Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Polyoxygenated Meroterpenoids and a Bioactive Illudalane Derivative from Co-culture of *Armillaria* sp. and *Epicoccum* sp.

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UPLC-QTOF-MS Analysis Conditions

The analysis of the extracts from the co-cultures was performed by an Agilent 1290 UPLC (6545)-QTOF-MS spectrometry system in the positive ion modes. The UPLC column was an Agilent ZORBAX RRHD Eclipse Plus-C18 column (1.8 μm, 2.1 × 50 mm) and kept at a temperature of 40 °C. The mobile phase consisted of A (water with 0.05% formic acid) and B (acetonitrile with 0.05% formic acid) at a flow rate of 0.4 mL/min. The injected sample (1 mg/mL) volume was set at 3 μL. The gradient elution started with 10% B, it was increased linearly to 70% B in 50 min, and then it was increased linearly to 95% B in 10 min and held for 5 min.

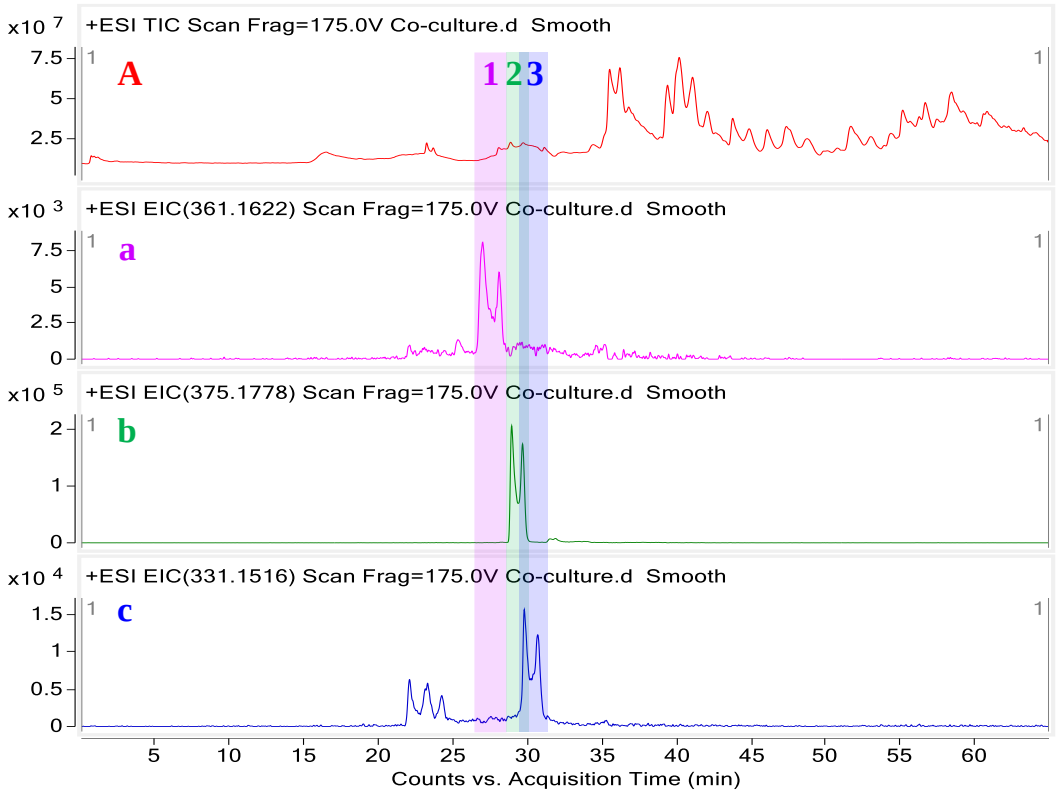

Figure S1. Total ion chromatograms (TIC) of extract from co-culture and extracted ion chromatogram (EIC) of compounds **1-3**. (TIC (positive) of the extract from co-culture (**A**); EIC of compound **1** at m/z 361.1622 $[M + Na]^+$ in the extract of co-culture (**a**); EIC of compound **2** at m/z 375.1778 $[M + Na]^+$ in the extract of co-culture (**b**); EIC of compound **3** at m/z 375.1516 $[M + Na]^+$ in the extract of co-culture (**c**)).

X-ray Crystal Structure Analysis

The crystal data of **1** was collected on a Bruker Apex DUO diffractometer with a graphite monochromator using Cu Kα radiation (λ = 1.54178 Å). The crystallographic data have been deposited in the Cambridge Crystallographic Data Centre with the deposition number CCDC 1918369. A copy of the data can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (via: www.ccdc.cam.ac.uk/data_request/cif).

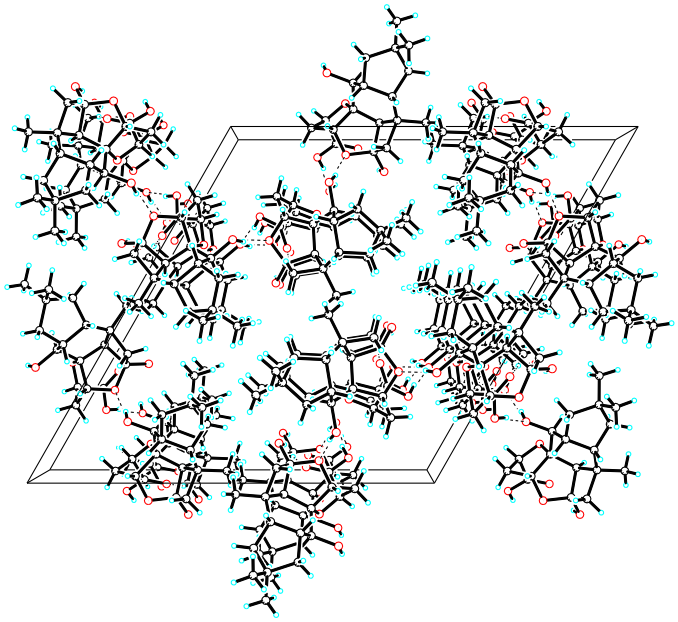

Figure S2. View of the pack drawing of **1** (Hydrogen-bonds are shown as dashed lines).

Table S1. Crystal Data and Structure Refinement for Compound 1

Identification code	global	
Empirical formula	$C_{18}\ H_{26}\ O_6$	
Formula weight	338.39	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Hexagonal	
Space group	$P6_5$	
Unit cell dimensions	a = 20.3875(7) Å	α= 90°
	b = 20.3875(7) Å	β= 90°
	c = 7.4174(3) Å	γ = 120°
Volume	2670.0(2) $Å^3$	
Z	6	
Density (calculated)	1.263 Mg/m^3	
Absorption coefficient	0.777 mm^{-1}	
F(000)	1092	
Crystal size	0.330 x 0.130 x 0.130 mm^3	
Theta range for data collection	2.50 to 72.41°	
Index ranges	-25<=h<=25, -23<=k<=25, -9<=l<=9	
Reflections collected	39060	
Independent reflections	3518 [R(int) = 0.0316]	
Completeness to theta = 72.41°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.91 and 0.84	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3518 / 1 / 223	
Goodness-of-fit on F^2	0.831	
Final R indices [I>2sigma(I)]	R1 = 0.0254, wR2 = 0.0844	
R indices (all data)	R1 = 0.0256, wR2 = 0.0852	
Absolute structure parameter	0.06(3)	
Largest diff. peak and hole	0.246 and -0.166 e.$Å^{-3}$	

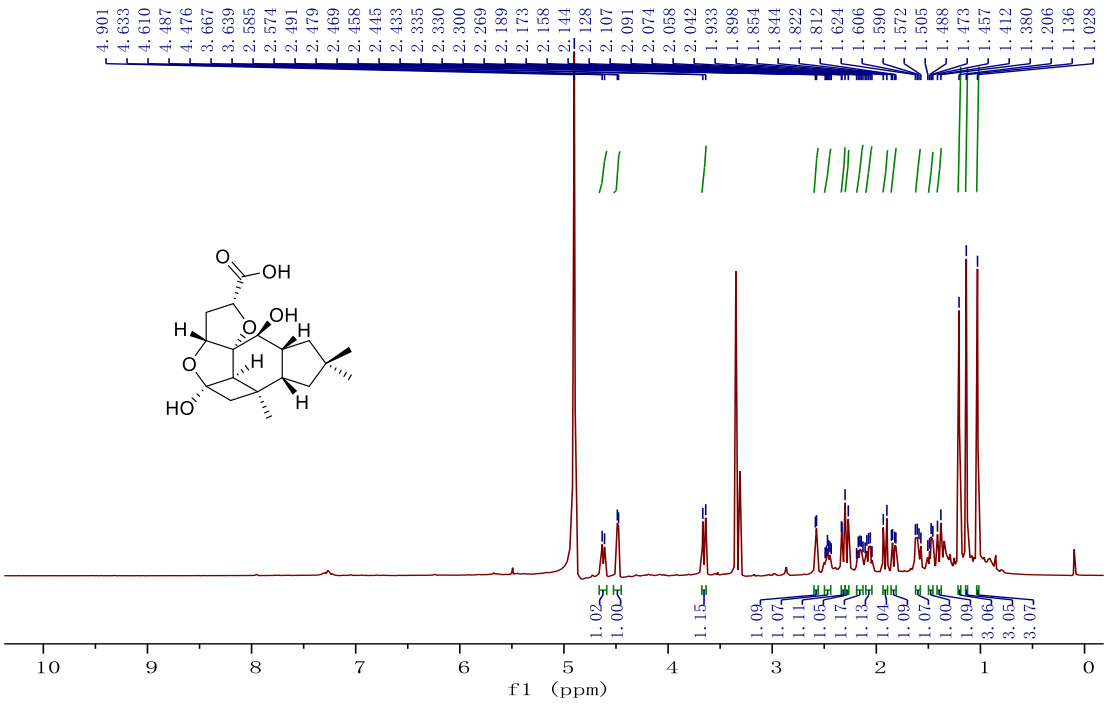

Figure S3. ^{1}H NMR spectrum of epiterenoid A (**1**) in methanol-d_4 (400 MHz).

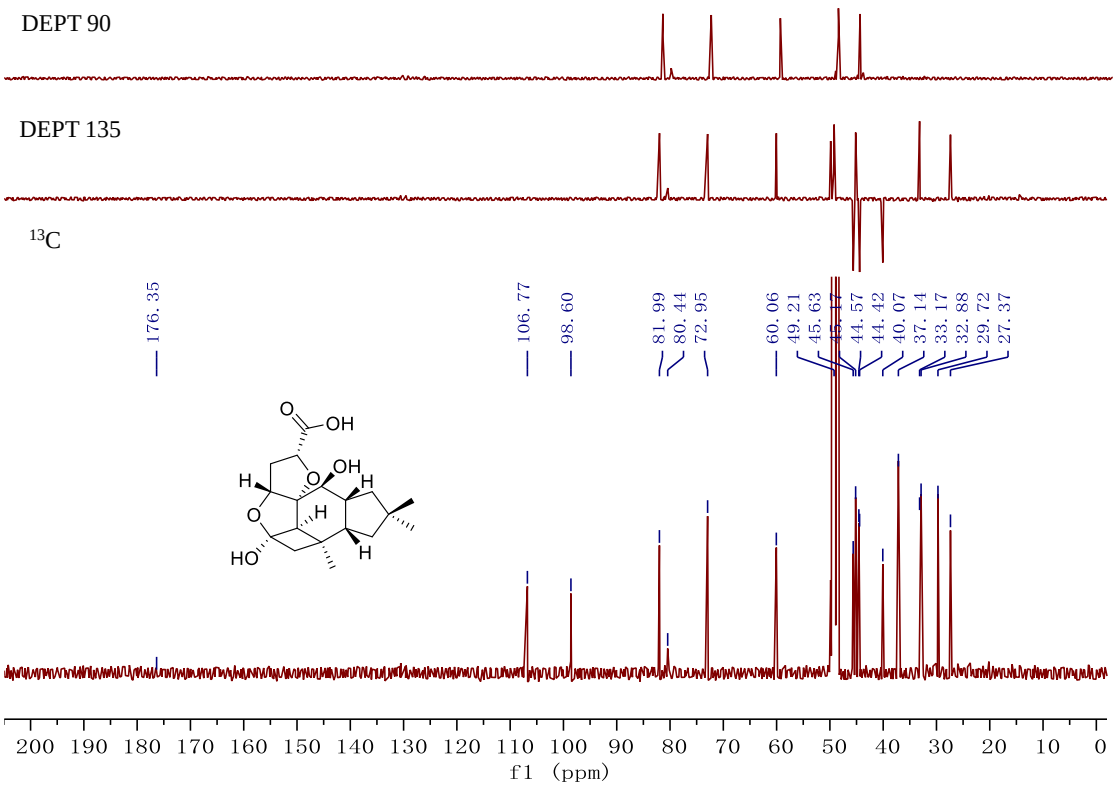

Figure S4. ^{13}C and DEPT NMR spectrum of epiterenoid A (**1**) in methanol-d_4 (100 MHz).

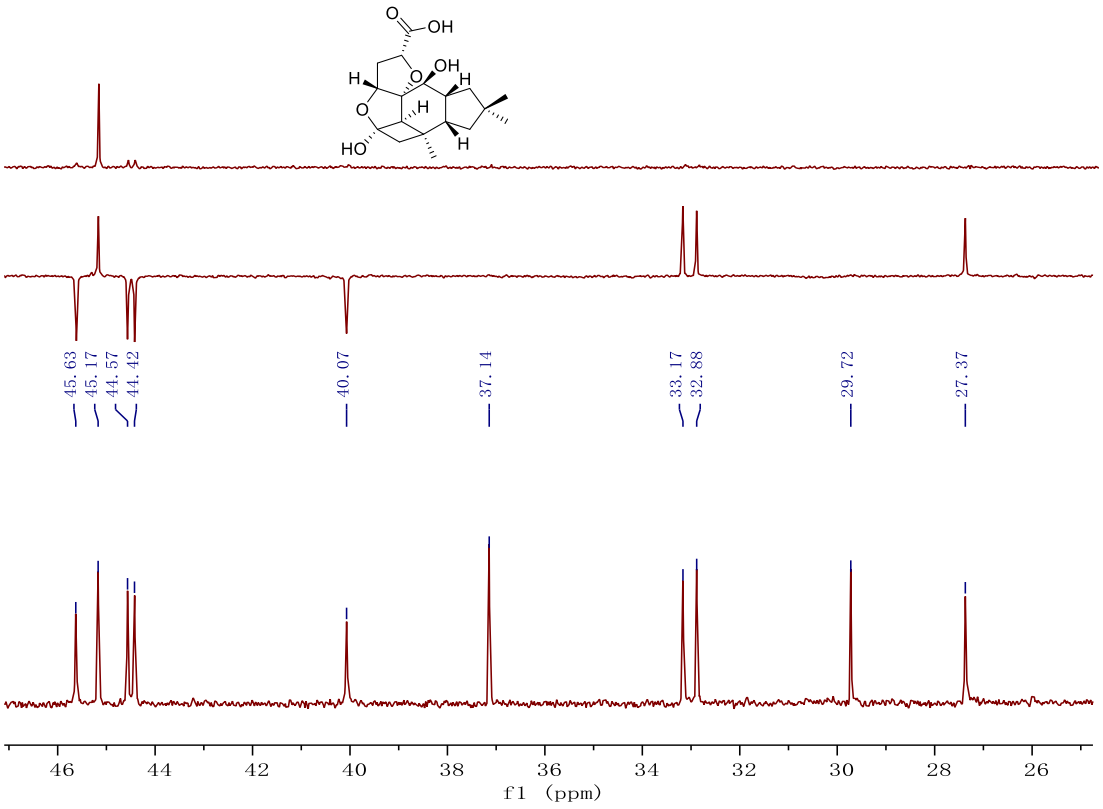

Figure S5. Partial enlarged ^{13}C and DEPT NMR spectrum of epiterenoid A (**1**) in methanol-d_4 (100 MHz).

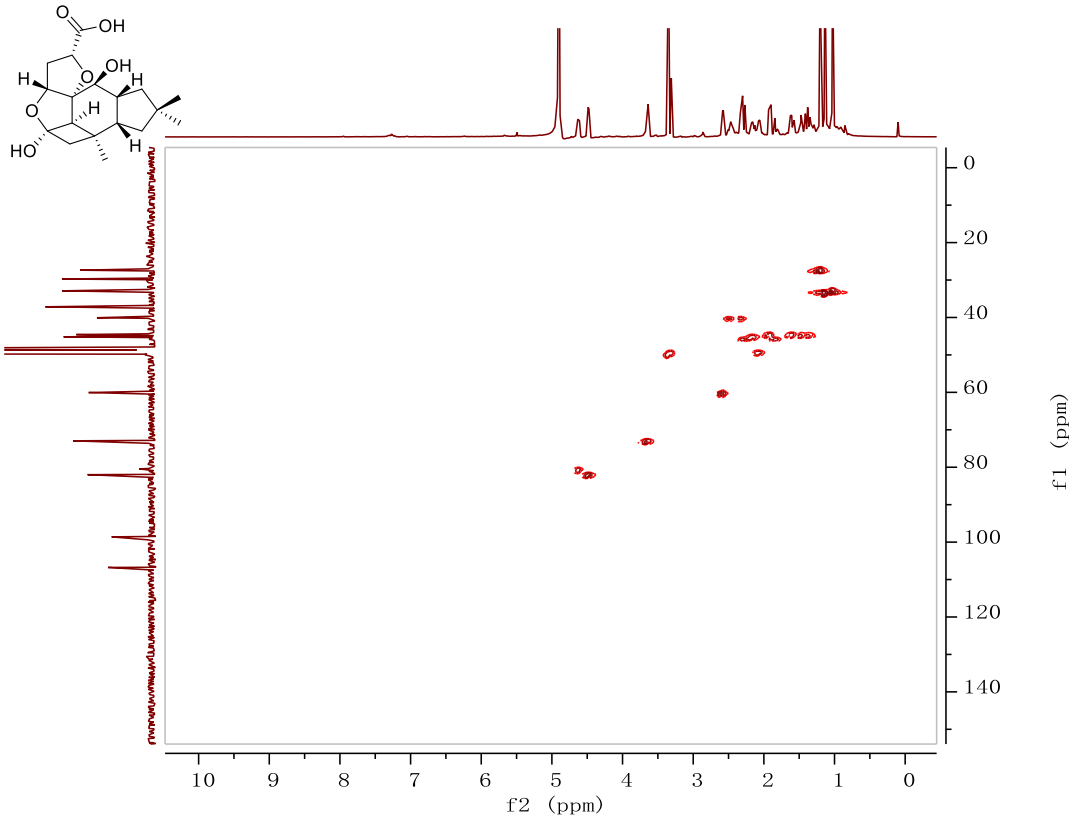

Figure S6. HSQC spectrum of epiterenoid A (**1**) in methanol-d_4 (^1H-400 MHz).

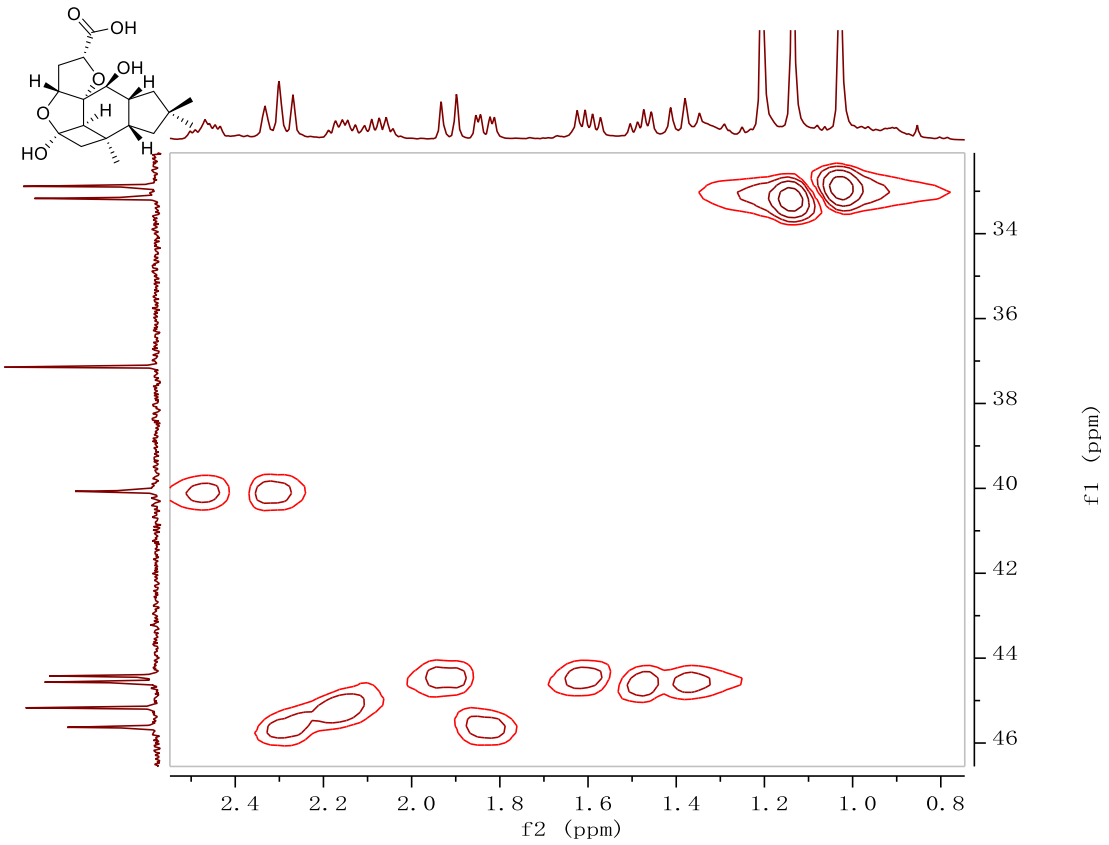

Figure S7. Partial enlarged HSQC spectrum of epiterenoid A (**1**) in methanol-d_4 (^{1}H-400 MHz).

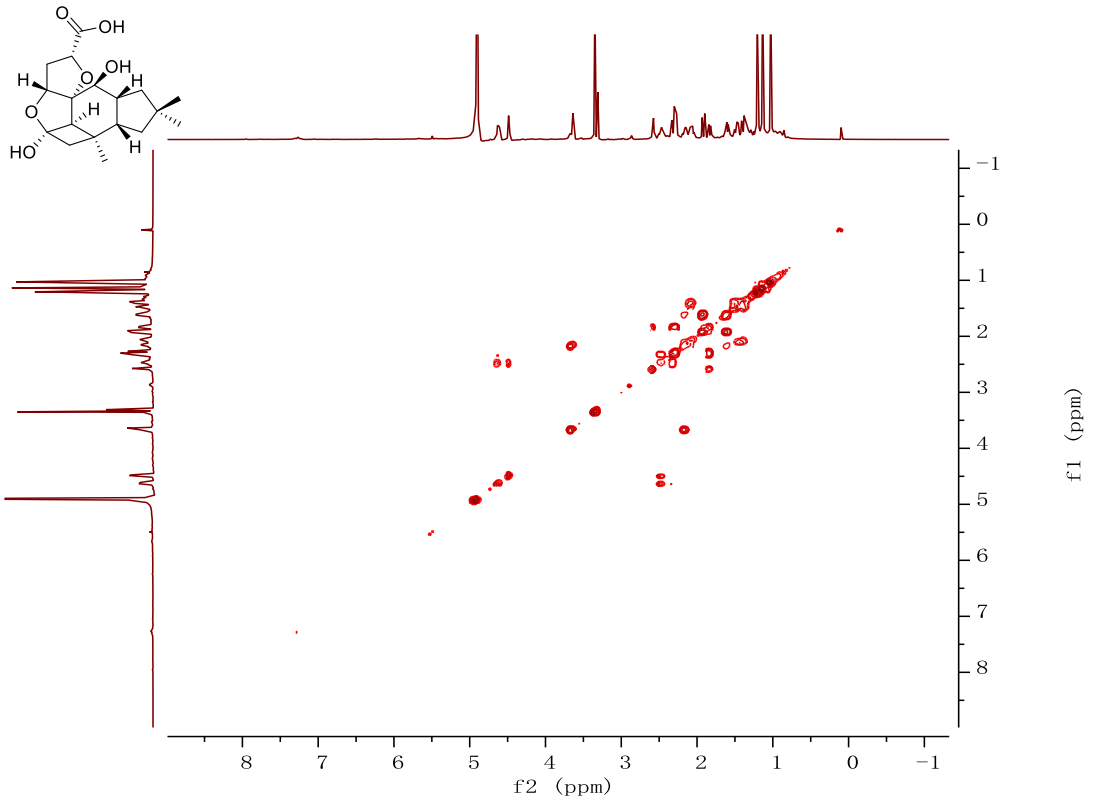

Figure S10. ^{1}H-^{1}H COSY spectrum of epiterenoid A (**1**) in methanol-d_4 (400 MHz).

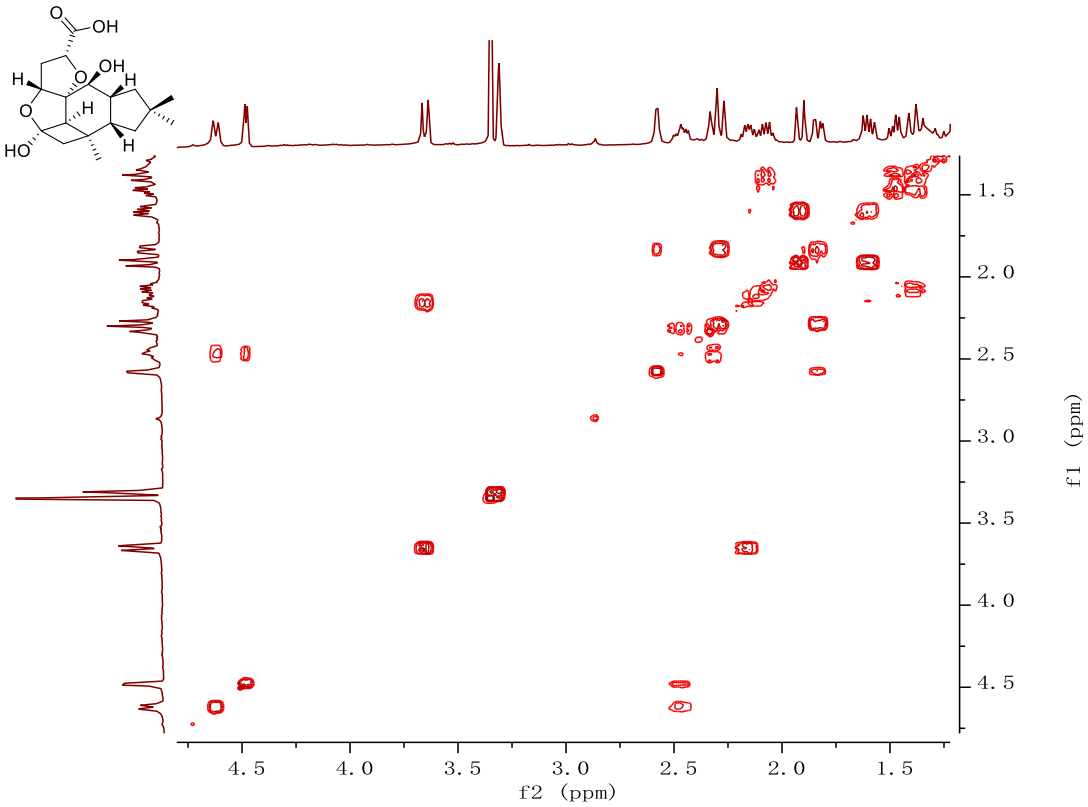

Figure S9. Partial enlarged ^{1}H-^{1}H COSY spectrum of epiterenoid A (**1**) in methanol-d_4 (400 MHz).

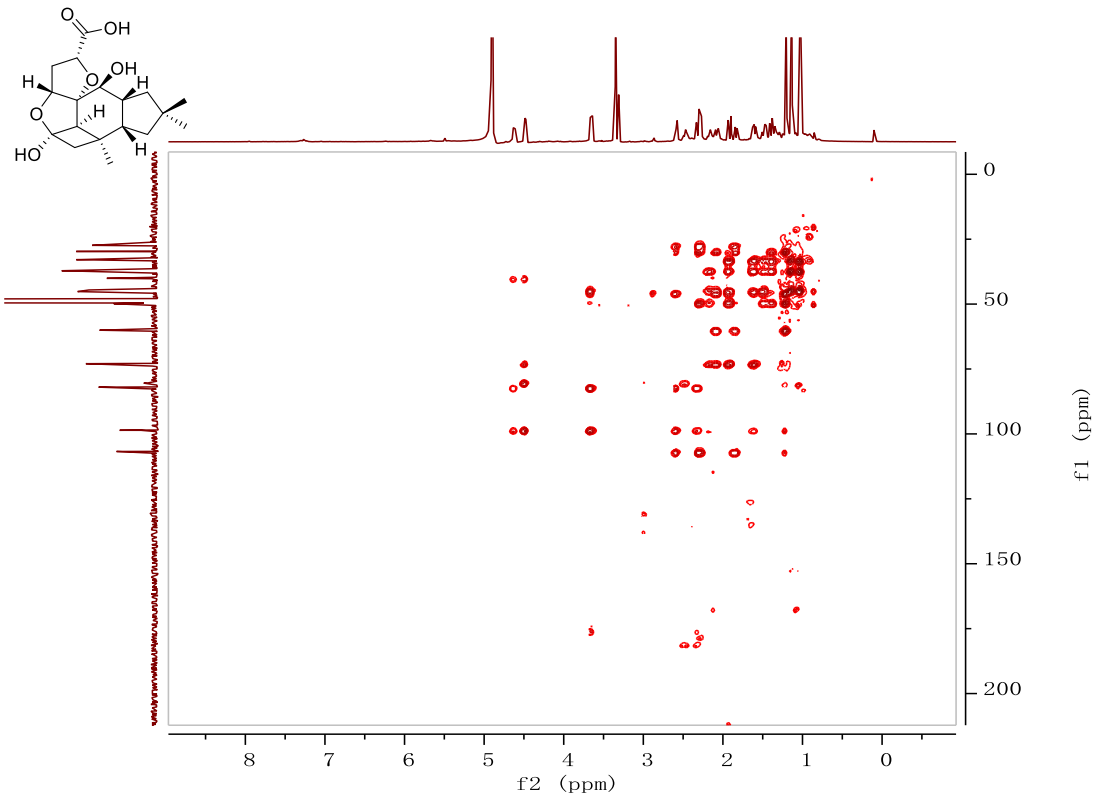

Figure S10. HMBC spectrum of epiterenoid A (**1**) in methanol-d_4 (^{1}H-400 MHz).

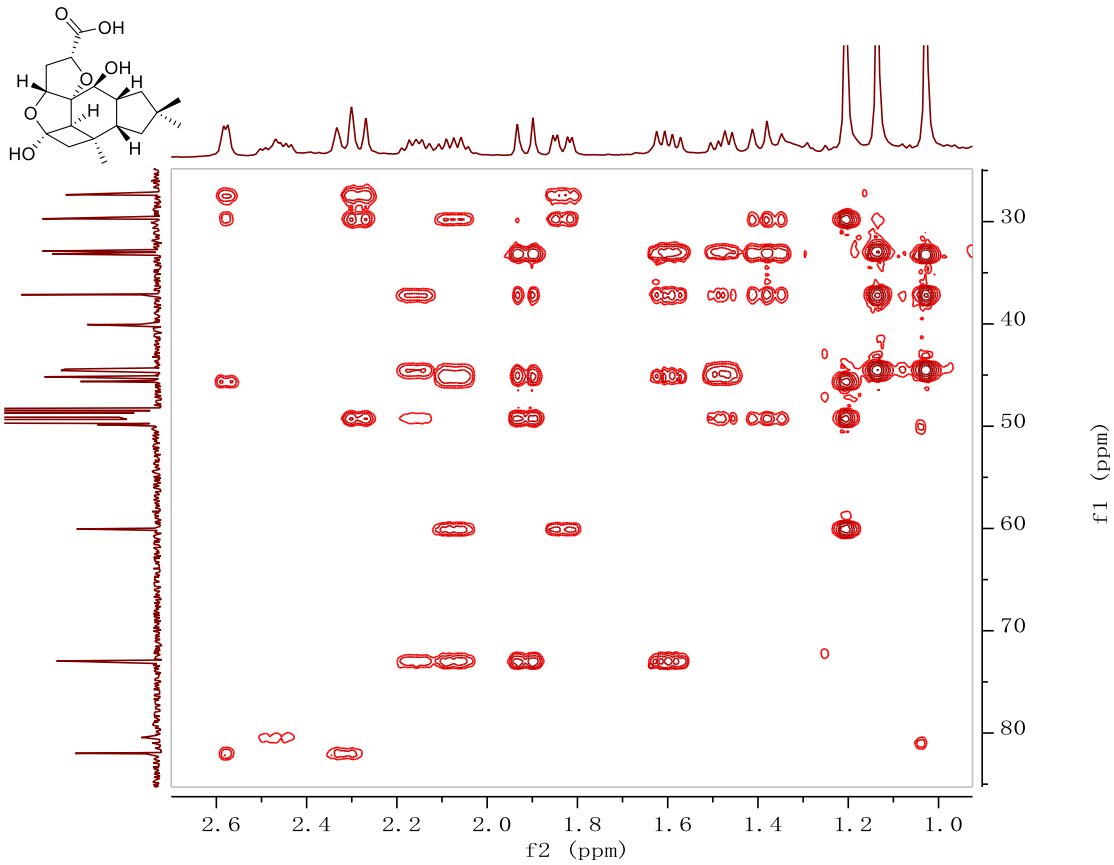

Figure S11. Partial enlarged HMBC spectrum of epiterenoid A (**1**) in methanol-d_4 (^{1}H-400 MHz).

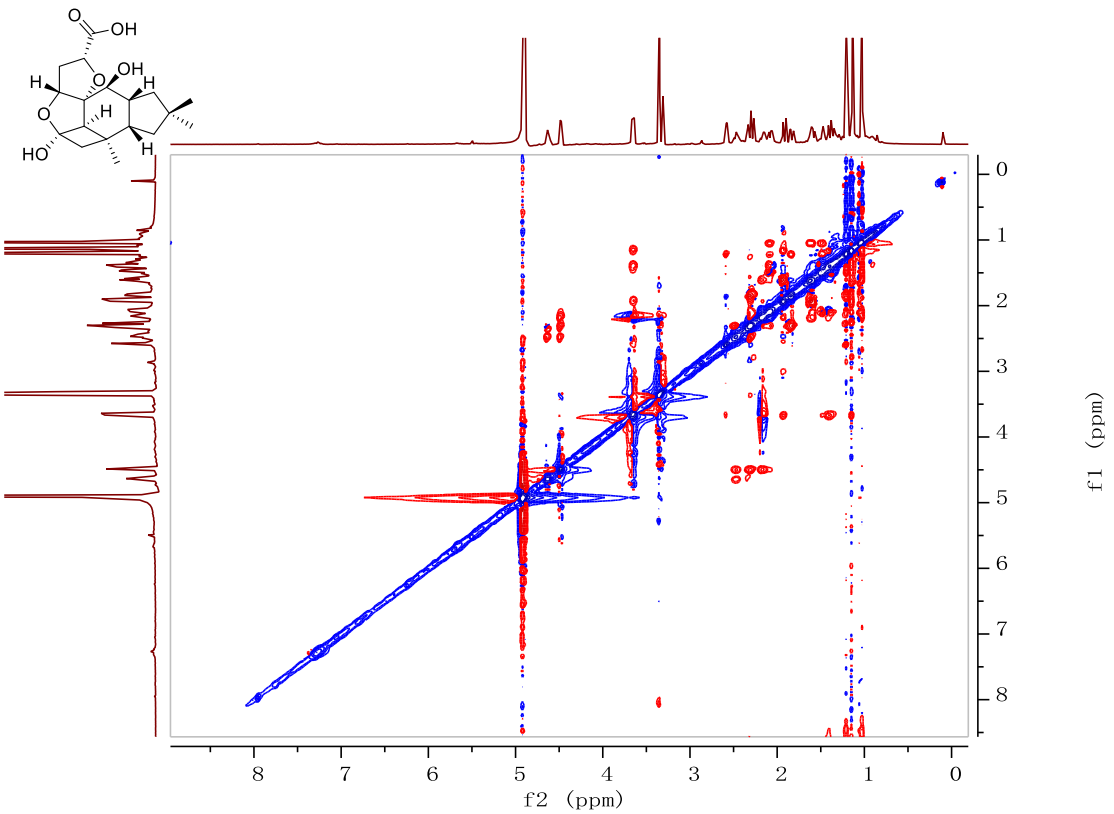

Figure S12. ROESY spectrum of epiterenoid A (**1**) in methanol-d_4 (400 MHz).

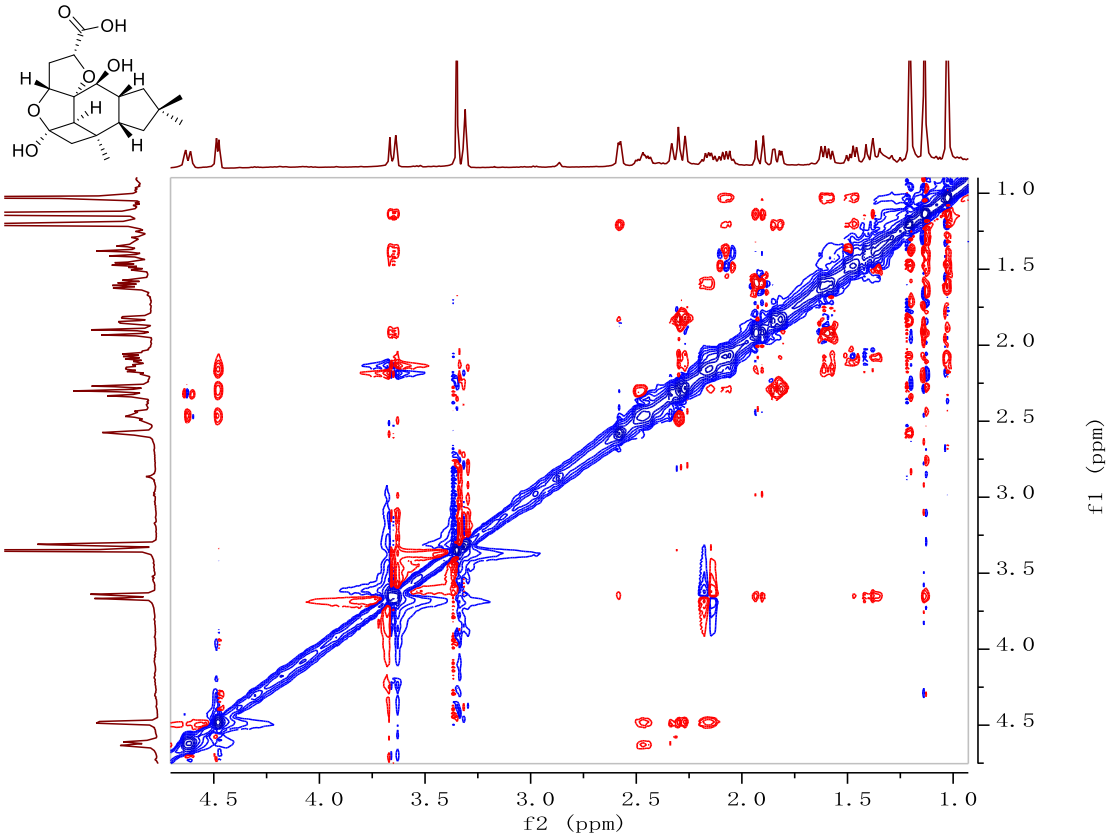

Figure S13. Partial enlarged ROESY spectrum of epiterenoid A (**1**) in methanol-d_4 (400 MHz).

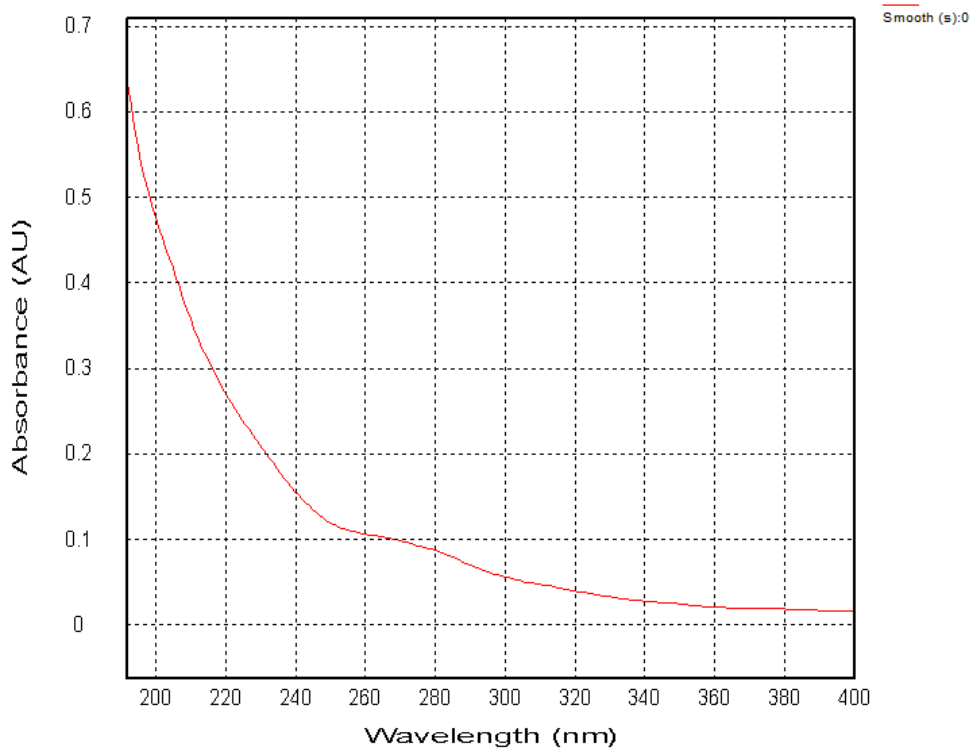

Figure S14. UV spectrum of epiterenoid A (**1**) in methanol.

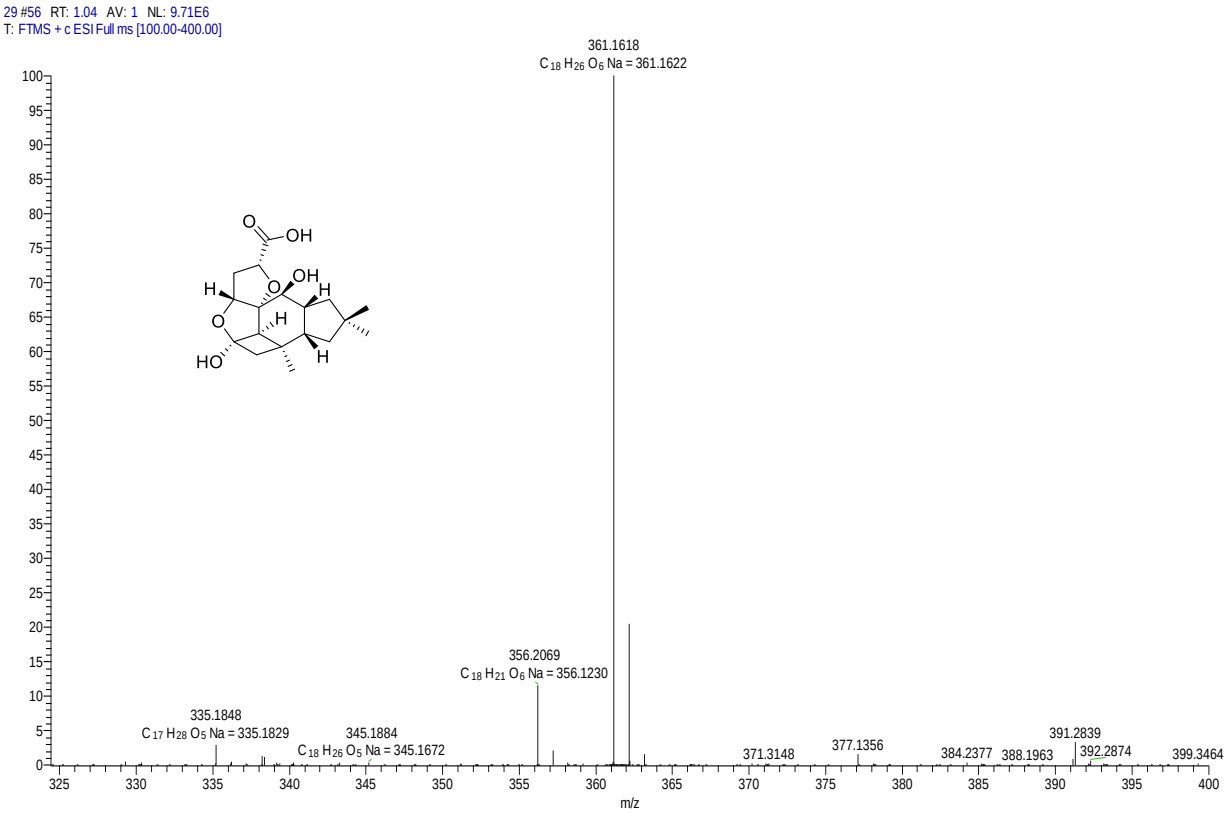

Figure S15. (+)-HRESIMS data of epiterenoid A (**1**).

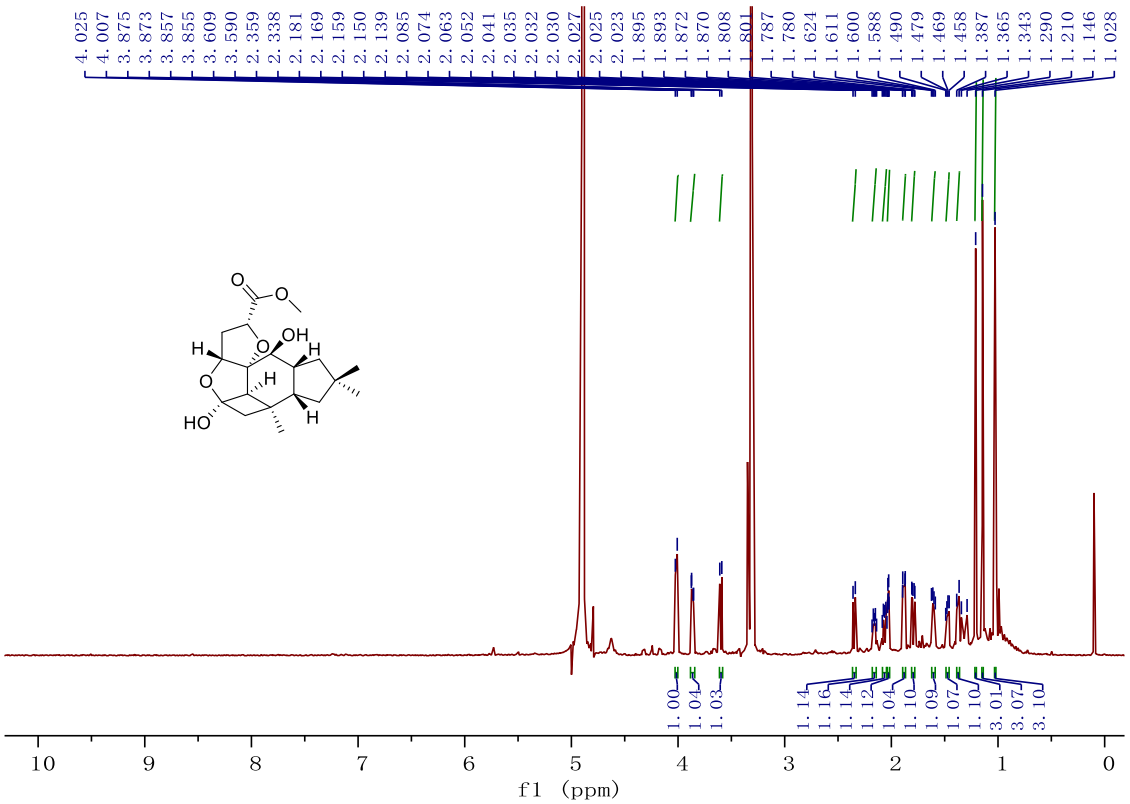

Figure S16. ^{1}H NMR spectrum of epiterenoid B (**2**) in methanol-d_4 (400 MHz).

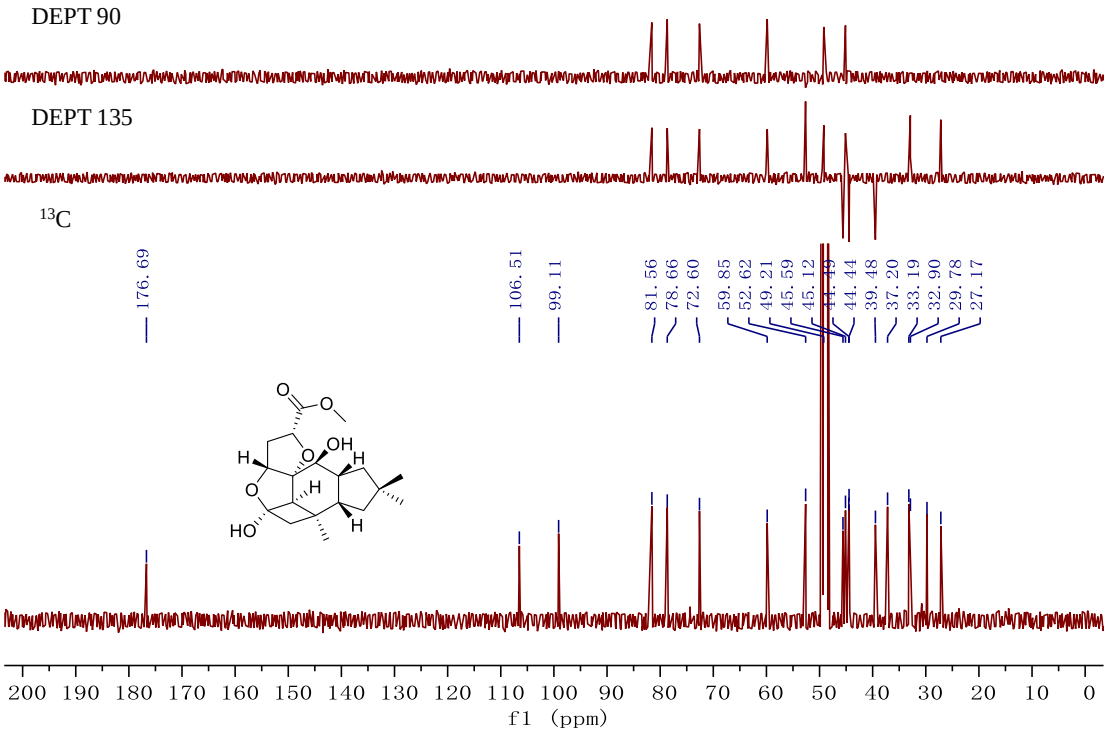

Figure S17. ^{13}C and DEPT NMR spectrum of epiterenoid B (**2**) in methanol-d_4 (100 MHz).

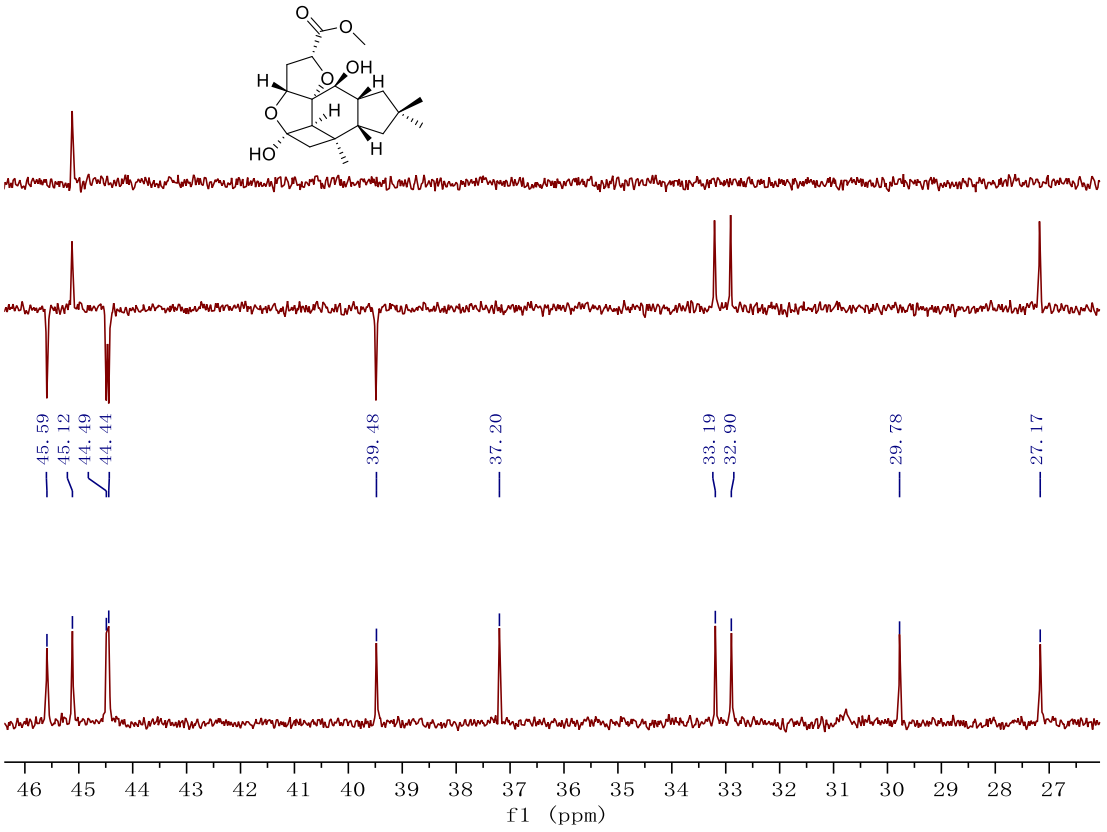

Figure S18. Partial enlarged ^{13}C and DEPT NMR spectrum of epiterenoid B (**2**) in methanol-d_4 (100 MHz).

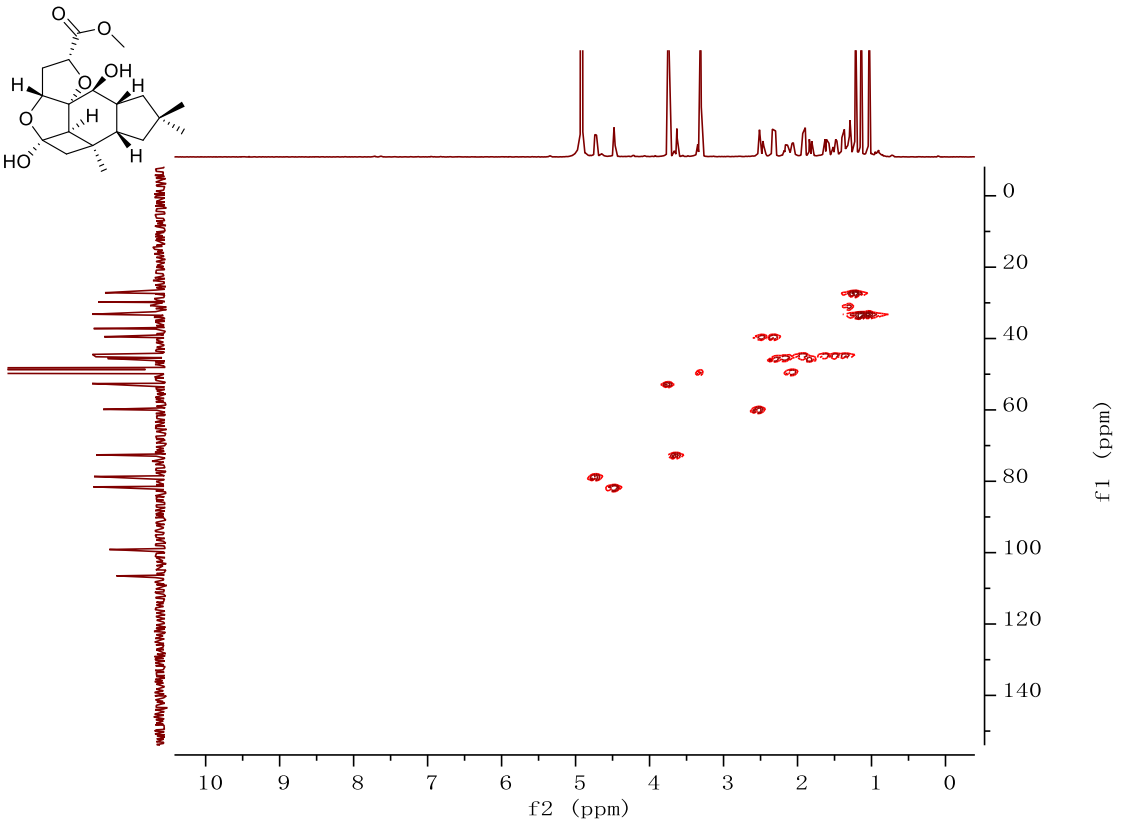

Figure S19. HSQC spectrum of epiterenoid B (**2**) in methanol-d_4 (^{1}H-400 MHz).

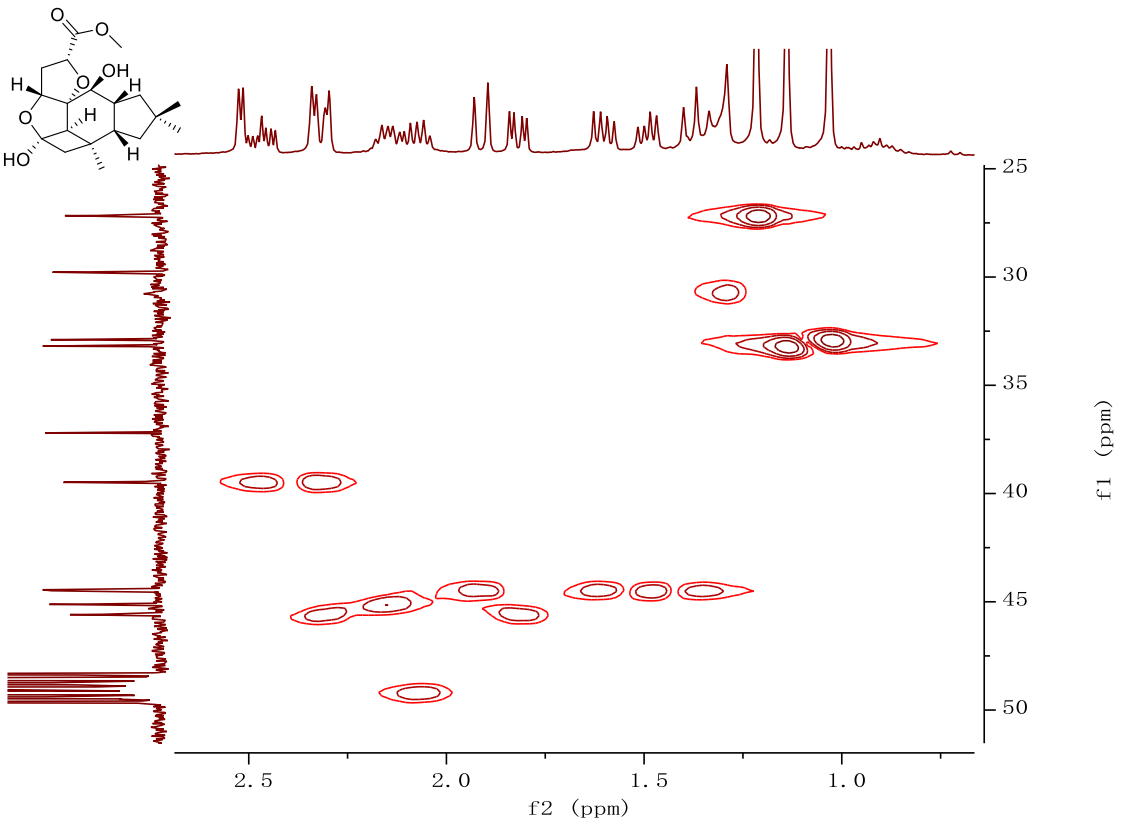

Figure S20. Partial enlarged HSQC spectrum of epiterenoid B (**2**) in methanol-d_4 (^{1}H-400 MHz).

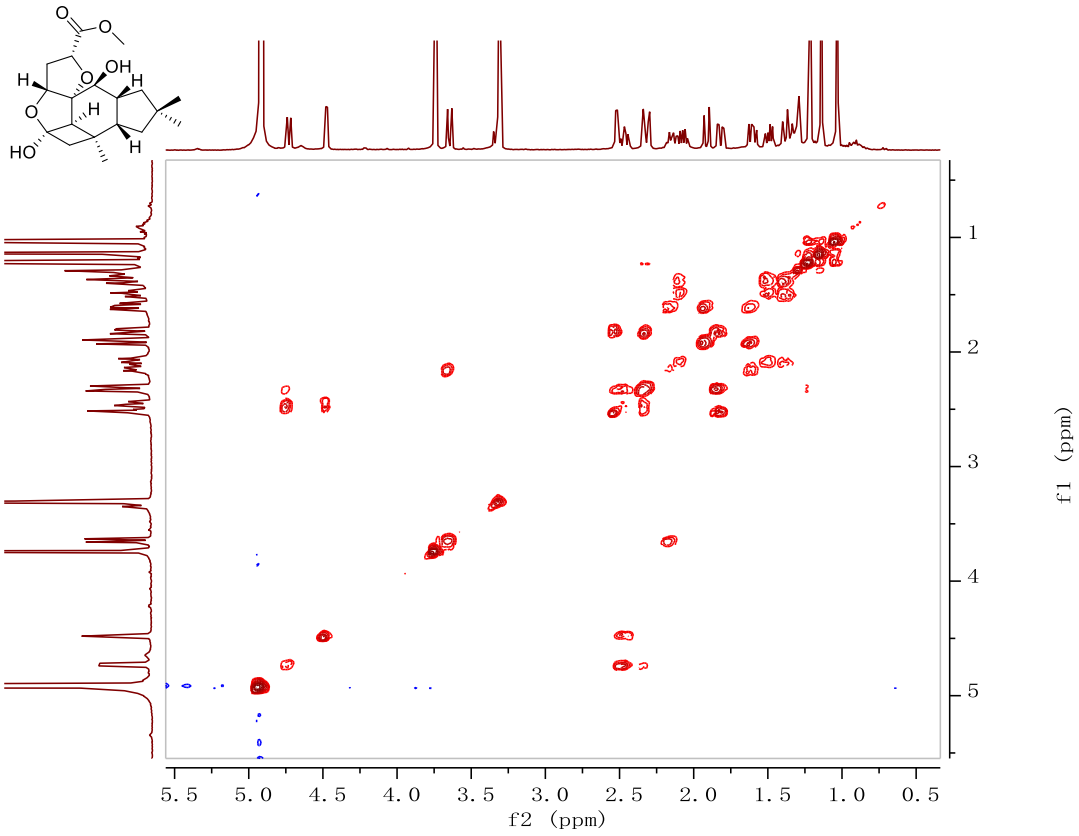

Figure S21. ^{1}H-^{1}H COSY spectrum of epiterenoid B (**2**) in methanol-d_4 (400 MHz).

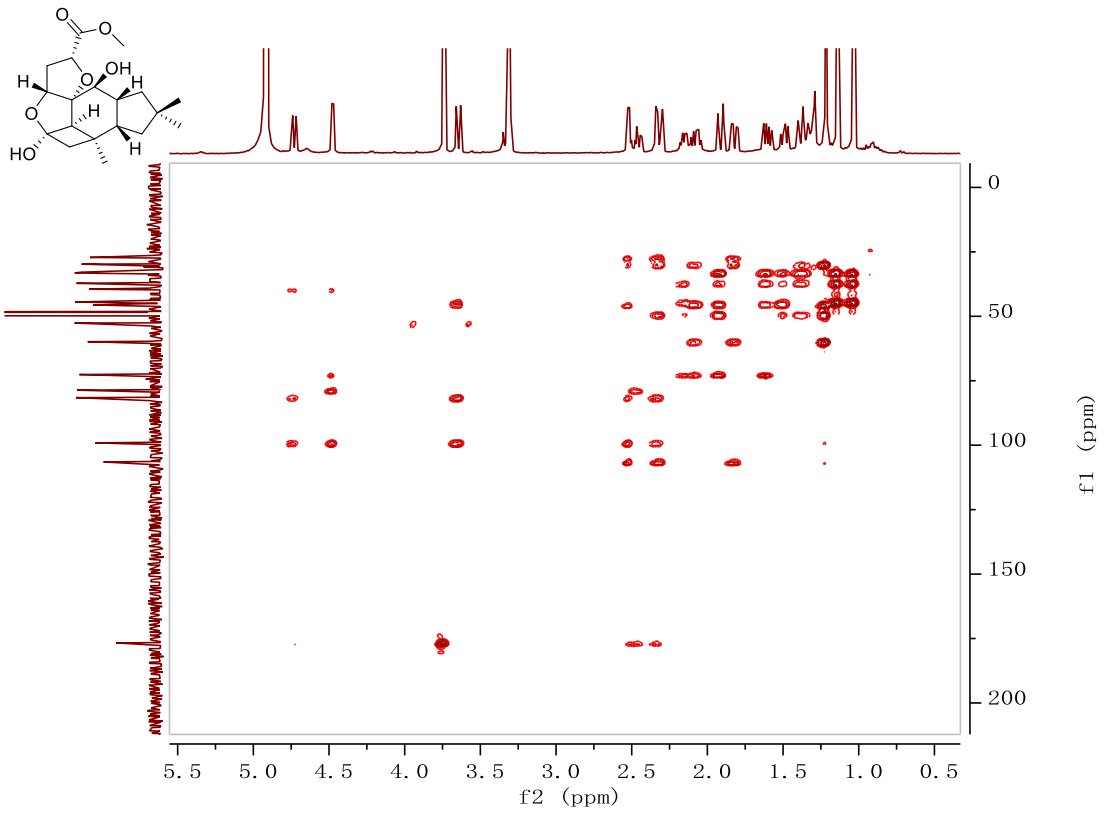

Figure S22. HMBC spectrum of epiterenoid B (**2**) in methanol-d_4 (^{1}H-400 MHz).

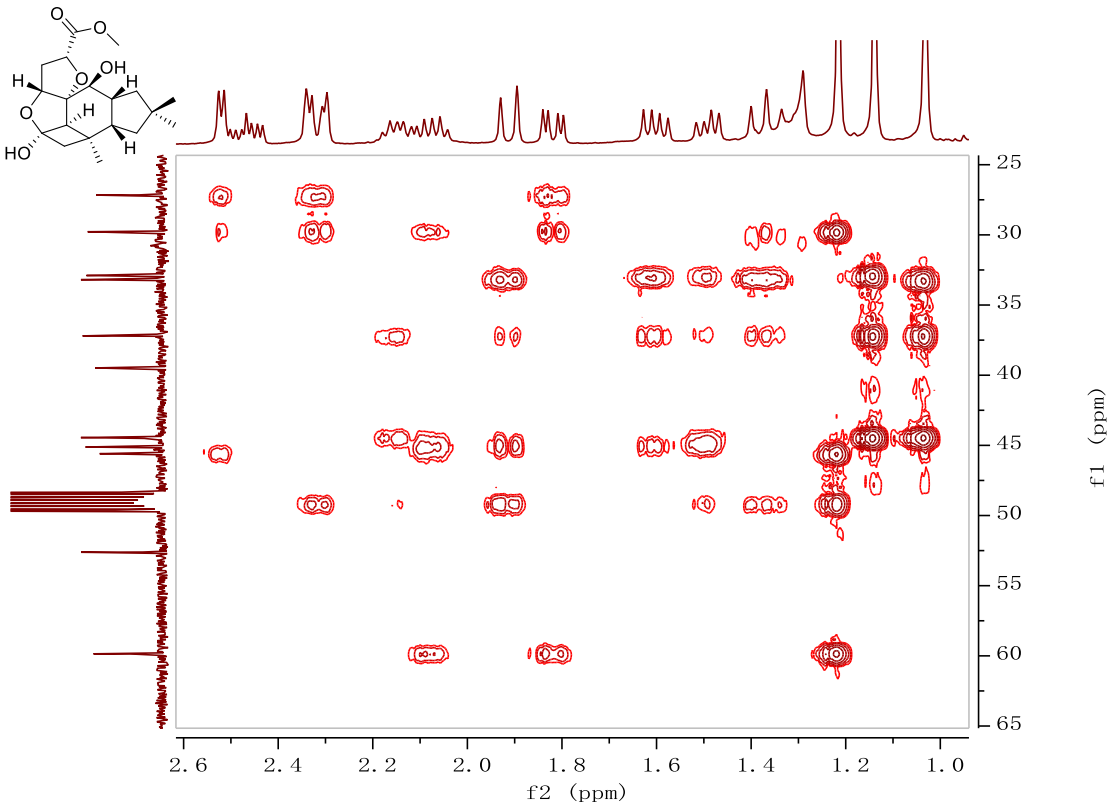

Figure S23. Partial enlarged HMBC spectrum of epiterenoid B (**2**) in methanol-d_4 (^{1}H-400 MHz).

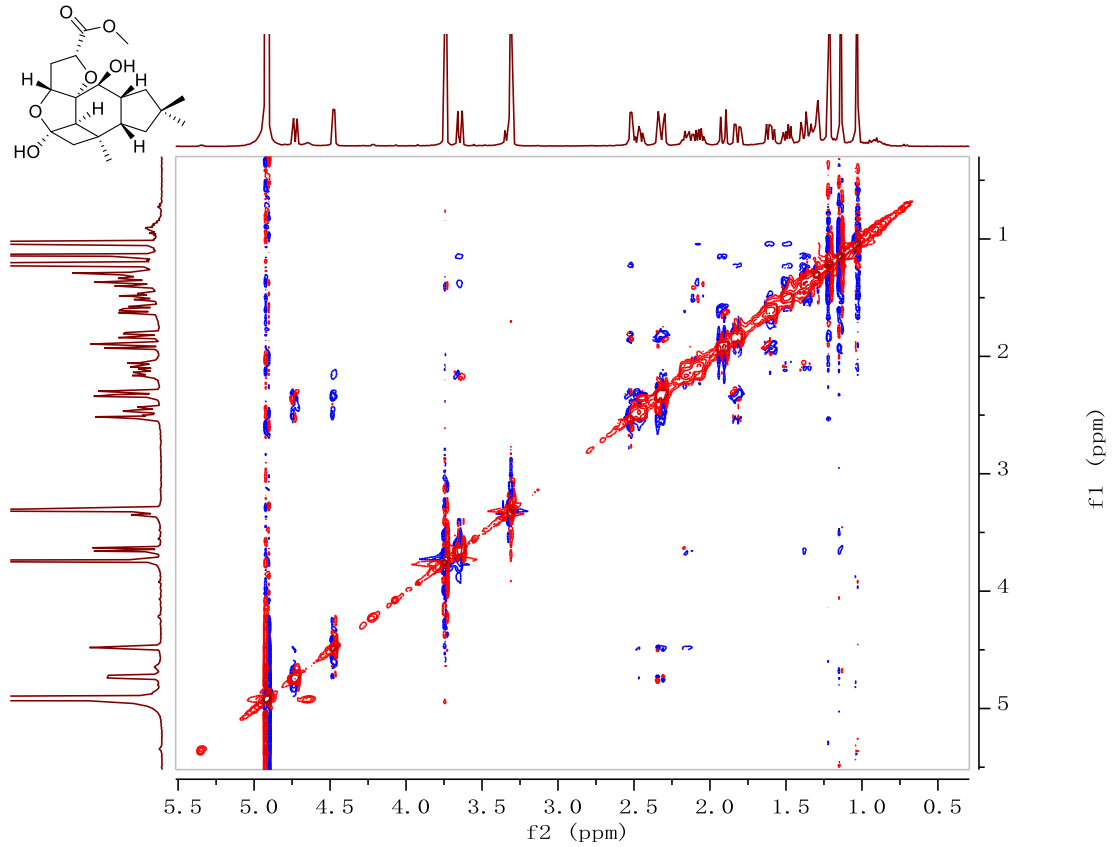

Figure S24. ROESY spectrum of epiterenoid B (**2**) in methanol-d_4 (400 MHz).

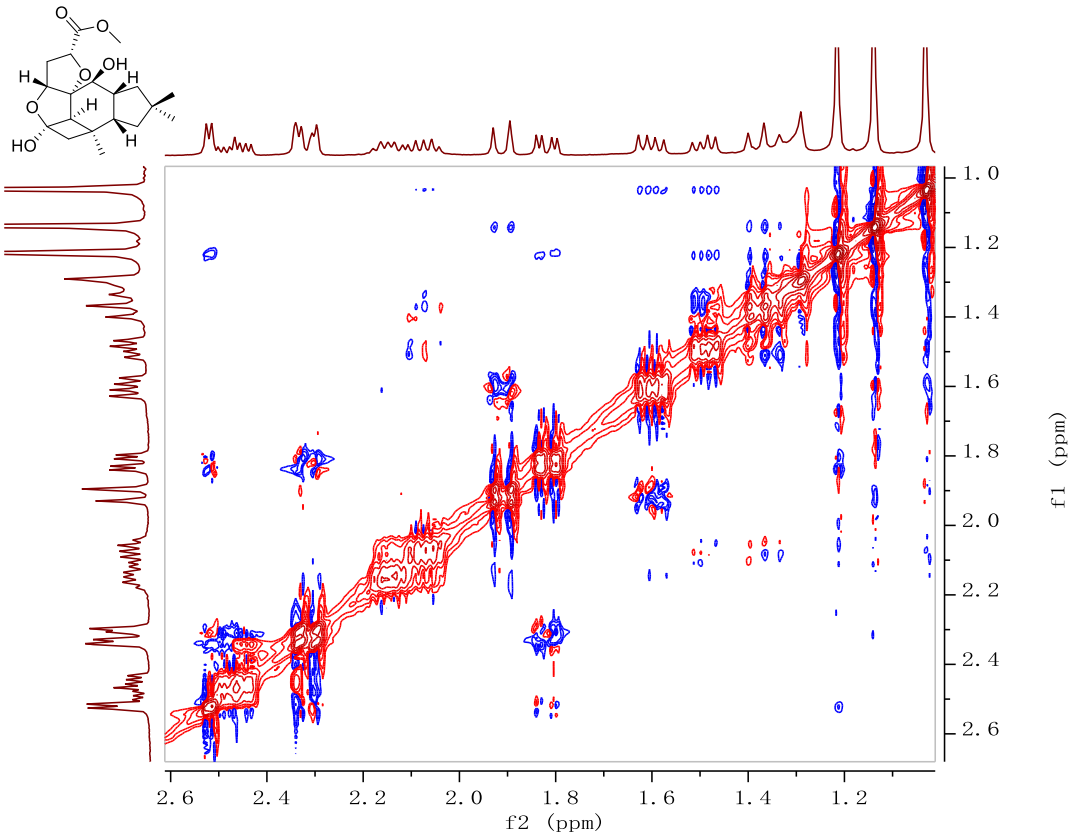

Figure S25. Partial enlarged ROESY spectrum of epiterenoid B (**2**) in methanol-d_4 (400 MHz).

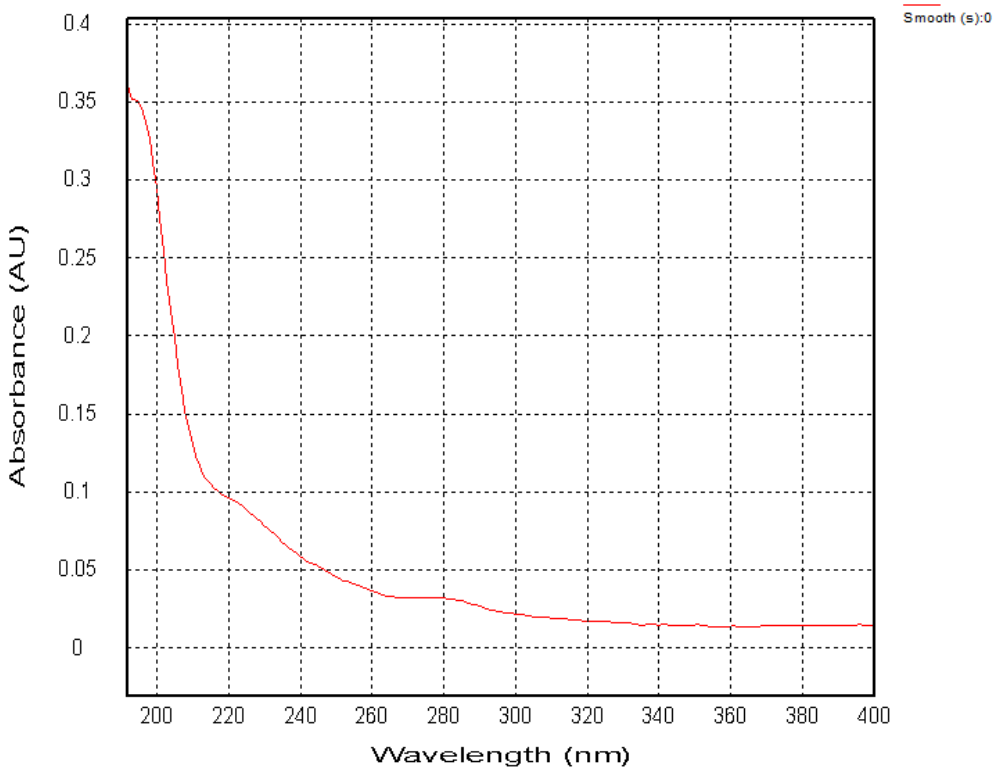

Figure S26. UV spectrum of epiterenoid B (**2**) in methanol.

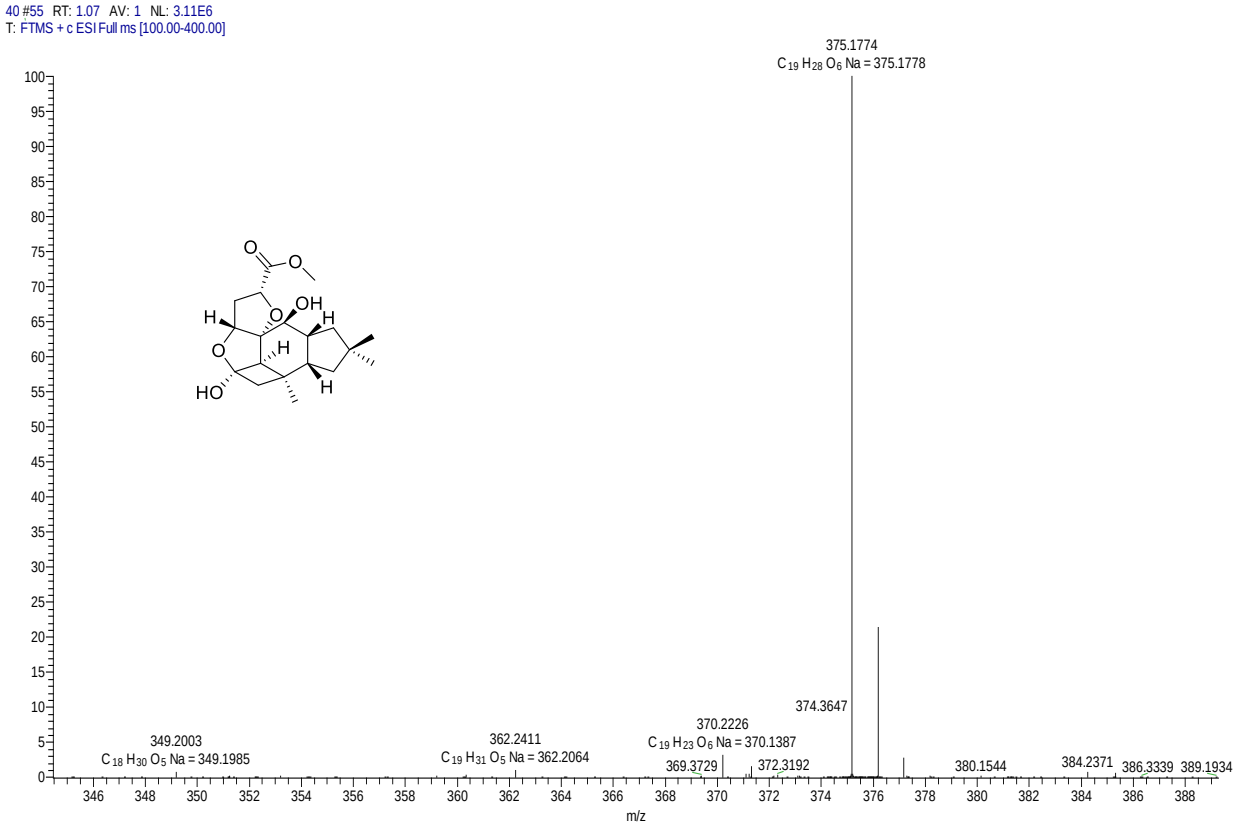

Figure S27. (+)-HRESIMS data of epiterenoid B (**2**).

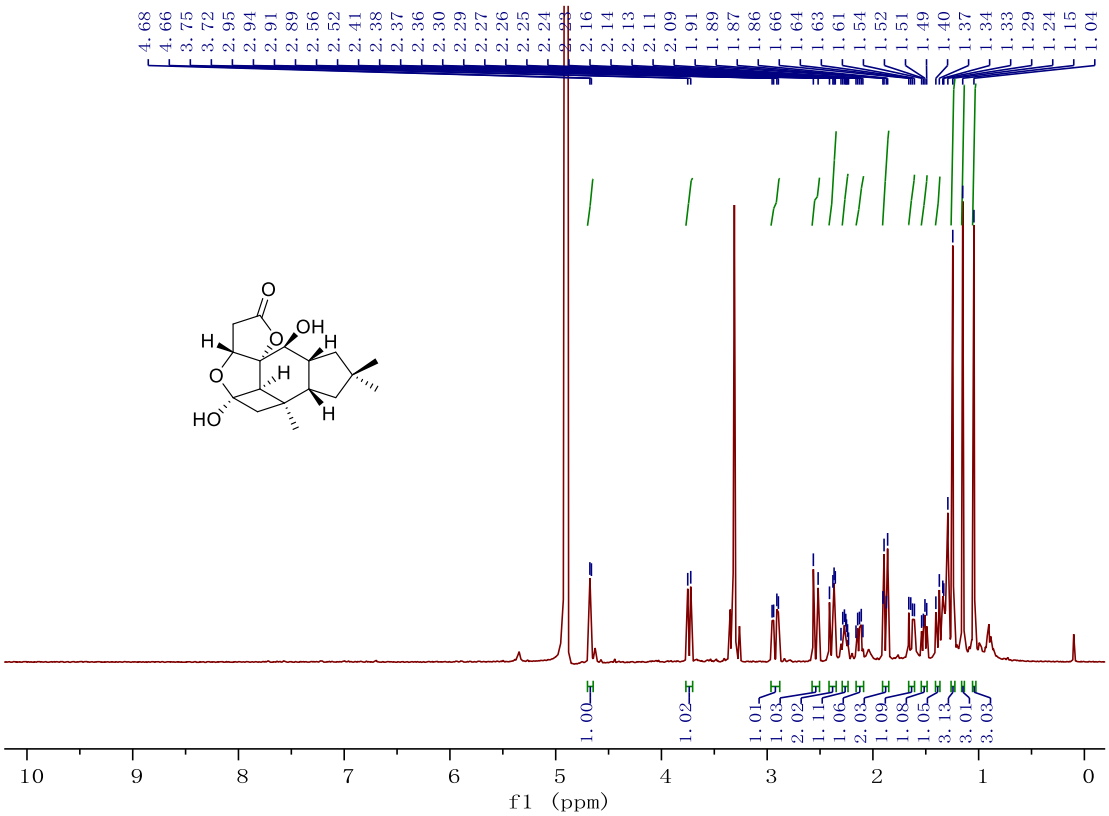

Figure S28. ^{1}H NMR spectrum of epiterenoid C (**3**) in methanol-d_4 (400 MHz).

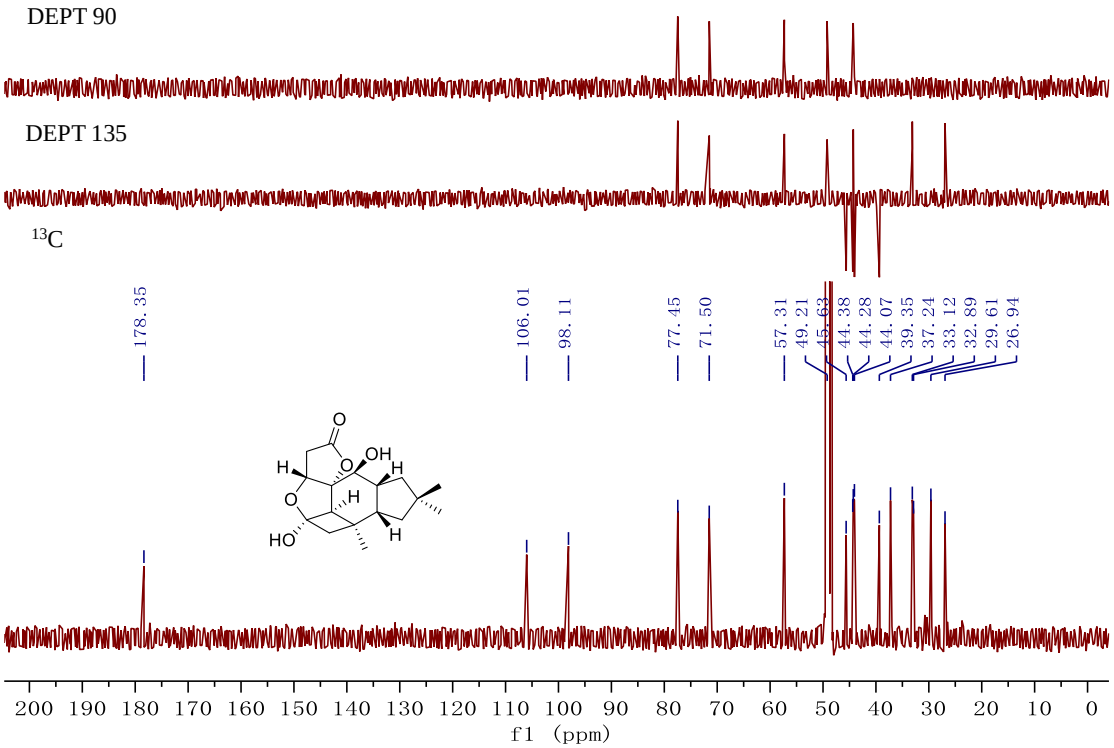

Figure S29. ^{13}C and DEPT NMR spectrum of epiterenoid C (**3**) in methanol-d_4 (100 MHz).

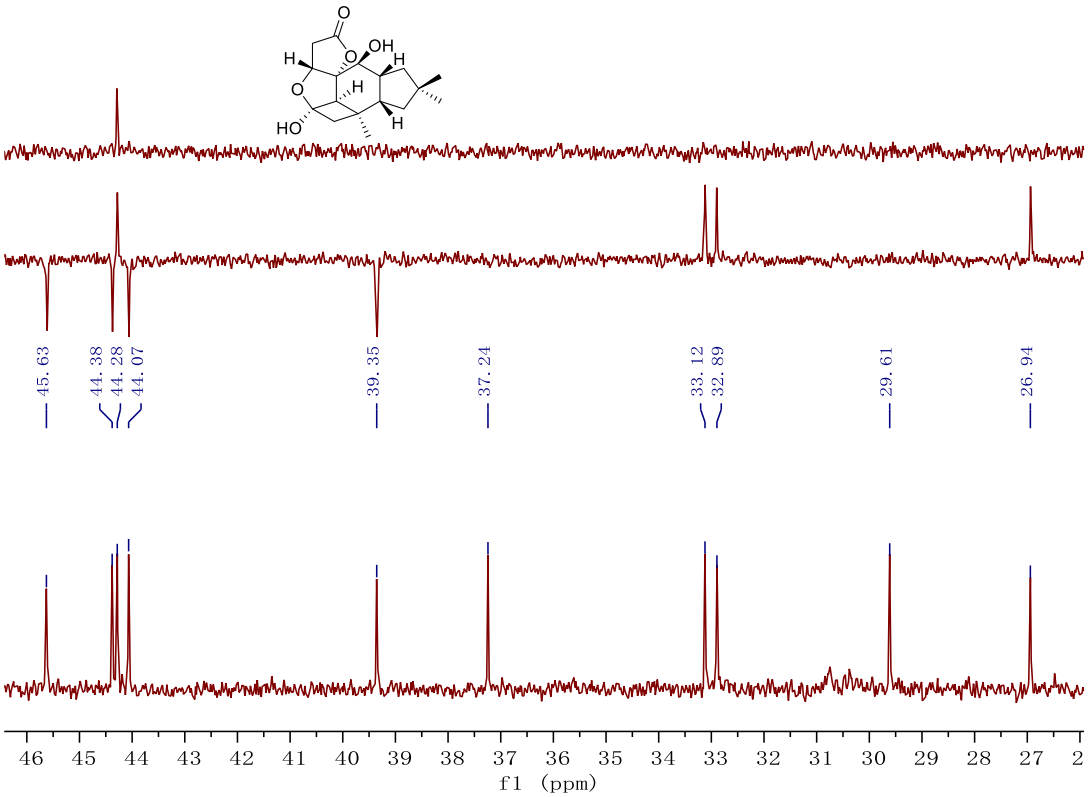

Figure S30. Partial enlarged ^{13}C and DEPT NMR spectrum of epiterenoid C (**3**) in methanol-d_4 (100 MHz).

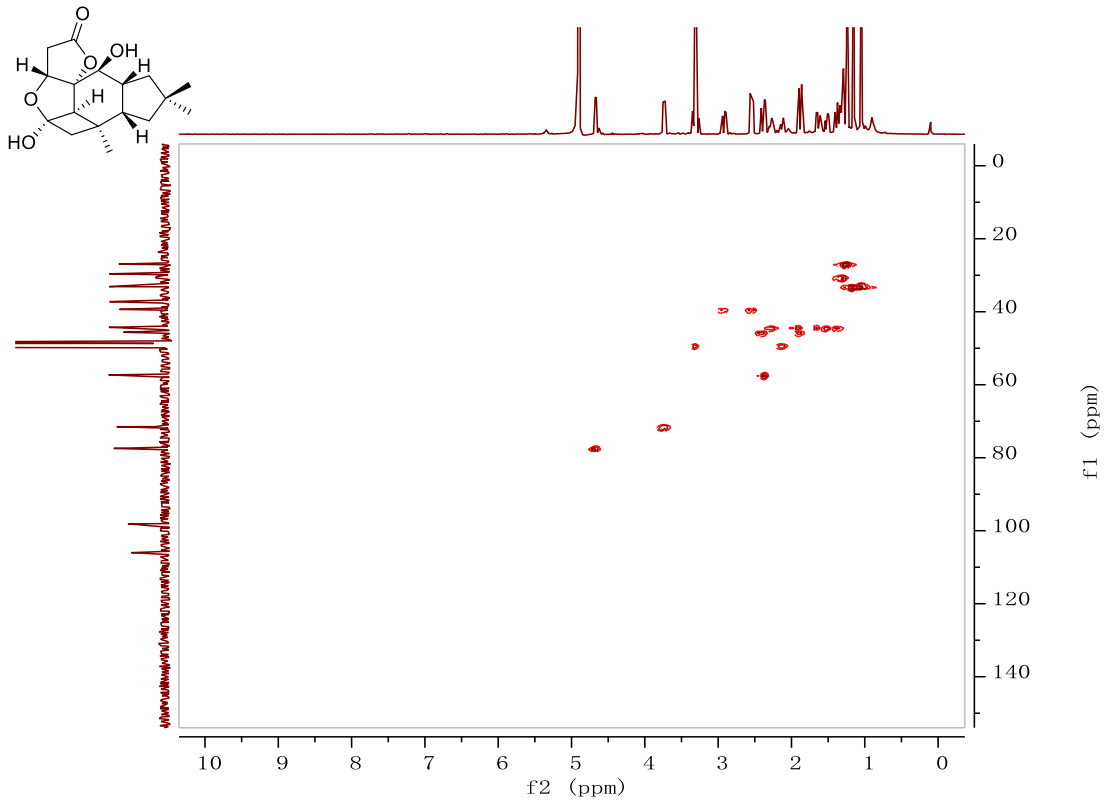

Figure S31. HSQC spectrum of epiterenoid C (**3**) in methanol-d_4 (^{1}H-400 MHz).

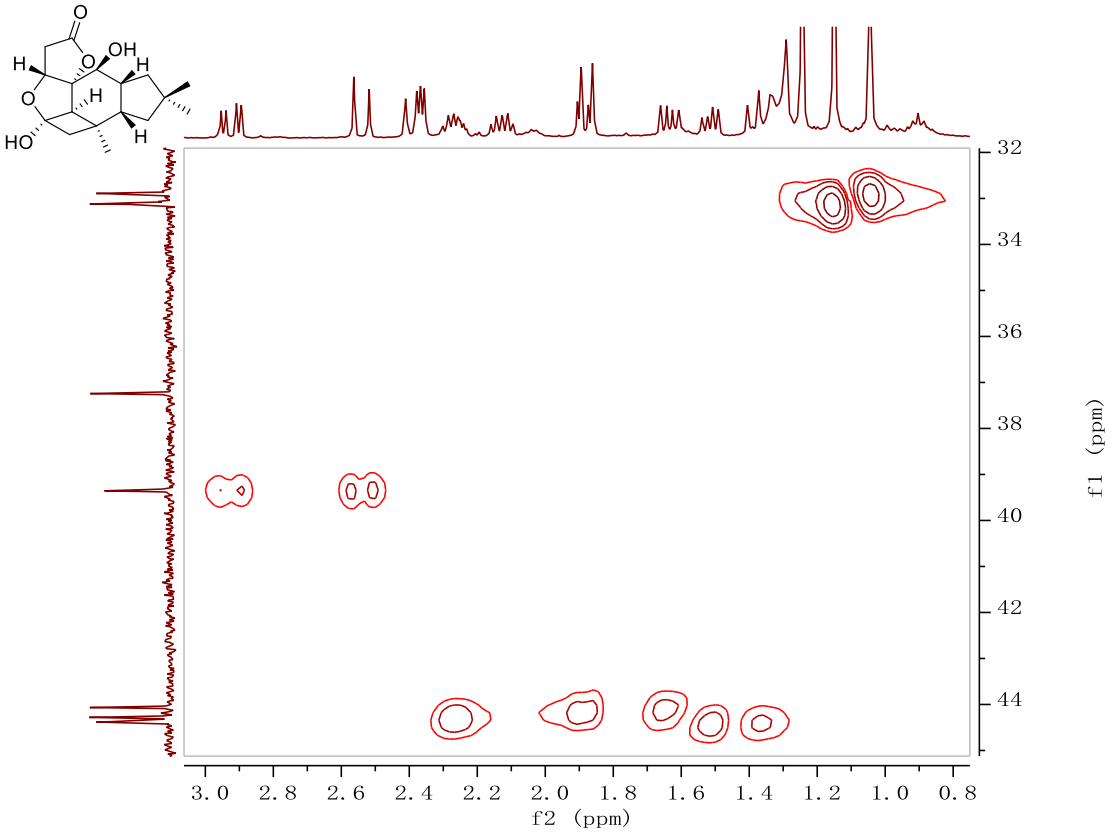

Figure S32. Partial enlarged HSQC spectrum of epiterenoid C (**3**) in methanol-d_4 (^{1}H-400 MHz).

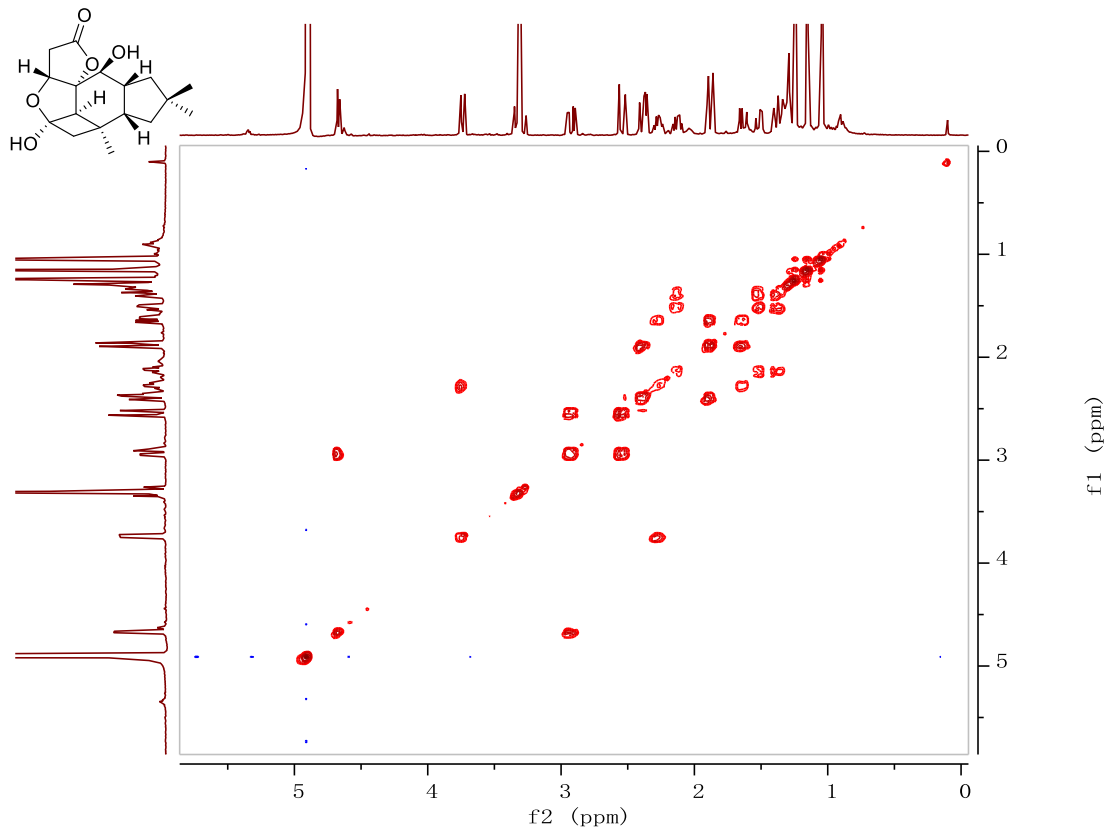

Figure S33. ^{1}H-^{1}H COSY spectrum of epiterenoid C (**3**) in methanol-d_4 (400 MHz).

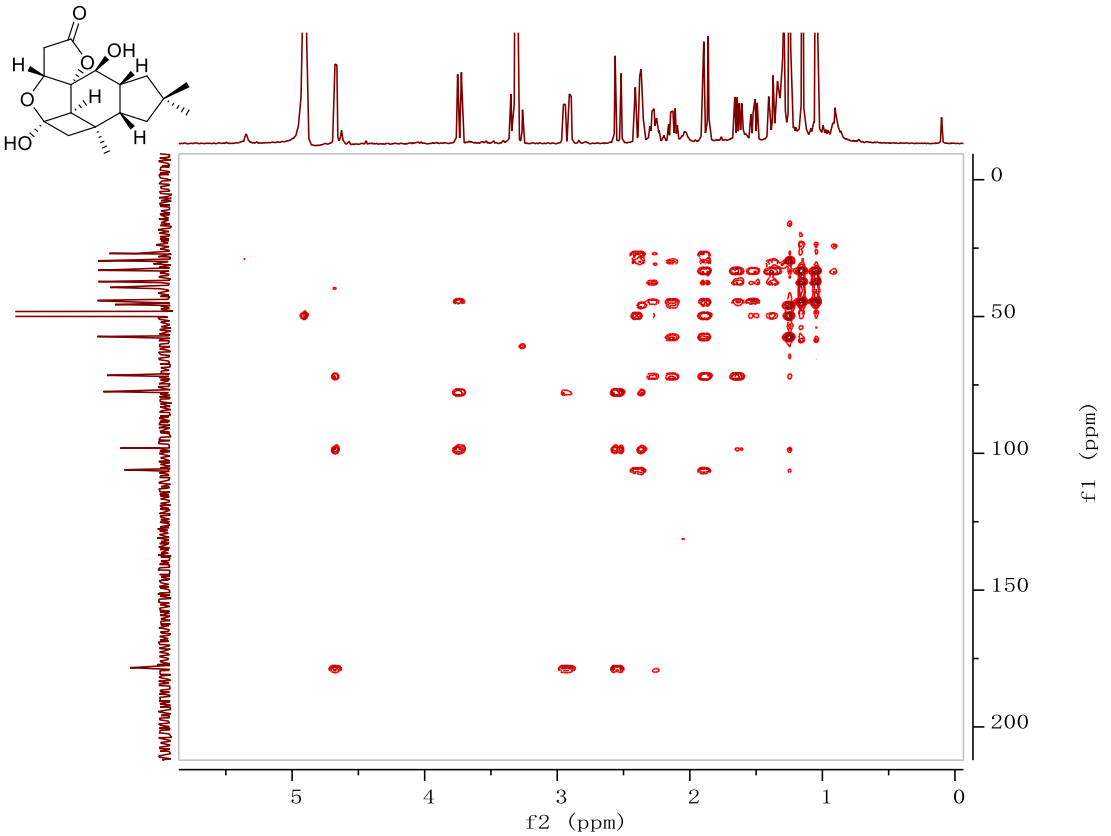

Figure S34. HMBC spectrum of epiterenoid C (**3**) in methanol-d_4 (^{1}H-400 MHz).

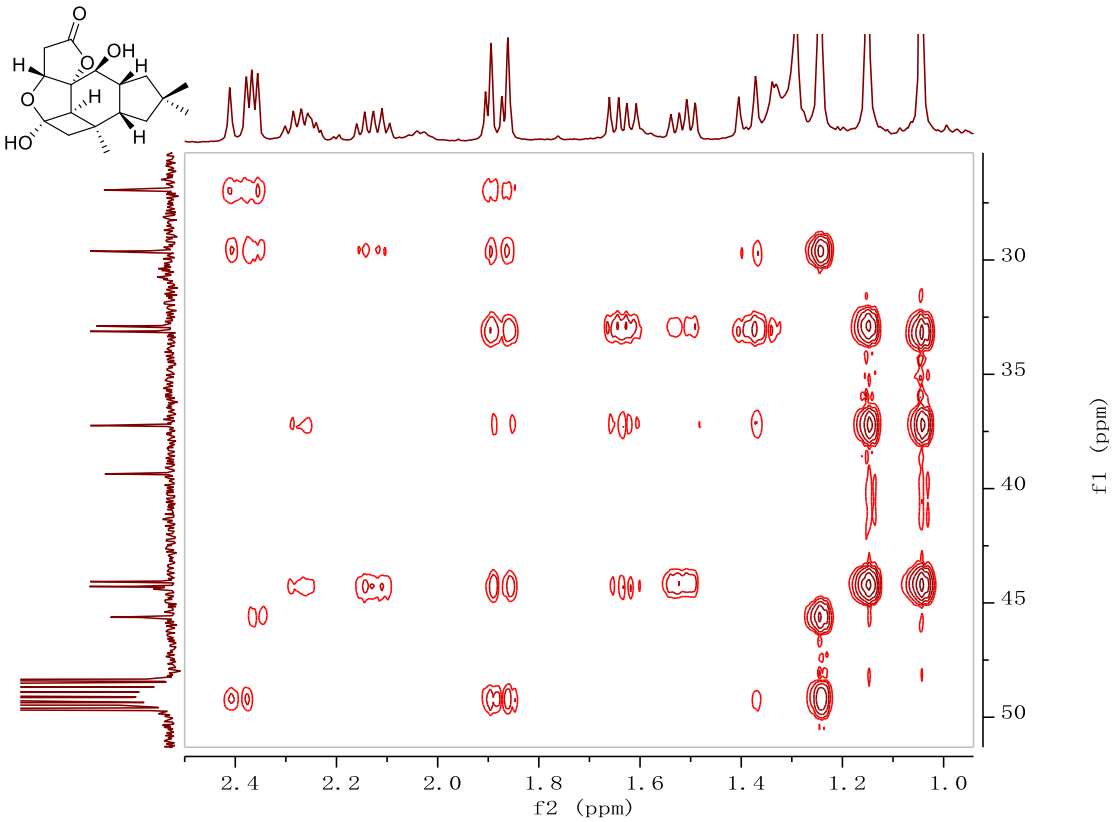

Figure S35. Partial enlarged HMBC spectrum of epiterenoid C (**3**) in methanol-d_4 (^{1}H-400 MHz).

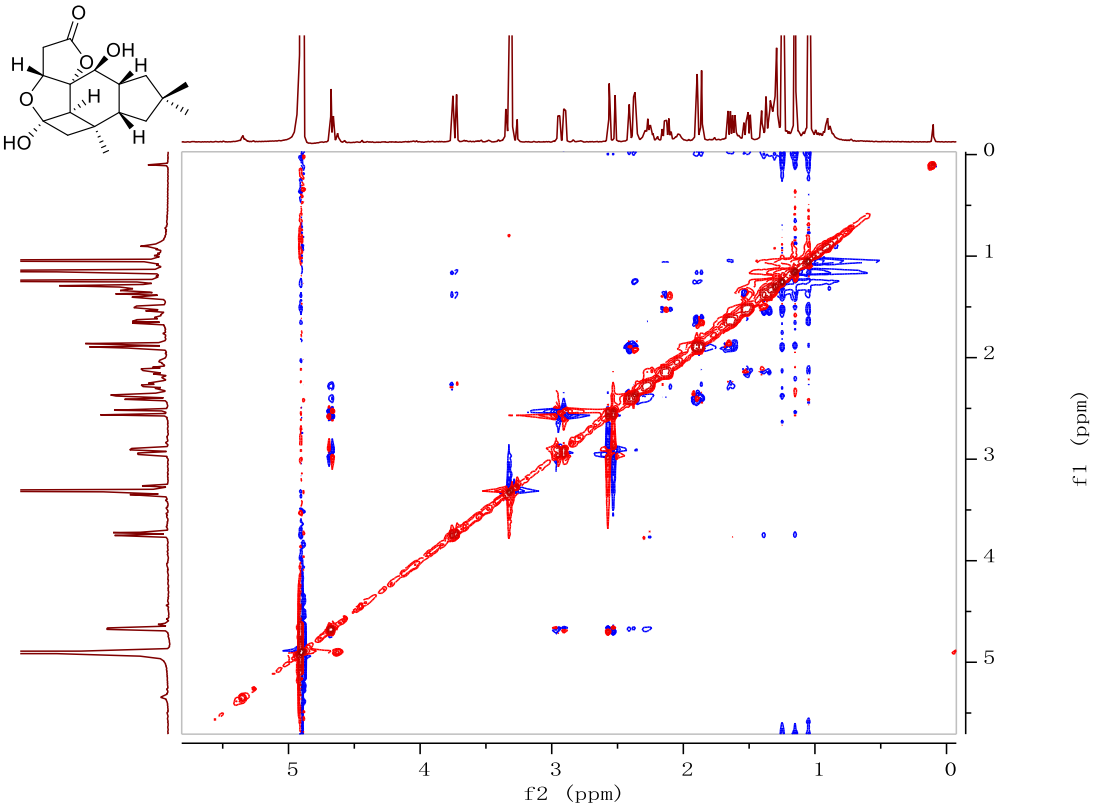

Figure S36. ROESY spectrum of epiterenoid C (**3**) in methanol-d_4 (400 MHz).

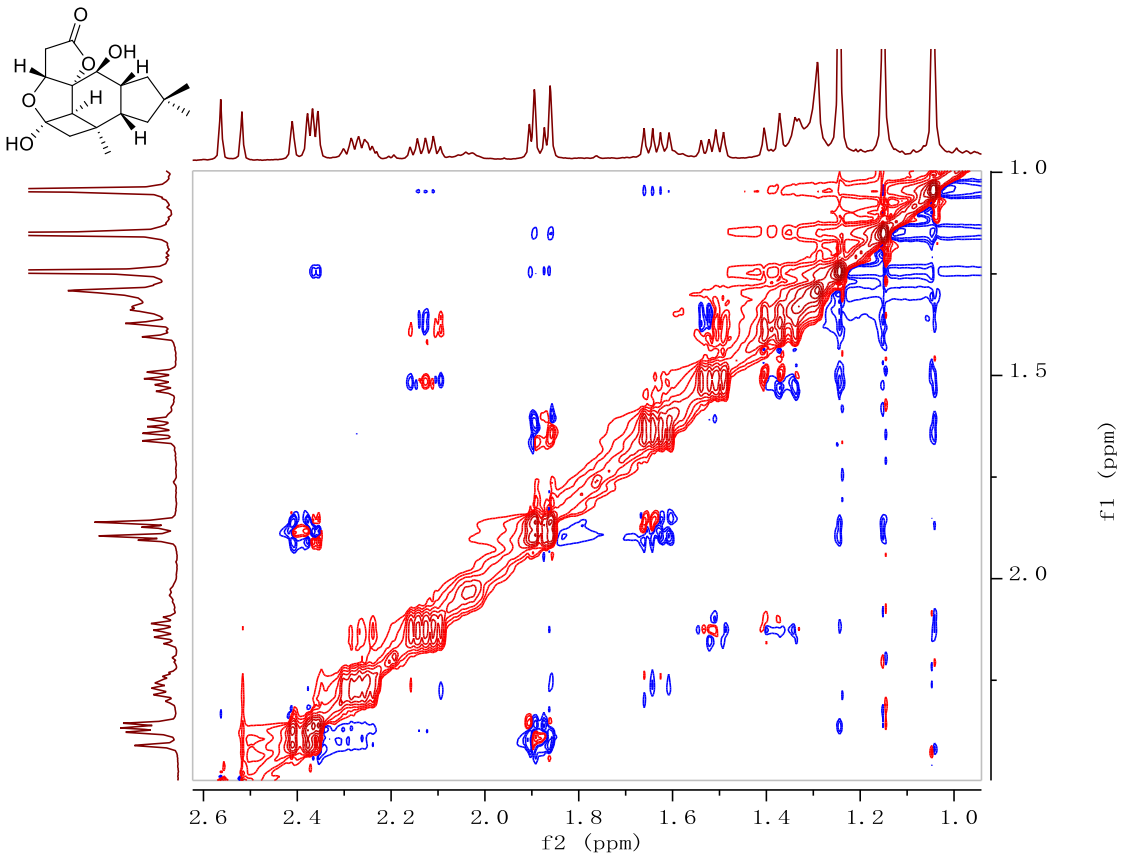

Figure S37. Partial enlarged ROESY spectrum of epiterenoid C (**3**) in methanol-d_4 (400 MHz).

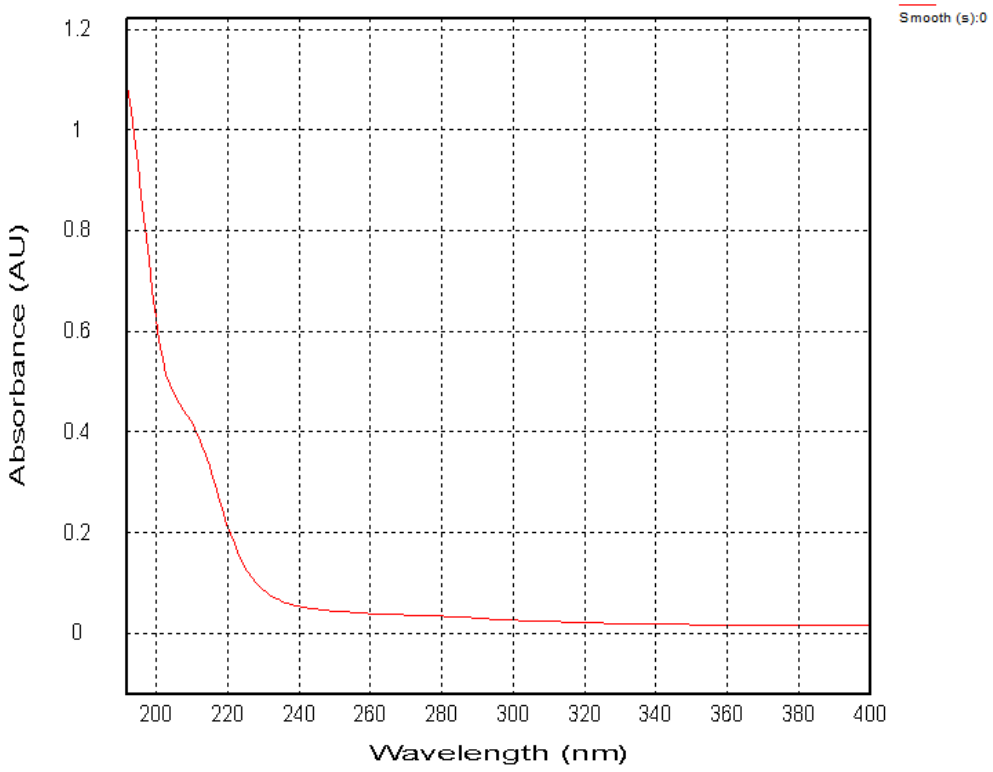

Figure S38. UV spectrum of epiterenoid C (**3**) in methanol.

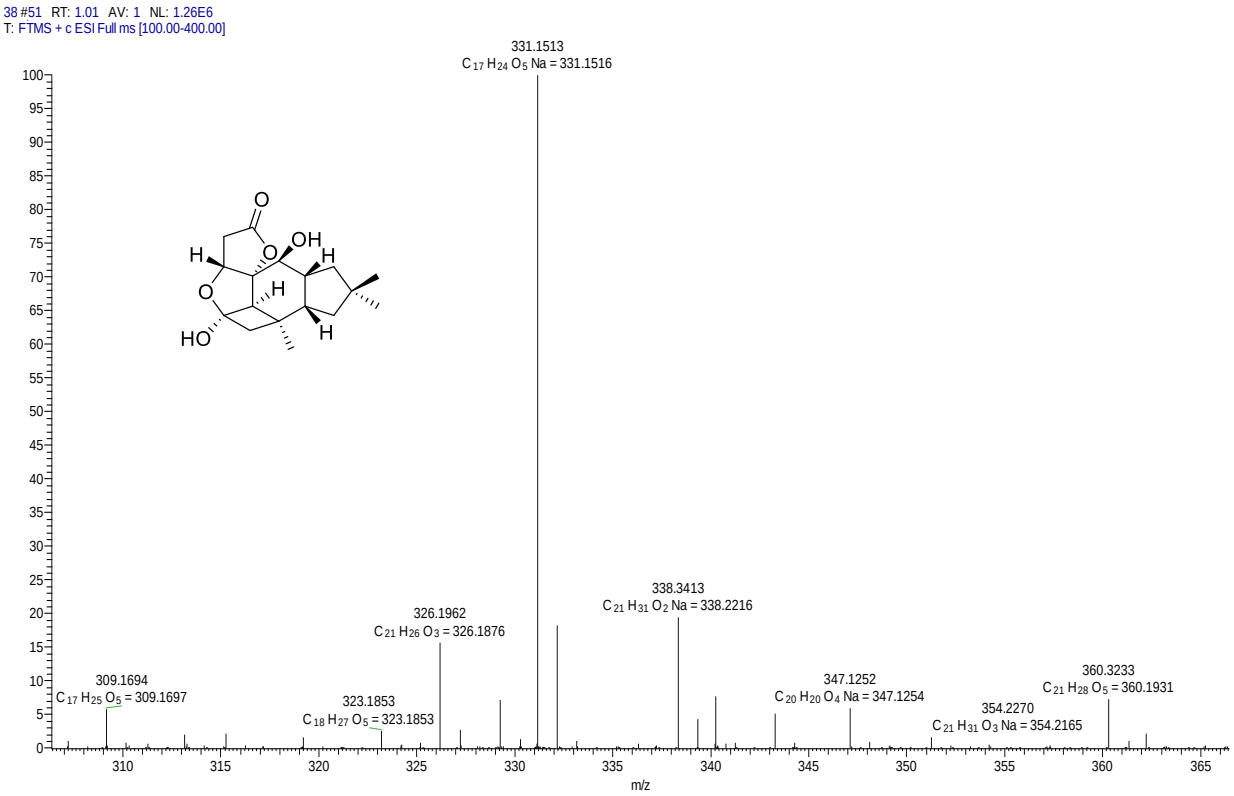

Figure S39. (+)-HRESIMS data of epiterenoid C (**3**).

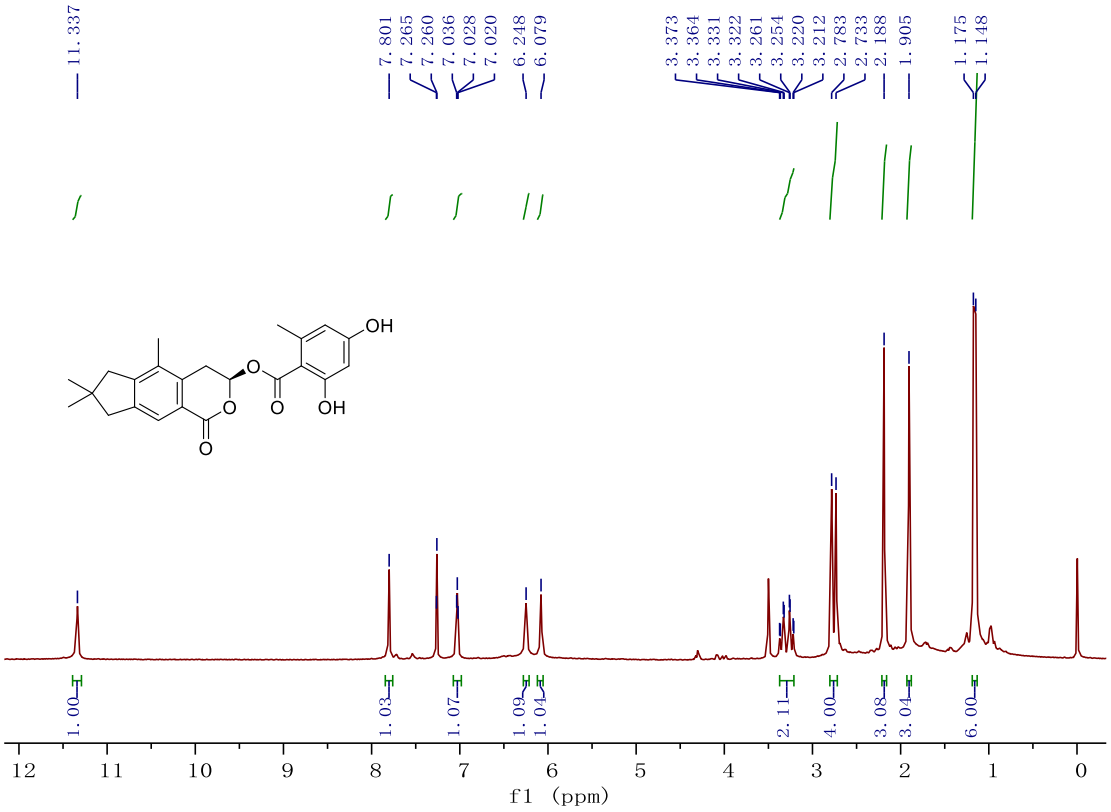

Figure S40. ^{1}H NMR spectrum of armiloid A (**4**) in methanol-d_4 (400 MHz).

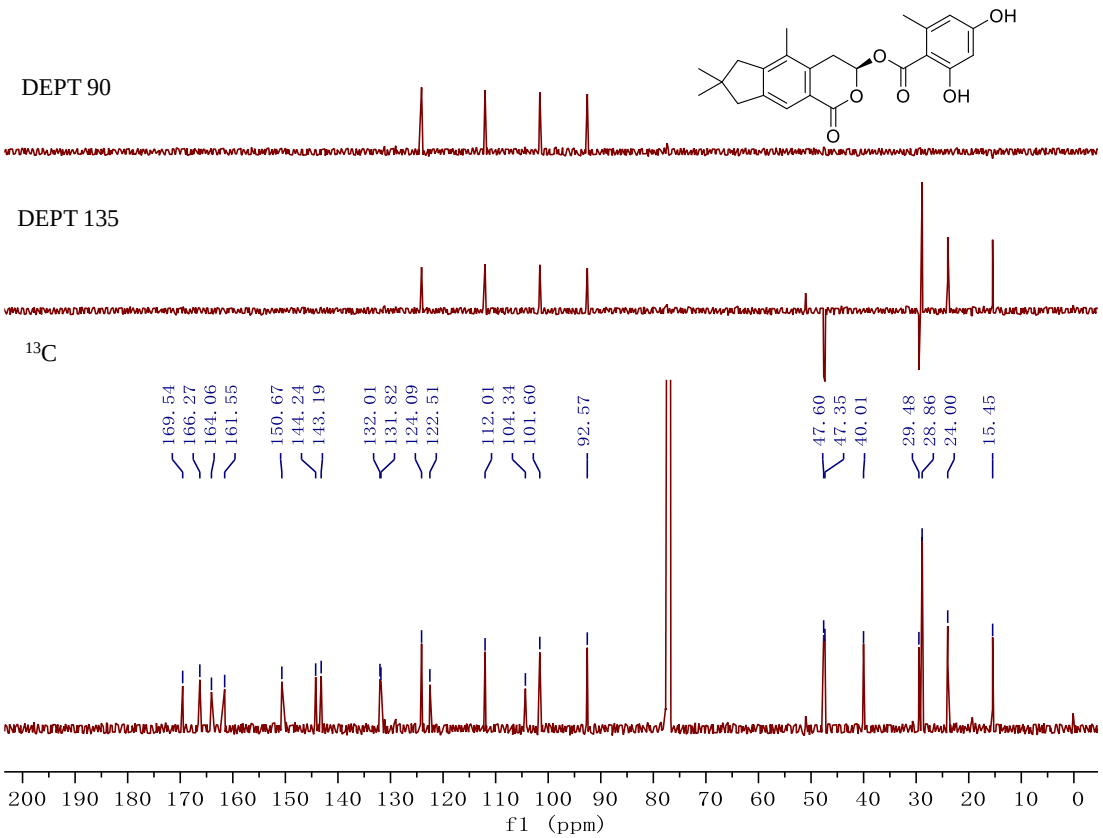

Figure S41. ^{13}C and DEPT NMR spectrum of armiloid A (**4**) in methanol-d_4 (100 MHz).

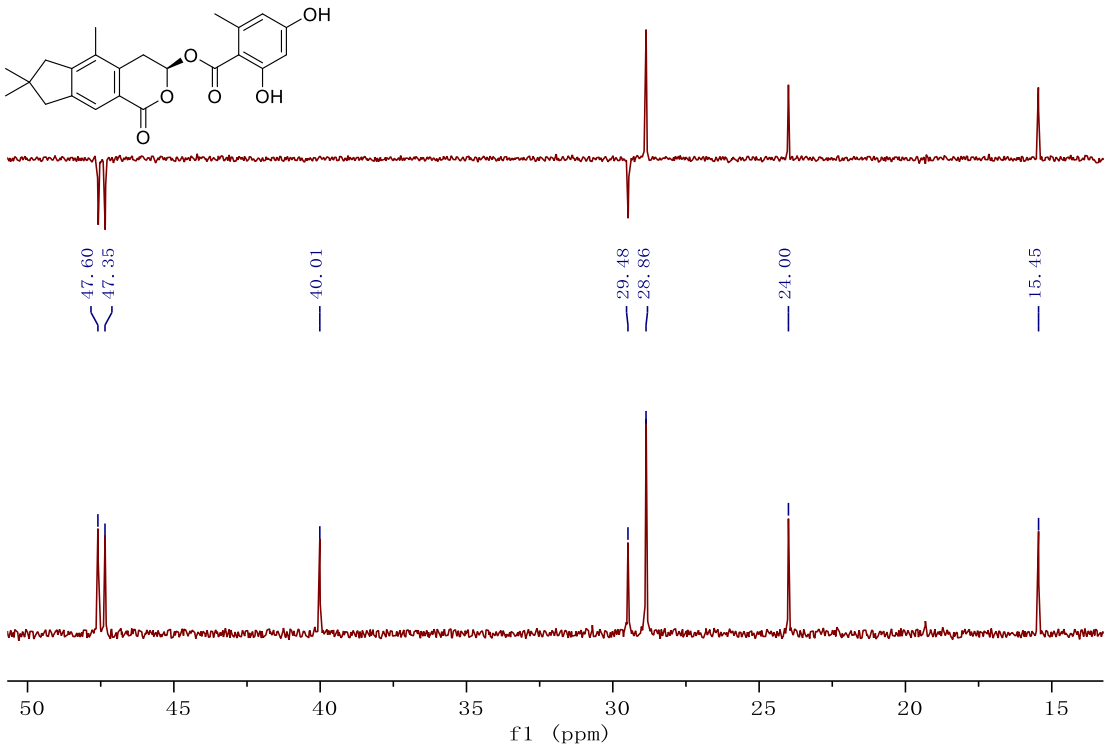

Figure S42. Partial enlarged ^{13}C and DEPT NMR of armiloid A (**4**) in methanol-d_4 (100 MHz).

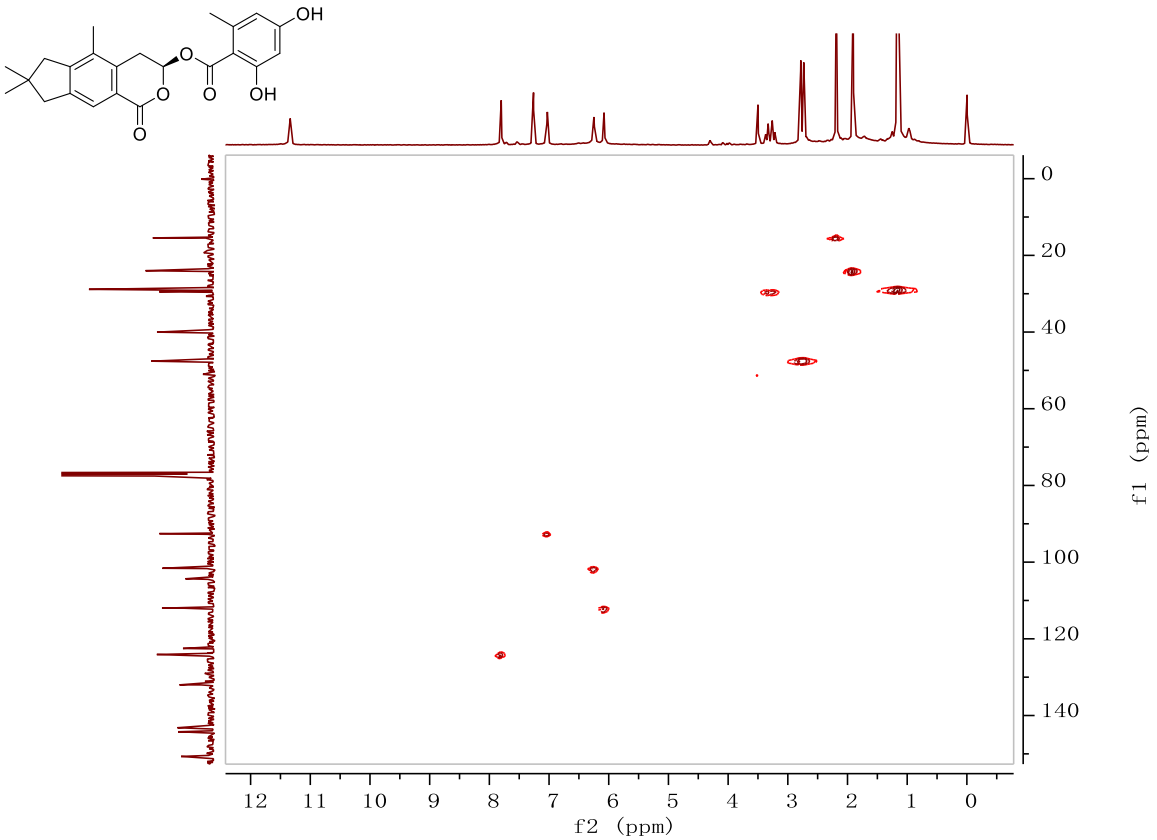

Figure S43. HSQC spectrum of armiloid A (**4**) in methanol-d_4 (^{1}H-400 MHz).

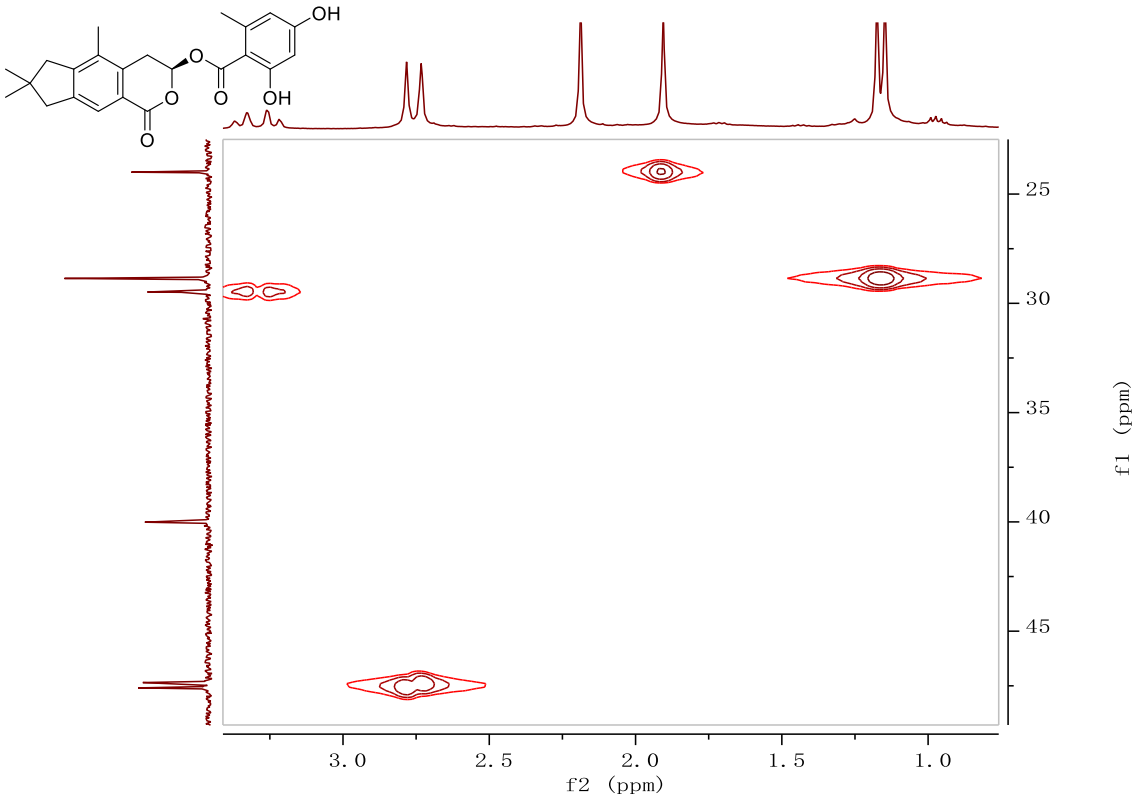

Figure S44. Partial enlarged HSQC spectrum of armiloid A (**4**) in methanol-d_4 (^{1}H-400 MHz).

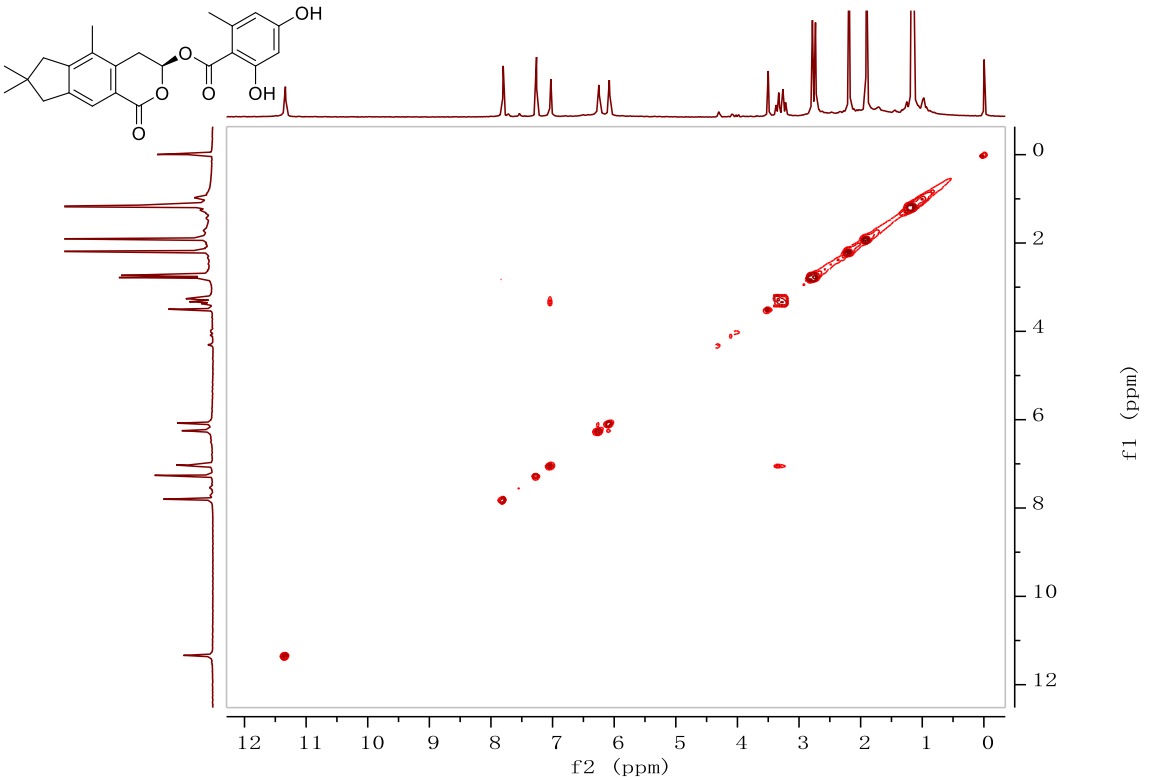

Figure S45. ^{1}H-^{1}H COSY spectrum of armiloid A (**4**) in methanol-d_4 (400 MHz).

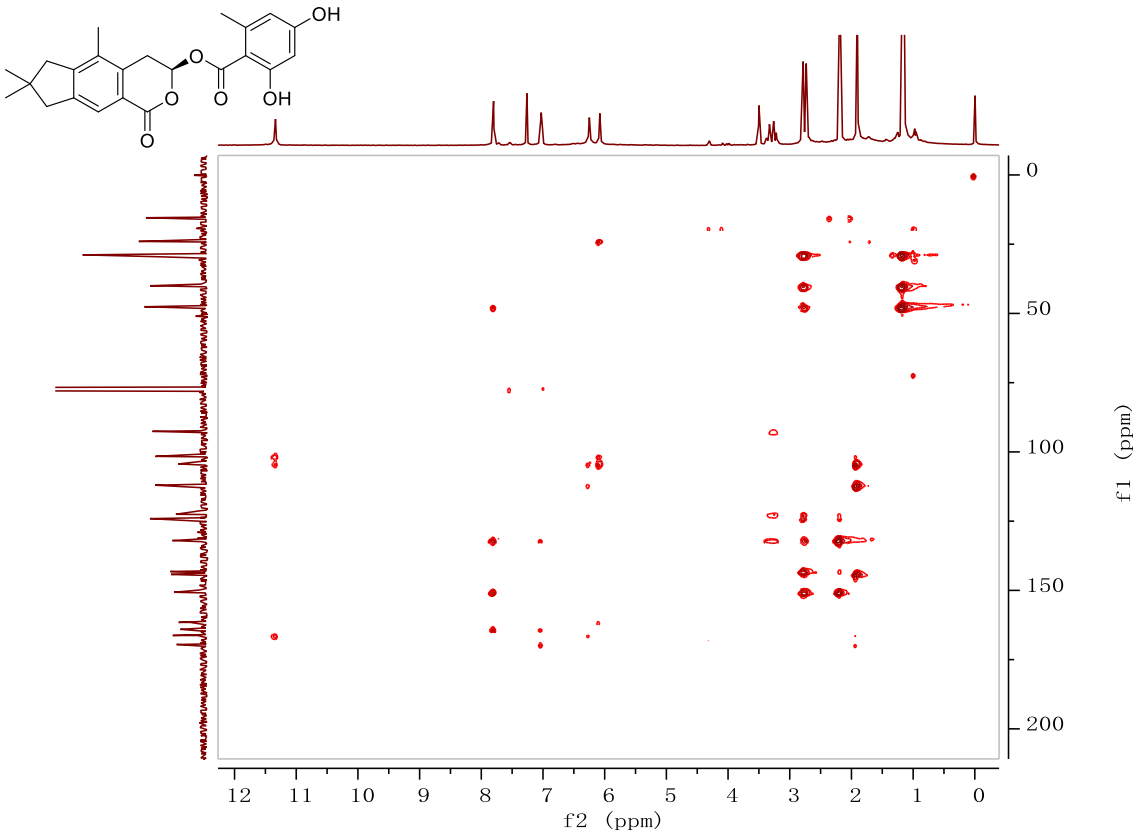

Figure S46. HMBC spectrum of armiloid A (**4**) in methanol-d_4 (^{1}H-400 MHz).

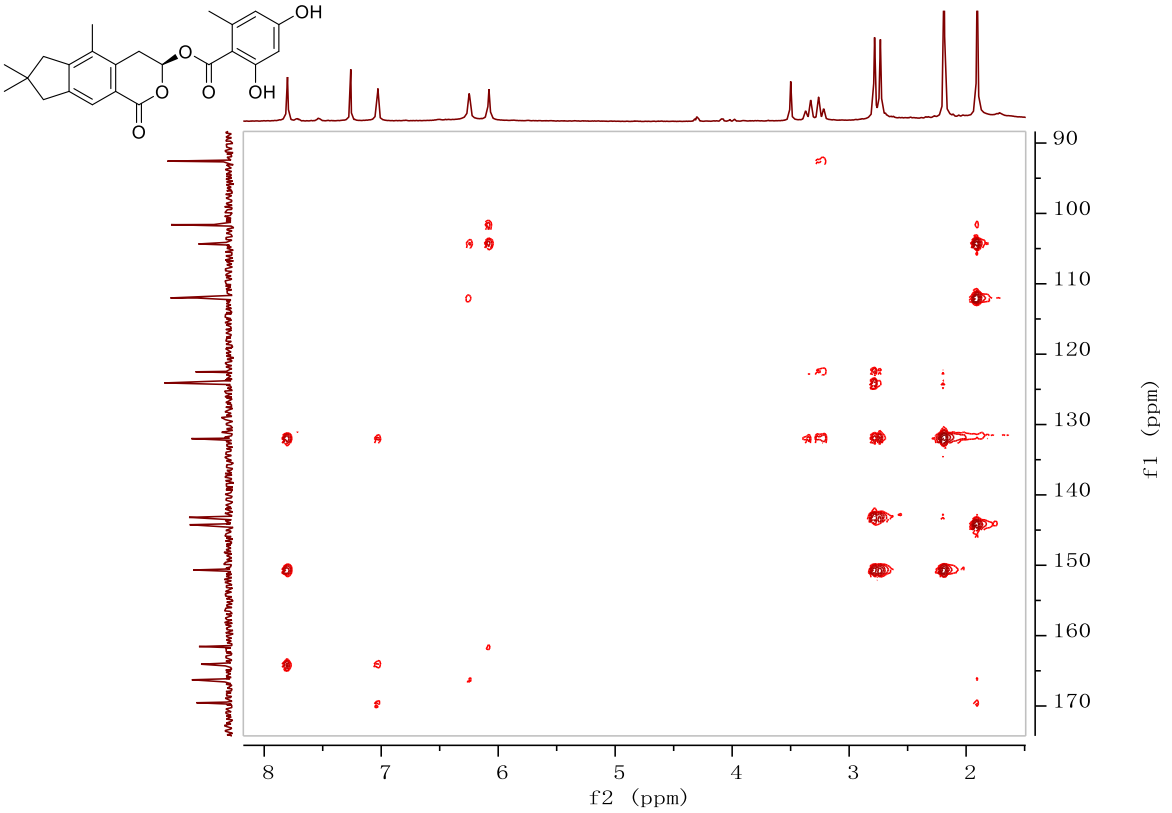

Figure S47. Partial enlarged HMBC spectrum of armiloid A (**4**) in methanol-d_4 (^{1}H-400 MHz).

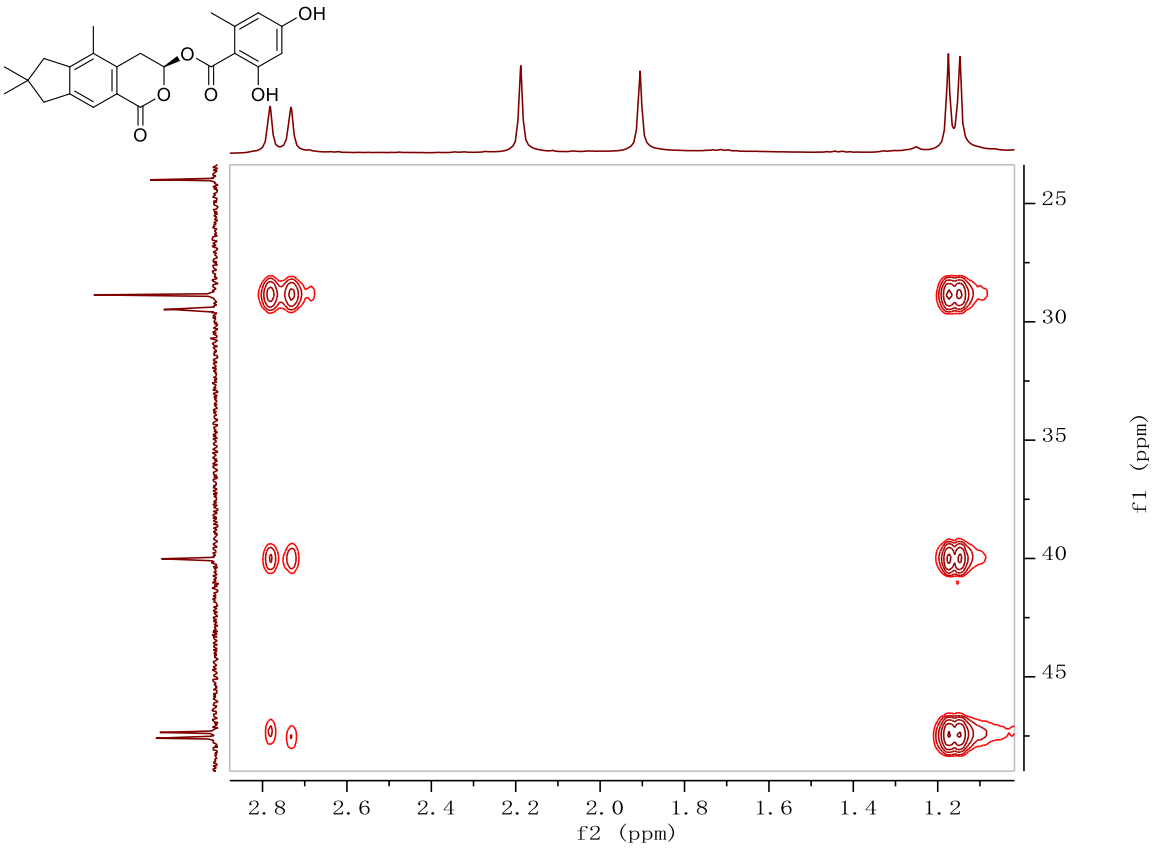

Figure S48. Partial enlarged HMBC spectrum of armiloid A (**4**) in methanol-d_4 (^{1}H-400 MHz).

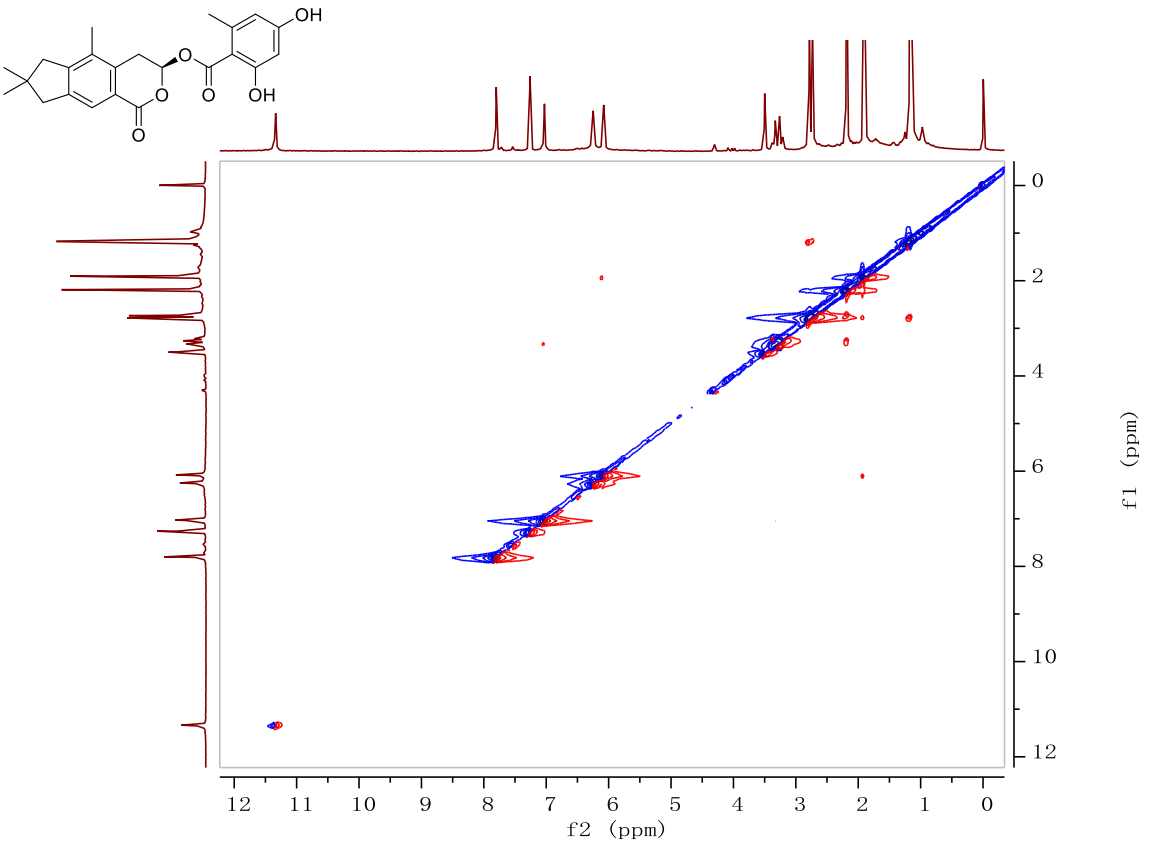

Figure S49. ROESY spectrum of armiloid A (**4**) in methanol-d_4 (400 MHz).

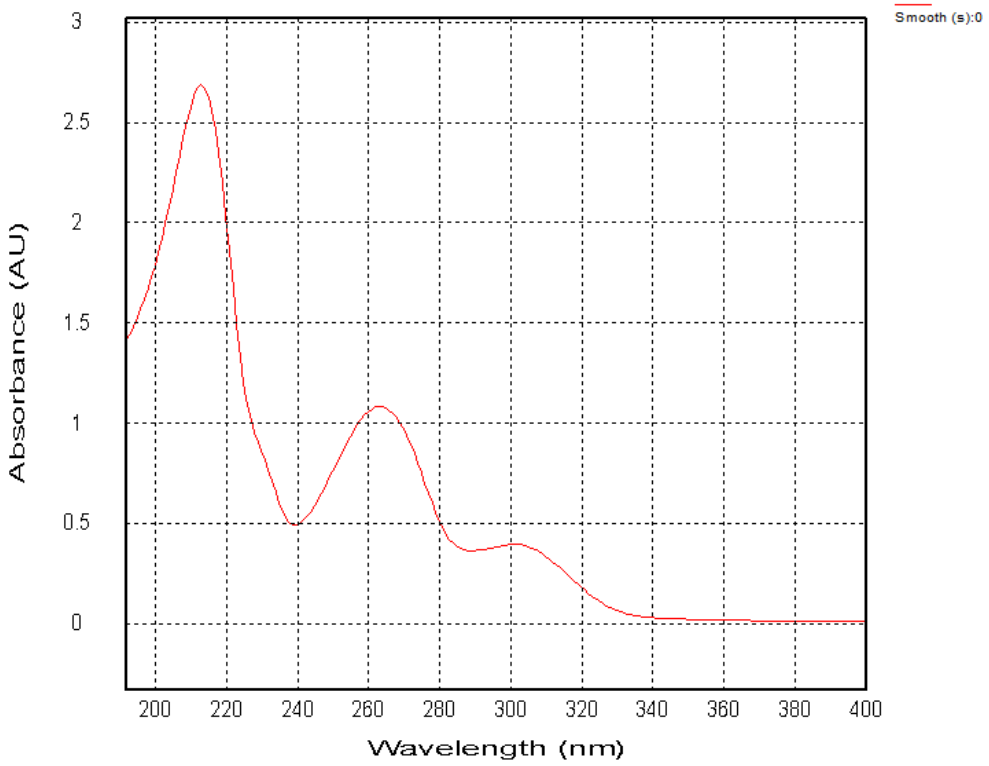

Figure S50. UV spectrum of armiloid A (**4**) in methanol.

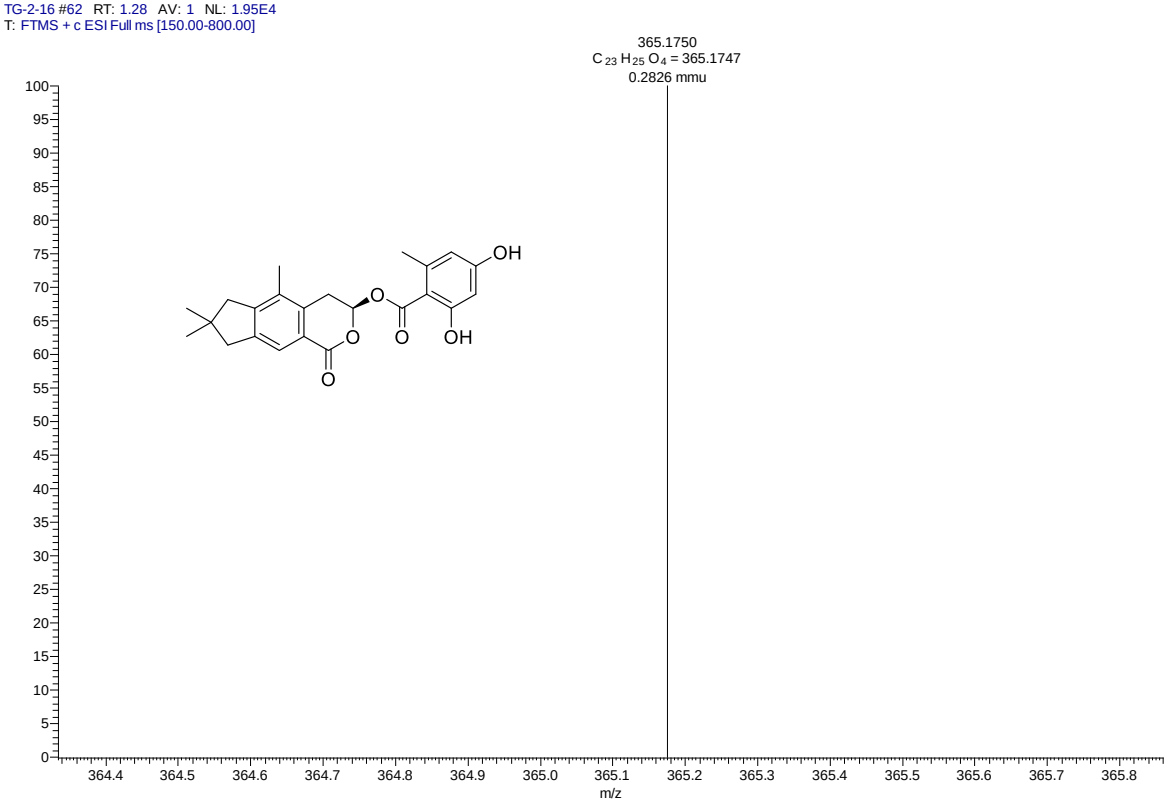

Figure S51. (+)-HRESIMS data of armiloid A (**4**).

ECD calculation details for compounds 1-4

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E)=\frac{1}{2.296\times10^{-39}\sqrt{\pi}\sigma}\sum_{i}^{A}\Delta E_i R_i e^{[-(E-\Delta Ei)^2/\sigma^2]}$$

The σ represented the width of the band at $1/e$ height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i, respectively. R_{vel} had been used in this work.

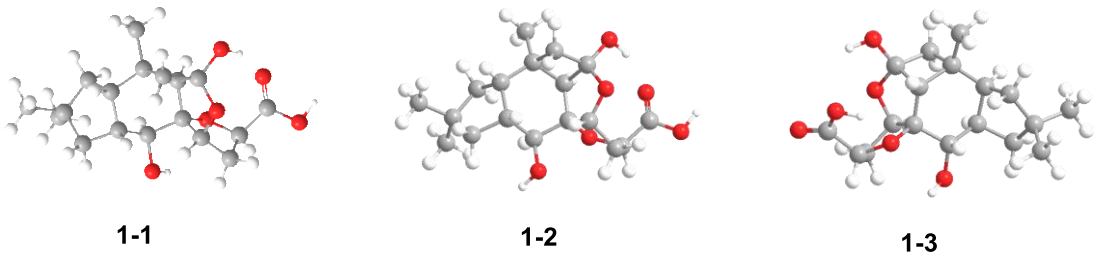

Figure S52. Optimized geometries of predominant conformers for **1**.

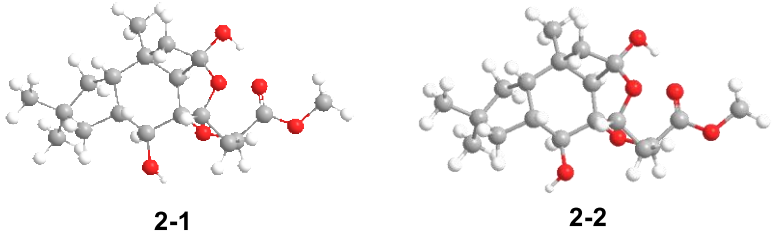

Figure S53. Optimized geometries of predominant conformers for **2**.

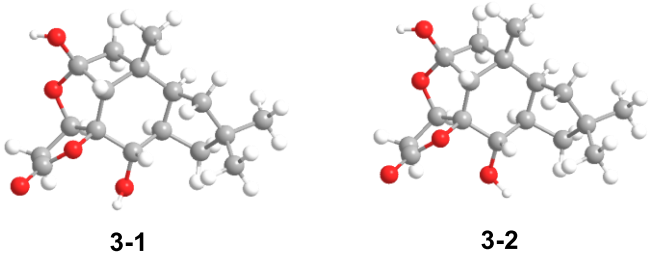

Figure S54. Optimized geometries of predominant conformers for **3**.

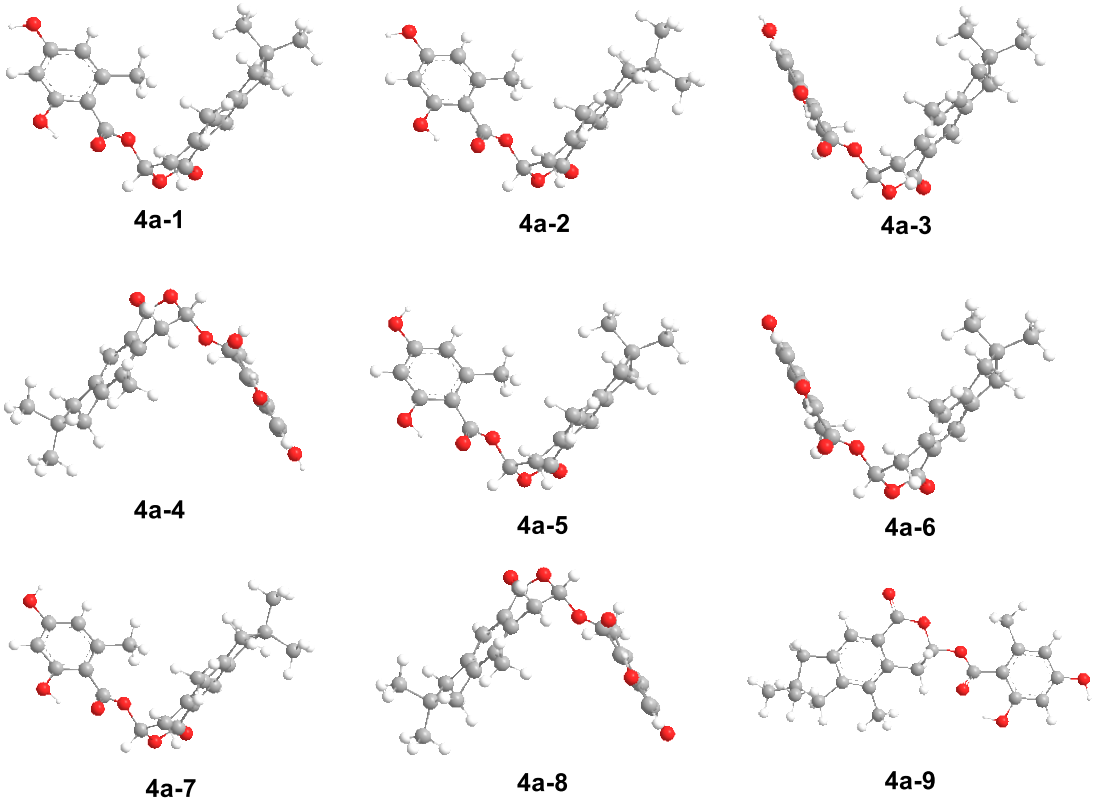

Figure S55. Optimized geometries of predominant conformers for (1*S*)-**4a.**

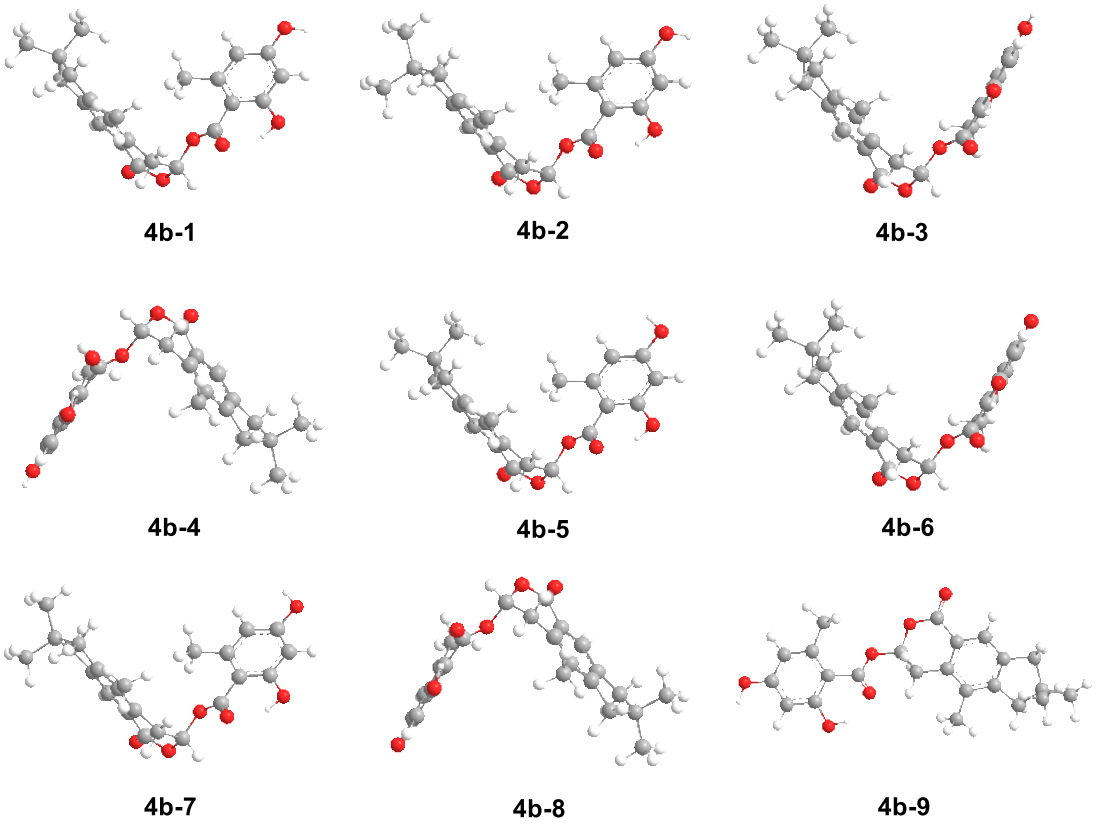

Figure S56. Optimized geometries of predominant conformers for (1*R*)-**4b.**

Table S2. Important Thermodynamic Parameters (a.u.) and Boltzmann Distributions of the Optimized Compounds 1-4 at B3LYP/6-311G (d, p) Level in Methanol

Conformations	Species	Gibbers	Ratio (%)
1	**1-1**	-1152.752780	92.20
	1-2	-1152.750789	5.47
	1-3	-1152.751728	1.60
2	**2-1**	-1192.056286	93.92
	2-2	-1192.054195	6.00
3	**3-1**	-1038.205386	59.40
	3-2	-1038.203327	46.60
(1*S*)-**4a**	**4a-1**	-1342.209717	34.93
	4a-2	-1342.209742	17.66
	4a-3	-1342.209719	17.38
	4a-4	-1342.209743	10.75
	4a-5	-1342.209412	5.26
	4a-6	-1342.209412	3.58
	4a-7	-1342.209356	2.64
	4a-8	-1342.209335	2.22
	4a-9	-1342.209352	1.06

(1*R*)-**4b**	**4b-1**	-1342.209717	34.93
	4b-2	-1342.209742	17.66
	4b-3	-1342.209719	17.38
	4b-4	-1342.209743	10.75
	4b-5	-1342.209412	5.26
	4b-6	-1342.209412	3.58
	4b-7	-1342.209356	2.64
	4b-8	-1342.209335	2.22
	4b-9	-1342.209352	1.06

Table S3. Cartesian Coordinates of the Lowest Energy Conformers for Compounds 1-4

1-1			
Atom	X	Y	Z
C	0.52710000	-0.57470000	-0.03770000
C	0.36090000	0.88150000	-0.46840000
C	-0.86720000	1.71700000	0.00460000
C	-2.13030000	0.92550000	0.36940000
C	-1.85910000	-0.50090000	0.87320000
C	-0.83590000	-1.27230000	0.01500000
C	-3.07890000	0.67900000	-0.80990000
C	-4.01660000	-0.45210000	-0.33580000
C	-3.25390000	-1.15240000	0.81550000
C	1.32260000	-0.59320000	1.27450000
O	1.98030000	0.67730000	1.34760000
C	1.25090000	1.63000000	0.54860000
O	1.34630000	-1.26670000	-1.01840000
C	2.61460000	-1.58990000	-0.42550000
C	2.36440000	-1.66620000	1.06960000
C	-0.02760000	2.18370000	1.22580000
C	3.70670000	-0.56570000	-0.75700000
O	3.56100000	0.52670000	-1.28620000
O	4.93660000	-0.98650000	-0.39160000
H	0.73280000	-0.72670000	2.18460000
O	2.13110000	2.61280000	-0.01010000
C	-1.16210000	2.92050000	-0.90640000
H	-2.68570000	1.47920000	1.13970000
H	-1.52130000	-0.49340000	1.91600000
C	-4.31980000	-1.42500000	-1.48130000
C	-5.34190000	0.12830000	0.18320000
O	-0.67550000	-2.59100000	0.54890000
H	0.61330000	1.04470000	-1.52350000

H	-1.21430000	-1.40140000	-1.00550000
H	-3.63190000	1.58630000	-1.07840000
H	-2.51510000	0.37880000	-1.70190000
H	-3.75990000	-0.97340000	1.77320000
H	-3.20710000	-2.23930000	0.68990000
H	2.93620000	-2.55250000	-0.83700000
H	3.26720000	-1.51120000	1.66790000
H	1.93930000	-2.64480000	1.31860000
H	-0.01880000	3.26340000	1.41230000
H	-0.27520000	1.69520000	2.17580000
H	5.52960000	-0.24450000	-0.63580000
H	2.78370000	2.06850000	-0.49610000
H	-1.50560000	2.59800000	-1.89460000
H	-1.93320000	3.56200000	-0.46590000
H	-0.27160000	3.53830000	-1.06770000
H	-4.97980000	-2.23330000	-1.14720000
H	-4.81290000	-0.91080000	-2.31380000
H	-3.40550000	-1.88540000	-1.87020000
H	-5.88640000	0.64420000	-0.61570000
H	-5.99160000	-0.66270000	0.57420000
H	-5.17390000	0.85120000	0.98930000
H	-0.16580000	-3.08800000	-0.11860000

1-2			
Atom	X	Y	Z
C	0.52460000	-0.57280000	-0.02840000
C	0.35400000	0.88510000	-0.45220000
C	-0.86720000	1.72390000	0.02200000
C	-2.13280000	0.93020000	0.36310000
C	-1.86820000	-0.49090000	0.88180000
C	-0.83420000	-1.28190000	0.05070000
C	-3.05540000	0.67180000	-0.83370000
C	-4.00230000	-0.45520000	-0.36710000
C	-3.26730000	-1.13340000	0.81520000
C	1.33490000	-0.59870000	1.27360000
O	1.98900000	0.67360000	1.35070000
C	1.25060000	1.62830000	0.56270000
O	1.33790000	-1.23780000	-1.03030000
C	2.60240000	-1.59030000	-0.44860000
C	2.37170000	-1.67220000	1.04920000
C	-0.02720000	2.17470000	1.24970000
C	3.70190000	-0.57550000	-0.78240000
O	3.56310000	0.52910000	-1.28840000

O	4.93320000	-1.01790000	-0.44690000
H	0.75380000	-0.73810000	2.18870000
O	2.12500000	2.61590000	0.00310000
C	-1.15410000	2.93660000	-0.87950000
H	-2.70590000	1.48700000	1.11840000
H	-1.54320000	-0.47170000	1.92900000
C	-4.27280000	-1.44710000	-1.50450000
C	-5.34270000	0.12840000	0.10780000
O	-0.65600000	-2.56900000	0.65770000
H	0.60370000	1.05210000	-1.50760000
H	-1.19560000	-1.45860000	-0.96890000
H	-3.60320000	1.57570000	-1.12330000
H	-2.47180000	0.36260000	-1.70980000
H	-3.78850000	-0.92370000	1.75850000
H	-3.23250000	-2.22330000	0.71990000
H	2.90680000	-2.55330000	-0.87200000
H	3.28240000	-1.52180000	1.63660000
H	1.94950000	-2.65180000	1.29890000
H	-0.01760000	3.25200000	1.44960000
H	-0.27460000	1.67410000	2.19330000
H	5.52890000	-0.27840000	-0.69120000
H	2.77960000	2.07270000	-0.48190000
H	-1.49240000	2.62410000	-1.87270000
H	-1.92690000	3.57510000	-0.43760000
H	-0.26190000	3.55460000	-1.02970000
H	-4.93910000	-2.25200000	-1.17470000
H	-4.74570000	-0.94770000	-2.35750000
H	-3.34800000	-1.91110000	-1.86260000
H	-5.86840000	0.62840000	-0.71350000
H	-5.99920000	-0.65860000	0.49560000
H	-5.19810000	0.86570000	0.90530000
H	-1.27440000	-3.18160000	0.22160000

1-3			
Atom	X	Y	Z
C	-0.55660000	-0.52460000	-0.00070000
C	-0.35710000	0.91750000	0.47040000
C	0.88700000	1.73620000	0.01230000
C	2.13500000	0.92330000	-0.35760000
C	1.83820000	-0.48730000	-0.89050000
C	0.78970000	-1.25530000	-0.05890000
C	3.06710000	0.63390000	0.82520000
C	3.98500000	-0.50780000	0.33830000

C	3.21820000	-1.17010000	-0.83230000
C	-1.33500000	-0.47980000	-1.32200000
O	-2.00390000	0.78740000	-1.31600000
C	-1.23420000	1.70920000	-0.52410000
O	-1.41290000	-1.21220000	0.95680000
C	-2.62160000	-1.63930000	0.28340000
C	-2.35620000	-1.58030000	-1.20640000
C	0.05580000	2.23780000	-1.20160000
C	-3.79410000	-0.75130000	0.71320000
O	-4.88710000	-0.71490000	0.17070000
O	-3.49280000	-0.01210000	1.81120000
H	-0.73110000	-0.54320000	-2.23050000
O	-2.08160000	2.70330000	0.05530000
C	1.20490000	2.92000000	0.94180000
H	2.70890000	1.47910000	-1.11270000
H	1.51270000	-0.45260000	-1.93660000
C	4.25730000	-1.50790000	1.46800000
C	5.32690000	0.05400000	-0.15830000
O	0.60500000	-2.55370000	-0.62980000
H	-0.59990000	1.05910000	1.53050000
H	1.15620000	-1.41770000	0.96120000
H	3.63680000	1.52360000	1.11640000
H	2.48820000	0.32870000	1.70590000
H	3.73690000	-0.98500000	-1.78200000
H	3.14660000	-2.25790000	-0.72700000
H	-2.85330000	-2.65550000	0.61870000
H	-3.25750000	-1.39830000	-1.79910000
H	-1.91370000	-2.52820000	-1.53190000
H	0.07390000	3.31960000	-1.37510000
H	0.28910000	1.75550000	-2.15810000
H	-2.56690000	-0.20600000	2.08030000
H	-2.97370000	2.37050000	-0.15310000
H	1.53810000	2.57590000	1.92620000
H	1.99120000	3.55070000	0.51280000
H	0.32790000	3.55490000	1.10960000
H	4.90310000	-2.32380000	1.12460000
H	4.75370000	-1.01980000	2.31420000
H	3.33000000	-1.95580000	1.84040000
H	5.87490000	0.54330000	0.65470000
H	5.96330000	-0.74330000	-0.55840000
H	5.18140000	0.79500000	-0.95220000
H	0.14080000	-3.08790000	0.04110000

2-1			
Atom	X	Y	Z
C	0.28780000	-0.57280000	-0.01050000
C	0.12620000	0.88350000	-0.44280000
C	-1.11180000	1.71590000	0.00960000
C	-2.37920000	0.92170000	0.35280000
C	-2.11350000	-0.50410000	0.86080000
C	-1.07450000	-1.27290000	0.01940000
C	-3.30740000	0.67370000	-0.84220000
C	-4.25050000	-0.45960000	-0.38420000
C	-3.50580000	-1.15860000	0.77960000
C	1.06150000	-0.59070000	1.31460000
O	1.71350000	0.68140000	1.40210000
C	0.99680000	1.63320000	0.59040000
O	1.12400000	-1.26470000	-0.97730000
C	2.38820000	-1.57380000	-0.36670000
C	2.11180000	-1.65820000	1.12390000
C	-0.29460000	2.18360000	1.24550000
C	3.48180000	-0.53780000	-0.67870000
O	3.29820000	0.54360000	-1.22720000
O	4.69390000	-0.99880000	-0.25150000
H	0.45750000	-0.72940000	2.21450000
O	1.88430000	2.61900000	0.04890000
C	-1.39370000	2.91930000	-0.90570000
H	-2.94870000	1.47400000	1.11390000
H	-1.79310000	-0.49630000	1.90910000
C	-4.53240000	-1.43280000	-1.53490000
C	-5.58560000	0.11790000	0.11260000
O	-0.92000000	-2.59170000	0.55520000
H	0.39600000	1.04800000	-1.49330000
C	5.77100000	-0.08640000	-0.46970000
H	-1.43580000	-1.40240000	-1.00730000
H	-3.85770000	1.57990000	-1.11970000
H	-2.72810000	0.37490000	-1.72480000
H	-4.02810000	-0.98090000	1.72870000
H	-3.45460000	-2.24540000	0.65450000
H	2.72410000	-2.53290000	-0.77530000
H	3.00230000	-1.50150000	1.73990000
H	1.68670000	-2.63980000	1.36080000
H	-0.29150000	3.26330000	1.43270000
H	-0.55750000	1.69400000	2.19070000
H	2.54210000	2.07770000	-0.43460000
H	-1.71980000	2.59650000	-1.89970000
H	-2.17350000	3.55890000	-0.47800000

H	-0.50180000	3.53890000	-1.05150000
H	-5.19620000	-2.24260000	-1.21210000
H	-5.01260000	-0.91940000	-2.37540000
H	-3.61070000	-1.89120000	-1.90850000
H	-6.11770000	0.63280000	-0.69520000
H	-6.24010000	-0.67470000	0.49250000
H	-5.43260000	0.84090000	0.92160000
H	-0.40130000	-3.08780000	-0.10610000
H	6.68490000	-0.54140000	-0.07810000
H	5.90590000	0.09710000	-1.54010000
H	5.59380000	0.85140000	0.06630000

2-2			
Atom	X	Y	Z
C	0.28570000	-0.56830000	0.00250000
C	0.11770000	0.88900000	-0.42450000
C	-1.11590000	1.72290000	0.02600000
C	-2.38460000	0.92420000	0.34340000
C	-2.12400000	-0.49540000	0.86800000
C	-1.07150000	-1.28260000	0.05690000
C	-3.28320000	0.66150000	-0.87060000
C	-4.23430000	-0.46900000	-0.42120000
C	-3.51930000	-1.14330000	0.77560000
C	1.07210000	-0.59110000	1.31900000
O	1.71760000	0.68430000	1.41080000
C	0.99150000	1.63610000	0.60770000
O	1.11940000	-1.23220000	-0.98370000
C	2.37960000	-1.56790000	-0.38170000
C	2.12010000	-1.65700000	1.11160000
C	-0.30180000	2.17730000	1.26960000
C	3.48030000	-0.54010000	-0.69410000
O	3.30240000	0.55470000	-1.21810000
O	4.69420000	-1.02360000	-0.29650000
H	0.47520000	-0.73600000	2.22310000
O	1.87240000	2.62790000	0.06600000
C	-1.39040000	2.93410000	-0.88130000
H	-2.97410000	1.47920000	1.08730000
H	-1.81870000	-0.47430000	1.92100000
C	-4.47890000	-1.46290000	-1.56260000
C	-5.58590000	0.10950000	0.02750000
O	-0.89890000	-2.56890000	0.66790000
H	0.38670000	1.05700000	-1.47500000
C	5.77840000	-0.12100000	-0.51830000

H	-1.41310000	-1.46170000	-0.96910000
H	-3.82900000	1.56300000	-1.17110000
H	-2.68180000	0.35400000	-1.73520000
H	-4.05900000	-0.93440000	1.70870000
H	-3.47880000	-2.23300000	0.68220000
H	2.70070000	-2.52740000	-0.80100000
H	3.01730000	-1.50270000	1.71830000
H	1.69930000	-2.64020000	1.34920000
H	-0.30060000	3.25470000	1.46930000
H	-0.56530000	1.67580000	2.20830000
H	2.53440000	2.08830000	-0.41410000
H	-1.70850000	2.61990000	-1.88060000
H	-2.17400000	3.56960000	-0.45440000
H	-0.49800000	3.55560000	-1.01470000
H	-5.14820000	-2.27030000	-1.24500000
H	-4.93740000	-0.96610000	-2.42500000
H	-3.54560000	-1.92350000	-1.90260000
H	-6.09780000	0.60660000	-0.80420000
H	-6.24640000	-0.67990000	0.40340000
H	-5.45960000	0.84800000	0.82700000
H	-1.51270000	-3.18220000	0.22640000
H	6.69370000	-0.59470000	-0.15290000
H	5.89560000	0.08090000	-1.58750000
H	5.62370000	0.80870000	0.03840000

3-1			
Atom	X	Y	Z
C	-0.99810000	-0.42300000	0.15770000
C	-0.70590000	0.98330000	0.67930000
C	0.52890000	1.77560000	0.15660000
C	1.70900000	0.93330000	-0.34580000
C	1.31240000	-0.43410000	-0.92370000
C	0.29840000	-1.20780000	-0.05430000
C	2.71210000	0.54490000	0.74680000
C	3.54250000	-0.60290000	0.13320000
C	2.66230000	-1.17250000	-1.00640000
C	-1.88900000	-0.29530000	-1.07450000
O	-2.49750000	1.00070000	-0.97300000
C	-1.62830000	1.85070000	-0.20230000
O	-1.80400000	-1.11450000	1.12830000
C	-2.88470000	-1.68670000	0.52790000
C	-2.93510000	-1.36690000	-0.93060000
C	-0.37610000	2.36020000	-0.96440000

O	-3.67500000	-2.40920000	1.11450000
H	-1.36980000	-0.33760000	-2.03580000
O	-2.38420000	2.85640000	0.47600000
C	0.96810000	2.90330000	1.10570000
H	2.24930000	1.50440000	-1.11430000
H	0.91030000	-0.33060000	-1.93830000
C	3.85800000	-1.67120000	1.18650000
C	4.86500000	-0.06610000	-0.43750000
O	0.00100000	-2.45170000	-0.69760000
H	-0.85980000	1.08130000	1.76090000
H	0.73840000	-1.45510000	0.91880000
H	3.33900000	1.39480000	1.03950000
H	2.18680000	0.21470000	1.65170000
H	3.11570000	-0.95830000	-1.98300000
H	2.55170000	-2.26060000	-0.94940000
H	-2.66320000	-2.26920000	-1.48540000
H	-3.93410000	-1.02060000	-1.20680000
H	-0.32760000	3.44700000	-1.09520000
H	-0.24120000	1.91120000	-1.95540000
H	-3.17120000	2.94320000	-0.08920000
H	1.36450000	2.50270000	2.04440000
H	1.74310000	3.52260000	0.64090000
H	0.13420000	3.56260000	1.37090000
H	4.44120000	-2.49140000	0.75310000
H	4.43730000	-1.24790000	2.01470000
H	2.94400000	-2.10320000	1.60730000
H	5.49270000	0.35840000	0.35400000
H	5.43580000	-0.86430000	-0.92520000
H	4.69080000	0.72100000	-1.17950000
H	-0.26130000	-3.08010000	0.00240000

3-2			
Atom	X	Y	Z
C	-0.99390000	-0.42570000	0.15260000
C	-0.70310000	0.98200000	0.67070000
C	0.52330000	1.78060000	0.14430000
C	1.70880000	0.93990000	-0.34310000
C	1.32090000	-0.42340000	-0.93530000
C	0.29930000	-1.21220000	-0.08720000
C	2.69420000	0.54390000	0.76260000
C	3.53510000	-0.59830000	0.15240000
C	2.67880000	-1.14770000	-1.01500000
C	-1.90330000	-0.30610000	-1.06620000

O	-2.51250000	0.98970000	-0.96300000
C	-1.63460000	1.84400000	-0.20670000
O	-1.78530000	-1.11030000	1.14020000
C	-2.86410000	-1.70160000	0.55600000
C	-2.94020000	-1.38480000	-0.90260000
C	-0.38720000	2.34900000	-0.98120000
O	-3.65150000	-2.41470000	1.15900000
H	-1.39620000	-0.35010000	-2.03410000
O	-2.38410000	2.85450000	0.47170000
C	0.95480000	2.91810000	1.08540000
H	2.26110000	1.51510000	-1.10000000
H	0.92670000	-0.31030000	-1.95230000
C	3.82340000	-1.68240000	1.19740000
C	4.87220000	-0.05860000	-0.38030000
O	-0.02580000	-2.42510000	-0.77760000
H	-0.85260000	1.08100000	1.75290000
H	0.72160000	-1.49990000	0.88230000
H	3.31570000	1.39180000	1.07220000
H	2.15400000	0.20590000	1.65590000
H	3.14500000	-0.90150000	-1.97820000
H	2.58380000	-2.23770000	-0.99040000
H	-2.67460000	-2.28660000	-1.46090000
H	-3.94530000	-1.04330000	-1.16200000
H	-0.34250000	3.43440000	-1.12460000
H	-0.25460000	1.88880000	-1.96730000
H	-3.21900000	2.86290000	-0.02770000
H	1.35130000	2.52700000	2.02800000
H	1.72790000	3.53720000	0.61730000
H	0.11750000	3.57580000	1.34360000
H	4.41410000	-2.49820000	0.76570000
H	4.38500000	-1.27270000	2.04440000
H	2.89930000	-2.11780000	1.59160000
H	5.48380000	0.35110000	0.43140000
H	5.45040000	-0.85170000	-0.86770000
H	4.71750000	0.74070000	-1.11370000
H	0.62610000	-3.09940000	-0.51240000

4a-1			
Atom	X	Y	Z
C	3.13960000	0.29070000	0.78330000
C	3.38290000	0.19980000	-0.59210000
C	2.72720000	-0.73030000	-1.37720000
C	1.77940000	-1.56080000	-0.77020000

C	1.51280000	-1.46690000	0.61670000
C	2.23230000	-0.55570000	1.42270000
C	4.01120000	1.35480000	1.39270000
C	4.47510000	2.16880000	0.15420000
C	4.43540000	1.17130000	-1.03220000
C	1.08010000	-2.56920000	-1.61410000
O	0.00480000	-3.18890000	-1.06940000
C	-0.60480000	-2.63690000	0.10950000
C	0.45880000	-2.38760000	1.18040000
O	-1.32410000	-1.43930000	-0.22650000
C	-2.26880000	-1.06030000	0.65770000
C	-3.00100000	0.14980000	0.20430000
O	-2.57480000	-1.66060000	1.67920000
C	-4.36190000	0.24580000	0.56010000
C	-5.14570000	1.31760000	0.13760000
C	-4.56490000	2.31680000	-0.62820000
C	-3.21530000	2.26590000	-0.96240000
C	-2.40640000	1.19470000	-0.53890000
C	-0.94810000	1.23010000	-0.90570000
O	-5.28680000	3.38560000	-1.06910000
O	-5.00980000	-0.68610000	1.33280000
O	1.47970000	-2.84380000	-2.73800000
C	1.99980000	-0.45440000	2.90370000
C	5.88960000	2.72010000	0.35980000
C	3.51230000	3.34550000	-0.10360000
H	2.94170000	-0.81050000	-2.43970000
H	3.45990000	1.97780000	2.10420000
H	4.85390000	0.87560000	1.90380000
H	4.17090000	1.65810000	-1.97630000
H	5.38600000	0.63930000	-1.15150000
H	-1.31070000	-3.39870000	0.46170000
H	0.94490000	-3.32860000	1.46260000
H	-0.00540000	-1.94770000	2.06720000
H	-6.19330000	1.35400000	0.41840000
H	-2.79370000	3.07720000	-1.55340000
H	-0.64190000	2.23300000	-1.22400000
H	-0.32720000	0.97890000	-0.04080000
H	-0.74310000	0.54320000	-1.73210000
H	-6.20860000	3.28050000	-0.77890000
H	-4.34390000	-1.27960000	1.74230000
H	2.83090000	0.04100000	3.41480000
H	1.08490000	0.11280000	3.10110000
H	1.91450000	-1.44930000	3.35260000
H	6.23020000	3.26970000	-0.52470000

H	5.92560000	3.40190000	1.21660000
H	6.60780000	1.91400000	0.54660000
H	3.50890000	4.04170000	0.74270000
H	3.81060000	3.90770000	-0.99560000
H	2.48230000	3.00430000	-0.25590000

4a-2			
Atom	X	Y	Z
C	3.06990000	0.47760000	0.71830000
C	3.29420000	0.36860000	-0.65920000
C	2.63010000	-0.57250000	-1.42450000
C	1.71200000	-1.41610000	-0.79110000
C	1.45770000	-1.30050000	0.59600000
C	2.15750000	-0.35020000	1.37610000
C	3.89810000	1.59740000	1.28760000
C	4.94630000	1.85720000	0.17110000
C	4.27340000	1.39340000	-1.14560000
C	1.02590000	-2.45400000	-1.60980000
O	-0.02110000	-3.09750000	-1.03850000
C	-0.63150000	-2.54430000	0.13930000
C	0.43730000	-2.24010000	1.19030000
O	-1.39630000	-1.37870000	-0.20800000
C	-2.34070000	-1.01520000	0.68290000
C	-3.12600000	0.15640000	0.21610000
O	-2.60660000	-1.60330000	1.72270000
C	-4.47930000	0.21710000	0.60730000
C	-5.31070000	1.24960000	0.17770000
C	-4.78600000	2.24510000	-0.63200000
C	-3.44530000	2.22930000	-1.00340000
C	-2.58870000	1.19830000	-0.57350000
C	-1.14360000	1.27170000	-0.98480000
O	-5.55590000	3.27610000	-1.08180000
O	-5.07440000	-0.71320000	1.42310000
O	1.41330000	-2.73180000	-2.73720000
C	1.89700000	-0.20400000	2.84900000
C	6.22380000	1.03540000	0.43590000
C	5.31680000	3.34230000	0.10360000
H	2.81960000	-0.65410000	-2.49170000
H	3.25310000	2.46800000	1.45230000
H	4.37980000	1.31800000	2.22950000
H	3.72510000	2.20720000	-1.63350000
H	4.99180000	0.96610000	-1.85250000
H	-1.30630000	-3.32260000	0.51540000

H	0.95560000	-3.16050000	1.48360000
H	-0.02880000	-1.80010000	2.07560000
H	-6.35090000	1.25910000	0.48700000
H	-3.06840000	3.03650000	-1.62920000
H	-0.88210000	2.27400000	-1.34230000
H	-0.48920000	1.06870000	-0.13200000
H	-0.93890000	0.56700000	-1.79620000
H	-6.46510000	3.14880000	-0.76230000
H	-4.37850000	-1.27580000	1.82630000
H	2.63500000	0.43300000	3.34360000
H	0.91010000	0.24100000	3.01140000
H	1.94290000	-1.17950000	3.34430000
H	6.95880000	1.18480000	-0.36300000
H	6.69360000	1.33390000	1.37990000
H	6.01250000	-0.03790000	0.49570000
H	5.76660000	3.67890000	1.04420000
H	6.03460000	3.53280000	-0.70190000
H	4.43460000	3.96450000	-0.08390000

4a-3			
Atom	X	Y	Z
C	3.05130000	0.50660000	0.71040000
C	3.31680000	0.21040000	-0.63120000
C	2.70500000	-0.85500000	-1.26580000
C	1.78170000	-1.61810000	-0.54300000
C	1.49340000	-1.31880000	0.81000000
C	2.16570000	-0.26280000	1.46710000
C	3.87720000	1.68350000	1.15330000
C	4.33670000	2.30780000	-0.19240000
C	4.34190000	1.13770000	-1.20970000
C	1.14260000	-2.78050000	-1.22140000
O	0.11330000	-3.38170000	-0.57590000
C	-0.54650000	-2.68300000	0.49190000
C	0.47990000	-2.18880000	1.51150000
O	-1.33050000	-1.60690000	-0.04490000
C	-2.33730000	-1.16860000	0.73580000
C	-3.03900000	-0.00300000	0.13540000
O	-2.60880000	-1.58900000	1.85270000
C	-3.61510000	0.92570000	1.02750000
C	-4.24600000	2.07910000	0.56530000
C	-4.32230000	2.30450000	-0.80030000
C	-3.79070000	1.39040000	-1.70420000
C	-3.15670000	0.21560000	-1.25650000

C	-2.63410000	-0.73530000	-2.29940000
O	-4.92550000	3.41760000	-1.30530000
O	-3.59920000	0.77530000	2.39250000
O	1.55210000	-3.19380000	-2.29840000
C	1.90860000	0.06060000	2.91190000
C	5.73250000	2.92550000	-0.06080000
C	3.34650000	3.40180000	-0.64010000
H	2.93770000	-1.09200000	-2.30070000
H	3.29370000	2.39130000	1.75060000
H	4.72590000	1.32060000	1.74420000
H	4.07240000	1.46310000	-2.21960000
H	5.31050000	0.62600000	-1.23960000
H	-1.20940000	-3.41880000	0.96300000
H	1.01200000	-3.03690000	1.95770000
H	-0.02660000	-1.63000000	2.30330000
H	-4.66840000	2.77770000	1.28020000
H	-3.88080000	1.59810000	-2.76910000
H	-3.07840000	-0.53150000	-3.28020000
H	-1.54900000	-0.63460000	-2.39930000
H	-2.89610000	-1.76890000	-2.05190000
H	-5.24950000	3.95960000	-0.56640000
H	-3.32150000	-0.14170000	2.60720000
H	2.70910000	0.66890000	3.34370000
H	0.96650000	0.60860000	3.01110000
H	1.86180000	-0.85380000	3.51230000
H	6.07090000	3.34090000	-1.01650000
H	5.73730000	3.73300000	0.67970000
H	6.46970000	2.17970000	0.25660000
H	3.31180000	4.22060000	0.08740000
H	3.64250000	3.82700000	-1.60570000
H	2.32870000	3.01100000	-0.74780000

4a-4			
Atom	X	Y	Z
C	-2.96510000	-0.68720000	0.58350000
C	-3.21010000	-0.31370000	-0.74330000
C	-2.59320000	0.78850000	-1.30640000
C	-1.70350000	1.52700000	-0.51960000
C	-1.42900000	1.14710000	0.81560000
C	-2.07900000	0.02950000	1.39060000
C	-3.73960000	-1.93280000	0.91890000
C	-4.78970000	-2.00760000	-0.22330000
C	-4.15180000	-1.26110000	-1.42220000

C	-1.07610000	2.74040000	-1.11470000
O	-0.07150000	3.32190000	-0.41470000
C	0.58400000	2.57400000	0.62180000
C	-0.44930000	1.99560000	1.58860000
O	1.40340000	1.55070000	0.03680000
C	2.40510000	1.08850000	0.81020000
C	3.14780000	-0.02000000	0.15360000
O	2.64360000	1.44400000	1.95680000
C	3.72620000	-0.99070000	0.99800000
C	4.39490000	-2.09730000	0.47810000
C	4.50700000	-2.23240000	-0.89690000
C	3.97360000	-1.27430000	-1.75290000
C	3.30170000	-0.14540000	-1.24620000
C	2.77960000	0.85880000	-2.23810000
O	5.14800000	-3.29660000	-1.45750000
O	3.67630000	-0.92870000	2.36900000
O	-1.47430000	3.20940000	-2.17300000
C	-1.79470000	-0.39830000	2.80310000
C	-6.09640000	-1.31040000	0.20570000
C	-5.10010000	-3.46340000	-0.58640000
H	-2.79810000	1.07320000	-2.33520000
H	-3.05750000	-2.79050000	0.90300000
H	-4.22100000	-1.86880000	1.89950000
H	-3.57630000	-1.93660000	-2.06530000
H	-4.89540000	-0.73200000	-2.02670000
H	1.22020000	3.29430000	1.15000000
H	-1.01060000	2.80310000	2.07300000
H	0.05520000	1.40470000	2.35760000
H	4.81810000	-2.83080000	1.15680000
H	4.09250000	-1.41070000	-2.82650000
H	3.25100000	0.72950000	-3.21890000
H	1.69980000	0.73980000	-2.37040000
H	3.01030000	1.88000000	-1.91820000
H	5.46890000	-3.87750000	-0.74730000
H	3.37370000	-0.03330000	2.63500000
H	-2.49480000	-1.15830000	3.15960000
H	-0.78550000	-0.81720000	2.87080000
H	-1.88210000	0.45360000	3.48550000
H	-6.83420000	-1.32760000	-0.60450000
H	-6.54230000	-1.81180000	1.07210000
H	-5.92830000	-0.26290000	0.47900000
H	-5.52460000	-4.00040000	0.26910000
H	-5.81910000	-3.51860000	-1.41120000
H	-4.19560000	-3.99750000	-0.89800000

4a-5			
Atom	X	Y	Z
C	3.14300000	0.28430000	0.78180000
C	3.38170000	0.20200000	-0.59480000
C	2.72090000	-0.72100000	-1.38410000
C	1.77320000	-1.55360000	-0.77970000
C	1.51150000	-1.46850000	0.60860000
C	2.23550000	-0.56420000	1.41830000
C	4.02040000	1.34080000	1.39610000
C	4.48390000	2.16140000	0.16180000
C	4.43680000	1.17240000	-1.03130000
C	1.06870000	-2.55450000	-1.62840000
O	-0.00200000	-3.18070000	-1.08220000
C	-0.60840000	-2.63530000	0.10160000
C	0.45890000	-2.39210000	1.17030000
O	-1.32890000	-1.43630000	-0.22770000
C	-2.26430000	-1.05510000	0.66560000
C	-3.00220000	0.15210000	0.21280000
O	-2.55650000	-1.65110000	1.69340000
C	-4.35960000	0.24610000	0.57820000
C	-5.14430000	1.31430000	0.15240000
C	-4.57490000	2.31030000	-0.62570000
C	-3.22680000	2.26330000	-0.97090000
C	-2.41470000	1.19490000	-0.54180000
C	-0.95700000	1.22780000	-0.91440000
O	-5.37480000	3.33800000	-1.02850000
O	-4.99880000	-0.68330000	1.36000000
O	1.46000000	-2.81630000	-2.75830000
C	2.00840000	-0.47320000	2.90090000
C	5.90120000	2.70570000	0.36700000
C	3.52510000	3.34380000	-0.08500000
H	2.93250000	-0.79520000	-2.44770000
H	3.47350000	1.96100000	2.11340000
H	4.86280000	0.85480000	1.90140000
H	4.17140000	1.66670000	-1.97130000
H	5.38490000	0.63750000	-1.15720000
H	-1.31410000	-3.39830000	0.45170000
H	0.94560000	-3.33500000	1.44520000
H	-0.00150000	-1.95750000	2.06160000
H	-6.19330000	1.36790000	0.42910000
H	-2.79310000	3.06140000	-1.56890000
H	-0.65080000	2.23010000	-1.23460000

H	-0.33280000	0.97720000	-0.05160000
H	-0.75630000	0.54000000	-1.74100000
H	-4.85880000	3.94450000	-1.58420000
H	-4.32980000	-1.26970000	1.77310000
H	1.92520000	-1.47140000	3.34310000
H	2.84120000	0.01890000	3.41250000
H	1.09410000	0.09230000	3.10570000
H	6.24140000	3.26010000	-0.51470000
H	5.94240000	3.38140000	1.22830000
H	6.61670000	1.89550000	0.54610000
H	3.52690000	4.03410000	0.76610000
H	3.82310000	3.91100000	-0.97400000
H	2.49330000	3.00780000	-0.23670000

4a-6			
Atom	X	Y	Z
C	3.04890000	0.49730000	0.70160000
C	3.30850000	0.19870000	-0.64060000
C	2.69030000	-0.86480000	-1.27190000
C	1.76670000	-1.62390000	-0.54510000
C	1.48510000	-1.32270000	0.80890000
C	2.16340000	-0.26830000	1.46230000
C	3.88030000	1.67170000	1.14060000
C	4.33770000	2.29280000	-0.20730000
C	4.33520000	1.12160000	-1.22330000
C	1.11920000	-2.78320000	-1.22110000
O	0.09430000	-3.38410000	-0.56820000
C	-0.55950000	-2.68270000	0.50160000
C	0.47220000	-2.18900000	1.51590000
O	-1.34320000	-1.60600000	-0.03450000
C	-2.34430000	-1.16270000	0.75120000
C	-3.03790000	0.00600000	0.14930000
O	-2.61300000	-1.57950000	1.86970000
C	-3.56800000	0.96180000	1.03880000
C	-4.18150000	2.11890000	0.56660000
C	-4.28940000	2.32340000	-0.80010000
C	-3.80500000	1.38090000	-1.70320000
C	-3.18790000	0.20000000	-1.24440000
C	-2.71350000	-0.78850000	-2.27630000
O	-4.89210000	3.46950000	-1.22600000
O	-3.51840000	0.83330000	2.40450000
O	1.51710000	-3.19340000	-2.30360000
C	1.91220000	0.05800000	2.90760000

C	5.73630000	2.90550000	-0.08100000
C	3.35010000	3.38990000	-0.65290000
H	2.91840000	-1.10370000	-2.30740000
H	3.30130000	2.38220000	1.73890000
H	4.72970000	1.30640000	1.72910000
H	4.06380000	1.44680000	-2.23270000
H	5.30180000	0.60620000	-1.25580000
H	-1.22210000	-3.41630000	0.97640000
H	1.00400000	-3.03760000	1.96160000
H	-0.02980000	-1.62750000	2.30880000
H	-4.57460000	2.85390000	1.26290000
H	-3.90860000	1.55190000	-2.77220000
H	-3.18930000	-0.60710000	-3.24660000
H	-1.63120000	-0.70560000	-2.41550000
H	-2.97970000	-1.81090000	-1.98990000
H	-4.89820000	3.48410000	-2.19700000
H	-3.27380000	-0.09000000	2.62870000
H	1.86500000	-0.85540000	3.50950000
H	2.71590000	0.66460000	3.33580000
H	0.97200000	0.60880000	3.00920000
H	6.07300000	3.31850000	-1.03830000
H	5.74650000	3.71380000	0.65860000
H	6.47170000	2.15720000	0.23480000
H	3.32090000	4.20970000	0.07370000
H	3.64450000	3.81300000	-1.62000000
H	2.33050000	3.00290000	-0.75690000

4a-7			
Atom	X	Y	Z
C	3.07330000	0.47230000	0.71940000
C	3.29330000	0.37390000	-0.65960000
C	2.62450000	-0.55950000	-1.43030000
C	1.70670000	-1.40650000	-0.80100000
C	1.45720000	-1.30170000	0.58770000
C	2.16100000	-0.35870000	1.37320000
C	3.90710000	1.58440000	1.29560000
C	4.95300000	1.84980000	0.17820000
C	4.27470000	1.39920000	-1.14020000
C	1.01590000	-2.43630000	-1.62620000
O	-0.02590000	-3.08760000	-1.05440000
C	-0.63360000	-2.54280000	0.12880000
C	0.43860000	-2.24570000	1.17840000
O	-1.39990000	-1.37570000	-0.21050000

C	-2.33540000	-1.01110000	0.68960000
C	-3.12690000	0.15750000	0.22480000
O	-2.58750000	-1.59570000	1.73450000
C	-4.47650000	0.21550000	0.62530000
C	-5.30930000	1.24430000	0.19350000
C	-4.79670000	2.23690000	-0.62700000
C	-3.45780000	2.22580000	-1.00930000
C	-2.59740000	1.19790000	-0.57480000
C	-1.15310000	1.27000000	-0.99160000
O	-5.64250000	3.22510000	-1.03430000
O	-5.06230000	-0.71310000	1.44890000
O	1.39490000	-2.69970000	-2.75990000
C	1.90590000	-0.22480000	2.84830000
C	6.22840000	1.02150000	0.43260000
C	5.32830000	3.33420000	0.12190000
H	2.81130000	-0.63350000	-2.49860000
H	3.26560000	2.45580000	1.46960000
H	4.39060000	1.29530000	2.23370000
H	3.72790000	2.21890000	-1.62000000
H	4.98960000	0.97520000	-1.85260000
H	-1.30780000	-3.32330000	0.50160000
H	0.95800000	-3.16810000	1.46320000
H	-0.02390000	-1.81230000	2.06880000
H	-6.35150000	1.26980000	0.49830000
H	-3.06900000	3.02090000	-1.64110000
H	-0.89220000	2.27210000	-1.35000000
H	-0.49540000	1.06720000	-0.14120000
H	-0.95210000	0.56510000	-1.80370000
H	-5.16350000	3.83320000	-1.62070000
H	-4.36320000	-1.26850000	1.85490000
H	2.64360000	0.41070000	3.34500000
H	0.91830000	0.21610000	3.01810000
H	1.95660000	-1.20410000	3.33560000
H	6.96170000	1.17500000	-0.36720000
H	6.70190000	1.31060000	1.37760000
H	6.01360000	-0.05150000	0.48410000
H	5.78200000	3.66150000	1.06400000
H	6.04450000	3.52890000	-0.68410000
H	4.44770000	3.96090000	-0.05790000

4a-8			
Atom	X	Y	Z
C	-2.96230000	-0.67990000	0.57580000

C	-3.20190000	-0.30410000	-0.75130000
C	-2.57950000	0.79670000	-1.31120000
C	-1.69000000	1.53160000	-0.52060000
C	-1.42180000	1.14970000	0.81520000
C	-2.07670000	0.03320000	1.38660000
C	-3.74150000	-1.92360000	0.90750000
C	-4.78840000	-1.99370000	-0.23800000
C	-4.14470000	-1.24780000	-1.43410000
C	-1.05530000	2.74240000	-1.11330000
O	-0.05560000	3.32390000	-0.40620000
C	0.59470000	2.57350000	0.63200000
C	-0.44330000	1.99490000	1.59350000
O	1.41460000	1.55030000	0.04750000
C	2.41090000	1.08320000	0.82550000
C	3.14640000	-0.02770000	0.16690000
O	2.64640000	1.43490000	1.97340000
C	3.67990000	-1.02640000	1.00570000
C	4.33230000	-2.13580000	0.47510000
C	4.47610000	-2.24880000	-0.89890000
C	3.98890000	-1.26120000	-1.75110000
C	3.33250000	-0.12730000	-1.23230000
C	2.85700000	0.91480000	-2.20940000
O	5.11650000	-3.35050000	-1.38290000
O	3.59640000	-0.98750000	2.37530000
O	-1.44220000	3.20870000	-2.17700000
C	-1.79770000	-0.39770000	2.79930000
C	-6.09420000	-1.29300000	0.18800000
C	-5.10230000	-3.44810000	-0.60380000
H	-2.78030000	1.08310000	-2.34020000
H	-3.06200000	-2.78330000	0.89250000
H	-4.22560000	-1.85930000	1.88660000
H	-3.56940000	-1.92420000	-2.07630000
H	-4.88480000	-0.71550000	-2.04010000
H	1.23010000	3.29180000	1.16380000
H	-1.00490000	2.80250000	2.07740000
H	0.05730000	1.40170000	2.36330000
H	4.72780000	-2.90510000	1.13200000
H	4.12090000	-1.36020000	-2.82600000
H	3.35940000	0.80850000	-3.17750000
H	1.78070000	0.81550000	-2.38020000
H	3.09050000	1.92240000	-1.85100000
H	5.14550000	-3.30170000	-2.35250000
H	3.32610000	-0.08600000	2.65220000
H	-1.88590000	0.45310000	3.48300000

H	-2.50020000	-1.15720000	3.15220000
H	-0.78950000	-0.81850000	2.86960000
H	-6.82960000	-1.30690000	-0.62440000
H	-6.54430000	-1.79400000	1.05250000
H	-5.92370000	-0.24640000	0.46310000
H	-5.53090000	-3.98490000	0.24970000
H	-5.81900000	-3.50010000	-1.43080000
H	-4.19850000	-3.98460000	-0.91340000

4a-9			
Atom	X	Y	Z
C	-4.04090000	-0.72790000	-0.44290000
C	-4.48730000	0.54250000	-0.06190000
C	-3.60640000	1.59790000	0.08770000
C	-2.24340000	1.36040000	-0.11980000
C	-1.77810000	0.07600000	-0.48970000
C	-2.69160000	-0.98280000	-0.69530000
C	-5.20760000	-1.66890000	-0.57150000
C	-6.33840000	-0.92200000	0.18710000
C	-5.97770000	0.58270000	0.08860000
C	-1.29860000	2.50520000	0.01210000
O	0.02560000	2.21440000	-0.00720000
C	0.44090000	0.86210000	0.24600000
C	-0.29630000	-0.08780000	-0.69430000
O	1.85400000	0.78210000	0.00480000
C	2.49290000	-0.22160000	0.63870000
C	3.94390000	-0.24820000	0.31840000
O	1.96230000	-1.08520000	1.32460000
C	4.57470000	-1.50950000	0.30840000
C	5.91880000	-1.64390000	-0.03370000
C	6.65050000	-0.50950000	-0.34940000
C	6.06250000	0.75090000	-0.31430000
C	4.70800000	0.90690000	0.03650000
C	4.15380000	2.30520000	0.08300000
O	7.96730000	-0.58490000	-0.69350000
O	3.93030000	-2.68010000	0.62470000
O	-1.70180000	3.65680000	0.10520000
C	-2.23460000	-2.34790000	-1.12660000
C	-6.37710000	-1.36750000	1.66270000
C	-7.70280000	-1.20130000	-0.45140000
H	-3.96720000	2.58740000	0.35650000
H	-5.44620000	-1.79710000	-1.63350000
H	-4.99630000	-2.64590000	-0.12520000

H	-6.41430000	1.05050000	-0.80110000
H	-6.28170000	1.14280000	0.97870000
H	0.22870000	0.65260000	1.30370000
H	0.02700000	-1.11520000	-0.50090000
H	-0.05550000	0.14160000	-1.73970000
H	6.36980000	-2.63090000	-0.04310000
H	6.67400000	1.61850000	-0.55640000
H	4.95760000	3.04840000	0.13350000
H	3.56450000	2.51280000	-0.81520000
H	3.54120000	2.45300000	0.97810000
H	8.24250000	-1.51690000	-0.67390000
H	3.07350000	-2.46440000	1.05290000
H	-3.05620000	-2.94520000	-1.53340000
H	-1.48710000	-2.27330000	-1.92310000
H	-1.80580000	-2.88570000	-0.27540000
H	-7.15000000	-0.82280000	2.21650000
H	-6.60150000	-2.43710000	1.74360000
H	-5.42090000	-1.19060000	2.16720000
H	-7.94600000	-2.26870000	-0.40930000
H	-8.49850000	-0.65230000	0.06420000
H	-7.71910000	-0.89840000	-1.50430000

4b-1			
Atom	X	Y	Z
C	-3.13960000	0.29070000	0.78330000
C	-3.38290000	0.19980000	-0.59210000
C	-2.72720000	-0.73030000	-1.37720000
C	-1.77940000	-1.56080000	-0.77020000
C	-1.51280000	-1.46690000	0.61670000
C	-2.23230000	-0.55570000	1.42270000
C	-4.01120000	1.35480000	1.39270000
C	-4.47510000	2.16880000	0.15420000
C	-4.43540000	1.17130000	-1.03220000
C	-1.08010000	-2.56920000	-1.61410000
O	-0.00480000	-3.18890000	-1.06940000
C	0.60480000	-2.63690000	0.10950000
C	-0.45880000	-2.38760000	1.18040000
O	1.32410000	-1.43930000	-0.22650000
C	2.26880000	-1.06030000	0.65770000
C	3.00100000	0.14980000	0.20430000
O	2.57480000	-1.66060000	1.67920000
C	4.36190000	0.24580000	0.56010000
C	5.14570000	1.31760000	0.13760000

C	4.56490000	2.31680000	-0.62820000
C	3.21530000	2.26590000	-0.96240000
C	2.40640000	1.19470000	-0.53890000
C	0.94810000	1.23010000	-0.90570000
O	5.28680000	3.38560000	-1.06910000
O	5.00980000	-0.68610000	1.33280000
O	-1.47970000	-2.84380000	-2.73800000
C	-1.99980000	-0.45440000	2.90370000
C	-3.51230000	3.34550000	-0.10360000
C	-5.88960000	2.72010000	0.35980000
H	-2.94170000	-0.81050000	-2.43970000
H	-4.85390000	0.87560000	1.90380000
H	-3.45990000	1.97780000	2.10420000
H	-5.38600000	0.63930000	-1.15150000
H	-4.17090000	1.65810000	-1.97630000
H	1.31070000	-3.39870000	0.46170000
H	0.00540000	-1.94770000	2.06720000
H	-0.94490000	-3.32860000	1.46260000
H	6.19330000	1.35400000	0.41840000
H	2.79370000	3.07720000	-1.55340000
H	0.64190000	2.23300000	-1.22400000
H	0.74310000	0.54320000	-1.73210000
H	0.32720000	0.97890000	-0.04080000
H	6.20860000	3.28050000	-0.77890000
H	4.34390000	-1.27960000	1.74230000
H	-2.83090000	0.04100000	3.41480000
H	-1.91450000	-1.44930000	3.35260000
H	-1.08490000	0.11280000	3.10110000
H	-3.50890000	4.04170000	0.74270000
H	-2.48230000	3.00430000	-0.25590000
H	-3.81060000	3.90770000	-0.99560000
H	-6.23020000	3.26970000	-0.52470000
H	-6.60780000	1.91400000	0.54660000
H	-5.92560000	3.40190000	1.21660000

4b-2			
Atom	X	Y	Z
C	-3.06990000	0.47760000	0.71830000
C	-3.29420000	0.36860000	-0.65920000
C	-2.63010000	-0.57250000	-1.42450000
C	-1.71200000	-1.41610000	-0.79110000
C	-1.45770000	-1.30050000	0.59600000
C	-2.15750000	-0.35020000	1.37610000

C	-3.89810000	1.59740000	1.28760000
C	-4.94630000	1.85720000	0.17110000
C	-4.27340000	1.39340000	-1.14560000
C	-1.02590000	-2.45400000	-1.60980000
O	0.02110000	-3.09750000	-1.03850000
C	0.63150000	-2.54430000	0.13930000
C	-0.43730000	-2.24010000	1.19030000
O	1.39630000	-1.37870000	-0.20800000
C	2.34070000	-1.01520000	0.68290000
C	3.12600000	0.15640000	0.21610000
O	2.60660000	-1.60330000	1.72270000
C	4.47930000	0.21710000	0.60730000
C	5.31070000	1.24960000	0.17770000
C	4.78600000	2.24510000	-0.63200000
C	3.44530000	2.22930000	-1.00340000
C	2.58870000	1.19830000	-0.57350000
C	1.14360000	1.27170000	-0.98480000
O	5.55590000	3.27610000	-1.08180000
O	5.07440000	-0.71320000	1.42310000
O	-1.41330000	-2.73180000	-2.73720000
C	-1.89700000	-0.20400000	2.84900000
C	-5.31680000	3.34230000	0.10360000
C	-6.22380000	1.03540000	0.43590000
H	-2.81960000	-0.65410000	-2.49170000
H	-4.37980000	1.31800000	2.22950000
H	-3.25310000	2.46800000	1.45230000
H	-4.99180000	0.96610000	-1.85250000
H	-3.72510000	2.20720000	-1.63350000
H	1.30630000	-3.32260000	0.51540000
H	0.02880000	-1.80010000	2.07560000
H	-0.95560000	-3.16050000	1.48360000
H	6.35090000	1.25910000	0.48700000
H	3.06840000	3.03650000	-1.62920000
H	0.88210000	2.27400000	-1.34230000
H	0.93890000	0.56700000	-1.79620000
H	0.48920000	1.06870000	-0.13200000
H	6.46510000	3.14880000	-0.76230000
H	4.37850000	-1.27580000	1.82630000
H	-2.63500000	0.43300000	3.34360000
H	-1.94290000	-1.17950000	3.34430000
H	-0.91010000	0.24100000	3.01140000
H	-5.76660000	3.67890000	1.04420000
H	-4.43460000	3.96450000	-0.08390000
H	-6.03460000	3.53280000	-0.70190000

H	-6.95880000	1.18480000	-0.36300000
H	-6.01250000	-0.03790000	0.49570000
H	-6.69360000	1.33390000	1.37990000

4b-3			
Atom	X	Y	Z
C	-3.05130000	0.50660000	0.71040000
C	-3.31680000	0.21040000	-0.63120000
C	-2.70500000	-0.85500000	-1.26580000
C	-1.78170000	-1.61810000	-0.54300000
C	-1.49340000	-1.31880000	0.81000000
C	-2.16570000	-0.26280000	1.46710000
C	-3.87720000	1.68350000	1.15330000
C	-4.33670000	2.30780000	-0.19240000
C	-4.34190000	1.13770000	-1.20970000
C	-1.14260000	-2.78050000	-1.22140000
O	-0.11330000	-3.38170000	-0.57590000
C	0.54650000	-2.68300000	0.49190000
C	-0.47990000	-2.18880000	1.51150000
O	1.33050000	-1.60690000	-0.04490000
C	2.33730000	-1.16860000	0.73580000
C	3.03900000	-0.00300000	0.13540000
O	2.60880000	-1.58900000	1.85270000
C	3.61510000	0.92570000	1.02750000
C	4.24600000	2.07910000	0.56530000
C	4.32230000	2.30450000	-0.80030000
C	3.79070000	1.39040000	-1.70420000
C	3.15670000	0.21560000	-1.25650000
C	2.63410000	-0.73530000	-2.29940000
O	4.92550000	3.41760000	-1.30530000
O	3.59920000	0.77530000	2.39250000
O	-1.55210000	-3.19380000	-2.29840000
C	-1.90860000	0.06060000	2.91190000
C	-3.34650000	3.40180000	-0.64010000
C	-5.73250000	2.92550000	-0.06080000
H	-2.93770000	-1.09200000	-2.30070000
H	-4.72590000	1.32060000	1.74420000
H	-3.29370000	2.39130000	1.75060000
H	-5.31050000	0.62600000	-1.23960000
H	-4.07240000	1.46310000	-2.21960000
H	1.20940000	-3.41880000	0.96300000
H	0.02660000	-1.63000000	2.30330000
H	-1.01200000	-3.03690000	1.95770000

H	4.66840000	2.77770000	1.28020000
H	3.88080000	1.59810000	-2.76910000
H	3.07840000	-0.53150000	-3.28020000
H	2.89610000	-1.76890000	-2.05190000
H	1.54900000	-0.63460000	-2.39930000
H	5.24950000	3.95960000	-0.56640000
H	3.32150000	-0.14170000	2.60720000
H	-2.70910000	0.66890000	3.34370000
H	-1.86180000	-0.85380000	3.51230000
H	-0.96650000	0.60860000	3.01110000
H	-3.31180000	4.22060000	0.08740000
H	-2.32870000	3.01100000	-0.74780000
H	-3.64250000	3.82700000	-1.60570000
H	-6.07090000	3.34090000	-1.01650000
H	-6.46970000	2.17970000	0.25660000
H	-5.73730000	3.73300000	0.67970000

4b-4			
Atom	X	Y	Z
C	2.96510000	-0.68720000	0.58350000
C	3.21010000	-0.31370000	-0.74330000
C	2.59320000	0.78850000	-1.30640000
C	1.70350000	1.52700000	-0.51960000
C	1.42900000	1.14710000	0.81560000
C	2.07900000	0.02950000	1.39060000
C	3.73960000	-1.93280000	0.91890000
C	4.78970000	-2.00760000	-0.22330000
C	4.15180000	-1.26110000	-1.42220000
C	1.07610000	2.74040000	-1.11470000
O	0.07150000	3.32190000	-0.41470000
C	-0.58400000	2.57400000	0.62180000
C	0.44930000	1.99560000	1.58860000
O	-1.40340000	1.55070000	0.03680000
C	-2.40510000	1.08850000	0.81020000
C	-3.14780000	-0.02000000	0.15360000
O	-2.64360000	1.44400000	1.95680000
C	-3.72620000	-0.99070000	0.99800000
C	-4.39490000	-2.09730000	0.47810000
C	-4.50700000	-2.23240000	-0.89690000
C	-3.97360000	-1.27430000	-1.75290000
C	-3.30170000	-0.14540000	-1.24620000
C	-2.77960000	0.85880000	-2.23810000
O	-5.14800000	-3.29660000	-1.45750000

O	-3.67630000	-0.92870000	2.36900000
O	1.47430000	3.20940000	-2.17300000
C	1.79470000	-0.39830000	2.80310000
C	5.10010000	-3.46340000	-0.58640000
C	6.09640000	-1.31040000	0.20570000
H	2.79810000	1.07320000	-2.33520000
H	4.22100000	-1.86880000	1.89950000
H	3.05750000	-2.79050000	0.90300000
H	4.89540000	-0.73200000	-2.02670000
H	3.57630000	-1.93660000	-2.06530000
H	-1.22020000	3.29430000	1.15000000
H	-0.05520000	1.40470000	2.35760000
H	1.01060000	2.80310000	2.07300000
H	-4.81810000	-2.83080000	1.15680000
H	-4.09250000	-1.41070000	-2.82650000
H	-3.25100000	0.72950000	-3.21890000
H	-3.01030000	1.88000000	-1.91820000
H	-1.69980000	0.73980000	-2.37040000
H	-5.46890000	-3.87750000	-0.74730000
H	-3.37370000	-0.03330000	2.63500000
H	2.49480000	-1.15830000	3.15960000
H	1.88210000	0.45360000	3.48550000
H	0.78550000	-0.81720000	2.87080000
H	5.52460000	-4.00040000	0.26910000
H	4.19560000	-3.99750000	-0.89800000
H	5.81910000	-3.51860000	-1.41120000
H	6.83420000	-1.32760000	-0.60450000
H	5.92830000	-0.26290000	0.47900000
H	6.54230000	-1.81180000	1.07210000

4b-5			
Atom	X	Y	Z
C	-3.14300000	0.28430000	0.78180000
C	-3.38170000	0.20200000	-0.59480000
C	-2.72090000	-0.72100000	-1.38410000
C	-1.77320000	-1.55360000	-0.77970000
C	-1.51150000	-1.46850000	0.60860000
C	-2.23550000	-0.56420000	1.41830000
C	-4.02040000	1.34080000	1.39610000
C	-4.48390000	2.16140000	0.16180000
C	-4.43680000	1.17240000	-1.03130000
C	-1.06870000	-2.55450000	-1.62840000
O	0.00200000	-3.18070000	-1.08220000

C	0.60840000	-2.63530000	0.10160000
C	-0.45890000	-2.39210000	1.17030000
O	1.32890000	-1.43630000	-0.22770000
C	2.26430000	-1.05510000	0.66560000
C	3.00220000	0.15210000	0.21280000
O	2.55650000	-1.65110000	1.69340000
C	4.35960000	0.24610000	0.57820000
C	5.14430000	1.31430000	0.15240000
C	4.57490000	2.31030000	-0.62570000
C	3.22680000	2.26330000	-0.97090000
C	2.41470000	1.19490000	-0.54180000
C	0.95700000	1.22780000	-0.91440000
O	5.37480000	3.33800000	-1.02850000
O	4.99880000	-0.68330000	1.36000000
O	-1.46000000	-2.81630000	-2.75830000
C	-2.00840000	-0.47320000	2.90090000
C	-3.52510000	3.34380000	-0.08500000
C	-5.90120000	2.70570000	0.36700000
H	-2.93250000	-0.79520000	-2.44770000
H	-4.86280000	0.85480000	1.90140000
H	-3.47350000	1.96100000	2.11340000
H	-5.38490000	0.63750000	-1.15720000
H	-4.17140000	1.66670000	-1.97130000
H	1.31410000	-3.39830000	0.45170000
H	0.00150000	-1.95750000	2.06160000
H	-0.94560000	-3.33500000	1.44520000
H	6.19330000	1.36790000	0.42910000
H	2.79310000	3.06140000	-1.56890000
H	0.65080000	2.23010000	-1.23460000
H	0.75630000	0.54000000	-1.74100000
H	0.33280000	0.97720000	-0.05160000
H	4.85880000	3.94450000	-1.58420000
H	4.32980000	-1.26970000	1.77310000
H	-2.84120000	0.01890000	3.41250000
H	-1.92520000	-1.47140000	3.34310000
H	-1.09410000	0.09230000	3.10570000
H	-3.52690000	4.03410000	0.76610000
H	-2.49330000	3.00780000	-0.23670000
H	-3.82310000	3.91100000	-0.97400000
H	-6.24140000	3.26010000	-0.51470000
H	-6.61670000	1.89550000	0.54610000
H	-5.94240000	3.38140000	1.22830000

4b-6			
Atom	X	Y	Z
C	-3.04890000	0.49730000	0.70160000
C	-3.30850000	0.19870000	-0.64060000
C	-2.69030000	-0.86480000	-1.27190000
C	-1.76670000	-1.62390000	-0.54510000
C	-1.48510000	-1.32270000	0.80890000
C	-2.16340000	-0.26830000	1.46230000
C	-3.88030000	1.67170000	1.14060000
C	-4.33770000	2.29280000	-0.20730000
C	-4.33520000	1.12160000	-1.22330000
C	-1.11920000	-2.78320000	-1.22110000
O	-0.09430000	-3.38410000	-0.56820000
C	0.55950000	-2.68270000	0.50160000
C	-0.47220000	-2.18900000	1.51590000
O	1.34320000	-1.60600000	-0.03450000
C	2.34430000	-1.16270000	0.75120000
C	3.03790000	0.00600000	0.14930000
O	2.61300000	-1.57950000	1.86970000
C	3.56800000	0.96180000	1.03880000
C	4.18150000	2.11890000	0.56660000
C	4.28940000	2.32340000	-0.80010000
C	3.80500000	1.38090000	-1.70320000
C	3.18790000	0.20000000	-1.24440000
C	2.71350000	-0.78850000	-2.27630000
O	4.89210000	3.46950000	-1.22600000
O	3.51840000	0.83330000	2.40450000
O	-1.51710000	-3.19340000	-2.30360000
C	-1.91220000	0.05800000	2.90760000
C	-3.35010000	3.38990000	-0.65290000
C	-5.73630000	2.90550000	-0.08100000
H	-2.91840000	-1.10370000	-2.30740000
H	-4.72970000	1.30640000	1.72910000
H	-3.30130000	2.38220000	1.73890000
H	-5.30180000	0.60620000	-1.25580000
H	-4.06380000	1.44680000	-2.23270000
H	1.22210000	-3.41630000	0.97640000
H	0.02980000	-1.62750000	2.30880000
H	-1.00400000	-3.03760000	1.96160000
H	4.57460000	2.85390000	1.26290000
H	3.90860000	1.55190000	-2.77220000
H	3.18930000	-0.60710000	-3.24660000
H	2.97970000	-1.81090000	-1.98990000
H	1.63120000	-0.70560000	-2.41550000

H	4.89820000	3.48410000	-2.19700000
H	3.27380000	-0.09000000	2.62870000
H	-2.71590000	0.66460000	3.33580000
H	-1.86500000	-0.85540000	3.50950000
H	-0.97200000	0.60880000	3.00920000
H	-3.32090000	4.20970000	0.07370000
H	-2.33050000	3.00290000	-0.75690000
H	-3.64450000	3.81300000	-1.62000000
H	-6.07300000	3.31850000	-1.03830000
H	-6.47170000	2.15720000	0.23480000
H	-5.74650000	3.71380000	0.65860000

4b-7			
Atom	X	Y	Z
C	-3.07330000	0.47230000	0.71940000
C	-3.29330000	0.37390000	-0.65960000
C	-2.62450000	-0.55950000	-1.43030000
C	-1.70670000	-1.40650000	-0.80100000
C	-1.45720000	-1.30170000	0.58770000
C	-2.16100000	-0.35870000	1.37320000
C	-3.90710000	1.58440000	1.29560000
C	-4.95300000	1.84980000	0.17820000
C	-4.27470000	1.39920000	-1.14020000
C	-1.01590000	-2.43630000	-1.62620000
O	0.02590000	-3.08760000	-1.05440000
C	0.63360000	-2.54280000	0.12880000
C	-0.43860000	-2.24570000	1.17840000
O	1.39990000	-1.37570000	-0.21050000
C	2.33540000	-1.01110000	0.68960000
C	3.12690000	0.15750000	0.22480000
O	2.58750000	-1.59570000	1.73450000
C	4.47650000	0.21550000	0.62530000
C	5.30930000	1.24430000	0.19350000
C	4.79670000	2.23690000	-0.62700000
C	3.45780000	2.22580000	-1.00930000
C	2.59740000	1.19790000	-0.57480000
C	1.15310000	1.27000000	-0.99160000
O	5.64250000	3.22510000	-1.03430000
O	5.06230000	-0.71310000	1.44890000
O	-1.39490000	-2.69970000	-2.75990000
C	-1.90590000	-0.22480000	2.84830000
C	-5.32830000	3.33420000	0.12190000
C	-6.22840000	1.02150000	0.43260000

H	-2.81130000	-0.63350000	-2.49860000
H	-4.39060000	1.29530000	2.23370000
H	-3.26560000	2.45580000	1.46960000
H	-4.98960000	0.97520000	-1.85260000
H	-3.72790000	2.21890000	-1.62000000
H	1.30780000	-3.32330000	0.50160000
H	0.02390000	-1.81230000	2.06880000
H	-0.95800000	-3.16810000	1.46320000
H	6.35150000	1.26980000	0.49830000
H	3.06900000	3.02090000	-1.64110000
H	0.89220000	2.27210000	-1.35000000
H	0.95210000	0.56510000	-1.80370000
H	0.49540000	1.06720000	-0.14120000
H	5.16350000	3.83320000	-1.62070000
H	4.36320000	-1.26850000	1.85490000
H	-2.64360000	0.41070000	3.34500000
H	-1.95660000	-1.20410000	3.33560000
H	-0.91830000	0.21610000	3.01810000
H	-5.78200000	3.66150000	1.06400000
H	-4.44770000	3.96090000	-0.05790000
H	-6.04450000	3.52890000	-0.68410000
H	-6.96170000	1.17500000	-0.36720000
H	-6.01360000	-0.05150000	0.48410000
H	-6.70190000	1.31060000	1.37760000

4b-8			
Atom	X	Y	Z
C	2.96230000	-0.67990000	0.57580000
C	3.20190000	-0.30410000	-0.75130000
C	2.57950000	0.79670000	-1.31120000
C	1.69000000	1.53160000	-0.52060000
C	1.42180000	1.14970000	0.81520000
C	2.07670000	0.03320000	1.38660000
C	3.74150000	-1.92360000	0.90750000
C	4.78840000	-1.99370000	-0.23800000
C	4.14470000	-1.24780000	-1.43410000
C	1.05530000	2.74240000	-1.11330000
O	0.05560000	3.32390000	-0.40620000
C	-0.59470000	2.57350000	0.63200000
C	0.44330000	1.99490000	1.59350000
O	-1.41460000	1.55030000	0.04750000
C	-2.41090000	1.08320000	0.82550000
C	-3.14640000	-0.02770000	0.16690000

O	-2.64640000	1.43490000	1.97340000
C	-3.67990000	-1.02640000	1.00570000
C	-4.33230000	-2.13580000	0.47510000
C	-4.47610000	-2.24880000	-0.89890000
C	-3.98890000	-1.26120000	-1.75110000
C	-3.33250000	-0.12730000	-1.23230000
C	-2.85700000	0.91480000	-2.20940000
O	-5.11650000	-3.35050000	-1.38290000
O	-3.59640000	-0.98750000	2.37530000
O	1.44220000	3.20870000	-2.17700000
C	1.79770000	-0.39770000	2.79930000
C	5.10230000	-3.44810000	-0.60380000
C	6.09420000	-1.29300000	0.18800000
H	2.78030000	1.08310000	-2.34020000
H	4.22560000	-1.85930000	1.88660000
H	3.06200000	-2.78330000	0.89250000
H	4.88480000	-0.71550000	-2.04010000
H	3.56940000	-1.92420000	-2.07630000
H	-1.23010000	3.29180000	1.16380000
H	-0.05730000	1.40170000	2.36330000
H	1.00490000	2.80250000	2.07740000
H	-4.72780000	-2.90510000	1.13200000
H	-4.12090000	-1.36020000	-2.82600000
H	-3.35940000	0.80850000	-3.17750000
H	-3.09050000	1.92240000	-1.85100000
H	-1.78070000	0.81550000	-2.38020000
H	-5.14550000	-3.30170000	-2.35250000
H	-3.32610000	-0.08600000	2.65220000
H	2.50020000	-1.15720000	3.15220000
H	1.88590000	0.45310000	3.48300000
H	0.78950000	-0.81850000	2.86960000
H	5.53090000	-3.98490000	0.24970000
H	4.19850000	-3.98460000	-0.91340000
H	5.81900000	-3.50010000	-1.43080000
H	6.82960000	-1.30690000	-0.62440000
H	5.92370000	-0.24640000	0.46310000
H	6.54430000	-1.79400000	1.05250000

4b-9			
Atom	X	Y	Z
C	4.04090000	-0.72790000	-0.44290000
C	4.48730000	0.54250000	-0.06190000
C	3.60640000	1.59790000	0.08770000

C	2.24340000	1.36040000	-0.11980000
C	1.77810000	0.07600000	-0.48970000
C	2.69160000	-0.98280000	-0.69530000
C	5.20760000	-1.66890000	-0.57150000
C	6.33840000	-0.92200000	0.18710000
C	5.97770000	0.58270000	0.08860000
C	1.29860000	2.50520000	0.01210000
O	-0.02560000	2.21440000	-0.00720000
C	-0.44090000	0.86210000	0.24600000
C	0.29630000	-0.08780000	-0.69430000
O	-1.85400000	0.78210000	0.00480000
C	-2.49290000	-0.22160000	0.63870000
C	-3.94390000	-0.24820000	0.31840000
O	-1.96230000	-1.08520000	1.32460000
C	-4.57470000	-1.50950000	0.30840000
C	-5.91880000	-1.64390000	-0.03370000
C	-6.65050000	-0.50950000	-0.34940000
C	-6.06250000	0.75090000	-0.31430000
C	-4.70800000	0.90690000	0.03650000
C	-4.15380000	2.30520000	0.08300000
O	-7.96730000	-0.58490000	-0.69350000
O	-3.93030000	-2.68010000	0.62470000
O	1.70180000	3.65680000	0.10520000
C	2.23460000	-2.34790000	-1.12660000
C	7.70280000	-1.20130000	-0.45140000
C	6.37710000	-1.36750000	1.66270000
H	3.96720000	2.58740000	0.35650000
H	4.99630000	-2.64590000	-0.12520000
H	5.44620000	-1.79710000	-1.63350000
H	6.28170000	1.14280000	0.97870000
H	6.41430000	1.05050000	-0.80110000
H	-0.22870000	0.65260000	1.30370000
H	0.05550000	0.14160000	-1.73970000
H	-0.02700000	-1.11520000	-0.50090000
H	-6.36980000	-2.63090000	-0.04310000
H	-6.67400000	1.61850000	-0.55640000
H	-4.95760000	3.04840000	0.13350000
H	-3.54120000	2.45300000	0.97810000
H	-3.56450000	2.51280000	-0.81520000
H	-8.24250000	-1.51690000	-0.67390000
H	-3.07350000	-2.46440000	1.05290000
H	3.05620000	-2.94520000	-1.53340000
H	1.80580000	-2.88570000	-0.27540000
H	1.48710000	-2.27330000	-1.92310000

H	7.94600000	-2.26870000	-0.40930000
H	7.71910000	-0.89840000	-1.50430000
H	8.49850000	-0.65230000	0.06420000
H	7.15000000	-0.82280000	2.21650000
H	5.42090000	-1.19060000	2.16720000
H	6.60150000	-2.43710000	1.74360000