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Supplementary Information

Clerodane Diterpenes from Bark of *Croton urucurana* Baillon

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **1**

	x	y	x	U(eq)
C(1)	1657(4)	499(3)	8363(1)	48(1)
C(2)	917(5)	–275(3)	7863(1)	53(1)
C(3)	1659(4)	53(3)	7272(1)	48(1)
C(4)	2948(4)	855(3)	7276(1)	45(1)
C(5)	3853(4)	1554(3)	7678(1)	41(1)
C(6)	5864(4)	1680(3)	7555(1)	47(1)
C(7)	6889(4)	2162(3)	8083(1)	48(1)
C(8)	6624(4)	1367(3)	8623(1)	41(1)
C(9)	4658(4)	1221(3)	8806(1)	40(1)
C(10)	3623(4)	774(3)	8250(1)	38(1)
C(11)	4687(4)	234(3)	9279(1)	45(1)
C(12)	5795(5)	576(3)	9814(1)	54(1)
C(13)	7762(4)	1739(3)	9142(2)	47(1)
C(14)	6180(5)	-445(3)	10216(1)	59(1)
C(15)	6581(9)	–1607(4)	10073(2)	113(2)
C(16)	6555(7)	–1458(5)	11052(2)	83(1)
C(17)	6206(6)	-411(5)	10836(2)	81(1)
C(18)	3884(5)	2398(3)	9073(2)	54(1)
C(19)	2998(5)	2837(3)	7694(2)	61(1)
C(20)	3440(5)	1133(3)	6550(1)	54(1)
C(21)	3726(7)	321(4)	5586(1)	73(1)
O(12)	7499(3)	1151(2)	9657(1)	63(1)
O(15)	6787(8)	–2279(4)	10582(2)	162(2)
O(20)	3797(5)	2123(2)	6360(1)	83(1)
O(21)	3422(4)	147(2)	6212(1)	62(1)
O(13)	8950(3)	2463(2)	9117(1)	64(1)

U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

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Table S2. Bond lengths (Å) and angles (degree) for compound **1**

C(1)-C(2)	1.522(4)	C(4)-C(5)-C(10)	106.5(2)
C(1)-C(10)	1.534(4)	C(6)-C(5)-C(10)	107.8(2)
C(2)-C(3)	1.492(4)	C(19)-C(5)-C(10)	115.9(3)
C(3)-C(4)	1.332(4)	C(7)-C(6)-C(5)	113.0(3)
C(4)-C(20)	1.493(5)	C(8)-C(7)-C(6)	111.2(2)
C(4)-C(5)	1.530(4)	C(13)-C(8)-C(7)	113.1(3)
C(5)-C(6)	1.547(4)	C(13)-C(8)-C(9)	111.4(2)
C(5)-C(19)	1.557(4)	C(7)-C(8)-C(9)	113.7(3)
C(5)-C(10)	1.561(4)	C(11)-C(9)-C(8)	104.4(2)
C(6)-C(7)	1.516(4)	C(11)-C(9)-C(18)	109.5(2)
C(7)-C(8)	1.515(4)	C(8)-C(9)-C(18)	112.2(3)
C(8)-C(13)	1.508(4)	C(11)-C(9)-C(10)	110.1(2)
C(8)-C(9)	1.547(4)	C(8)-C(9)-C(10)	107.3(2)
C(9)-C(11)	1.526(4)	C(18)-C(9)-C(10)	113.0(3)
C(9)-C(18)	1.547(4)	C(1)-C(10)-C(9)	114.3(2)
C(9)-C(10)	1.559(4)	C(1)-C(10)-C(5)	110.7(2)
C(11)-C(12)	1.517(4)	C(9)-C(10)-C(5)	115.8(2)
C(12)-O(12)	1.476(4)	C(12)-C(11)-C(9)	112.7(3)
C(12)-C(14)	1.477(5)	O(12)-C(12)-C(14)	107.8(3)
C(13)-0(13)	1.202(4)	O(12)-C(12)-C(11)	113.3(3)
C(13)-O(12)	1.347(4)	C(14)-C(12)-C(11)	114.1(3)
C(14)-C(15)	1.357(6)	0(13)-C(13)-O(12)	118.1(3)
C(14)-C(17)	1.399(5)	0(13)-C(13)-C(8)	124.6(3)
C(15)-O(15)	1.378(5)	O(12)-C(13)-C(8)	117.2(3)
C(16)-C(17)	1.283(6)	C(15)-C(14)-C(17)	105.1(4)
C(16)-O(15)	1.406(6)	C(15)-C(14)-C(12)	128.2(3)
C(20)-O(20)	1.205(4)	C(17)-C(14)-C(12)	126.6(4)
C(20)-O(21)	1.330(4)	C(14)-C(15)-O(15)	109.6(4)
C(21)-O(21)	1.445(4)	C(17)-C(16)-O(15)	108.6(4)
C(2)-C(1)-C(10)	110.0(3)	C(16)-C(17)-C(14)	111.1(4)
C(3)-C(2)-C(1)	113.0(3)	O(20)-C(20)-O(21)	122.7(3)
C(4)-C(3)-C(2)	125.4(3)	O(20)-C(20)-C(4)	125.4(3)
C(20)-C(4)-C(5)	119.1(3)	O(21)-C(20)-C(4)	111.9(3)
C(4)-C(5)-C(6)	110.5(3)	C(13)-O(12)-C(12)	122.8(3)
C(4)-C(5)-C(19)	107.0(3)	C(15)-O(15)-C(16)	105.6(4)
C(6)-C(5)-C(19)	109.1(3)	C(20)-O(21)-C(21)	116.8(3)

Symmetry transformations used to generate equivalent atoms.

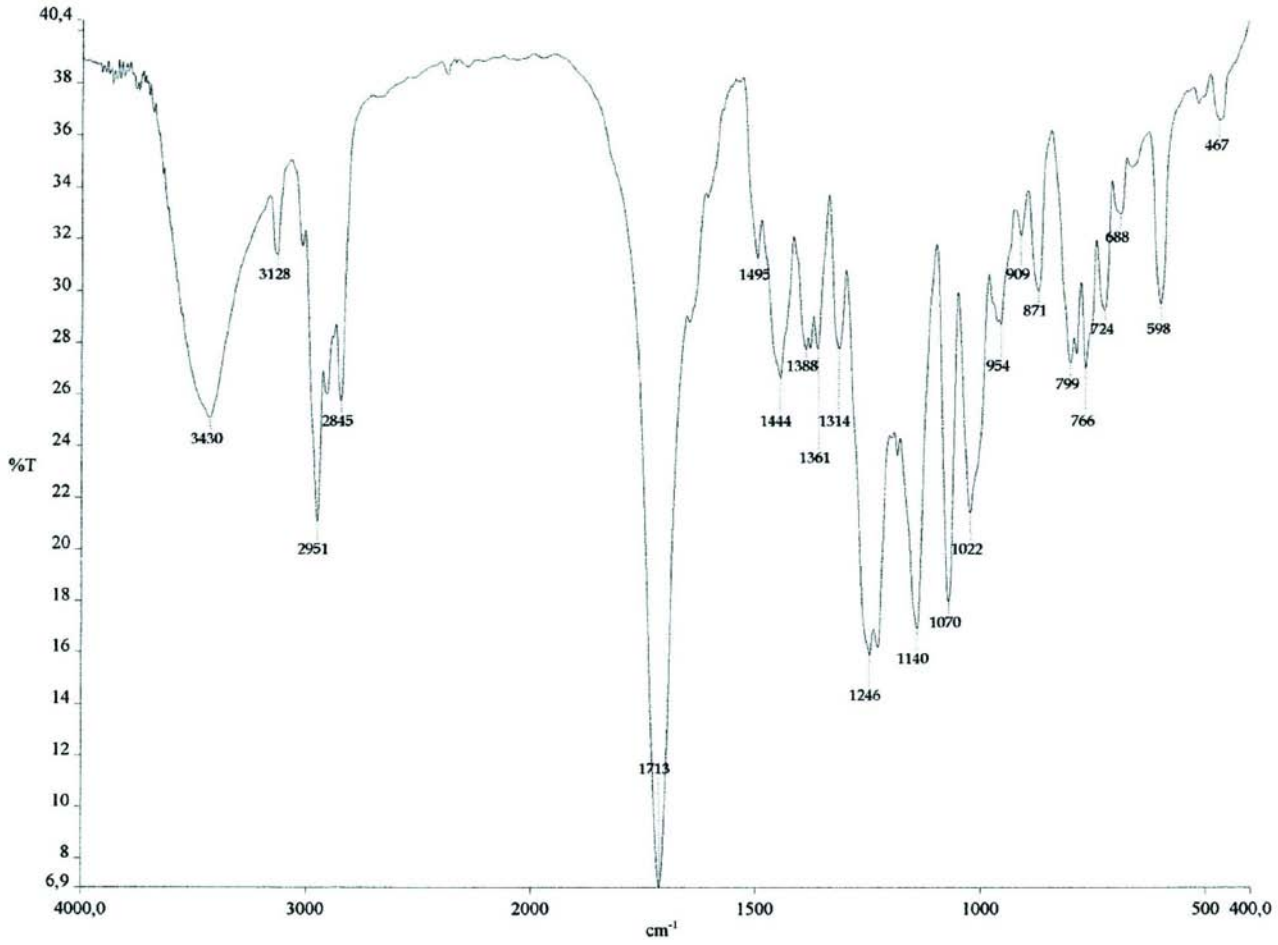

Figure S1. Infrared spectrum (KBr disks) of compound **1**.

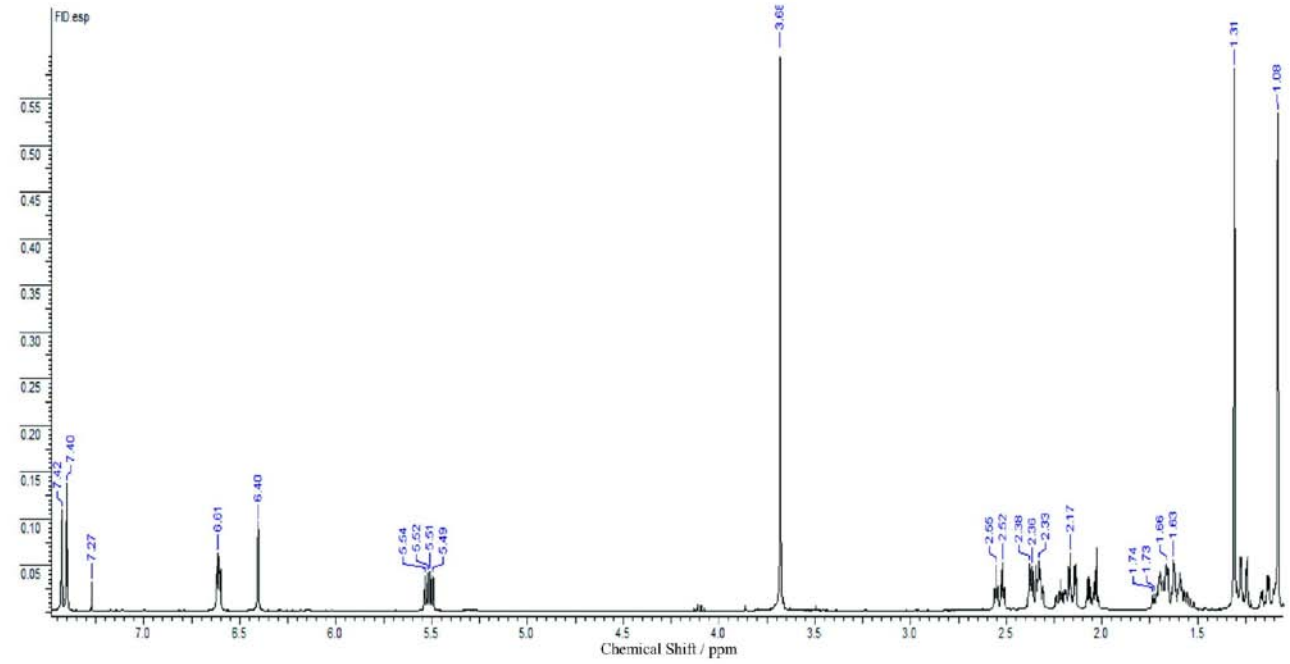

Figure S2. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **1**.

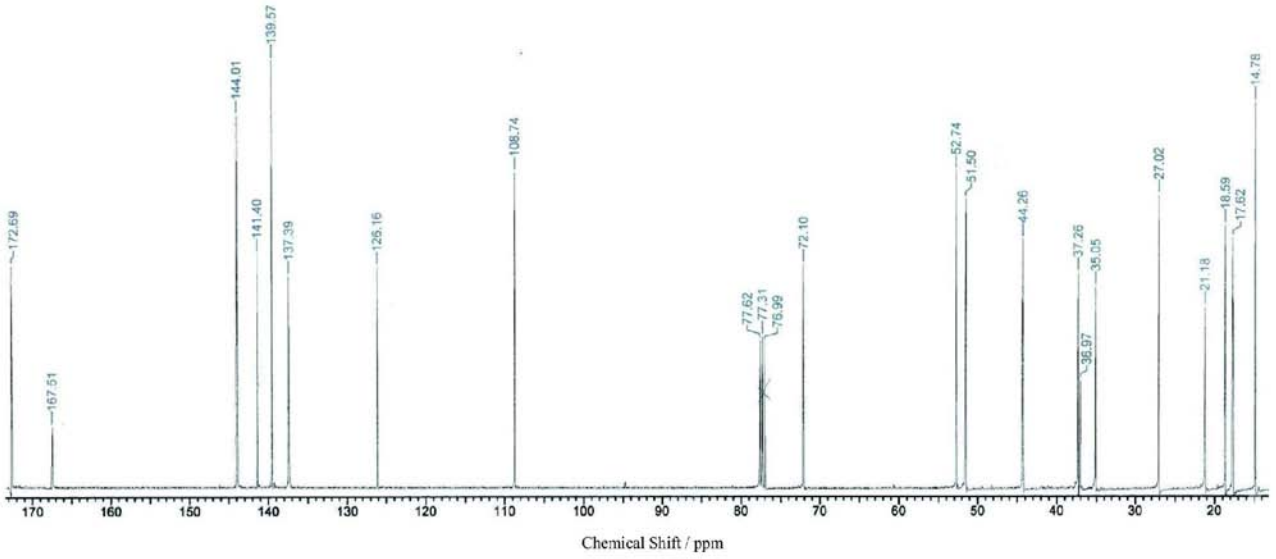

Figure S3. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **1**.

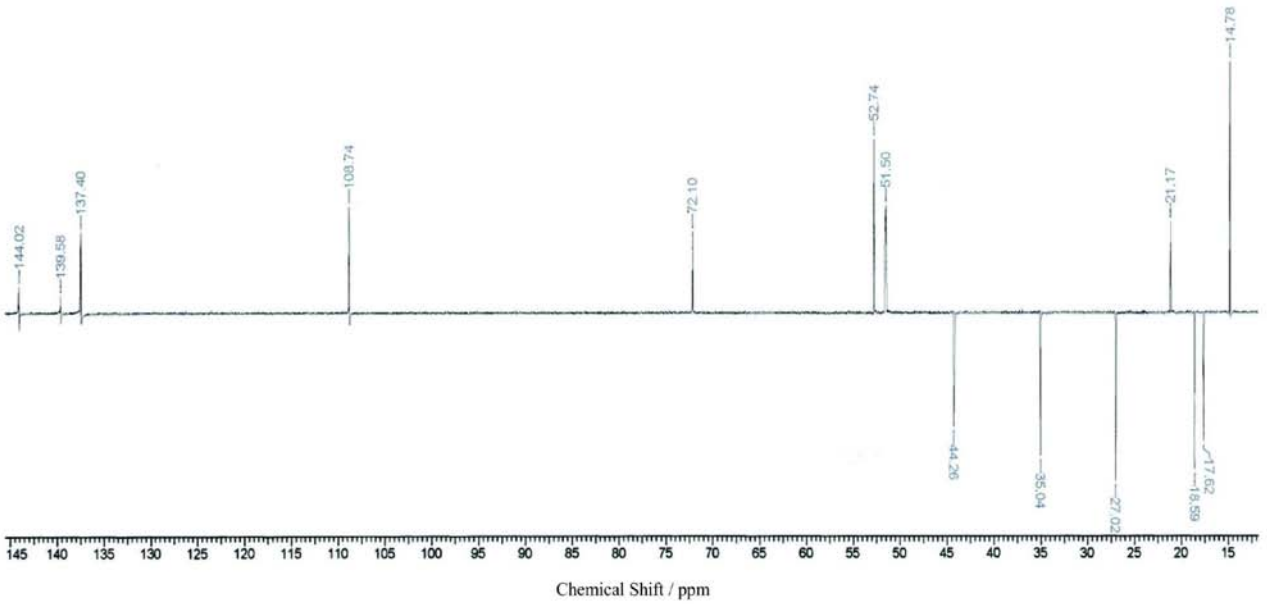

Figure S4. ^{13}C NMR DEPT spectrum (100 MHz, $CDCl_3$) of compound **1**.

Table S3. Bond lengths (Å) and angles (degree) for compound **4**

C(1)-C(10)	1.531(3)	C(6)-C(5)-C(4)	109.01(19)
C(1)-C(2)	1.532(4)	C(19)-C(5)-C(4)	109.33(18)
C(2)-C(3)	1.498(4)	C(6)-C(5)-C(10)	109.69(17)
C(3)-O(3)	1.208(3)	C(19)-C(5)-C(10)	113.95(19)
C(3)-C(4)	1.531(4)	C(4)-C(5)-C(10)	104.99(18)
C(4)-C(18)	1.523(4)	C(7)-C(6)-C(5)	113.4(2)
C(4)-C(5)	1.566(3)	C(8)-C(7)-C(6)	109.3(2)
C(5)-C(6)	1.535(3)	C(17)-C(8)-C(7)	112.9(2)
C(5)-C(19)	1.548(3)	C(17)-C(8)-C(9)	111.07(18)
C(5)-C(10)	1.569(3)	C(7)-C(8)-C(9)	113.16(19)
C(6)-C(7)	1.526(4)	C(11)-C(9)-C(20)	109.6(2)
C(7)-C(8)	1.517(4)	C(11)-C(9)-C(8)	104.03(18)
C(8)-C(17)	1.511(3)	C(20)-C(9)-C(8)	111.4(2)
C(8)-C(9)	1.547(3)	C(11)-C(9)-C(10)	108.49(18)
C(9)-C(11)	1.538(3)	C(20)-C(9)-C(10)	114.09(19)
C(9)-C(20)	1.543(3)	C(8)-C(9)-C(10)	108.70(17)
C(9)-C(10)	1.557(3)	C(1)-C(10)-C(9)	113.59(18)
C(11)-C(12)	1.523(3)	C(1)-C(10)-C(5)	110.40(17)
C(12)-O(12)	1.467(3)	C(9)-C(10)-C(5)	116.72(17)
C(12)-C(13)	1.498(4)	C(12)-C(11)-C(9)	113.2(2)
C(13)-C(16)	1.352(4)	O(12)-C(12)-C(13)	106.9(2)
C(13)-C(14)	1.434(4)	O(12)-C(12)-C(11)	115.5(2)
C(14)-C(15)	1.336(6)	C(13)-C(12)-C(11)	113.1(2)
C(15)-O(16)	1.365(5)	C(16)-C(13)-C(14)	105.0(3)
C(16)-O(16)	1.369(3)	C(16)-C(13)-C(12)	127.7(2)
C(17)-O(17)	1.208(3)	C(14)-C(13)-C(12)	127.1(3)
C(17)-O(12)	1.351(3)	C(15)-C(14)-C(13)	106.8(3)
C(18)-O(18)	1.195(4)	C(14)-C(15)-O(16)	111.4(3)
C(18)-O(21)	1.344(4)	C(13)-C(16)-O(16)	111.7(3)
C(21)-O(21)	1.450(3)	O(17)-C(17)-O(12)	117.7(2)
C(10)-C(1)-C(2)	111.3(2)	O(17)-C(17)-C(8)	124.8(3)
C(3)-C(2)-C(1)	113.6(2)	O(12)-C(17)-C(8)	117.5(2)
O(3)-C(3)-C(2)	123.3(2)	O(18)-C(18)-O(21)	122.7(3)
O(3)-C(3)-C(4)	122.1(2)	O(18)-C(18)-C(4)	127.6(3)
C(2)-C(3)-C(4)	114.6(2)	O(21)-C(18)-C(4)	109.7(2)
C(18)-C(4)-C(3)	109.67(19)	C(17)-O(12)-C(12)	122.83(19)
C(18)-C(4)-C(5)	116.8(2)	C(15)-O(16)-C(16)	105.1(3)
C(3)-C(4)-C(5)	109.8(2)	C(18)-O(21)-C(21)	116.7(3)
C(6)-C(5)-C(19)	109.7(2)		

Symmetry transformations used to generate equivalent atoms.

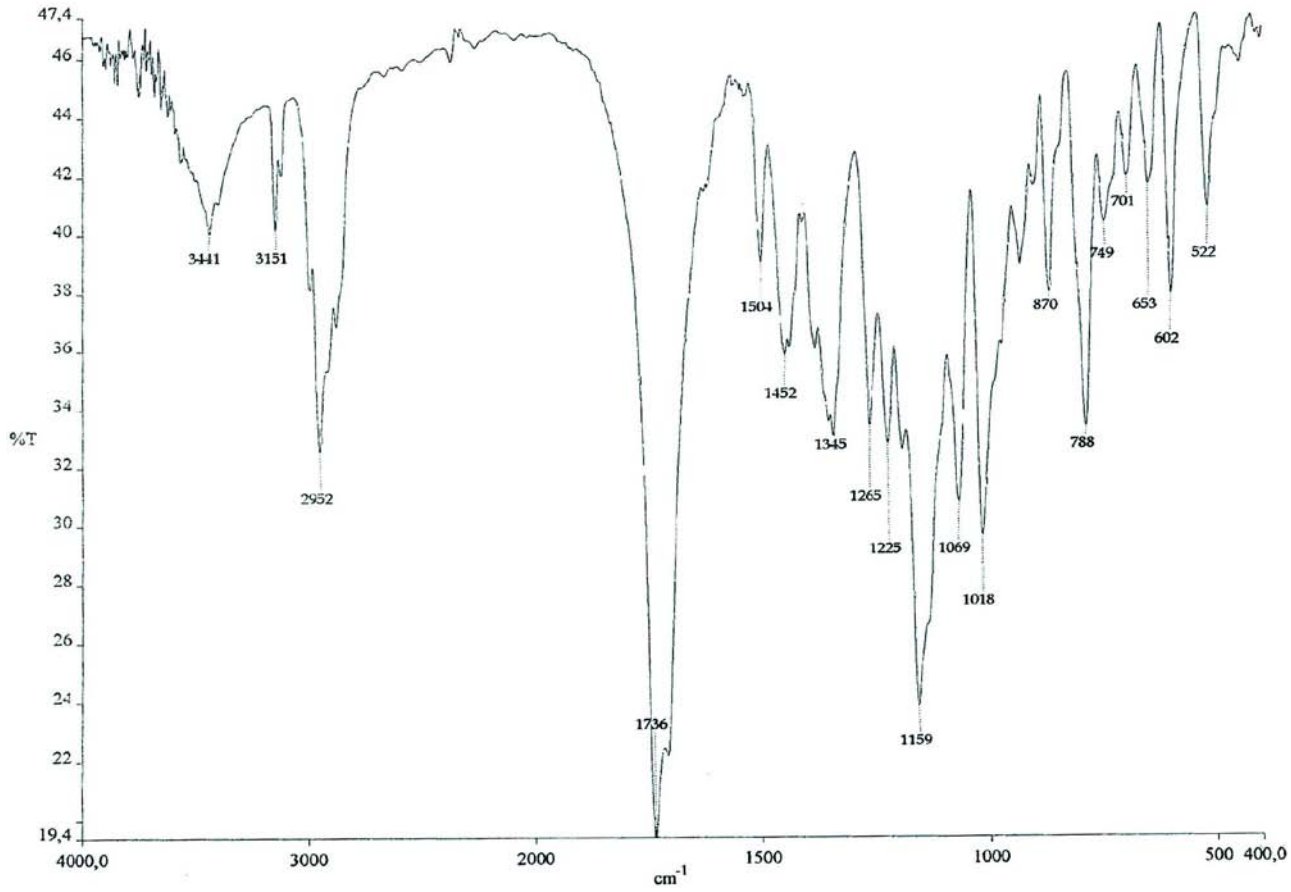

Figure S5. Infrared spectrum (KBr disks) of compound **4.**

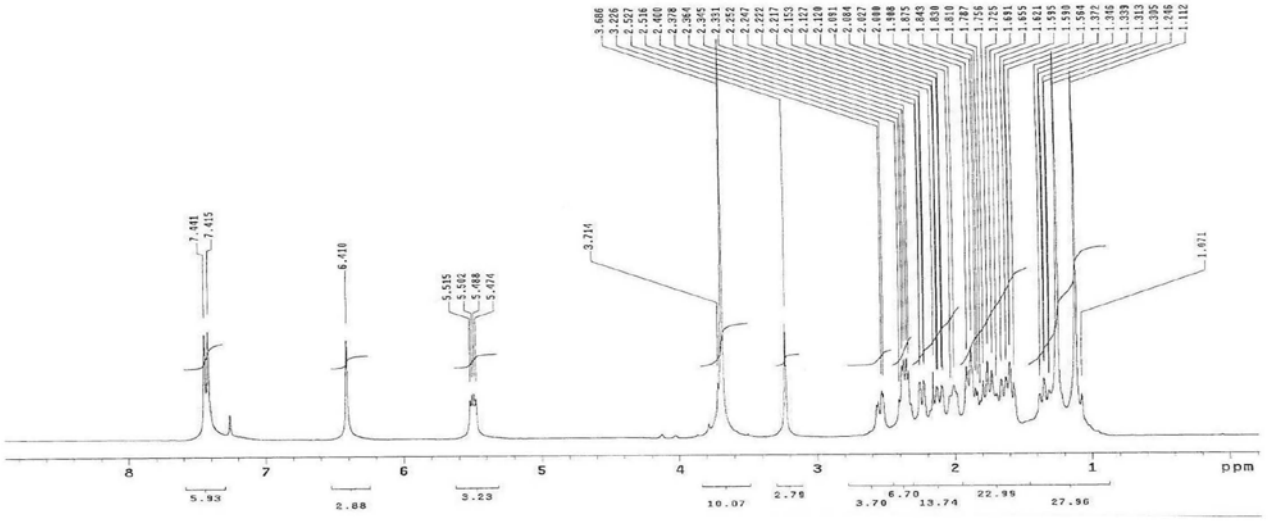

Figure S6. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **4.**

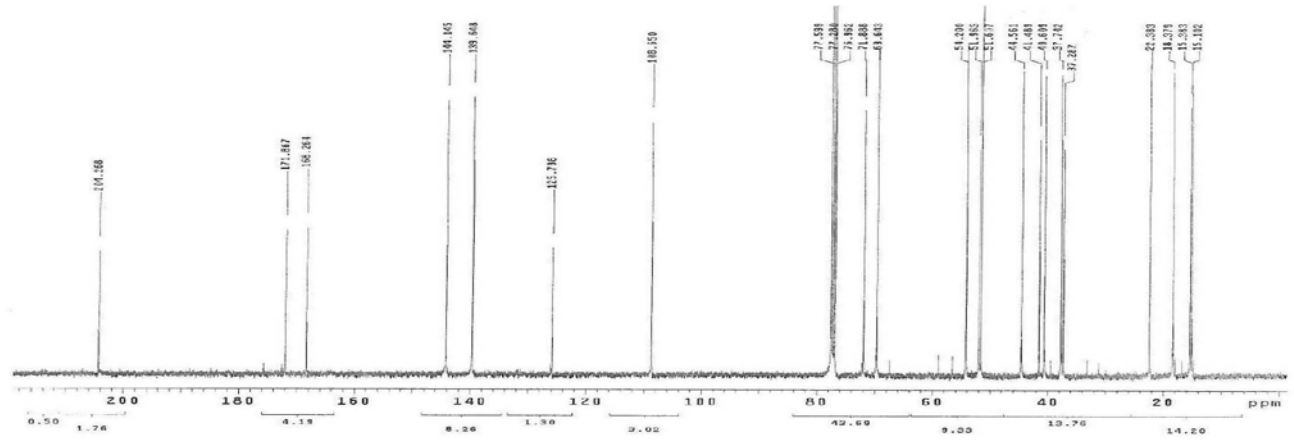

Figure S7. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **4.**

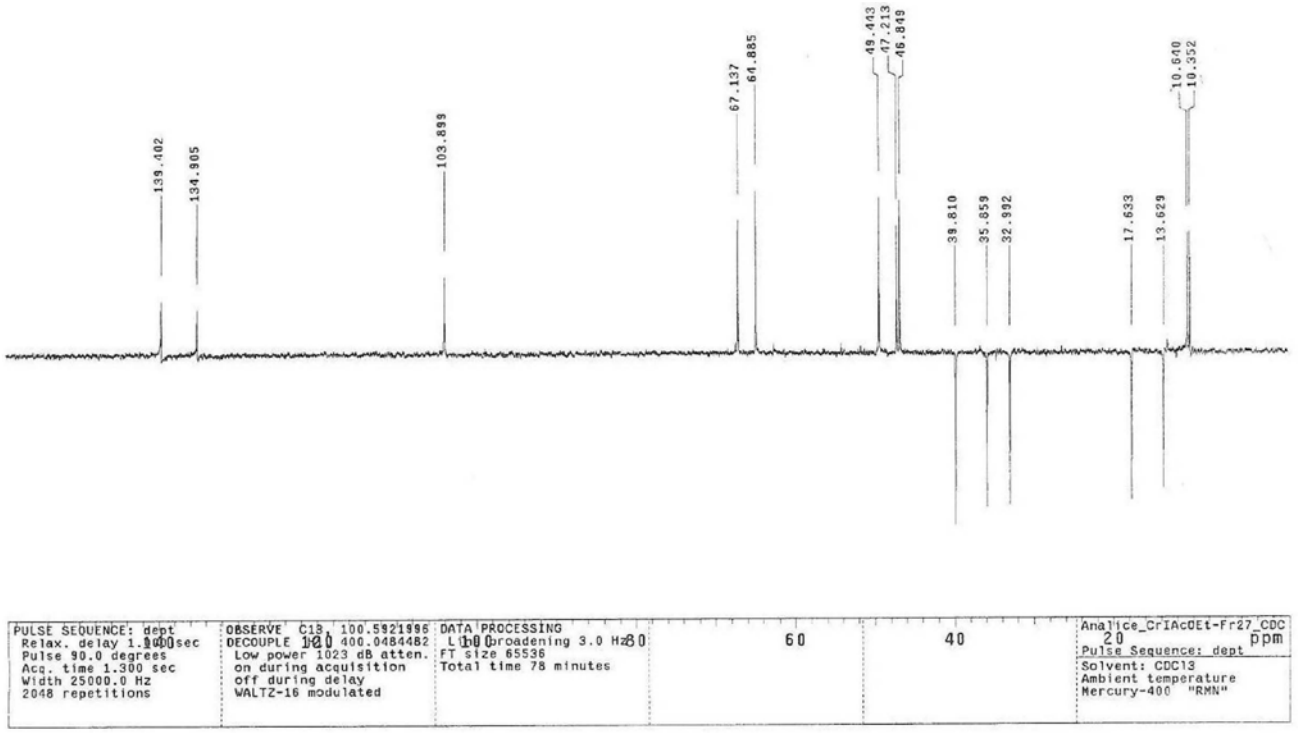

Figure S8. ^{13}C NMR DEPT spectrum (100 MHz, $CDCl_3$) of compound **4.**

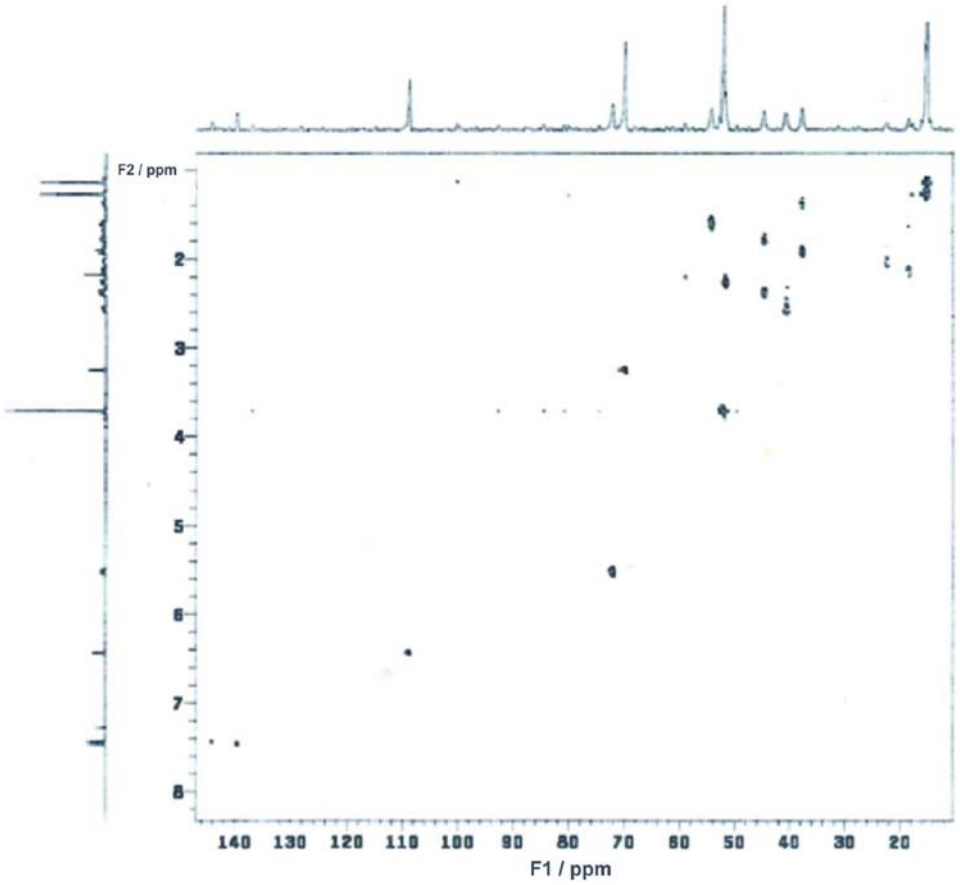

Figure S9. HMQC bidimensional spectrum (400 MHz, $CDCl_3$) of compound **4.**

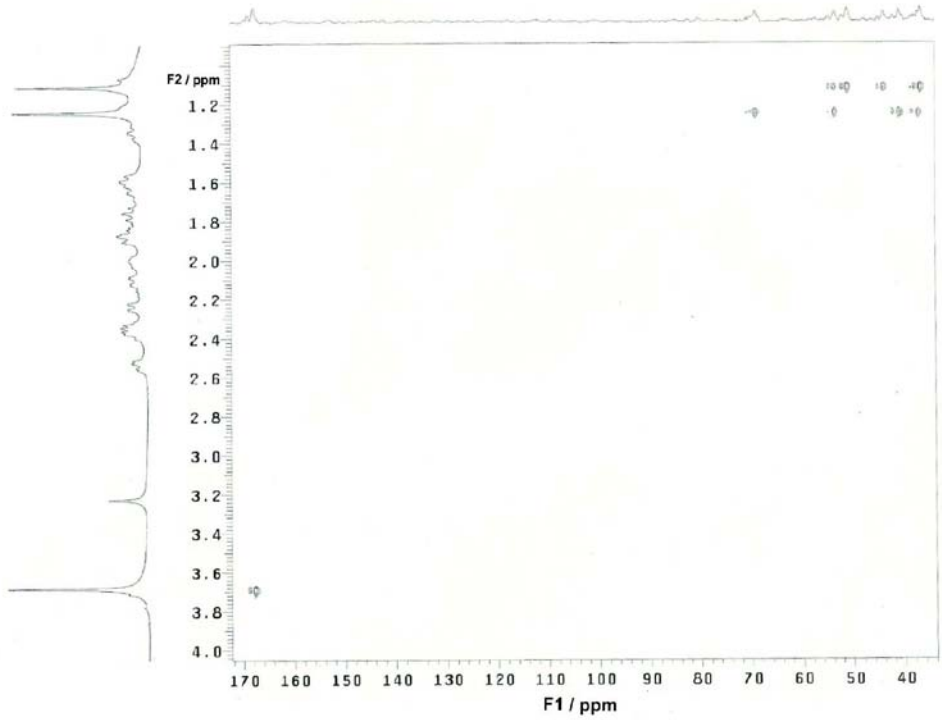

Figure S10. HMBC bidimensional spectrum (400 MHz, $CDCl_3$) of compound **4.**

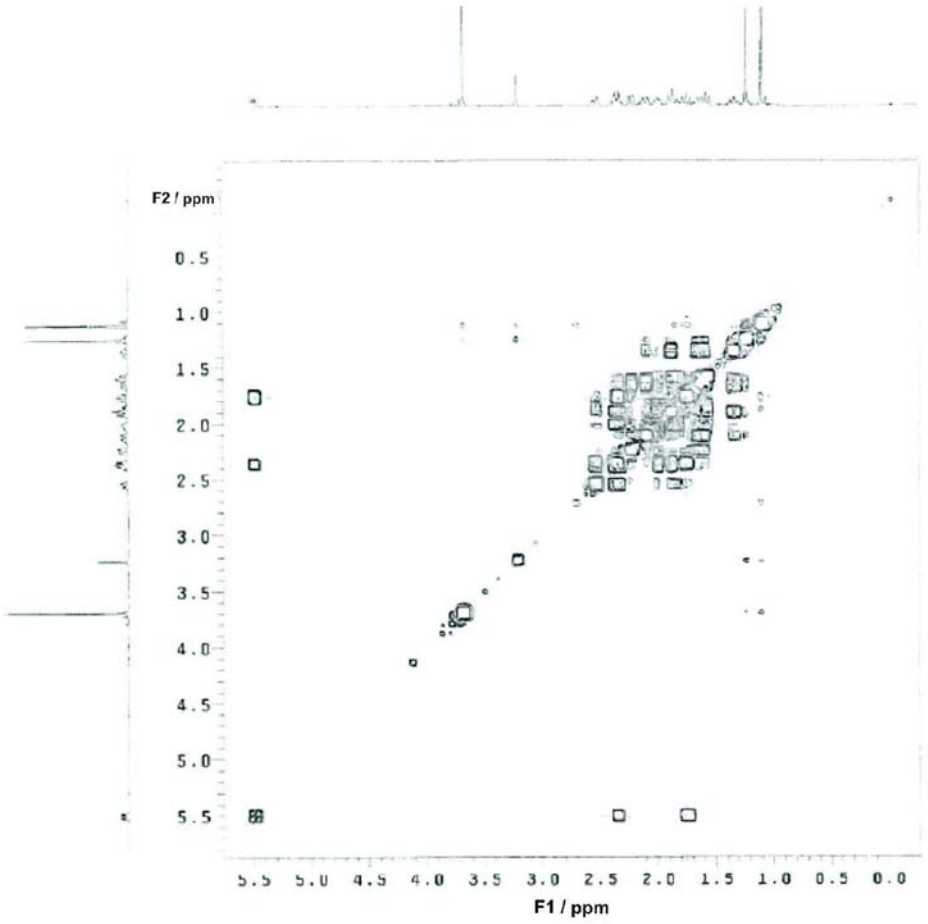

Figure S11. ^{1}H-^{1}H COSY spectrum (400 MHz, $CDCl_3$) of compound **4.**

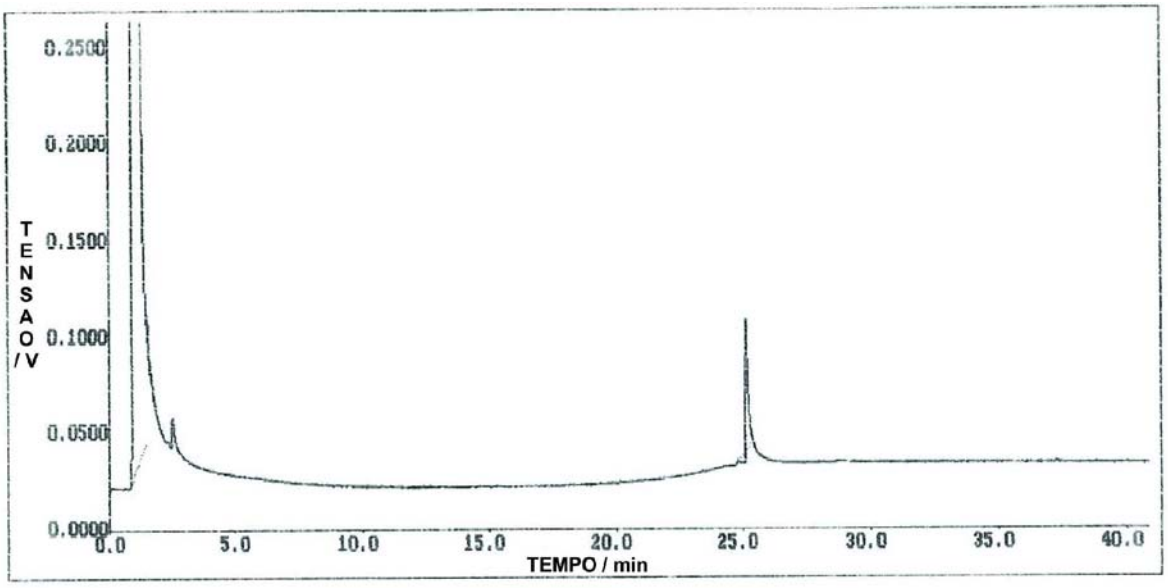

Figure S12. Gas chromatography of compound **4.**

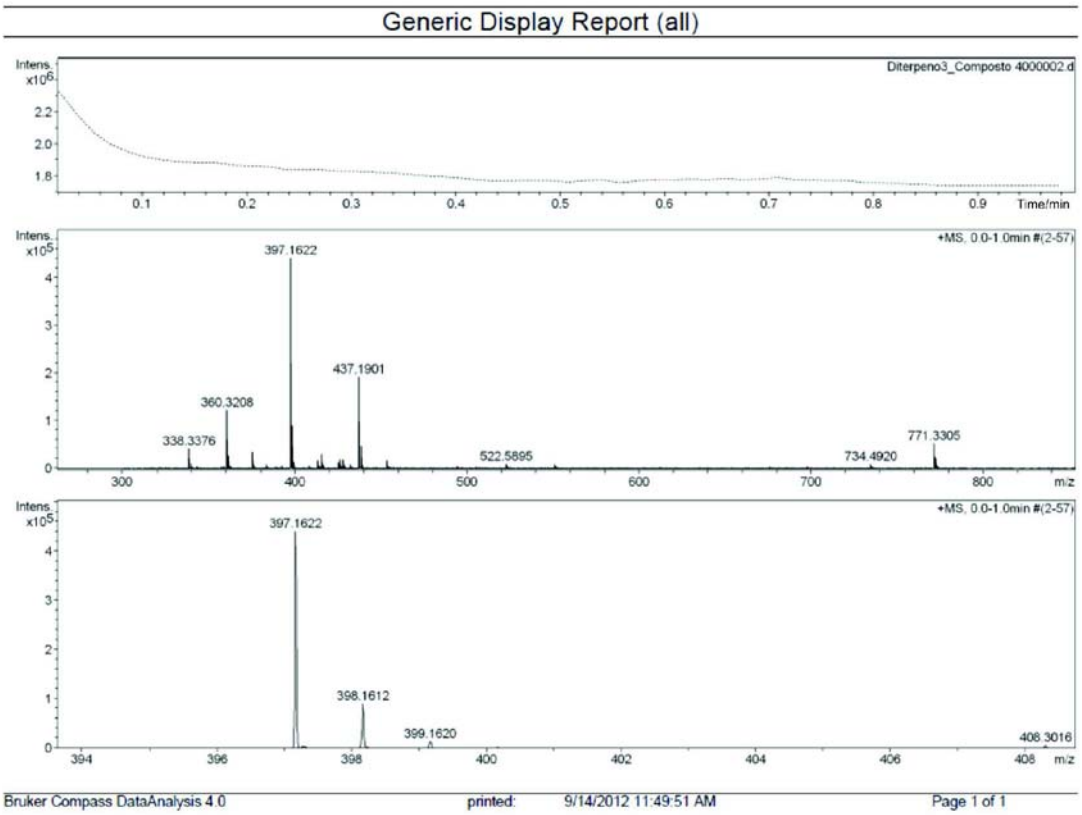

Figure S13. HRMS for the compound **4**.