J. Braz. Chem. Soc., Vol. 21, No. 4, S1-S9, 2010.
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0103 - 5053 $6.00+0.00

Isolation, X-ray Crystal Structure and Theoretical Calculations of the New Compound 8-epicordatin and Identification of Others Terpenes and Steroids from the Bark and Leaves of *Croton palanostigma* Klotzsch

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **2** U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(4)	2238(2)	4025(2)	774(1)	57(1)
O(5)	2280(2)	5725(2)	438(1)	73(1)
C(2)	2821(3)	4243(3)	2029(1)	53(1)
C(19)	2505(2)	5093(2)	781(1)	49(1)
C(9)	5490(2)	3141(3)	1335(1)	52(1)
O(6)	3060(3)	6646(2)	1274(1)	80(1)
C(1)	3861(2)	3587(2)	1948(1)	49(1)
C(5)	4368(2)	5055(3)	1284(1)	49(1)
O(1)	7063(2)	1733(4)	825(1)	96(1)
C(10)	4370(2)	3781(2)	1419(1)	42(1)
C(8)	5963(2)	3455(3)	806(1)	63(1)
C(11)	5223(2)	1897(3)	1284(1)	60(1)
C(3)	2486(3)	5056(3)	1727(1)	56(1)
C(4)	3117(3)	5450(2)	1269(1)	51(1)
C(13)	5926(3)	123(4)	880(1)	73(1)
C(7)	6060(3)	4715(4)	720(1)	77(1)
C(20)	6359(3)	3319(4)	1759(1)	73(1)
O(2)	7815(2)	3222(4)	483(1)	119(1)
C(18)	4970(3)	5775(3)	1692(1)	72(1)
C(14)	5757(4)	−36(4)	359(2)	92(1)
C(17)	7009(3)	2817(6)	695(1)	90(2)
O(10)	5358(4)	−1610(3)	747(2)	130(1)
C(6)	4921(3)	5245(3)	762(1)	66(1)
C(12)	6241(3)	1182(4)	1146(1)	78(1)
C(15)	5419(5)	−1082(4)	295(2)	104(2)
C(16)	5672(5)	−853(6)	1105(2)	111(2)
C(21)	1641(3)	3616(3)	336(1)	68(1)

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Table S2. Bond lengths [Å] and angles [°] for **2**

O(4)-C(19)	1.317(4)	C(20)-C(9)-C(10)	114.2(2)
O(4)-C(21)	1.437(3)	C(8)-C(9)-C(10)	108.9(2)
O(5)-C(19)	1.205(3)	C(2)-C(1)-C(10)	112.4(2)
C(2)-C(3)	1.315(4)	C(6)-C(5)-C(18)	109.3(2)
C(2)-C(1)	1.486(4)	C(6)-C(5)-C(10)	110.2(3)
C(19)-C(4)	1.533(4)	C(18)-C(5)-C(10)	112.6(2)
C(9)-C(11)	1.528(5)	C(6)-C(5)-C(4)	110.1(2)
C(9)-C(20)	1.536(4)	C(18)-C(5)-C(4)	107.1(3)
C(9)-C(8)	1.541(4)	C(10)-C(5)-C(4)	107.5(2)
C(9)-C(10)	1.558(4)	C(17)-O(1)-C(12)	123.5(3)
O(6)-C(4)	1.432(4)	C(1)-C(10)-C(9)	113.3(2)
C(1)-C(10)	1.530(3)	C(1)-C(10)-C(5)	110.6(2)
C(5)-C(6)	1.535(4)	C(9)-C(10)-C(5)	116.6(2)
C(5)-C(18)	1.549(4)	C(17)-C(8)-C(7)	114.3(3)
C(5)-C(10)	1.565(4)	C(17)-C(8)-C(9)	111.0(3)
C(5)-C(4)	1.570(4)	C(7)-C(8)-C(9)	113.6(3)
O(1)-C(17)	1.344(6)	C(9)-C(11)-C(12)	113.4(3)
O(1)-C(12)	1.451(5)	C(2)-C(3)-C(4)	124.1(3)
C(8)-C(17)	1.493(6)	O(6)-C(4)-C(3)	106.5(3)
C(8)-C(7)	1.529(6)	O(6)-C(4)-C(19)	105.3(2)
C(11)-C(12)	1.531(5)	C(3)-C(4)-C(19)	109.9(2)
C(3)-C(4)	1.494(4)	O(6)-C(4)-C(5)	110.2(2)
C(13)-C(16)	1.342(7)	C(3)-C(4)-C(5)	111.5(2)
C(13)-C(14)	1.393(6)	C(19)-C(4)-C(5)	113.1(2)
C(13)-C(12)	1.494(6)	C(16)-C(13)-C(14)	106.1(5)
C(7)-C(6)	1.507(6)	C(16)-C(13)-C(12)	126.3(4)
O(2)-C(17)	1.214(5)	C(14)-C(13)-C(12)	127.5(4)
C(14)-C(15)	1.326(7)	C(6)-C(7)-C(8)	109.6(3)
O(10)-C(15)	1.342(7)	C(15)-C(14)-C(13)	107.3(4)
O(10)-C(16)	1.356(7)	O(2)-C(17)-O(1)	117.6(4)
C(19)-O(4)-C(21)	117.5(2)	O(2)-C(17)-C(8)	123.5(6)
C(3)-C(2)-C(1)	124.1(3)	O(1)-C(17)-C(8)	118.9(4)
O(5)-C(19)-O(4)	123.0(3)	C(15)-O(10)-C(16)	106.3(4)
O(5)-C(19)-C(4)	123.6(3)	C(7)-C(6)-C(5)	113.1(3)
O(4)-C(19)-C(4)	113.4(2)	O(1)-C(12)-C(13)	106.6(3)
C(11)-C(9)-C(20)	109.8(3)	O(1)-C(12)-C(11)	115.0(4)
C(11)-C(9)-C(8)	103.6(2)	C(13)-C(12)-C(11)	112.5(3)
C(20)-C(9)-C(8)	111.5(2)	C(14)-C(15)-O(10)	110.4(5)
C(11)-C(9)-C(10)	108.1(2)	C(13)-C(16)-O(10)	109.9(4)

Symmetry transformations used to generate equivalent atoms

Table S3. Anisotropic displacement parameters ($Å^2$x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(4)	69(1)	50(1)	53(1)	3(1)	−18(1)	−9(1)
O(5)	95(2)	63(1)	61(1)	13(1)	−22(1)	−3(1)
C(2)	60(2)	60(2)	37(1)	−7(1)	13(1)	3(1)
C(19)	54(2)	51(2)	43(1)	3(1)	1(1)	−1(1)
C(9)	33(1)	88(2)	35(1)	−9(1)	−1(1)	−5(1)
O(6)	123(2)	44(1)	73(1)	−6(1)	−14(2)	−7(1)
C(1)	49(2)	57(2)	40(1)	3(1)	8(1)	0(1)
C(5)	53(2)	59(2)	35(1)	−1(1)	−1(1)	−20(1)
O(1)	41(1)	150(3)	96(2)	−35(2)	12(1)	15(2)
C(10)	35(1)	59(2)	32(1)	−3(1)	1(1)	-6(1)
C(8)	39(2)	114(3)	36(1)	−12(2)	3(1)	−19(2)
C(11)	39(2)	87(2)	53(2)	−9(2)	0(1)	13(2)
C(3)	62(2)	64(2)	41(1)	−8(1)	5(1)	10(2)
C(4)	67(2)	42(2)	45(1)	−3(1)	−4(1)	−6(1)
C(13)	62(2)	97(3)	58(2)	11(2)	5(2)	47(2)
C(7)	59(2)	128(3)	44(2)	3(2)	8(2)	−39(2)
C(20)	42(2)	134(3)	44(2)	−10(2)	−7(1)	−7(2)
O(2)	55(2)	211(4)	92(2)	−36(2)	37(2)	−28(2)
C(18)	89(3)	78(2)	48(2)	−8(2)	−5(2)	−39(2)
C(14)	118(4)	82(3)	77(3)	8(2)	0(2)	32(3)
C(17)	47(2)	173(5)	52(2)	−38(3)	11(2)	−4(3)
O(10)	149(3)	99(3)	142(3)	26(3)	40(3)	40(2)
C(6)	69(2)	82(2)	46(2)	7(2)	4(2)	−33(2)
C(12)	49(2)	129(4)	57(2)	−8(2)	−4(2)	34(2)
C(15)	133(4)	69(3)	111(4)	−17(3)	−10(3)	28(3)
C(16)	118(4)	125(4)	89(3)	27(3)	33(3)	52(3)
C(21)	73(2)	68(2)	62(2)	−4(2)	−24(2)	−11(2)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **2**

	x	y	z	U(eq)
H(2)	2379	4068	2310	63
H(6)	2917	6874	986	120
H(1A)	3696	2798	1989	59
H(1B)	4404	3792	2207	59
H(10)	3841	3439	1180	50
H(8)	5411	3191	557	75
H(11A)	4656	1800	1023	72
H(11B)	4914	1631	1604	72
H(3)	1813	5408	1804	67
H(7A)	6558	5037	973	92
H(7B)	6371	4859	384	92
H(20A)	6035	3130	2083	110
H(20B)	6590	4087	1762	110
H(20C)	6996	2850	1697	110
H(18A)	5725	5516	1732	108
H(18B)	4583	5712	2012	108
H(18C)	4976	6542	1584	108
H(14)	5861	494	103	111
H(6A)	4441	4940	497	79
H(6B)	4990	6042	702	79
H(12)	6613	977	1466	94
H(15)	5248	-1405	-19	125
H(16)	5705	-991	1454	133
H(21A)	941	4001	306	102
H(21B)	1507	2829	374	102
H(21C)	2078	3743	33	102

Table S5. Theoretical and Experimental NMR Chemical Shifts for **2**

Position	8-*epi*-cordatin (**2**) calculated[a]		8-*epi*-cordatin (**2**) experimental	
	δ_C	δ_H	δ_C	δ_H
1	28.0	1.95	22.9	2.1
2	137.6	6.14	130.0	5.95
3	139.5	5.71	128.7	5.36
4	88.8		81.2	
5	46.7		40.5	
6	37.0	α - 1.87 β - 0.71	33.2	α - 1.86 β - 0.91
7	22.5	α - 1.43 β - 2.22	18.1	α - 1.60 β - 2.10
8	57.7	1.90	51.4	2.07
9	40.7		36.4	
10	50.1	2.28	44.7	2.33
11	51.3	α - 1.79 β - 1.54	44.4	α - 2.29 β - 1.67
12	77.0	5.26	71.9	5.48
13	131.5		125.8	
14	113.2	6.57	108.5	6.41
15	149.5	7.45	143.7	7.41
16	146.4	7.26	139.3	7.44
17	177.1		171.9	
18	17.5	1.15	15.2	1.12
19	187.7		175.5	
20	18.7	1.04	15.4	1.17
21	59.4	3.66	53.2	3.81

[a] NMR chemical shifts calculated at B3PW91/DGDZVP.

Table S6. Predicted, calculated and Experimental ^{1}H NMR coupling constant [^nJ(H-H)] (Hz) for **2**

Coupling	experimental	B3PW91/ DGDZVP	Predicted[a]
2 - 1α	2.9	3.2	2.9
2 - 1β	4.6	5.3	4.8
2 - 3	10	10.5	9.7
3 - 1α	1.8	4.5	4.2
3 - 1β	2.5	3.2	2.9
6α - 6β	13.3	16.5	15.3
6α - 7α	2.7	3.2	2.9
6α - 7β	2.7	3.2	2.9
6β - 7α	13.3	12.7	11.7
6β - 7α	3.0	4.1	3.8
10 - 1α	11.0	10.4	9.6
10 - 1β	5.2	5.2	4.8
11α - 11β	13.6	16.2	15.0
11α - 12	5.4	4.8	4.4
12 - 11β	11.7	12.1	11.2
14 - 15	1.9	1.4	1.3
14 - 16	0.9	0.1	0.0
15 - 16	1.9	0.9	0.8

[a]Predicted after linear regression using the equation: $J_{calcd} = a + bJ_{expt}$.

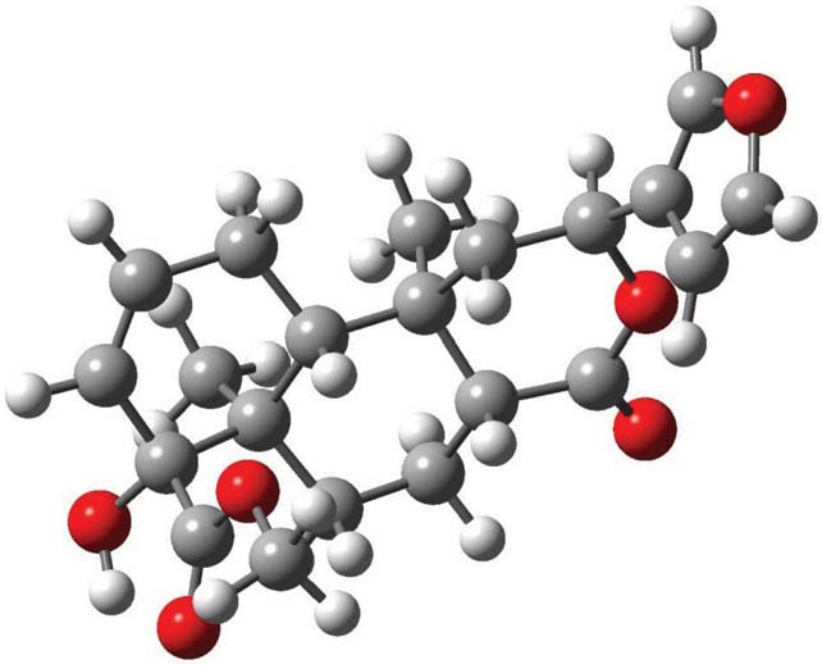

Figure S1. B3LYP/6-31G(*d,p*) optimized structure of **2**.

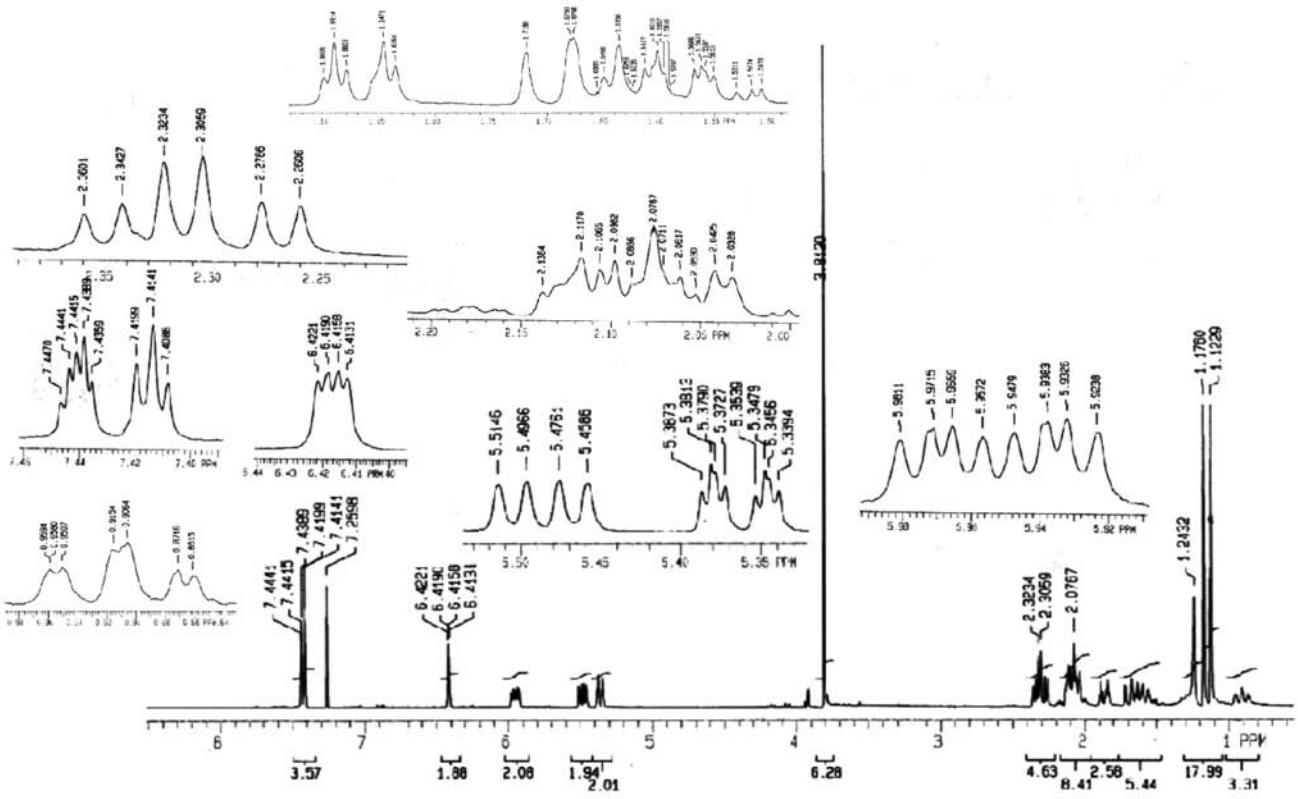

Figure S2. ^{1}H NMR (300 MHz, $CDCl_3$) of the new compound **2**.

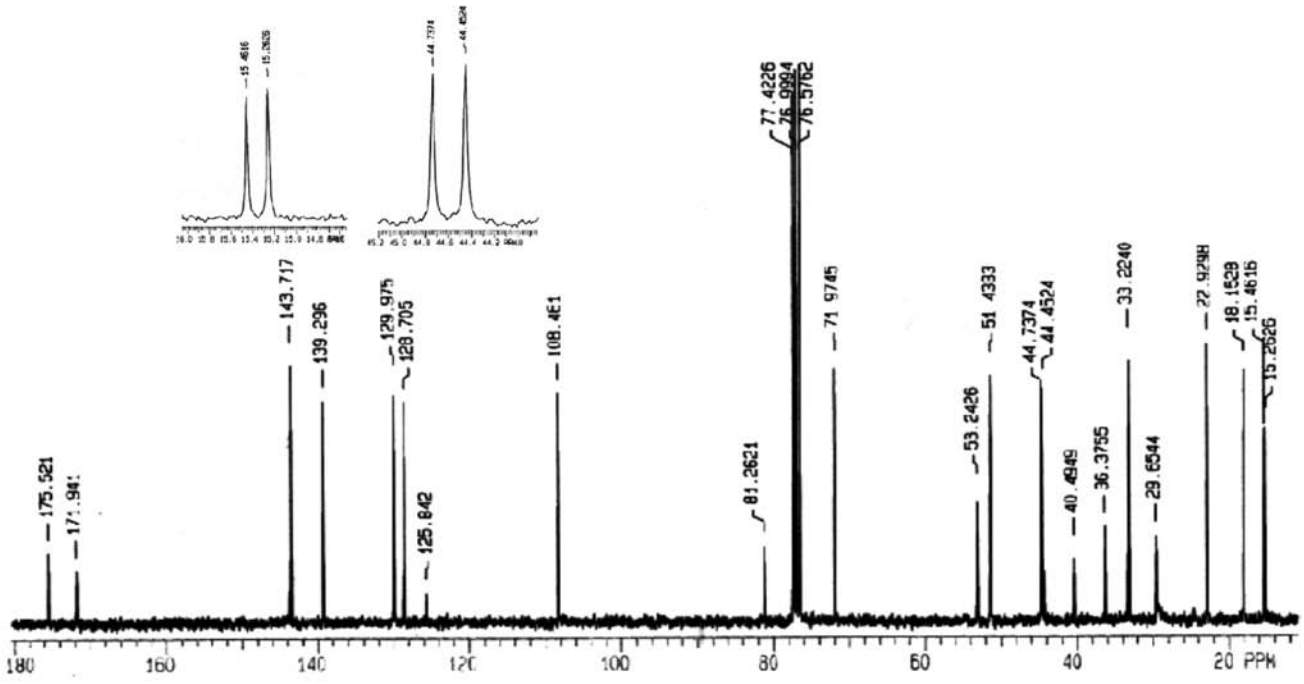

Figure S3. ^{13}C NMR (75.4 MHz, $CDCl_3$) of the new compound **2**.

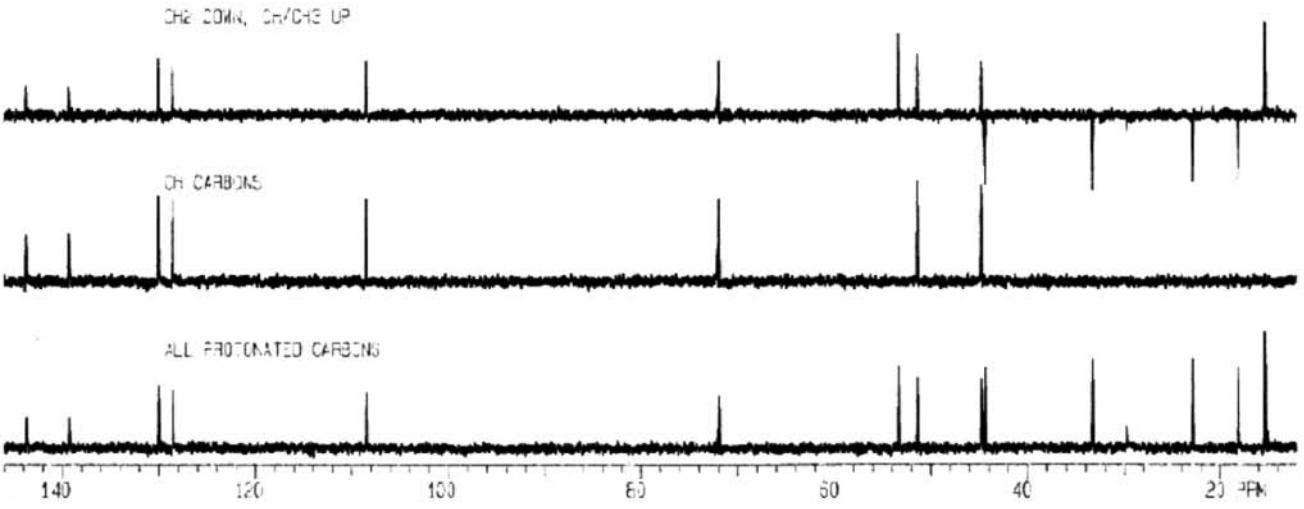

Figure S4. DEPT spectrum of the new compound **2**.

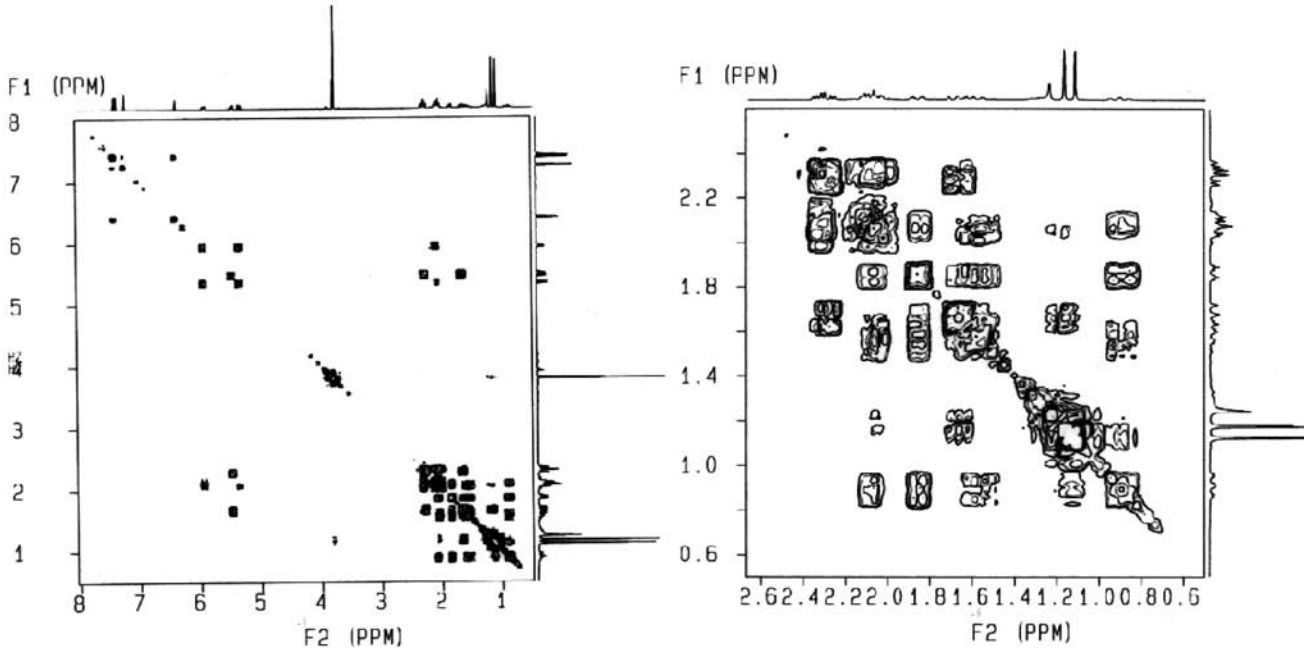

Figure S5. ^{1}H, ^{1}H- COSY spectrum of the new compound **2**.

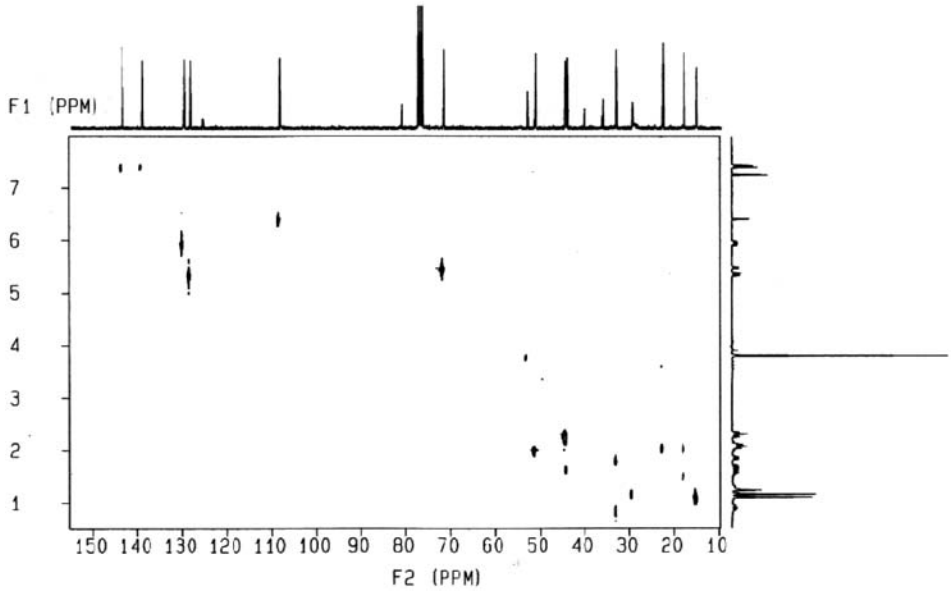

Figure S6. HETCOR spectrum of the new compound **2**.

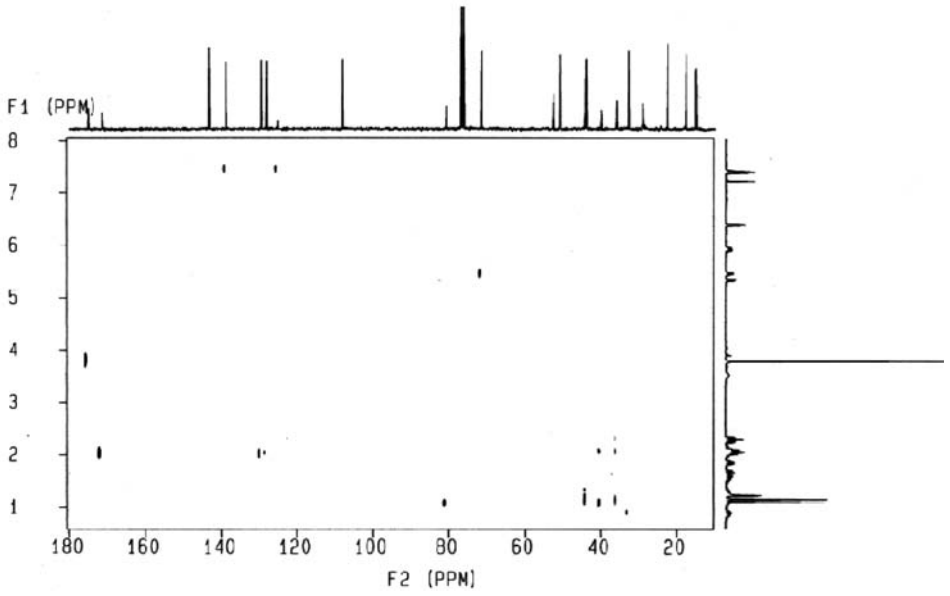

Figure S7. COLOC spectrum of the new compound **2**.

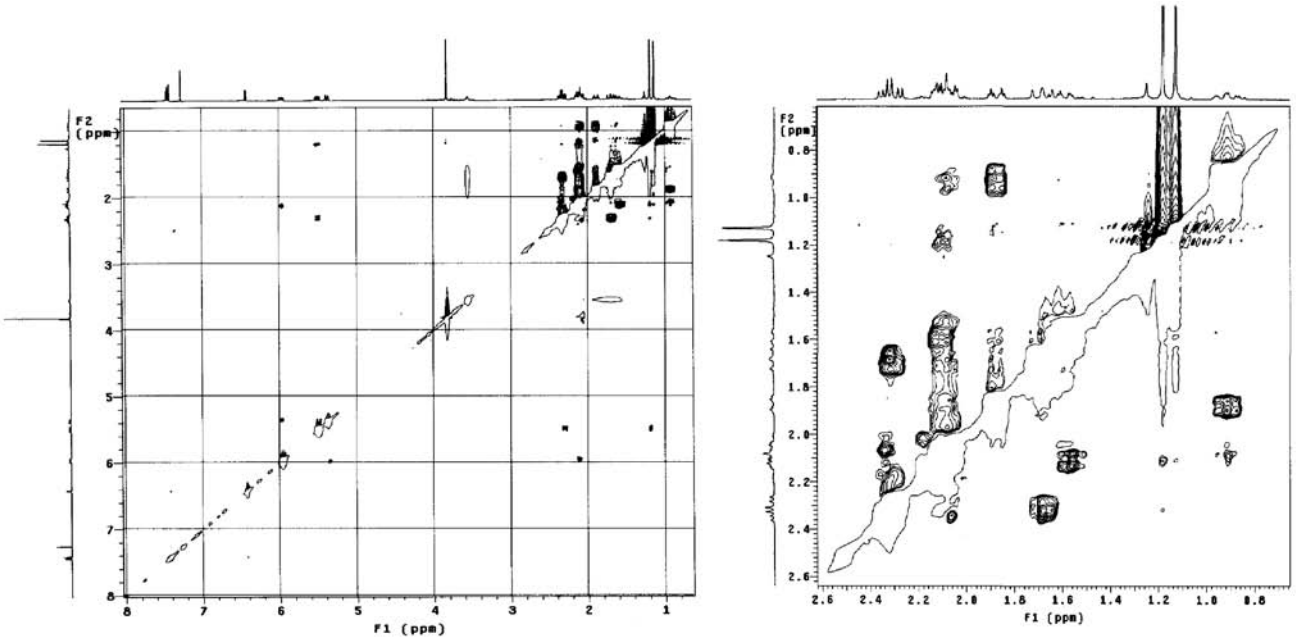

Figure S8. NOESY spectrum of the new compound **2**.

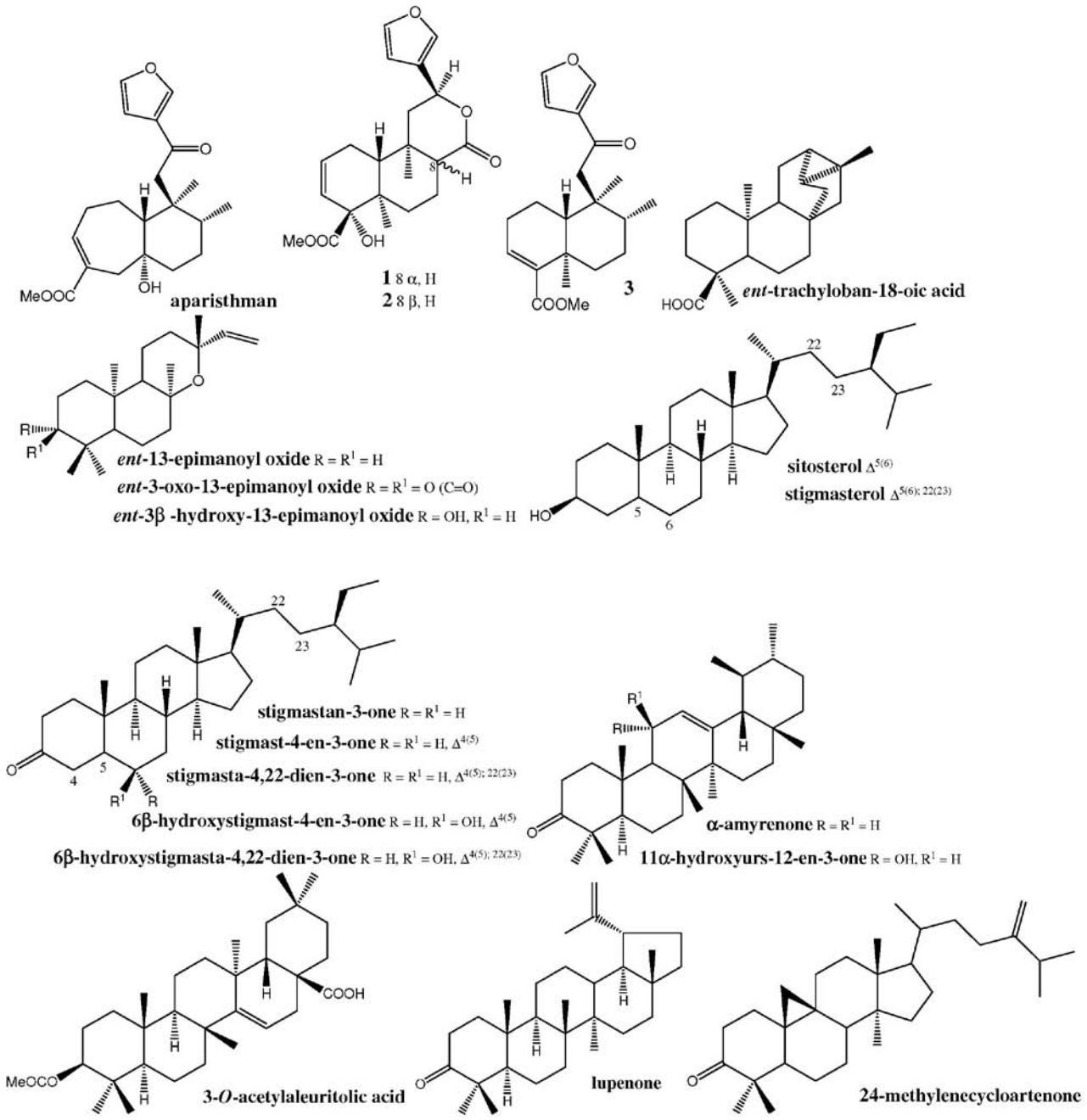

Figure S9. Structures of all identified compounds.