Supporting Information

Insights into the Structural Diversity of Cembranoids and Their Bioactivity from *Sarcophyton glaucum*

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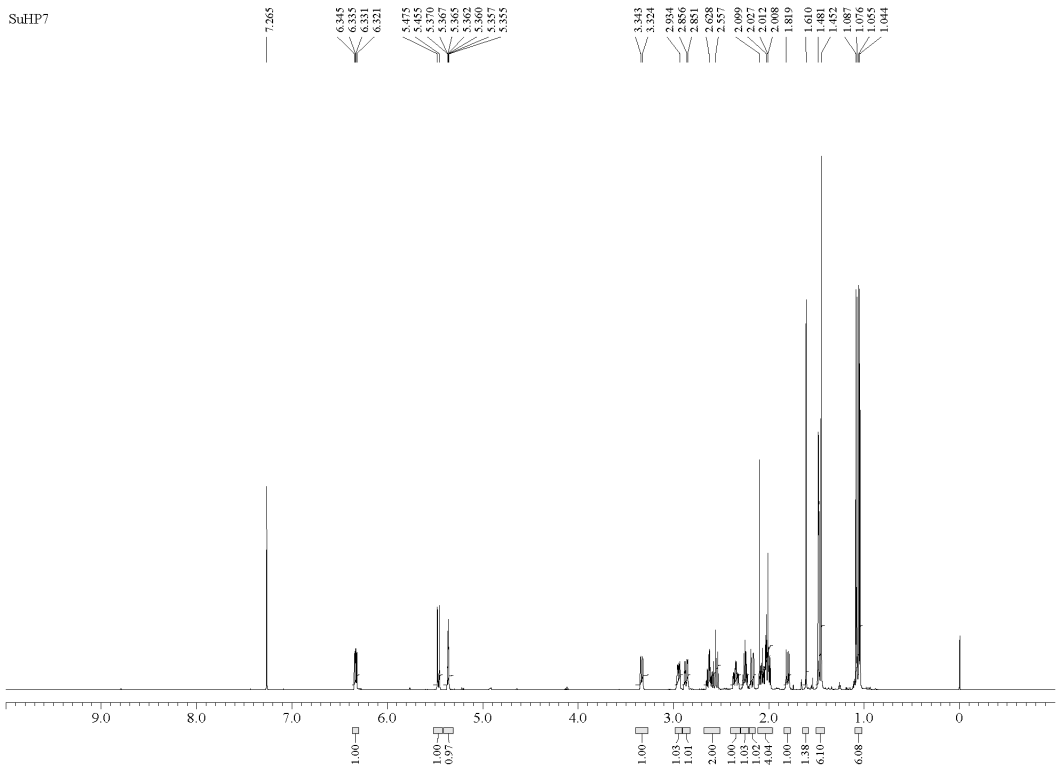

Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$ at 600 MHz

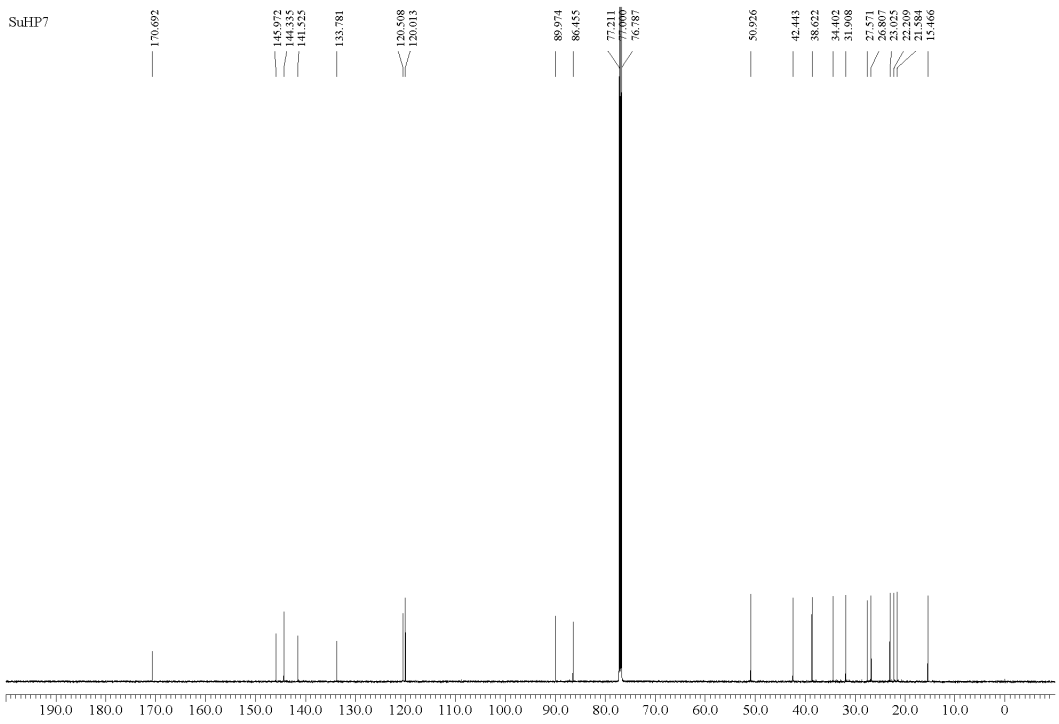

Figure S2. ^{13}C NMR spectrum of **1** in $CDCl_3$ at 150 MHz

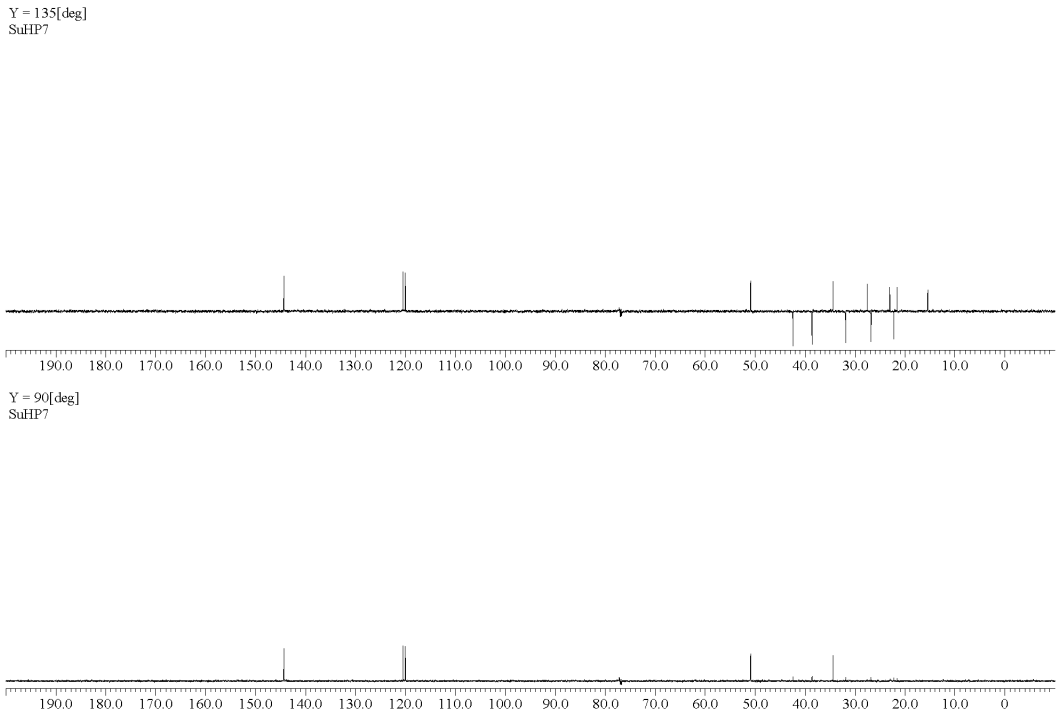

Figure S3. DEPT spectrum of **1**

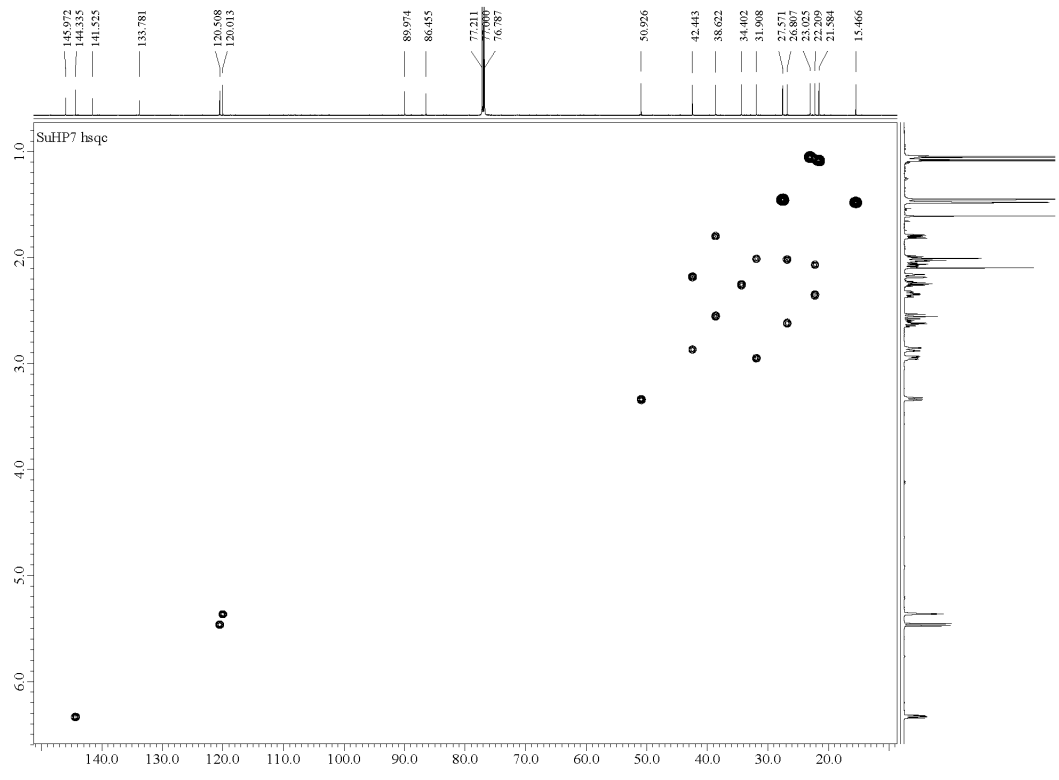

Figure S4. HSQC spectrum of **1**

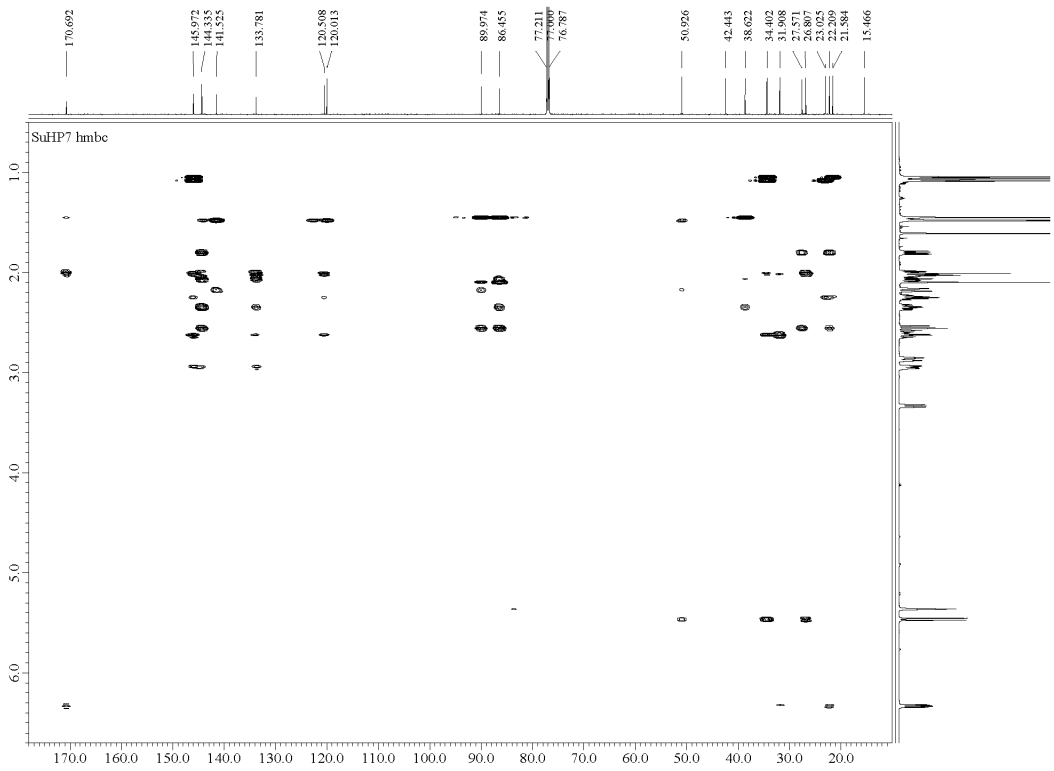

Figure S5. HMBC spectrum of **1**

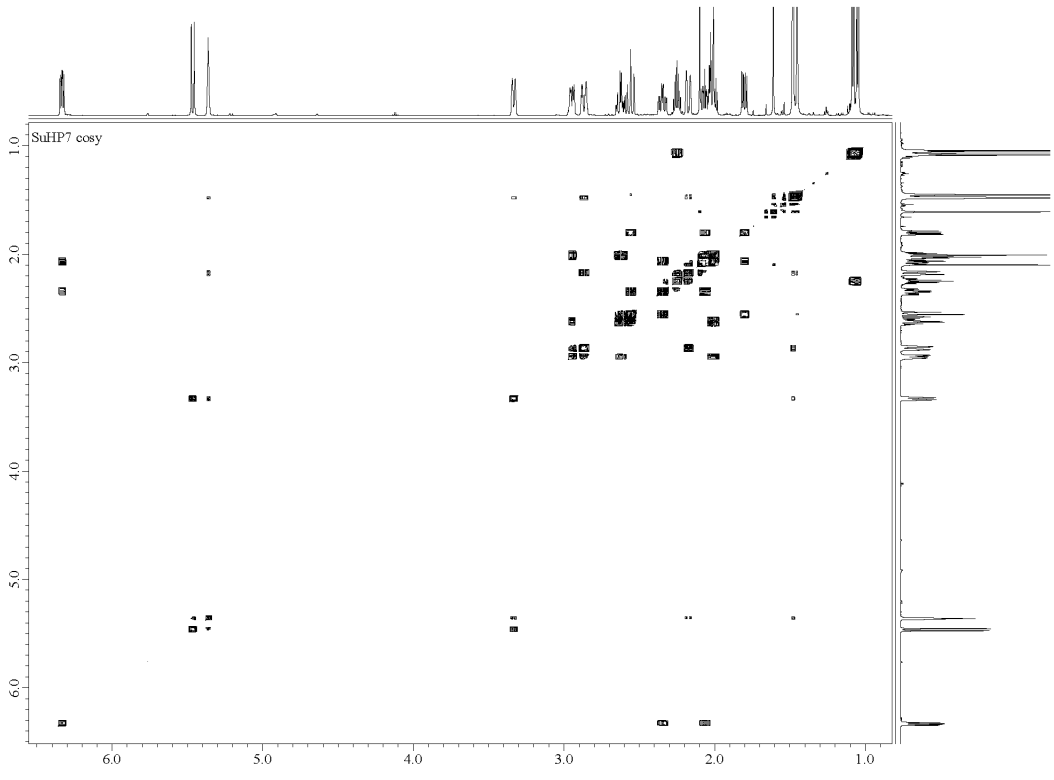

Figure S6. COSY spectrum of **1**

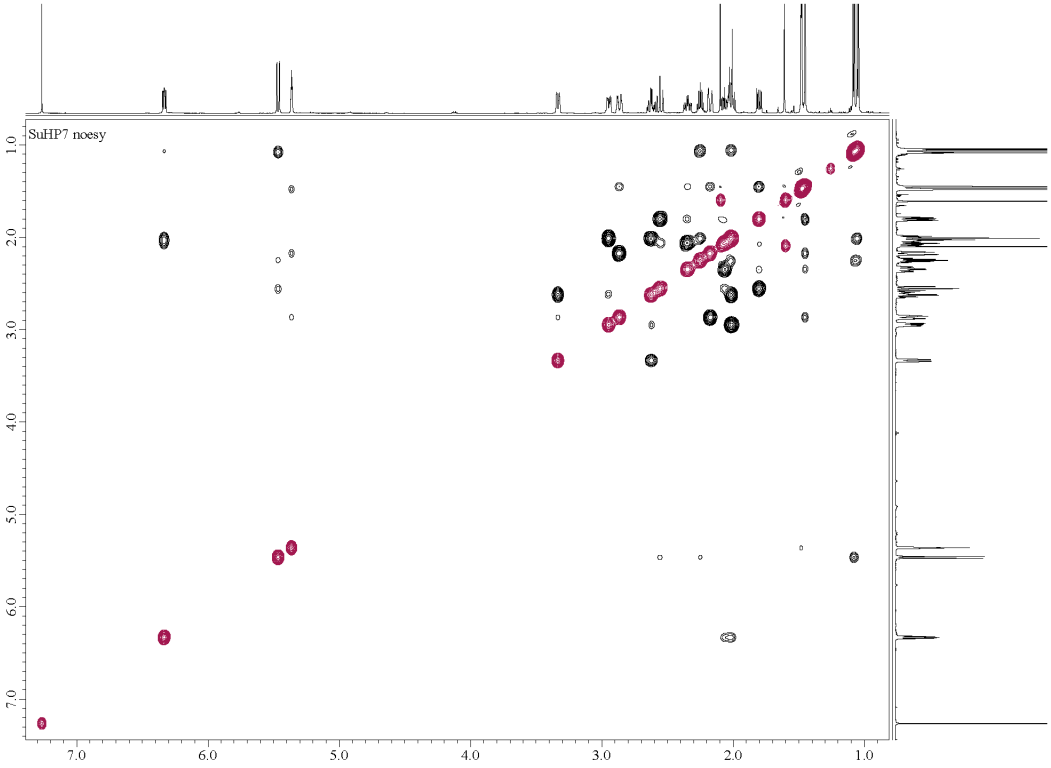

Figure S7. NOESY spectrum of **1**

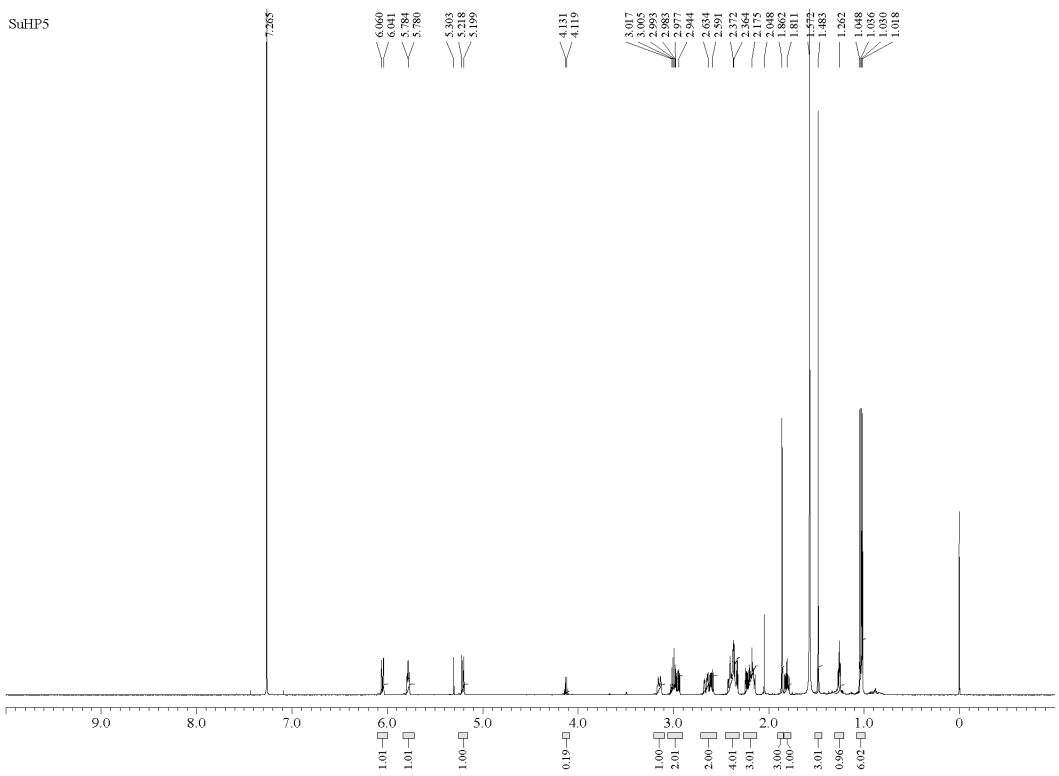

Figure S8. ^{1}H NMR spectrum of **4** in $CDCl_3$ at 600 MHz

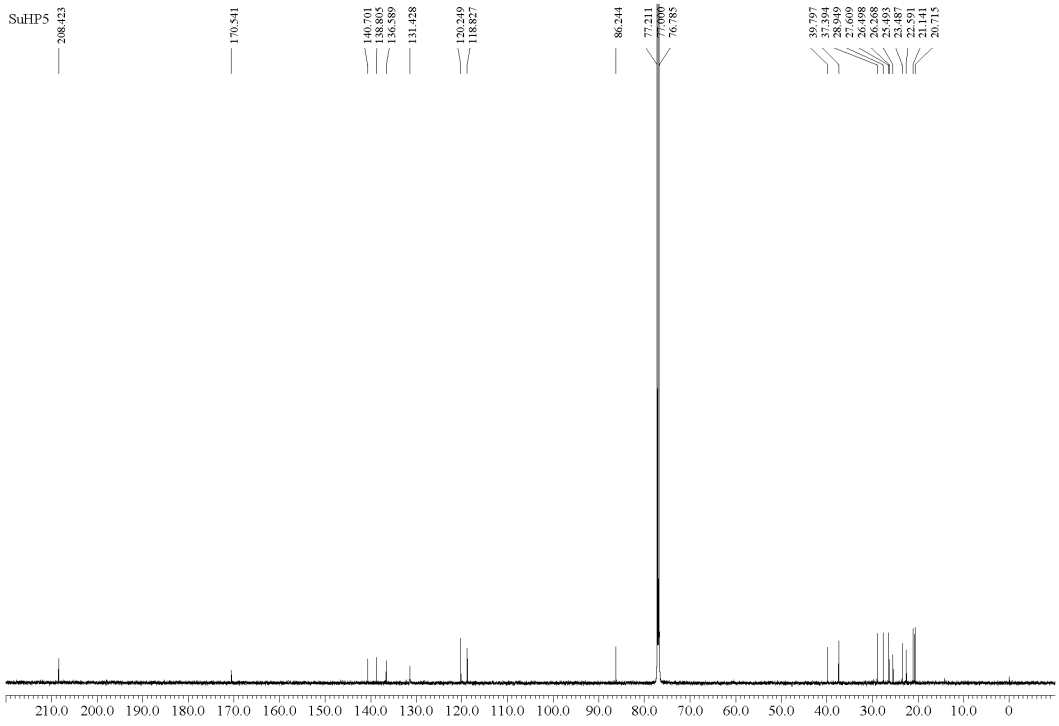

Figure S9. ^{13}C NMR spectrum of **4** in $CDCl_3$ at 150 MHz

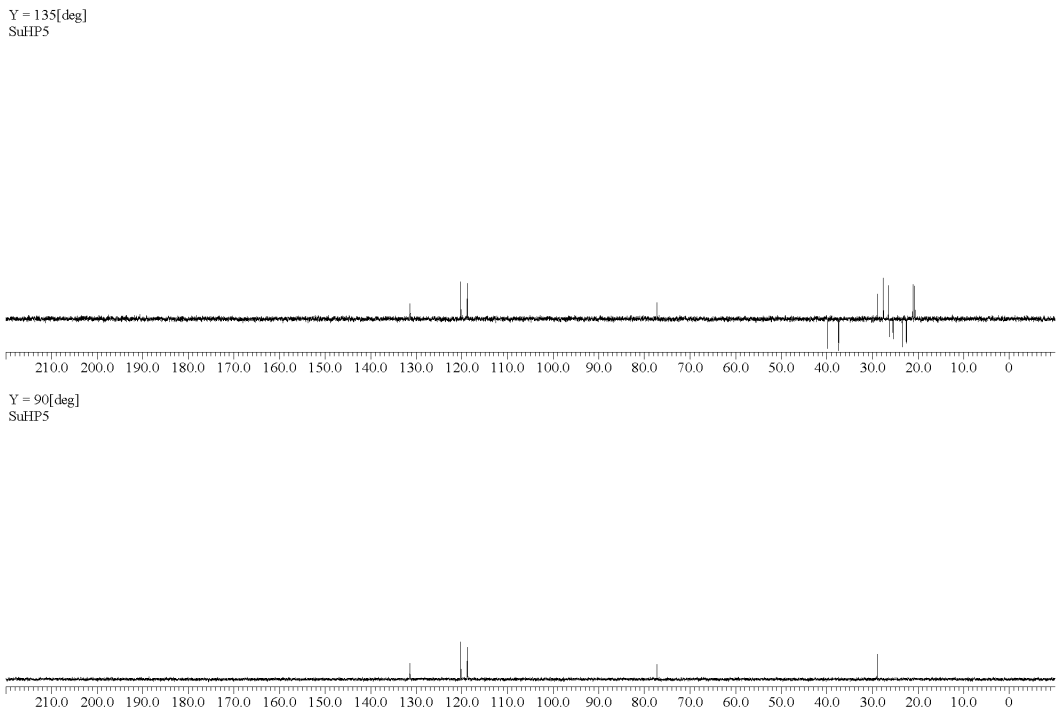

Figure S10. DEPT spectrum of **4**

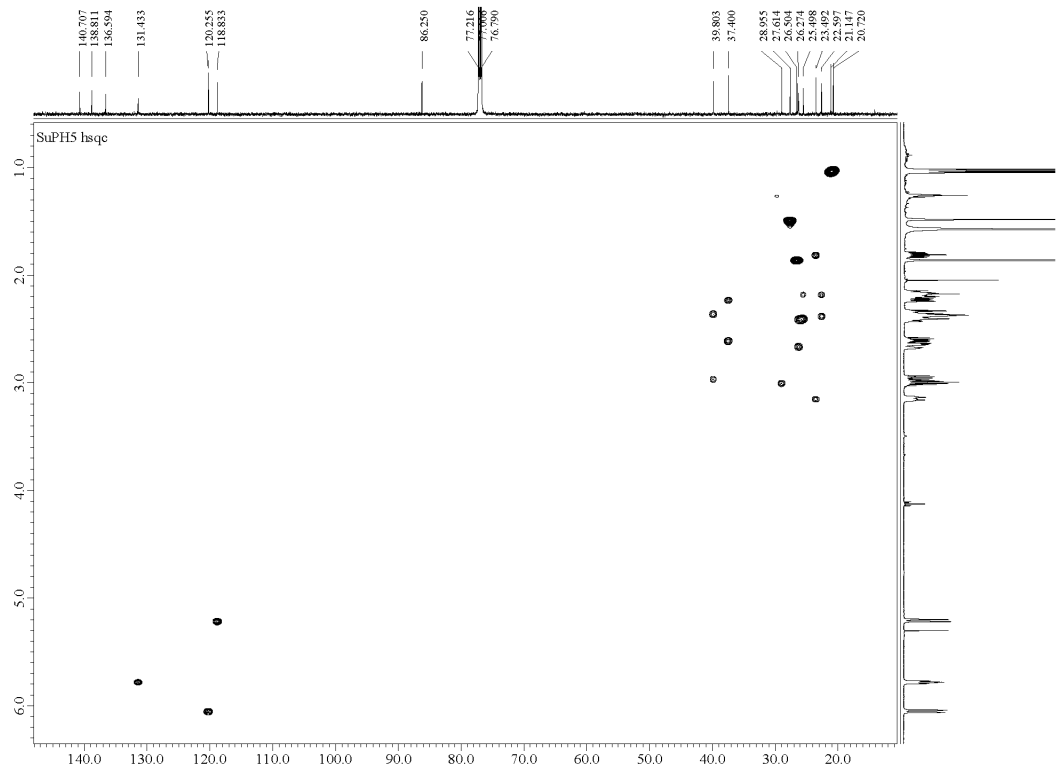

Figure S11. HSQC spectrum of **4**

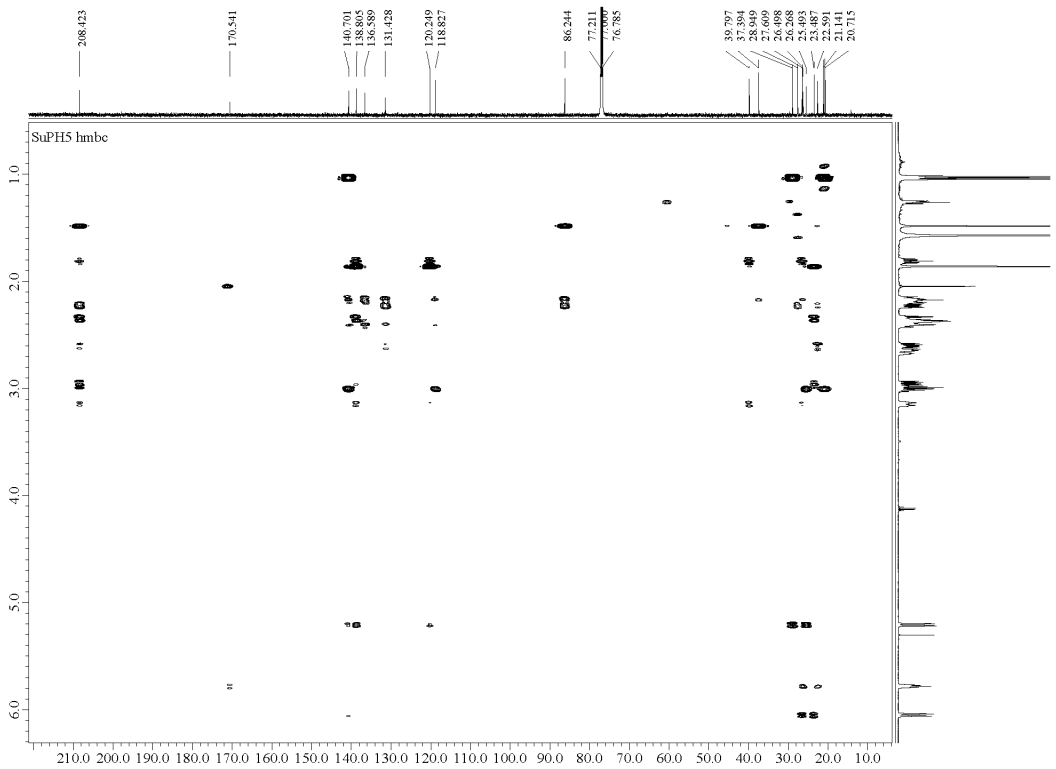

Figure S12. HMBC spectrum of **4**

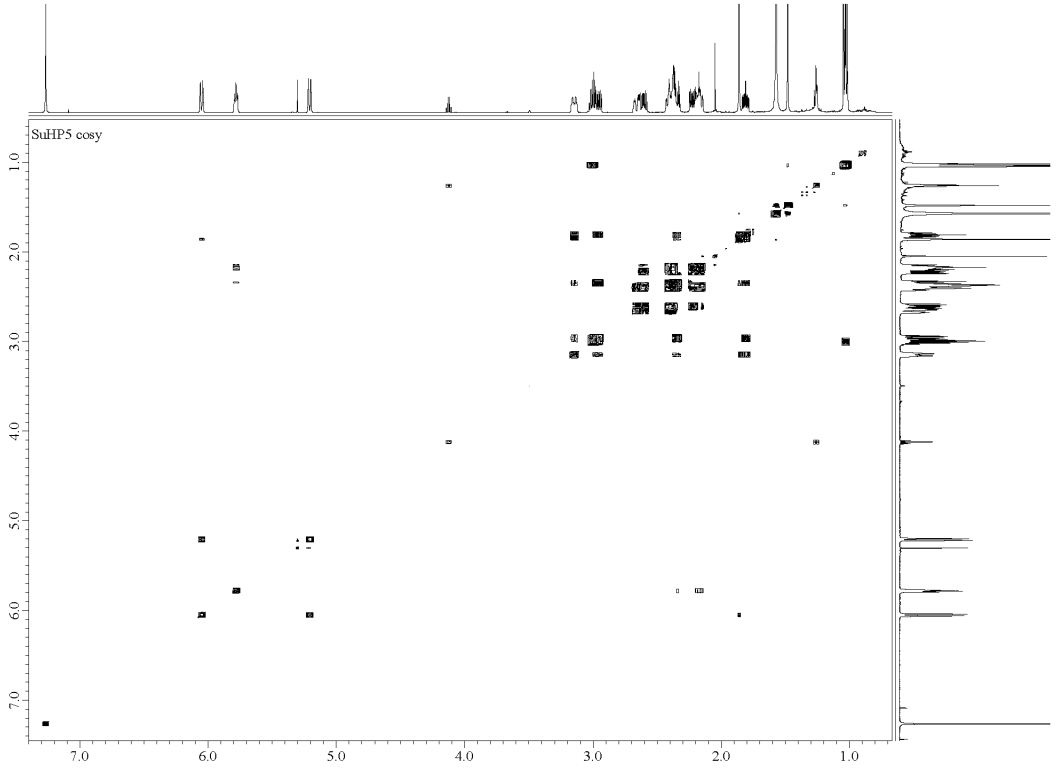

Figure S13. COSY spectrum of **4**

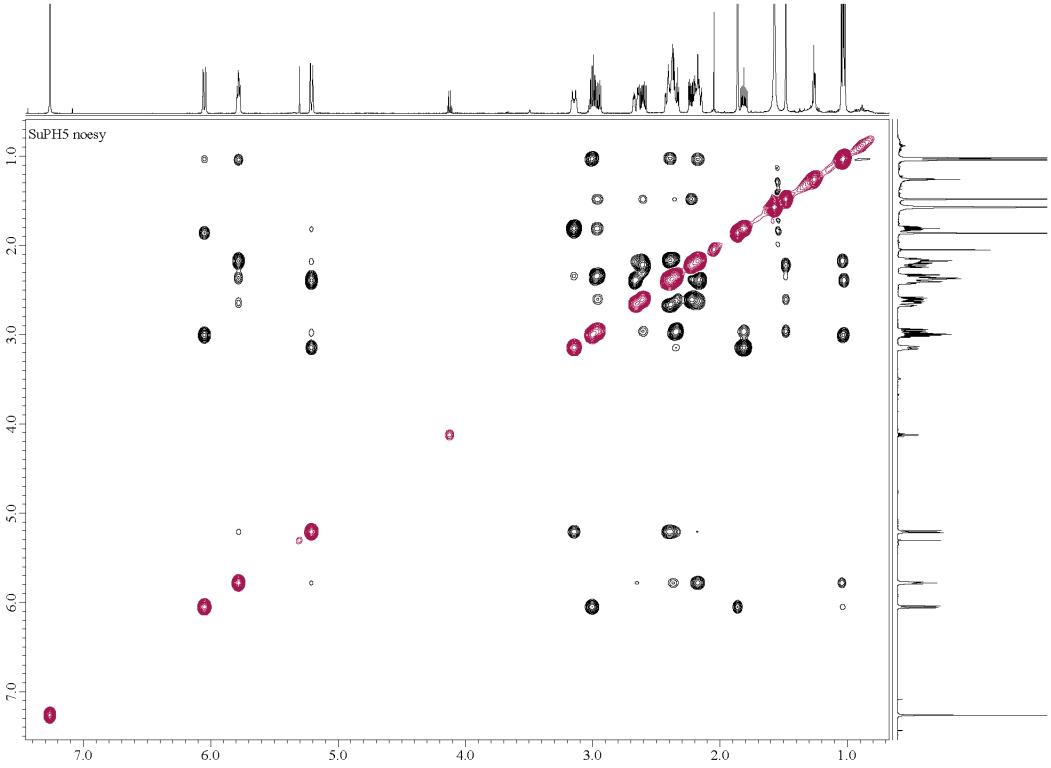

Figure S14. NOESY spectrum of **4**

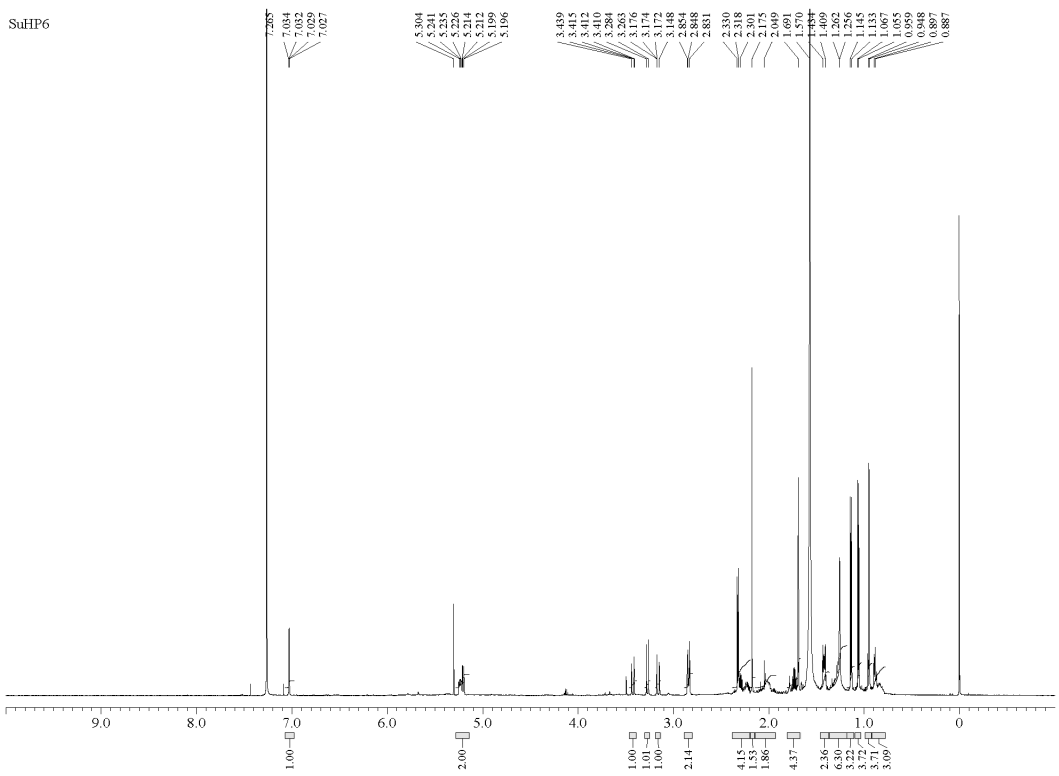

Figure S15. ^{1}H NMR spectrum of **7** in $CDCl_3$ at 600 MHz

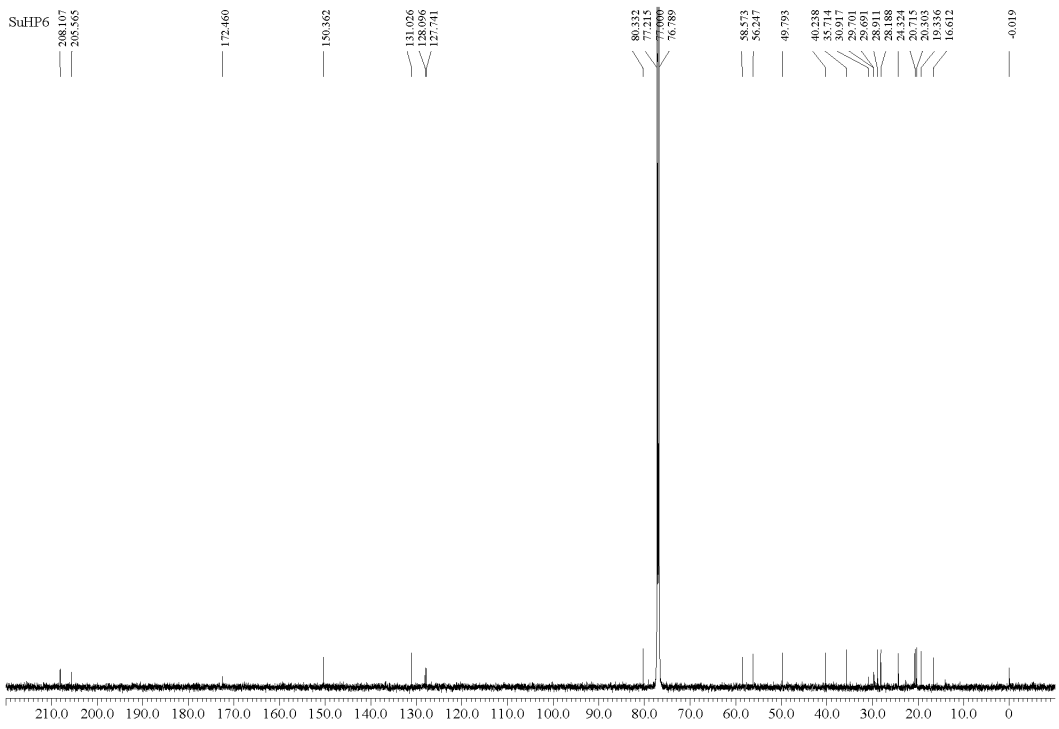

Figure S16. ^{13}C NMR spectrum of **7** in $CDCl_3$ at 150 MHz

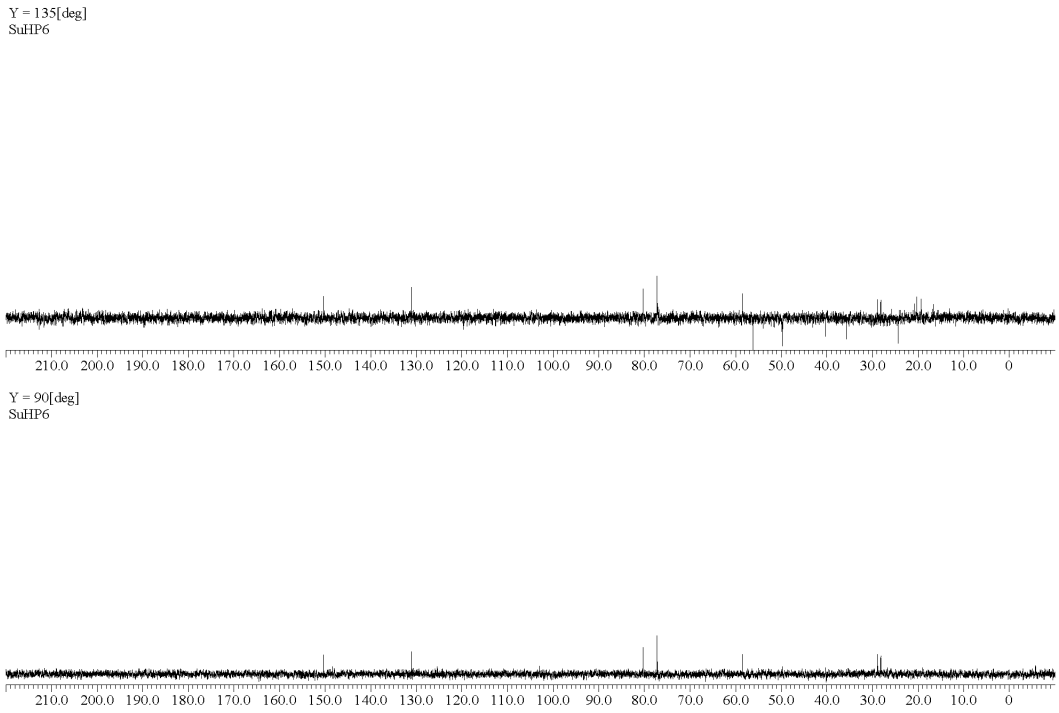

Figure S17. DEPT spectrum of **7**

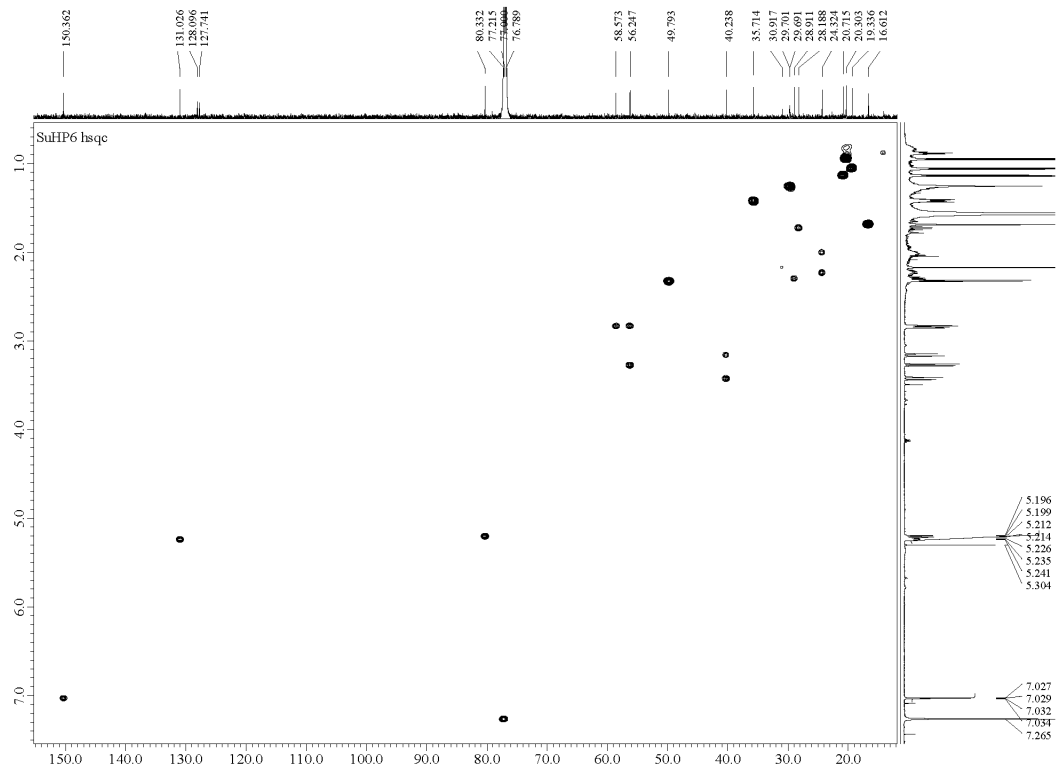

Figure S18. HSQC spectrum of **7**

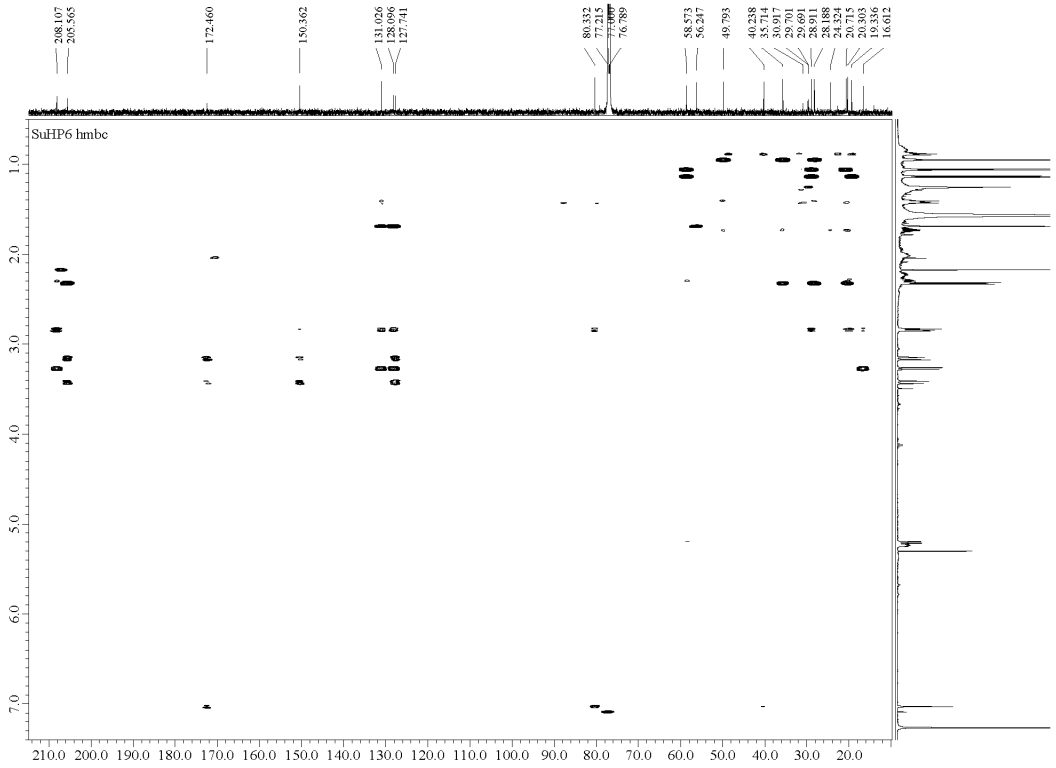

Figure S19. HMBC spectrum of **7**

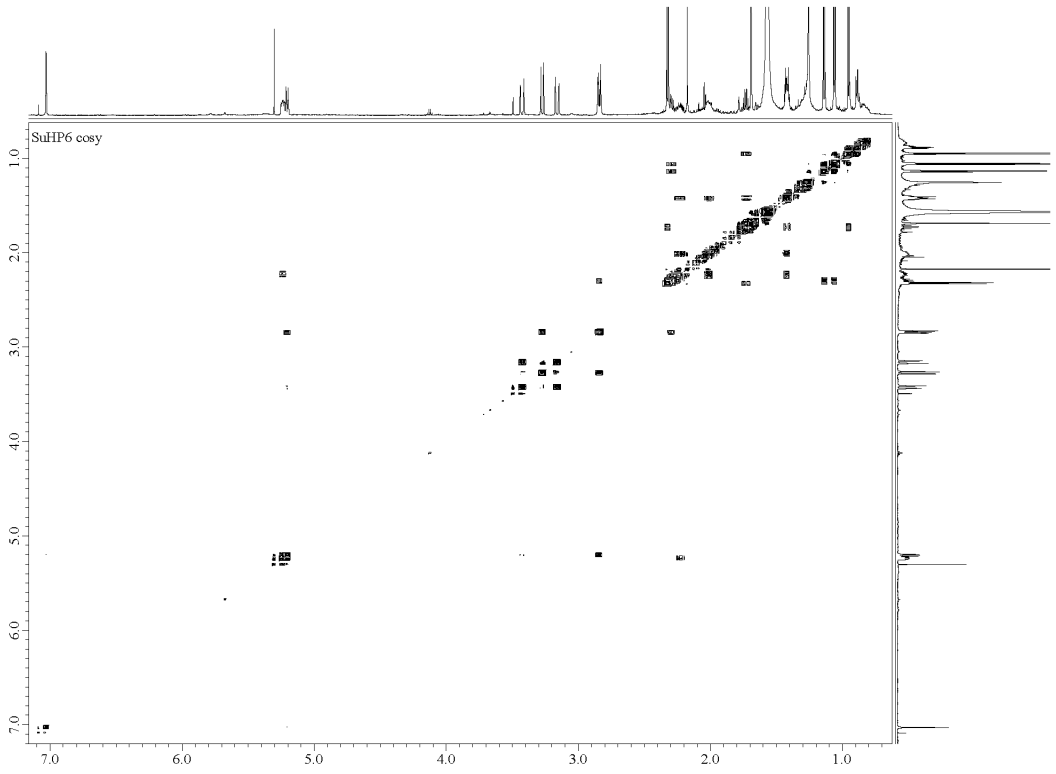

Figure S20. COSY spectrum of **7**

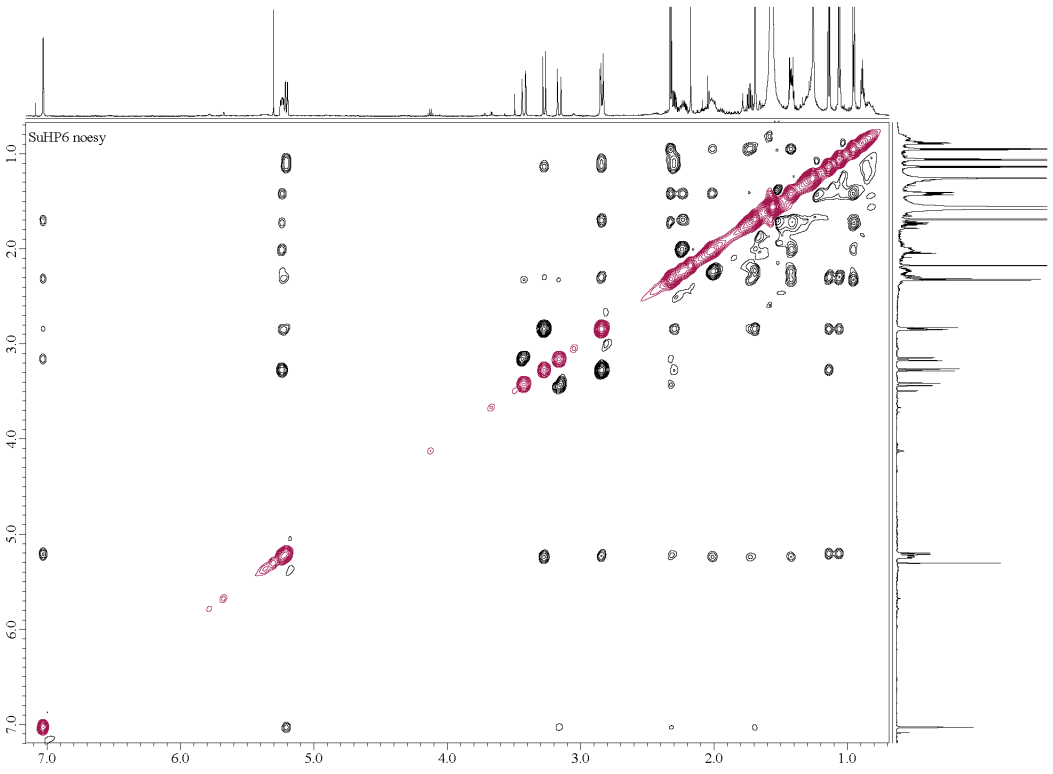

Figure S21. NOESY spectrum of **7**

Table S1. Crystal data and structure refinement for **1** (ic22957).

Identification code	ic22957	
Empirical formula	C20 H28 O3	
Formula weight	316.42	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.9787(4) Å	a= 90°.
	b = 11.8275(4) Å	b= 90°.
	c = 13.8005(5) Å	g = 90°.
Volume	1792.00(11) $Å^3$	
Z	4	
Density (calculated)	1.173 Mg/m^3	
Absorption coefficient	0.609 mm^{-1}	
F(000)	688	
Crystal size	0.330 x 0.289 x 0.110 mm^3	
Theta range for data collection	4.924 to 74.417°.	
Index ranges	-13<=h<=13, -13<=k<=14, -17<=l<=16	
Reflections collected	18753	
Independent reflections	3646 [R(int) = 0.0333]	
Completeness to theta = 67.679°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9288 and 0.7389	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3646 / 0 / 216	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0859	
R indices (all data)	R1 = 0.0326, wR2 = 0.0866	
Absolute structure parameter	0.16(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.207 and -0.145 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **1** (ic22957). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8480(1)	4857(1)	8120(1)	34(1)
O(2)	9905(1)	6768(1)	6343(1)	31(1)
O(3)	9629(1)	8556(1)	6021(1)	38(1)
C(1)	6094(2)	7272(2)	7032(1)	32(1)
C(2)	6782(1)	6584(2)	7570(1)	31(1)
C(3)	8050(1)	6834(1)	7916(1)	28(1)
C(4)	8170(2)	7137(2)	8984(1)	34(1)
C(5)	9255(2)	6835(2)	9315(1)	37(1)
C(6)	10008(2)	6270(2)	8540(1)	34(1)
C(7)	9027(1)	5888(1)	7806(1)	28(1)
C(8)	9520(2)	5674(1)	6759(1)	30(1)
C(9)	8611(2)	4999(2)	6126(1)	36(1)
C(10)	8567(2)	5416(2)	5075(1)	41(1)
C(11)	7784(2)	6444(2)	5053(1)	37(1)
C(12)	8003(2)	7397(2)	5539(1)	31(1)
C(13)	7075(2)	8325(2)	5623(1)	37(1)
C(14)	6540(2)	8403(2)	6661(1)	35(1)
C(15)	4806(2)	6976(2)	6715(2)	44(1)
C(16)	4589(2)	5725(2)	6533(2)	66(1)
C(17)	3876(2)	7468(4)	7408(3)	91(1)
C(18)	7194(2)	7762(2)	9512(2)	47(1)
C(19)	10726(2)	5039(2)	6783(2)	43(1)
C(20)	9202(2)	7605(1)	5999(1)	28(1)

Table S3. Bond lengths [Å] and angles [°] for **1** (ic22957).

O(1)-C(7)	1.427(2)
O(2)-C(20)	1.342(2)
O(2)-C(8)	1.4785(19)
O(3)-C(20)	1.218(2)
C(1)-C(2)	1.336(2)
C(1)-C(14)	1.514(3)
C(1)-C(15)	1.521(2)
C(2)-C(3)	1.501(2)
C(3)-C(4)	1.523(2)
C(3)-C(7)	1.558(2)
C(4)-C(5)	1.324(3)
C(4)-C(18)	1.492(3)
C(5)-C(6)	1.508(3)
C(6)-C(7)	1.547(2)
C(7)-C(8)	1.563(2)
C(8)-C(19)	1.523(2)
C(8)-C(9)	1.548(2)
C(9)-C(10)	1.532(3)
C(10)-C(11)	1.489(3)
C(11)-C(12)	1.334(3)
C(12)-C(20)	1.482(2)
C(12)-C(13)	1.501(3)
C(13)-C(14)	1.551(3)
C(15)-C(17)	1.515(4)
C(15)-C(16)	1.519(4)
C(20)-O(2)-C(8)	128.20(13)
C(2)-C(1)-C(14)	122.91(15)
C(2)-C(1)-C(15)	123.04(17)
C(14)-C(1)-C(15)	114.02(15)
C(1)-C(2)-C(3)	125.50(16)
C(2)-C(3)-C(4)	115.75(14)
C(2)-C(3)-C(7)	117.74(14)
C(4)-C(3)-C(7)	101.76(13)
C(5)-C(4)-C(18)	127.67(18)

C(5)-C(4)-C(3)	110.37(15)
C(18)-C(4)-C(3)	121.82(16)
C(4)-C(5)-C(6)	111.62(16)
C(5)-C(6)-C(7)	102.24(14)
O(1)-C(7)-C(6)	110.12(13)
O(1)-C(7)-C(3)	107.16(13)
C(6)-C(7)-C(3)	101.86(13)
O(1)-C(7)-C(8)	106.72(13)
C(6)-C(7)-C(8)	114.33(13)
C(3)-C(7)-C(8)	116.40(13)
O(2)-C(8)-C(19)	101.02(13)
O(2)-C(8)-C(9)	114.62(14)
C(19)-C(8)-C(9)	108.57(15)
O(2)-C(8)-C(7)	108.45(13)
C(19)-C(8)-C(7)	111.15(15)
C(9)-C(8)-C(7)	112.48(13)
C(10)-C(9)-C(8)	112.87(15)
C(11)-C(10)-C(9)	107.49(15)
C(12)-C(11)-C(10)	125.13(17)
C(11)-C(12)-C(20)	121.06(17)
C(11)-C(12)-C(13)	122.30(16)
C(20)-C(12)-C(13)	116.60(15)
C(12)-C(13)-C(14)	111.81(14)
C(1)-C(14)-C(13)	112.47(15)
C(17)-C(15)-C(16)	111.9(2)
C(17)-C(15)-C(1)	110.9(2)
C(16)-C(15)-C(1)	114.64(18)
O(3)-C(20)-O(2)	116.78(15)
O(3)-C(20)-C(12)	120.39(15)
O(2)-C(20)-C(12)	122.66(14)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1** (ic22957). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	29(1)	33(1)	40(1)	11(1)	-1(1)	-2(1)
O(2)	26(1)	31(1)	34(1)	3(1)	4(1)	-5(1)
O(3)	40(1)	31(1)	42(1)	0(1)	-4(1)	-10(1)
C(1)	26(1)	41(1)	30(1)	2(1)	-1(1)	1(1)
C(2)	24(1)	36(1)	32(1)	5(1)	3(1)	-1(1)
C(3)	26(1)	32(1)	27(1)	3(1)	1(1)	2(1)
C(4)	35(1)	36(1)	30(1)	1(1)	3(1)	-3(1)
C(5)	36(1)	47(1)	29(1)	0(1)	-5(1)	-4(1)
C(6)	26(1)	38(1)	38(1)	4(1)	-5(1)	0(1)
C(7)	24(1)	29(1)	31(1)	4(1)	0(1)	0(1)
C(8)	29(1)	26(1)	35(1)	2(1)	5(1)	-1(1)
C(9)	43(1)	29(1)	37(1)	-3(1)	4(1)	-7(1)
C(10)	52(1)	38(1)	32(1)	-10(1)	4(1)	-12(1)
C(11)	41(1)	44(1)	26(1)	0(1)	-3(1)	-13(1)
C(12)	32(1)	34(1)	25(1)	5(1)	-2(1)	-7(1)
C(13)	37(1)	40(1)	36(1)	10(1)	-6(1)	-2(1)
C(14)	33(1)	35(1)	38(1)	3(1)	-7(1)	5(1)
C(15)	28(1)	56(1)	48(1)	10(1)	-8(1)	-1(1)
C(16)	46(1)	64(2)	88(2)	14(1)	-23(1)	-19(1)
C(17)	31(1)	135(3)	107(3)	-27(2)	10(1)	6(2)
C(18)	48(1)	51(1)	42(1)	-5(1)	10(1)	5(1)
C(19)	36(1)	41(1)	51(1)	3(1)	10(1)	10(1)
C(20)	30(1)	30(1)	24(1)	-1(1)	3(1)	-5(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1** (ic22957).

	x	y	z	U(eq)
H(1)	9050(20)	4440(20)	8350(20)	50(7)
H(2)	6440	5876	7749	37
H(3)	8347	7501	7537	34
H(5)	9524	6958	9960	45
H(6A)	10464	5616	8803	41
H(6B)	10589	6808	8242	41
H(9A)	8846	4191	6131	44
H(9B)	7787	5060	6412	44
H(10A)	9398	5600	4845	49
H(10B)	8223	4823	4649	49
H(11)	7073	6419	4661	44
H(13A)	6407	8184	5157	45
H(13B)	7460	9055	5452	45
H(14A)	7174	8696	7105	42
H(14B)	5855	8946	6661	42
H(15)	4675	7364	6080	53
H(16A)	3773	5617	6261	99
H(16B)	4656	5310	7145	99
H(16C)	5200	5441	6075	99
H(17A)	3059	7388	7131	136
H(17B)	4053	8271	7514	136
H(17C)	3916	7064	8027	136
H(18A)	7447	7888	10184	70
H(18B)	6441	7316	9503	70
H(18C)	7051	8492	9196	70
H(19A)	10626	4333	7147	64
H(19B)	11345	5509	7098	64
H(19C)	10983	4866	6119	64

Table S6. Crystal data and structure refinement for **2** (ic22934).

Identification code	ic22934	
Empirical formula	C20 H28 O3	
Formula weight	316.42	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.9227(3) Å	a= 90°.
	b = 11.4366(3) Å	b= 90°.
	c = 14.0387(4) Å	g = 90°.
Volume	1753.69(8) $Å^3$	
Z	4	
Density (calculated)	1.198 Mg/m^3	
Absorption coefficient	0.622 mm^{-1}	
F(000)	688	
Crystal size	0.171 x 0.142 x 0.109 mm^3	
Theta range for data collection	4.988 to 74.394°.	
Index ranges	-12<=h<=13, -13<=k<=11, -17<=l<=17	
Reflections collected	15840	
Independent reflections	3550 [R(int) = 0.0292]	
Completeness to theta = 67.679°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9154 and 0.7309	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3550 / 6 / 212	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0296, wR2 = 0.0799	
R indices (all data)	R1 = 0.0302, wR2 = 0.0804	
Absolute structure parameter	0.08(6)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.167 and -0.165 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2** (ic22934). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1532(1)	5040(1)	1774(1)	30(1)
O(2)	180(1)	6911(1)	3643(1)	26(1)
O(3)	457(1)	8738(1)	4026(1)	31(1)
C(1)	3969(2)	7468(2)	2982(1)	28(1)
C(2)	3286(1)	6783(2)	2425(1)	28(1)
C(3)	2018(1)	7048(1)	2078(1)	24(1)
C(4)	1957(2)	7387(2)	1028(1)	30(1)
C(5)	723(2)	7036(2)	642(1)	36(1)
C(6)	18(2)	6565(2)	1499(1)	30(1)
C(7)	1022(1)	6083(1)	2162(1)	24(1)
C(8)	562(1)	5800(1)	3186(1)	25(1)
C(9)	1489(2)	5073(2)	3766(1)	30(1)
C(10)	1528(2)	5421(2)	4824(1)	34(1)
C(11)	2304(2)	6489(2)	4901(1)	31(1)
C(12)	2084(1)	7502(1)	4468(1)	26(1)
C(13)	3014(2)	8472(2)	4420(1)	31(1)
C(14)	3520(2)	8612(2)	3396(1)	31(1)
C(15)	5268(2)	7143(2)	3281(2)	41(1)
C(16)	5466(2)	5846(2)	3465(2)	52(1)
C(17)	6195(2)	7619(4)	2581(3)	91(1)
C(18)	2844(2)	7922(2)	553(1)	43(1)
C(19)	-654(2)	5144(2)	3164(1)	36(1)
C(20)	884(1)	7755(1)	4018(1)	23(1)

Table S8. Bond lengths [Å] and angles [°] for **2** (ic22934).

O(1)-C(7)	1.4254(19)
O(2)-C(20)	1.3419(19)
O(2)-C(8)	1.4828(19)
O(3)-C(20)	1.2165(19)
C(1)-C(2)	1.334(2)
C(1)-C(14)	1.514(2)
C(1)-C(15)	1.526(2)
C(2)-C(3)	1.500(2)
C(3)-C(4)	1.525(2)
C(3)-C(7)	1.554(2)
C(4)-C(18)	1.326(3)
C(4)-C(5)	1.508(2)
C(5)-C(6)	1.526(3)
C(6)-C(7)	1.540(2)
C(7)-C(8)	1.557(2)
C(8)-C(19)	1.526(2)
C(8)-C(9)	1.542(2)
C(9)-C(10)	1.537(2)
C(10)-C(11)	1.491(3)
C(11)-C(12)	1.330(2)
C(12)-C(20)	1.484(2)
C(12)-C(13)	1.506(2)
C(13)-C(14)	1.548(2)
C(15)-C(17)	1.512(4)
C(15)-C(16)	1.521(3)
C(20)-O(2)-C(8)	128.69(12)
C(2)-C(1)-C(14)	123.46(15)
C(2)-C(1)-C(15)	122.53(17)
C(14)-C(1)-C(15)	113.99(15)
C(1)-C(2)-C(3)	126.02(16)
C(2)-C(3)-C(4)	113.92(13)
C(2)-C(3)-C(7)	118.60(14)
C(4)-C(3)-C(7)	102.94(13)
C(18)-C(4)-C(5)	126.48(17)

C(18)-C(4)-C(3)	124.91(17)
C(5)-C(4)-C(3)	108.60(14)
C(4)-C(5)-C(6)	105.12(14)
C(5)-C(6)-C(7)	104.13(14)
O(1)-C(7)-C(6)	110.32(13)
O(1)-C(7)-C(3)	106.97(12)
C(6)-C(7)-C(3)	101.42(13)
O(1)-C(7)-C(8)	107.74(13)
C(6)-C(7)-C(8)	113.78(13)
C(3)-C(7)-C(8)	116.33(12)
O(2)-C(8)-C(19)	100.67(12)
O(2)-C(8)-C(9)	114.74(13)
C(19)-C(8)-C(9)	108.48(14)
O(2)-C(8)-C(7)	108.17(12)
C(19)-C(8)-C(7)	111.35(13)
C(9)-C(8)-C(7)	112.82(13)
C(10)-C(9)-C(8)	112.87(14)
C(11)-C(10)-C(9)	107.36(14)
C(12)-C(11)-C(10)	125.28(15)
C(11)-C(12)-C(20)	121.62(15)
C(11)-C(12)-C(13)	122.72(15)
C(20)-C(12)-C(13)	115.64(14)
C(12)-C(13)-C(14)	111.04(13)
C(1)-C(14)-C(13)	112.50(14)
C(17)-C(15)-C(16)	111.5(2)
C(17)-C(15)-C(1)	110.85(19)
C(16)-C(15)-C(1)	114.64(17)
O(3)-C(20)-O(2)	116.65(14)
O(3)-C(20)-C(12)	121.00(14)
O(2)-C(20)-C(12)	122.20(13)

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2** (ic22934). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	26(1)	28(1)	36(1)	-11(1)	-1(1)	1(1)
O(2)	21(1)	26(1)	30(1)	-4(1)	3(1)	3(1)
O(3)	35(1)	25(1)	34(1)	-1(1)	-4(1)	7(1)
C(1)	22(1)	35(1)	28(1)	0(1)	-1(1)	-3(1)
C(2)	21(1)	32(1)	29(1)	-4(1)	3(1)	0(1)
C(3)	22(1)	27(1)	24(1)	-4(1)	2(1)	-2(1)
C(4)	31(1)	31(1)	26(1)	-3(1)	2(1)	3(1)
C(5)	35(1)	45(1)	29(1)	0(1)	-5(1)	1(1)
C(6)	24(1)	33(1)	34(1)	-3(1)	-5(1)	0(1)
C(7)	21(1)	24(1)	28(1)	-5(1)	0(1)	1(1)
C(8)	24(1)	21(1)	31(1)	-3(1)	3(1)	1(1)
C(9)	33(1)	22(1)	36(1)	2(1)	2(1)	4(1)
C(10)	41(1)	29(1)	31(1)	8(1)	3(1)	7(1)
C(11)	32(1)	36(1)	23(1)	1(1)	-2(1)	9(1)
C(12)	26(1)	29(1)	22(1)	-3(1)	-1(1)	3(1)
C(13)	30(1)	34(1)	30(1)	-6(1)	-5(1)	-1(1)
C(14)	29(1)	30(1)	32(1)	-1(1)	-5(1)	-6(1)
C(15)	25(1)	48(1)	50(1)	-9(1)	-8(1)	0(1)
C(16)	38(1)	58(1)	59(1)	-10(1)	-12(1)	15(1)
C(17)	25(1)	118(3)	128(3)	45(2)	12(1)	-2(1)
C(18)	41(1)	54(1)	35(1)	6(1)	9(1)	-1(1)
C(19)	30(1)	34(1)	45(1)	-4(1)	7(1)	-9(1)
C(20)	25(1)	25(1)	20(1)	1(1)	3(1)	3(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2** (ic22934).

	x	y	z	U(eq)
H(1)	968	4616	1559	45
H(2)	3636	6061	2231	33
H(3)	1719	7736	2450	29
H(5A)	811	6425	147	44
H(5B)	296	7718	361	44
H(6A)	-555	5939	1305	36
H(6B)	-450	7196	1815	36
H(9A)	1270	4236	3716	36
H(9B)	2314	5175	3487	36
H(10A)	691	5584	5059	40
H(10B)	1882	4779	5208	40
H(11)	3012	6443	5292	37
H(13A)	3698	8298	4861	38
H(13B)	2630	9214	4625	38
H(14A)	2867	8932	2981	37
H(14B)	4203	9181	3403	37
H(15)	5423	7550	3900	49
H(16A)	6291	5723	3720	78
H(16B)	5376	5413	2867	78
H(16C)	4859	5567	3926	78
H(17A)	7023	7493	2830	136
H(17B)	6056	8458	2490	136
H(17C)	6107	7213	1970	136
H(18A)	2731	8121	-99	52
H(18B)	3592	8107	863	52
H(19A)	-577	4454	2756	55
H(19B)	-1294	5659	2911	55
H(19C)	-873	4900	3811	55

Table S11. Crystal data and structure refinement for **6** (ic22883).

Identification code	ic22883	
Empirical formula	C20 H30 O3	
Formula weight	318.44	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.6524(2) Å	a= 90°.
	b = 13.8446(3) Å	b= 90°.
	c = 17.0676(4) Å	g = 90°.
Volume	1808.22(7) $Å^3$	
Z	4	
Density (calculated)	1.170 Mg/m^3	
Absorption coefficient	0.604 mm^{-1}	
F(000)	696	
Crystal size	0.332 x 0.118 x 0.100 mm^3	
Theta range for data collection	4.111 to 74.422°.	
Index ranges	-8<=h<=9, -15<=k<=17, -19<=l<=21	
Reflections collected	14037	
Independent reflections	3676 [R(int) = 0.0327]	
Completeness to theta = 67.679°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9819 and 0.8779	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3676 / 0 / 213	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0296, wR2 = 0.0777	
R indices (all data)	R1 = 0.0315, wR2 = 0.0790	
Absolute structure parameter	-0.07(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole0.149 and -0.141 $e.Å^{-3}$		

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6** (ic22883). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1215(1)	3162(1)	8786(1)	40(1)
O(2)	5959(1)	3189(1)	8510(1)	41(1)
O(3)	8294(2)	3176(1)	7794(1)	54(1)
C(1)	5444(2)	3963(1)	5606(1)	30(1)
C(2)	3965(2)	4351(1)	5889(1)	32(1)
C(3)	3550(2)	4507(1)	6711(1)	31(1)
C(4)	2130(2)	4953(1)	6999(1)	33(1)
C(5)	1777(2)	5060(1)	7866(1)	37(1)
C(6)	3011(2)	4545(1)	8427(1)	37(1)
C(7)	2782(2)	3450(1)	8398(1)	30(1)
C(8)	4240(2)	2868(1)	8806(1)	36(1)
C(9)	4040(2)	1786(1)	8693(1)	42(1)
C(10)	3514(2)	1464(1)	7878(1)	40(1)
C(11)	4593(2)	1812(1)	7208(1)	34(1)
C(12)	5927(2)	2433(1)	7178(1)	30(1)
C(13)	6893(2)	2597(1)	6412(1)	36(1)
C(14)	6958(2)	3652(1)	6116(1)	31(1)
C(15)	5694(2)	3890(1)	4721(1)	36(1)
C(16)	6929(3)	4681(2)	4431(1)	50(1)
C(17)	6323(2)	2896(1)	4452(1)	41(1)
C(18)	750(2)	5408(2)	6490(1)	48(1)
C(19)	4364(3)	3119(2)	9672(1)	54(1)
C(20)	6769(2)	2935(1)	7853(1)	35(1)

Table S13. Bond lengths [Å] and angles [°] for **6** (ic22883).

O(1)-C(7)	1.4269(17)
O(2)-C(20)	1.329(2)
O(2)-C(8)	1.4775(18)
O(3)-C(20)	1.218(2)
C(1)-C(2)	1.343(2)
C(1)-C(14)	1.511(2)
C(1)-C(15)	1.526(2)
C(2)-C(3)	1.454(2)
C(3)-C(4)	1.343(2)
C(4)-C(18)	1.506(2)
C(4)-C(5)	1.512(2)
C(5)-C(6)	1.523(2)
C(6)-C(7)	1.527(2)
C(7)-C(8)	1.543(2)
C(8)-C(9)	1.518(3)
C(8)-C(19)	1.521(2)
C(9)-C(10)	1.515(3)
C(10)-C(11)	1.489(2)
C(11)-C(12)	1.336(2)
C(12)-C(20)	1.491(2)
C(12)-C(13)	1.518(2)
C(13)-C(14)	1.547(2)
C(15)-C(16)	1.529(3)
C(15)-C(17)	1.529(2)

C(20)-O(2)-C(8)	128.56(13)
C(2)-C(1)-C(14)	123.54(14)
C(2)-C(1)-C(15)	119.23(14)
C(14)-C(1)-C(15)	117.08(13)
C(1)-C(2)-C(3)	126.21(15)
C(4)-C(3)-C(2)	126.72(15)
C(3)-C(4)-C(18)	123.27(16)
C(3)-C(4)-C(5)	123.24(15)
C(18)-C(4)-C(5)	113.48(14)
C(4)-C(5)-C(6)	117.32(13)

C(5)-C(6)-C(7)	111.89(13)
O(1)-C(7)-C(6)	111.04(13)
O(1)-C(7)-C(8)	104.56(12)
C(6)-C(7)-C(8)	114.87(13)
O(2)-C(8)-C(9)	110.09(14)
O(2)-C(8)-C(19)	101.95(13)
C(9)-C(8)-C(19)	110.77(16)
O(2)-C(8)-C(7)	109.45(13)
C(9)-C(8)-C(7)	112.69(13)
C(19)-C(8)-C(7)	111.36(15)
C(10)-C(9)-C(8)	115.62(14)
C(11)-C(10)-C(9)	117.55(14)
C(12)-C(11)-C(10)	131.41(16)
C(11)-C(12)-C(20)	126.84(14)
C(11)-C(12)-C(13)	120.14(15)
C(20)-C(12)-C(13)	112.63(13)
C(12)-C(13)-C(14)	116.00(13)
C(1)-C(14)-C(13)	115.61(13)
C(1)-C(15)-C(16)	110.54(15)
C(1)-C(15)-C(17)	113.30(14)
C(16)-C(15)-C(17)	110.71(14)
O(3)-C(20)-O(2)	116.29(16)
O(3)-C(20)-C(12)	118.57(15)
O(2)-C(20)-C(12)	125.05(13)

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6** (ic22883). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	25(1)	59(1)	36(1)	14(1)	1(1)	-4(1)
O(2)	25(1)	63(1)	34(1)	-3(1)	-2(1)	-8(1)
O(3)	24(1)	97(1)	42(1)	8(1)	-4(1)	-14(1)
C(1)	30(1)	30(1)	30(1)	2(1)	2(1)	0(1)
C(2)	31(1)	32(1)	33(1)	3(1)	3(1)	3(1)
C(3)	31(1)	28(1)	33(1)	2(1)	5(1)	2(1)
C(4)	31(1)	27(1)	41(1)	1(1)	8(1)	-1(1)
C(5)	38(1)	31(1)	42(1)	-3(1)	13(1)	2(1)
C(6)	39(1)	41(1)	32(1)	-9(1)	6(1)	-5(1)
C(7)	26(1)	40(1)	25(1)	1(1)	0(1)	-4(1)
C(8)	24(1)	58(1)	27(1)	6(1)	0(1)	-3(1)
C(9)	34(1)	50(1)	43(1)	19(1)	4(1)	5(1)
C(10)	32(1)	32(1)	56(1)	7(1)	3(1)	-2(1)
C(11)	31(1)	31(1)	39(1)	1(1)	-2(1)	4(1)
C(12)	27(1)	33(1)	31(1)	5(1)	0(1)	5(1)
C(13)	36(1)	36(1)	34(1)	3(1)	6(1)	8(1)
C(14)	28(1)	33(1)	31(1)	1(1)	5(1)	0(1)
C(15)	31(1)	48(1)	29(1)	1(1)	1(1)	6(1)
C(16)	61(1)	50(1)	38(1)	9(1)	12(1)	2(1)
C(17)	36(1)	51(1)	35(1)	-10(1)	4(1)	1(1)
C(18)	38(1)	54(1)	53(1)	6(1)	7(1)	15(1)
C(19)	39(1)	95(2)	28(1)	2(1)	-4(1)	2(1)
C(20)	23(1)	49(1)	32(1)	7(1)	-3(1)	-2(1)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6** (ic22883).

	x	y	z	U(eq)
H(1A)	362	3232	8482	48
H(2)	3108	4541	5517	38
H(3)	4368	4269	7083	37
H(5A)	577	4825	7969	45
H(5B)	1797	5758	7994	45
H(6A)	2789	4774	8968	45
H(6B)	4232	4710	8291	45
H(7)	2713	3244	7837	36
H(9A)	5164	1473	8828	51
H(9B)	3154	1548	9069	51
H(10A)	3519	750	7868	48
H(10B)	2294	1675	7787	48
H(11)	4276	1544	6716	41
H(13A)	6335	2195	6003	43
H(13B)	8108	2364	6476	43
H(14A)	7010	4086	6576	37
H(14B)	8053	3742	5816	37
H(15)	4530	4007	4472	44
H(16A)	7013	4652	3859	75
H(16B)	8090	4585	4660	75
H(16C)	6476	5314	4588	75
H(17A)	6340	2873	3878	61
H(17B)	5528	2398	4652	61
H(17C)	7503	2778	4654	61
H(18A)	774	6111	6558	72
H(18B)	-402	5160	6640	72
H(18C)	980	5250	5940	72
H(19A)	3218	3034	9918	81
H(19B)	4740	3792	9729	81
H(19C)	5215	2693	9925	81