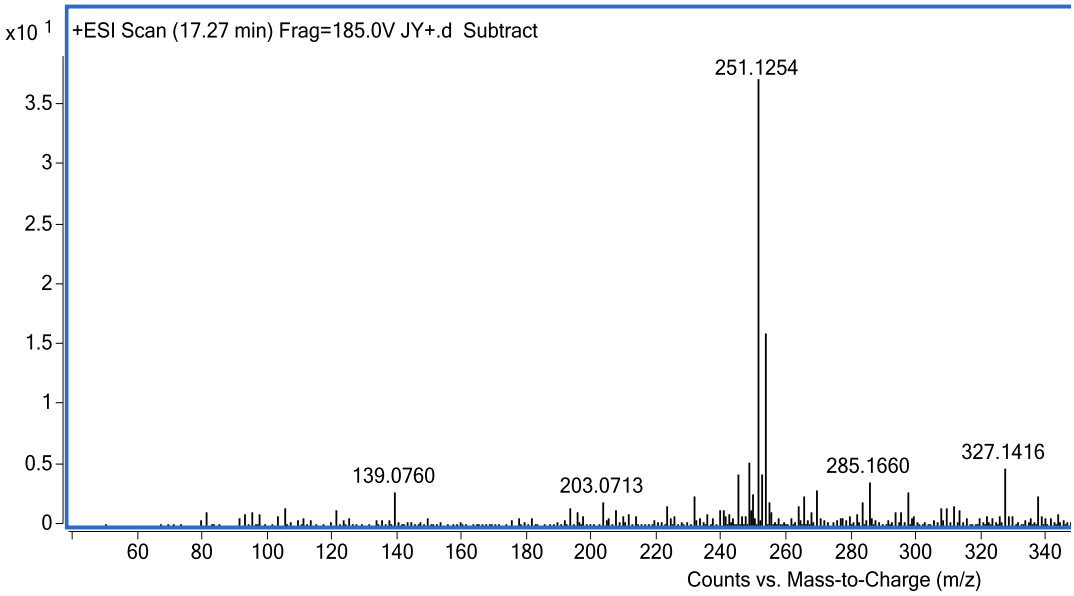

Fig. S26. (+)-HRESIMS data of phomretone C (**3**).

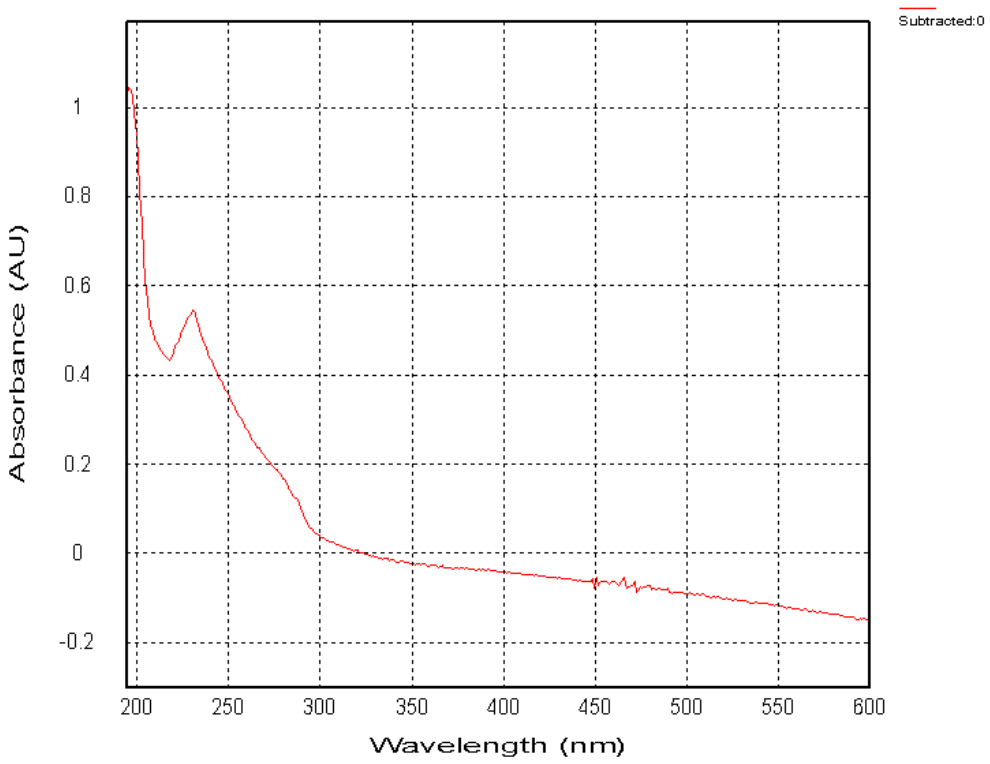

Fig. S27. UV absorption spectrum of phomretone C (**3**) in MeOH.

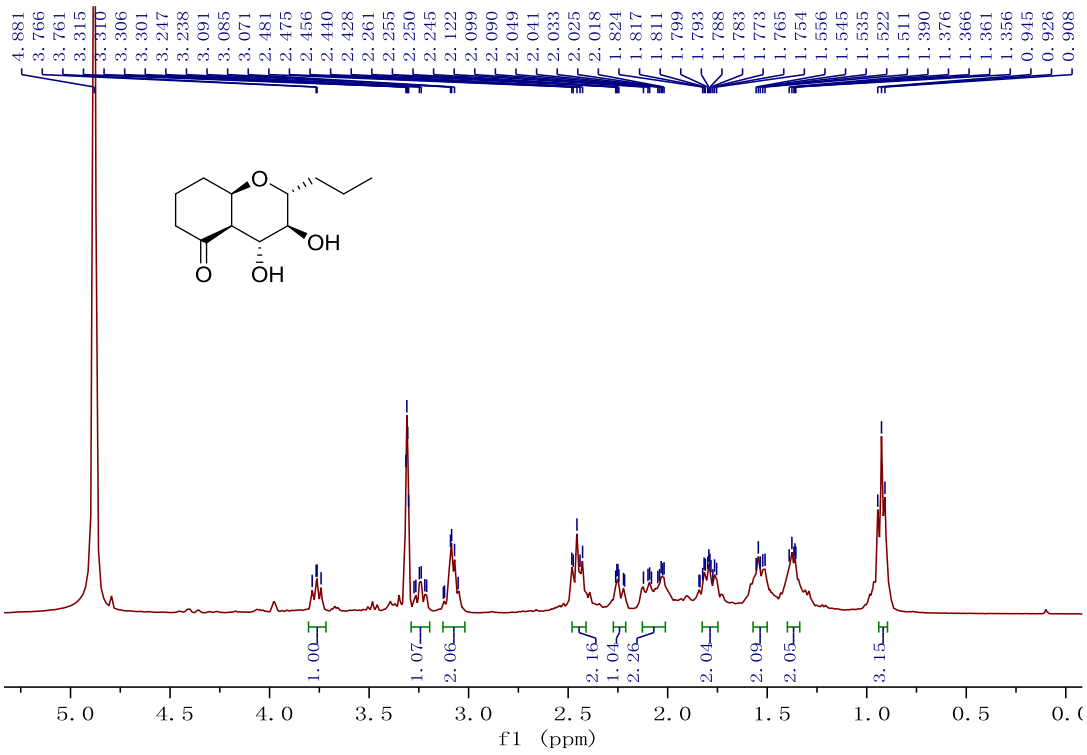

Fig. S28. ^{1}H NMR spectrum of phomretone D (**4**) in methanol-d_4 (400 MHz).

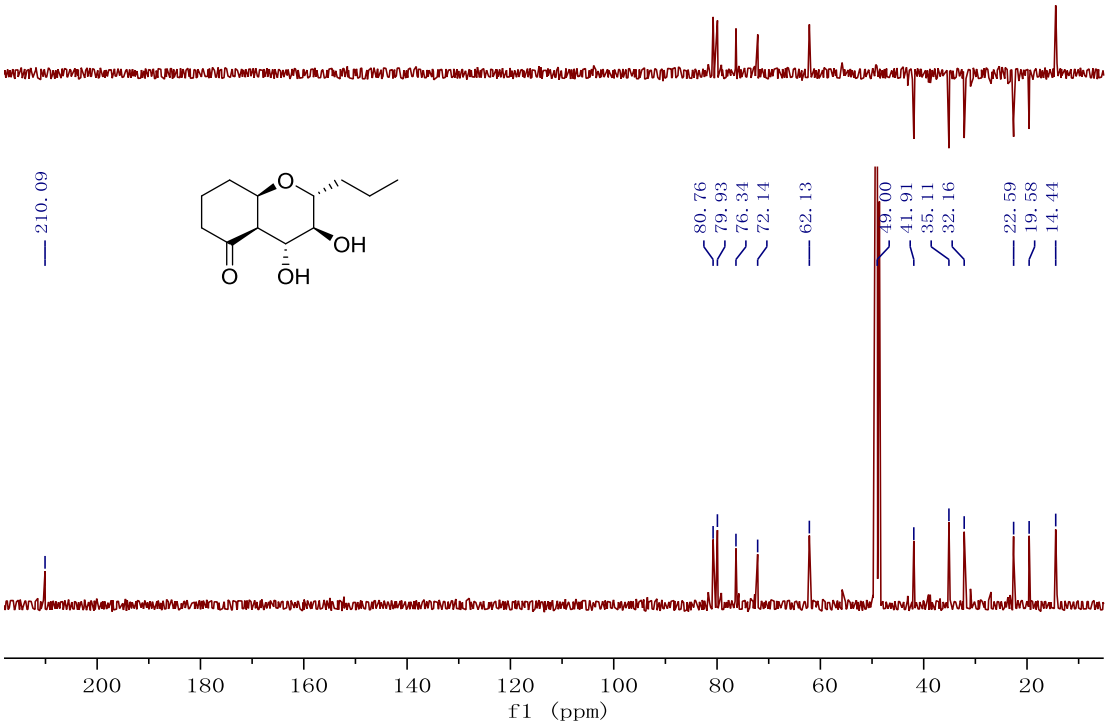

Fig. S29. ^{13}C NMR and DEPT spectrum of phomretone D (**4**) in methanol-d_4 (100 MHz).

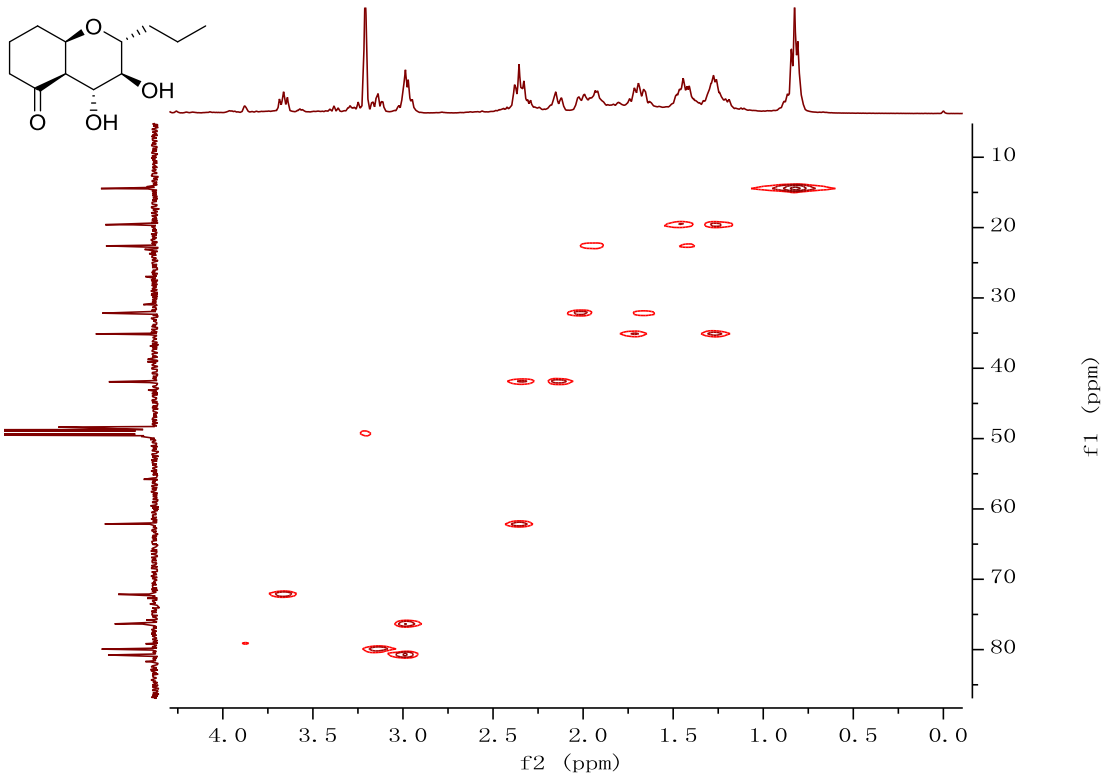

Fig. S30. HSQC spectrum of phomretone D (**4**) in methanol-d_4 (^{1}H-400 MHz).

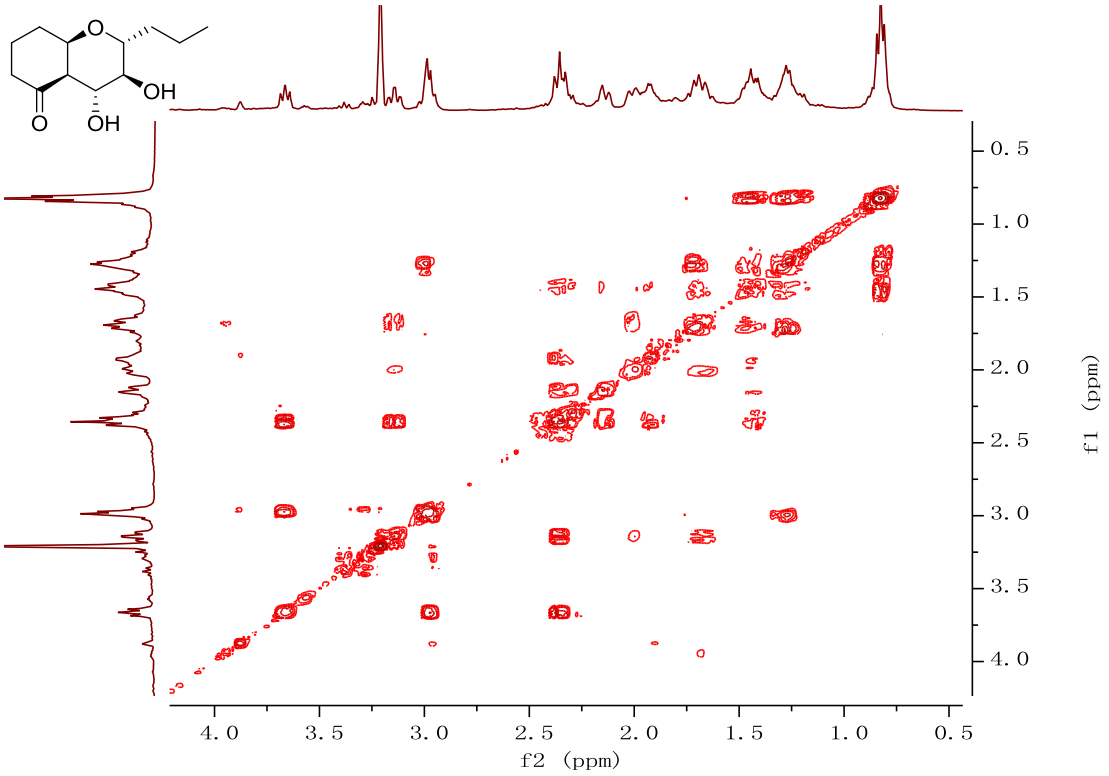

Fig. S31. ^{1}H-^{1}H COSY spectrum of phomretone D (**4**) in methanol-d_4 (400 MHz).

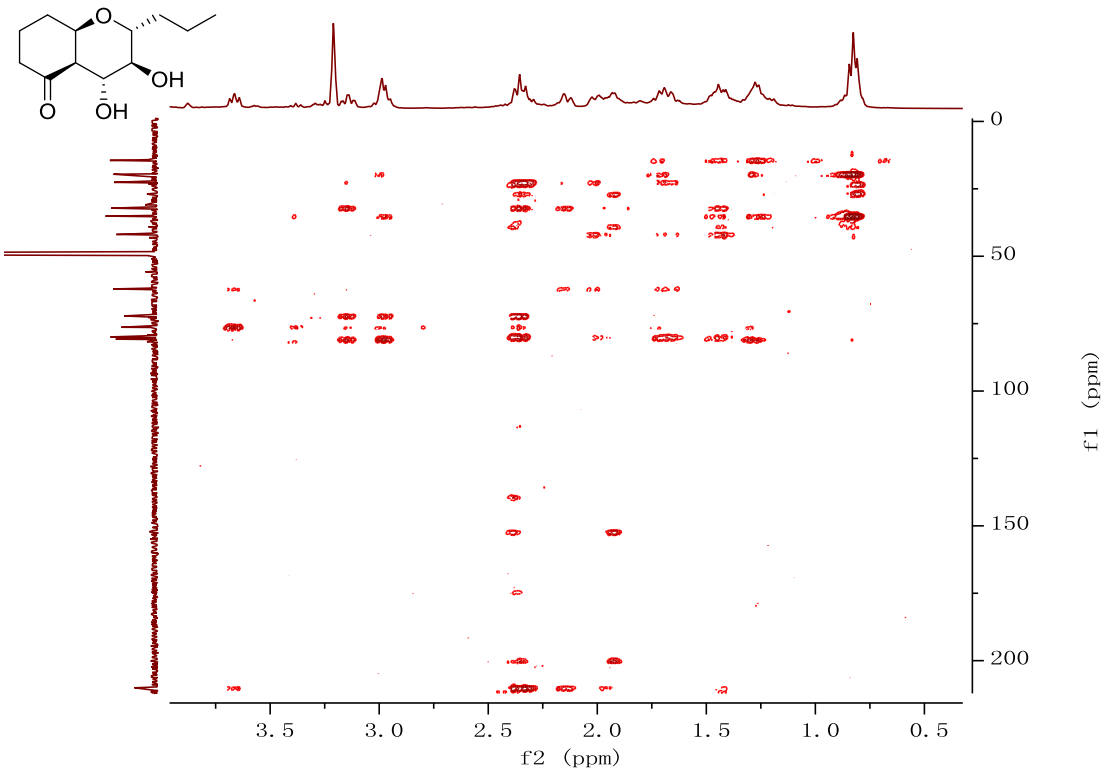

Fig. S32. HMBC spectrum of phomretone D (**4**) in methanol-d_4 (^{1}H-400 MHz).

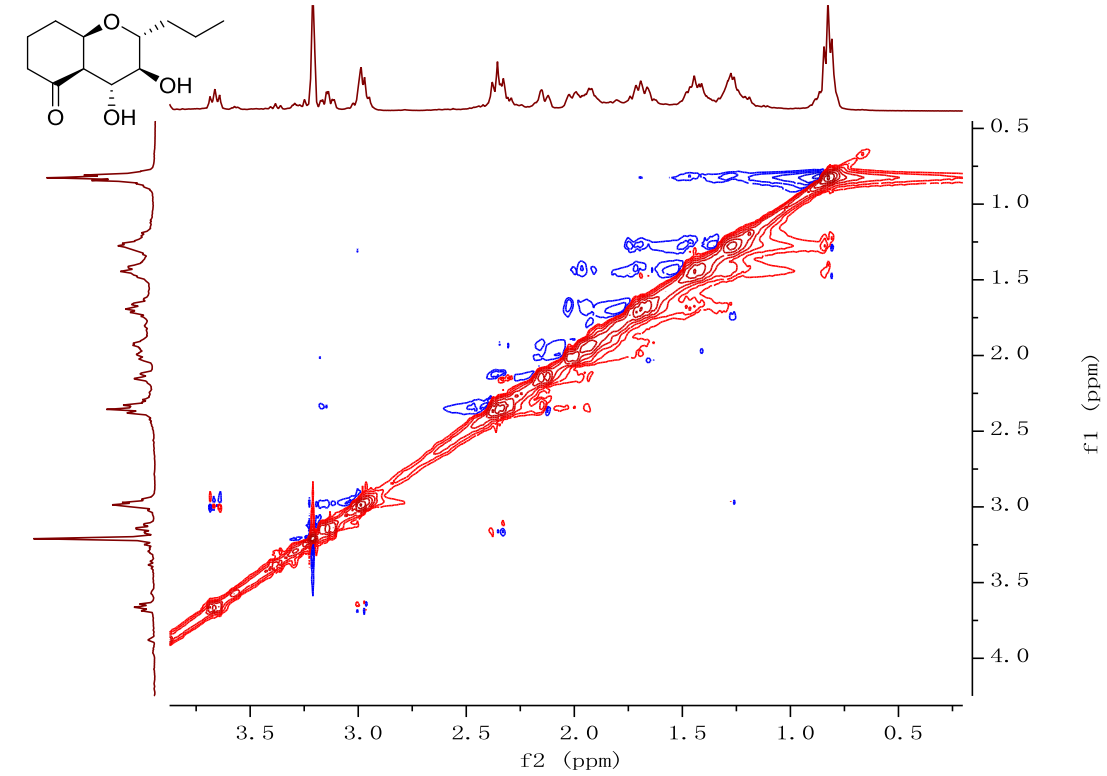

Fig. S33. ROESY spectrum of phomretone D (**4**) in methanol-d_4 (400 MHz).

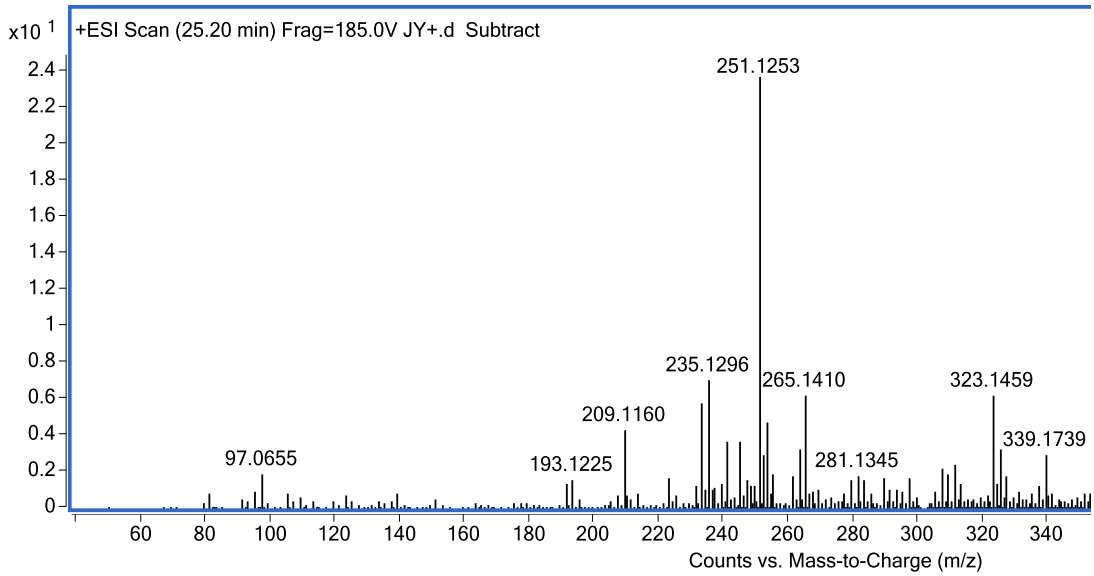

Fig. S34. (+)-HRESIMS data of phomretone D (**4**).

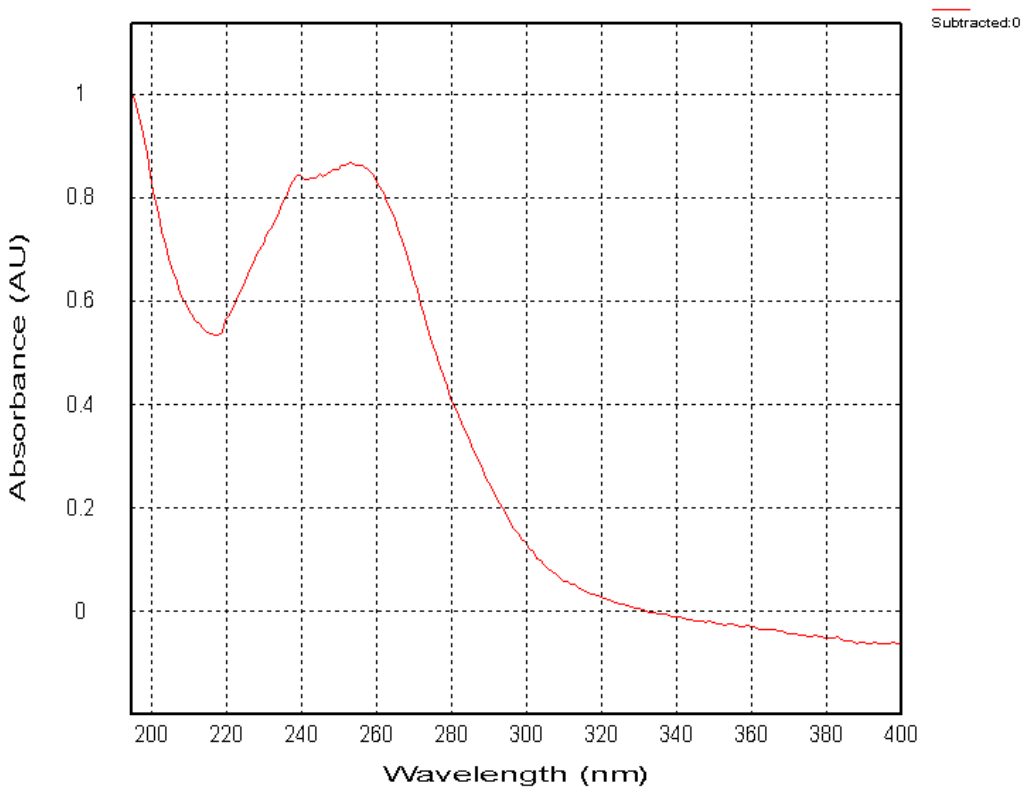

Fig. S35. UV absorption spectrum of phomretone D (**4**) in MeOH.

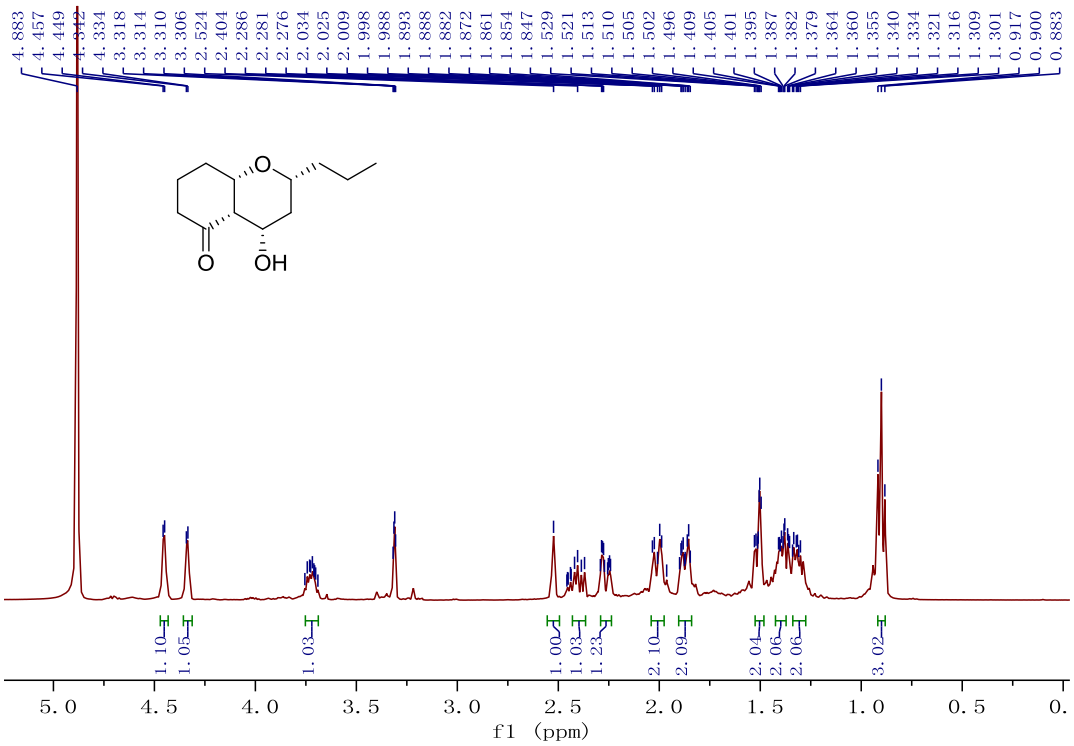

Fig. S36. ^{1}H NMR spectrum of phomretone E (**5**) in methanol-d_4 (400 MHz).

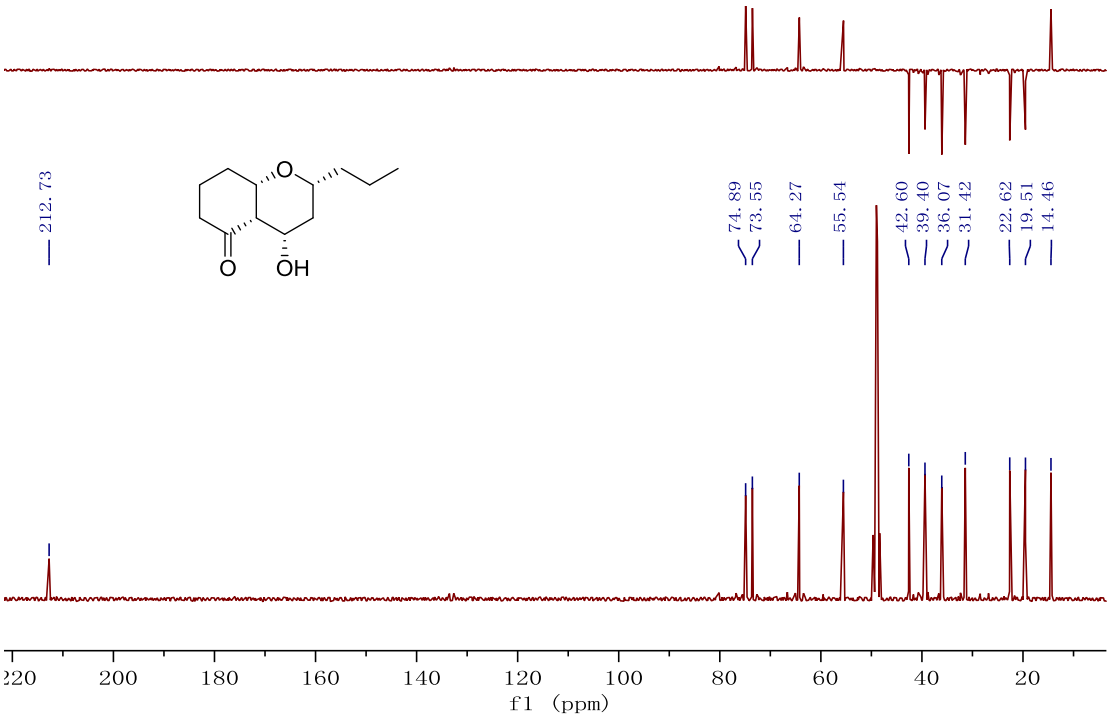

Fig. S37. ^{13}C NMR and DEPT spectrum of phomretone E (**5**) in methanol-d_4 (100 MHz).

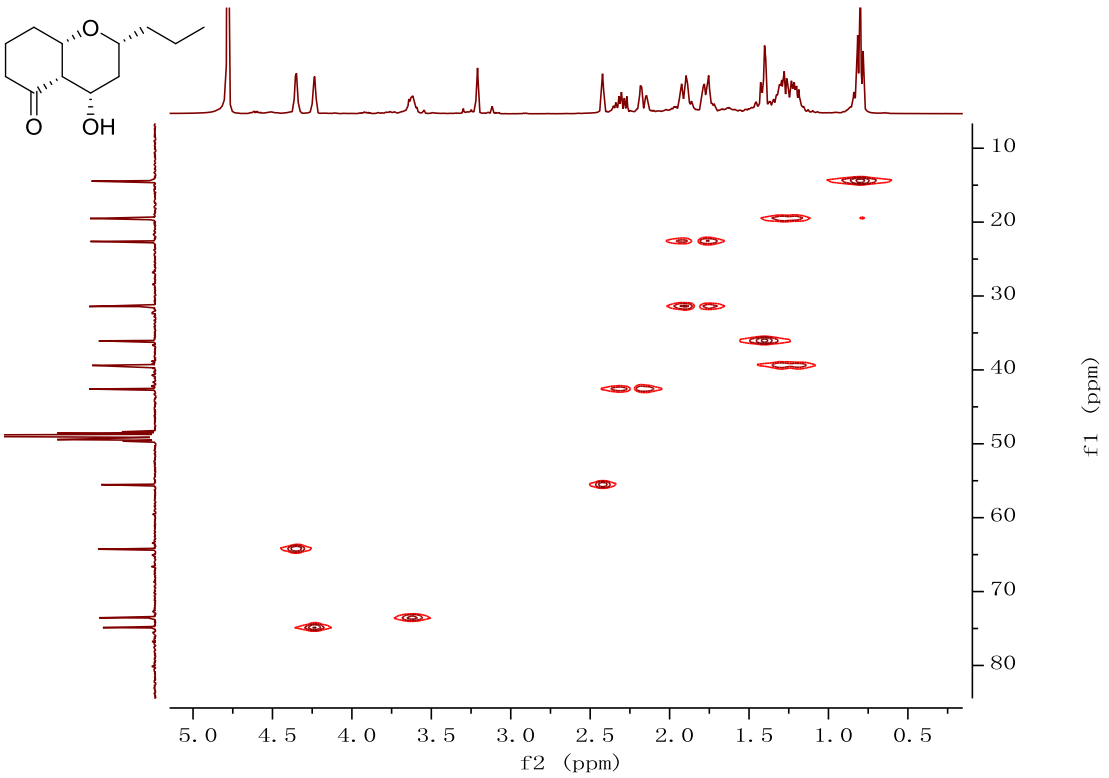

Fig. S38. HSQC spectrum of phomretone E (**5**) in methanol-d_4 (^{1}H-400 MHz).

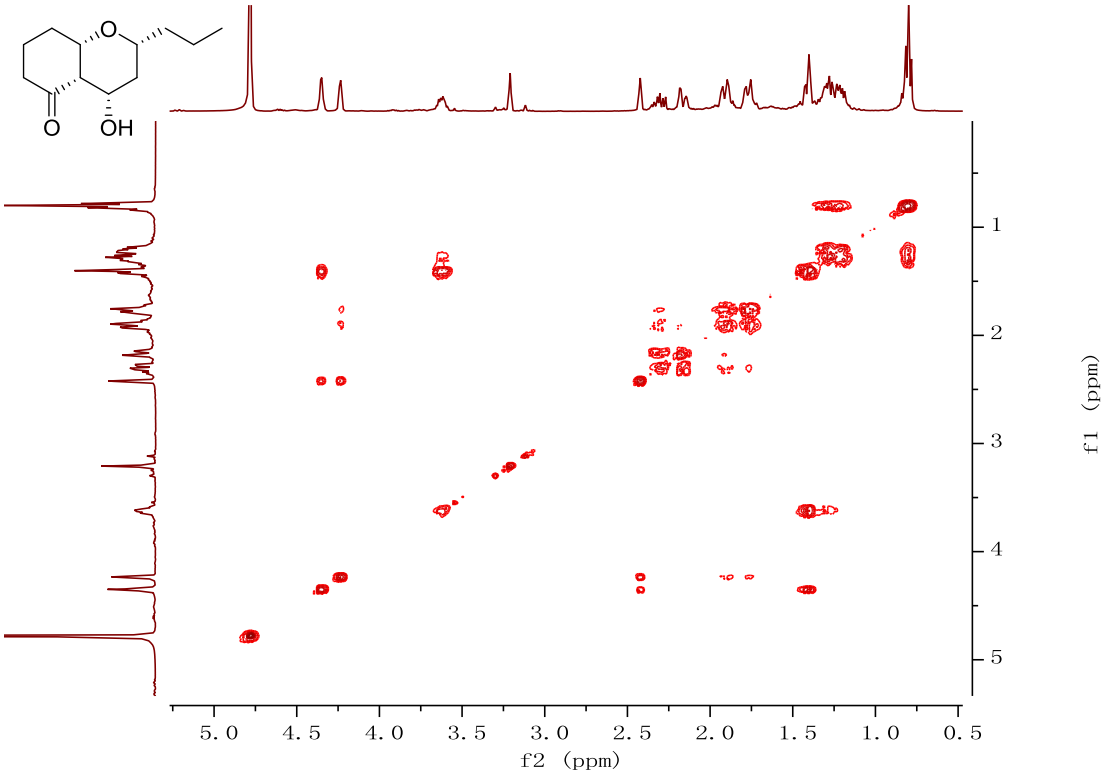

Fig. S39. ^{1}H-^{1}H COSY spectrum of phomretone E (**5**) in methanol-d_4 (400 MHz).

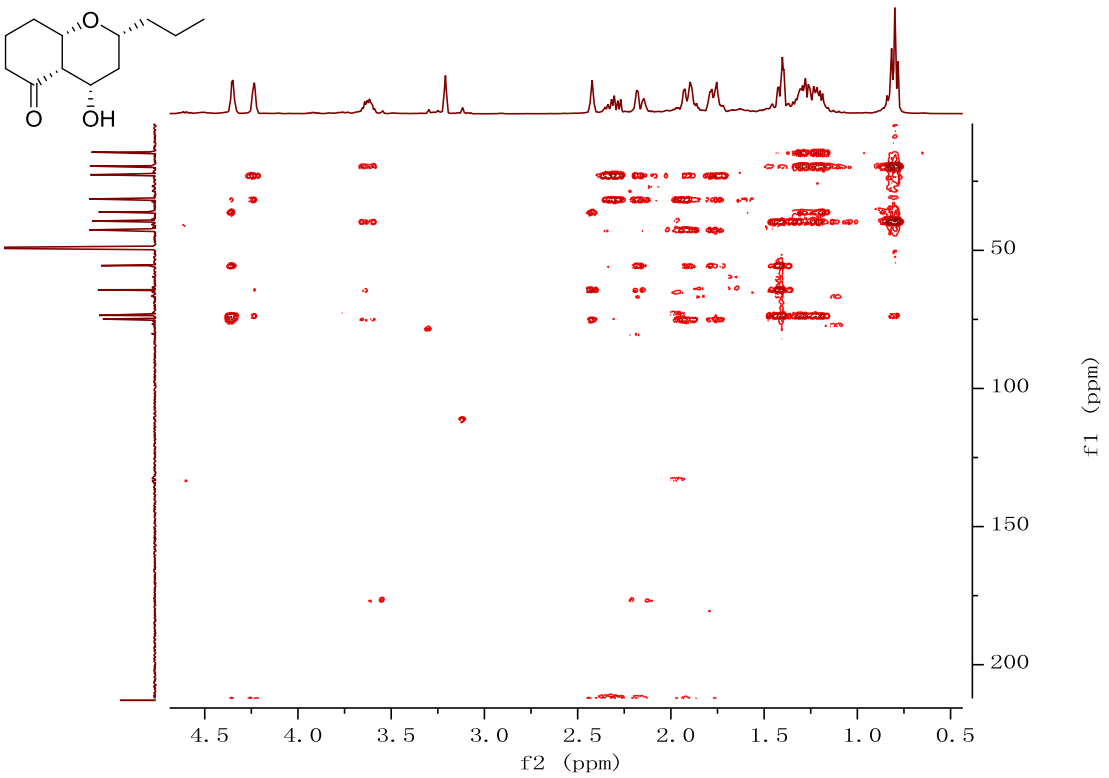

Fig. S40. HMBC spectrum of phomretone E (**5**) in methanol-d_4 (^{1}H-400 MHz).

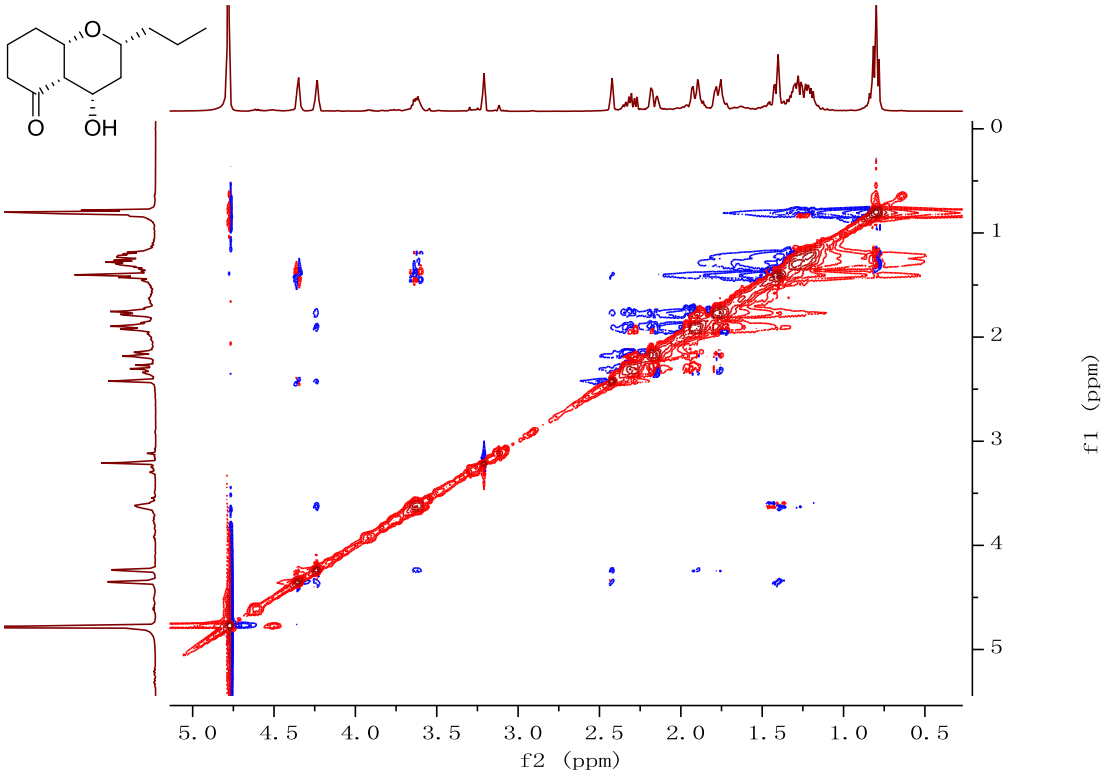

Fig. S41. ROESY spectrum of phomretone E (**5**) in methanol-d_4 (400 MHz).

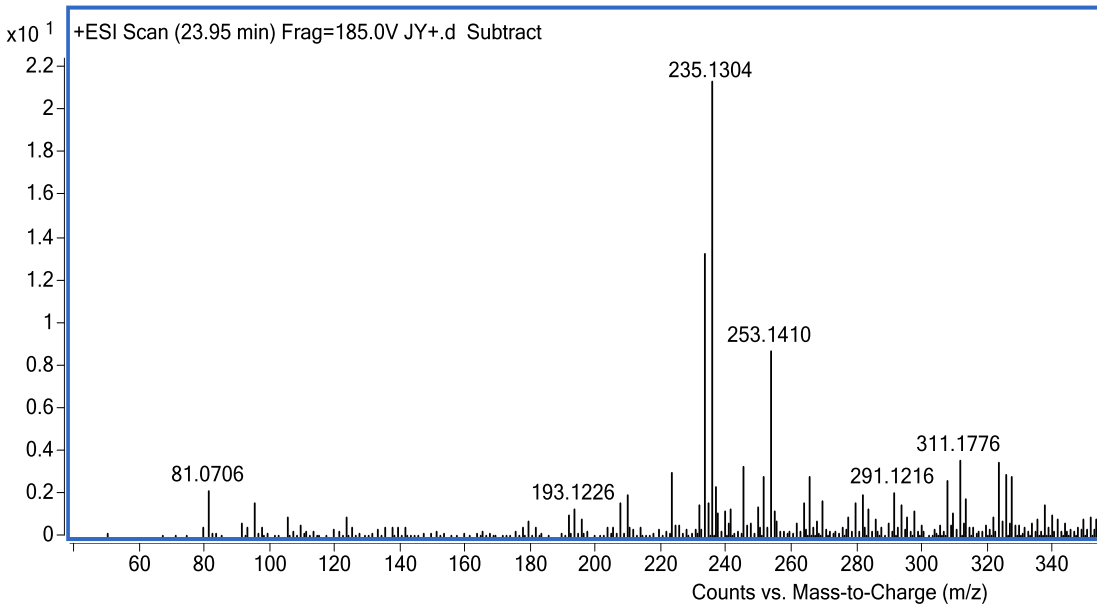

Fig. S42. (+)-HRESIMS data of phomretone E (**5**).

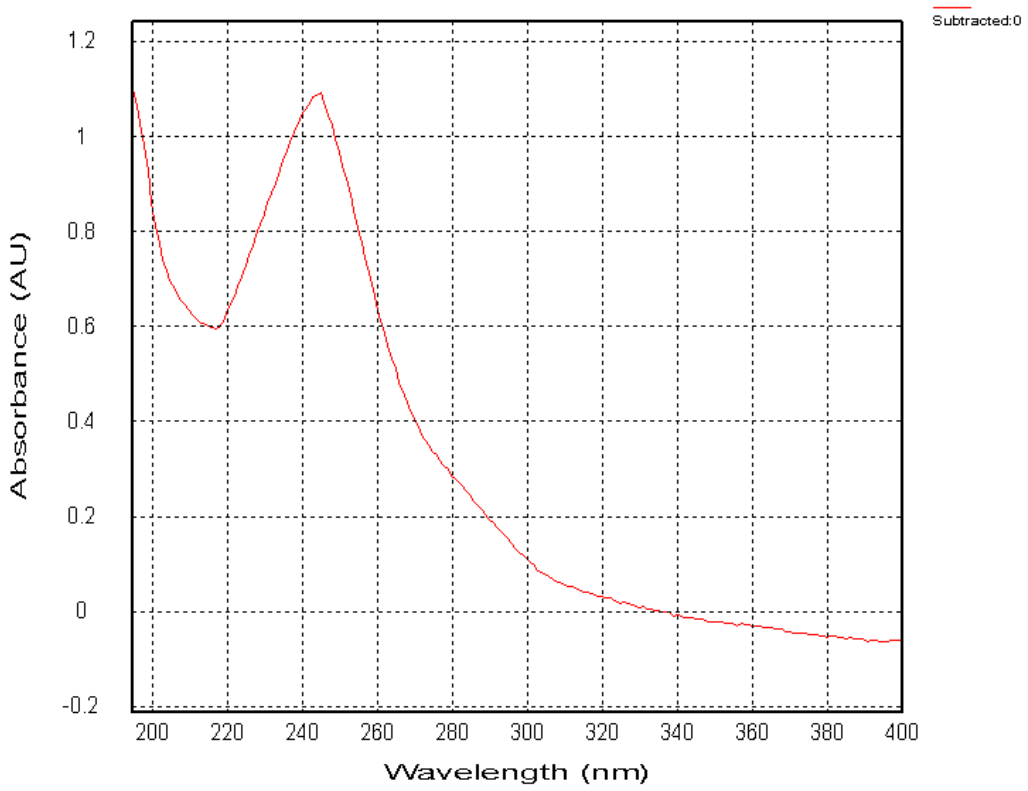

Fig. S43. UV absorption spectrum of phomretone E (**5**) in MeOH.

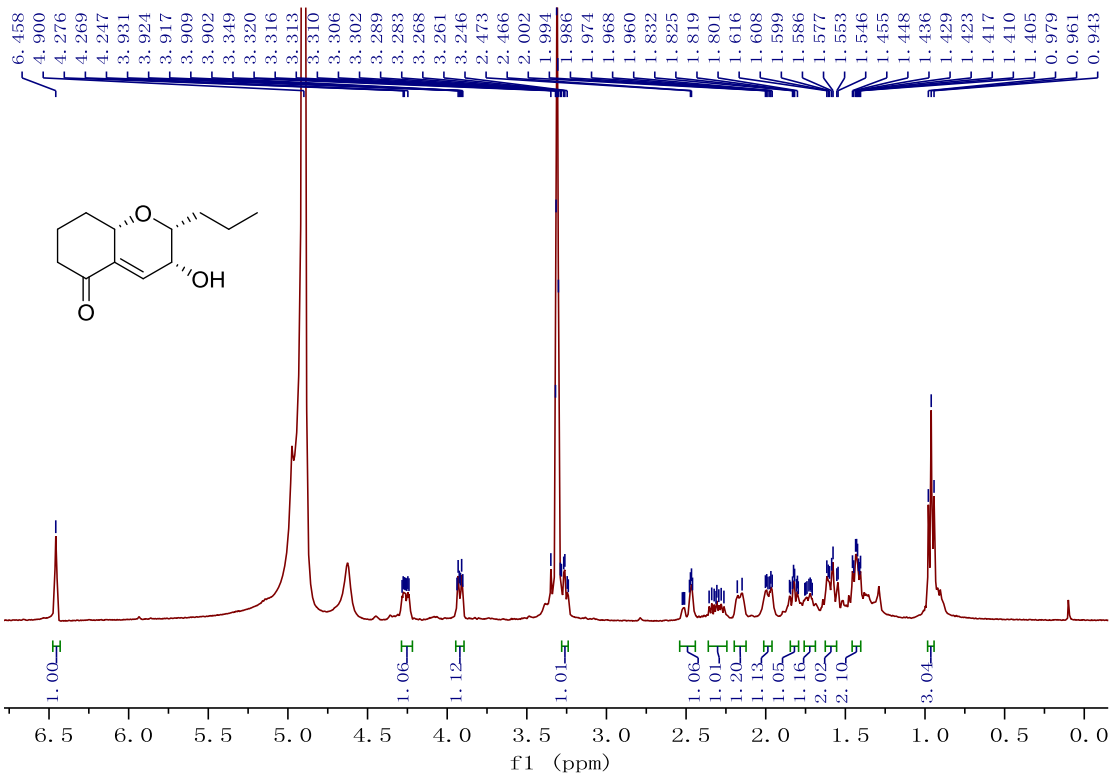

Fig. S44. ^{1}H NMR spectrum of phomretone F (**6**) in methanol-d_4 (400 MHz).

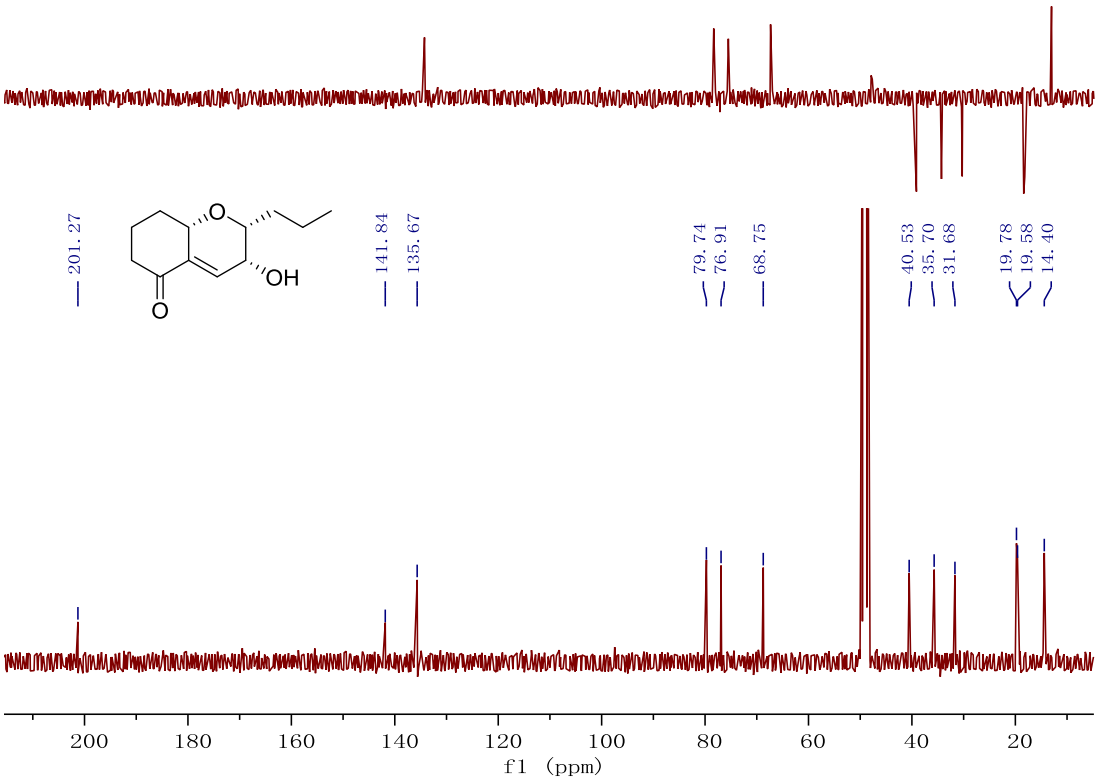

Fig. S45. ^{13}C NMR and DEPT spectrum of phomretone F (**6**) in methanol-d_4 (100 MHz).

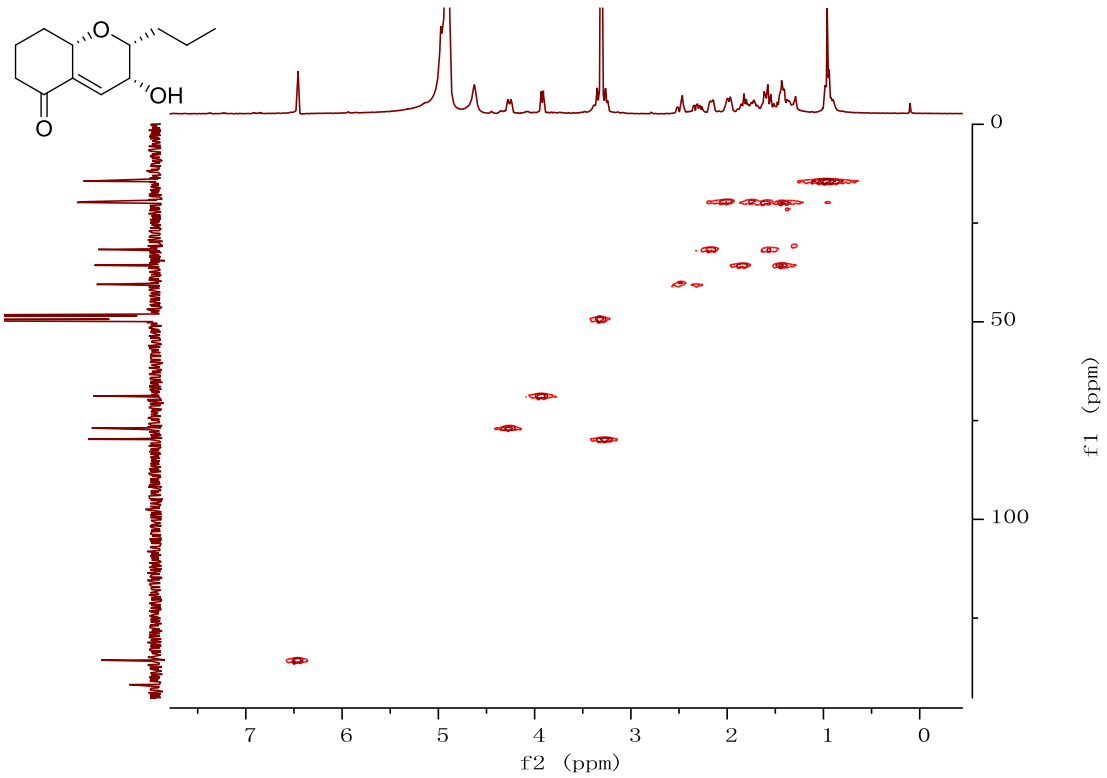

Fig. S46. HSQC spectrum of phomretone F (**6**) in methanol-d_4 (^{1}H-400 MHz).

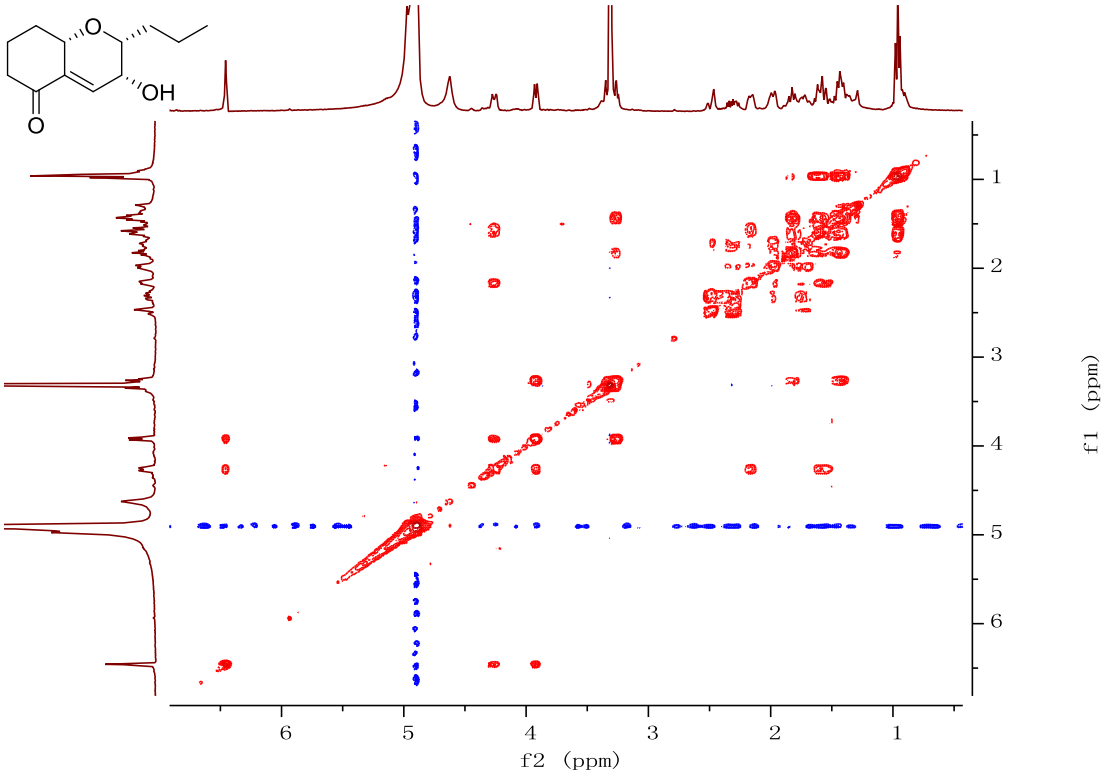

Fig. S47. ^{1}H-^{1}H COSY spectrum of phomretone F (**6**) in methanol-d_4 (400 MHz).

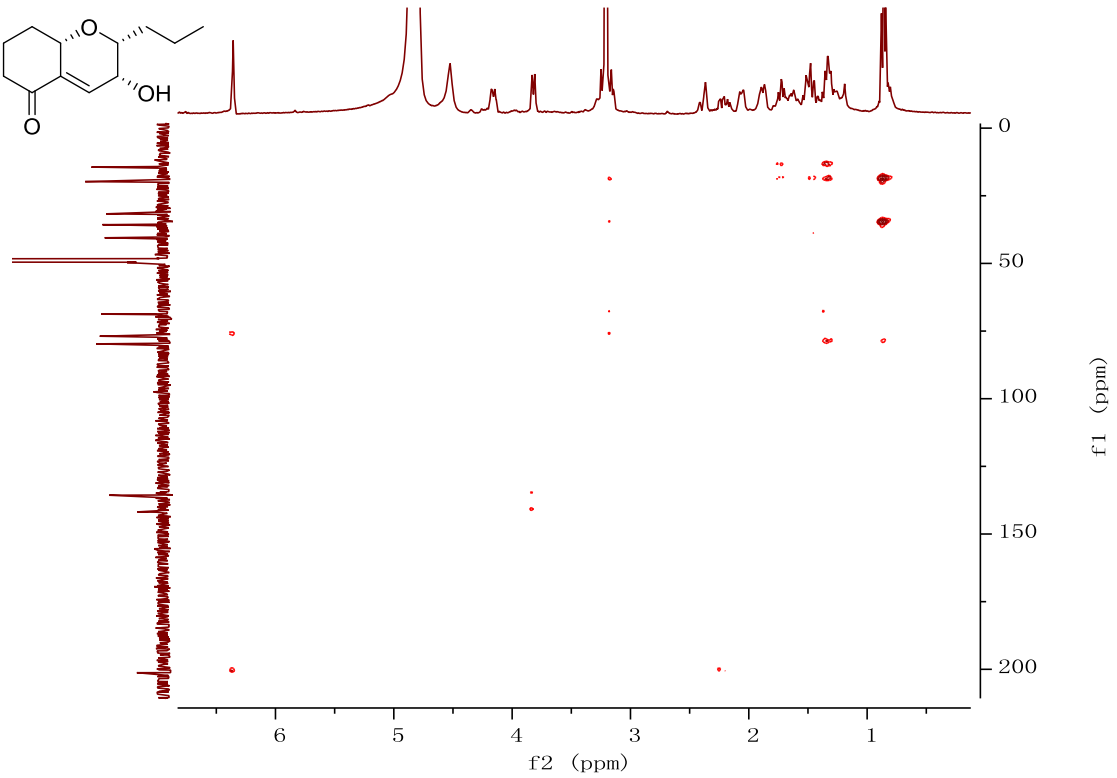

Fig. S48. HMBC spectrum of phomretone F (**6**) in methanol-d_4 (^{1}H-400 MHz).

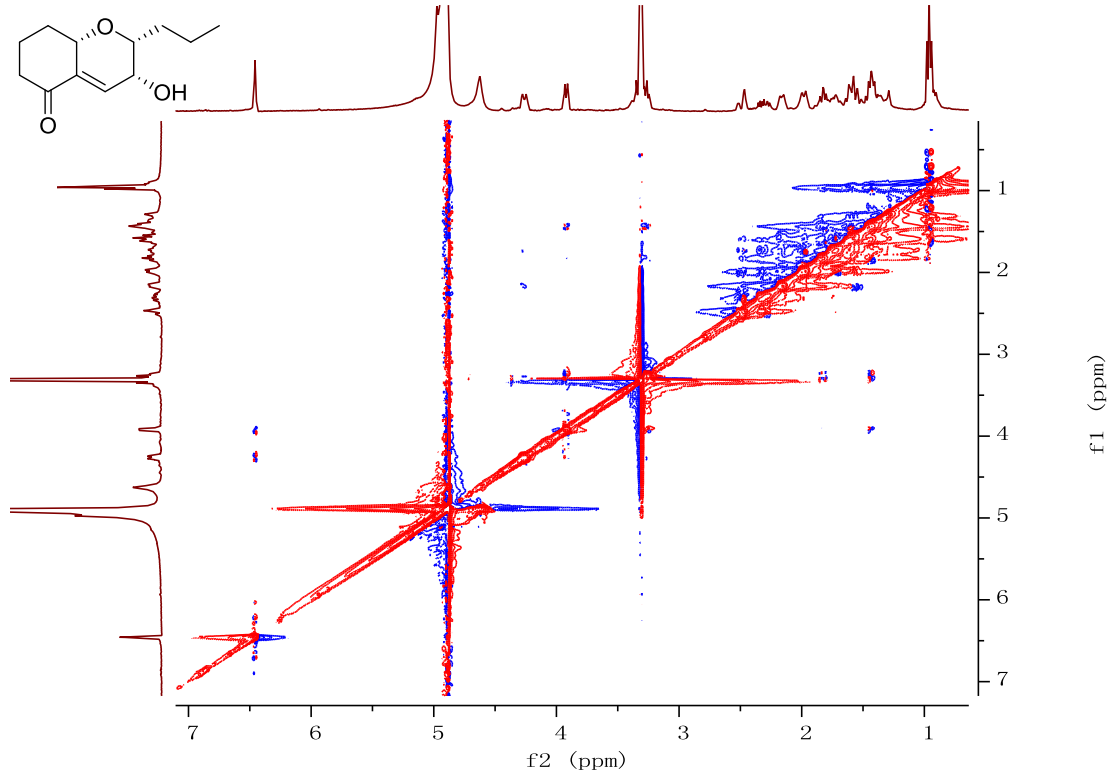

Fig. S49. ROESY spectrum of phomretone F (**6**) in methanol-d_4 (400 MHz).

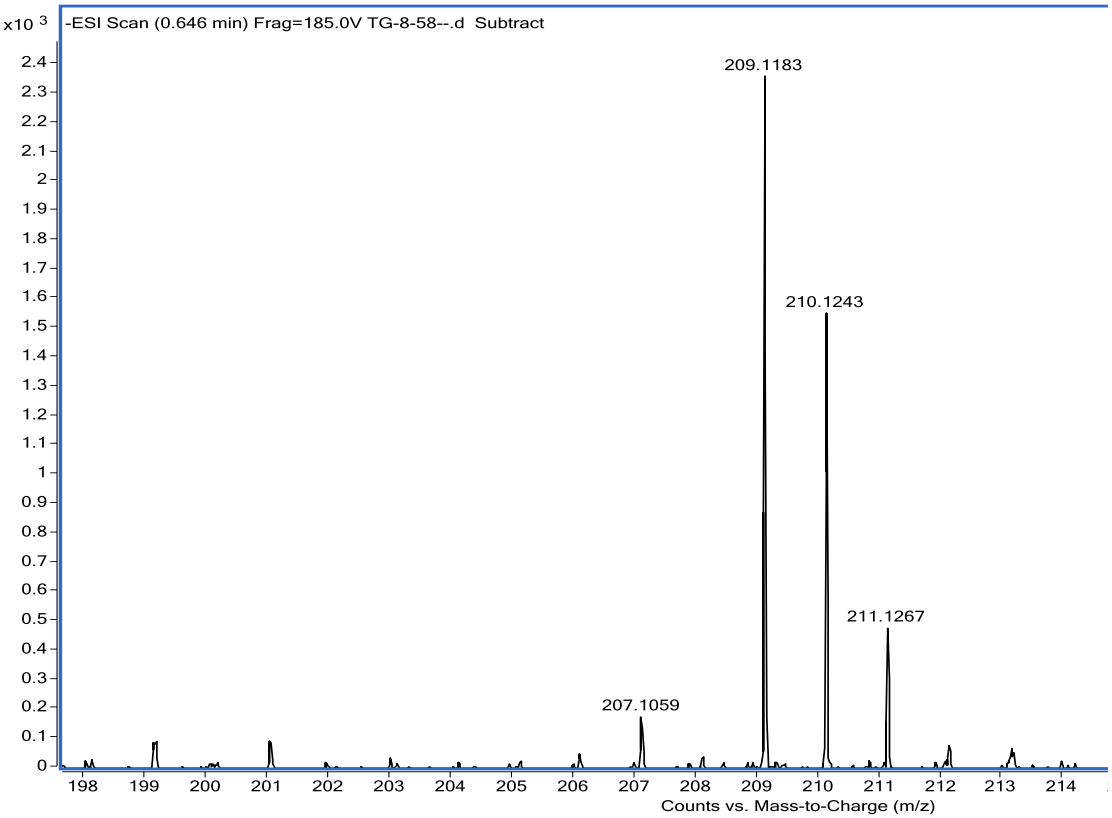

Fig. S50. (+)-HRESIMS data of phomretone F (**6**).

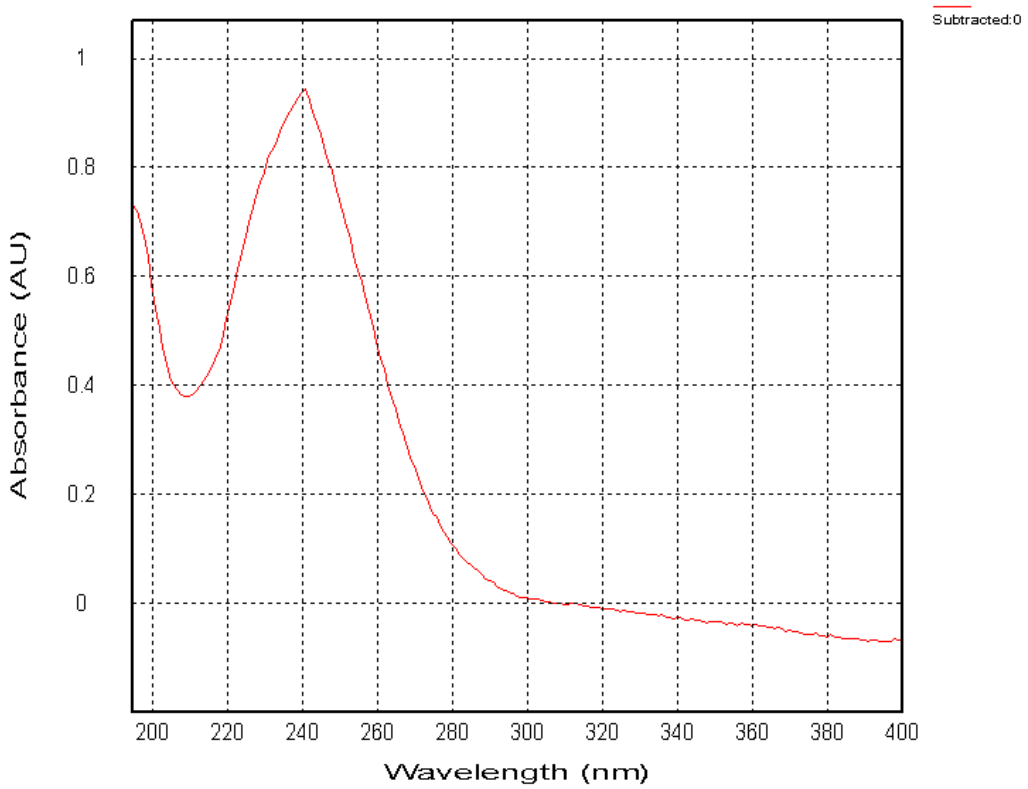

Fig. S51. UV absorption spectrum of phomretone F (**6**) in MeOH.

References

[1] C. Li, A. M. Sarotti, J. Turkson, S. Cao, *Tetrahedron lett.*, 2017, **58**, 2290-2293.