X-Ray Structural Characterization of New Compound 12

General procedures.

A single crystal of suitable size of **12**, coated with dry perfluoropolyether was mounted on a glass fiber and fixed in a cold nitrogen stream [T = 173(2) K] to the goniometer head. Data collections were performed on Bruker-Nonius X8APEX-II CCD diffractometer, using monochromatic radiation λ(Mo $K_{\alpha 1}$) = 0.71073 Å, by means of ω and φ scans. The data were reduced (SAINT)[1] and corrected for Lorentz polarization effects and absorption by multiscan method applied by SADABS[2] . The structure were solved by direct methods (SIR-2002)[3] and refined against all F^2 data by full-matrix least-squares techniques (SHELXTL-6.12).[4] All the non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were included from calculated positions and refined riding on their respective carbon atoms with isotropic displacement parameters.

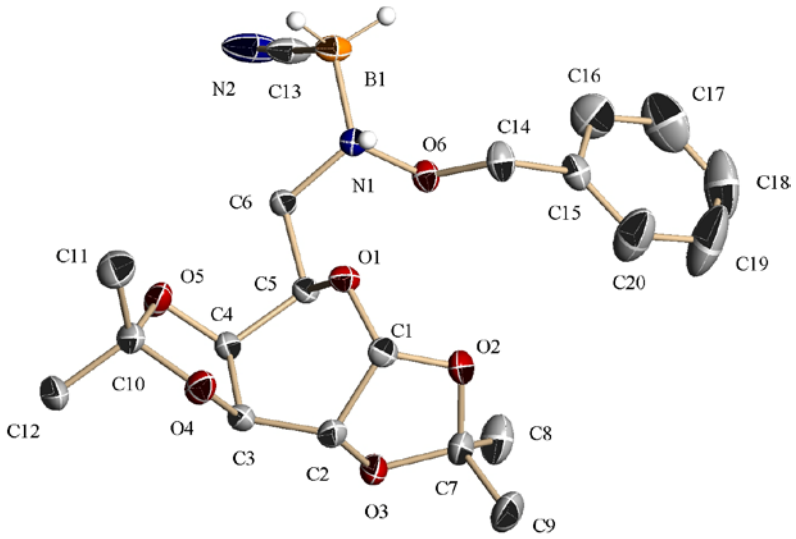


Figure 1. ORTEP drawing of **12** showing thermal ellipsoids at the 50% probability level.

1. SAINT 6.02, BRUKER-AXS, Inc., Madison, WI 53711-5373 USA, 1997–1999.

2. SADABS George Sheldrick, Bruker AXS, Inc., Madison,Wisconsin, USA, 1999.

3. M.C.Burla, M. Camalli, B. Carrozzini, G.L. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna SIR2002: the program; *J. Appl. Cryst*, 2003, **36**, 1103.

4. SHELXTL 6.14, Bruker AXS, Inc., Madison, Wisconsin, USA, 2000–2003.

Table 1. Crystal data and structure refinement for **12**.

Empirical formula	$C_{20}H_{29}BN_2O_6$	
Formula weight	404.26	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 8.5632(3) Å	α= 90°.
	b = 11.8122(4) Å	β= 91.6900(10)°.
	c = 10.9084(4) Å	γ = 90°.
Volume	1102.91(7) $Å^3$	
Z	2	
Density (calculated)	1.217 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	432	
Crystal size	0.50 x 0.50 x 0.45 mm^3	
Theta range for data collection	2.54 to 30.51°.	
Index ranges	-12<=h<=7, -12<=k<=16, -15<=l<=12	
Reflections collected	15535	
Independent reflections	3469 [R(int) = 0.0188]	
Completeness to theta = 30.51°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9612 and 0.9570	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3469 / 1 / 266	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0339, wR2 = 0.0863	
R indices (all data)	R1 = 0.0368, wR2 = 0.0889	
Largest diff. peak and hole	0.232 and -0.155 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12** U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3102(1)	3280(1)	1173(1)	23(1)
O(2)	3990(1)	2918(1)	3168(1)	32(1)
O(3)	6373(1)	3528(1)	2612(1)	31(1)
O(4)	5704(1)	2540(1)	-482(1)	29(1)
O(5)	4607(1)	4196(1)	-1108(1)	32(1)
O(6)	1113(1)	5239(1)	2285(1)	23(1)
N(1)	851(1)	4910(1)	1015(1)	19(1)
N(2)	130(2)	7709(1)	-187(2)	52(1)
C(1)	4104(2)	2614(1)	1918(1)	25(1)
C(2)	5848(2)	2784(1)	1660(1)	26(1)
C(3)	6138(2)	3345(1)	446(1)	24(1)
C(4)	5083(2)	4370(1)	148(1)	22(1)
C(5)	3672(1)	4399(1)	968(1)	19(1)
C(6)	2335(1)	5065(1)	376(1)	21(1)
C(7)	5484(2)	3271(2)	3658(1)	32(1)
C(8)	5290(3)	4338(2)	4390(2)	48(1)
C(9)	6231(3)	2307(2)	4395(2)	50(1)
C(10)	5291(2)	3171(1)	-1550(1)	28(1)
C(11)	4051(2)	2517(2)	-2267(2)	44(1)
C(12)	6729(2)	3446(2)	-2276(1)	38(1)
C(13)	-151(2)	6811(1)	119(2)	33(1)
C(14)	326(2)	4440(1)	3061(1)	30(1)
C(15)	188(2)	4957(1)	4306(1)	30(1)
C(16)	-762(3)	5882(2)	4478(2)	51(1)
C(17)	-974(4)	6312(2)	5644(3)	68(1)
C(18)	-228(4)	5838(3)	6629(2)	73(1)
C(19)	696(5)	4920(3)	6481(2)	91(1)
C(20)	929(4)	4485(2)	5317(2)	63(1)
B(1)	-615(2)	5550(1)	420(2)	26(1)

Table 3. Bond lengths [Å] and angles [°] for **12**.

O(1)-C(1)	1.4052(16)	C(10)-C(11)	1.512(2)
O(1)-C(5)	1.4282(15)	C(10)-C(12)	1.519(2)
O(2)-C(1)	1.4162(18)	C(11)-H(11A)	0.9800
O(2)-C(7)	1.4339(19)	C(11)-H(11B)	0.9800
O(3)-C(2)	1.4232(18)	C(11)-H(11C)	0.9800
O(3)-C(7)	1.4233(18)	C(12)-H(12A)	0.9800
O(4)-C(10)	1.4194(18)	C(12)-H(12B)	0.9800
O(4)-C(3)	1.4303(17)	C(12)-H(12C)	0.9800
O(5)-C(4)	1.4320(17)	C(13)-B(1)	1.578(2)
O(5)-C(10)	1.4353(19)	C(14)-C(15)	1.497(2)
O(6)-C(14)	1.4472(17)	C(14)-H(14A)	0.9900
O(6)-N(1)	1.4506(14)	C(14)-H(14B)	0.9900
N(1)-C(6)	1.4787(16)	C(15)-C(20)	1.374(3)
N(1)-B(1)	1.5872(18)	C(15)-C(16)	1.378(3)
N(1)-H(1N)	0.9300	C(16)-C(17)	1.387(3)
N(2)-C(13)	1.141(2)	C(16)-H(16)	0.9500
C(1)-C(2)	1.5405(19)	C(17)-C(18)	1.355(5)
C(1)-H(1)	1.0000	C(17)-H(17)	0.9500
C(2)-C(3)	1.5081(19)	C(18)-C(19)	1.355(5)
C(2)-H(2)	1.0000	C(18)-H(18)	0.9500
C(3)-C(4)	1.5404(19)	C(19)-C(20)	1.390(3)
C(3)-H(3)	1.0000	C(19)-H(19)	0.9500
C(4)-C(5)	1.5247(17)	C(20)-H(20)	0.9500
C(4)-H(4)	1.0000	B(1)-H(1A)	0.9900
C(5)-C(6)	1.5173(16)	B(1)-H(1B)	0.9900
C(5)-H(5)	1.0000		
C(6)-H(6A)	0.9900	C(1)-O(1)-C(5)	113.79(9)
C(6)-H(6B)	0.9900	C(1)-O(2)-C(7)	110.29(11)
C(7)-C(8)	1.504(3)	C(2)-O(3)-C(7)	106.73(12)
C(7)-C(9)	1.524(2)	C(10)-O(4)-C(3)	106.58(12)
C(8)-H(8A)	0.9800	C(4)-O(5)-C(10)	109.60(11)
C(8)-H(8B)	0.9800	C(14)-O(6)-N(1)	108.80(10)
C(8)-H(8C)	0.9800	O(6)-N(1)-C(6)	107.85(9)
C(9)-H(9A)	0.9800	O(6)-N(1)-B(1)	111.19(10)
C(9)-H(9B)	0.9800	C(6)-N(1)-B(1)	115.38(11)
C(9)-H(9C)	0.9800	O(6)-N(1)-H(1N)	107.4

C(6)-N(1)-H(1N)	107.4	O(3)-C(7)-O(2)	104.81(11)
B(1)-N(1)-H(1N)	107.4	O(3)-C(7)-C(8)	108.50(15)
O(1)-C(1)-O(2)	110.89(12)	O(2)-C(7)-C(8)	109.29(14)
O(1)-C(1)-C(2)	113.57(11)	O(3)-C(7)-C(9)	110.87(14)
O(2)-C(1)-C(2)	103.73(11)	O(2)-C(7)-C(9)	109.56(16)
O(1)-C(1)-H(1)	109.5	C(8)-C(7)-C(9)	113.44(15)
O(2)-C(1)-H(1)	109.5	C(7)-C(8)-H(8A)	109.5
C(2)-C(1)-H(1)	109.5	C(7)-C(8)-H(8B)	109.5
O(3)-C(2)-C(3)	108.18(12)	H(8A)-C(8)-H(8B)	109.5
O(3)-C(2)-C(1)	103.58(11)	C(7)-C(8)-H(8C)	109.5
C(3)-C(2)-C(1)	113.80(11)	H(8A)-C(8)-H(8C)	109.5
O(3)-C(2)-H(2)	110.3	H(8B)-C(8)-H(8C)	109.5
C(3)-C(2)-H(2)	110.3	C(7)-C(9)-H(9A)	109.5
C(1)-C(2)-H(2)	110.3	C(7)-C(9)-H(9B)	109.5
O(4)-C(3)-C(2)	106.44(12)	H(9A)-C(9)-H(9B)	109.5
O(4)-C(3)-C(4)	103.56(10)	C(7)-C(9)-H(9C)	109.5
C(2)-C(3)-C(4)	114.83(11)	H(9A)-C(9)-H(9C)	109.5
O(4)-C(3)-H(3)	110.6	H(9B)-C(9)-H(9C)	109.5
C(2)-C(3)-H(3)	110.6	O(4)-C(10)-O(5)	105.15(11)
C(4)-C(3)-H(3)	110.6	O(4)-C(10)-C(11)	108.11(14)
O(5)-C(4)-C(5)	110.86(10)	O(5)-C(10)-C(11)	108.51(14)
O(5)-C(4)-C(3)	103.76(11)	O(4)-C(10)-C(12)	110.69(12)
C(5)-C(4)-C(3)	111.33(11)	O(5)-C(10)-C(12)	109.89(15)
O(5)-C(4)-H(4)	110.2	C(11)-C(10)-C(12)	114.07(13)
C(5)-C(4)-H(4)	110.2	C(10)-C(11)-H(11A)	109.5
C(3)-C(4)-H(4)	110.2	C(10)-C(11)-H(11B)	109.5
O(1)-C(5)-C(6)	106.82(9)	H(11A)-C(11)-H(11B)	109.5
O(1)-C(5)-C(4)	110.58(10)	C(10)-C(11)-H(11C)	109.5
C(6)-C(5)-C(4)	111.25(10)	H(11A)-C(11)-H(11C)	109.5
O(1)-C(5)-H(5)	109.4	H(11B)-C(11)-H(11C)	109.5
C(6)-C(5)-H(5)	109.4	C(10)-C(12)-H(12A)	109.5
C(4)-C(5)-H(5)	109.4	C(10)-C(12)-H(12B)	109.5
N(1)-C(6)-C(5)	112.53(10)	H(12A)-C(12)-H(12B)	109.5
N(1)-C(6)-H(6A)	109.1	C(10)-C(12)-H(12C)	109.5
C(5)-C(6)-H(6A)	109.1	H(12A)-C(12)-H(12C)	109.5
N(1)-C(6)-H(6B)	109.1	H(12B)-C(12)-H(12C)	109.5
C(5)-C(6)-H(6B)	109.1	N(2)-C(13)-B(1)	174.6(2)
H(6A)-C(6)-H(6B)	107.8	O(6)-C(14)-C(15)	108.34(12)

O(6)-C(14)-H(14A)	110.0	C(17)-C(18)-H(18)	120.0
C(15)-C(14)-H(14A)	110.0	C(19)-C(18)-H(18)	120.0
O(6)-C(14)-H(14B)	110.0	C(18)-C(19)-C(20)	120.4(3)
C(15)-C(14)-H(14B)	110.0	C(18)-C(19)-H(19)	119.8
H(14A)-C(14)-H(14B)	108.4	C(20)-C(19)-H(19)	119.8
C(20)-C(15)-C(16)	118.17(18)	C(15)-C(20)-C(19)	120.5(2)
C(20)-C(15)-C(14)	121.04(16)	C(15)-C(20)-H(20)	119.7
C(16)-C(15)-C(14)	120.67(16)	C(19)-C(20)-H(20)	119.7
C(15)-C(16)-C(17)	120.7(2)	C(13)-B(1)-N(1)	109.48(11)
C(15)-C(16)-H(16)	119.7	C(13)-B(1)-H(1A)	109.8
C(17)-C(16)-H(16)	119.7	N(1)-B(1)-H(1A)	109.8
C(18)-C(17)-C(16)	120.3(3)	C(13)-B(1)-H(1B)	109.8
C(18)-C(17)-H(17)	119.9	N(1)-B(1)-H(1B)	109.8
C(16)-C(17)-H(17)	119.9	H(1A)-B(1)-H(1B)	108.2
C(17)-C(18)-C(19)	119.9(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **12**. 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(1)	19(1)	20(1)	29(1)	5(1)	-1(1)	-1(1)
O(2)	29(1)	44(1)	25(1)	9(1)	6(1)	-1(1)
O(3)	25(1)	48(1)	20(1)	2(1)	0(1)	-5(1)
O(4)	33(1)	31(1)	23(1)	-3(1)	1(1)	7(1)
O(5)	38(1)	40(1)	19(1)	3(1)	2(1)	14(1)
O(6)	26(1)	22(1)	21(1)	-2(1)	3(1)	-3(1)
N(1)	20(1)	16(1)	21(1)	-1(1)	0(1)	0(1)
N(2)	26(1)	27(1)	103(2)	20(1)	-13(1)	1(1)
C(1)	25(1)	22(1)	27(1)	6(1)	2(1)	1(1)
C(2)	24(1)	31(1)	23(1)	3(1)	0(1)	7(1)
C(3)	20(1)	31(1)	21(1)	0(1)	2(1)	4(1)
C(4)	21(1)	25(1)	21(1)	2(1)	3(1)	0(1)
C(5)	19(1)	18(1)	21(1)	1(1)	1(1)	0(1)
C(6)	20(1)	22(1)	22(1)	3(1)	2(1)	3(1)
C(7)	32(1)	43(1)	20(1)	7(1)	2(1)	3(1)
C(8)	67(1)	51(1)	28(1)	-4(1)	6(1)	-4(1)
C(9)	54(1)	66(1)	29(1)	16(1)	1(1)	21(1)
C(10)	26(1)	38(1)	20(1)	-3(1)	2(1)	3(1)
C(11)	40(1)	57(1)	34(1)	-5(1)	-6(1)	-10(1)
C(12)	29(1)	62(1)	23(1)	-3(1)	6(1)	3(1)
C(13)	20(1)	22(1)	56(1)	6(1)	-6(1)	2(1)
C(14)	40(1)	24(1)	27(1)	0(1)	9(1)	-5(1)
C(15)	31(1)	30(1)	28(1)	-1(1)	10(1)	0(1)
C(16)	59(1)	43(1)	50(1)	-9(1)	4(1)	16(1)
C(17)	82(2)	53(1)	72(2)	-25(1)	31(1)	7(1)
C(18)	119(2)	63(2)	40(1)	-19(1)	34(1)	-20(2)
C(19)	160(3)	85(2)	28(1)	0(1)	-1(2)	22(2)
C(20)	92(2)	62(1)	35(1)	-3(1)	-1(1)	29(1)
B(1)	21(1)	19(1)	37(1)	3(1)	-4(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **12**.

	x	y	z	U(eq)
H(1N)	624	4140	1006	23
H(1)	3825	1797	1811	30
H(2)	6417	2046	1720	31
H(3)	7264	3556	387	29
H(4)	5692	5089	235	27
H(5)	3978	4753	1772	23
H(6A)	2610	5879	376	25
H(6B)	2190	4821	-489	25
H(8A)	6319	4620	4663	73
H(8B)	4661	4178	5106	73
H(8C)	4763	4912	3878	73
H(9A)	6361	1648	3861	74
H(9B)	5557	2104	5071	74
H(9C)	7254	2548	4726	74
H(11A)	4476	1786	-2517	65
H(11B)	3724	2950	-2997	65
H(11C)	3148	2393	-1751	65
H(12A)	7494	3843	-1746	57
H(12B)	6432	3929	-2975	57
H(12C)	7191	2742	-2574	57
H(14A)	931	3726	3121	36
H(14B)	-724	4265	2708	36
H(16)	-1276	6228	3792	61
H(17)	-1646	6942	5753	82
H(18)	-353	6149	7424	88
H(19)	1189	4573	7176	109
H(20)	1605	3856	5219	75
H(1A)	-966	5158	-342	31
H(1B)	-1486	5543	996	31

Table 6. Torsion angles [°] for **12**.

C(14)-O(6)-N(1)-C(6)	-138.87(11)
C(14)-O(6)-N(1)-B(1)	93.70(13)
C(5)-O(1)-C(1)-O(2)	76.88(13)
C(5)-O(1)-C(1)-C(2)	-39.45(16)
C(7)-O(2)-C(1)-O(1)	-121.01(13)
C(7)-O(2)-C(1)-C(2)	1.25(15)
C(7)-O(3)-C(2)-C(3)	153.48(12)
C(7)-O(3)-C(2)-C(1)	32.40(14)
O(1)-C(1)-C(2)-O(3)	100.11(13)
O(2)-C(1)-C(2)-O(3)	-20.36(14)
O(1)-C(1)-C(2)-C(3)	-17.11(18)
O(2)-C(1)-C(2)-C(3)	-137.58(13)
C(10)-O(4)-C(3)-C(2)	154.15(10)
C(10)-O(4)-C(3)-C(4)	32.71(13)
O(3)-C(2)-C(3)-O(4)	175.81(10)
C(1)-C(2)-C(3)-O(4)	-69.67(14)
O(3)-C(2)-C(3)-C(4)	-70.24(14)
C(1)-C(2)-C(3)-C(4)	44.28(17)
C(10)-O(5)-C(4)-C(5)	-119.60(13)
C(10)-O(5)-C(4)-C(3)	0.01(14)
O(4)-C(3)-C(4)-O(5)	-19.71(13)
C(2)-C(3)-C(4)-O(5)	-135.34(12)
O(4)-C(3)-C(4)-C(5)	99.58(12)
C(2)-C(3)-C(4)-C(5)	-16.04(16)
C(1)-O(1)-C(5)-C(6)	-168.99(11)
C(1)-O(1)-C(5)-C(4)	69.81(13)
O(5)-C(4)-C(5)-O(1)	76.99(13)
C(3)-C(4)-C(5)-O(1)	-37.99(14)
O(5)-C(4)-C(5)-C(6)	-41.55(15)
C(3)-C(4)-C(5)-C(6)	-156.52(11)
O(6)-N(1)-C(6)-C(5)	56.98(13)
B(1)-N(1)-C(6)-C(5)	-178.04(11)
O(1)-C(5)-C(6)-N(1)	47.16(14)
C(4)-C(5)-C(6)-N(1)	167.93(11)
C(2)-O(3)-C(7)-O(2)	-32.04(16)
C(2)-O(3)-C(7)-C(8)	-148.70(13)

C(2)-O(3)-C(7)-C(9)	86.09(17)
C(1)-O(2)-C(7)-O(3)	18.42(17)
C(1)-O(2)-C(7)-C(8)	134.55(14)
C(1)-O(2)-C(7)-C(9)	-100.60(15)
C(3)-O(4)-C(10)-O(5)	-33.24(14)
C(3)-O(4)-C(10)-C(11)	-149.00(13)
C(3)-O(4)-C(10)-C(12)	85.39(15)
C(4)-O(5)-C(10)-O(4)	20.00(15)
C(4)-O(5)-C(10)-C(11)	135.49(14)
C(4)-O(5)-C(10)-C(12)	-99.16(13)
N(1)-O(6)-C(14)-C(15)	-163.29(11)
O(6)-C(14)-C(15)-C(20)	-116.3(2)
O(6)-C(14)-C(15)-C(16)	67.6(2)
C(20)-C(15)-C(16)-C(17)	-0.8(4)
C(14)-C(15)-C(16)-C(17)	175.5(2)
C(15)-C(16)-C(17)-C(18)	1.1(4)
C(16)-C(17)-C(18)-C(19)	-1.8(5)
C(17)-C(18)-C(19)-C(20)	2.3(6)
C(16)-C(15)-C(20)-C(19)	1.2(4)
C(14)-C(15)-C(20)-C(19)	-175.0(3)
C(18)-C(19)-C(20)-C(15)	-2.0(6)
N(2)-C(13)-B(1)-N(1)	132.1(17)
O(6)-N(1)-B(1)-C(13)	76.33(15)
C(6)-N(1)-B(1)-C(13)	-46.89(17)

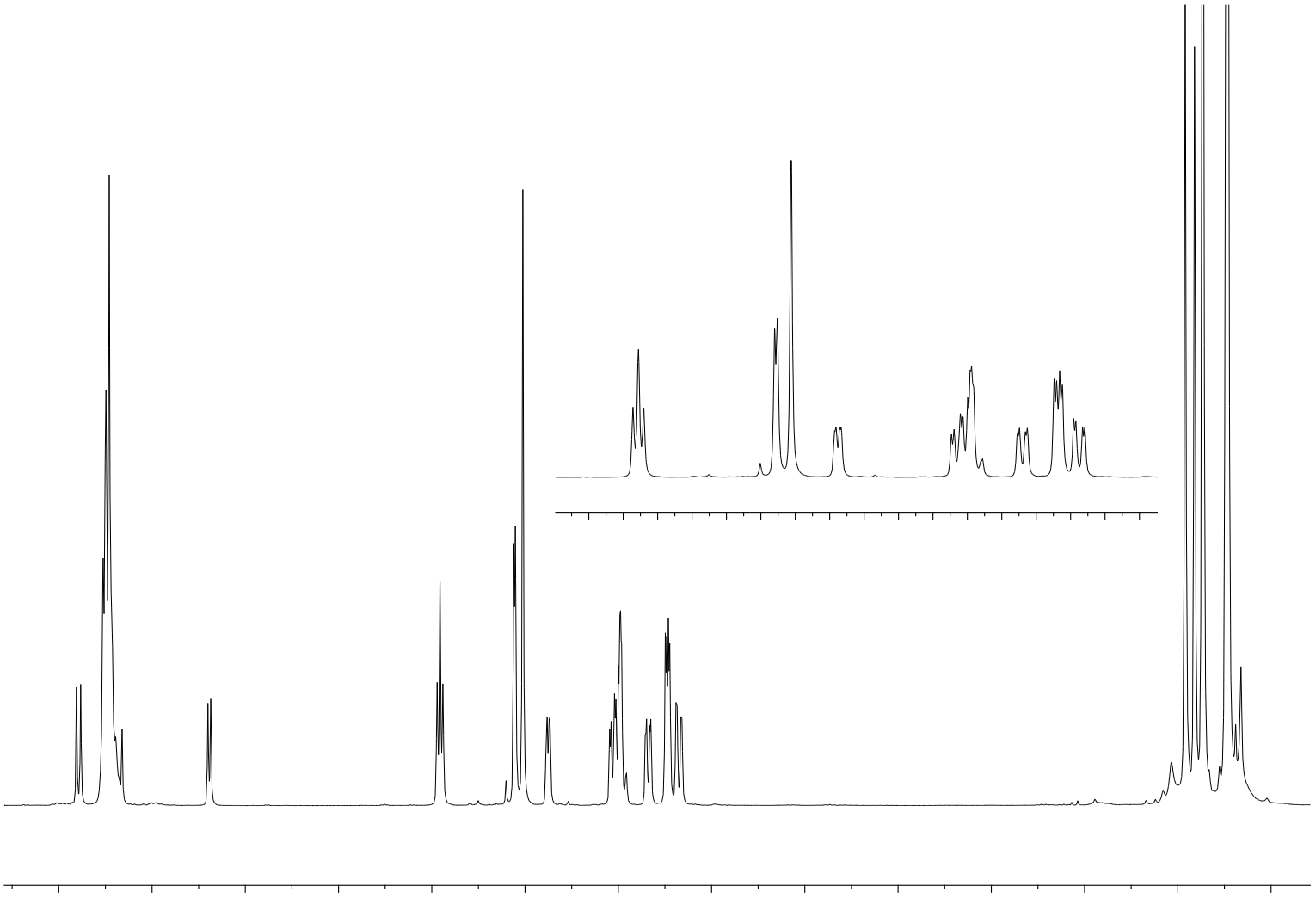
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **12** [Å and °].

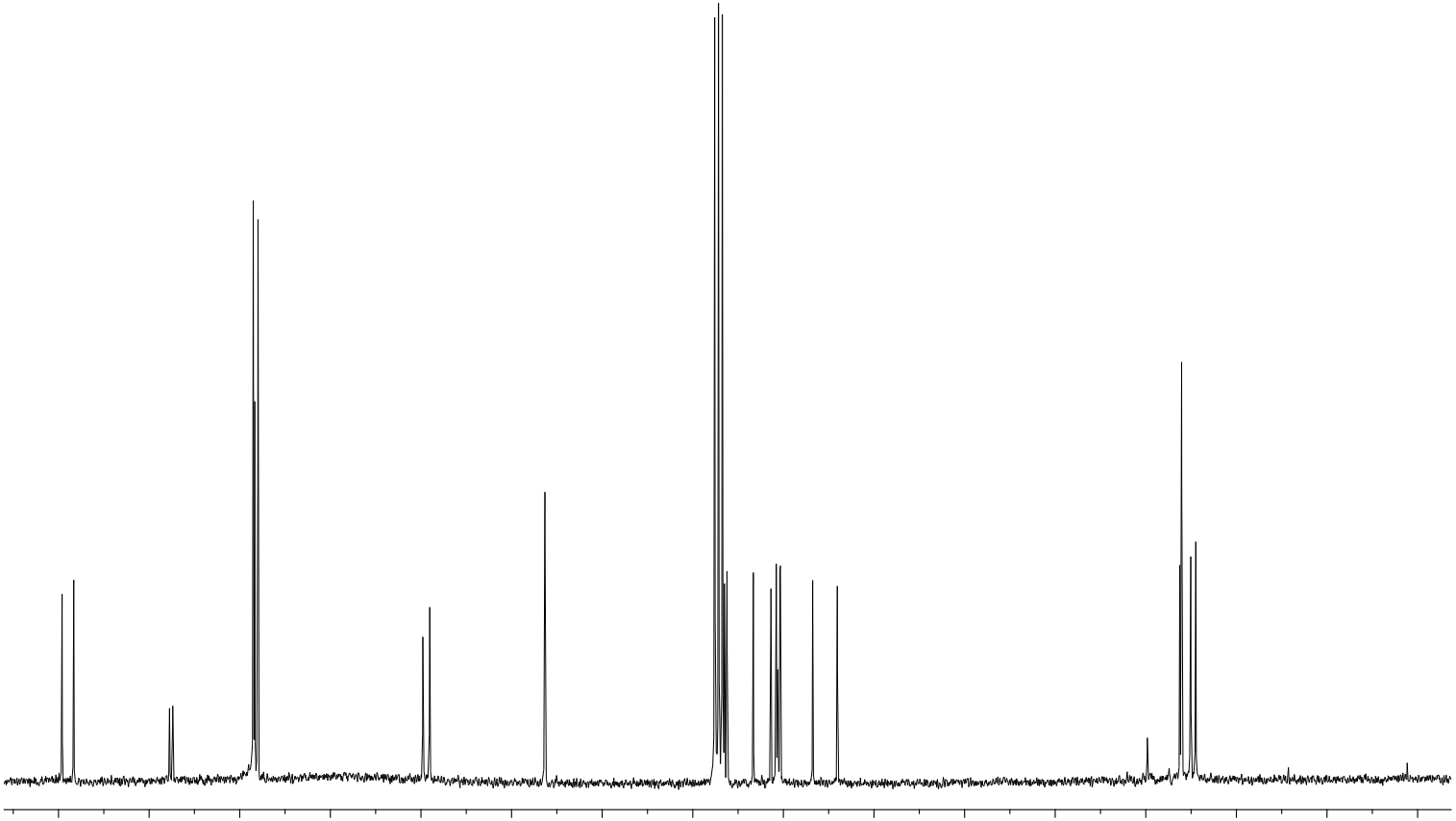
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...N(2)#1	0.93	2.01	2.8698(18)	153.1

Symmetry transformations used to generate equivalent atoms:

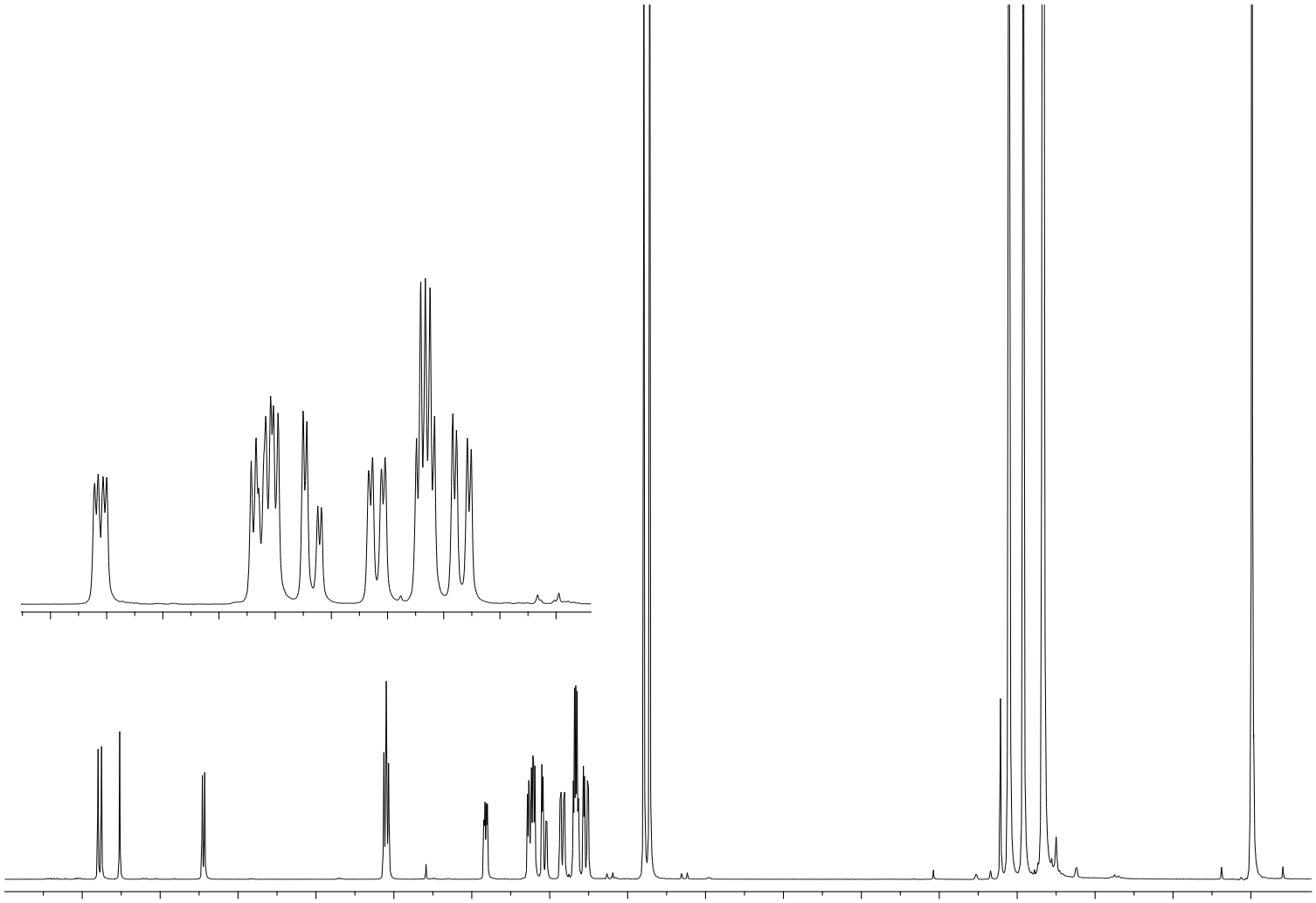
#1 -x,y-1/2,-z



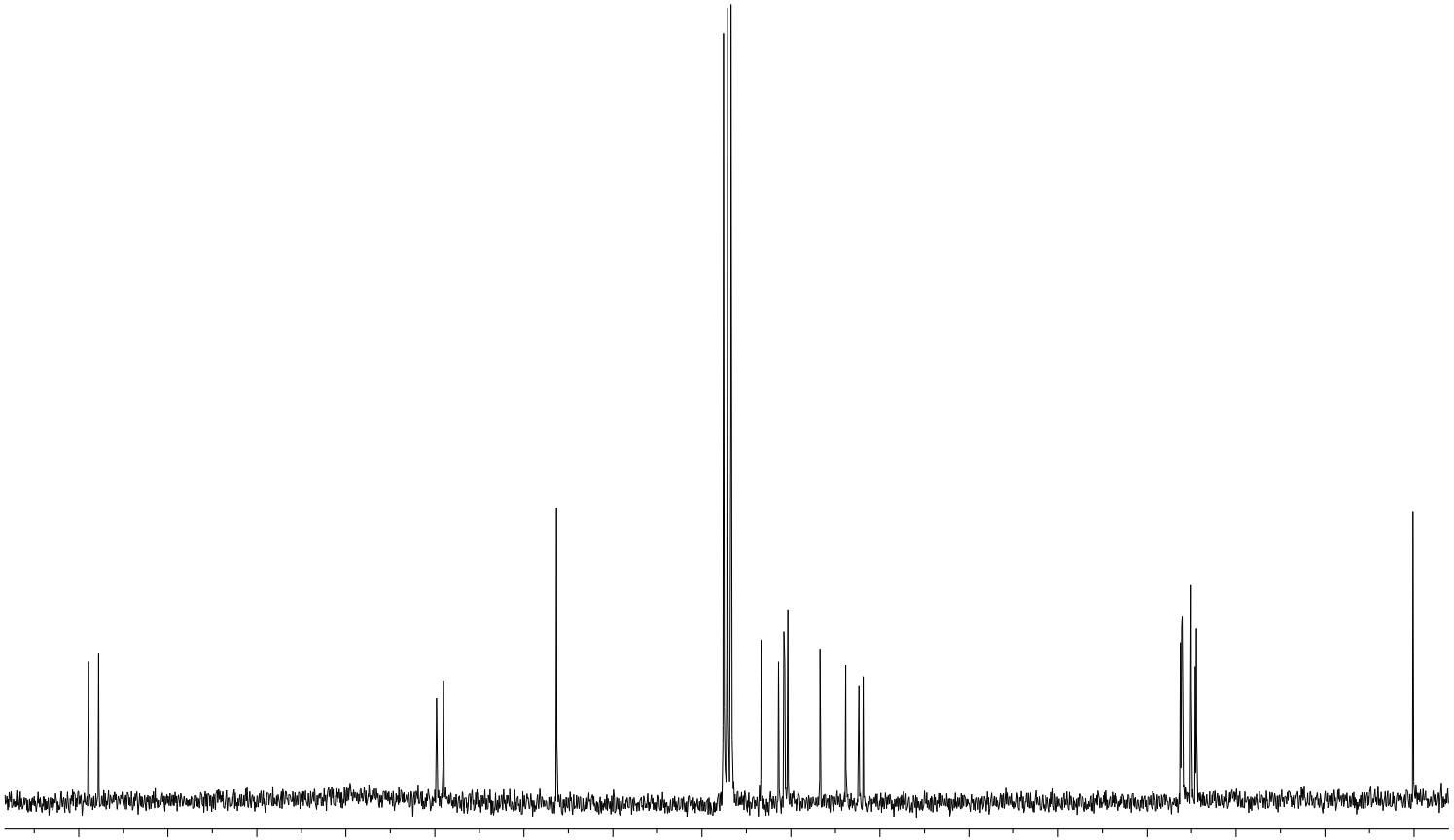
^{1}H-NMR ($CDCl_3$, 300 MHz) of **8**



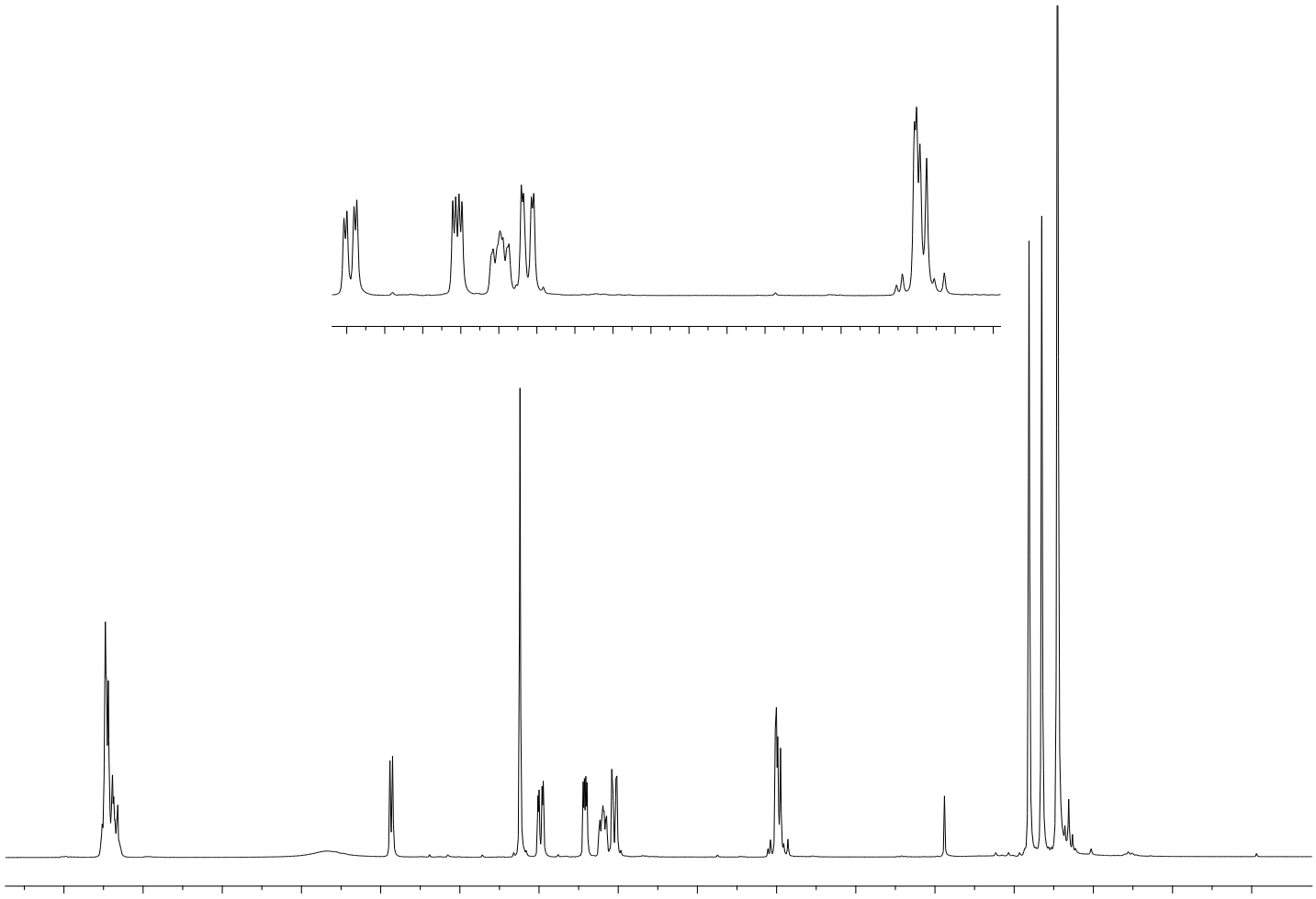
^{13}C-NMR (75.5 MHz, $CDCl_3$) of **8**



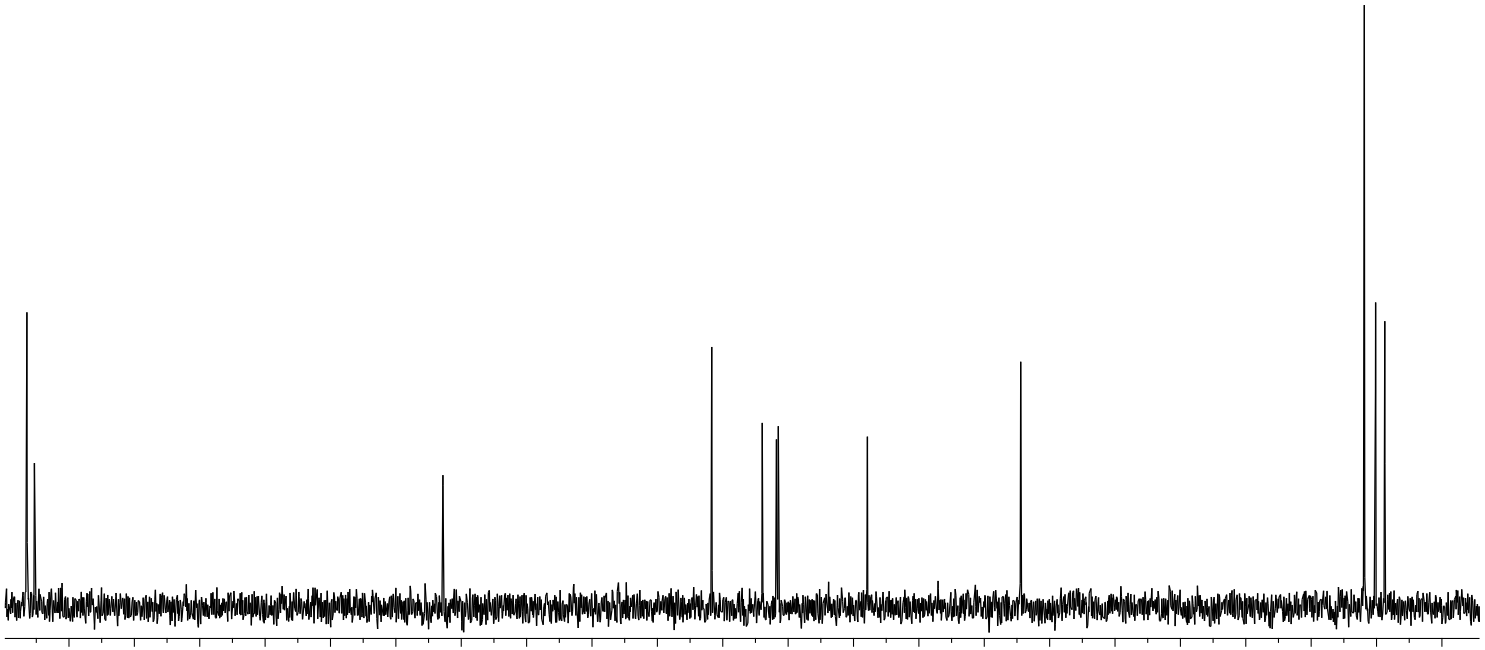
^{1}H-NMR (300 MHz, $CDCl_3$) of **9**



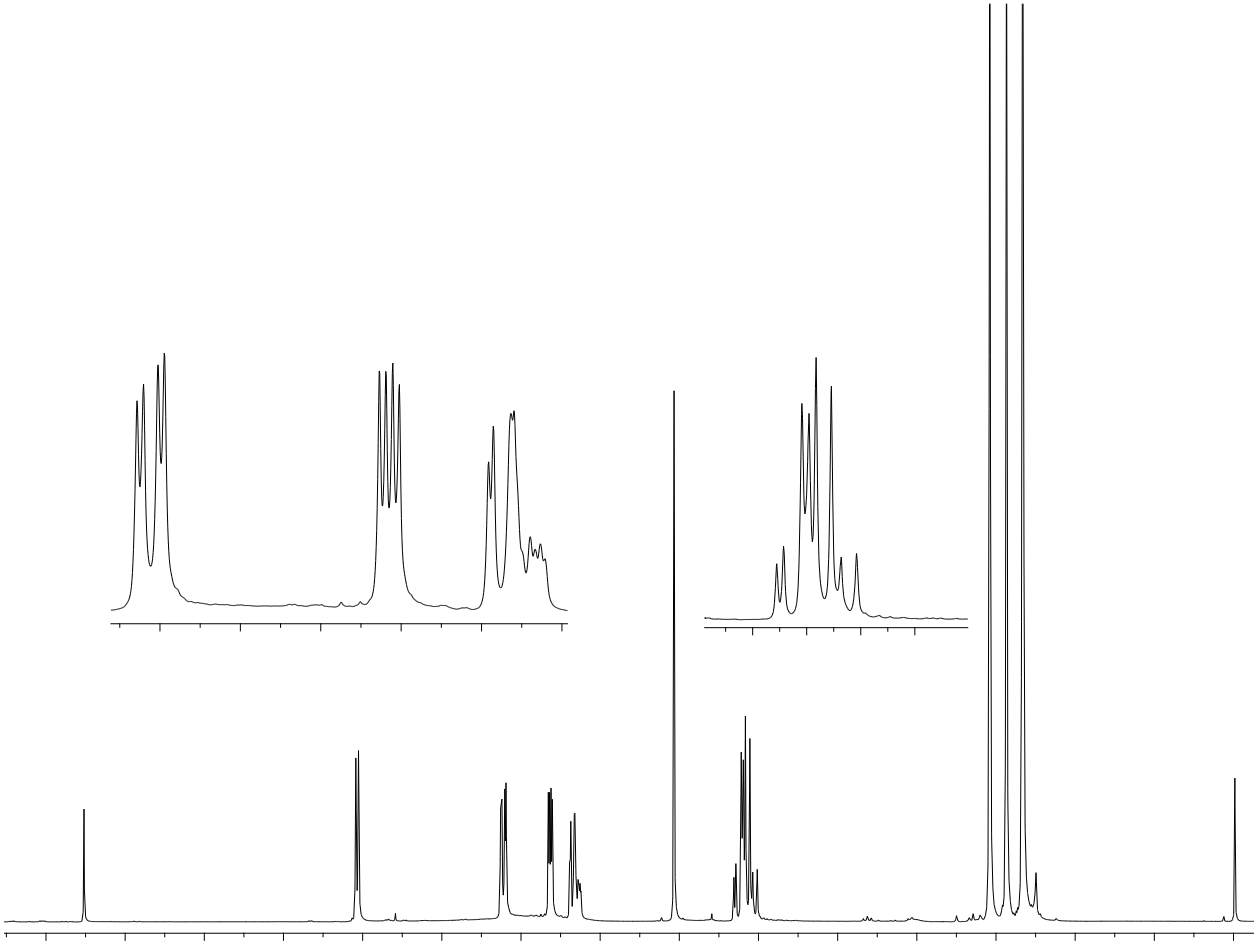
^{13}C-NMR (75.5 MHz, $CDCl_3$) of **9**



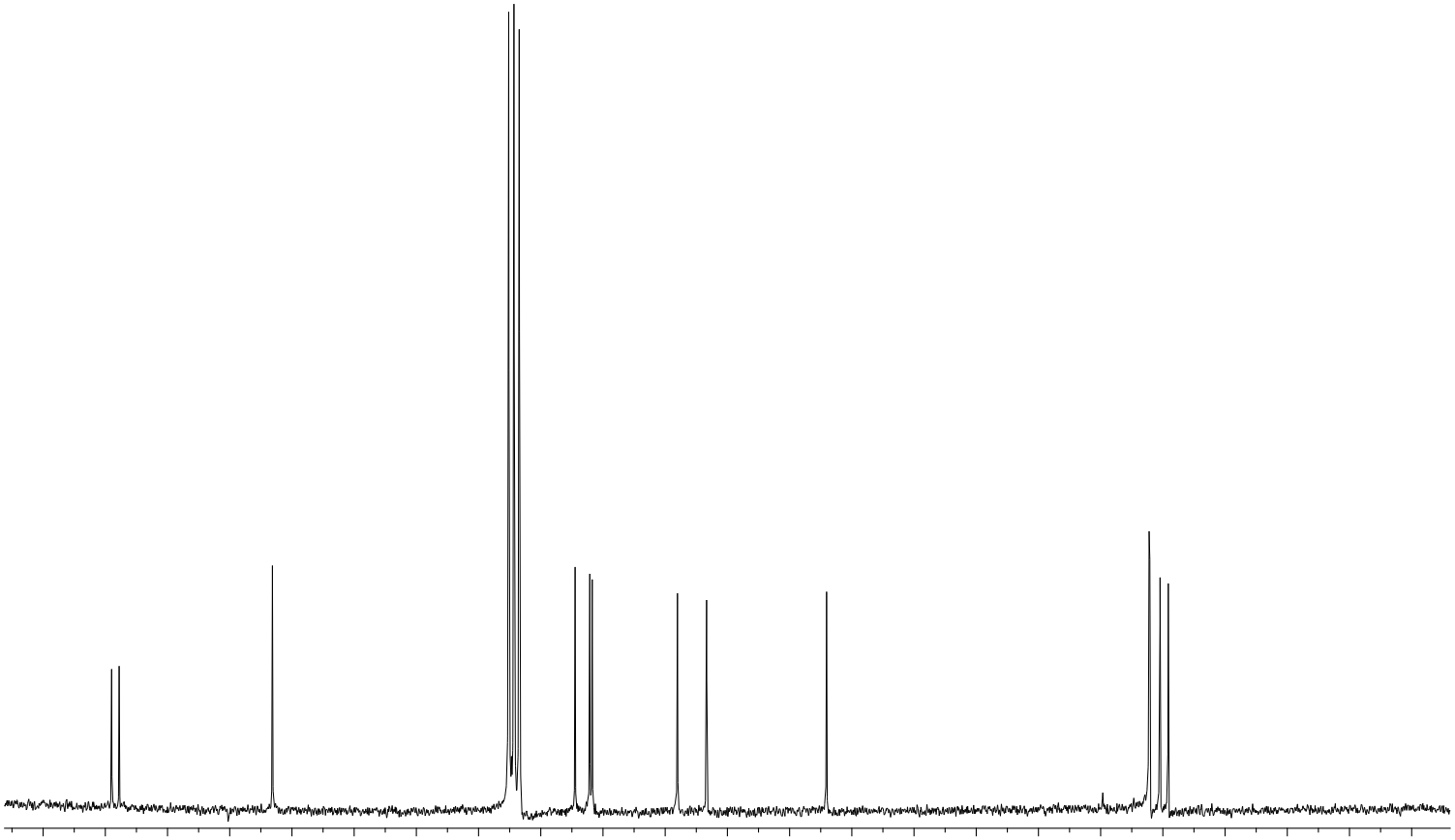
^{1}H-NMR (300 MHz, $CDCl_3$) of **10**



^{13}C-NMR (75.5 MHz, $CDCl_3$) of **10**



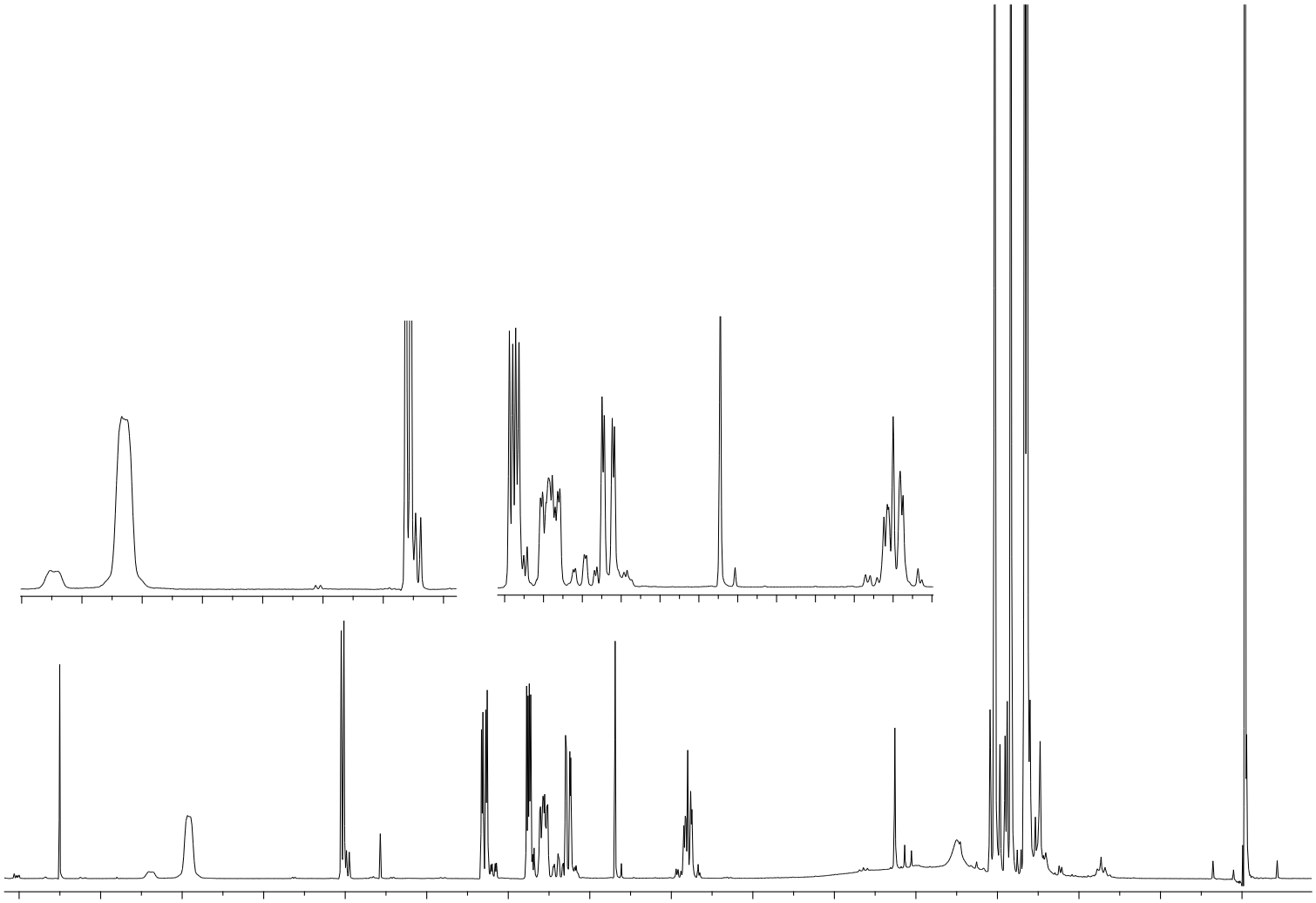
^{1}H-NMR (300 MHz, $CDCl_3$) of **11**



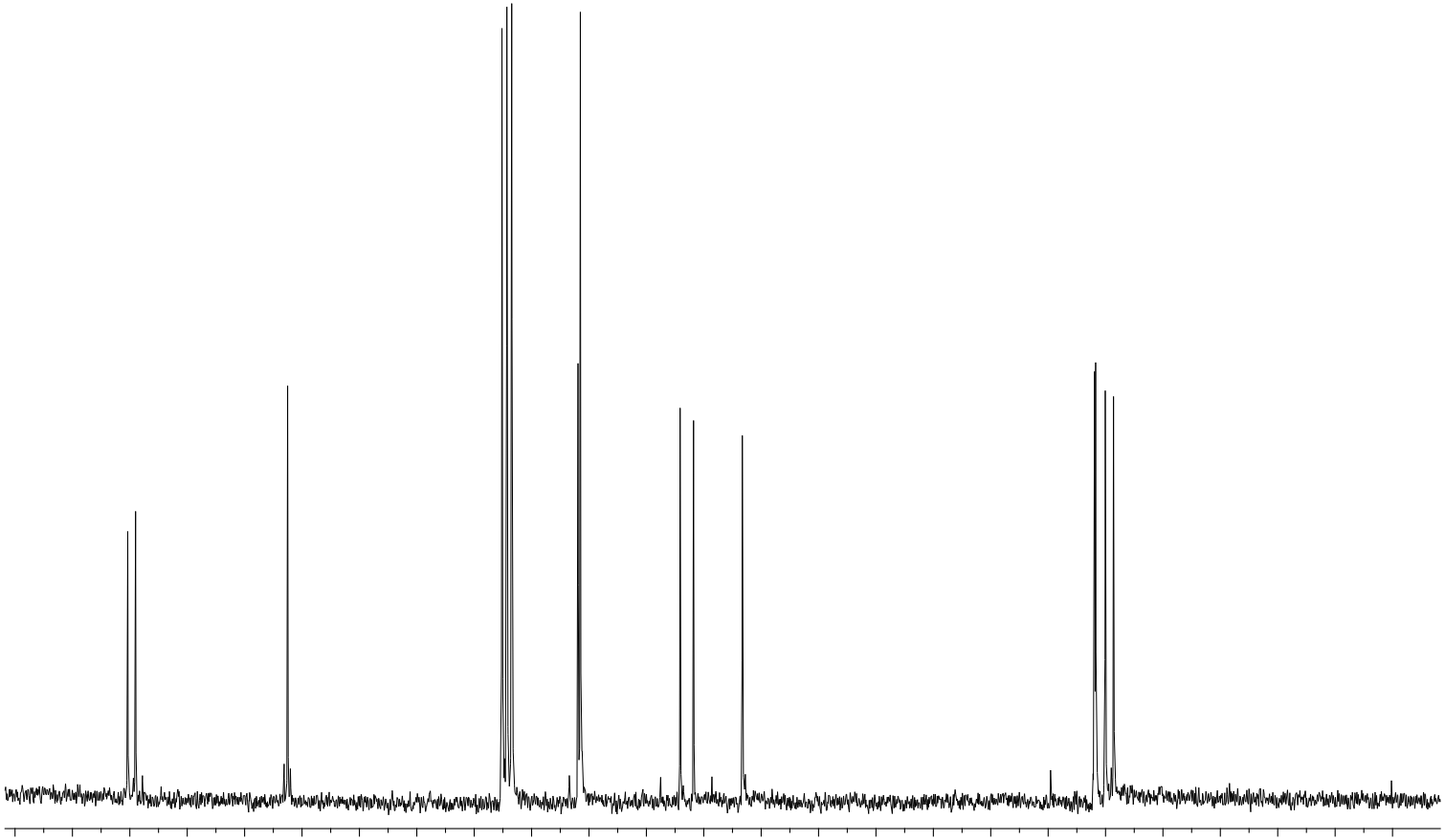
^{13}C-NMR (75.5 MHz, $CDCl_3$) of **11**

^{1}H-NMR (300 MHz, $CDCl_3$) of **12**

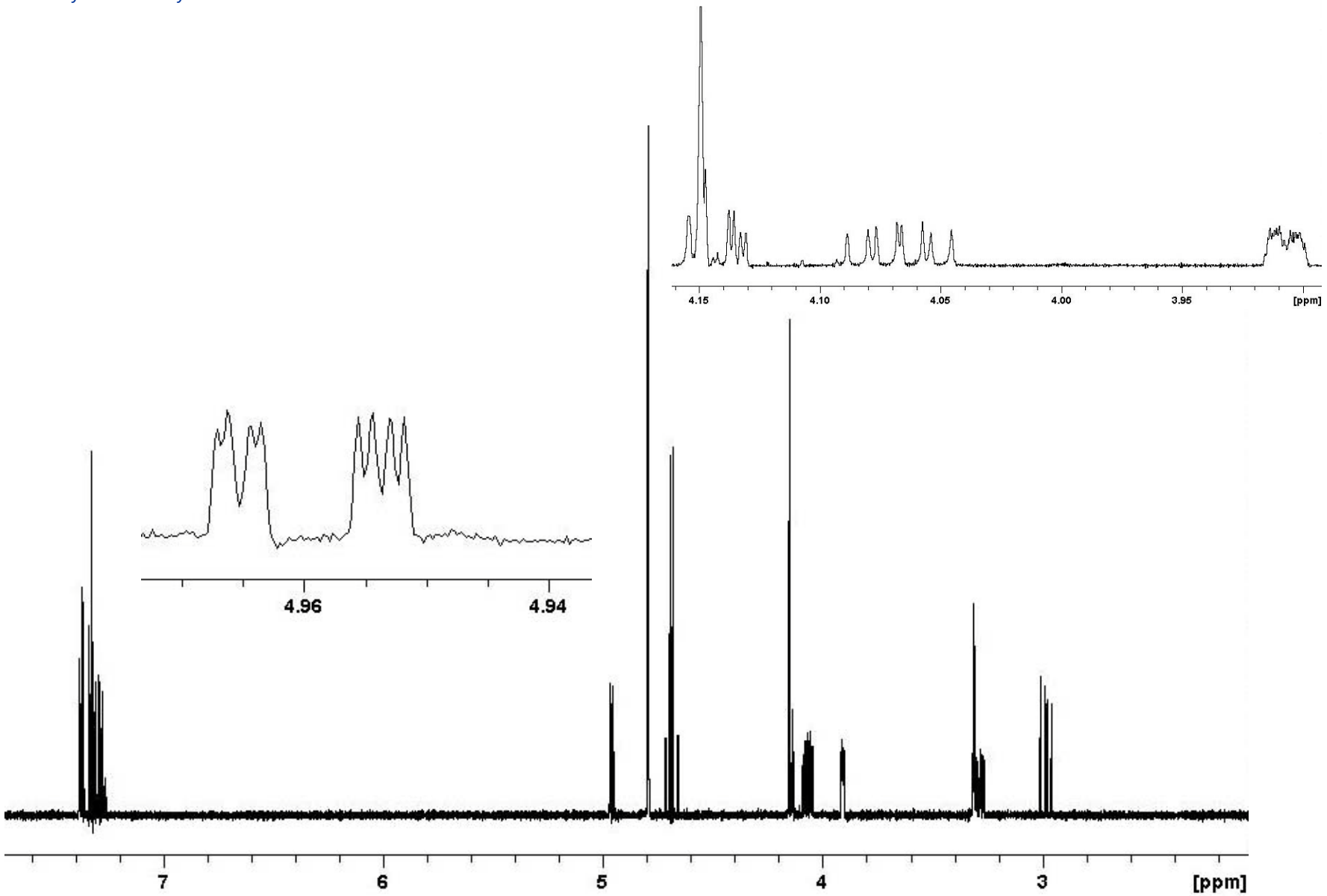
^{13}C-NMR (75.5 MHz, $CDCl_3$) of **12**



^{1}H-NMR (300 MHz, $CDCl_3$) of **13**

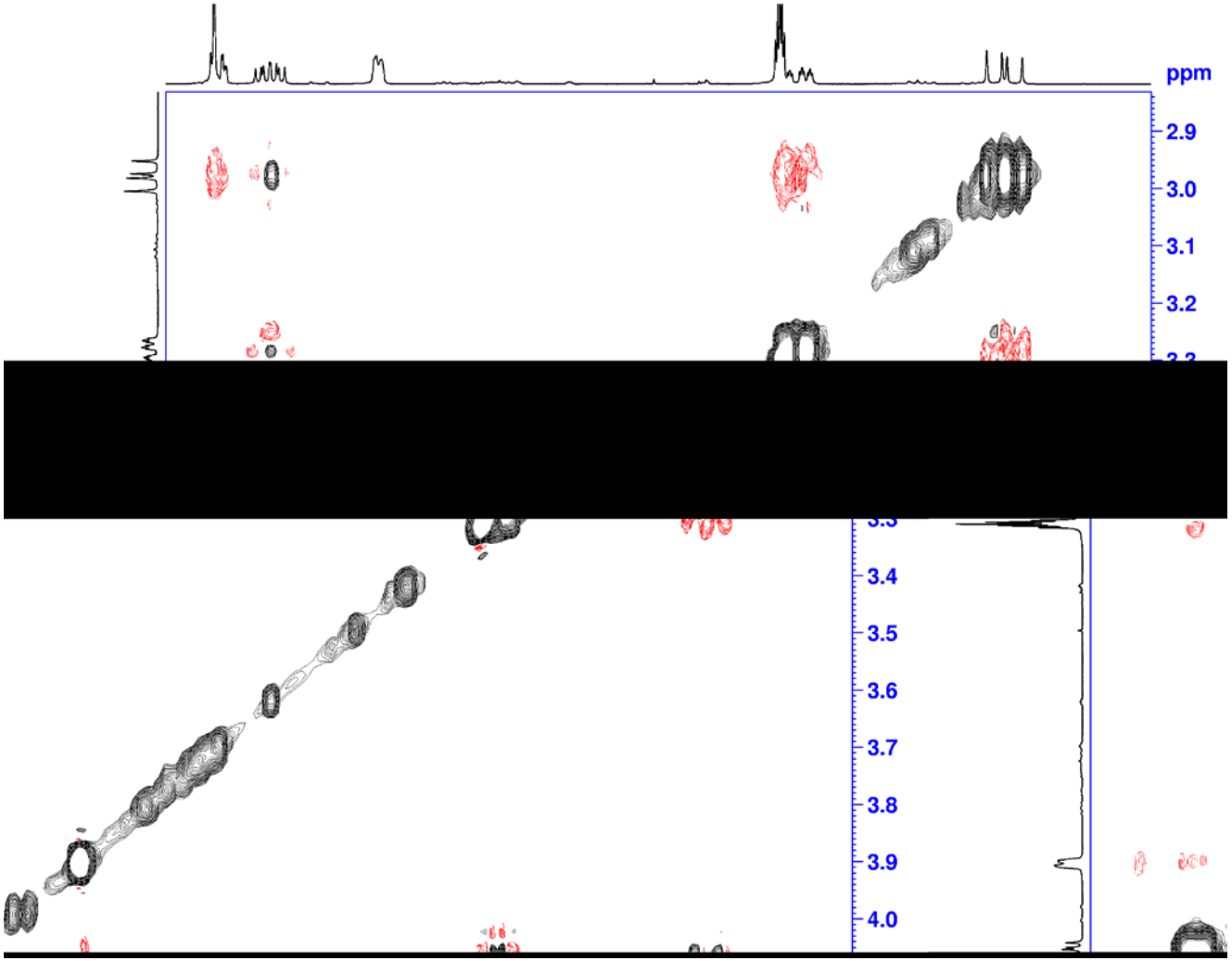


^{13}C-NMR (75.5 MHz, $CDCl_3$) of **13**



^{1}H-NMR (500 MHz, CD_3OD) of **19**

^{13}C-NMR (75.5 MHz, CD_3OD) of **19**



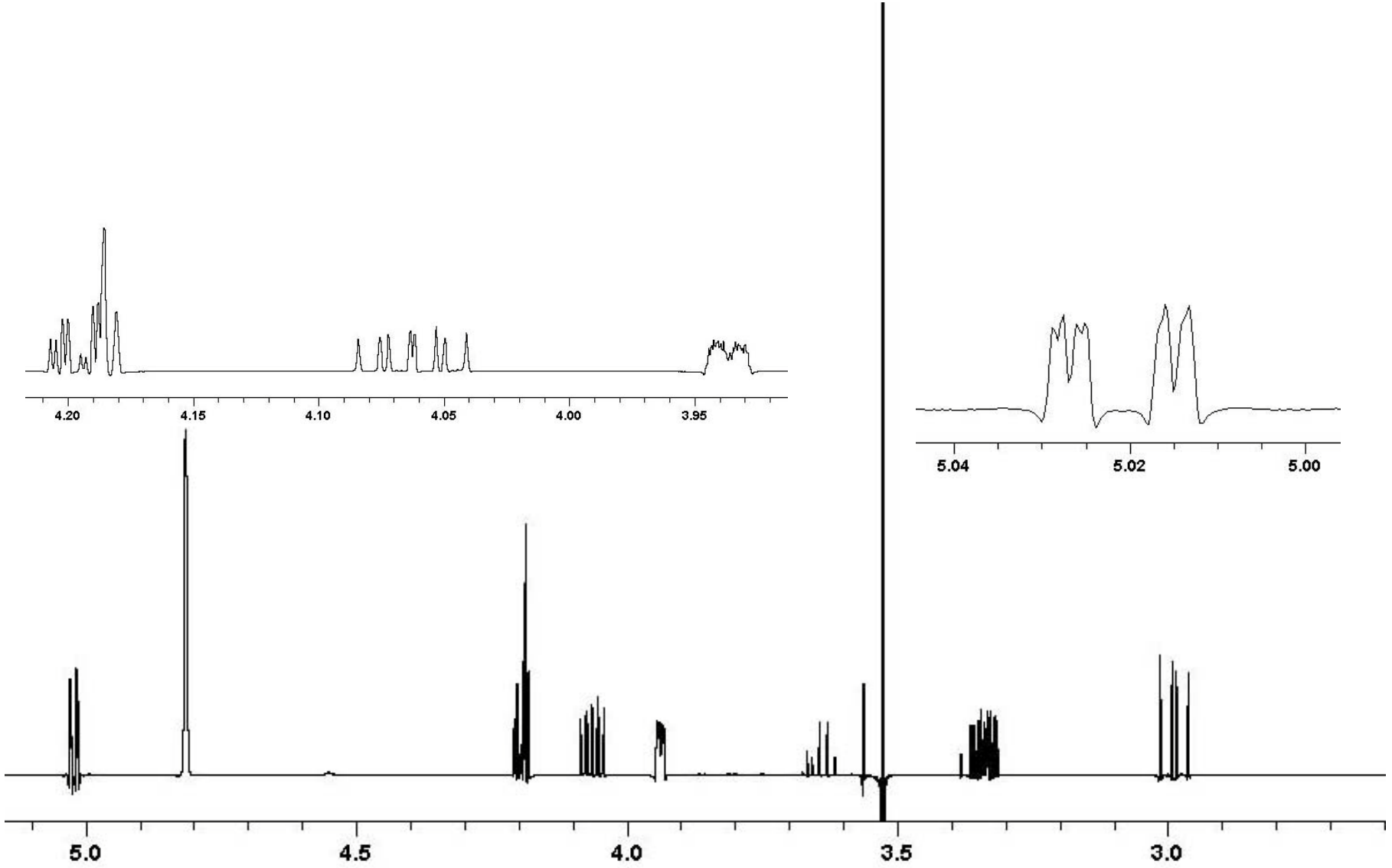
2D-NOESY of **19**

^{1}H-NMR (500 MHz, $CDCl_3$) of **21**

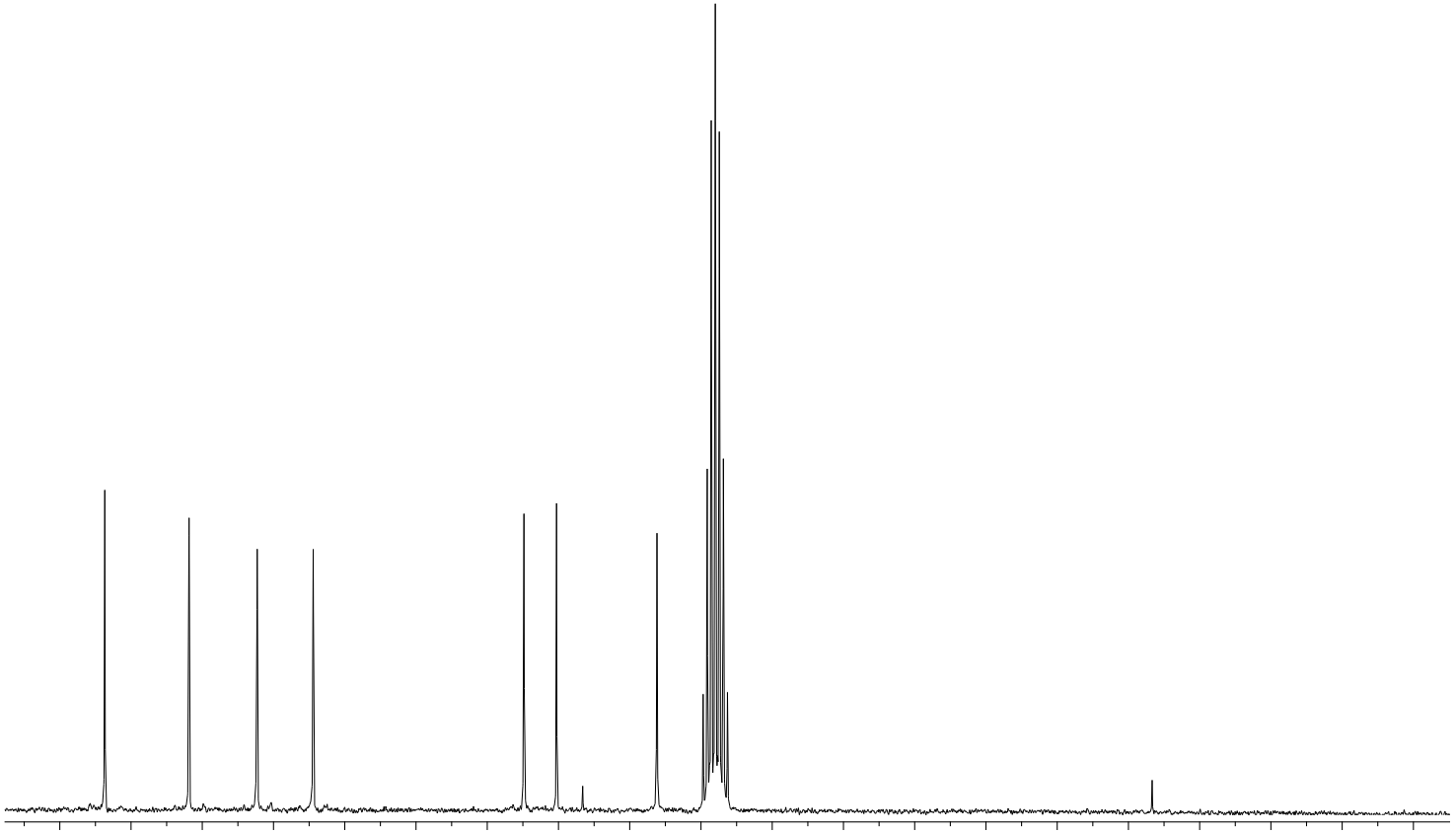
^{13}C-NMR (75.5 MHz, $CDCl_3$) of **21**

^{1}H-NMR (300 MHz, CD_3OD) of **22**

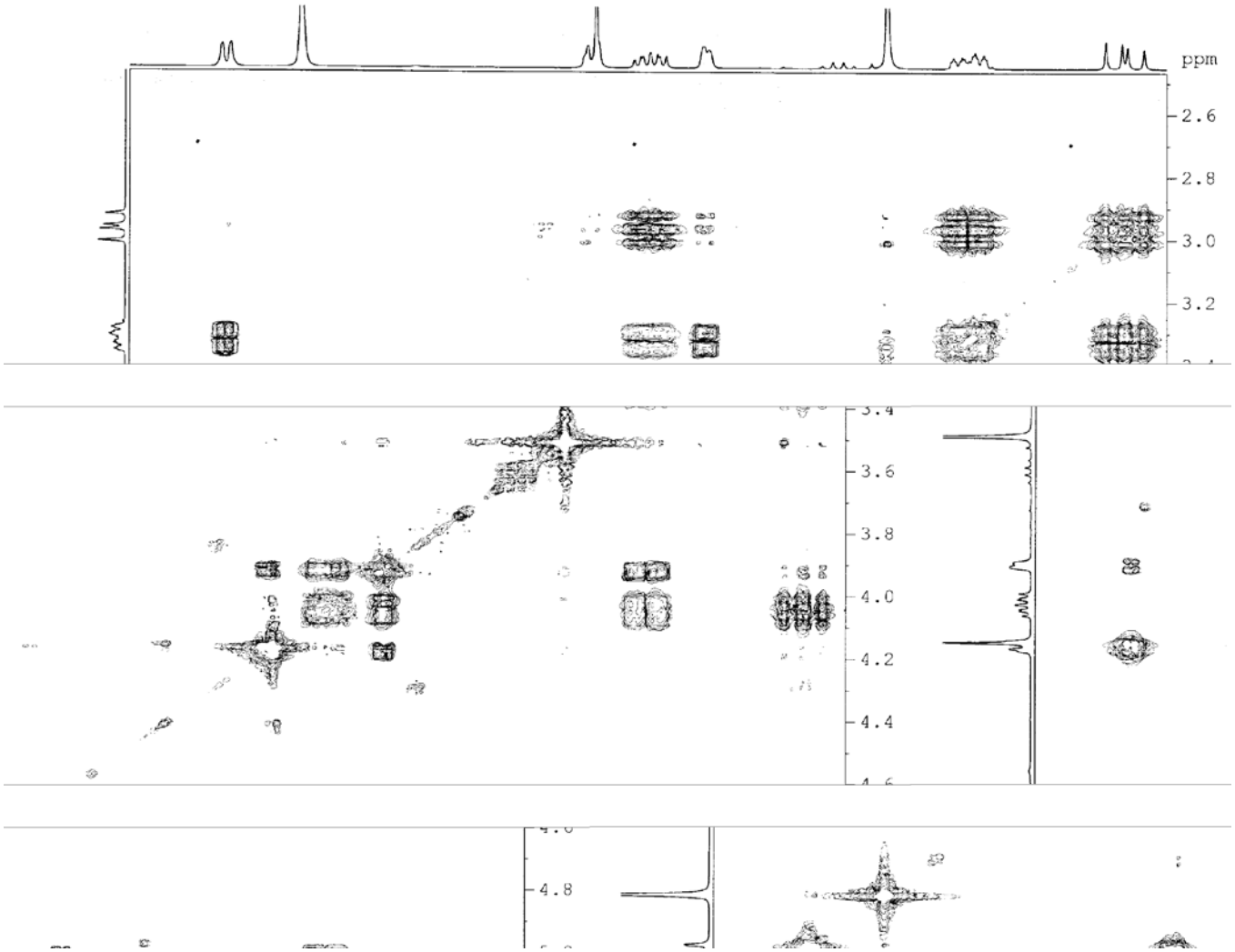
^{13}C-NMR (75.5 MHz, CD_3OD) of **22**



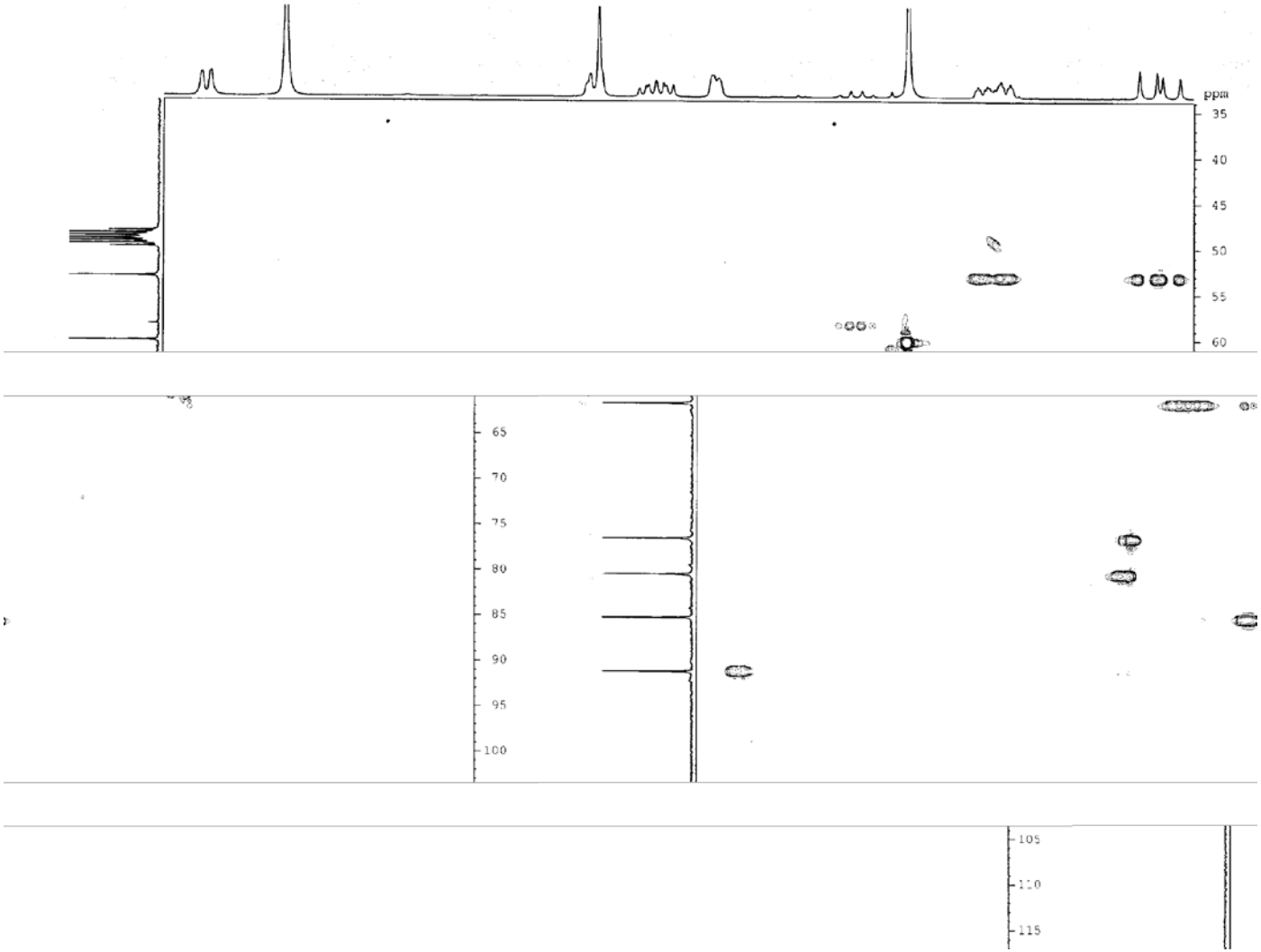
^{1}H-NMR (500 MHz, CD_3OD) of **23**



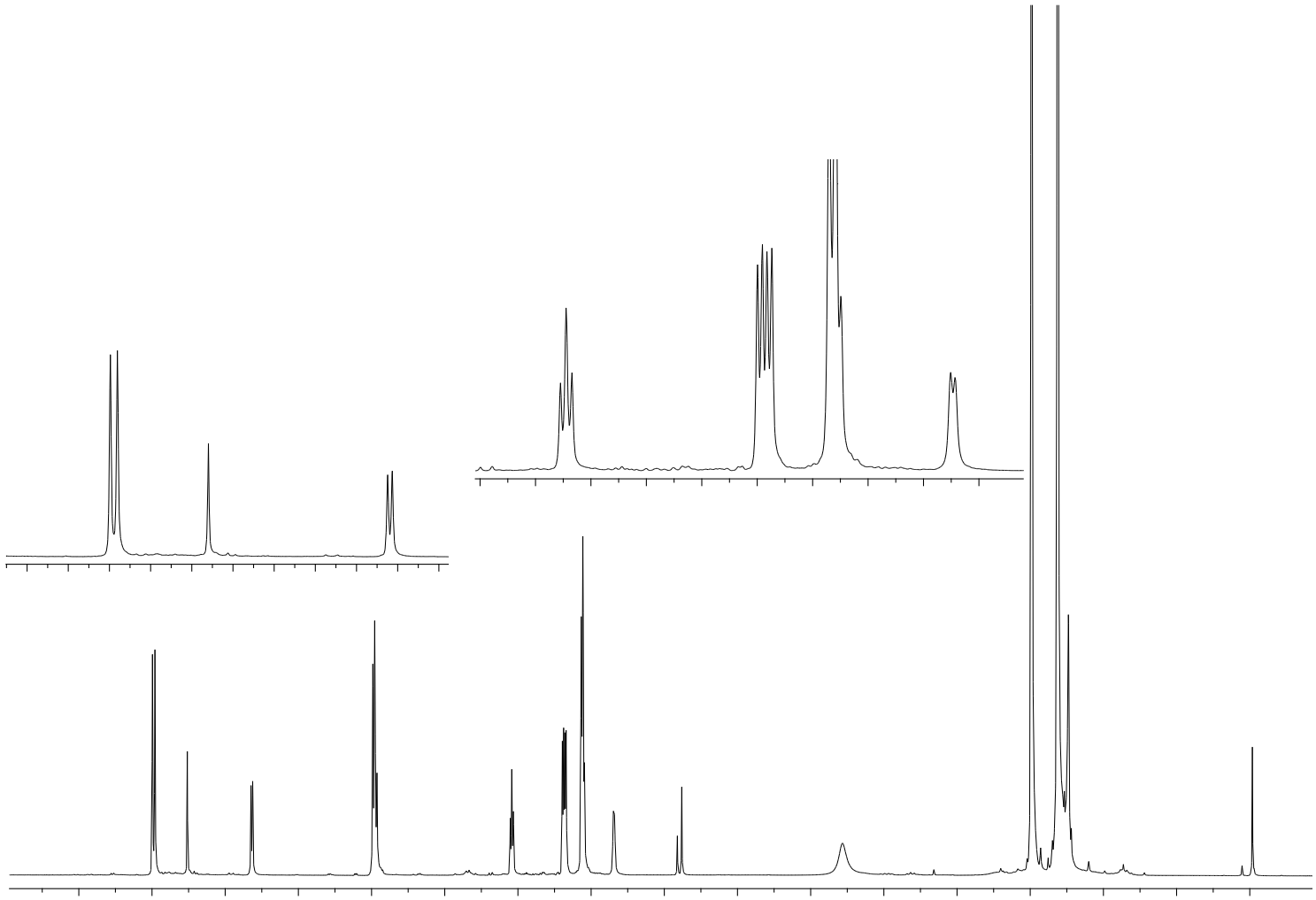
^{13}C-NMR (75.5 MHz, CD_3OD) of **23**



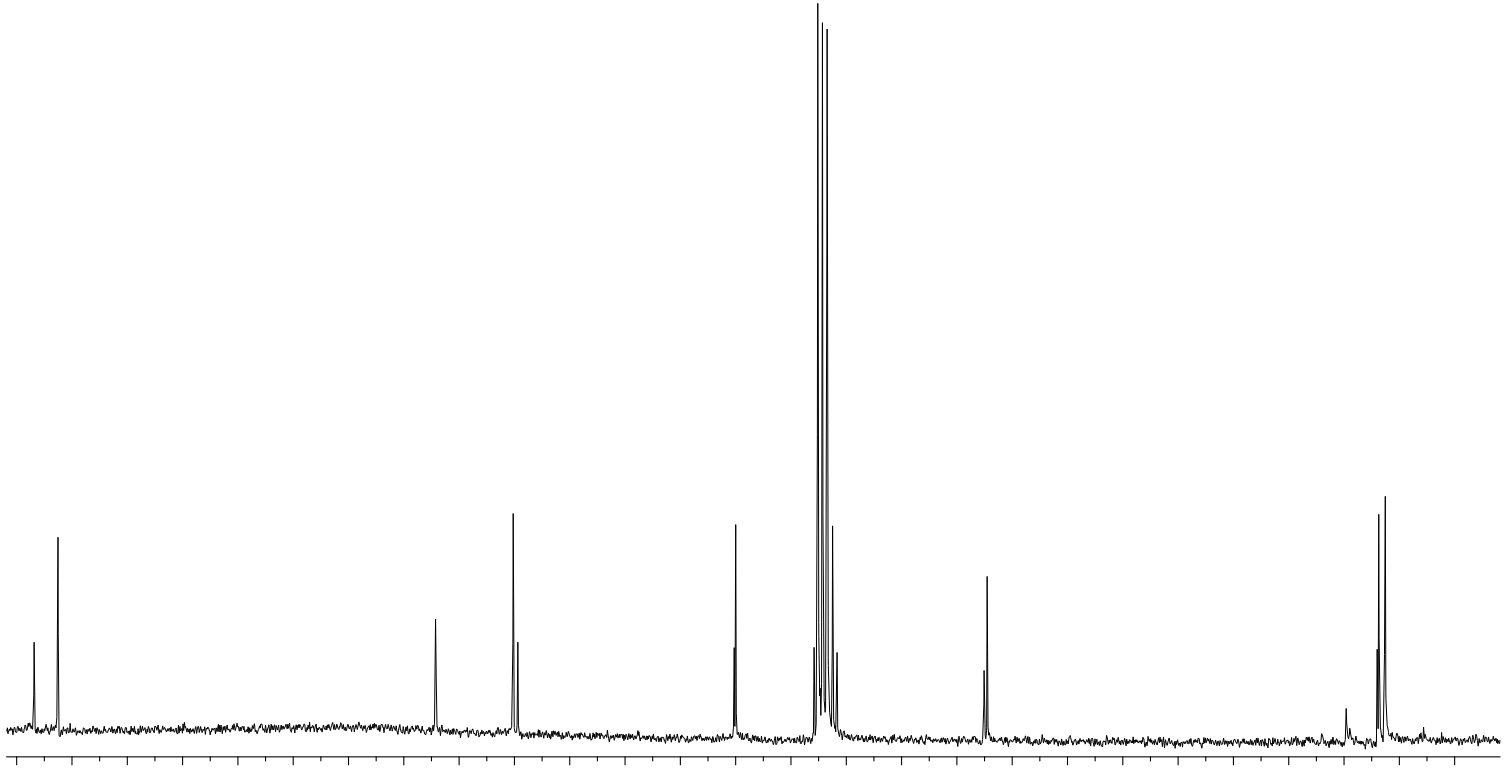
2D-COSY spectrum of **23**



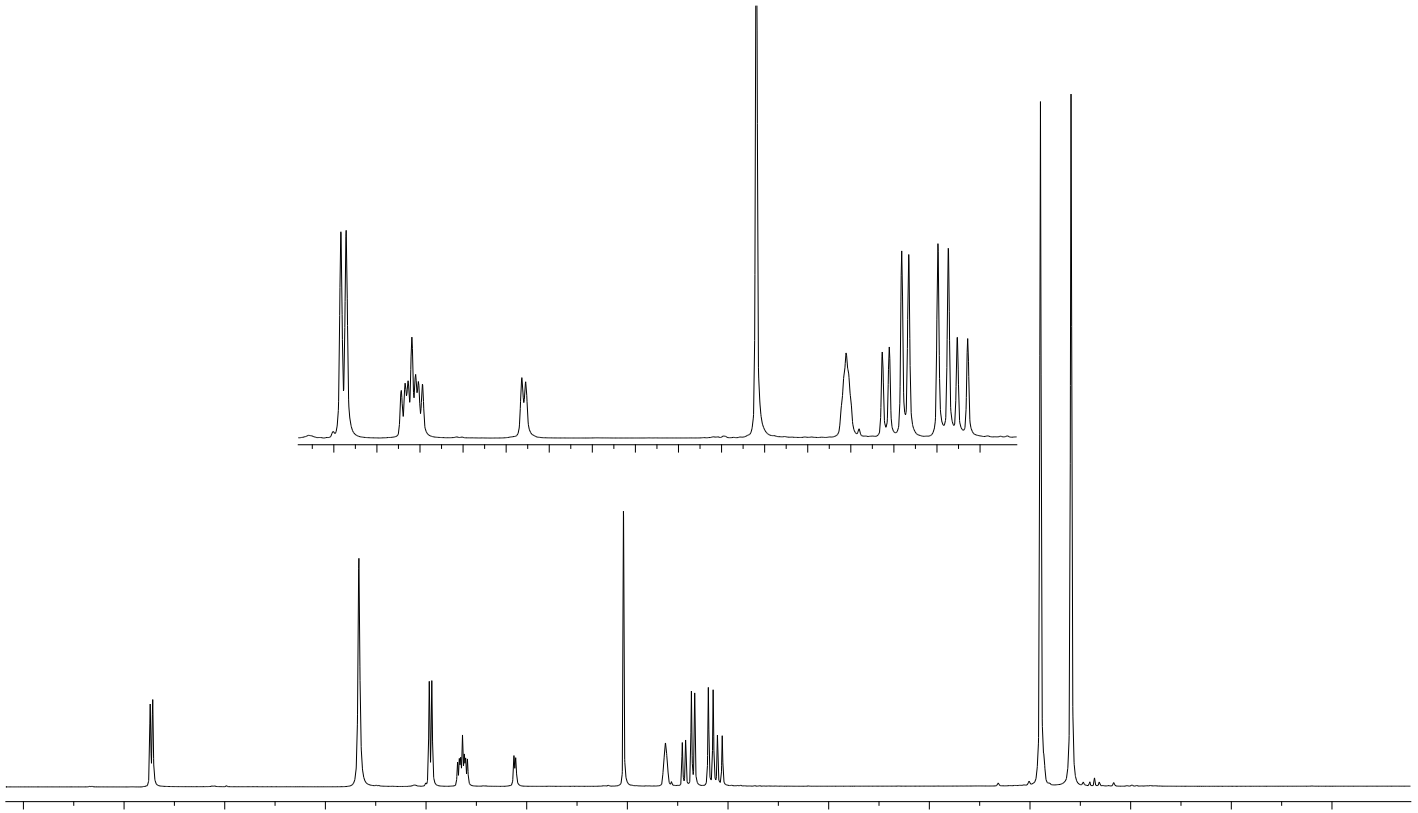
2D-HSQC spectrum of **23**



^{1}H-NMR (300 MHz, $CDCl_3$) of **27**



^{13}C-NMR (75.5 MHz, $CDCl_3$) of **27**



^{1}H-NMR (300 MHz, CD_3OD) of **29**

^{13}C-NMR (75.5 MHz, CD_3OD) of **29**

^{13}C-NMR (75.5 MHz, CD_3OD) of **29**

^{1}H-NMR (500 MHz, DMSO-d_6/D_2O) of **33**

^{13}C-NMR (125.5 MHz, DMSO-d_6/D_2O) of **33**