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Supplementary Information

Pyrrolizidine Alkaloids and Diterpenes from *Villasenoria orcuttii*

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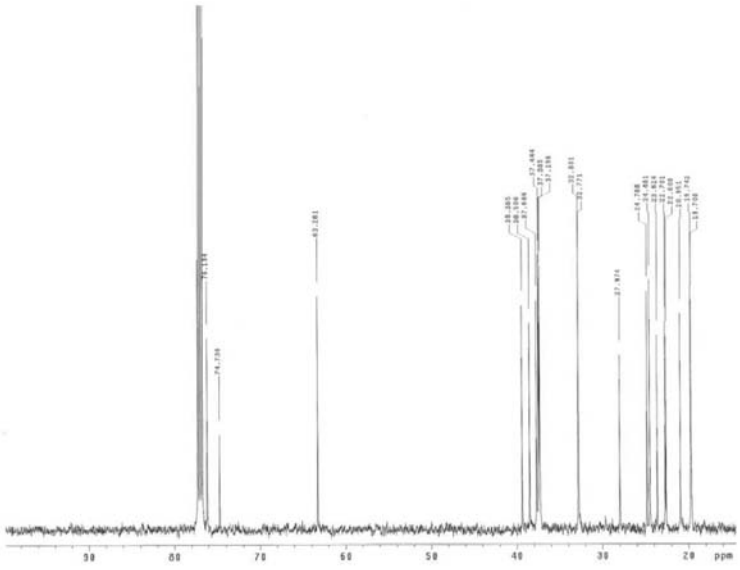

Figure S1. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **1**.

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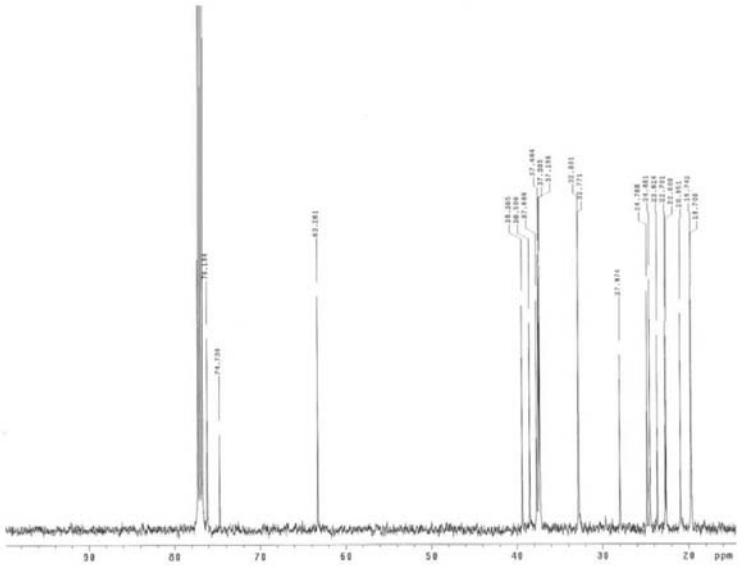


Figure S2. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **1**.

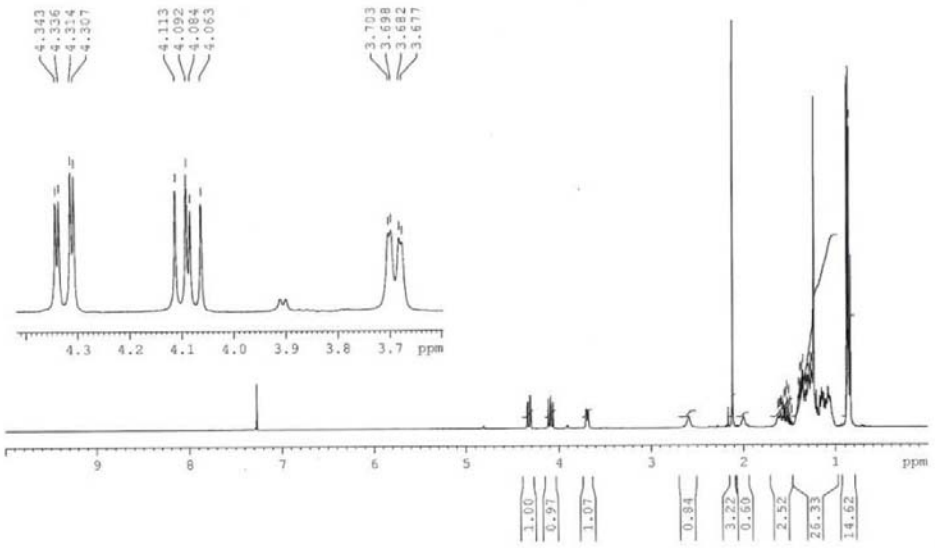


Figure S3. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **2**.

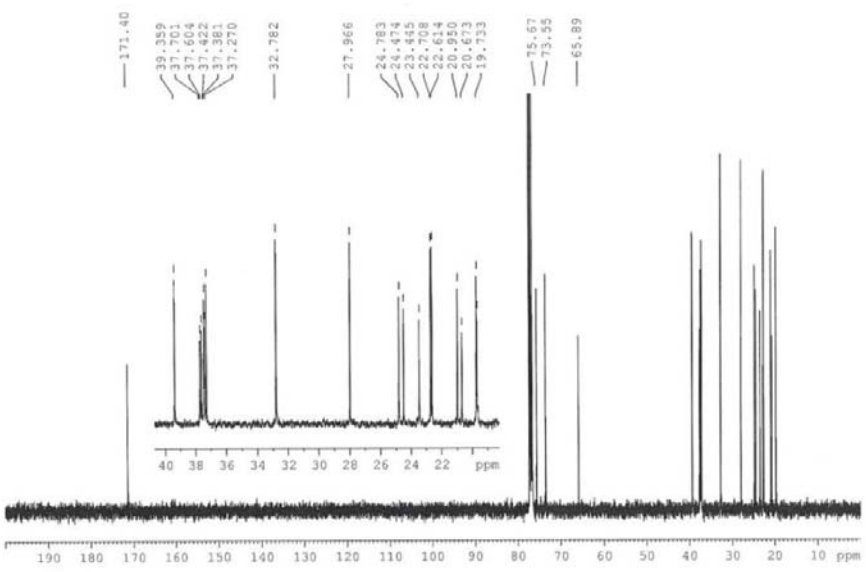


Figure S4. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **2**.

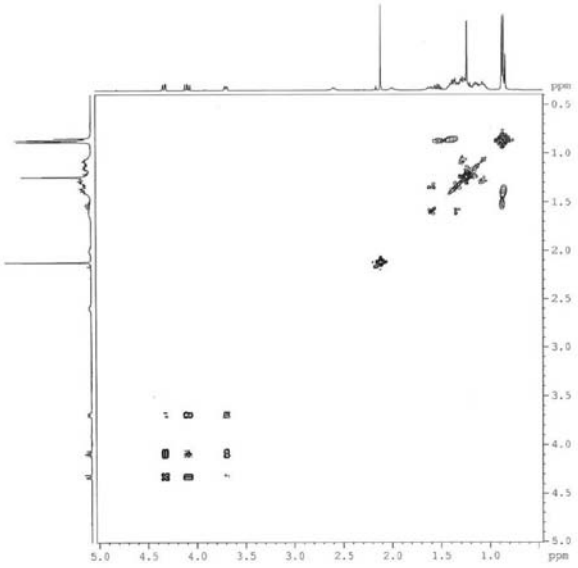


Figure S5. COSY spectrum of compound **2**.

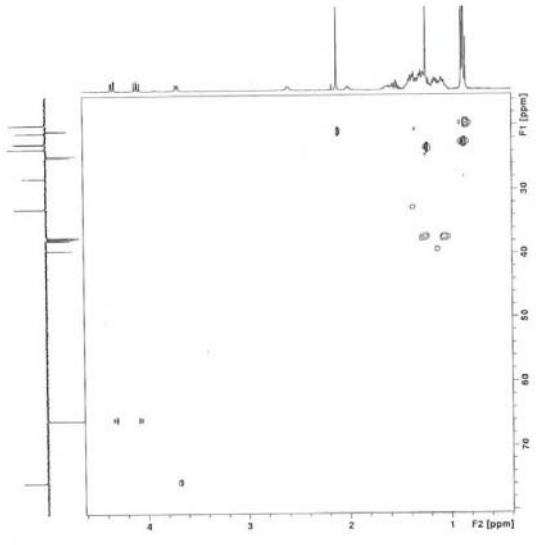


Figure S6. HSQC spectrum of compound **2**.

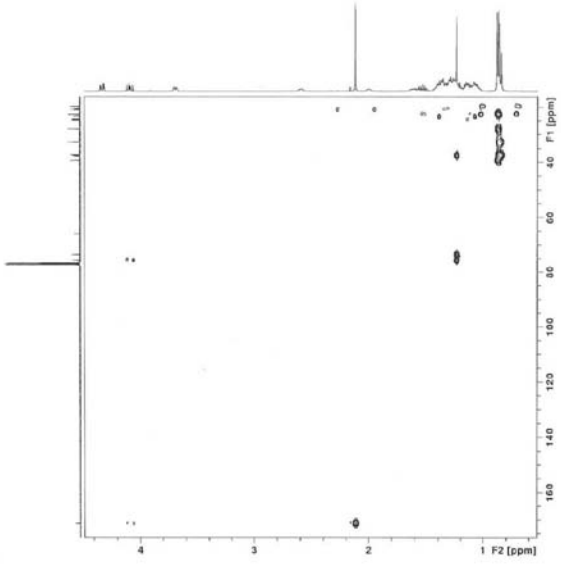


Figure S7. HMBC spectrum of compound **2**.

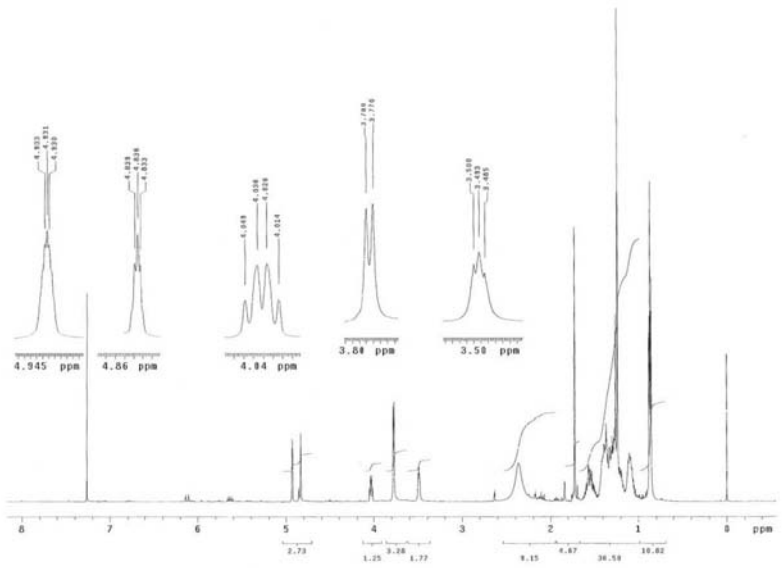


Figure S8. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **3**.

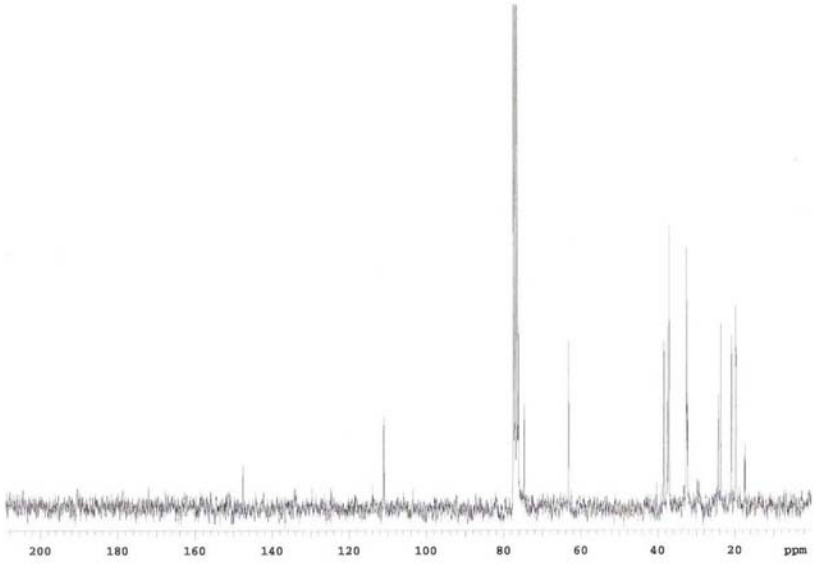


Figure S9. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **3**.

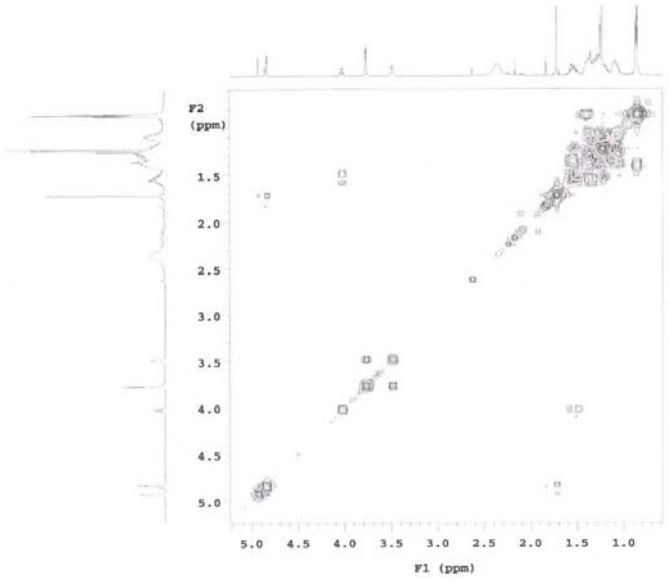


Figure S10. COSY spectrum of compound **3**.

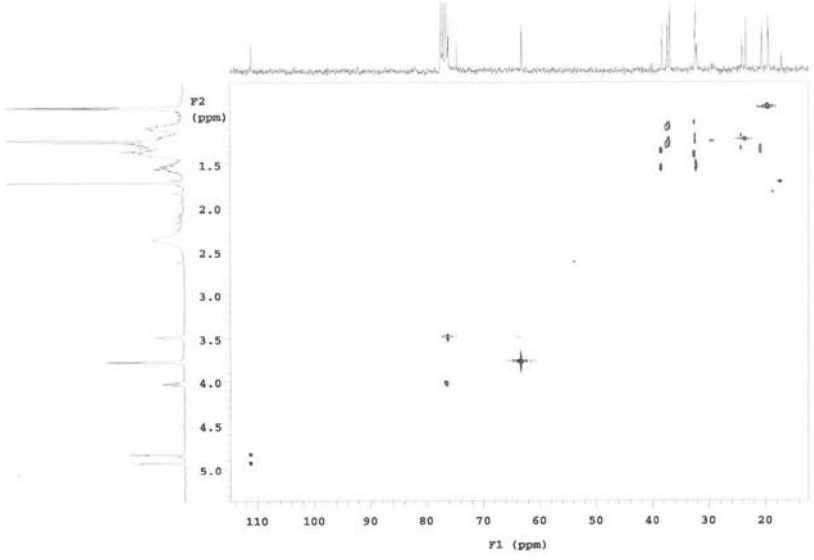


Figure S11. HSQC spectrum of compound **3**.

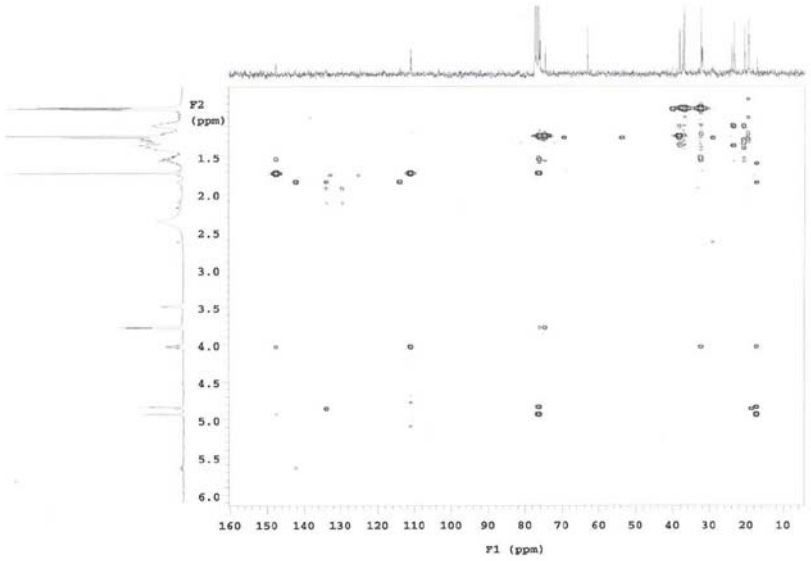


Figure S12. HMBC spectrum of compound **3**.

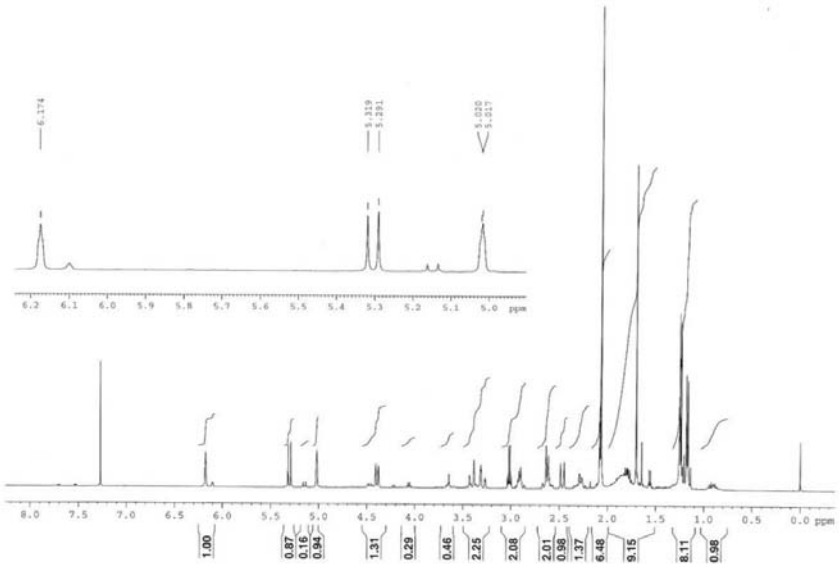


Figure S13. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **4**.

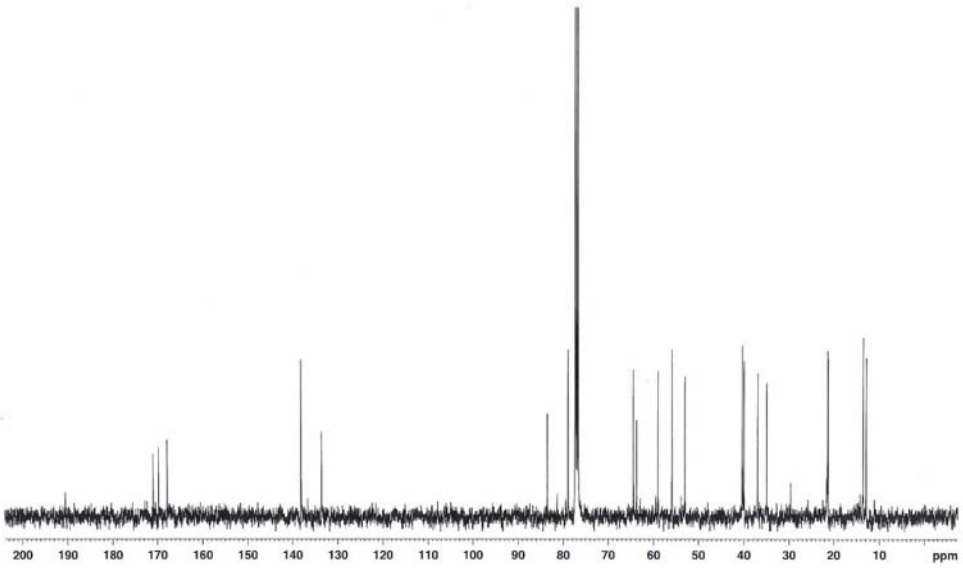


Figure S14. ^{13}C NMR (125 MHz, $CDCl_3$) of compound **4**.

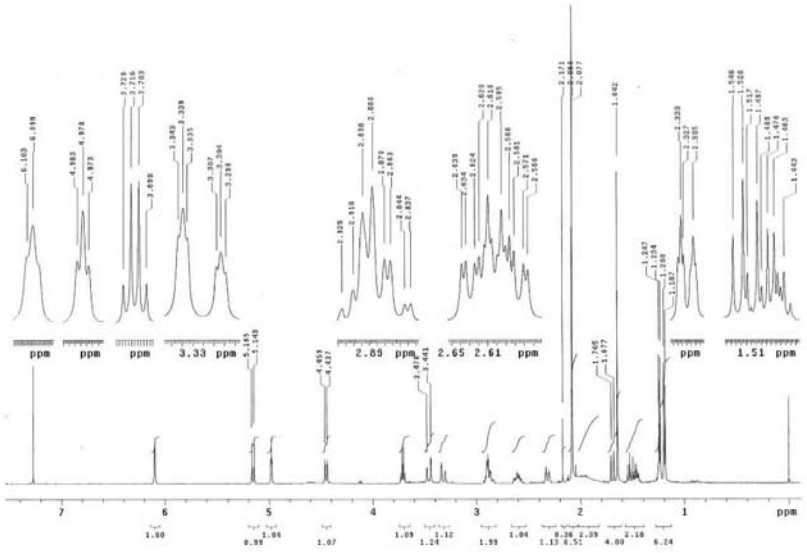


Figure S15. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **5**.

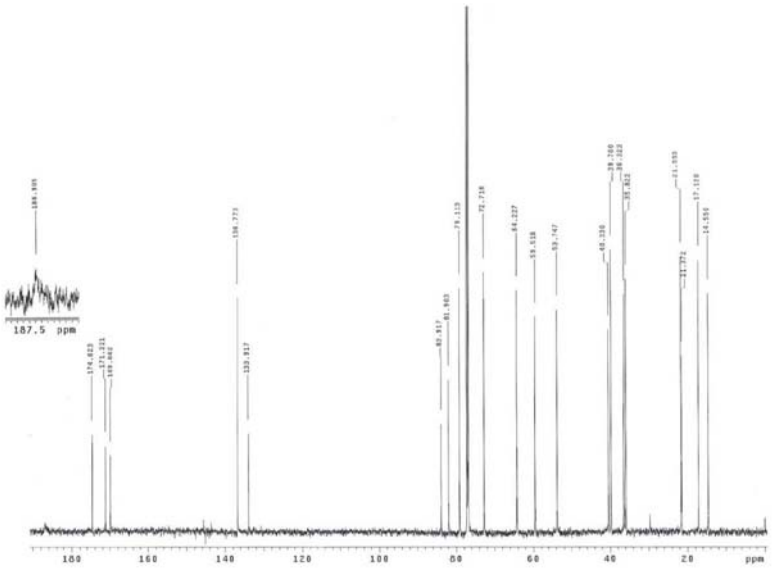


Figure S16. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **5**.

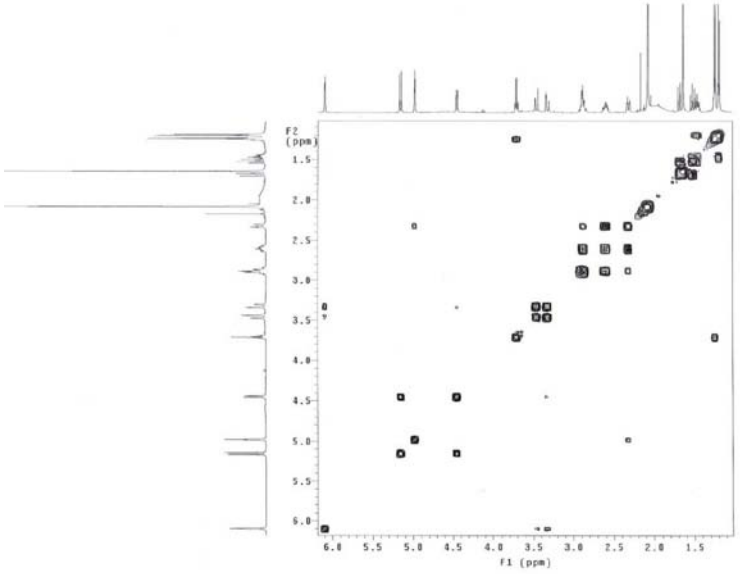


Figure S17. COSY spectrum of compound **5**.

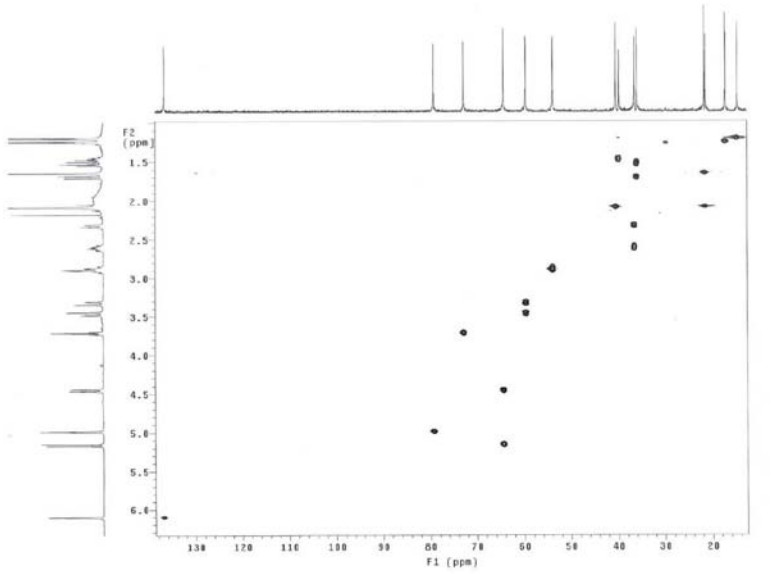


Figure S18. HSQC spectrum of compound **5**.

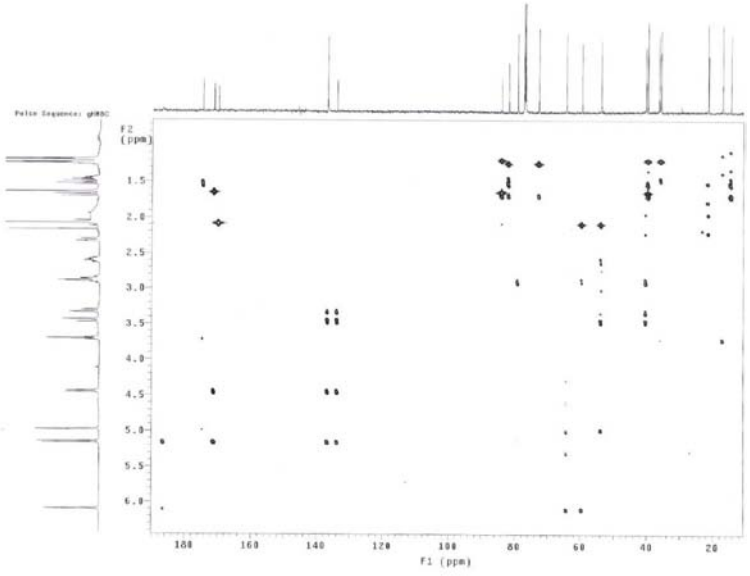
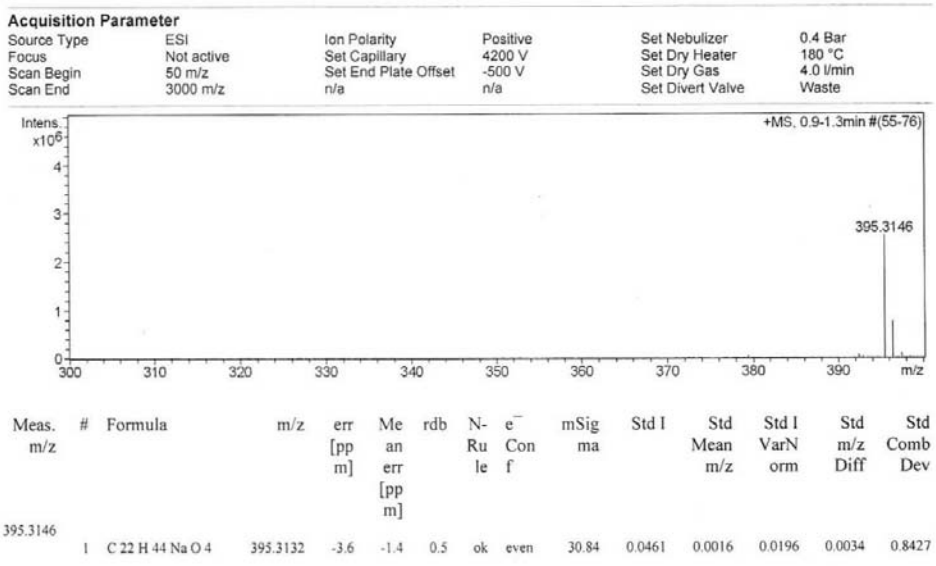
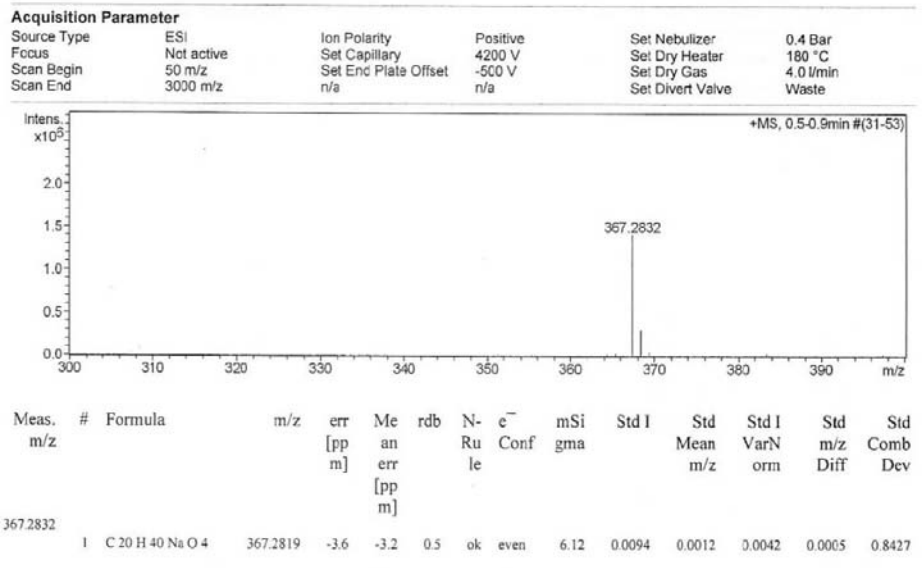


Figure S19. HMBC spectrum of compound **5**.



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
395.3146	1	C 22 H 44 Na O 4	395.3132	-3.6	-1.4	0.5	ok	even	30.84	0.0461	0.0016	0.0196	0.0034	0.8427

Figure S20. HRESIMS spectrum of compound **2**.



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
367.2832	1	C 20 H 40 Na O 4	367.2819	-3.6	-3.2	0.5	ok	even	6.12	0.0094	0.0012	0.0042	0.0005	0.8427

Figure S21. HRESIMS spectrum of compound **3**.

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
N(4)	2906(3)	8625(2)	3206(1)	68(1)
C(22)	2548(5)	8800(3)	3776(1)	102(1)
O(8)	2091(5)	10844(4)	3113(2)	65(1)
O(10)	966(4)	10305(3)	1548(1)	60(1)
O(11)	2267(4)	11793(3)	1783(1)	79(1)
O(12)	1410(20)	10581(12)	500(4)	57(2)
O(23)	–783(7)	11425(6)	710(2)	74(1)
C(1)	1273(8)	9560(6)	2468(3)	49(1)
C(2)	932(14)	8524(5)	2556(5)	65(2)
C(3)	1646(9)	7950(8)	2978(4)	69(2)
C(5)	4580(16)	8510(8)	3117(5)	76(2)
C(6)	5251(9)	9623(6)	3017(4)	67(2)
C(7)	4208(12)	10174(8)	2603(4)	50(1)
C(8)	2484(8)	10110(8)	2794(3)	51(1)
C(9)	308(4)	10229(4)	2094(2)	63(1)
C(11)	1829(4)	11164(3)	1448(2)	54(1)
C(12)	2343(7)	11264(7)	857(3)	55(1)
C(13)	4016(9)	10798(8)	800(3)	64(2)
C(19)	4678(12)	10992(9)	245(4)	102(3)
C(18)	2271(8)	12476(4)	697(3)	71(1)
C(23)	–87(10)	10776(9)	444(2)	56(1)
C(24)	–757(12)	10023(10)	41(3)	80(2)
O(8A)	2541(10)	10688(6)	3290(3)	62(2)
O(10A)	1394(5)	11157(3)	1841(2)	60(1)
O(11A)	239(5)	9882(4)	1338(2)	64(1)
O(12A)	1400(40)	10690(20)	425(8)	58(2)
O(23A)	–1020(12)	11431(9)	515(3)	70(2)
C(1A)	1434(18)	9777(10)	2561(5)	53(2)
C(2A)	850(20)	8786(10)	2574(8)	59(2)
C(3A)	2053(17)	7886(15)	2857(7)	74(2)
C(5A)	4470(30)	8229(12)	3049(8)	69(3)
C(6A)	5365(18)	9261(9)	3013(6)	64(2)
C(7A)	4380(20)	10031(14)	2685(7)	53(2)
C(8A)	2780(14)	10054(11)	2902(5)	50(2)
C(9A)	599(9)	10734(6)	2314(3)	63(1)
C(11A)	1064(10)	10658(7)	1382(3)	51(1)
C(12A)	1973(12)	11180(11)	908(5)	54(2)
C(13A)	3720(14)	10870(11)	919(6)	56(2)
C(19A)	4614(13)	11338(10)	444(6)	80(3)
C(18A)	1742(11)	12419(7)	898(4)	67(2)
C(23A)	–187(19)	10800(15)	296(5)	61(2)
C(24A)	–650(20)	10063(13)	–130(5)	76(3)
C(14)	4029(3)	9589(2)	952(1)	56(1)
C(15)	5507(2)	9278(2)	1264(1)	52(1)
C(16)	5548(2)	9884(1)	1799(1)	49(1)
C(20)	5566(3)	8050(2)	1389(1)	62(1)
C(21)	5763(5)	7361(2)	889(1)	92(1)
O(15)	6816(2)	9588(2)	962(1)	70(1)
O(16)	6531(2)	10524(1)	1923(1)	67(1)
O(17)	4322(2)	9632(1)	2105(1)	49(1)
O(20)	6823(3)	7919(1)	1753(1)	79(1)
C(25)	457(13)	6995(12)	1163(4)	159(2)
Cl(1)	731(5)	7016(4)	506(1)	204(2)
Cl(2)	1811(2)	6320(3)	1547(1)	162(1)
C(25A)	1290(40)	6811(15)	1350(8)	171(3)
Cl(1A)	538(15)	7663(10)	914(6)	196(3)
Cl(2A)	1437(11)	5457(9)	1169(5)	178(3)

Table S2. Bond lengths (Å) and angles (degree) for compound **5**

N(4)-C(3A)	1.456(19)	C(20)-O(20)	1.422(3)	C(2A)-C(1A)-C(8A)	120.0(13)
N(4)-C(22)	1.465(4)	C(20)-C(21)	1.514(3)	C(2A)-C(1A)-C(9A)	122.9(12)
N(4)-C(5)	1.471(14)	C(25)-Cl(1)	1.650(9)	C(8A)-C(1A)-C(9A)	115.5(9)
N(4)-C(3)	1.482(9)	C(25)-Cl(2)	1.724(10)	C(1A)-C(2A)-C(3A)	112.3(14)
N(4)-C(5A)	1.49(2)	C(25A)-Cl(1A)	1.639(14)	N(4)-C(3A)-C(2A)	98.9(12)
N(4)-C(8A)	1.911(13)	C(25A)-Cl(2A)	1.726(14)	C(6A)-C(5A)-N(4)	102.2(11)
O(8)-C(8)	1.246(9)	C(3A)-N(4)-C(22)	124.0(6)	C(5A)-C(6A)-C(7A)	105.7(12)
O(10)-C(11)	1.316(6)	C(3A)-N(4)-C(5)	110.5(7)	C(8A)-C(7A)-C(6A)	110.0(12)
O(10)-C(9)	1.474(5)	C(22)-N(4)-C(5)	111.6(5)	C(8A)-C(7A)-O(17)	108.8(12)
O(11)-C(11)	1.197(5)	C(3A)-N(4)-C(3)	18.4(6)	C(6A)-C(7A)-O(17)	109.1(14)
O(12)-C(23)	1.325(18)	C(22)-N(4)-C(3)	107.2(4)	O(8A)-C(8A)-C(1A)	116.9(11)
O(12)-C(12)	1.462(16)	C(5)-N(4)-C(3)	127.8(5)	O(8A)-C(8A)-C(7A)	116.4(11)
O(23)-C(23)	1.198(10)	C(3A)-N(4)-C(5A)	95.8(8)	C(1A)-C(8A)-C(7A)	121.2(11)
C(1)-C(2)	1.323(9)	C(22)-N(4)-C(5A)	119.5(8)	O(8A)-C(8A)-N(4)	105.9(9)
C(1)-C(8)	1.486(7)	C(5)-N(4)-C(5A)	15.4(7)	C(1A)-C(8A)-N(4)	93.5(8)
C(1)-C(9)	1.494(8)	C(3)-N(4)-C(5A)	112.6(6)	C(7A)-C(8A)-N(4)	94.2(8)
C(2)-C(3)	1.407(15)	C(3A)-N(4)-C(8A)	107.9(8)	O(10A)-C(9A)-C(1A)	112.2(7)
C(5)-C(6)	1.504(9)	C(22)-N(4)-C(8A)	103.6(5)	O(11A)-C(11A)-O(10A)	125.1(8)
C(6)-C(7)	1.527(8)	C(5)-N(4)-C(8A)	94.9(6)	O(11A)-C(11A)-C(12A)	124.1(8)
C(7)-O(17)	1.409(12)	C(3)-N(4)-C(8A)	108.7(5)	O(10A)-C(11A)-C(12A)	110.7(9)
C(7)-C(8)	1.568(11)	C(5A)-N(4)-C(8A)	104.4(8)	O(12A)-C(12A)-C(18A)	110.8(14)
C(11)-C(12)	1.539(7)	C(11)-O(10)-C(9)	116.4(4)	O(12A)-C(12A)-C(11A)	106.9(13)
C(12)-C(18)	1.540(9)	C(23)-O(12)-C(12)	119.9(12)	C(18A)-C(12A)-C(11A)	110.7(9)
C(12)-C(13)	1.562(8)	C(2)-C(1)-C(8)	120.2(7)	O(12A)-C(12A)-C(13A)	104.4(16)
C(13)-C(19)	1.514(8)	C(2)-C(1)-C(9)	120.4(6)	C(18A)-C(12A)-C(13A)	111.6(9)
C(13)-C(14)	1.530(10)	C(8)-C(1)-C(9)	118.9(6)	C(11A)-C(12A)-C(13A)	112.1(9)
C(23)-C(24)	1.481(9)	C(1)-C(2)-C(3)	120.4(9)	C(19A)-C(13A)-C(12A)	112.7(10)
O(8A)-C(8A)	1.255(15)	C(2)-C(3)-N(4)	109.2(7)	C(19A)-C(13A)-C(14)	109.0(8)
O(10A)-C(11A)	1.326(9)	N(4)-C(5)-C(6)	108.5(7)	C(12A)-C(13A)-C(14)	113.8(10)
O(10A)-C(9A)	1.459(8)	C(5)-C(6)-C(7)	106.6(7)	O(23A)-C(23A)-O(12A)	123.0(14)
O(11A)-C(11A)	1.194(12)	O(17)-C(7)-C(6)	110.0(7)	O(23A)-C(23A)-C(24A)	124.9(14)
O(12A)-C(23A)	1.42(3)	O(17)-C(7)-C(8)	108.0(7)	O(12A)-C(23A)-C(24A)	112.1(16)
O(12A)-C(12A)	1.43(3)	C(6)-C(7)-C(8)	109.6(6)	C(13)-C(14)-C(15)	111.6(4)
O(23A)-C(23A)	1.188(19)	O(8)-C(8)-C(1)	118.9(6)	C(13)-C(14)-C(13A)	14.5(5)
C(1A)-C(2A)	1.317(16)	O(8)-C(8)-C(7)	114.6(7)	C(15)-C(14)-C(13A)	114.0(5)
C(1A)-C(8A)	1.480(13)	C(1)-C(8)-C(7)	121.8(7)	O(15)-C(15)-C(16)	108.30(17)
C(1A)-C(9A)	1.509(15)	O(10)-C(9)-C(1)	113.0(4)	O(15)-C(15)-C(20)	110.19(18)
C(2A)-C(3A)	1.67(2)	O(11)-C(11)-O(10)	124.3(4)	C(16)-C(15)-C(20)	107.42(16)
C(5A)-C(6A)	1.488(13)	O(11)-C(11)-C(12)	121.4(4)	O(15)-C(15)-C(14)	109.37(16)
C(6A)-C(7A)	1.512(14)	O(10)-C(11)-C(12)	114.2(4)	C(16)-C(15)-C(14)	109.70(16)
C(7A)-C(8A)	1.48(2)	O(12)-C(12)-C(11)	111.9(7)	C(20)-C(15)-C(14)	111.78(18)
C(7A)-O(17)	1.52(2)	O(12)-C(12)-C(18)	112.0(8)	O(16)-C(16)-O(17)	124.43(19)
C(11A)-C(12A)	1.555(15)	C(11)-C(12)-C(18)	108.1(6)	O(16)-C(16)-C(15)	124.20(19)
C(12A)-C(18A)	1.534(15)	O(12)-C(12)-C(13)	104.3(10)	O(17)-C(16)-C(15)	111.35(16)
C(12A)-C(13A)	1.558(13)	C(11)-C(12)-C(13)	108.9(5)	O(20)-C(20)-C(21)	111.9(2)
C(13A)-C(19A)	1.524(14)	C(18)-C(12)-C(13)	111.6(5)	O(20)-C(20)-C(15)	105.32(19)
C(13A)-C(14)	1.596(13)	C(19)-C(13)-C(14)	112.0(7)	C(21)-C(20)-C(15)	112.5(2)
C(23A)-C(24A)	1.451(16)	C(19)-C(13)-C(12)	111.9(6)	C(16)-O(17)-C(7)	116.4(5)
C(14)-C(15)	1.543(3)	C(14)-C(13)-C(12)	109.8(6)	C(16)-O(17)-C(7A)	116.0(8)
C(15)-O(15)	1.410(3)	O(23)-C(23)-O(12)	123.7(8)	C(7)-O(17)-C(7A)	11.1(9)
C(15)-C(16)	1.524(3)	O(23)-C(23)-C(24)	126.3(8)	Cl(1)-C(25)-Cl(2)	117.3(6)
C(15)-C(20)	1.540(3)	O(12)-C(23)-C(24)	109.9(9)	Cl(1A)-C(25A)-Cl(2A)	118.1(11)
C(16)-O(16)	1.198(3)	C(11A)-O(10A)-C(9A)	115.3(6)		
C(16)-O(17)	1.342(2)	C(23A)-O(12A)-C(12A)	119(2)		

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **5.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \ldots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(4)	74(1)	56(1)	73(1)	12(1)	−17(1)	-8(1)
C(22)	110(2)	121(3)	74(2)	26(2)	0(2)	−30(2)
O(8)	71(2)	52(2)	73(3)	−12(2)	15(2)	−3(2)
O(10)	57(2)	64(2)	58(2)	14(1)	−2(1)	−3(1)
O(11)	92(2)	77(2)	69(2)	–4(1)	−1(2)	−19(2)
O(12)	53(2)	60(3)	58(3)	6(2)	4(2)	6(2)
O(23)	55(2)	85(2)	81(3)	–9(3)	−3(2)	13(2)
C(1)	38(2)	52(3)	57(2)	6(2)	−2(2)	1(2)
C(2)	66(3)	48(3)	80(3)	–6(3)	−13(2)	–5(3)
C(3)	71(4)	42(2)	94(4)	–1(2)	-5(3)	−10(3)
C(5)	81(4)	65(5)	83(3)	13(4)	−20(3)	13(4)
C(6)	56(2)	74(4)	70(2)	0(3)	-8(2)	−2(3)
C(7)	49(3)	45(3)	57(3)	0(2)	1(2)	–7(2)
C(8)	50(3)	44(2)	60(3)	–3(2)	7(2)	−2(2)
C(9)	47(2)	78(2)	65(2)	20(2)	4(1)	8(2)
C(11)	51(2)	53(2)	59(2)	6(1)	−1(1)	6(2)
C(12)	54(3)	53(2)	59(2)	14(2)	−2(2)	0(2)
C(13)	53(3)	67(3)	71(3)	23(3)	1(2)	8(2)
C(19)	94(4)	112(6)	99(5)	52(4)	39(4)	25(4)
C(18)	65(3)	56(2)	93(4)	25(2)	–9(2)	2(2)
C(23)	51(2)	66(2)	52(3)	7(3)	1(2)	3(2)
C(24)	74(3)	106(4)	60(4)	–6(4)	2(3)	−13(3)
O(8A)	84(4)	39(2)	64(3)	–7(2)	12(2)	−12(3)
O(10A)	66(2)	55(2)	59(2)	5(2)	–3(2)	13(2)
O(11A)	59(2)	70(2)	63(2)	10(2)	0(2)	−10(2)
O(12A)	56(2)	60(4)	58(4)	10(3)	3(3)	3(3)
O(23A)	61(3)	69(3)	79(5)	2(4)	−12(3)	9(3)
C(1A)	52(3)	49(3)	59(3)	5(2)	3(3)	2(3)
C(2A)	56(3)	52(4)	69(3)	–7(4)	-6(3)	−2(3)
C(3A)	76(5)	48(3)	97(5)	2(4)	−1(4)	−1(4)
C(5A)	76(4)	40(5)	90(5)	6(4)	−22(4)	–5(4)
C(6A)	66(3)	49(5)	77(3)	1(4)	−18(3)	0(3)
C(7A)	60(3)	40(4)	59(4)	–4(3)	–5(3)	–5(3)
C(8A)	58(3)	29(3)	64(4)	–2(3)	–5(2)	–4(3)
C(9A)	64(3)	63(3)	61(3)	4(2)	5(2)	21(3)
C(11A)	50(3)	47(3)	55(3)	6(2)	0(2)	12(2)
C(12A)	52(3)	46(3)	63(3)	9(2)	1(2)	8(3)
C(13A)	51(3)	44(3)	74(5)	10(3)	3(3)	0(3)
C(19A)	62(4)	72(5)	107(7)	35(5)	16(4)	5(4)
C(18A)	63(4)	51(3)	86(5)	15(3)	−12(4)	1(3)
C(23A)	58(3)	64(3)	61(5)	9(4)	0(3)	0(3)
C(24A)	95(7)	79(4)	55(6)	3(4)	−14(5)	−1(4)
C(14)	54(1)	52(1)	62(1)	6(1)	−2(1)	1(1)
C(15)	44(1)	50(1)	63(1)	5(1)	6(1)	3(1)
C(16)	39(1)	39(1)	68(1)	5(1)	1(1)	2(1)
C(20)	72(1)	46(1)	68(1)	0(1)	2(1)	10(1)
C(21)	129(3)	64(1)	85(2)	−16(1)	–5(2)	26(2)
O(15)	53(1)	80(1)	76(1)	10(1)	19(1)	2(1)
O(16)	49(1)	61(1)	92(1)	–7(1)	4(1)	−13(1)
O(17)	43(1)	44(1)	59(1)	–4(1)	2(1)	–5(1)
O(20)	94(1)	59(1)	84(1)	2(1)	−17(1)	29(1)
C(25)	136(4)	225(5)	115(2)	59(4)	40(3)	54(4)
Cl(1)	222(3)	278(4)	110(1)	15(2)	34(2)	64(3)
Cl(2)	94(1)	219(3)	172(2)	49(2)	−1(1)	11(2)
C(25A)	140(6)	228(5)	143(5)	41(4)	40(5)	39(5)
Cl(1A)	184(5)	231(6)	172(5)	41(5)	12(5)	47(5)
Cl(2A)	125(5)	222(5)	188(7)	40(5)	9(5)	25(6)

Table S4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for compound **5**

	x	y	z	U(eq)		x	y	z	U(eq)
H(22A)	3335	9274	3936	153	H(6AB)	5557	9564	3376	77
H(22B)	2539	8097	3963	153	H(7A)	4830	10780	2697	64
H(22C)	1530	9145	3808	153	H(9AA)	–459	10507	2212	75
H(2)	200	8165	2332	78	H(9AB)	507	11321	2586	75
H(3A)	2072	7254	2842	83	H(13A)	4169	11200	1252	67
H(3B)	877	7782	3261	83	H(19D)	4647	12134	473	120
H(5A)	4774	8033	2803	91	H(19E)	4098	11131	108	120
H(5B)	5072	8177	3437	91	H(19F)	5670	11048	445	120
H(6A)	6320	9561	2878	80	H(18D)	2220	12742	1218	100
H(6B)	5273	10051	3355	80	H(18E)	633	12585	896	100
H(7)	4520	10954	2559	60	H(18F)	2225	12722	574	100
H(9A)	–738	9905	2072	76	H(24D)	–878	9344	23	114
H(9B)	201	10973	2244	76	H(24E)	184	9998	–394	114
H(13)	4688	11191	1064	76	H(24F)	–1581	10348	–307	114
H(19A)	4079	10578	–21	153	H(14A)	3960	9143	621	68
H(19B)	5758	10752	236	153	H(14B)	3112	9424	1176	68
H(19C)	4624	11771	159	153	H(14C)	3130	9236	1127	68
H(18A)	2375	12543	306	107	H(14D)	4105	9296	582	68
H(18B)	3114	12872	873	107	H(20)	4586	7833	1574	74
H(18C)	1277	12783	810	107	H(21A)	4784	7335	691	139
H(24A)	–1115	10441	–271	120	H(21B)	6068	6620	992	139
H(24B)	–1631	9632	201	120	H(21C)	6566	7681	660	139
H(24C)	32	9499	–74	120	H(15A)	7170(40)	10208(11)	1023(13)	105
H(2A)	–148	8604	2439	71	H(20A)	7150(60)	7278(17)	1794(18)	119
H(3AA)	1492	7322	3064	88	H(25A)	-564	6659	1233	190
H(3AB)	2732	7533	2588	88	H(25B)	404	7759	1290	190
H(5AA)	4904	7735	3326	82	H(25C)	664	6850	1683	205
H(5AB)	4440	7845	2699	82	H(25D)	2339	7075	1441	205
H(6AA)	6371	9134	2834	77					

Table S5. Hydrogen bonds for compound **5** (Å and degree)

D-H...A	d(D-H)	d(H...A)	d(D...A)	< (DHA)
O(15)-H(15A)...O(23A)[a]	0.835(11)	2.51(3)	3.138(12)	133(3)
O(20)-H(20A)...O(8)[b]	0.842(11)	1.892(12)	2.734(5)	179(6)
O(20)-H(20A)...O(8A)[b]	0.842(11)	1.979(19)	2.793(7)	162(5)
O(15)-H(15A)...O(23)[a]	0.835(11)	2.44(3)	3.127(8)	140(4)

Symmetry transformations used to generate equivalent atoms: [a] x + 1, y, z [b] –x + 1, y – 1/2, –z + 1/2.