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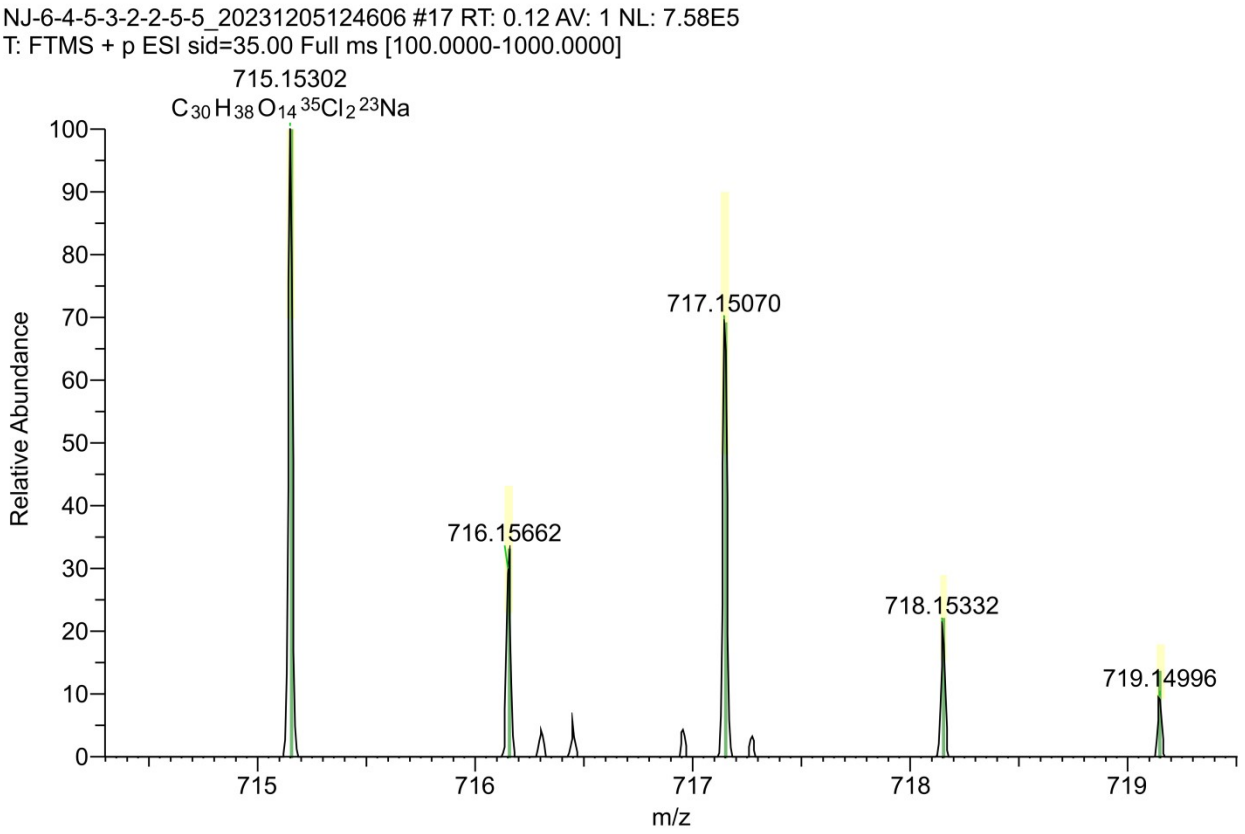
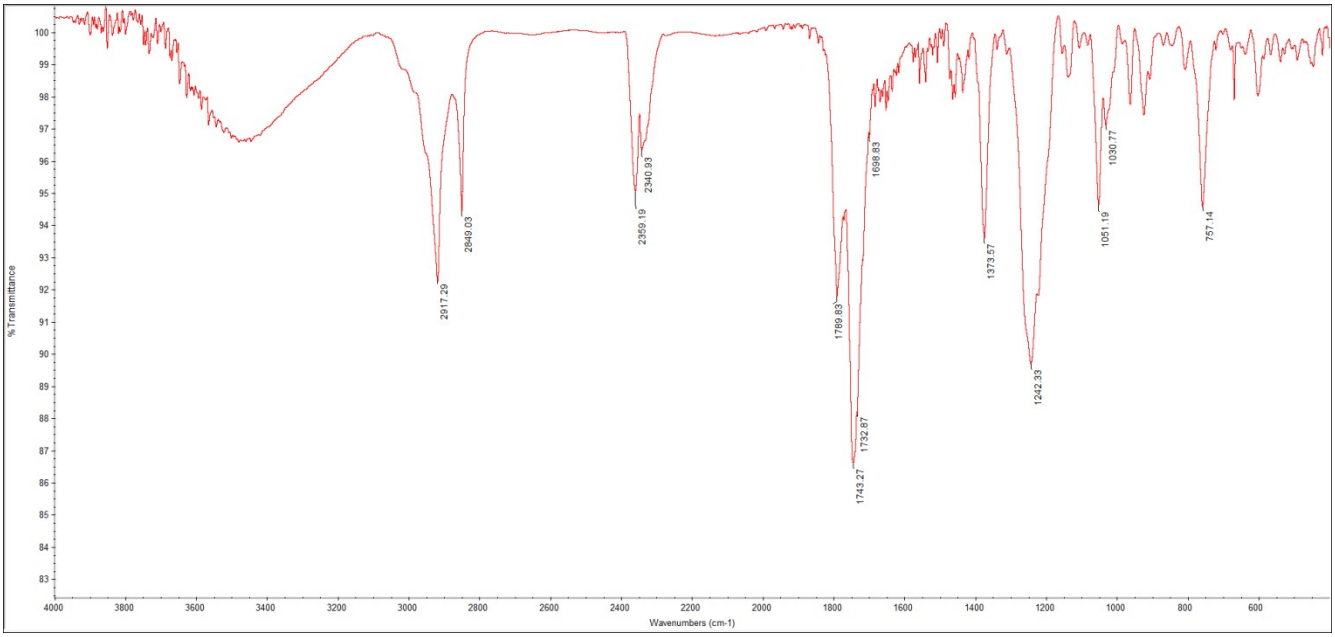
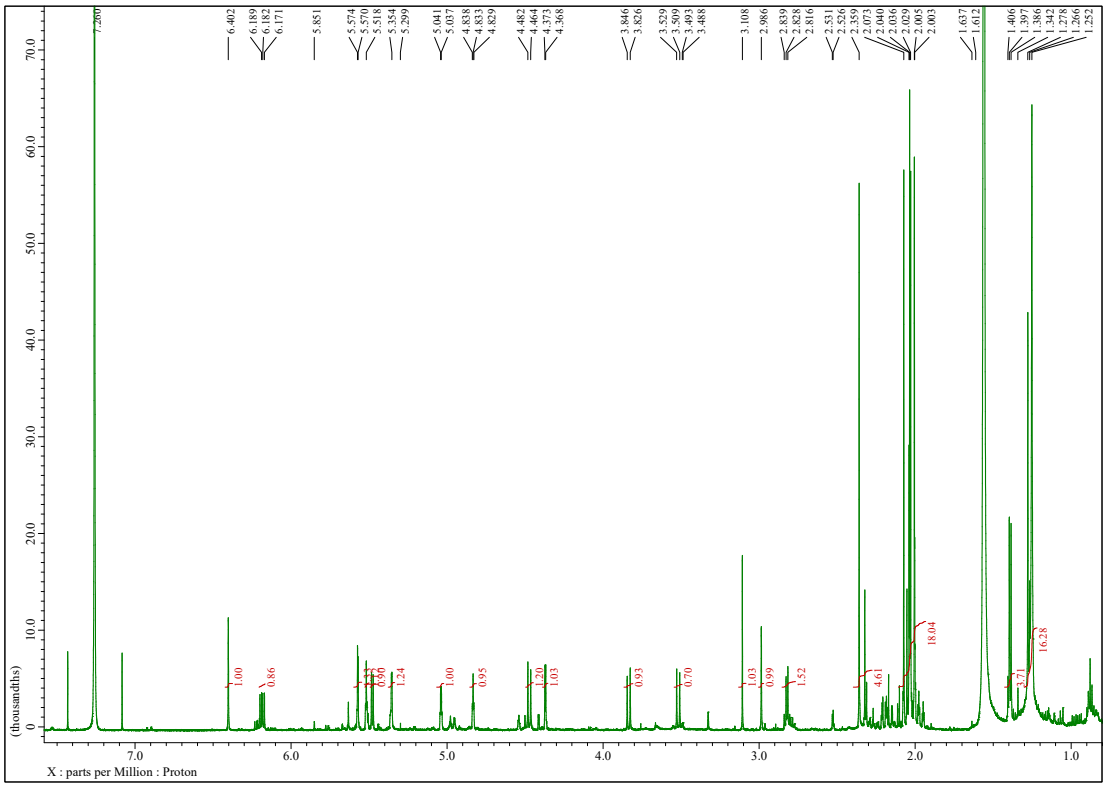
Supporting information



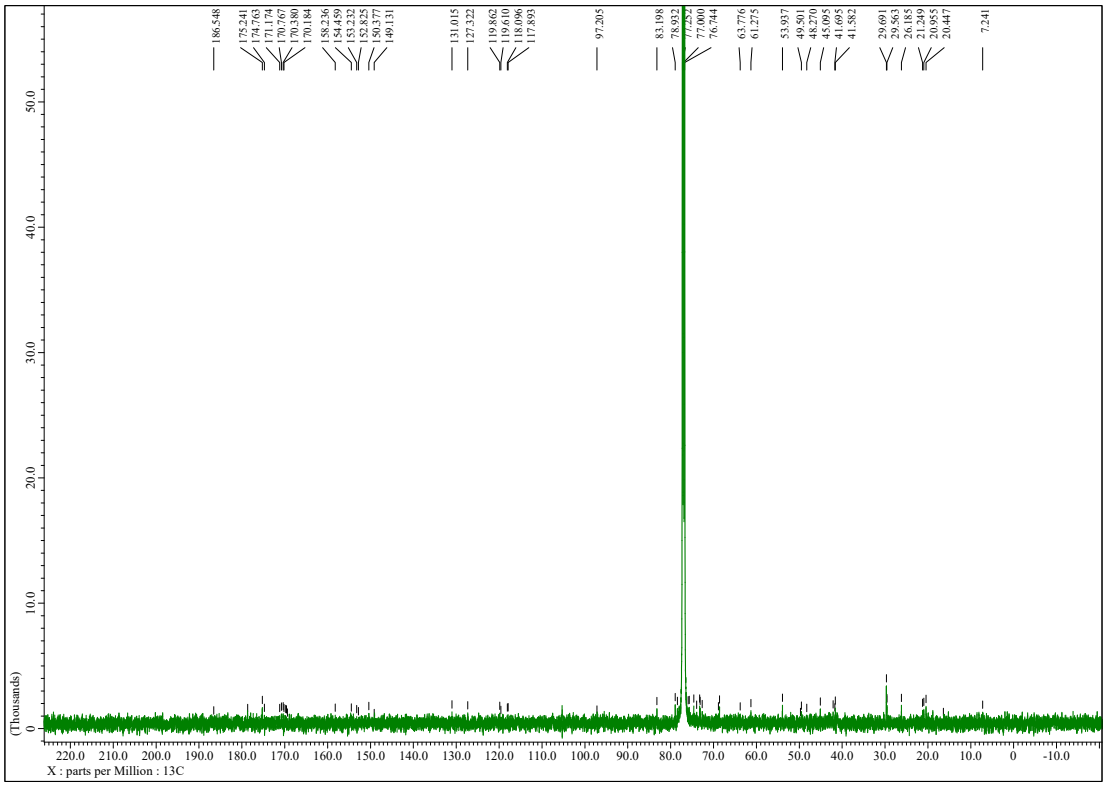
S1. HRESIMS spectrum of compound **4**



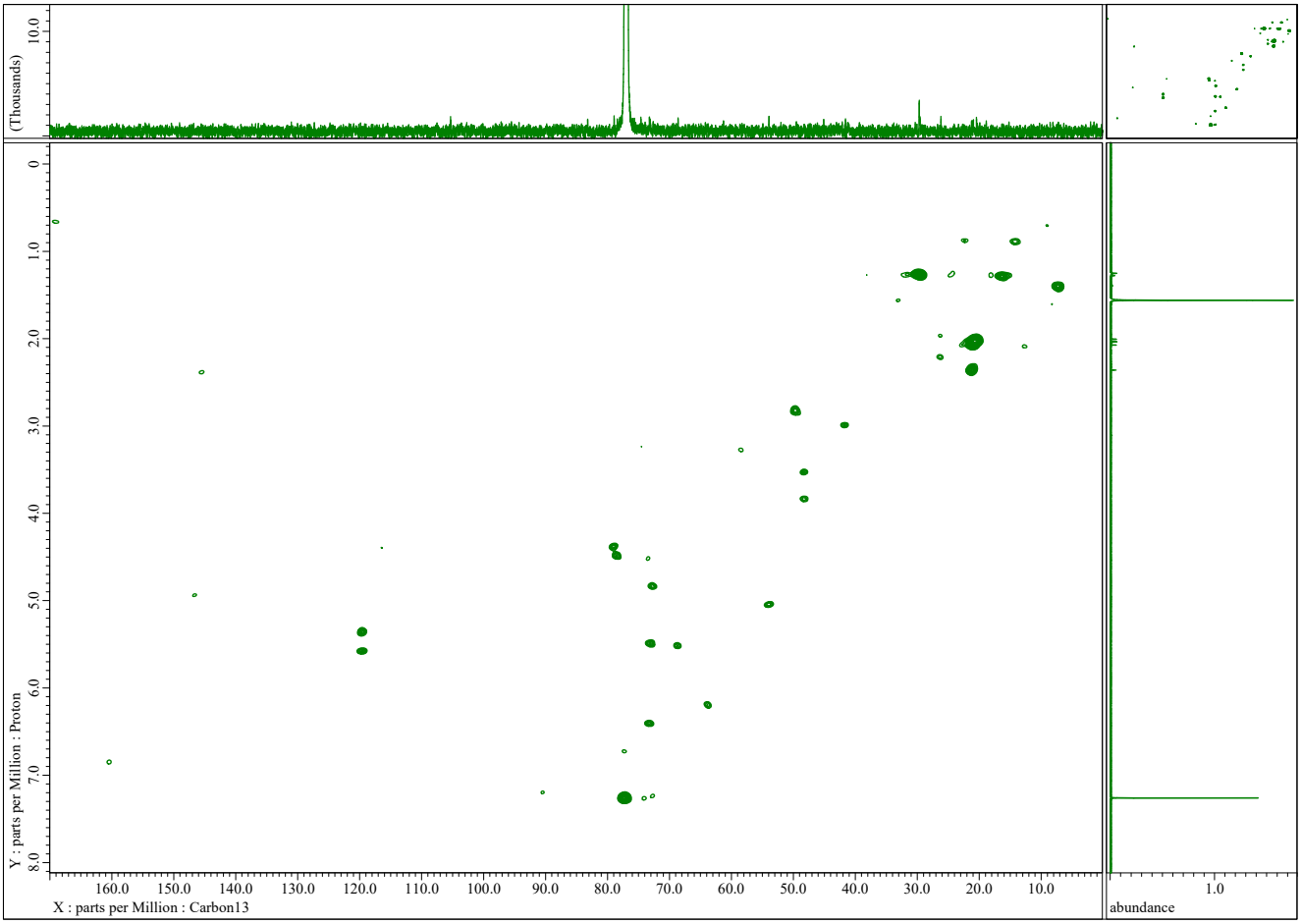
S2. IR spectrum of compound **4**



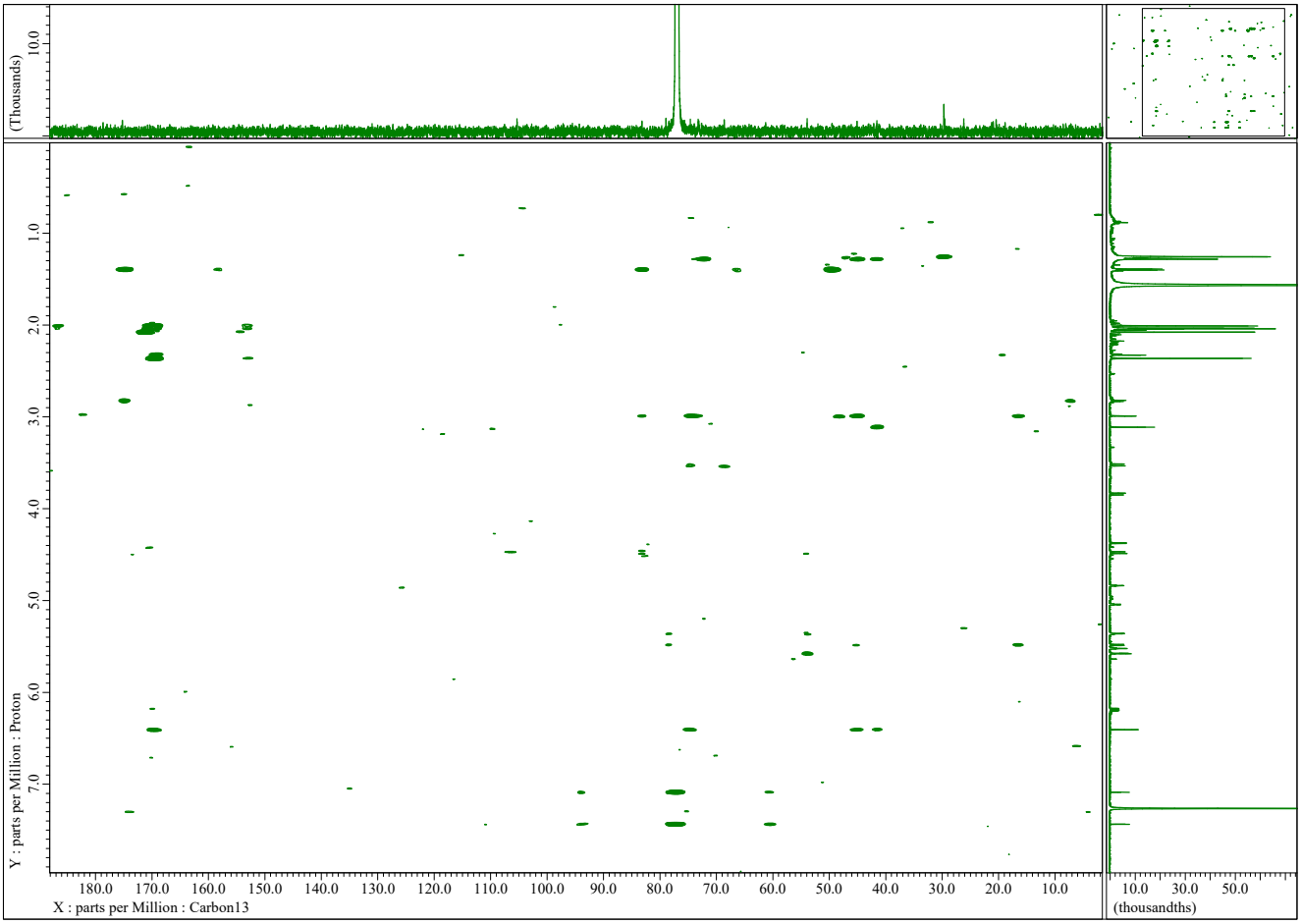
S3. ^{1}H NMR spectrum (400 MHz) of compound **4** in $CDCl_3$



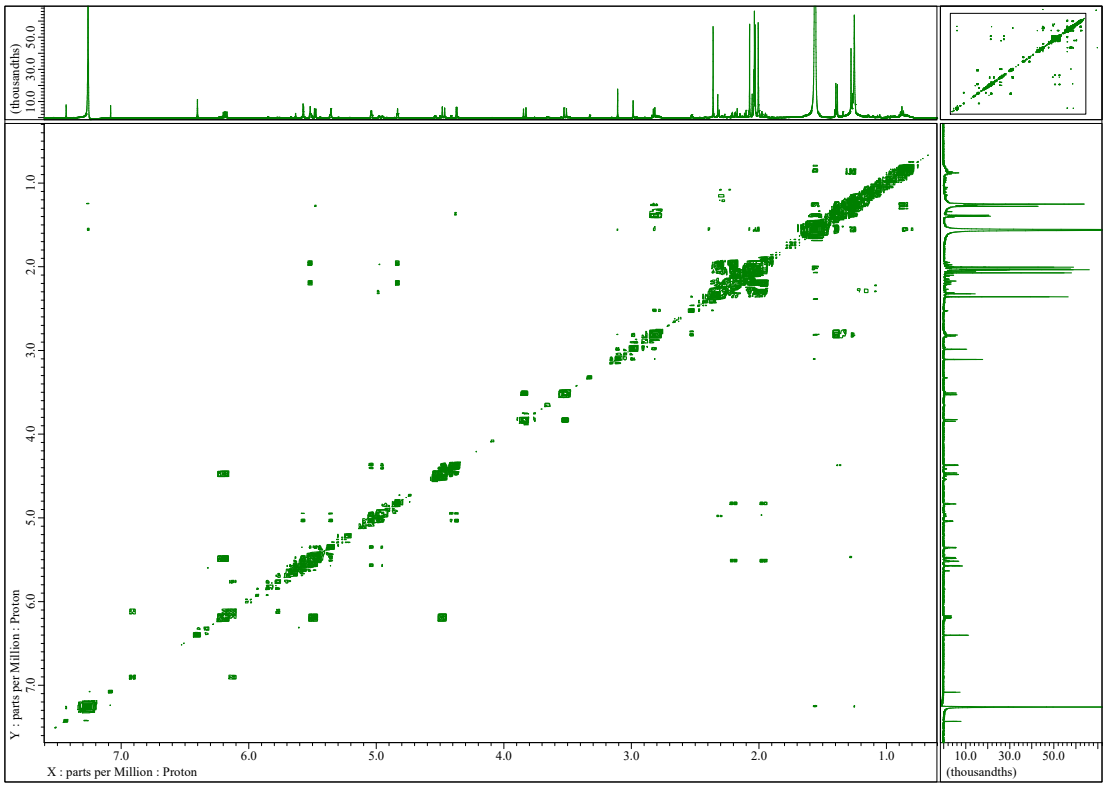
S4. ^{13}C NMR spectrum (100 MHz) of compound **4** in $CDCl_3$



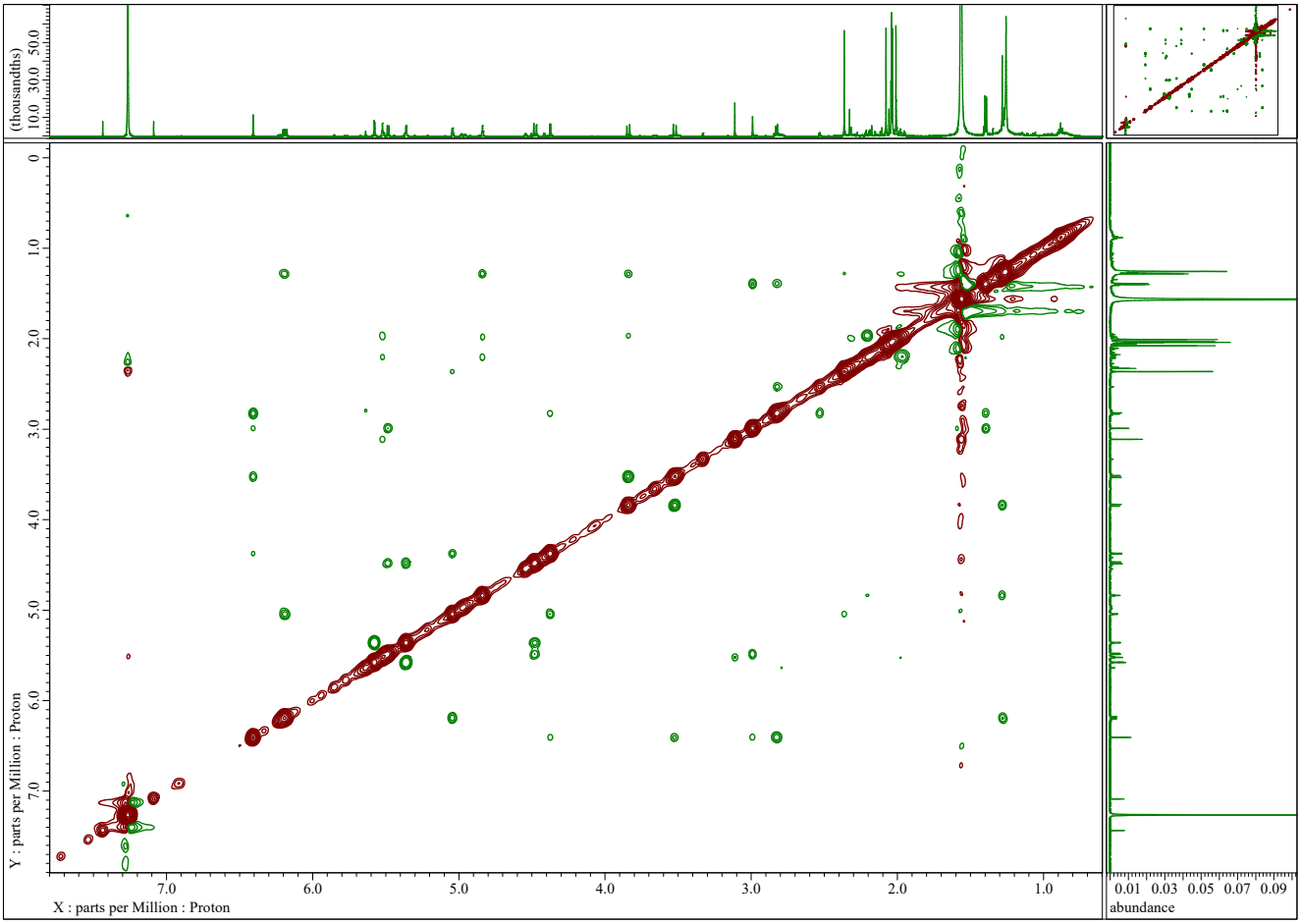
S5. HSQC spectrum of compound **4** in $CDCl_3$



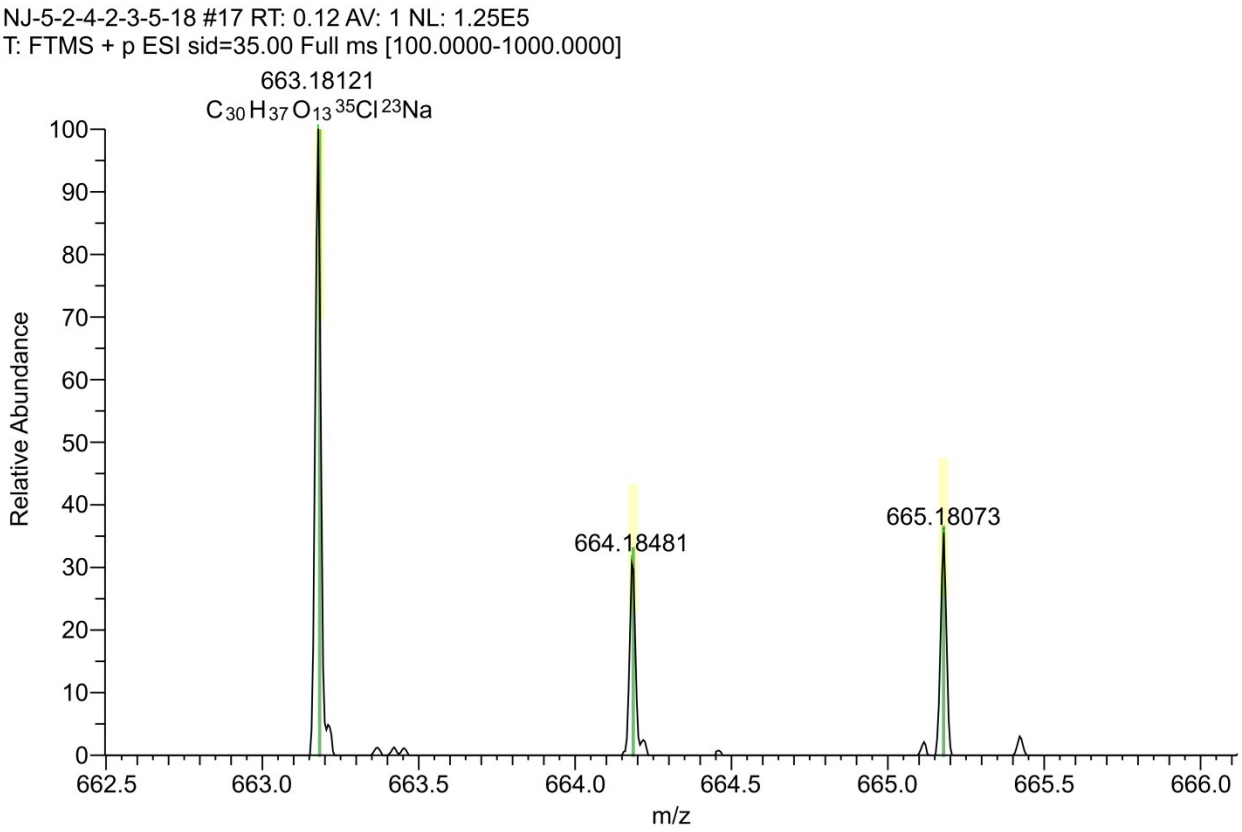
S6. HMBC spectrum of compound **4** in $CDCl_3$



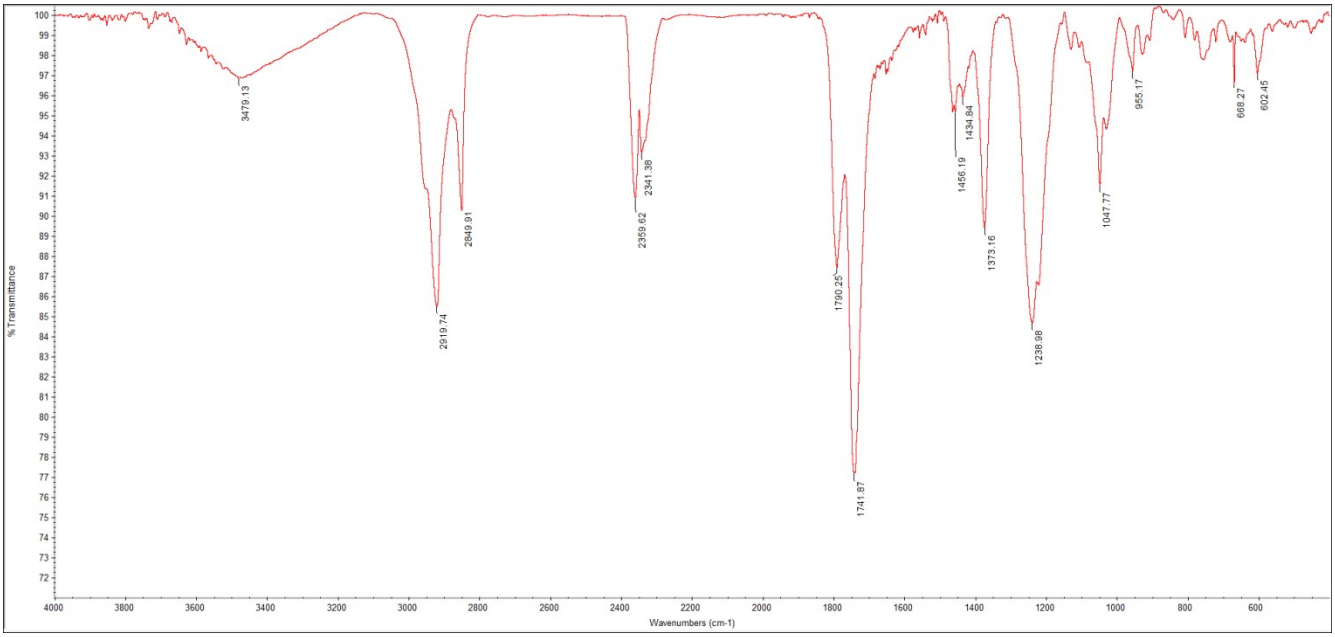
S7. ^{1}H-^{1}H COSY spectrum of compound **4** in $CDCl_3$



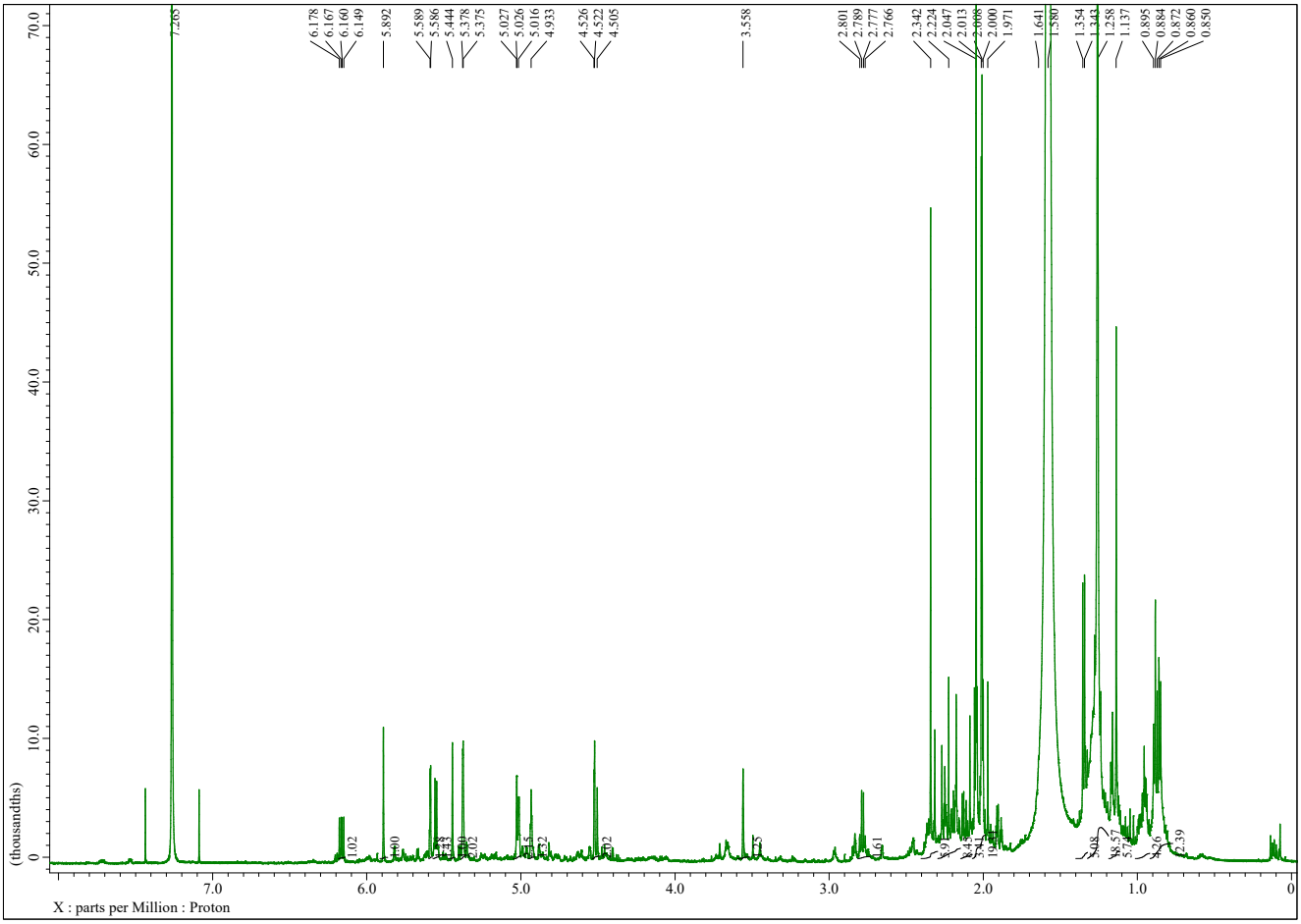
S8. NOESY spectrum of compound **4** in $CDCl_3$



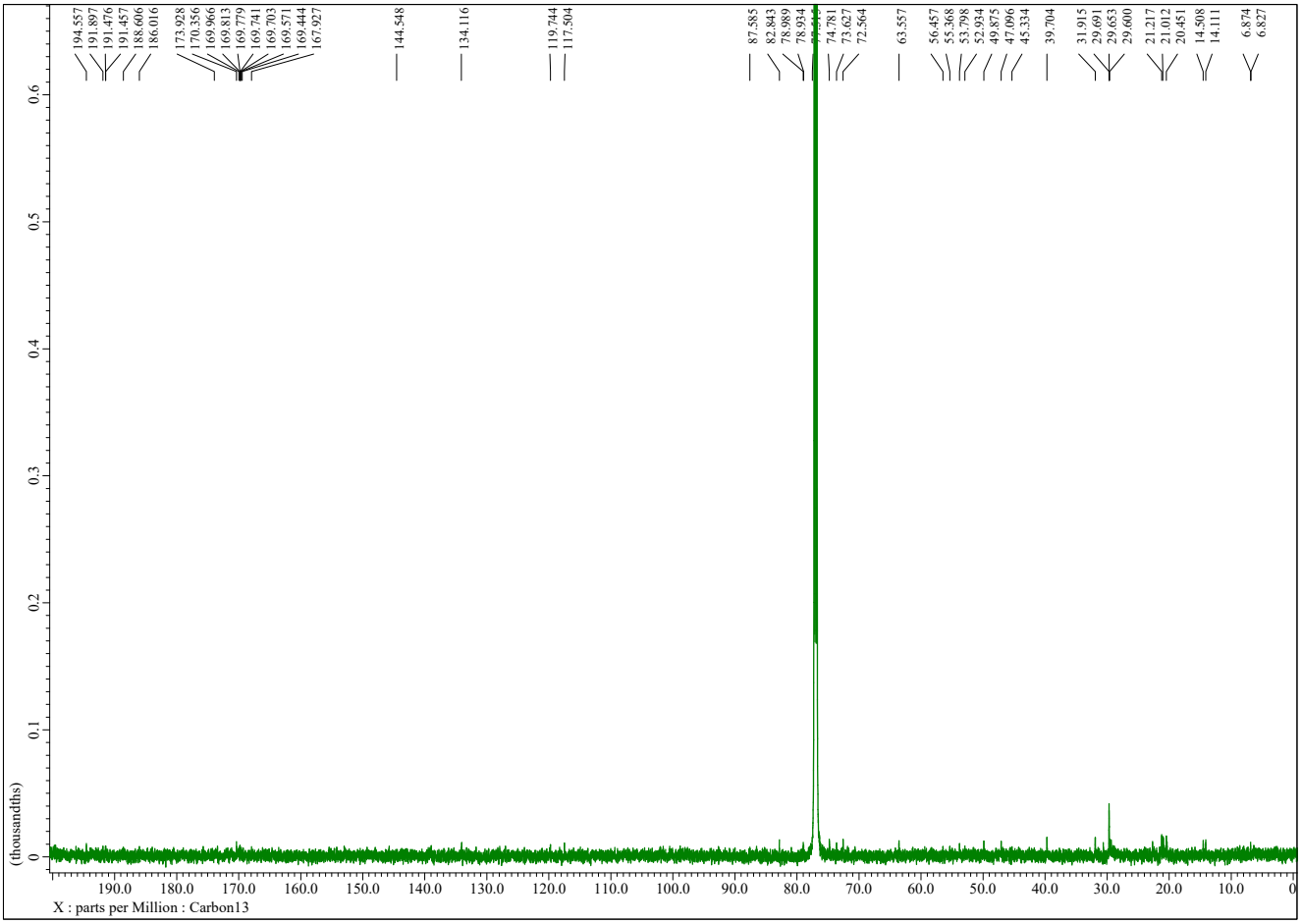
S9. HRESIMS spectrum of compound **5**



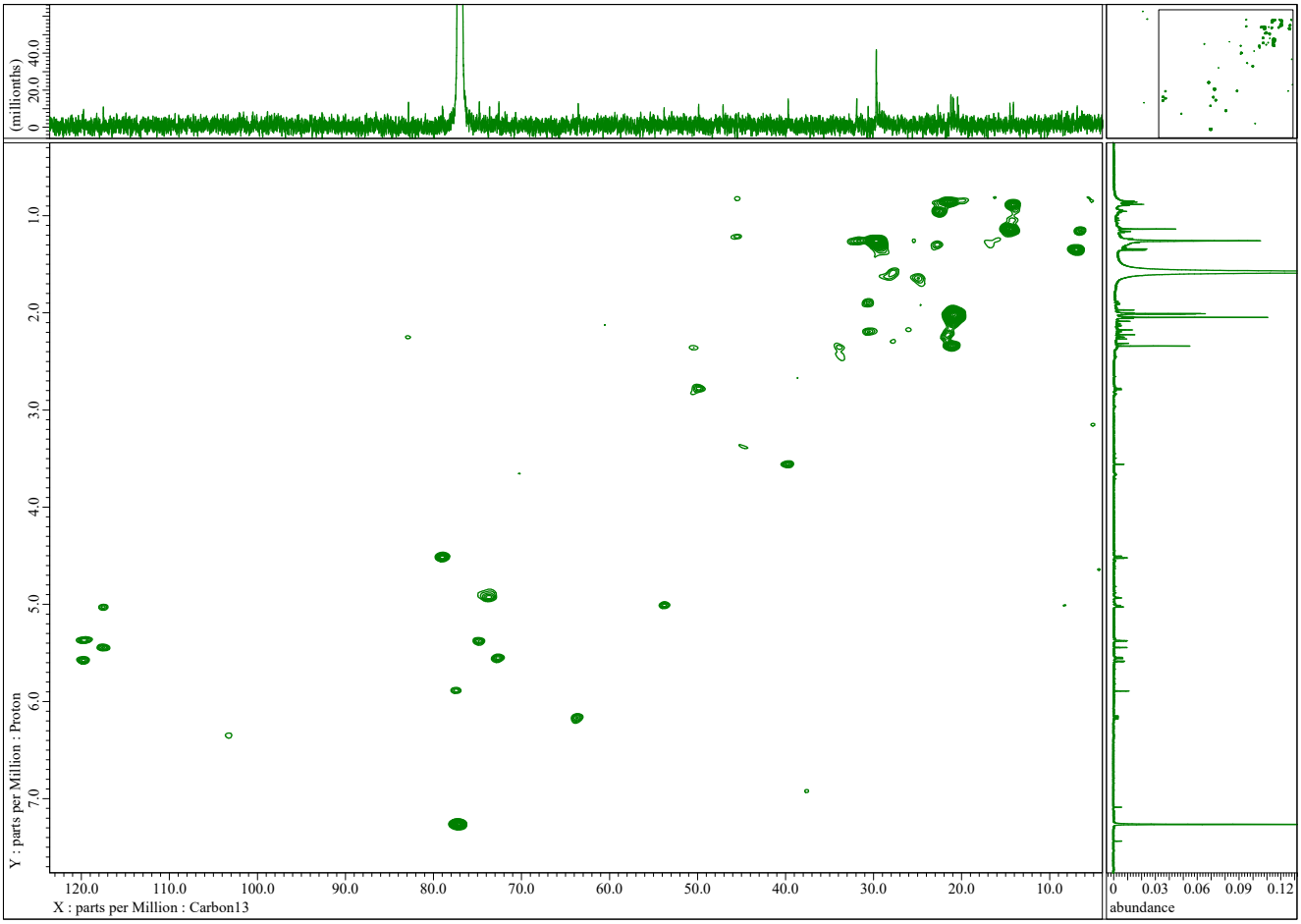
S10. IR spectrum of compound **5**



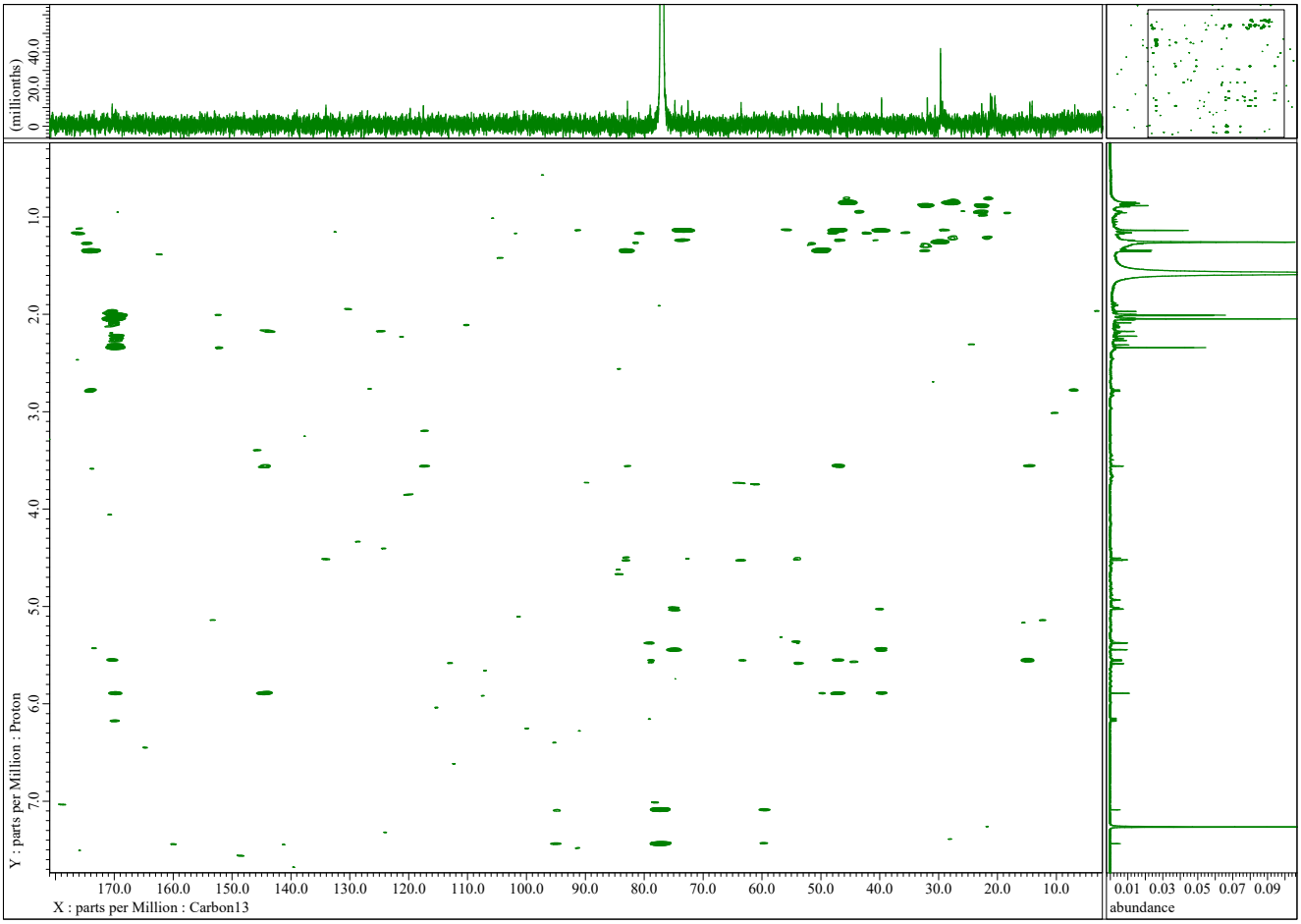
S11. ^{1}H NMR spectrum (600 MHz) of compound **5** in $CDCl_3$



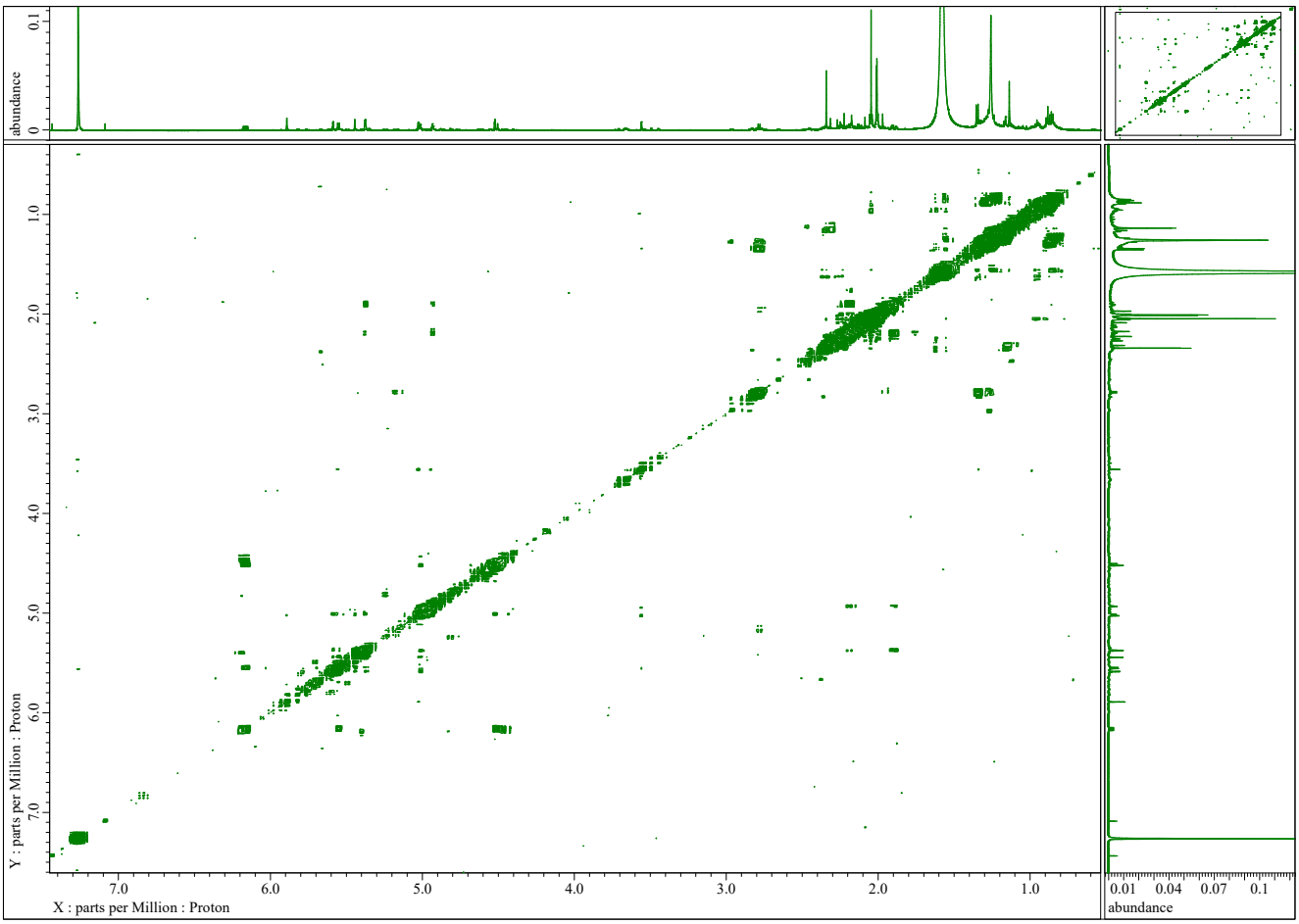
S12. ^{13}C NMR spectrum (600 MHz) of compound **5** in $CDCl_3$



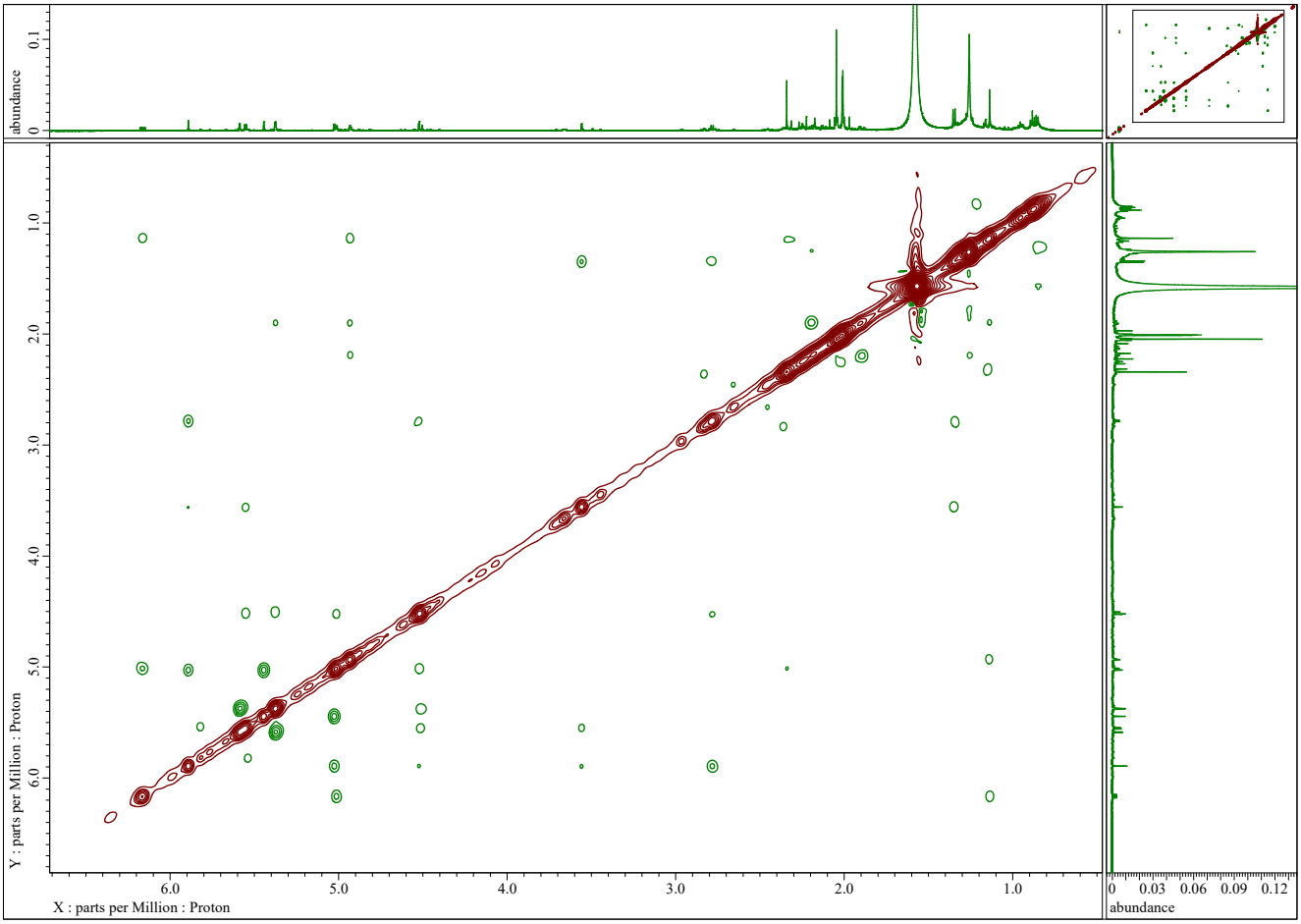
S13. HSQC spectrum of compound **5** in $CDCl_3$



S14. HMBC spectrum of compound **5** in $CDCl_3$



S15. ^{1}H-^{1}H COSY spectrum of compound **5** in $CDCl_3$



S16. NOESY spectrum of compound **5** in $CDCl_3$

S17. Single-crystal X-ray Crystallography of compound **1**

Table 1. Crystal data and structure refinement for ic22450.

Identification code	ic22450	
Empirical formula	$C_{30}\ H_{38}\ Cl\ O_{14.50}$	
Formula weight	666.05	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 12.2945(2) Å	a= 90°.
	b = 12.4454(2) Å	b= 90°.
	c = 22.2997(4) Å	g = 90°.
Volume	3412.08(10) $Å^3$	
Z	4	
Density (calculated)	1.297 Mg/m^3	
Absorption coefficient	1.567 mm^{-1}	
F(000)	1404	
Crystal size	0.363 x 0.235 x 0.198 mm^3	
Theta range for data collection	4.068 to 68.349°.	
Index ranges	-14<=h<=13, -15<=k<=15, -26<=l<=26	
Reflections collected	34394	
Independent reflections	6232 [R(int) = 0.0329]	
Completeness to theta = 67.679°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9798 and 0.7879	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6232 / 6 / 425	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0292, wR2 = 0.0758	
R indices (all data)	R1 = 0.0310, wR2 = 0.0772	
Absolute structure parameter	0.000(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.224 and -0.201 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ic22450. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	11115(1)	7069(1)	6745(1)	49(1)
O(1)	7588(2)	2488(1)	6082(1)	45(1)
O(2)	7107(2)	2483(2)	7053(1)	70(1)
O(3)	9367(1)	3220(1)	6504(1)	36(1)
O(4)	10795(2)	3752(2)	5945(1)	52(1)
O(5)	7754(1)	5669(1)	6612(1)	30(1)
O(6)	8841(1)	7750(1)	6771(1)	36(1)
O(7)	8854(1)	5602(1)	5282(1)	30(1)
O(8)	9133(2)	7002(2)	4660(1)	53(1)
O(9)	6154(1)	6617(1)	4702(1)	41(1)
O(10)	4470(1)	5301(1)	5288(1)	39(1)
O(11)	3203(2)	5834(2)	4629(1)	61(1)
O(12)	5381(1)	3653(1)	5953(1)	38(1)
O(13)	4785(2)	1951(2)	6012(1)	69(1)
O(14)	7391(2)	8523(1)	7180(1)	46(1)
C(1)	7114(2)	3988(2)	5466(1)	30(1)
C(2)	7568(2)	3647(2)	6088(1)	32(1)
C(3)	8711(2)	4073(2)	6256(1)	31(1)
C(4)	8593(2)	4909(2)	6759(1)	32(1)
C(5)	9638(2)	5449(2)	6925(1)	36(1)
C(6)	9995(2)	6279(2)	6476(1)	36(1)
C(7)	9074(2)	7017(2)	6283(1)	32(1)
C(8)	7979(2)	6449(2)	6160(1)	28(1)
C(9)	7841(2)	6045(2)	5508(1)	27(1)
C(10)	6893(2)	5235(2)	5434(1)	27(1)
C(11)	6238(2)	5500(2)	4864(1)	31(1)
C(12)	5168(2)	4921(2)	4809(1)	35(1)
C(13)	5329(2)	3722(2)	4869(1)	39(1)
C(14)	5995(2)	3410(2)	5414(1)	35(1)
C(15)	7833(2)	3552(2)	4954(1)	36(1)
C(16)	10193(2)	5142(2)	7404(1)	51(1)

C(17)	7176(2)	7370(2)	6299(1)	32(1)
C(18)	6000(2)	7102(2)	6453(1)	42(1)
C(19)	7762(2)	7948(2)	6800(1)	34(1)
C(20)	6724(2)	5893(2)	4306(1)	40(1)
C(21)	7324(2)	2004(2)	6606(1)	56(1)
C(22)	7335(4)	813(2)	6540(2)	92(1)
C(23)	10417(2)	3182(2)	6326(1)	38(1)
C(24)	11023(2)	2346(2)	6672(1)	53(1)
C(25)	9412(2)	6152(2)	4851(1)	35(1)
C(26)	10376(2)	5515(2)	4654(1)	51(1)
C(27)	3501(2)	5710(2)	5138(1)	41(1)
C(28)	2850(2)	5956(2)	5685(1)	54(1)
C(29)	4814(2)	2844(2)	6209(1)	50(1)
C(30)	4264(3)	3227(3)	6765(2)	80(1)
O(15)	6829(11)	5507(10)	8431(6)	116(3)
O(15')	6412(13)	3418(13)	8147(6)	116(3)

Table 3. Bond lengths [Å] and angles [°] for ic22450.

Cl(1)-C(6)	1.794(2)
O(1)-C(21)	1.352(3)
O(1)-C(2)	1.443(2)
O(2)-C(21)	1.193(4)
O(3)-C(23)	1.351(3)
O(3)-C(3)	1.444(2)
O(4)-C(23)	1.201(3)
O(5)-C(8)	1.426(2)
O(5)-C(4)	1.438(2)
O(6)-C(19)	1.351(3)
O(6)-C(7)	1.450(2)
O(7)-C(25)	1.365(3)
O(7)-C(9)	1.452(2)
O(8)-C(25)	1.190(3)
O(9)-C(11)	1.440(3)
O(9)-C(20)	1.443(3)
O(10)-C(27)	1.339(3)
O(10)-C(12)	1.450(3)
O(11)-C(27)	1.202(3)
O(12)-C(29)	1.351(3)
O(12)-C(14)	1.452(3)
O(13)-C(29)	1.196(4)
O(14)-C(19)	1.200(3)
C(1)-C(15)	1.542(3)
C(1)-C(2)	1.553(3)
C(1)-C(14)	1.557(3)
C(1)-C(10)	1.577(3)
C(2)-C(3)	1.548(3)
C(3)-C(4)	1.537(3)
C(4)-C(5)	1.497(3)
C(5)-C(16)	1.325(3)
C(5)-C(6)	1.504(3)
C(6)-C(7)	1.519(3)
C(7)-C(8)	1.545(3)

C(8)-C(17)	1.544(3)
C(8)-C(9)	1.546(3)
C(9)-C(10)	1.550(3)
C(10)-C(11)	1.540(3)
C(11)-C(20)	1.465(3)
C(11)-C(12)	1.505(3)
C(12)-C(13)	1.512(3)
C(13)-C(14)	1.515(3)
C(17)-C(19)	1.510(3)
C(17)-C(18)	1.523(3)
C(21)-C(22)	1.490(4)
C(23)-C(24)	1.495(3)
C(25)-C(26)	1.492(3)
C(27)-C(28)	1.490(4)
C(29)-C(30)	1.489(4)

C(21)-O(1)-C(2)	115.7(2)
C(23)-O(3)-C(3)	116.52(17)
C(8)-O(5)-C(4)	118.08(16)
C(19)-O(6)-C(7)	110.13(16)
C(25)-O(7)-C(9)	119.05(16)
C(11)-O(9)-C(20)	61.06(14)
C(27)-O(10)-C(12)	117.79(18)
C(29)-O(12)-C(14)	117.56(19)
C(15)-C(1)-C(2)	110.97(17)
C(15)-C(1)-C(14)	106.74(17)
C(2)-C(1)-C(14)	104.99(17)
C(15)-C(1)-C(10)	114.28(17)
C(2)-C(1)-C(10)	111.79(16)
C(14)-C(1)-C(10)	107.44(16)
O(1)-C(2)-C(3)	109.24(17)
O(1)-C(2)-C(1)	105.75(17)
C(3)-C(2)-C(1)	116.67(18)
O(3)-C(3)-C(4)	105.66(16)
O(3)-C(3)-C(2)	110.35(16)
C(4)-C(3)-C(2)	108.82(17)

O(5)-C(4)-C(5)	112.08(17)
O(5)-C(4)-C(3)	110.22(16)
C(5)-C(4)-C(3)	113.78(18)
C(16)-C(5)-C(4)	120.8(2)
C(16)-C(5)-C(6)	125.8(2)
C(4)-C(5)-C(6)	113.26(18)
C(5)-C(6)-C(7)	112.74(19)
C(5)-C(6)-Cl(1)	112.19(15)
C(7)-C(6)-Cl(1)	109.62(16)
O(6)-C(7)-C(6)	108.31(16)
O(6)-C(7)-C(8)	104.42(16)
C(6)-C(7)-C(8)	115.04(17)
O(5)-C(8)-C(17)	103.82(15)
O(5)-C(8)-C(7)	110.76(16)
C(17)-C(8)-C(7)	100.45(16)
O(5)-C(8)-C(9)	114.94(16)
C(17)-C(8)-C(9)	111.13(16)
C(7)-C(8)-C(9)	114.26(16)
O(7)-C(9)-C(8)	110.82(16)
O(7)-C(9)-C(10)	111.16(15)
C(8)-C(9)-C(10)	113.22(15)
C(11)-C(10)-C(9)	110.04(16)
C(11)-C(10)-C(1)	109.74(16)
C(9)-C(10)-C(1)	120.41(17)
O(9)-C(11)-C(20)	59.58(14)
O(9)-C(11)-C(12)	112.25(18)
C(20)-C(11)-C(12)	116.52(19)
O(9)-C(11)-C(10)	116.77(17)
C(20)-C(11)-C(10)	123.97(19)
C(12)-C(11)-C(10)	115.04(18)
O(10)-C(12)-C(11)	107.49(17)
O(10)-C(12)-C(13)	109.50(19)
C(11)-C(12)-C(13)	110.51(19)
C(12)-C(13)-C(14)	113.25(19)
O(12)-C(14)-C(13)	109.27(18)
O(12)-C(14)-C(1)	107.46(16)

C(13)-C(14)-C(1)	114.80(18)
C(19)-C(17)-C(18)	113.01(18)
C(19)-C(17)-C(8)	101.41(17)
C(18)-C(17)-C(8)	119.27(18)
O(14)-C(19)-O(6)	121.0(2)
O(14)-C(19)-C(17)	128.7(2)
O(6)-C(19)-C(17)	110.29(18)
O(9)-C(20)-C(11)	59.37(13)
O(2)-C(21)-O(1)	123.6(3)
O(2)-C(21)-C(22)	125.6(3)
O(1)-C(21)-C(22)	110.8(3)
O(4)-C(23)-O(3)	123.9(2)
O(4)-C(23)-C(24)	125.7(2)
O(3)-C(23)-C(24)	110.4(2)
O(8)-C(25)-O(7)	123.5(2)
O(8)-C(25)-C(26)	126.5(2)
O(7)-C(25)-C(26)	110.0(2)
O(11)-C(27)-O(10)	123.7(2)
O(11)-C(27)-C(28)	125.6(2)
O(10)-C(27)-C(28)	110.6(2)
O(13)-C(29)-O(12)	123.6(3)
O(13)-C(29)-C(30)	126.1(3)
O(12)-C(29)-C(30)	110.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ic22450. 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}
Cl(1)	35(1)	61(1)	51(1)	-6(1)	-9(1)	-9(1)
O(1)	53(1)	27(1)	54(1)	3(1)	-15(1)	-2(1)
O(2)	83(2)	69(1)	59(1)	29(1)	-3(1)	-10(1)
O(3)	36(1)	34(1)	38(1)	5(1)	-5(1)	7(1)
O(4)	40(1)	59(1)	58(1)	9(1)	5(1)	6(1)
O(5)	31(1)	31(1)	27(1)	4(1)	1(1)	3(1)
O(6)	41(1)	35(1)	33(1)	-5(1)	-2(1)	-1(1)
O(7)	24(1)	35(1)	29(1)	2(1)	4(1)	2(1)
O(8)	50(1)	47(1)	62(1)	18(1)	20(1)	3(1)
O(9)	40(1)	40(1)	41(1)	6(1)	-8(1)	6(1)
O(10)	27(1)	52(1)	38(1)	-1(1)	-1(1)	7(1)
O(11)	40(1)	81(1)	63(1)	8(1)	-13(1)	15(1)
O(12)	34(1)	43(1)	38(1)	1(1)	6(1)	-6(1)
O(13)	80(2)	58(1)	70(1)	5(1)	4(1)	-32(1)
O(14)	60(1)	38(1)	40(1)	-9(1)	7(1)	4(1)
C(1)	27(1)	32(1)	29(1)	-3(1)	1(1)	0(1)
C(2)	35(1)	26(1)	35(1)	3(1)	-2(1)	1(1)
C(3)	32(1)	28(1)	34(1)	4(1)	-5(1)	4(1)
C(4)	34(1)	32(1)	31(1)	3(1)	-4(1)	5(1)
C(5)	36(1)	37(1)	36(1)	-6(1)	-6(1)	6(1)
C(6)	29(1)	43(1)	35(1)	-7(1)	-4(1)	-1(1)
C(7)	34(1)	33(1)	27(1)	-2(1)	0(1)	-3(1)
C(8)	28(1)	32(1)	25(1)	2(1)	1(1)	2(1)
C(9)	24(1)	30(1)	27(1)	1(1)	1(1)	3(1)
C(10)	24(1)	33(1)	24(1)	-1(1)	1(1)	2(1)
C(11)	28(1)	36(1)	29(1)	0(1)	-2(1)	5(1)
C(12)	27(1)	49(1)	30(1)	-2(1)	-4(1)	2(1)
C(13)	31(1)	47(1)	39(1)	-9(1)	-2(1)	-3(1)
C(14)	34(1)	34(1)	36(1)	-5(1)	2(1)	-1(1)
C(15)	33(1)	38(1)	37(1)	-6(1)	2(1)	6(1)
C(16)	56(2)	50(1)	47(1)	-1(1)	-21(1)	5(1)

C(17)	37(1)	30(1)	28(1)	2(1)	3(1)	6(1)
C(18)	35(1)	46(1)	44(1)	-6(1)	4(1)	6(1)
C(19)	44(1)	26(1)	32(1)	5(1)	3(1)	2(1)
C(20)	38(1)	53(1)	31(1)	4(1)	-2(1)	0(1)
C(21)	52(2)	45(1)	69(2)	23(1)	-26(1)	-13(1)
C(22)	113(3)	42(2)	120(3)	29(2)	-59(3)	-17(2)
C(23)	38(1)	39(1)	37(1)	-8(1)	-8(1)	7(1)
C(24)	52(2)	61(2)	47(1)	-3(1)	-12(1)	23(1)
C(25)	29(1)	42(1)	32(1)	0(1)	5(1)	-5(1)
C(26)	35(1)	63(2)	55(1)	2(1)	17(1)	4(1)
C(27)	26(1)	38(1)	58(2)	4(1)	-2(1)	-1(1)
C(28)	33(1)	57(2)	72(2)	3(1)	12(1)	5(1)
C(29)	41(1)	63(2)	46(1)	9(1)	-1(1)	-14(1)
C(30)	72(2)	109(3)	60(2)	4(2)	28(2)	-23(2)
O(15)	116(6)	112(6)	119(6)	-20(5)	-16(5)	24(5)
O(15')	116(6)	112(6)	119(6)	-20(5)	-16(5)	24(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ic22450.

	x	y	z	U(eq)
H(2)	7043	3886	6403	39
H(3)	9075	4398	5898	38
H(4)	8340	4511	7124	39
H(6)	10250	5887	6111	43
H(7)	9300	7434	5920	38
H(9)	7664	6685	5256	33
H(10)	6388	5389	5775	33
H(12)	4828	5088	4412	42
H(13A)	5696	3450	4504	47
H(13B)	4608	3370	4894	47
H(14)	6126	2617	5400	42
H(15A)	7530	3777	4568	54
H(15B)	8572	3837	4997	54
H(15C)	7852	2766	4974	54
H(16A)	9929	4572	7648	62
H(16B)	10856	5492	7505	62
H(17)	7167	7860	5944	38
H(18A)	5983	6511	6744	62
H(18B)	5614	6886	6088	62
H(18C)	5646	7736	6626	62
H(20A)	7526	5948	4287	48
H(20B)	6366	5694	3924	48
H(22A)	7200	478	6930	137
H(22B)	8046	582	6388	137
H(22C)	6766	594	6257	137
H(24A)	11694	2161	6459	80
H(24B)	10569	1703	6714	80
H(24C)	11203	2626	7071	80
H(26A)	10186	5094	4297	77
H(26B)	10599	5030	4977	77

H(26C)	10976	6004	4557	77
H(28A)	2357	6557	5601	81
H(28B)	3340	6152	6014	81
H(28C)	2425	5322	5799	81
H(30A)	3989	2609	6991	121
H(30B)	3656	3698	6656	121
H(30C)	4785	3626	7012	121
H(15D)	6411	5588	8762	173
H(15E)	6358	5192	8120	173
H(15F)	6969	2983	8041	173
H(15G)	6720	4240	8039	173

S18. Single-crystal X-ray Crystallography of compound **2**

Table 1. Crystal data and structure refinement for ic22479.

Identification code	.ic22479	
Empirical formula	$C_{28}\ H_{35}\ Cl\ O_{12}$	
Formula weight	599.01	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Hexagonal	
Space group	$P6_1$	
Unit cell dimensions	a = 22.8317(3) Å	a= 90°.
	b = 22.8317(3) Å	b= 90°.
	c = 10.2937(2) Å	g = 120°.
Volume	4647.06(15) $Å^3$	
Z	6	
Density (calculated)	1.284 Mg/m^3	
Absorption coefficient	1.605 mm^{-1}	
F(000)	1896	
Crystal size	0.191 x 0.102 x 0.049 mm^3	
Theta range for data collection	3.872 to 74.402°.	
Index ranges	-28<=h<=27, -28<=k<=27, -12<=l<=11	
Reflections collected	47636	
Independent reflections	6221 [R(int) = 0.0562]	
Completeness to theta = 67.679°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9819 and 0.8637	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6221 / 1 / 377	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0960	
R indices (all data)	R1 = 0.0393, wR2 = 0.0989	
Absolute structure parameter	-0.002(13)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.199 and -0.224 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ic22479. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	8378(1)	6762(1)	397(1)	46(1)
O(1)	8199(1)	7200(1)	6527(2)	36(1)
O(2)	7695(2)	7609(2)	5234(3)	77(1)
O(3)	8551(1)	5564(1)	536(2)	43(1)
O(4)	7626(1)	5721(1)	2634(2)	31(1)
O(5)	9004(1)	6040(1)	4397(2)	31(1)
O(6)	9423(1)	5336(1)	4238(3)	58(1)
O(7)	7497(1)	4237(1)	5296(2)	45(1)
O(8)	6447(1)	5025(1)	8371(2)	34(1)
O(9)	6980(1)	5411(2)	10248(2)	60(1)
O(10)	6828(1)	5869(1)	6393(2)	30(1)
O(11)	6682(1)	6445(1)	8025(3)	54(1)
O(12)	7828(2)	4548(1)	-225(2)	60(1)
C(1)	7991(1)	6062(1)	6199(2)	25(1)
C(2)	8122(1)	6722(1)	5506(2)	29(1)
C(3)	8741(1)	7047(1)	4670(3)	32(1)
C(4)	8682(1)	7072(1)	3398(3)	34(1)
C(5)	9216(1)	7171(1)	2473(3)	38(1)
C(6)	8989(1)	6672(2)	1382(3)	38(1)
C(7)	8727(1)	5930(1)	1756(2)	33(1)
C(8)	8111(1)	5510(1)	2688(2)	28(1)
C(9)	8318(1)	5501(1)	4146(2)	26(1)
C(10)	7800(1)	5471(1)	5185(2)	25(1)
C(11)	7521(1)	4802(1)	5952(3)	32(1)
C(12)	6892(1)	4624(1)	6721(3)	36(1)
C(13)	7075(1)	5169(1)	7727(2)	30(1)
C(14)	7375(1)	5867(1)	7114(2)	26(1)
C(15)	8583(1)	6190(1)	7094(3)	32(1)
C(16)	9864(2)	7627(2)	2586(4)	62(1)
C(17)	7829(1)	4792(1)	2088(3)	36(1)
C(18)	7081(2)	4286(2)	2276(3)	48(1)

C(19)	8039(2)	4924(2)	681(3)	43(1)
C(20)	7949(2)	4532(2)	6380(3)	45(1)
C(21)	7984(2)	7636(2)	6217(4)	49(1)
C(22)	8173(3)	8157(2)	7267(5)	74(1)
C(23)	9503(1)	5888(2)	4421(3)	37(1)
C(24)	10172(2)	6514(2)	4651(3)	49(1)
C(25)	6482(1)	5205(1)	9608(3)	37(1)
C(26)	5826(2)	5129(2)	10077(4)	56(1)
C(27)	6481(1)	6115(1)	7050(3)	37(1)
C(28)	5809(2)	5889(2)	6434(4)	50(1)

Table 3. Bond lengths [Å] and angles [°] for ic22479.

Cl(1)-C(6)	1.818(3)
O(1)-C(21)	1.351(4)
O(1)-C(2)	1.461(3)
O(2)-C(21)	1.192(5)
O(3)-C(19)	1.348(4)
O(3)-C(7)	1.450(3)
O(4)-C(8)	1.410(3)
O(5)-C(23)	1.347(3)
O(5)-C(9)	1.452(3)
O(6)-C(23)	1.195(4)
O(7)-C(11)	1.434(3)
O(7)-C(20)	1.439(4)
O(8)-C(25)	1.328(3)
O(8)-C(13)	1.460(3)
O(9)-C(25)	1.190(4)
O(10)-C(27)	1.360(3)
O(10)-C(14)	1.455(3)
O(11)-C(27)	1.199(4)
O(12)-C(19)	1.193(4)
C(1)-C(15)	1.537(3)
C(1)-C(2)	1.556(3)
C(1)-C(14)	1.561(3)
C(1)-C(10)	1.585(3)
C(2)-C(3)	1.496(4)
C(3)-C(4)	1.321(4)
C(4)-C(5)	1.473(4)
C(5)-C(16)	1.322(5)
C(5)-C(6)	1.496(4)
C(6)-C(7)	1.536(4)
C(7)-C(8)	1.572(3)
C(8)-C(17)	1.558(4)
C(8)-C(9)	1.577(3)
C(9)-C(10)	1.570(3)
C(10)-C(11)	1.545(3)

C(11)-C(20)	1.462(4)
C(11)-C(12)	1.507(4)
C(12)-C(13)	1.509(4)
C(13)-C(14)	1.522(4)
C(17)-C(19)	1.508(4)
C(17)-C(18)	1.522(4)
C(21)-C(22)	1.501(5)
C(23)-C(24)	1.500(4)
C(25)-C(26)	1.498(4)
C(27)-C(28)	1.493(4)

C(21)-O(1)-C(2)	115.4(2)
C(19)-O(3)-C(7)	111.7(2)
C(23)-O(5)-C(9)	118.5(2)
C(11)-O(7)-C(20)	61.18(19)
C(25)-O(8)-C(13)	117.8(2)
C(27)-O(10)-C(14)	115.2(2)
C(15)-C(1)-C(2)	111.5(2)
C(15)-C(1)-C(14)	105.85(19)
C(2)-C(1)-C(14)	105.17(18)
C(15)-C(1)-C(10)	113.53(19)
C(2)-C(1)-C(10)	111.12(19)
C(14)-C(1)-C(10)	109.20(18)
O(1)-C(2)-C(3)	108.2(2)
O(1)-C(2)-C(1)	106.66(19)
C(3)-C(2)-C(1)	114.8(2)
C(4)-C(3)-C(2)	120.0(2)
C(3)-C(4)-C(5)	123.5(3)
C(16)-C(5)-C(4)	125.4(3)
C(16)-C(5)-C(6)	119.4(3)
C(4)-C(5)-C(6)	115.1(2)
C(5)-C(6)-C(7)	116.6(2)
C(5)-C(6)-Cl(1)	109.0(2)
C(7)-C(6)-Cl(1)	111.5(2)
O(3)-C(7)-C(6)	105.2(2)
O(3)-C(7)-C(8)	105.7(2)

C(6)-C(7)-C(8)	124.2(2)
O(4)-C(8)-C(17)	111.3(2)
O(4)-C(8)-C(7)	112.6(2)
C(17)-C(8)-C(7)	100.0(2)
O(4)-C(8)-C(9)	109.43(19)
C(17)-C(8)-C(9)	109.4(2)
C(7)-C(8)-C(9)	113.9(2)
O(5)-C(9)-C(10)	112.68(18)
O(5)-C(9)-C(8)	111.21(18)
C(10)-C(9)-C(8)	115.12(19)
C(11)-C(10)-C(9)	108.67(19)
C(11)-C(10)-C(1)	107.88(19)
C(9)-C(10)-C(1)	122.02(19)
O(7)-C(11)-C(20)	59.6(2)
O(7)-C(11)-C(12)	113.7(2)
C(20)-C(11)-C(12)	118.4(2)
O(7)-C(11)-C(10)	117.4(2)
C(20)-C(11)-C(10)	122.6(2)
C(12)-C(11)-C(10)	113.7(2)
C(11)-C(12)-C(13)	107.7(2)
O(8)-C(13)-C(12)	106.8(2)
O(8)-C(13)-C(14)	107.6(2)
C(12)-C(13)-C(14)	112.0(2)
O(10)-C(14)-C(13)	106.02(19)
O(10)-C(14)-C(1)	110.11(18)
C(13)-C(14)-C(1)	114.71(19)
C(19)-C(17)-C(18)	113.4(2)
C(19)-C(17)-C(8)	104.4(2)
C(18)-C(17)-C(8)	117.7(2)
O(12)-C(19)-O(3)	120.8(3)
O(12)-C(19)-C(17)	129.4(3)
O(3)-C(19)-C(17)	109.8(2)
O(7)-C(20)-C(11)	59.24(19)
O(2)-C(21)-O(1)	123.8(3)
O(2)-C(21)-C(22)	125.9(3)
O(1)-C(21)-C(22)	110.3(3)

O(6)-C(23)-O(5)	124.4(3)
O(6)-C(23)-C(24)	125.2(3)
O(5)-C(23)-C(24)	110.3(3)
O(9)-C(25)-O(8)	123.4(3)
O(9)-C(25)-C(26)	124.7(3)
O(8)-C(25)-C(26)	111.8(3)
O(11)-C(27)-O(10)	123.8(3)
O(11)-C(27)-C(28)	125.2(3)
O(10)-C(27)-C(28)	110.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ic22479. 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}
Cl(1)	58(1)	58(1)	31(1)	7(1)	3(1)	35(1)
O(1)	39(1)	33(1)	36(1)	-7(1)	2(1)	18(1)
O(2)	99(2)	82(2)	86(2)	-12(2)	-24(2)	73(2)
O(3)	58(1)	53(1)	26(1)	-1(1)	6(1)	33(1)
O(4)	32(1)	43(1)	22(1)	-1(1)	-2(1)	23(1)
O(5)	26(1)	37(1)	30(1)	-2(1)	0(1)	17(1)
O(6)	44(1)	57(1)	87(2)	9(1)	7(1)	34(1)
O(7)	60(1)	32(1)	45(1)	2(1)	19(1)	25(1)
O(8)	28(1)	42(1)	28(1)	-3(1)	6(1)	14(1)
O(9)	54(1)	97(2)	28(1)	-11(1)	-5(1)	36(1)
O(10)	26(1)	37(1)	29(1)	-2(1)	-3(1)	18(1)
O(11)	50(1)	56(1)	66(2)	-21(1)	0(1)	34(1)
O(12)	92(2)	63(2)	34(1)	-17(1)	-7(1)	44(2)
C(1)	25(1)	31(1)	20(1)	-2(1)	-1(1)	14(1)
C(2)	30(1)	31(1)	26(1)	-3(1)	-2(1)	16(1)
C(3)	31(1)	29(1)	32(1)	-1(1)	1(1)	12(1)
C(4)	37(1)	31(1)	34(1)	1(1)	2(1)	17(1)
C(5)	38(1)	38(1)	34(1)	8(1)	6(1)	15(1)
C(6)	37(1)	48(2)	30(1)	6(1)	10(1)	22(1)
C(7)	38(1)	44(1)	23(1)	2(1)	6(1)	24(1)
C(8)	31(1)	34(1)	24(1)	1(1)	2(1)	19(1)
C(9)	26(1)	30(1)	21(1)	-1(1)	2(1)	14(1)
C(10)	28(1)	31(1)	19(1)	-1(1)	1(1)	16(1)
C(11)	40(1)	29(1)	28(1)	2(1)	10(1)	18(1)
C(12)	40(1)	30(1)	33(1)	2(1)	11(1)	16(1)
C(13)	28(1)	39(1)	22(1)	2(1)	5(1)	16(1)
C(14)	25(1)	34(1)	21(1)	-4(1)	-2(1)	16(1)
C(15)	28(1)	44(1)	25(1)	-2(1)	-1(1)	19(1)
C(16)	48(2)	65(2)	50(2)	-4(2)	9(2)	11(2)
C(17)	45(2)	40(1)	27(1)	-6(1)	-4(1)	24(1)
C(18)	48(2)	38(2)	46(2)	-7(1)	-7(1)	13(1)

C(19)	59(2)	49(2)	33(2)	-4(1)	-2(1)	35(2)
C(20)	62(2)	50(2)	40(2)	15(1)	18(1)	39(2)
C(21)	50(2)	40(2)	64(2)	4(1)	13(2)	28(1)
C(22)	88(3)	50(2)	87(3)	-9(2)	28(2)	37(2)
C(23)	33(1)	54(2)	29(1)	4(1)	2(1)	27(1)
C(24)	32(1)	67(2)	46(2)	-3(2)	-2(1)	22(1)
C(25)	37(1)	40(1)	28(1)	-2(1)	6(1)	14(1)
C(26)	42(2)	58(2)	54(2)	-16(2)	16(1)	17(2)
C(27)	32(1)	36(1)	47(2)	5(1)	6(1)	21(1)
C(28)	37(2)	63(2)	61(2)	15(2)	4(1)	32(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ic22479.

	x	y	z	U(eq)
H(4)	7452	5643	1891	46
H(2)	7719	6622	4964	35
H(3)	9176	7235	5054	39
H(4A)	8272	7024	3061	41
H(6)	9395	6810	819	46
H(7)	9120	5905	2121	40
H(9)	8327	5070	4251	31
H(10)	7408	5433	4680	31
H(12A)	6721	4179	7149	43
H(12B)	6534	4597	6140	43
H(13)	7398	5161	8373	36
H(14)	7521	6212	7824	31
H(15A)	8997	6358	6578	48
H(15B)	8483	5767	7523	48
H(15C)	8646	6527	7752	48
H(16A)	10017	7925	3311	75
H(16B)	10177	7657	1944	75
H(17)	8086	4590	2493	43
H(18A)	6810	4464	1885	72
H(18B)	6980	4210	3207	72
H(18C)	6971	3857	1858	72
H(20A)	8440	4802	6197	55
H(20B)	7830	4274	7205	55
H(22A)	8628	8537	7099	111
H(22B)	8167	7954	8109	111
H(22C)	7848	8318	7277	111
H(24A)	10494	6388	4995	74
H(24B)	10116	6805	5278	74
H(24C)	10344	6759	3830	74
H(26A)	5686	4855	10871	83

H(26B)	5480	4905	9406	83
H(26C)	5885	5576	10261	83
H(28A)	5498	5415	6657	76
H(28B)	5862	5935	5489	76
H(28C)	5625	6169	6753	76