Supporting Information for

Quorumolides A-C, Three Cembranoids from *Euphorbia antiquorum*

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Table S1. X-ray crystal data for quorumolide A (1) [A]

Empirical formula	$C_{20}H_{30}O_4$
Formula weight	336.464.44
Temperature	293 (2) K
Wavelength	1.54178 Å
Crystal system, space group	Monoclinic, P2 (1)
Unit cell dimensions	a = 6.14420 (10) Å, α = 90°
	b = 11.10470 (10) Å, β = 91.6320 (10)°
	c = 13.24270 (10) Å, γ = 90°
Volume	903.176 (18) $Å^3$
Z, calculated density	2, 1.230 Mg/m^3
Absorption cofficient	0.672 mm^{-1}
F (000)	364
Crystal size	0.30 × 0.05 × 0.04 mm
Theta rage for data collection	3.34 to 68.98°
Limiting indices	$-7 \leq h \leq 5, -13 \leq k \leq 13, -15 \leq l \leq 15$
Reflections collected / unique	11695/ 3109 [R (int) = 0.0283]
Completeness to theta = 68.98	96.7%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9736 and 0.8239
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3109 / 1 / 222
Goodness-of-fit on F^2	1.064
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0339, wR2 = 0.0900
R indices (all data)	R1 = 0.0346, wR2 = 0.0907
Absolute structure parameter	−0.10 (17)
Largest diff. peak and hole	0.127 and −0.163 e. $Å^{-3}$

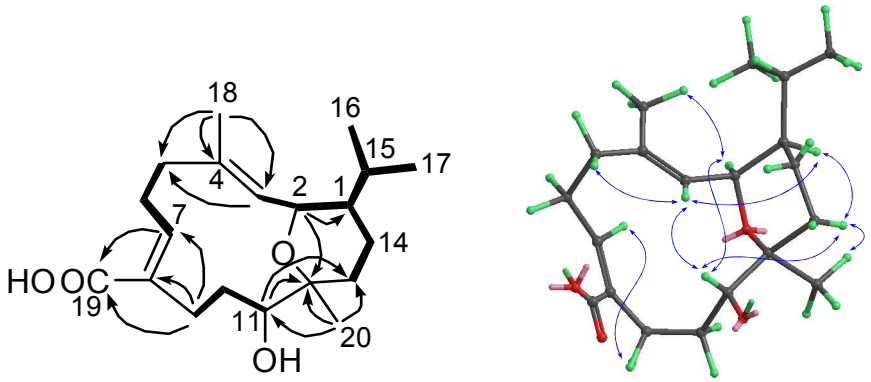
[A]Colorless crystals of 1 were obtained in the solvent of MeOH

Table S2. X-ray crastal data for quorumolide B (2)

Empirical formula	$C_{20}H_{32}O_4$
Formula weight	336.46
Temperature	140 (2) K
Wavelength	1.54178 Å
Crystal system, space group	Monoclinic, P2 (1)
Unit cell dimensions	a = 9.21880 (10) Å, α = 90°
	b = 10.6982 (2) Å, β = 101.6680 (10)°
	c = 19.9113 (3) Å, γ = 90°
Volume	1923.16 (5) $Å^3$
Z, calculated density	4, 1.162 Mg/m^3
Absorption cofficient	0.631 mm^{-1}
F (000)	736
Crystal size	0.25× 0.15 × 0.12 mm
Theta rage for data collection	2.27 to 69.79°
Limiting indices	$-10 \le h \le 11$, $-13 \le k \le 12$, $-23 \le l \le 24$
Reflections collected / unique	15318 / 6186 [R (int) = 0.0369]
Completeness to theta = 69.79	97.1%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9281 and 0.8581
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6186 / 1 / 445
Goodness-of-fit on F^2	1.033
Final R indices [I＞2σ (I)]	R1 = 0.0385, wR2 = 0.1024
R indices (all data)	R1 = 0.0407, wR2 = 0.1048
Absolute structure parameter	−0.15 (14)
Largest diff. peak and hole	0.181 and −0.168 e. $Å^{-3}$

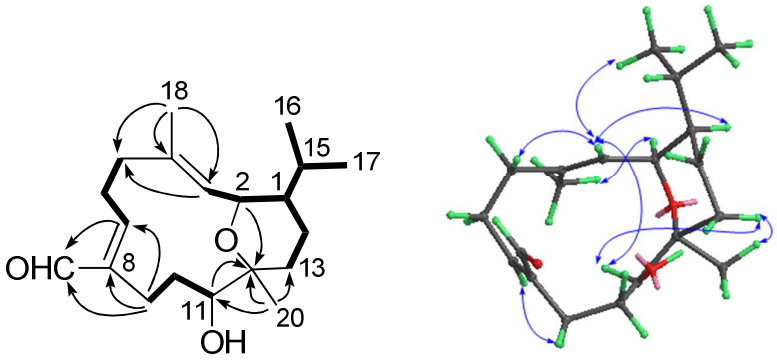
[A]Colorless crystals of 1 were obtained in the solvent of MeOH

Figure S1. Key (a) ^{1}H-^{1}H COSY (—), HMBC (H⟶C), and (b) ROESY correlations of **2**



a **b**

Figure S2. Key (a) ^{1}H-^{1}H COSY (—), HMBC (H⟶C), and (b) ROESY correlations of **3**



a **b**

Figure S3. CD and UV spectra of compounds **2** and **3**.

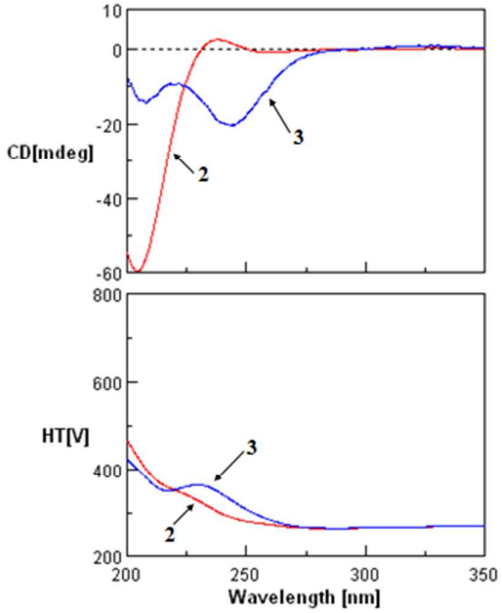


Figure S4. ^{1}H NMR spectrum of quorumolide A (**1**) in $CDCl_3$.

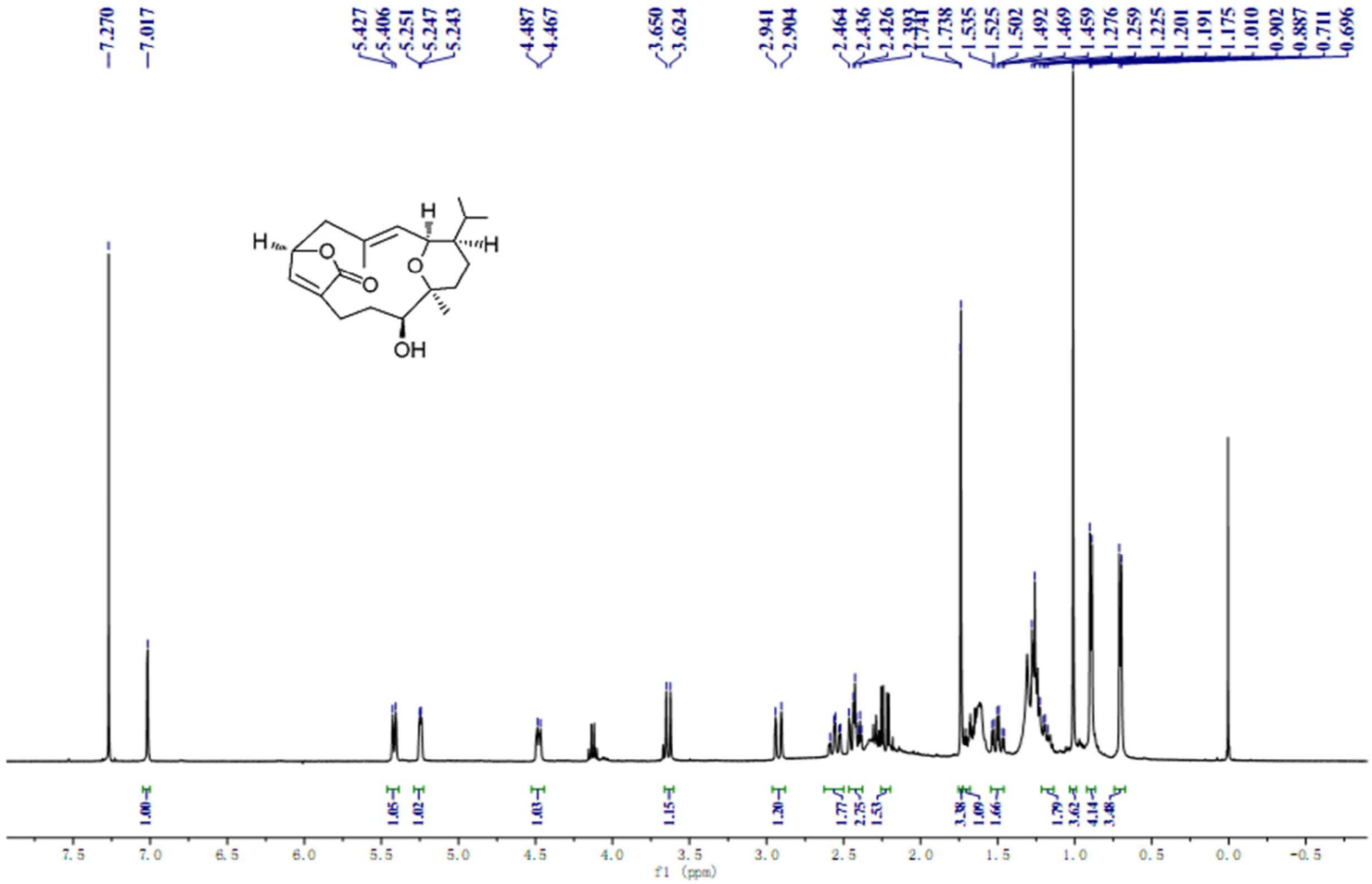


Figure S5. ^{13}C NMR spectrum of quorumolide A (**1**) in $CDCl_3$.

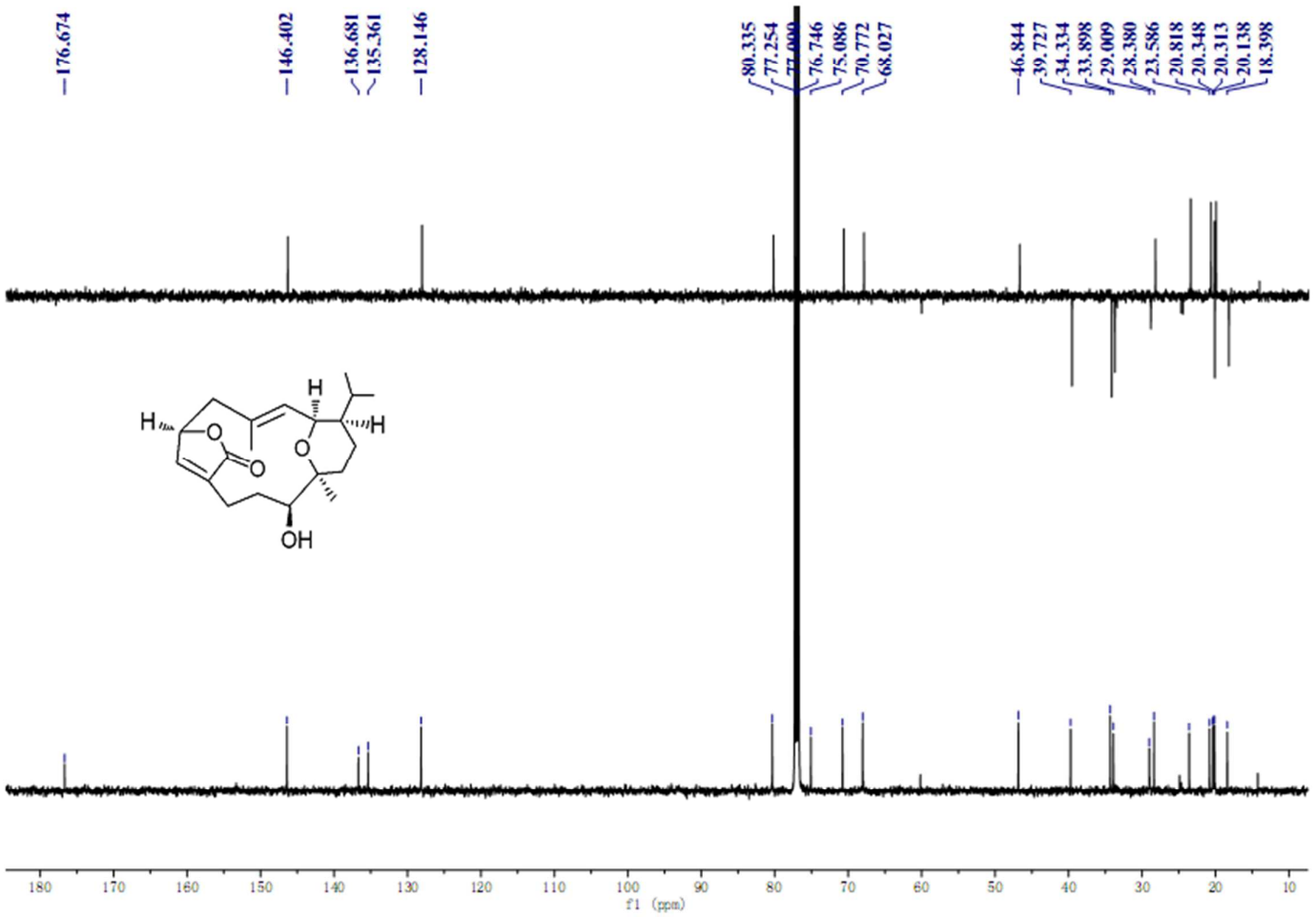


Figure S6. HSQC spectrum of quorumolide A (**1**) in $CDCl_3$.

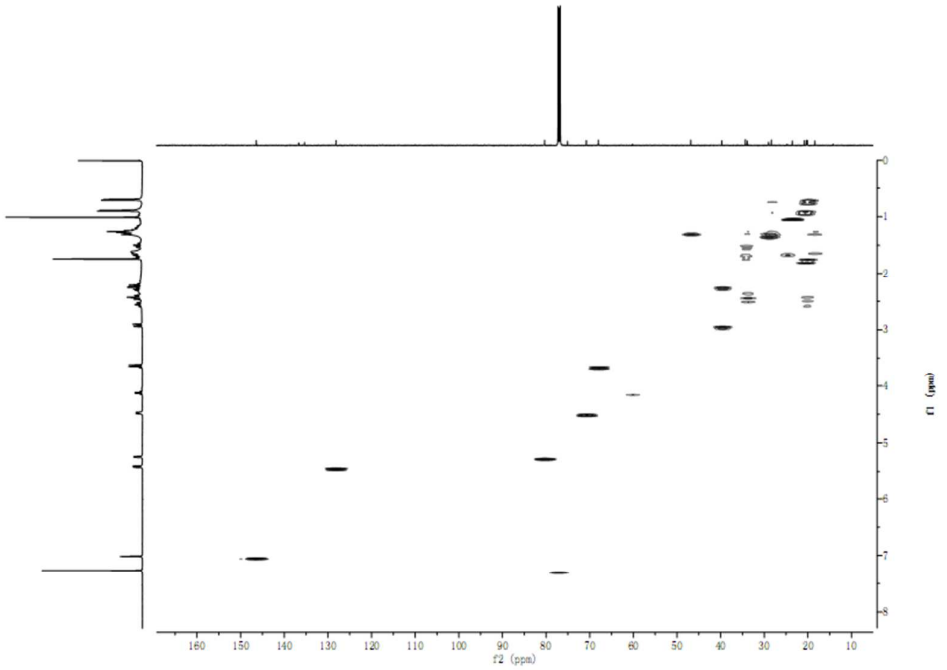


Figure S7. HMBC spectrum of quorumolide A (**1**) in $CDCl_3$.

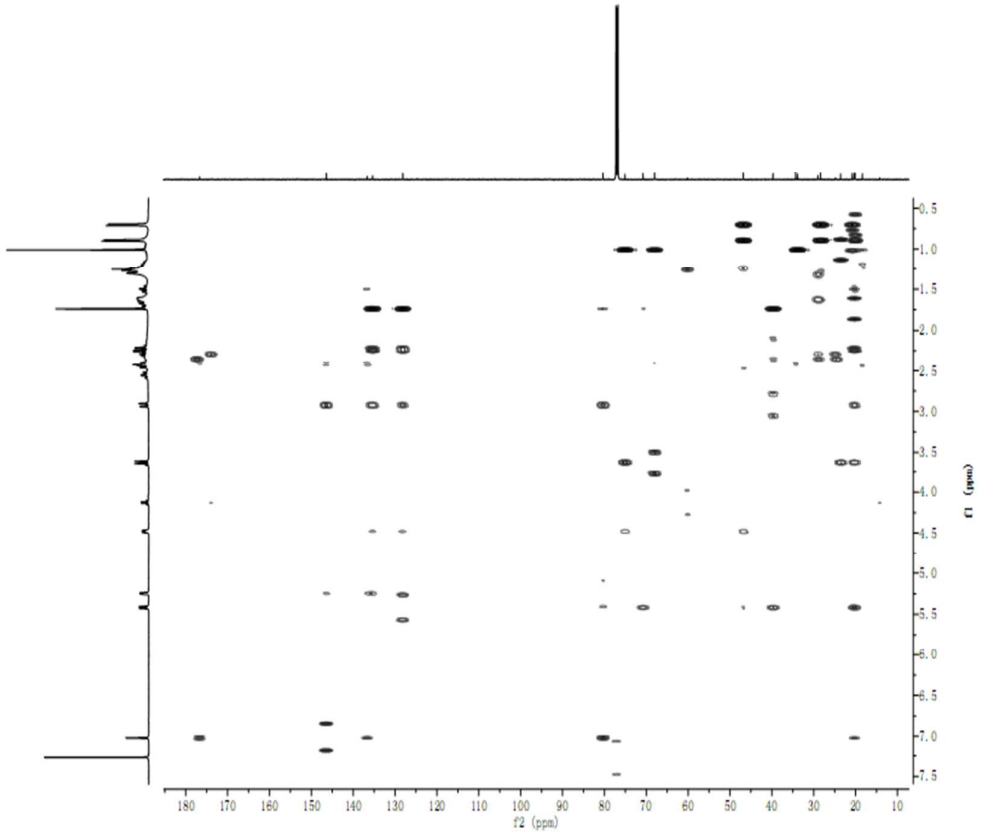


Figure S8. ^{1}H-^{1}H COSY spectrum of quorumolide A (**1**) in $CDCl_3$.

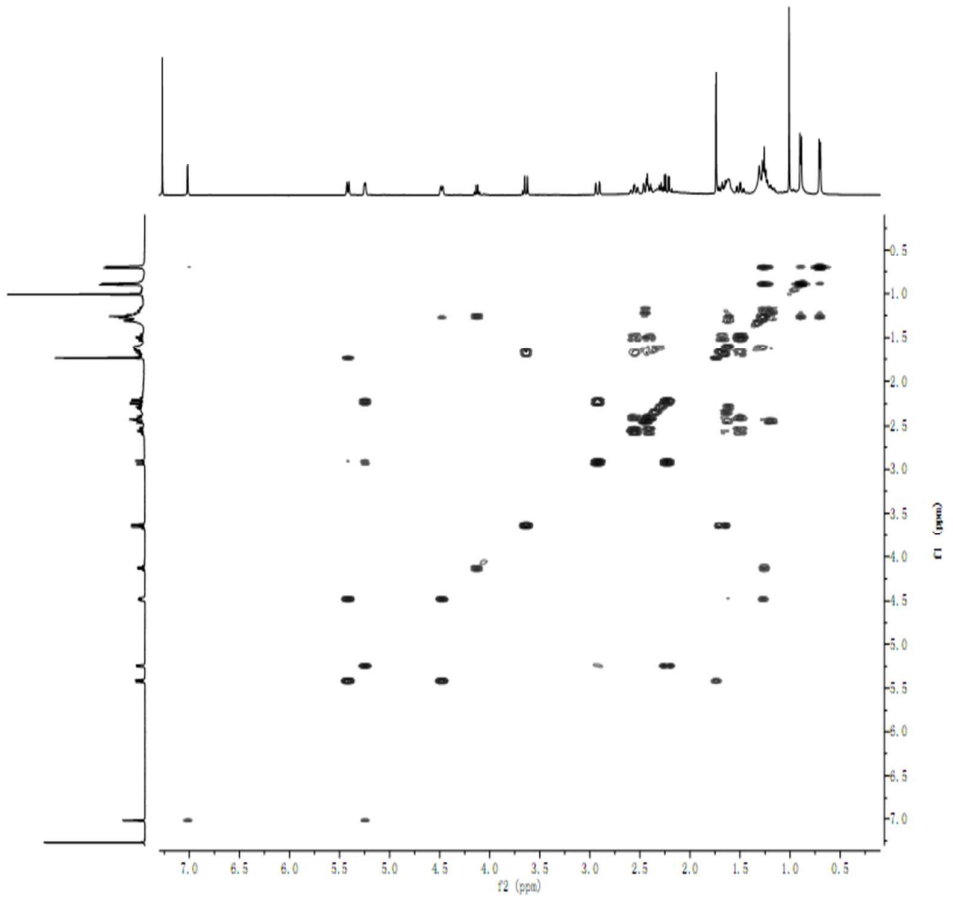


Figure S9. ROESY spectrum of quorumolide A (**1**) in $CDCl_3$.

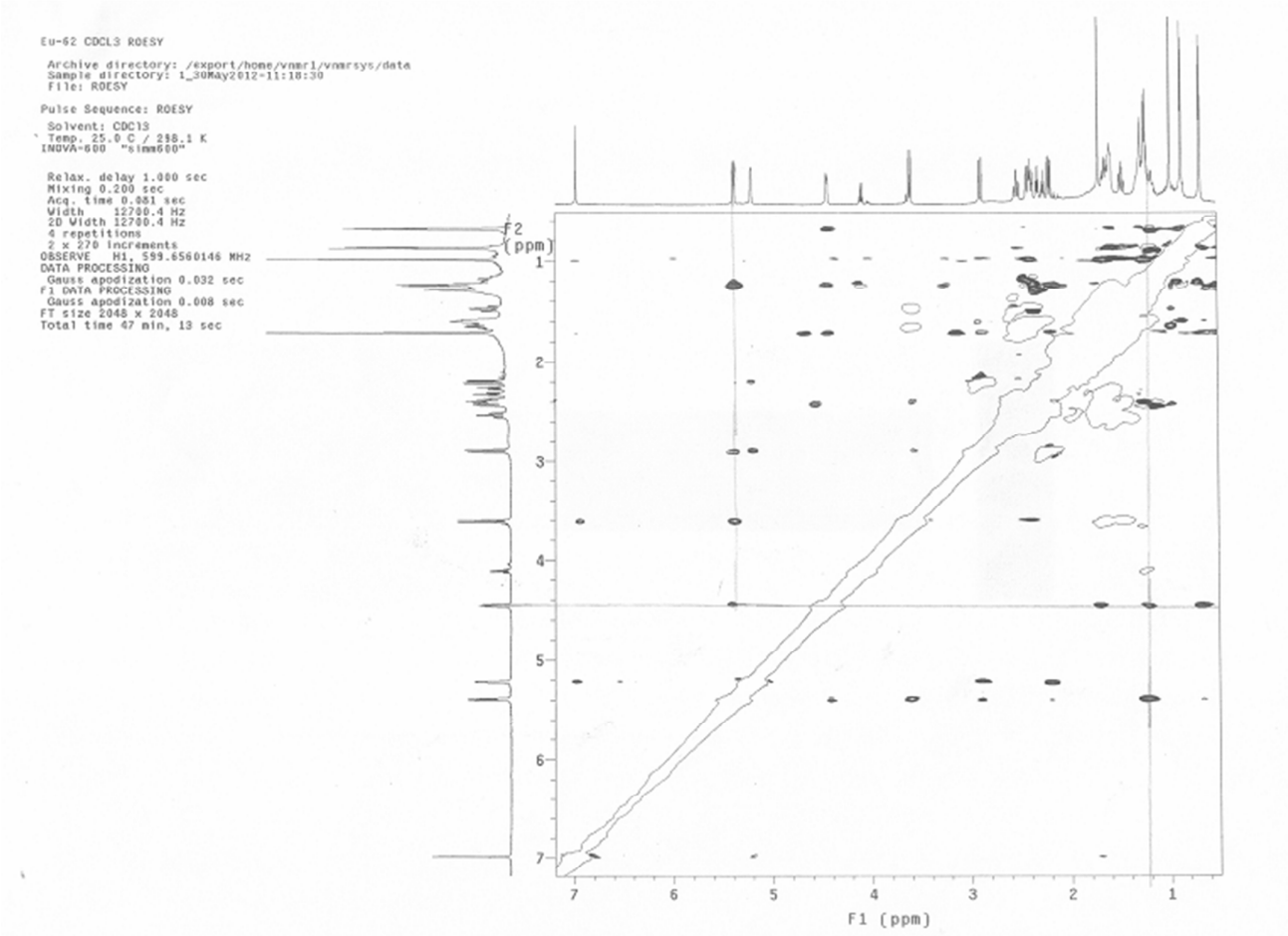

Eu-62 CDCL3 ROESY
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: 1_30May2012-11:18:30
File: ROESY
Pulse Sequence: ROESY
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-600 "sinm600"
Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.081 sec
Width 12780.4 Hz
2D Width 12780.4 Hz
4 repetitions
2 x 270 increments
OBSERVE H1, 599.6560146 MHz
DATA PROCESSING
Gauss apodization 0.032 sec
F1 DATA PROCESSING
Gauss apodization 0.008 sec
FT size 2048 x 2048
Total time 47 min, 13 sec
F2 (ppm)
1
2
3
4
5
6
7
7
6
5
4
3
2
1
F1 (ppm)

Figure S10. HRMS (ESI-TOF) spectrum of quorumolide A (**1**).

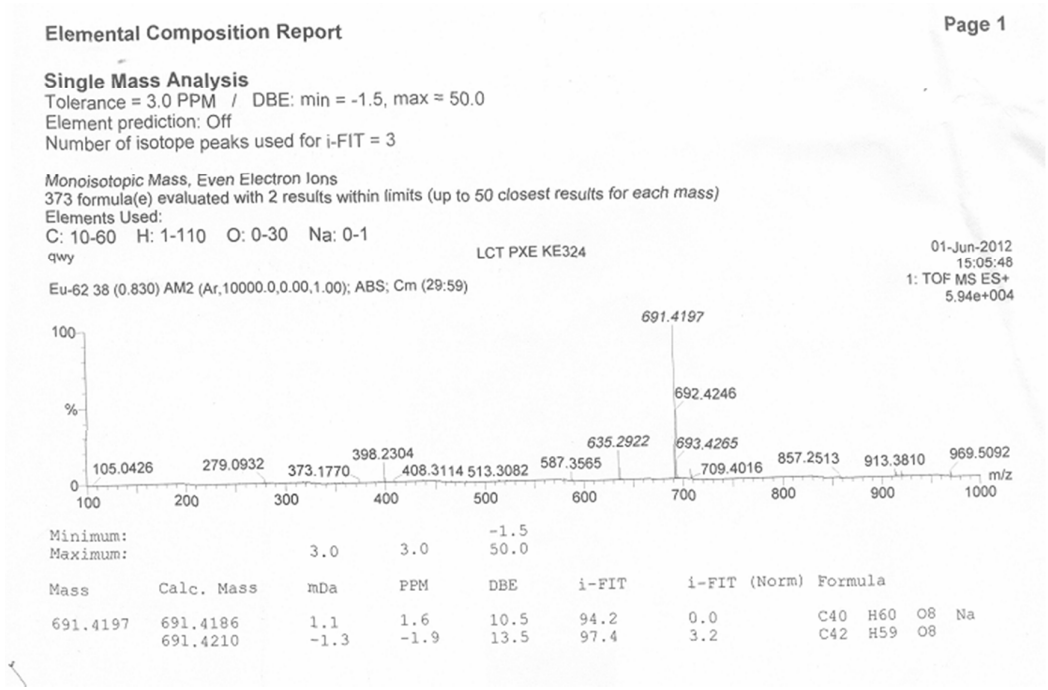


Figure S11. IR spectrum of quorumolide A (**1**).

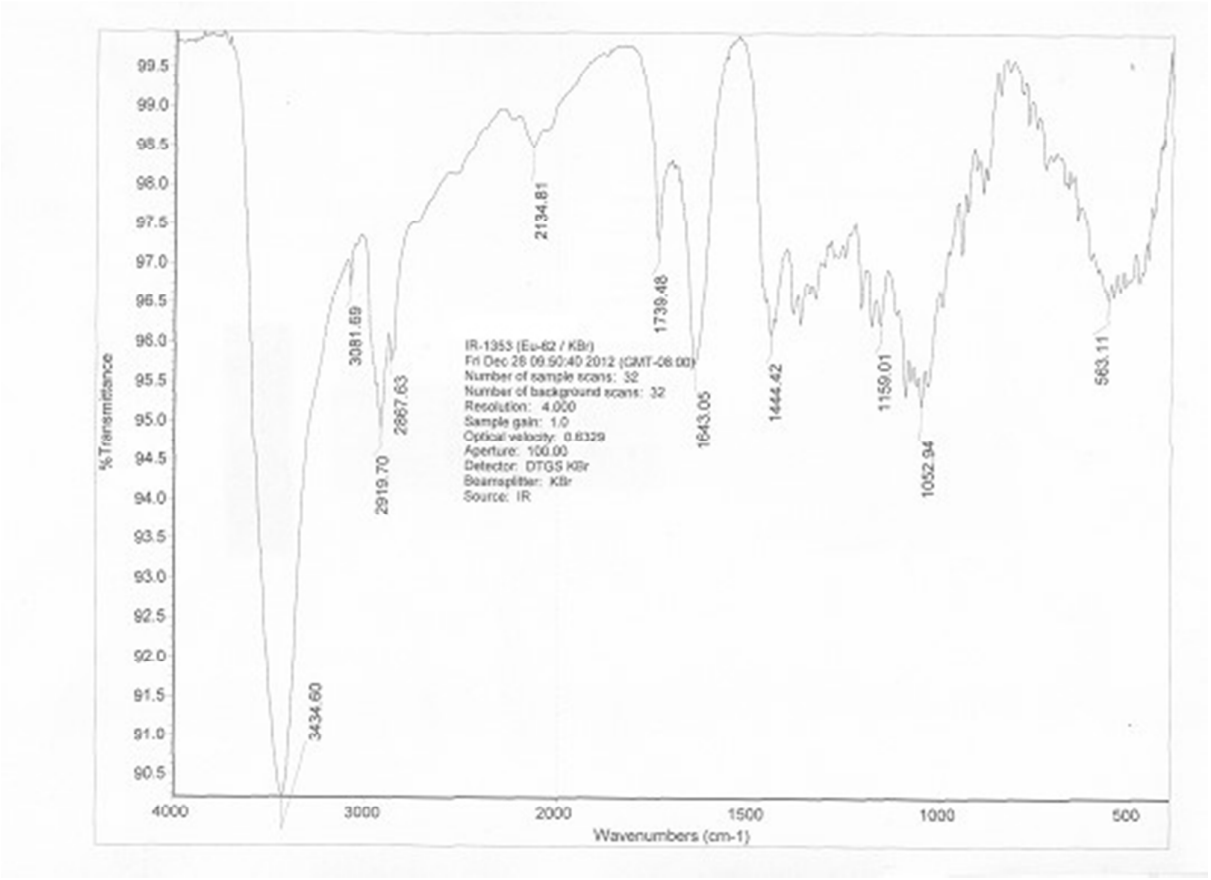


Figure S12. ^{1}H NMR spectrum of quorumolide B (**2**) in $CDCl_3$

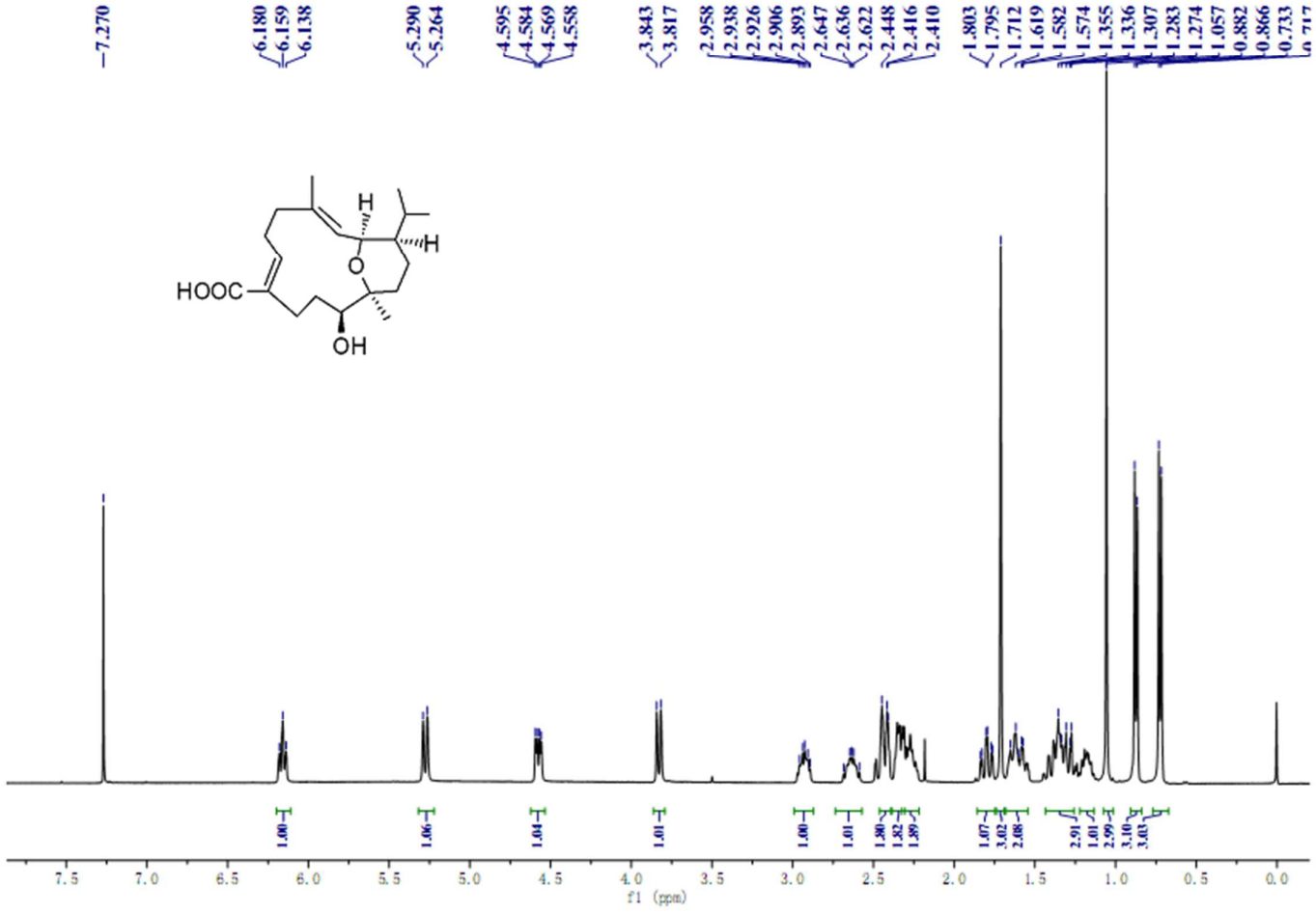


Figure S13. ^{13}C NMR spectrum of quorumolide B (**2**) in $CDCl_3$.

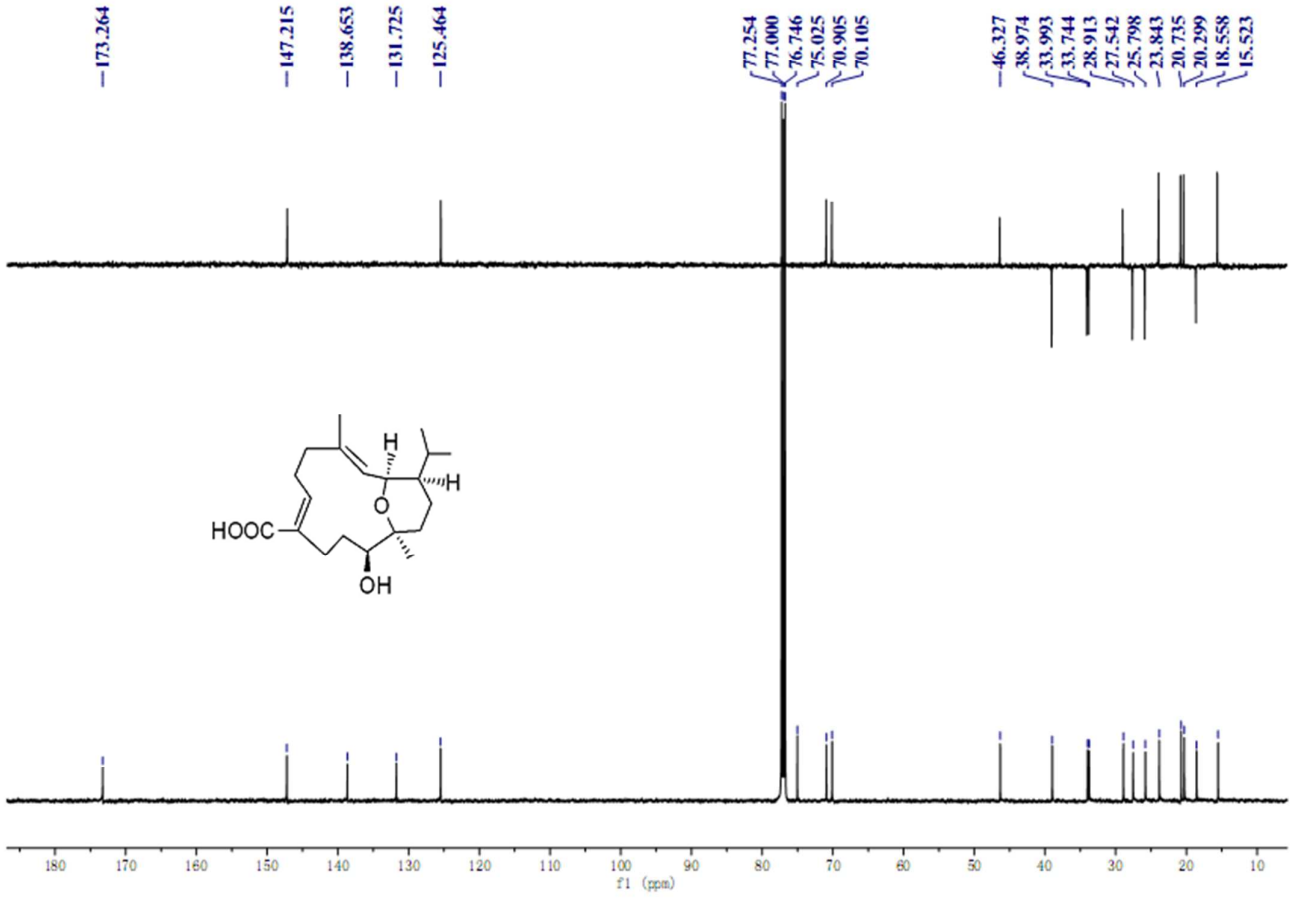


Figure S14. HSQC spectrum of quorumolide B (**2**) in $CDCl_3$.

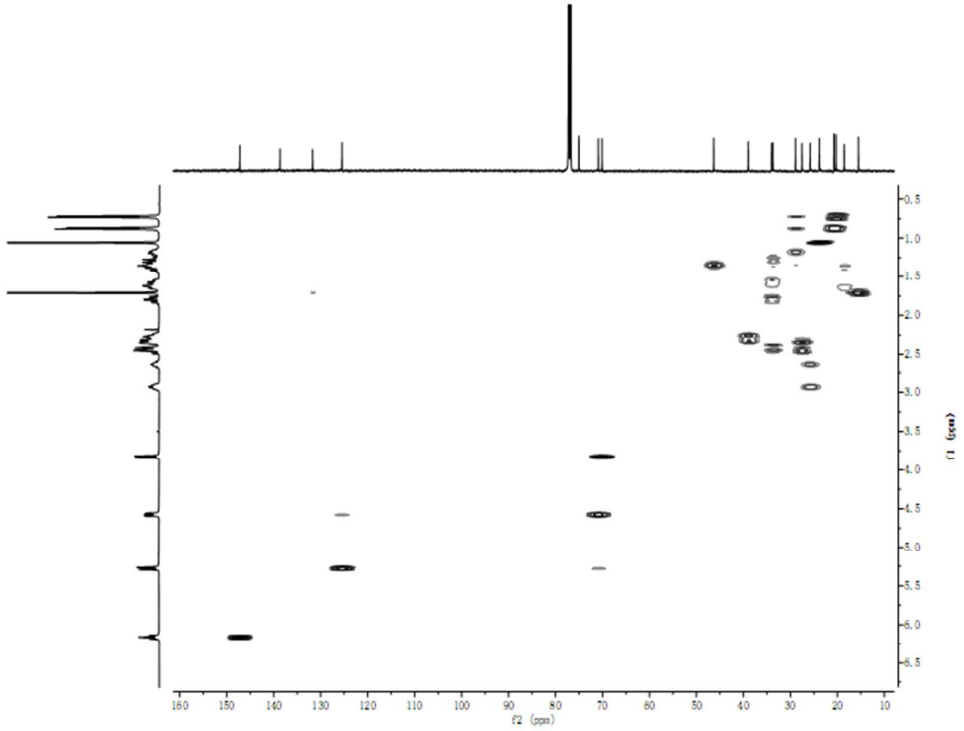


Figure S15. HMBC spectrum of quorumolide B (**2**) in $CDCl_3$.

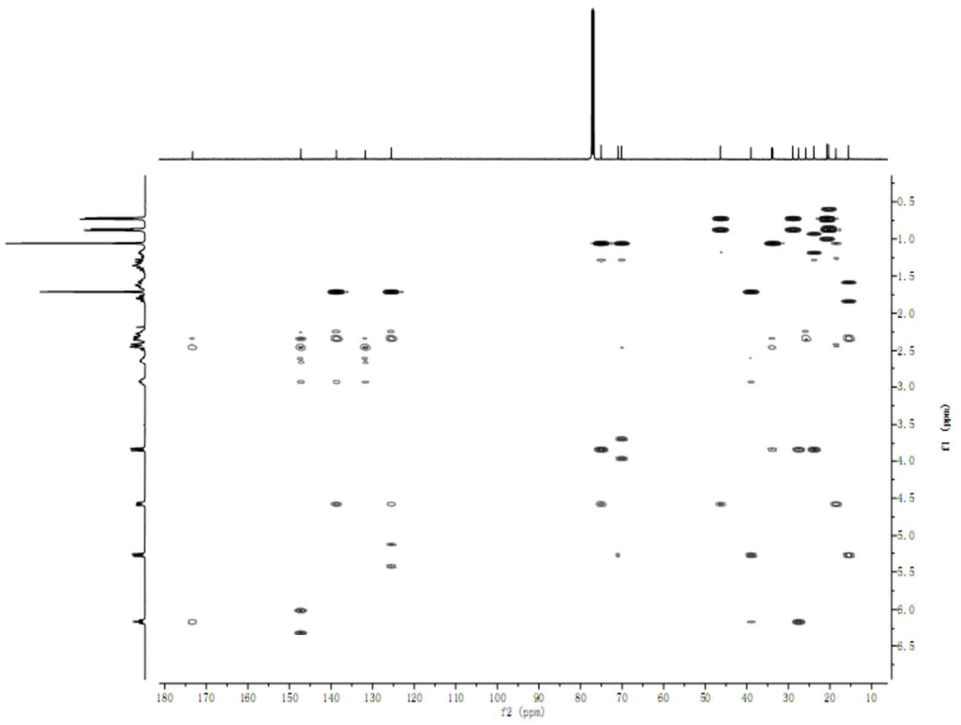

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f2 (ppm)
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
f1 (ppm)

Figure S16. ^{1}H-^{1}H COSY spectrum of quorumolide B (**2**) in $CDCl_3$.

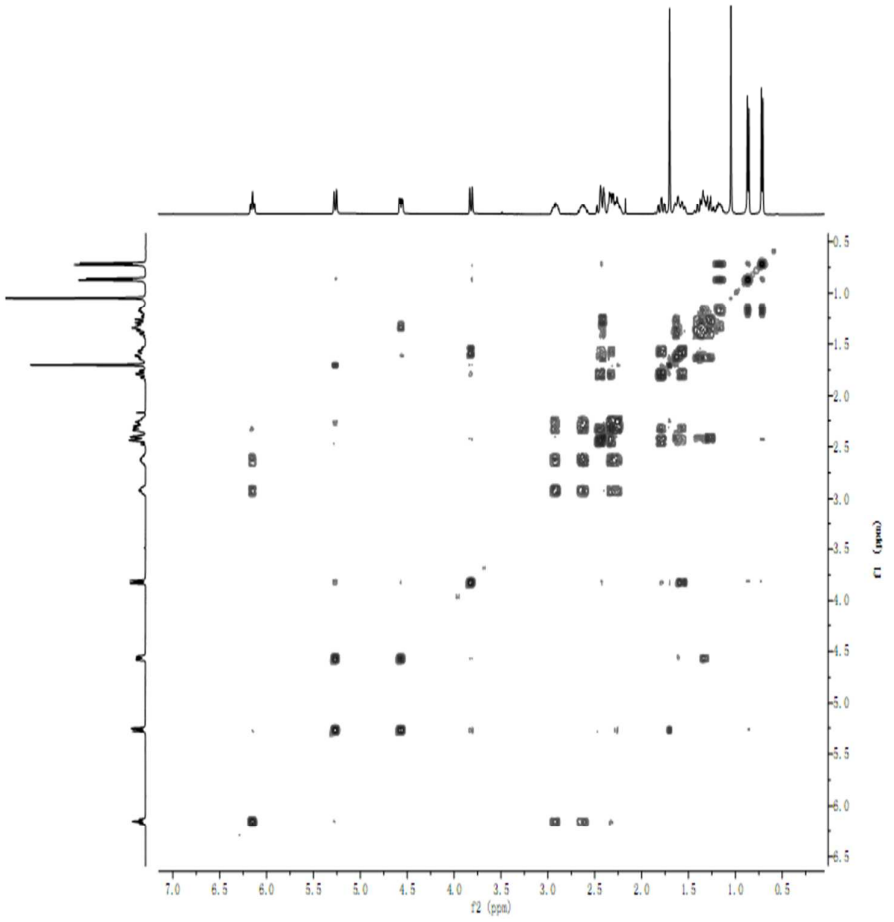


Figure S17. ROESY spectrum of quorumolide B (**2**) in $CDCl_3$.

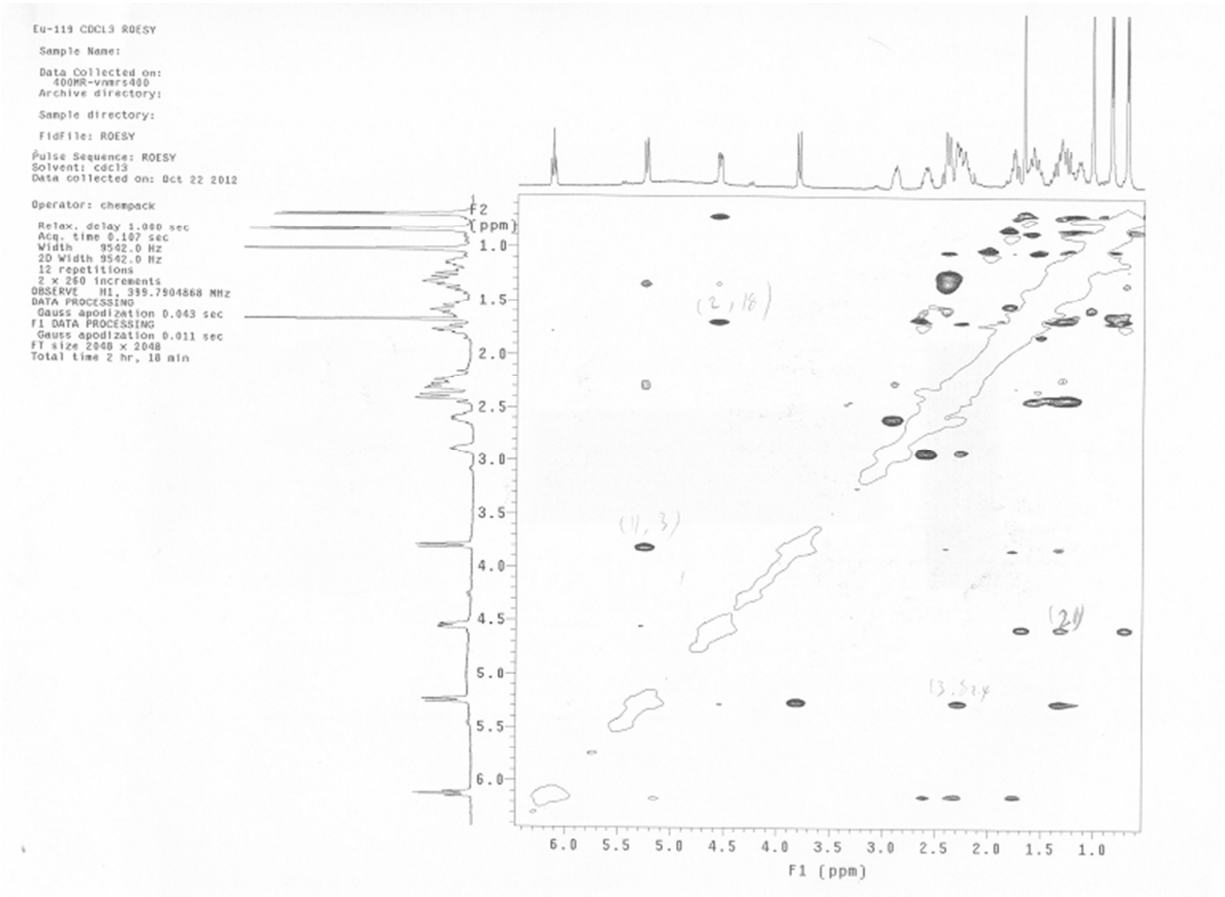


Figure S18. HRMS (ESI-TOF) spectrum of quorumolide B (**2**).

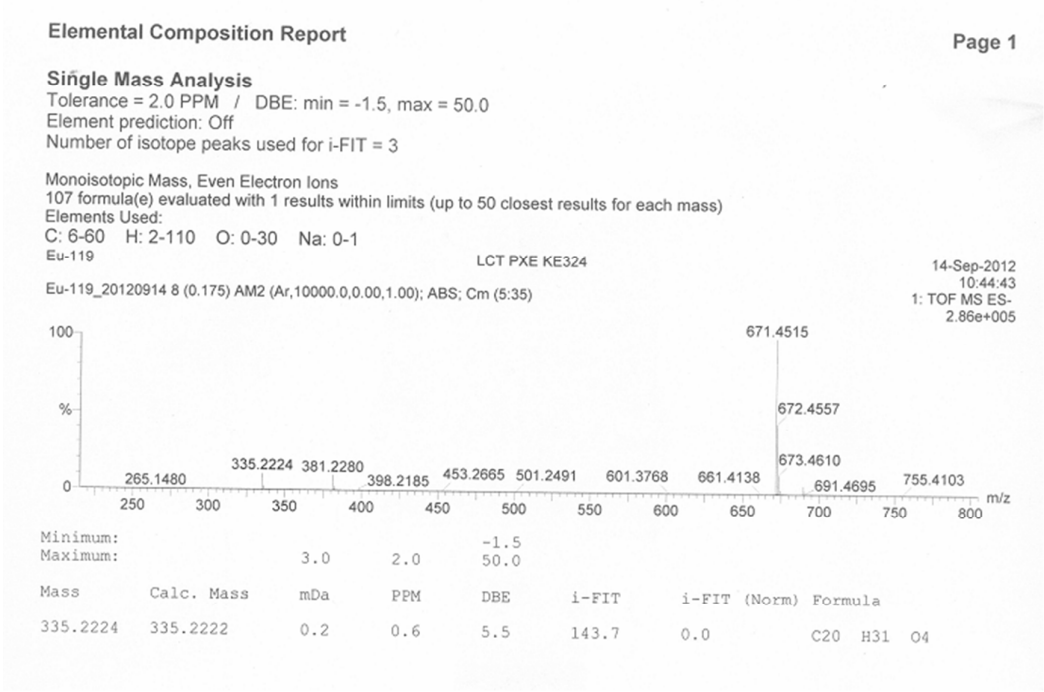


Figure S19. IR spectrum of quorumolide B (**2**).

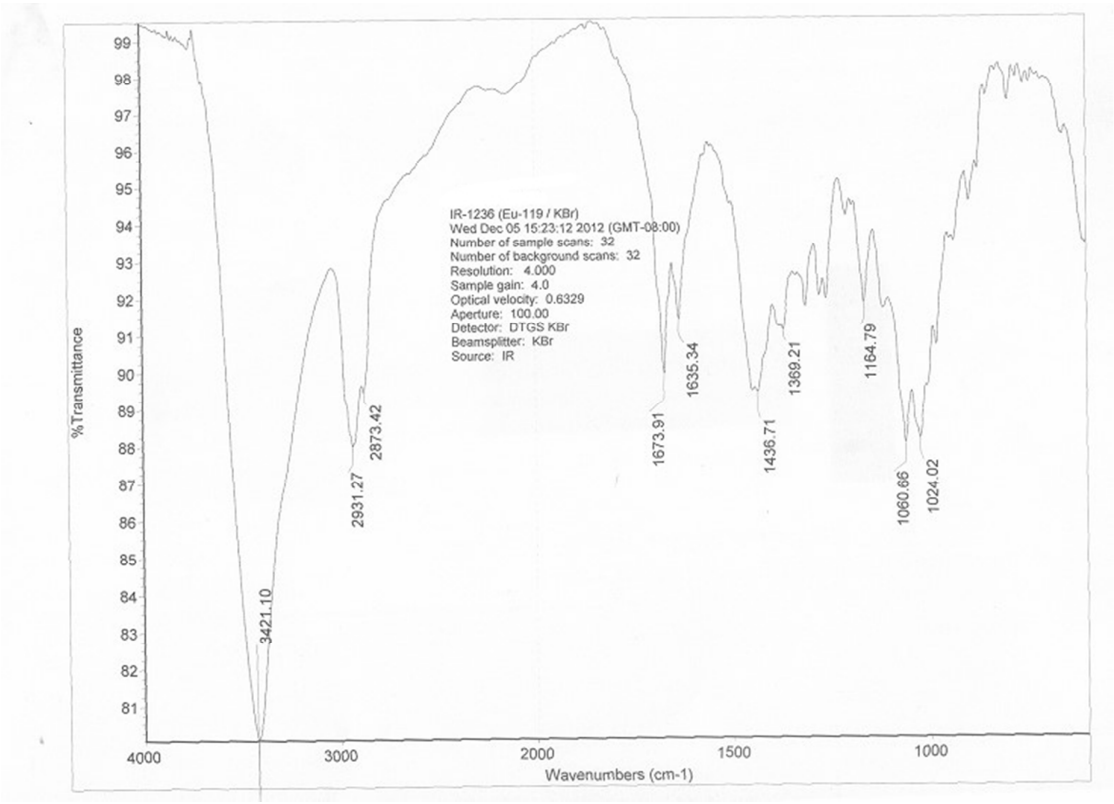


Figure S20. ^{1}H NMR spectrum of quorumolide C (**3**) in $CDCl_3$.

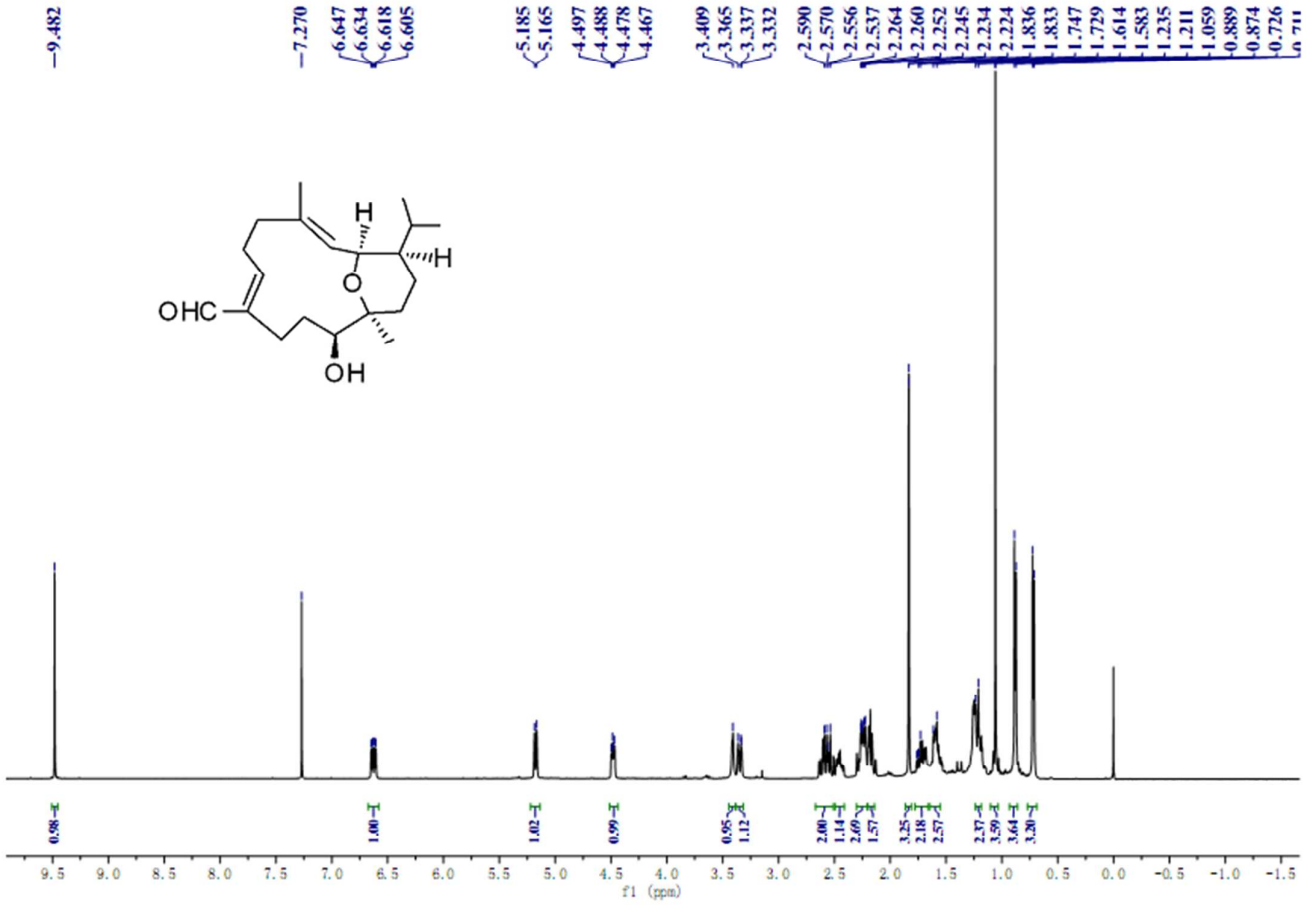


Figure S21. ^{13}C NMR spectrum of quorumolide C (**3**) in $CDCl_3$.

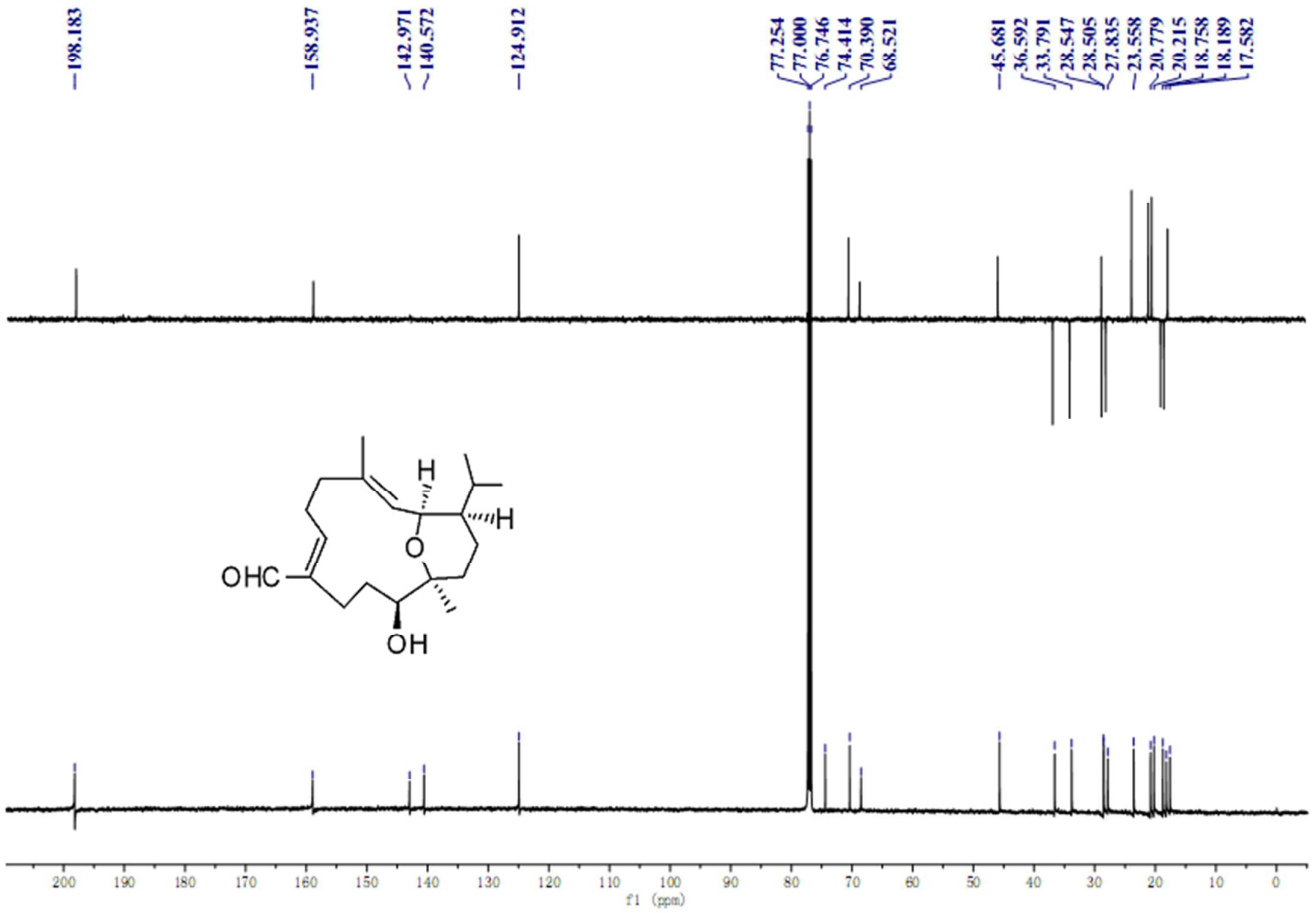


Figure S22. HSQC spectrum of quorumolide C (**3**) in $CDCl_3$.

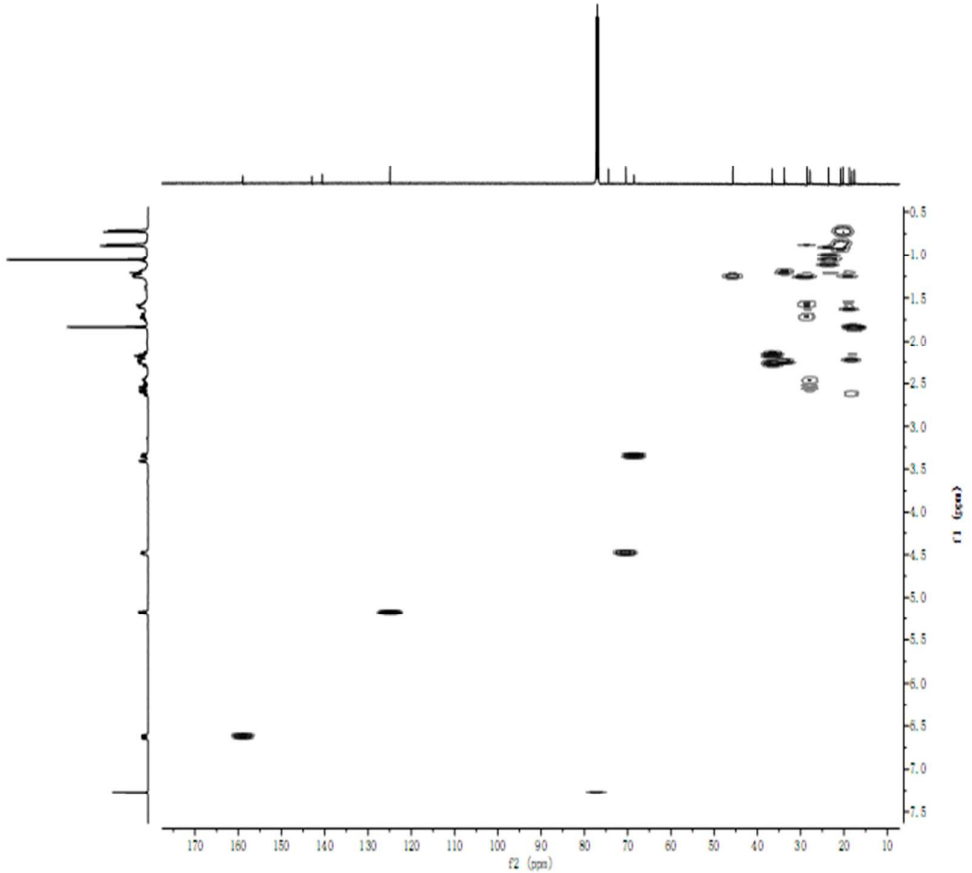


Figure S23. HMBC spectrum of quorumolide C (**3**) in $CDCl_3$

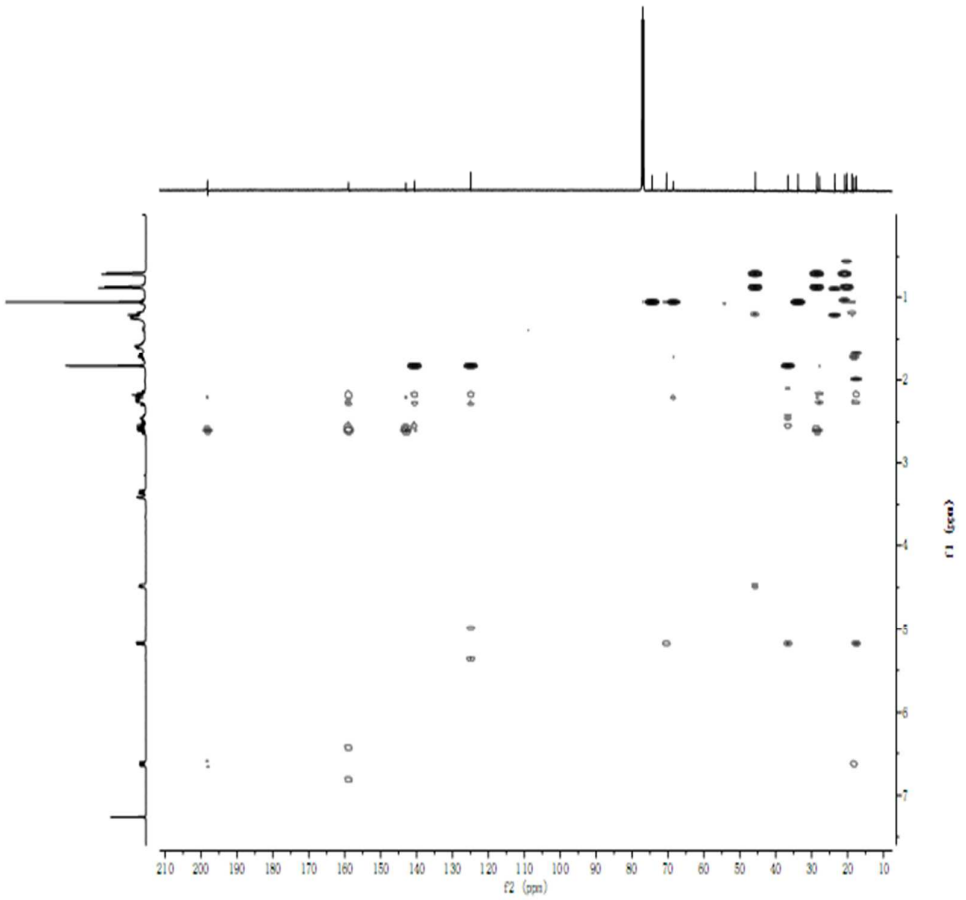

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f2 (ppm)
1
2
3
4
5
6
7
f1 (ppm)

Figure S24. ^{1}H-^{1}H COSY spectrum of quorumolide C (**3**) in $CDCl_3$.

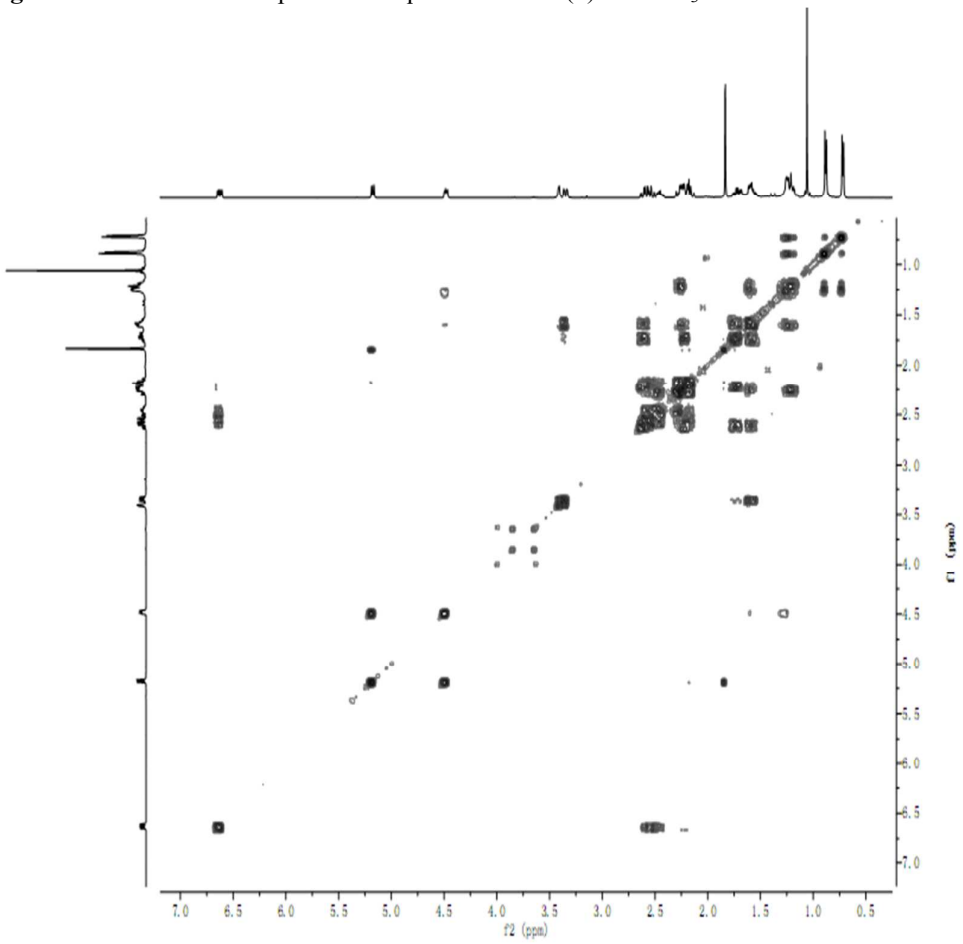


Figure S25. ROESY spectrum of quorumolide C (**3**) in $CDCl_3$.

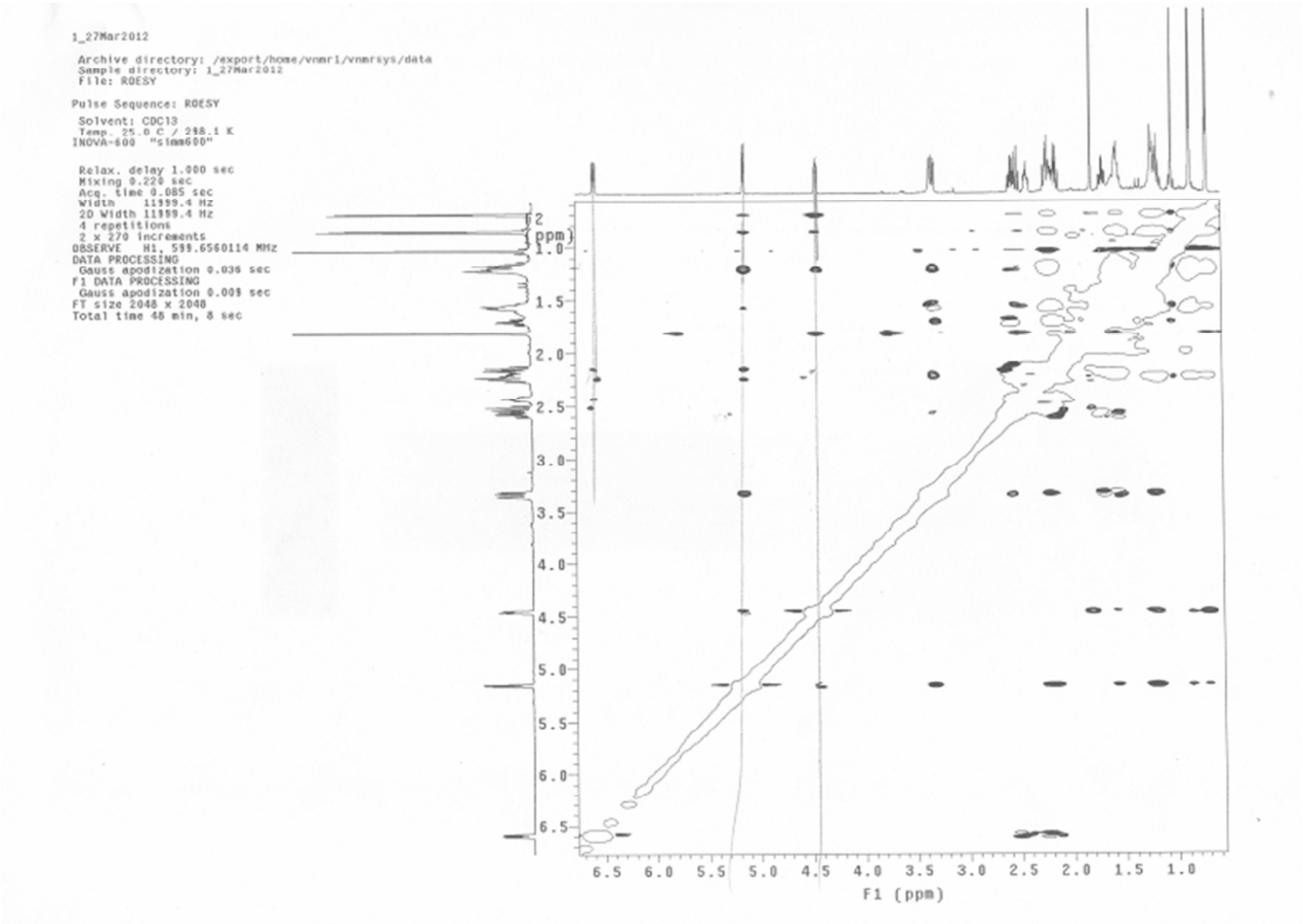


Figure S26. HRMS (ESI-TOF) spectrum of quorumolide C (**3**).

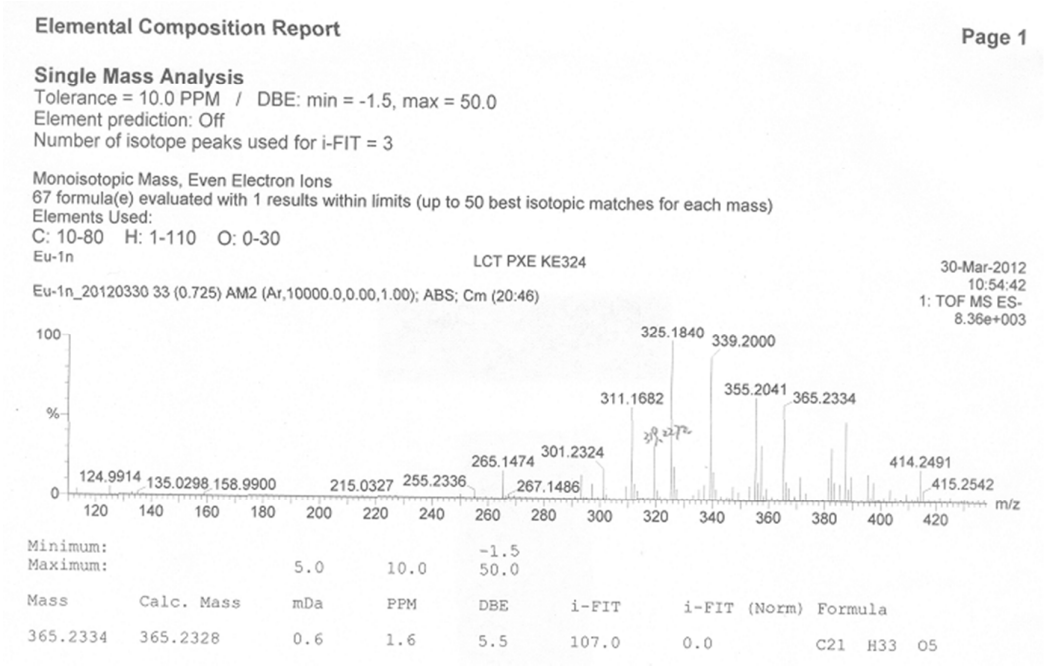


Figure S27. IR spectrum of quorumolide C (**3**).

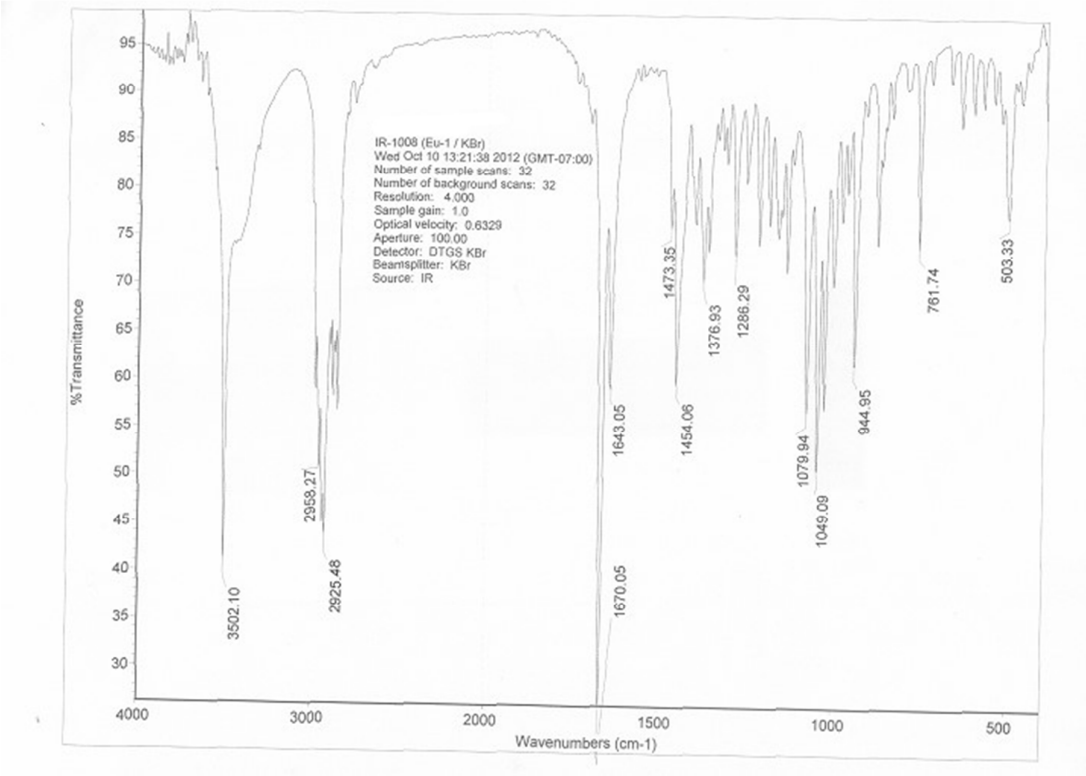


Figure S28. ORTEP diagram of **1** (thermal ellipsoids at the 50% probability level)

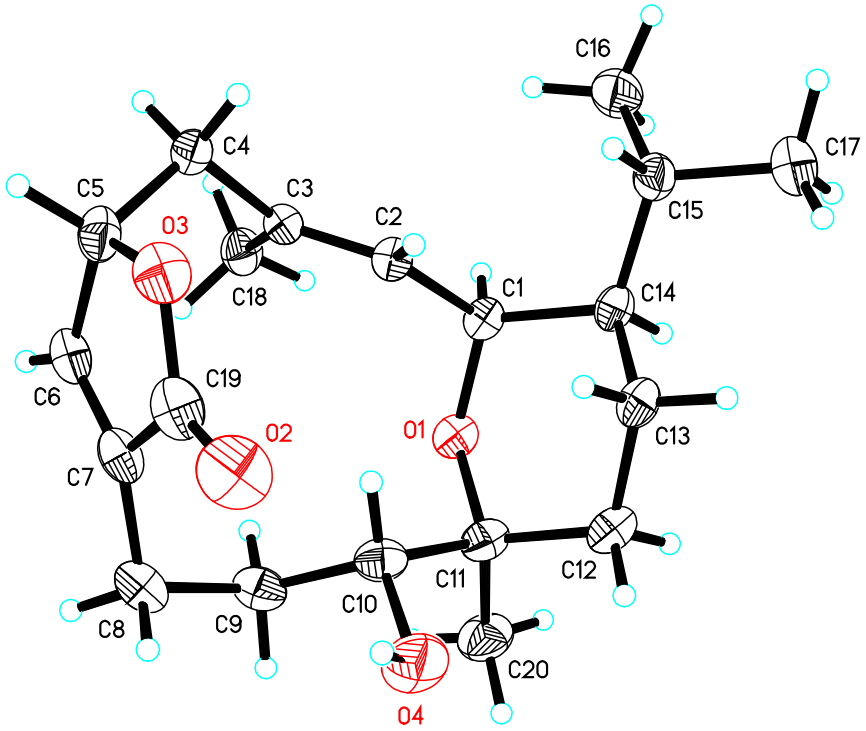


Figure S29. ORTEP diagram of **2** (thermal ellipsoids at the 50% probability level)