Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Supporting Information

Synthesis of Tetrahydroxy Perhydroaza-azulenes: Tandem Johnson-Claisen Rearrangement of D-Glucose Derived Allylic Alcohols

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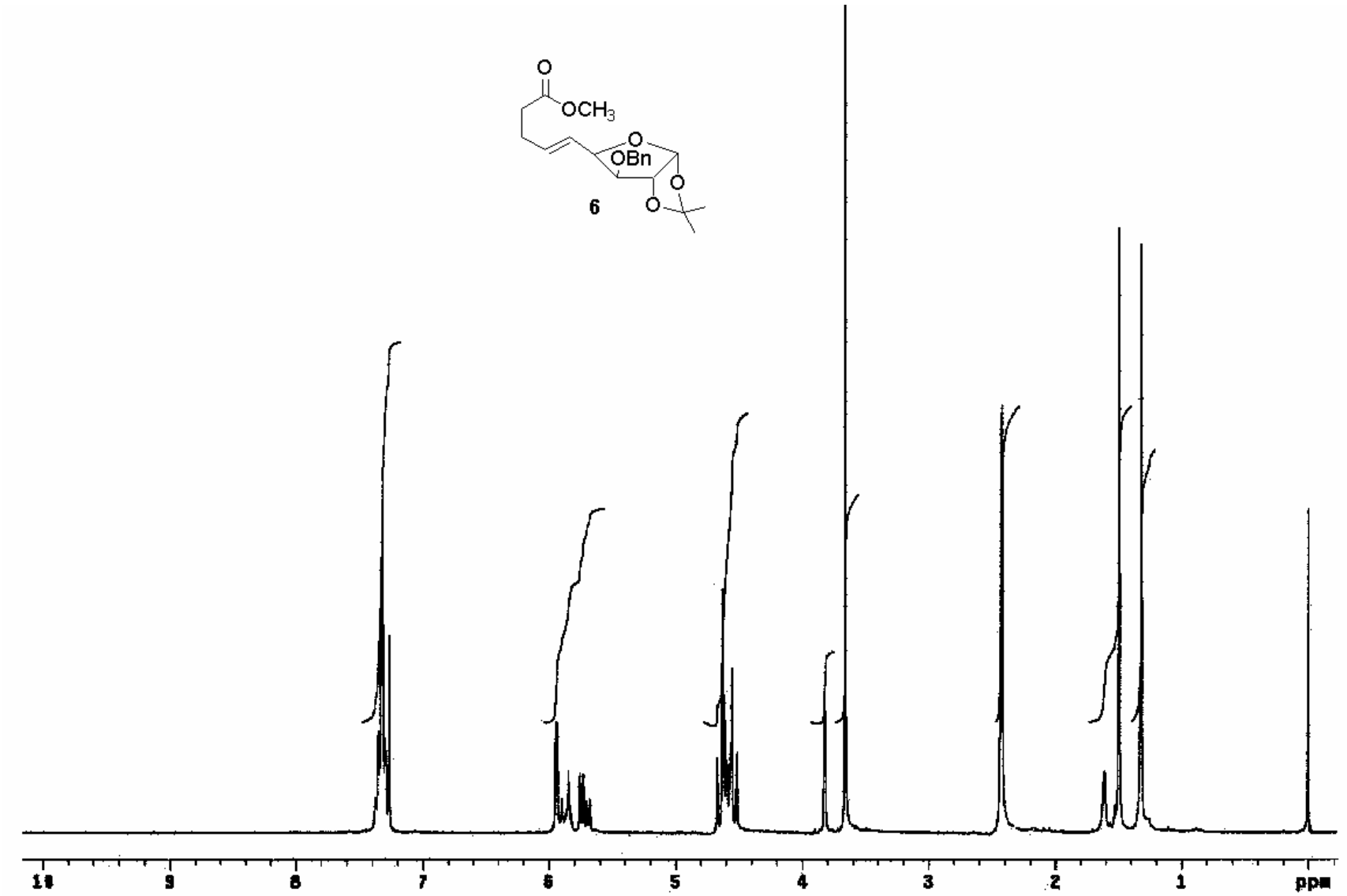

Figure 1: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6

Figure 2: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6

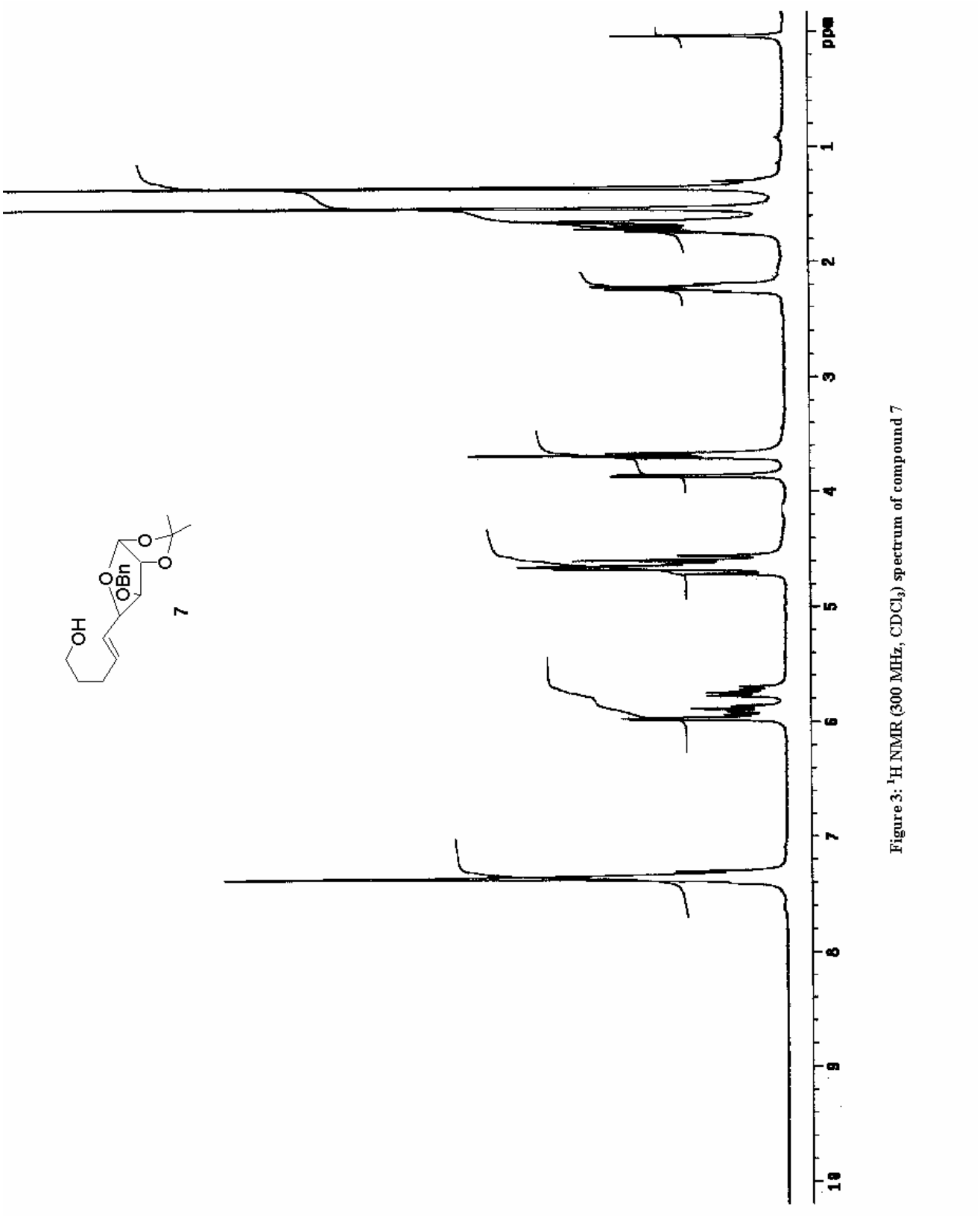

Figure 3: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 7

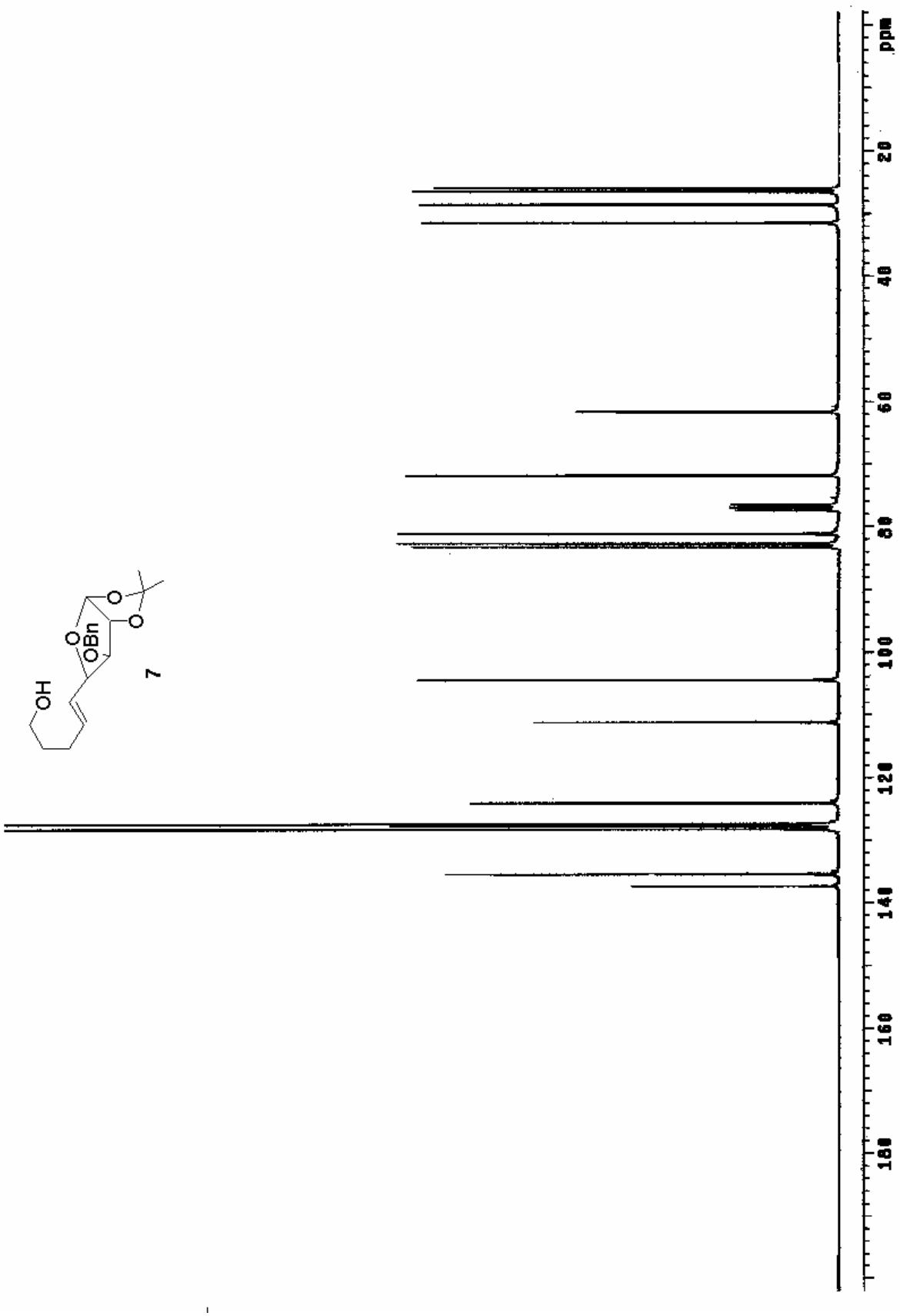

Figure 4: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 7

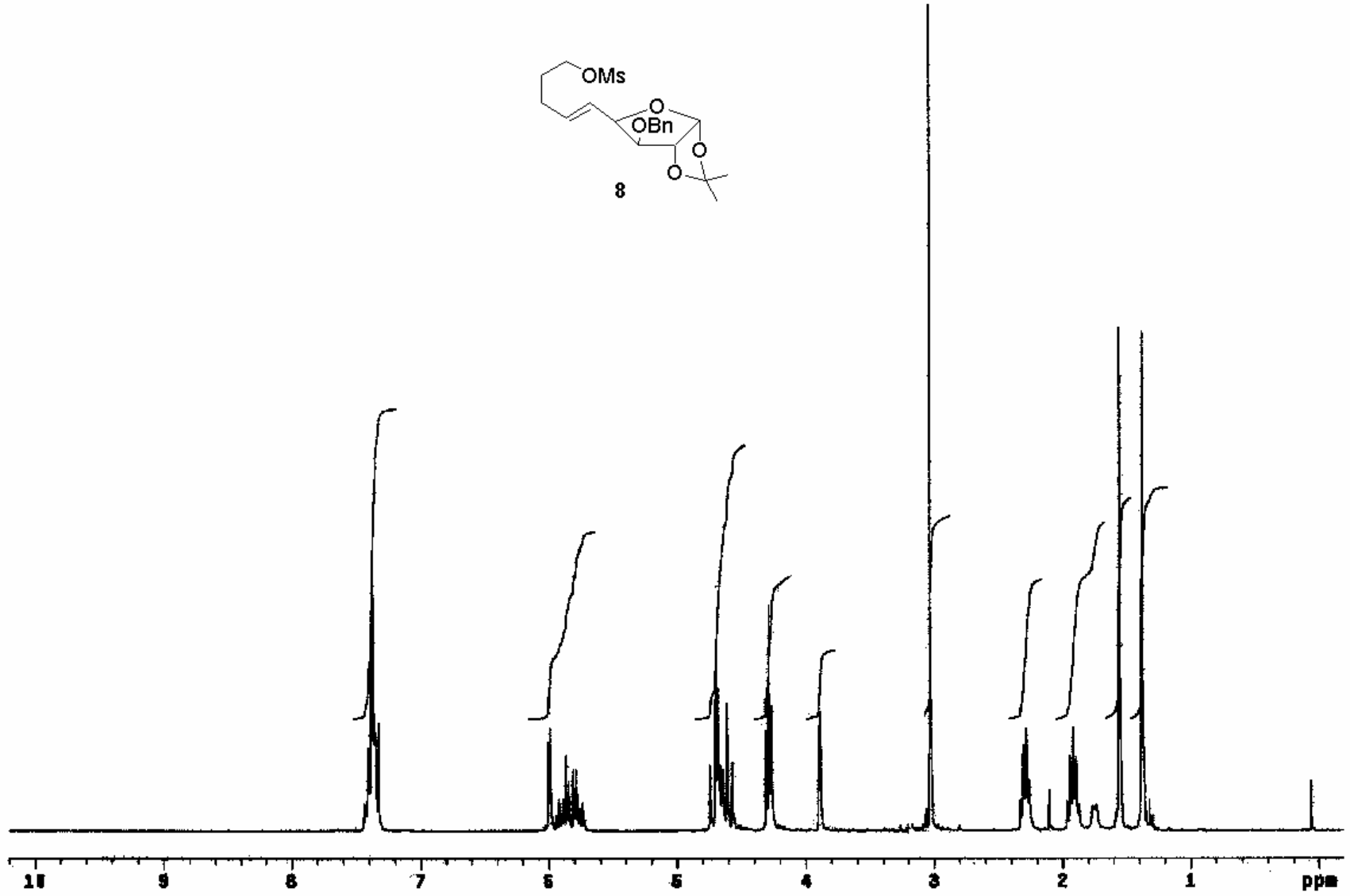

Figure 5: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 8

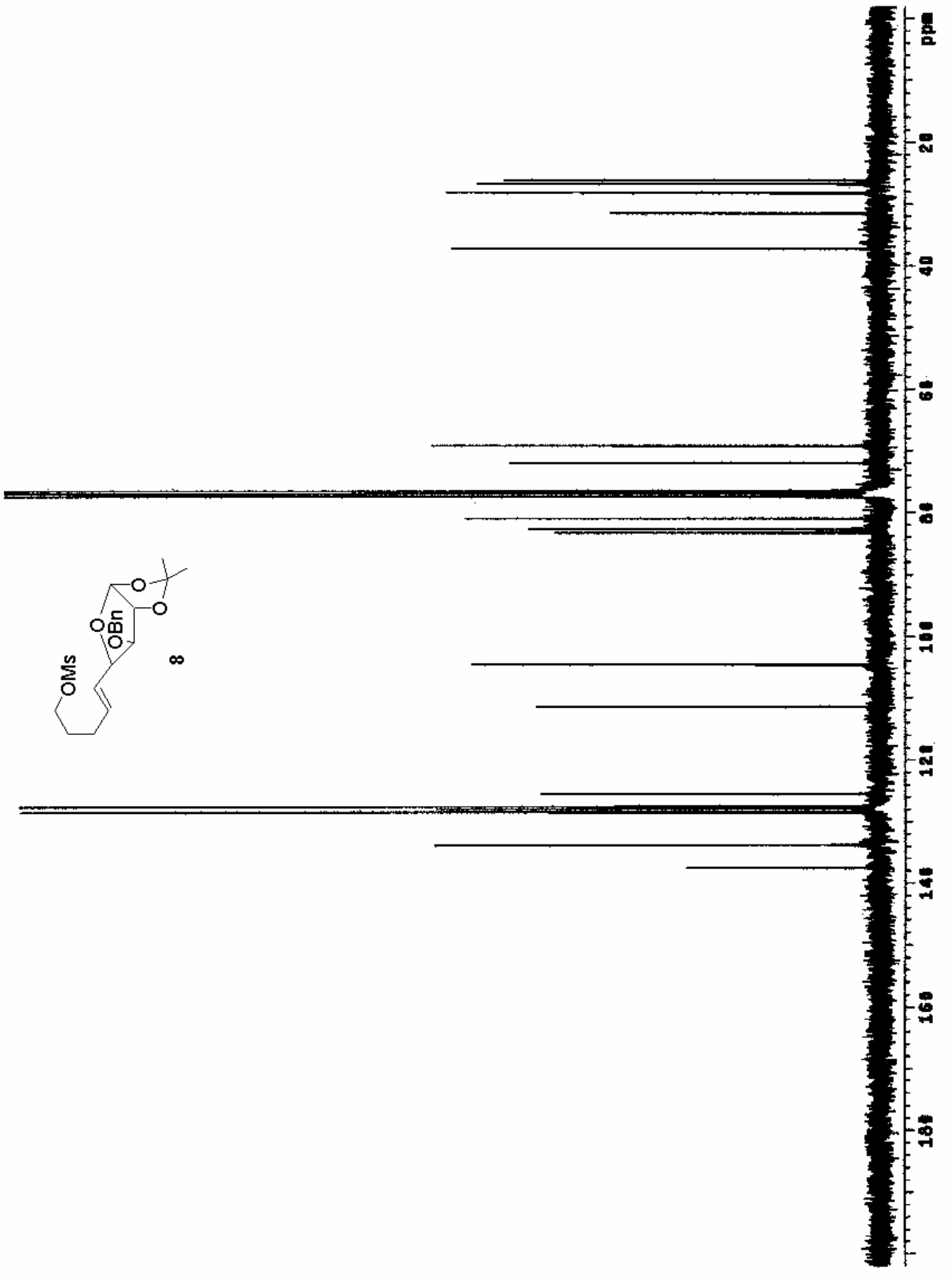

Figure 6: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 8

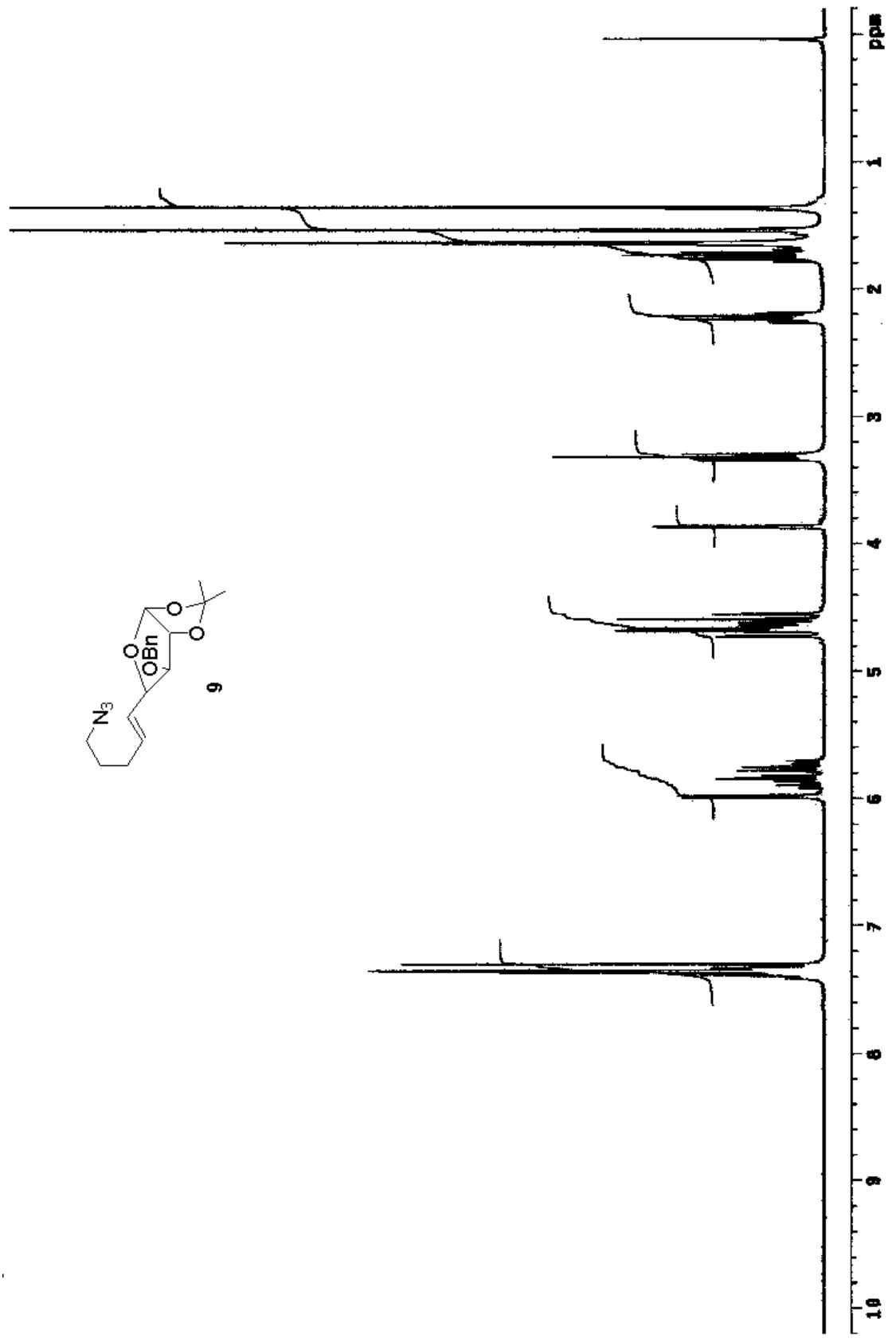

Figure 7: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 9

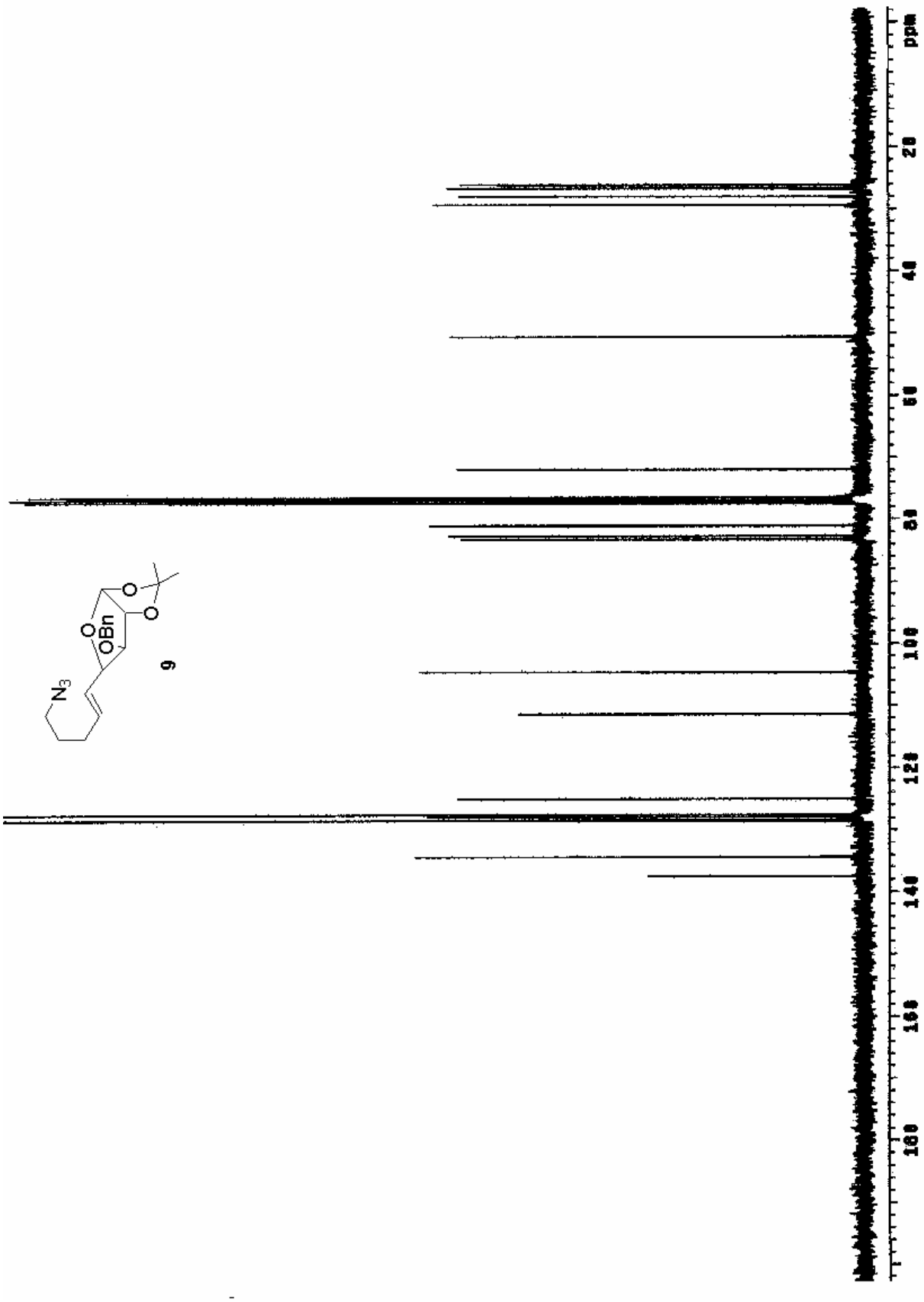

Figure 8: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 9

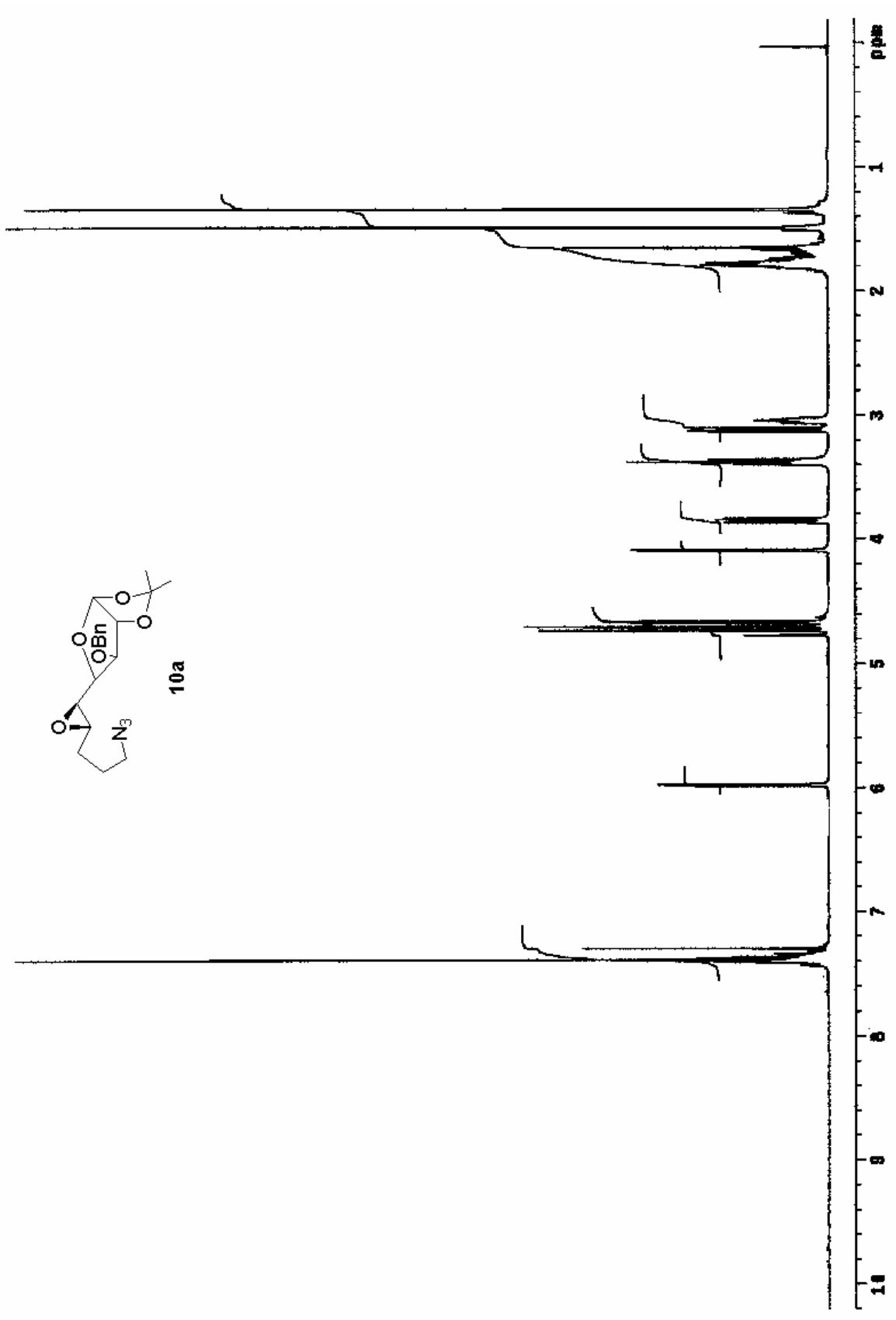

Figure 9: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 10a

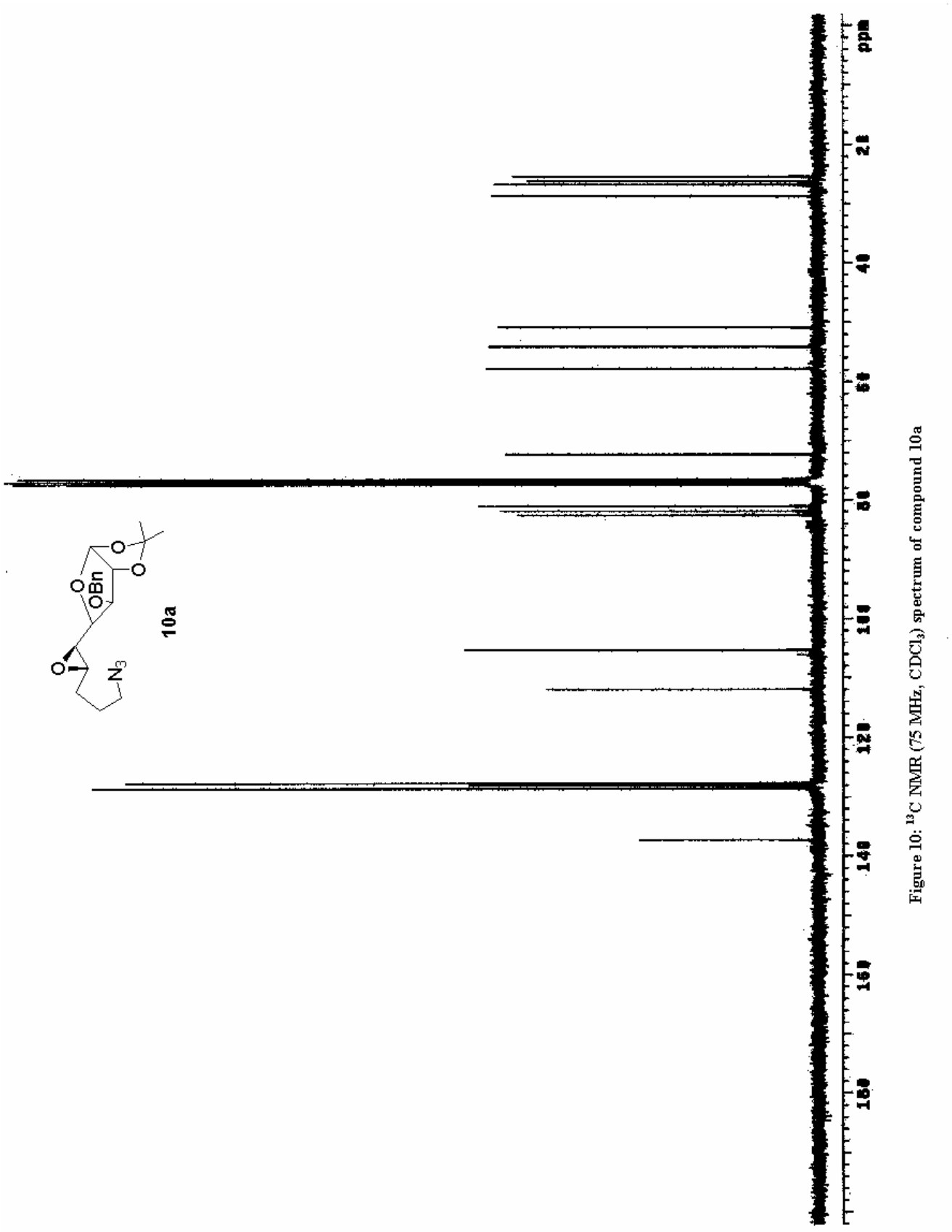

Figure 10: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 10a

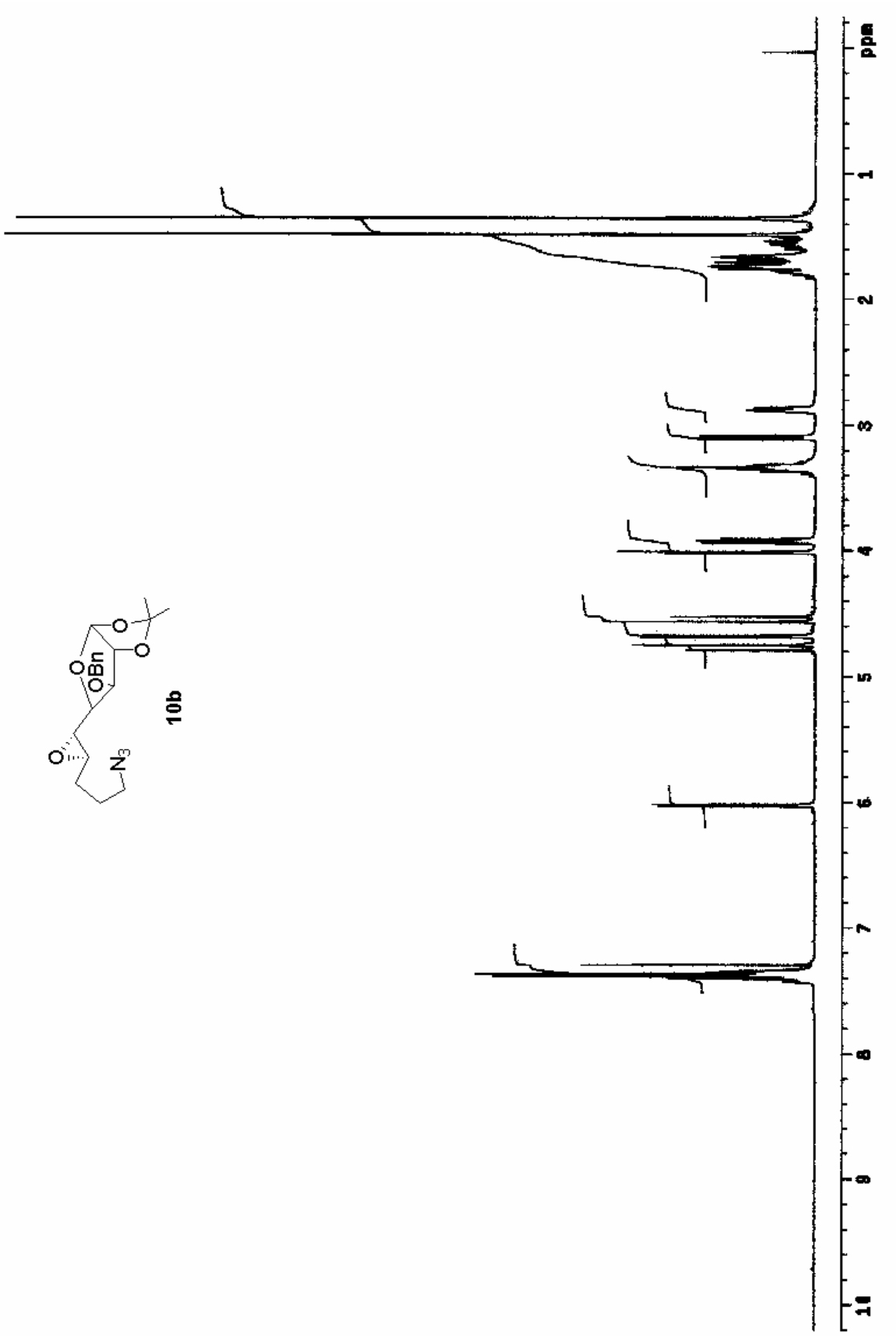

Figure 11: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 10b

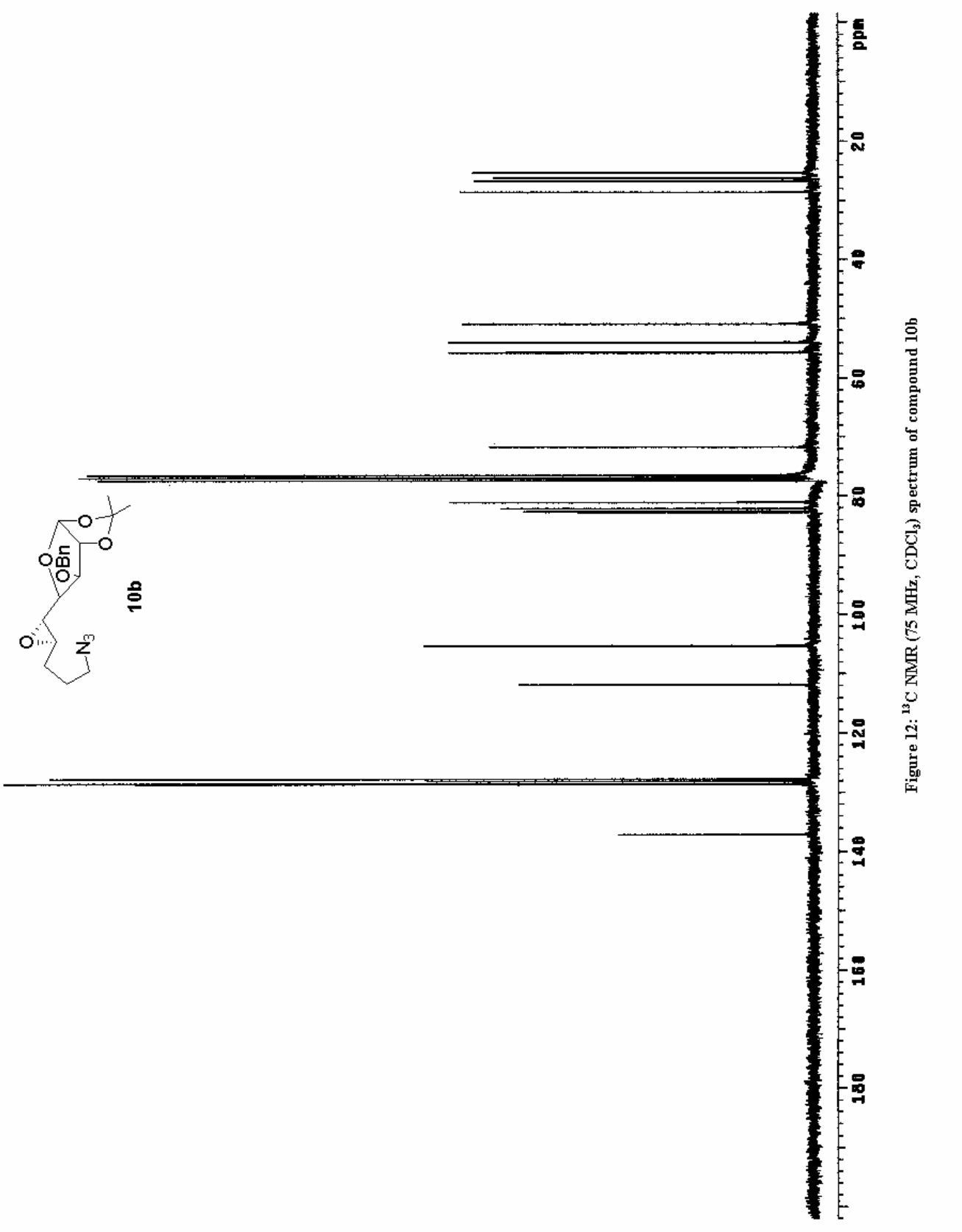

Figure 12: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 10b

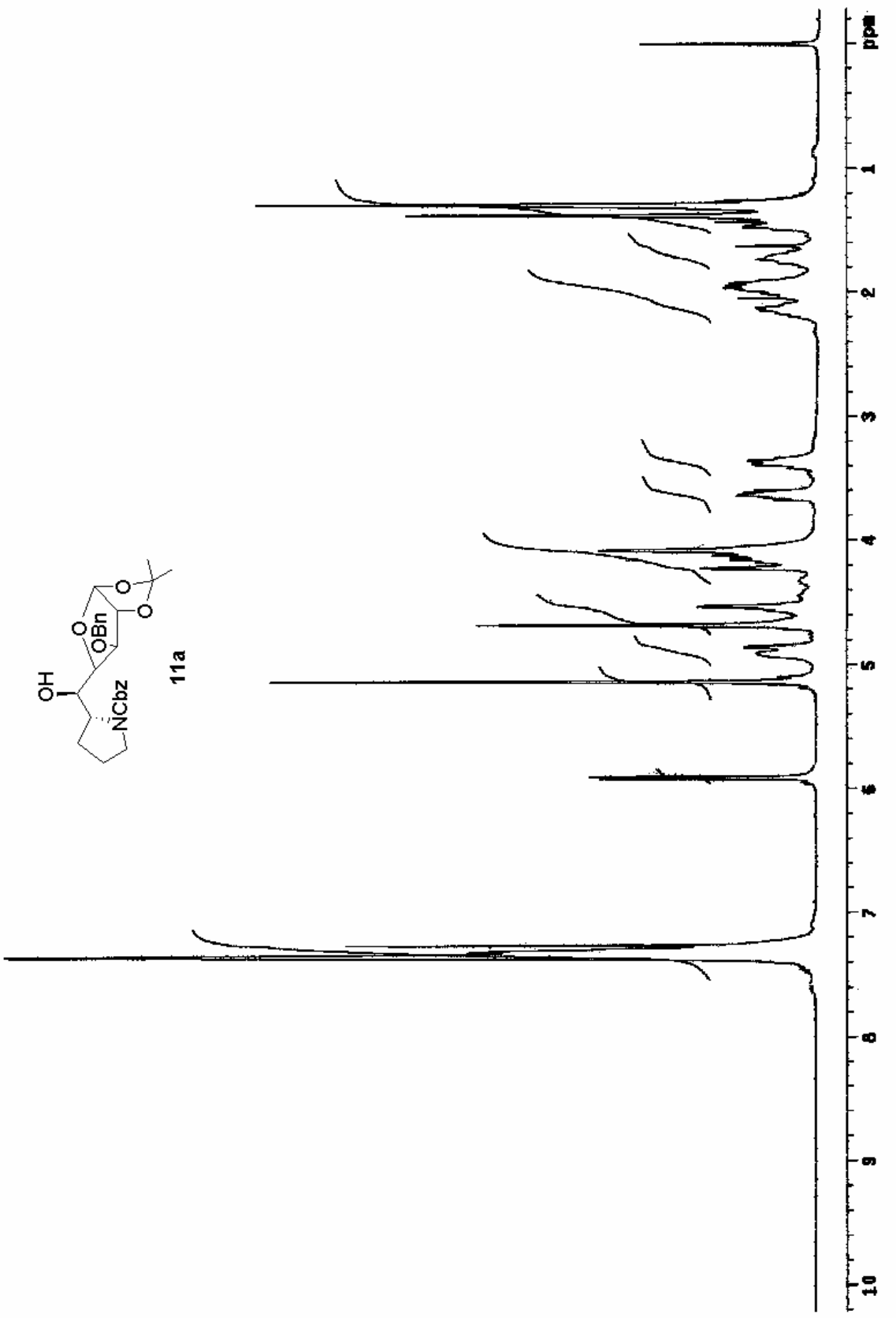

Figure 13: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 11a

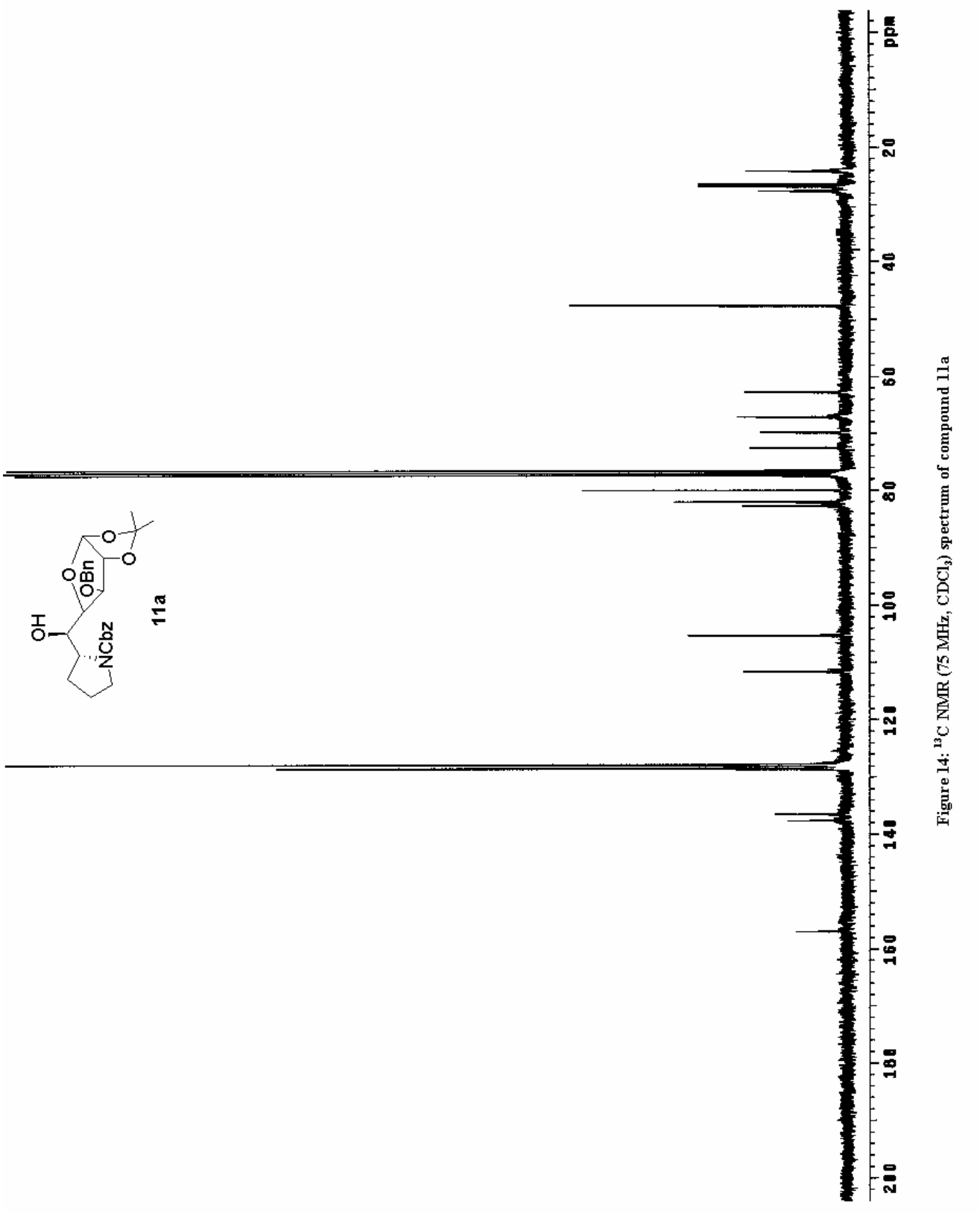

Figure 14: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 11a

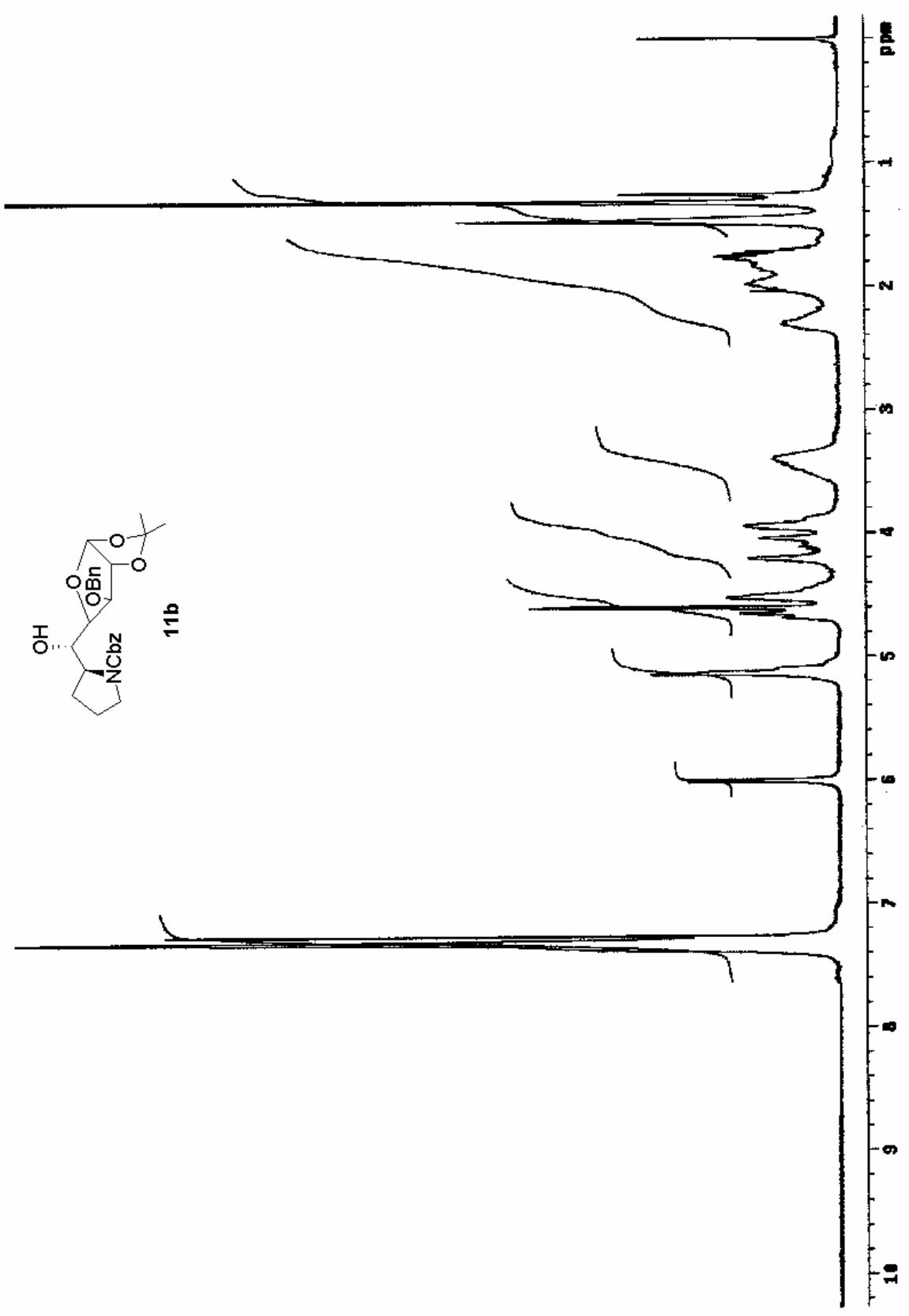

Figure 15: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 11b

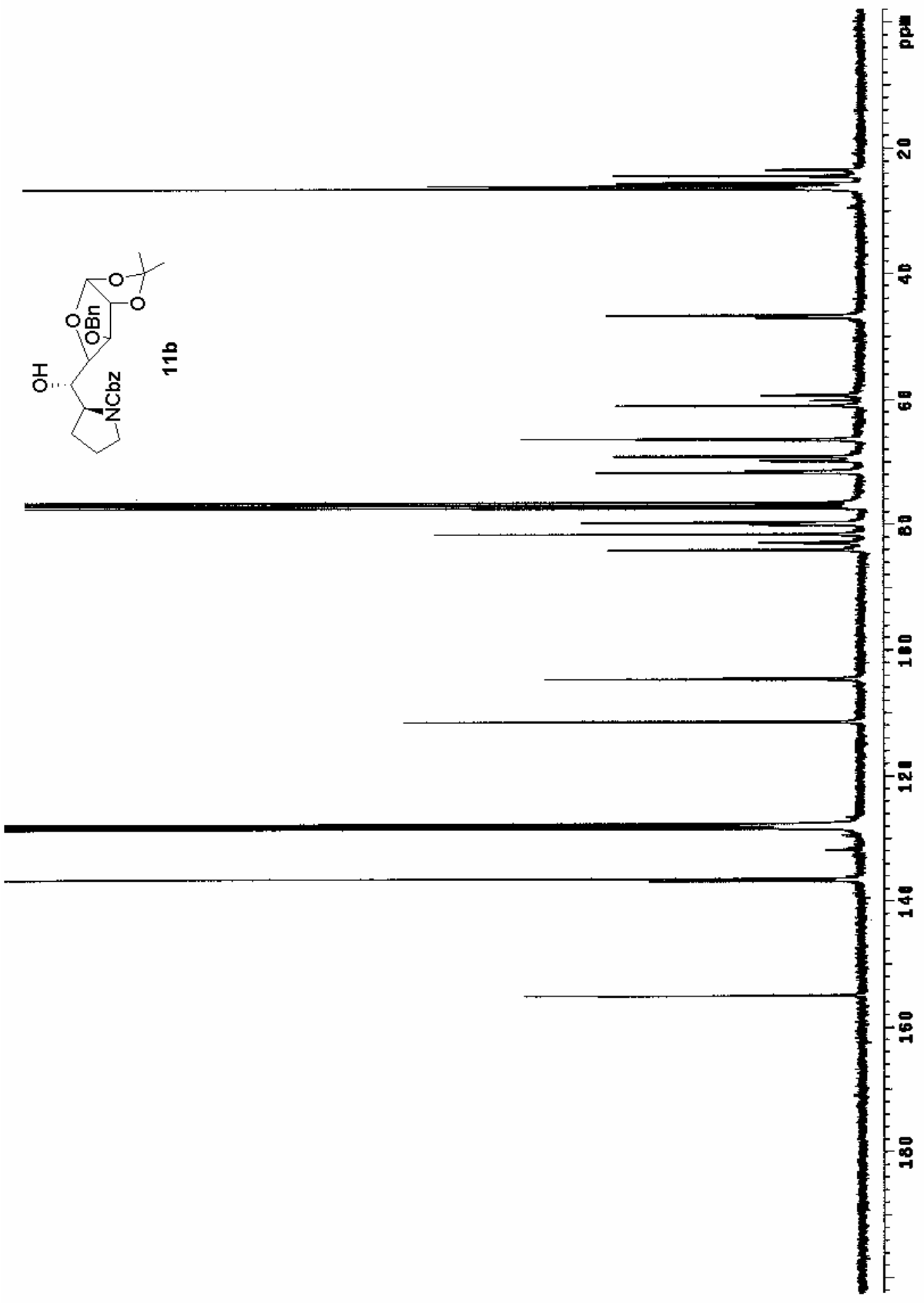

Figure 16: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 11b

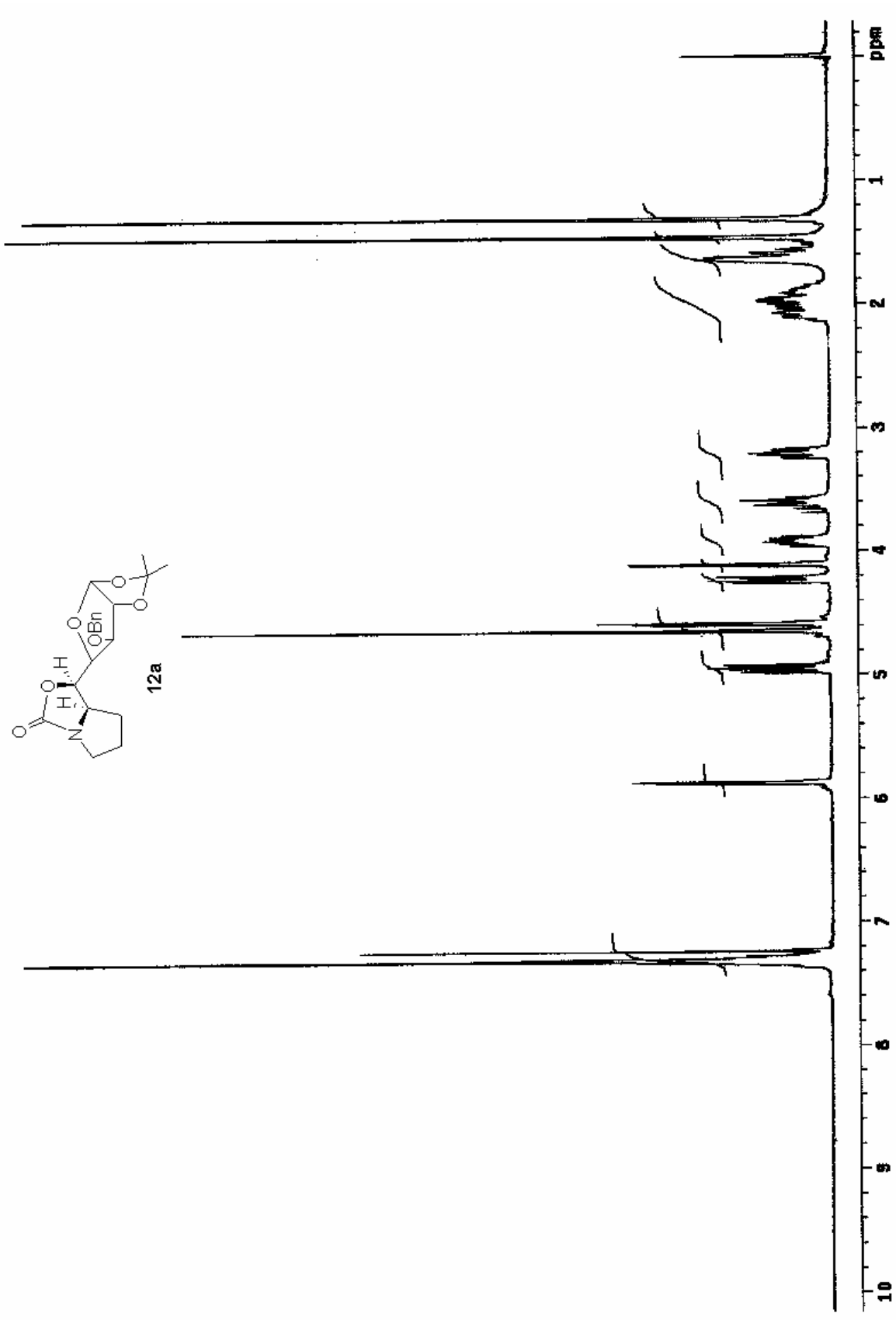

Figure 17: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 12a

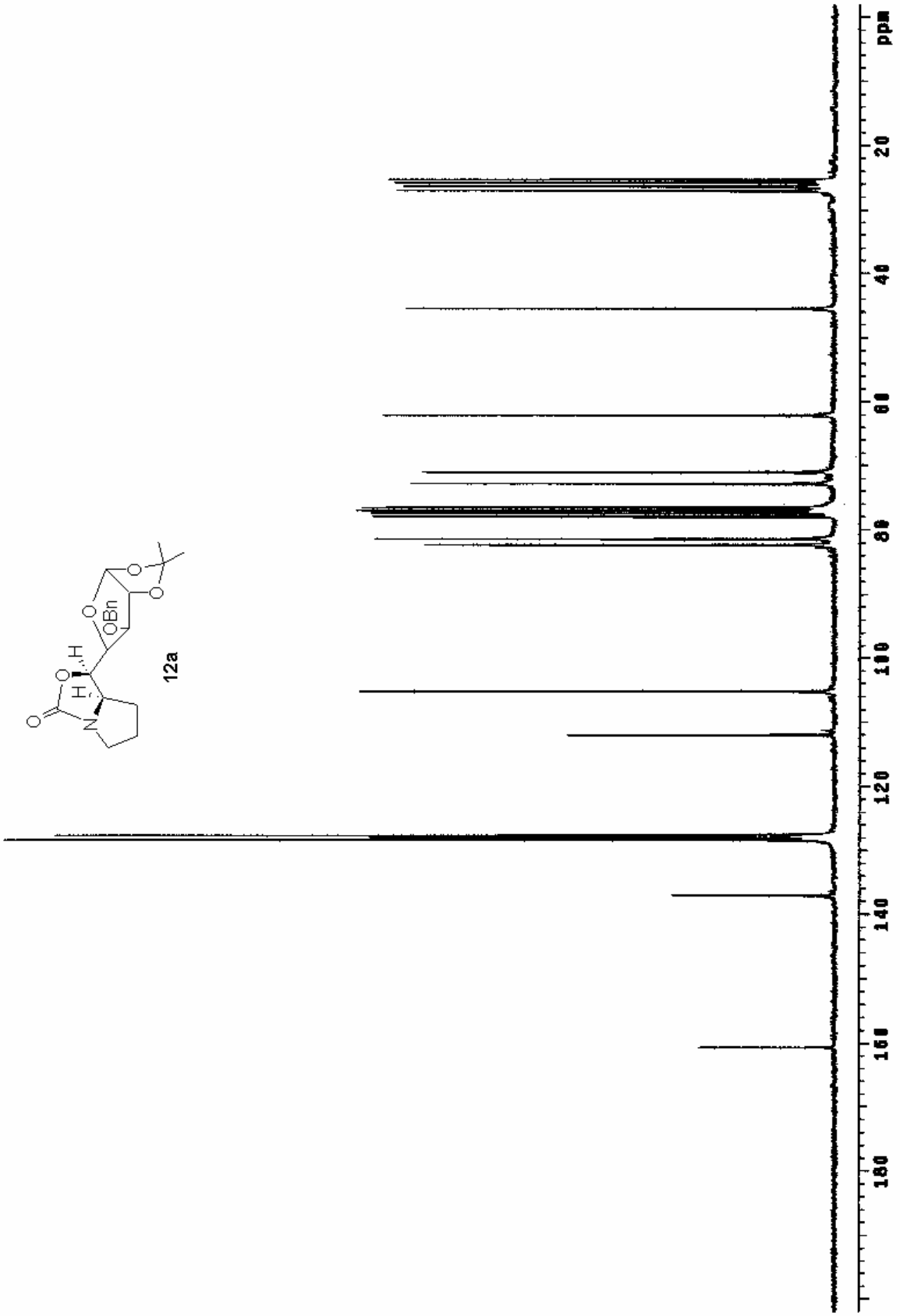

Figure 18: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 12a

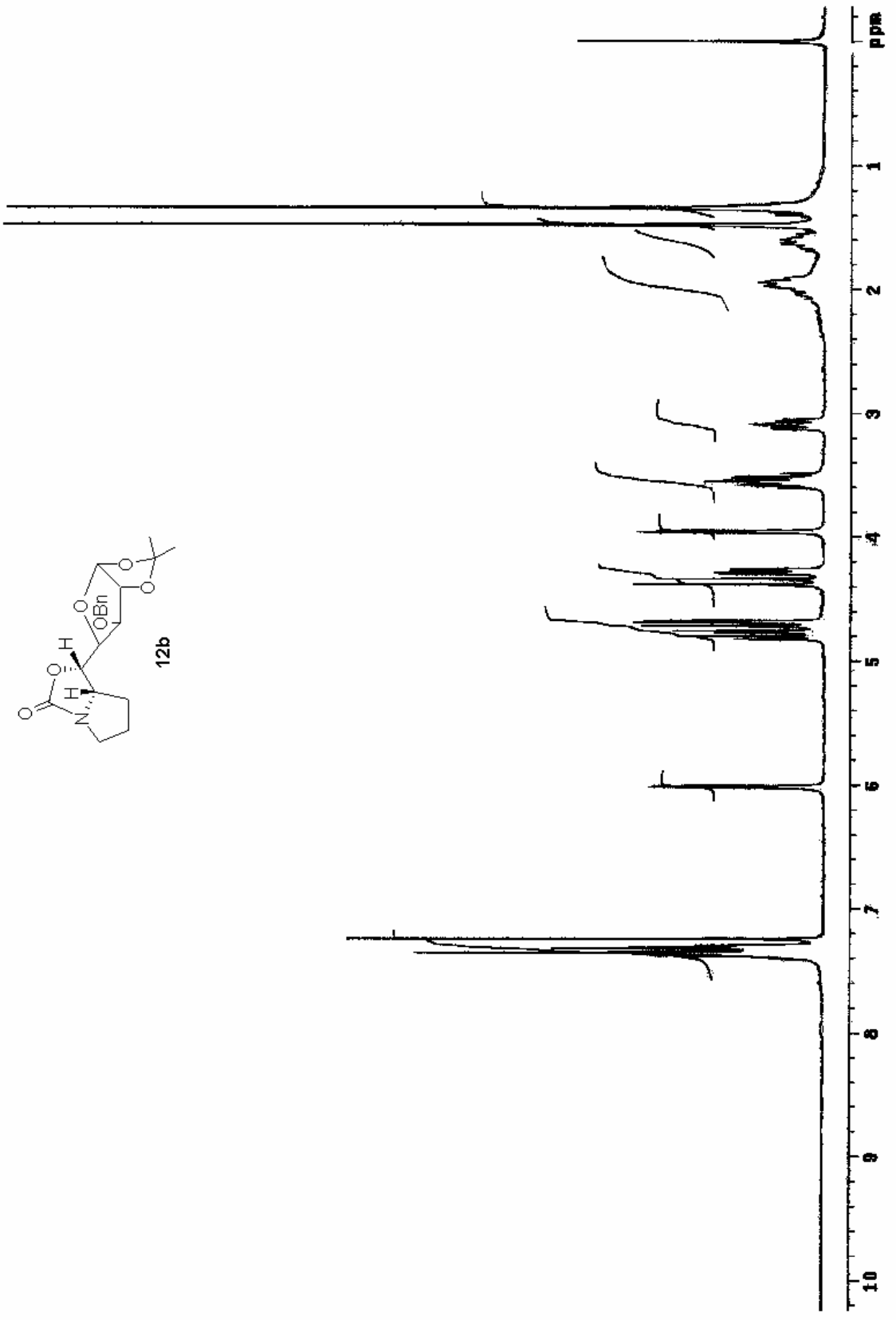

Figure 19: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 12b

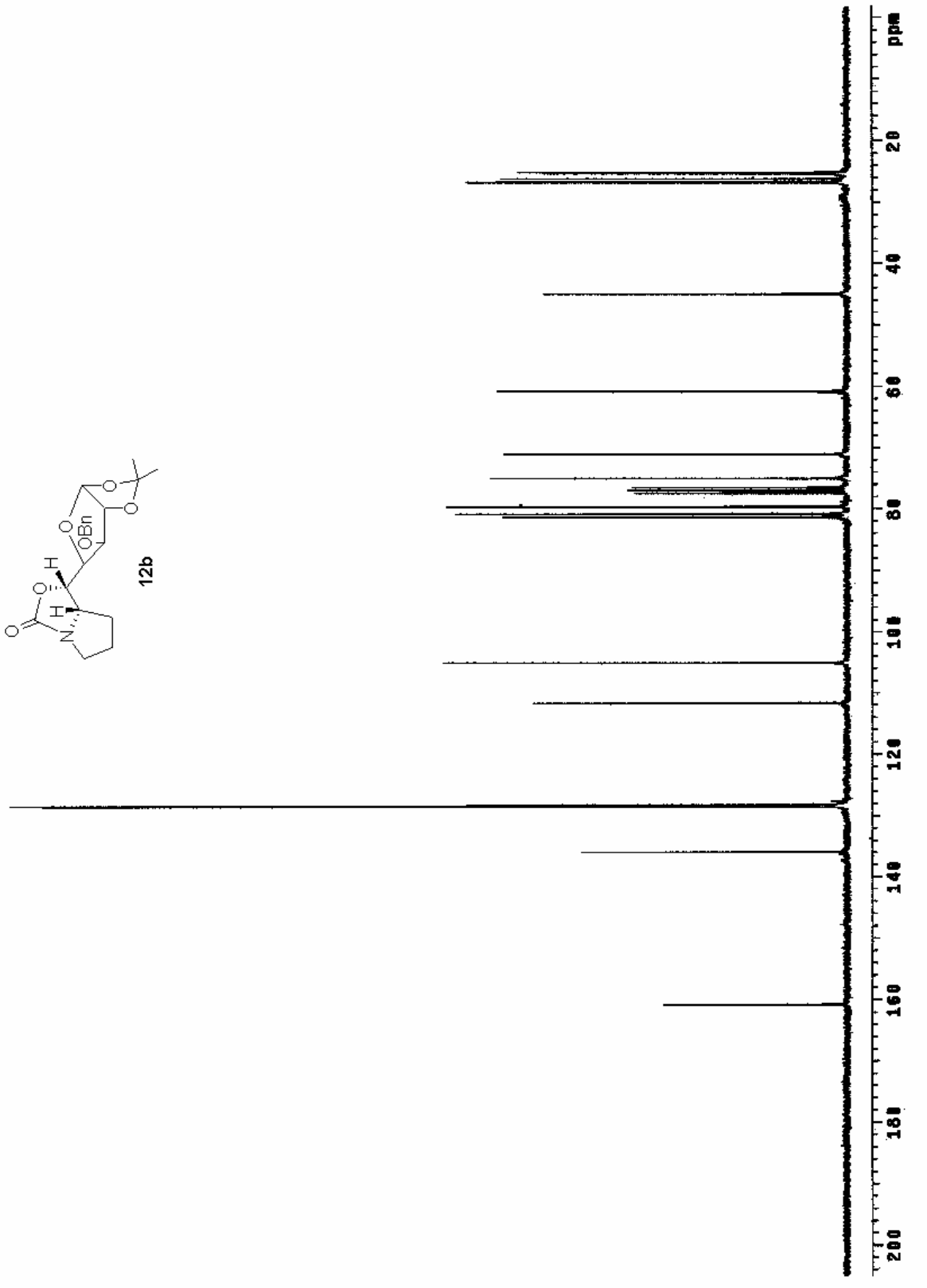

Figure 20: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 12b

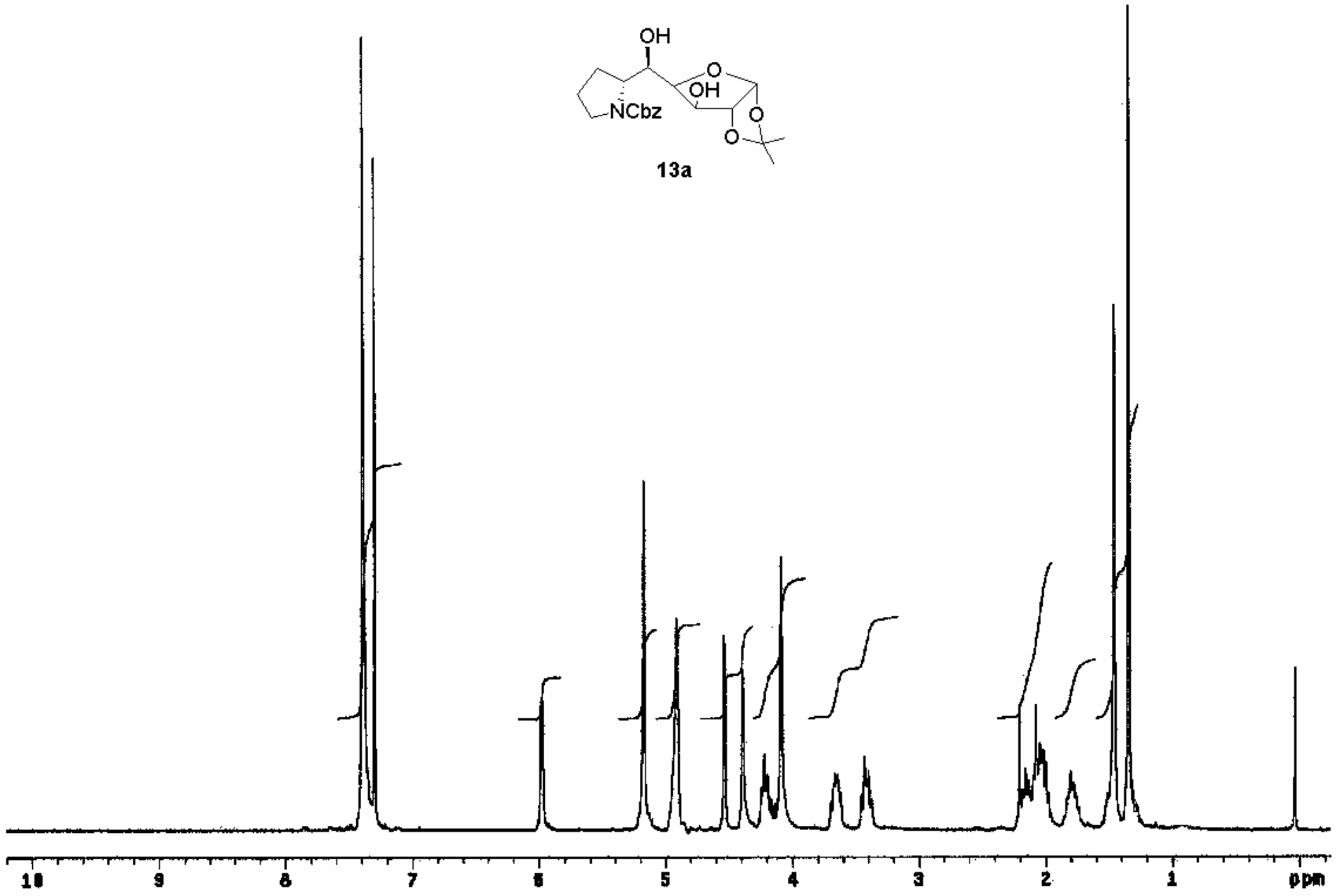

Figure 21: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 13a

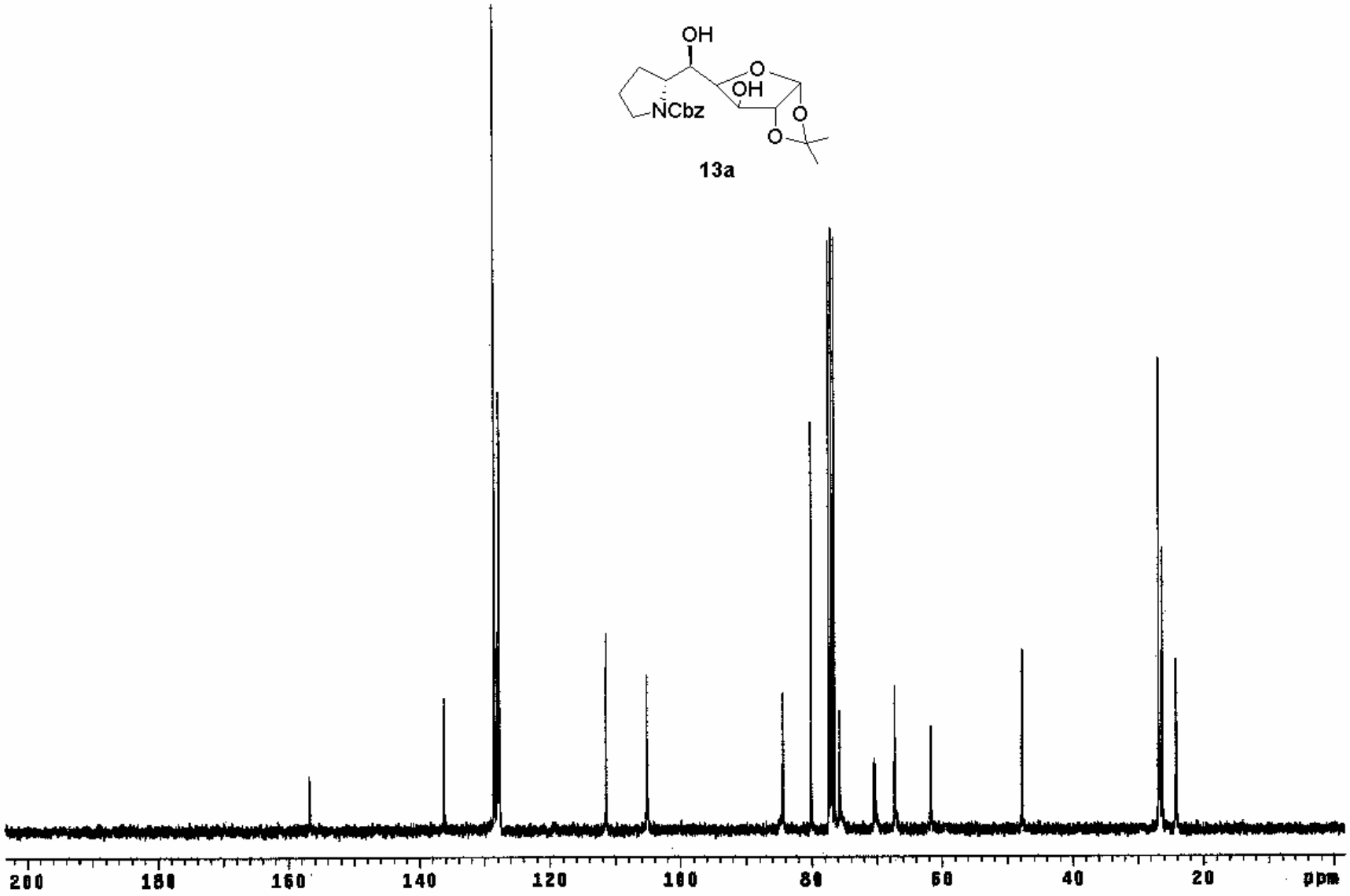

Figure 22: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 13a

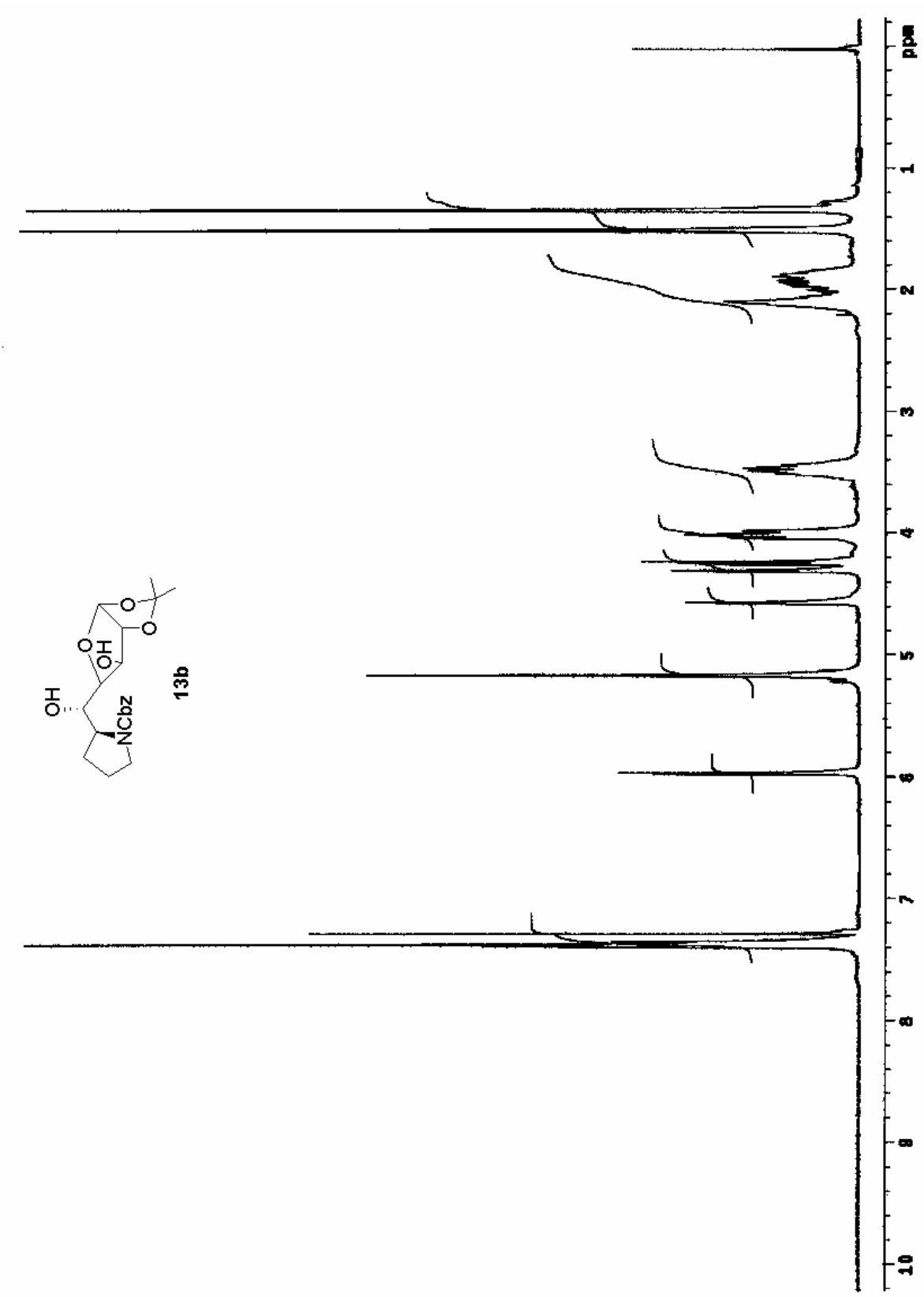

Figure 23: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 13b

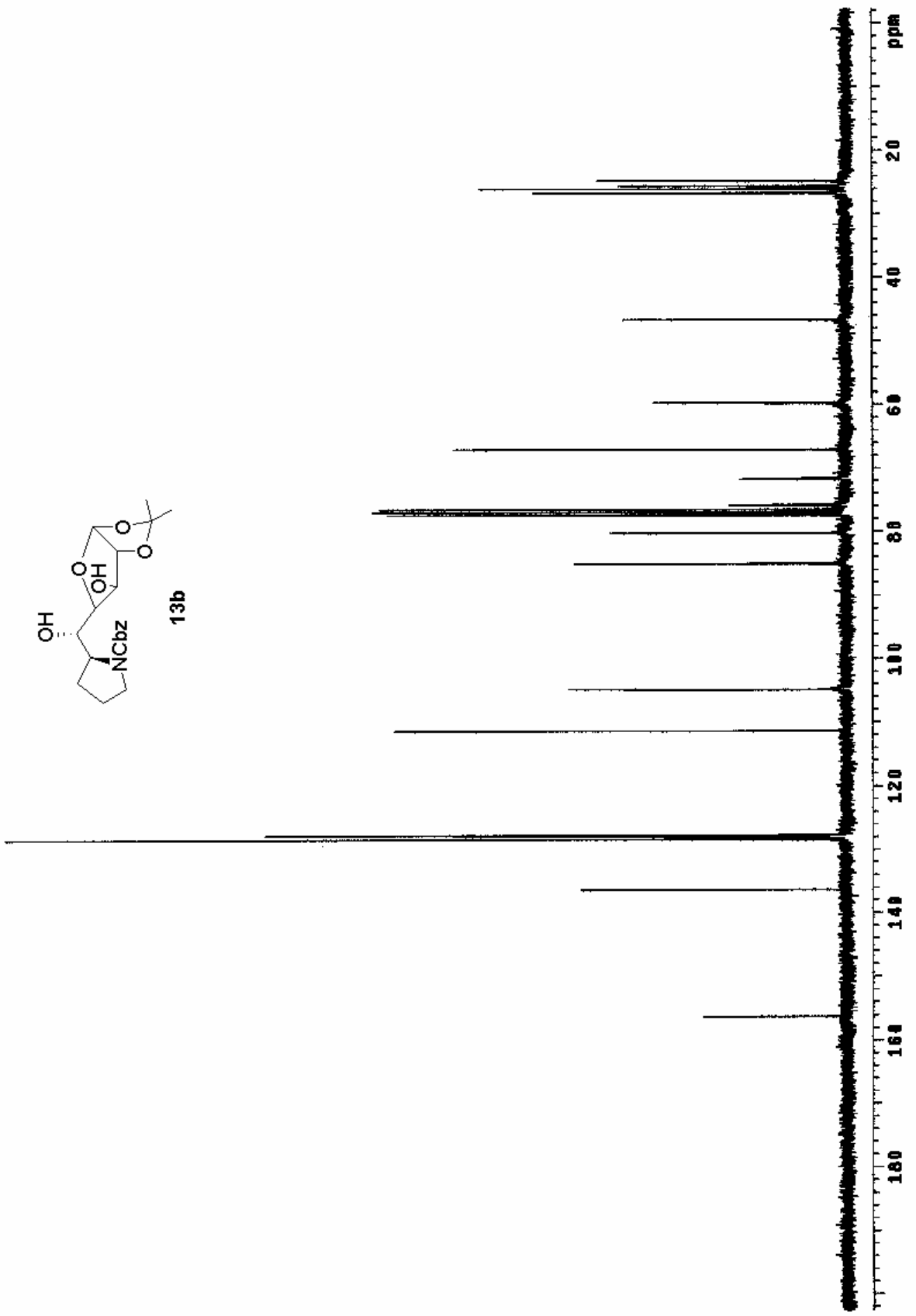

Figure 24: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 13b

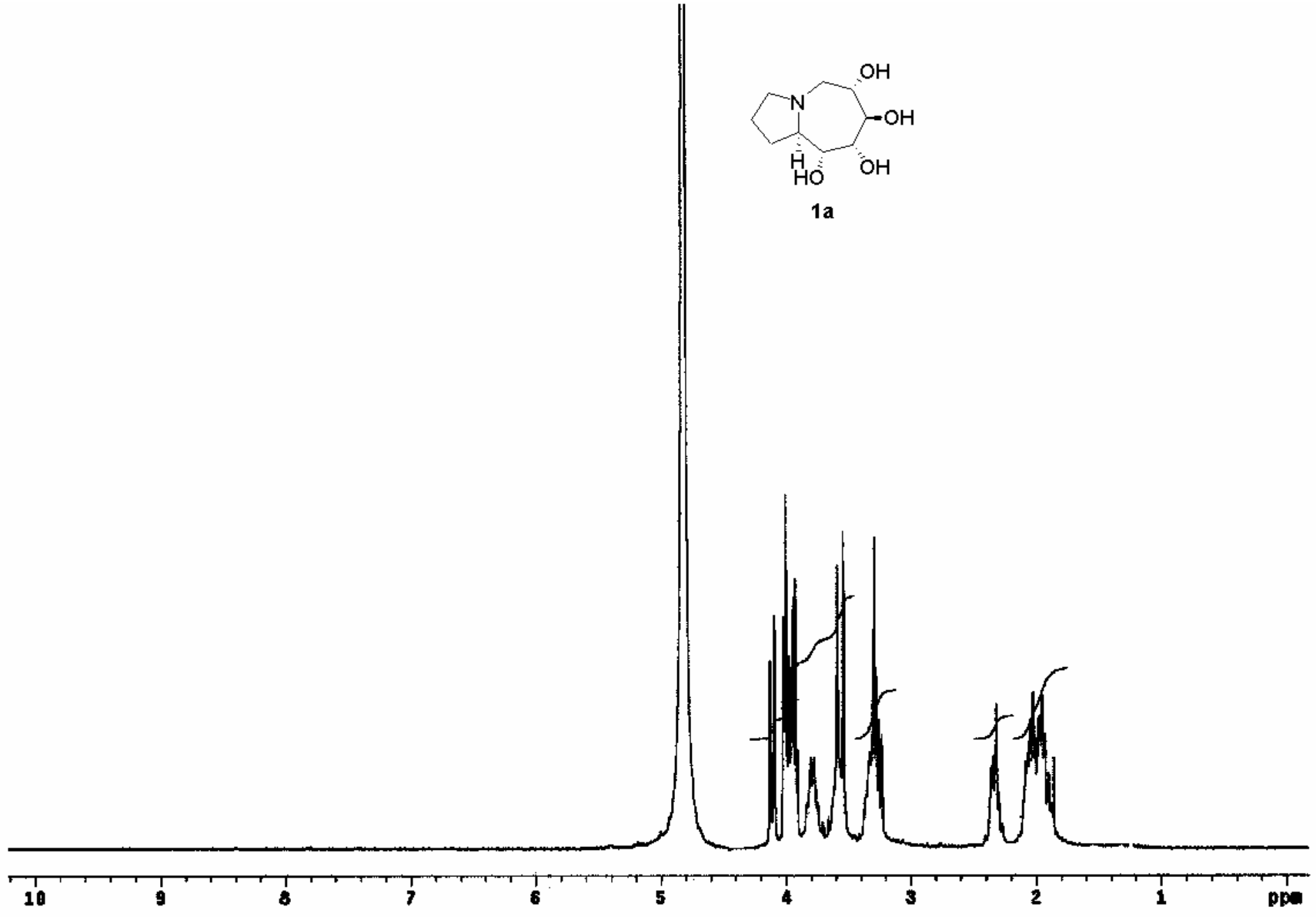

Figure 25: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 1a

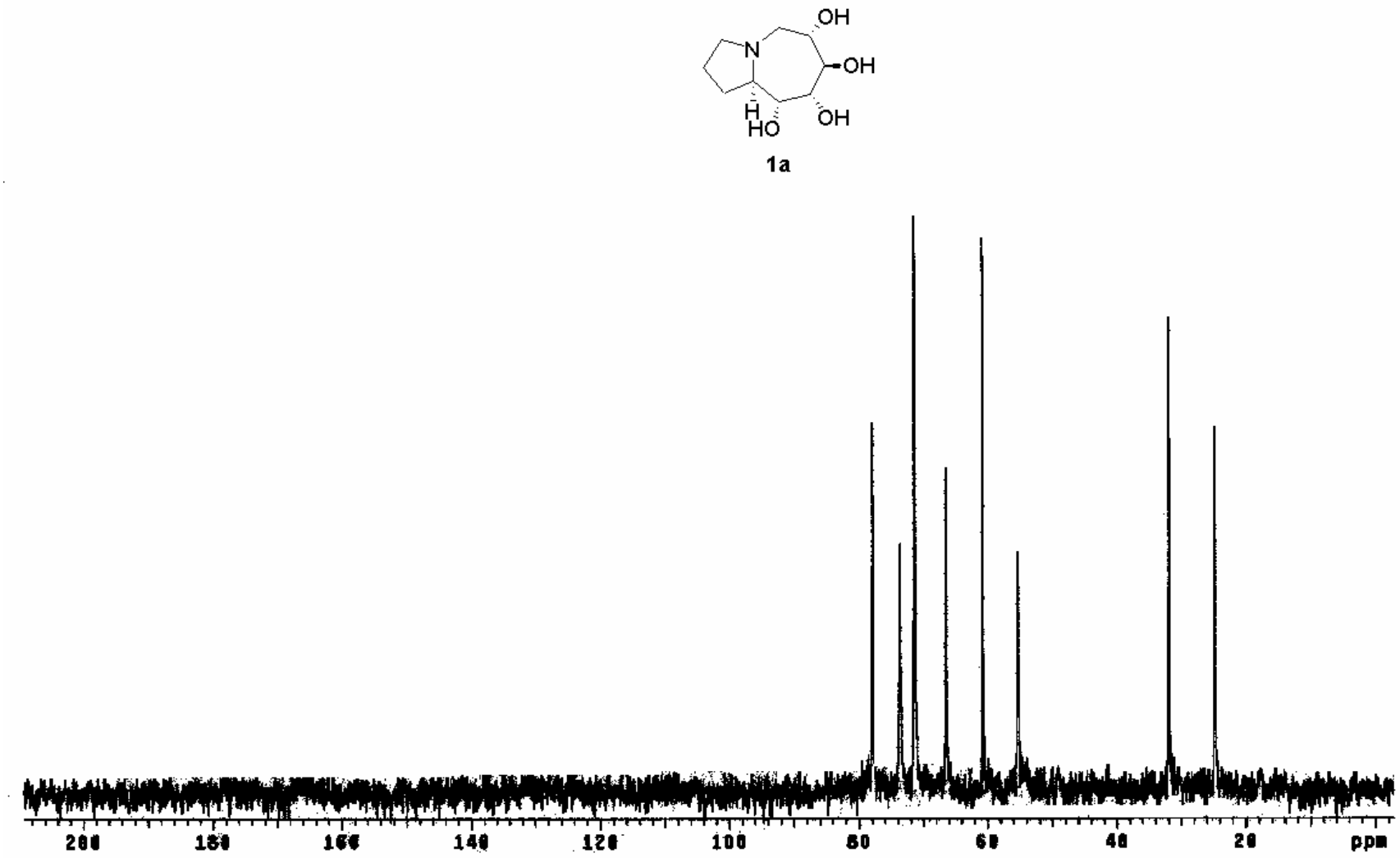

Figure 26: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 1a

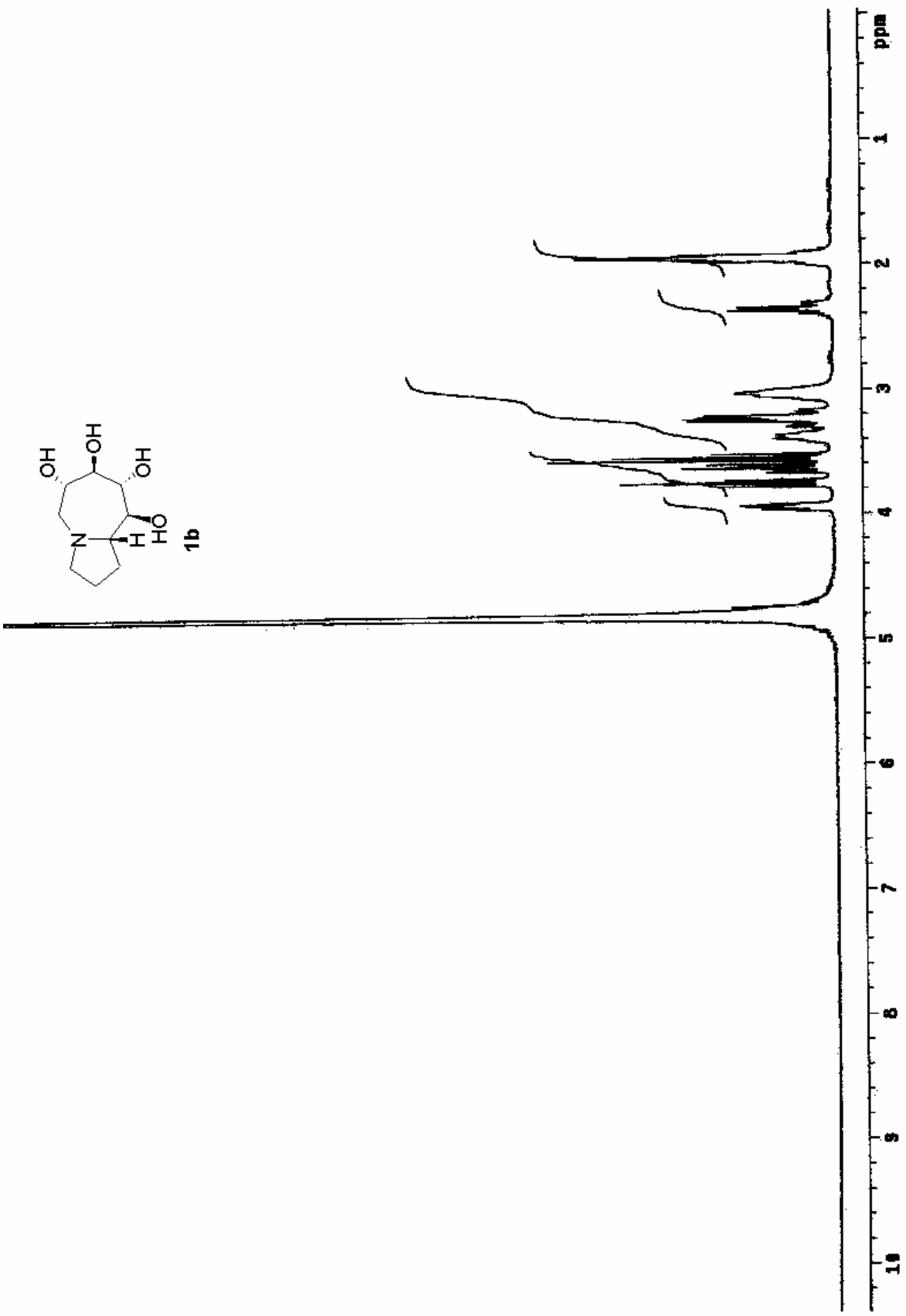

Figure 27: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 1b

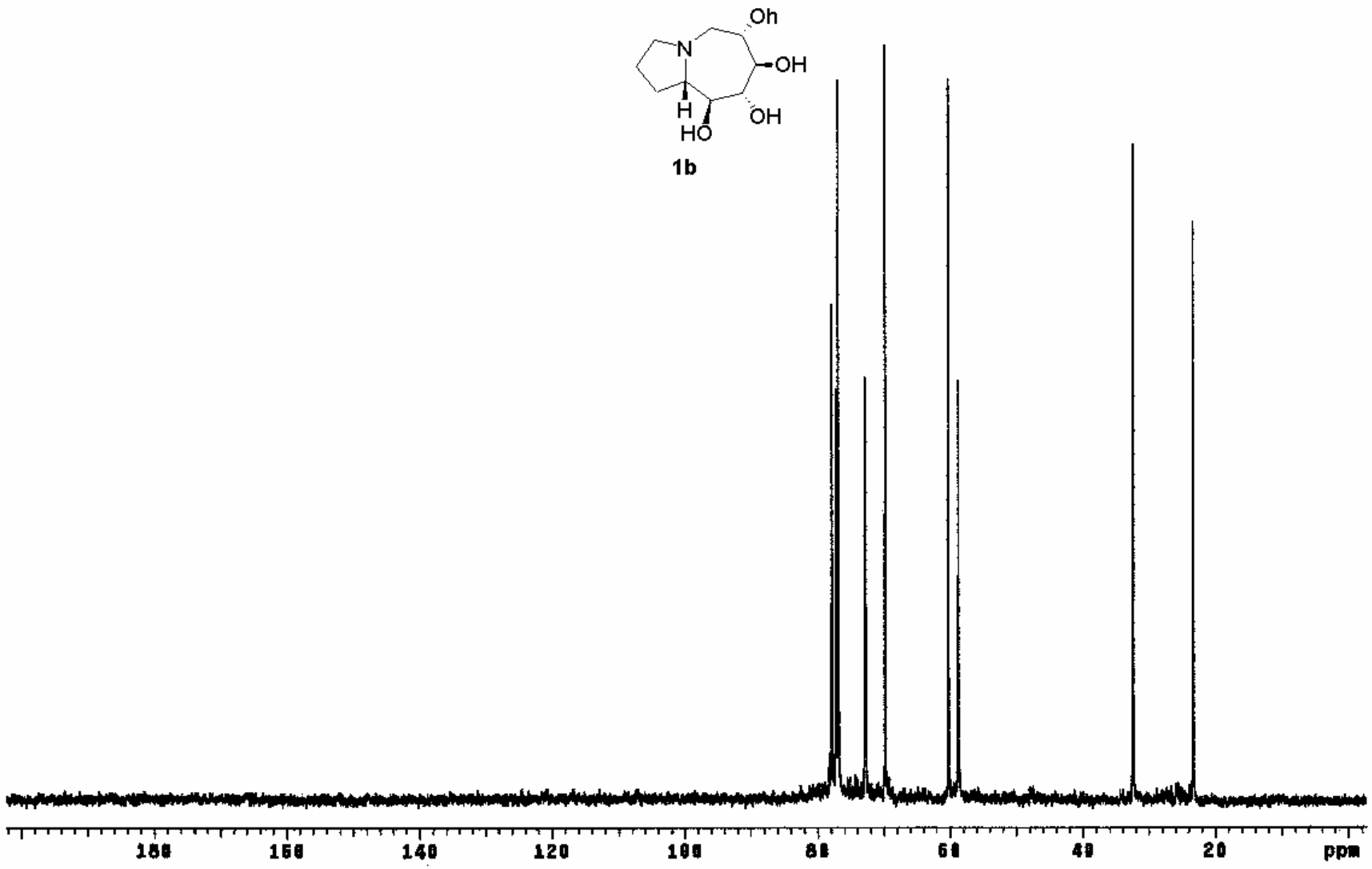

Figure 28: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 1b

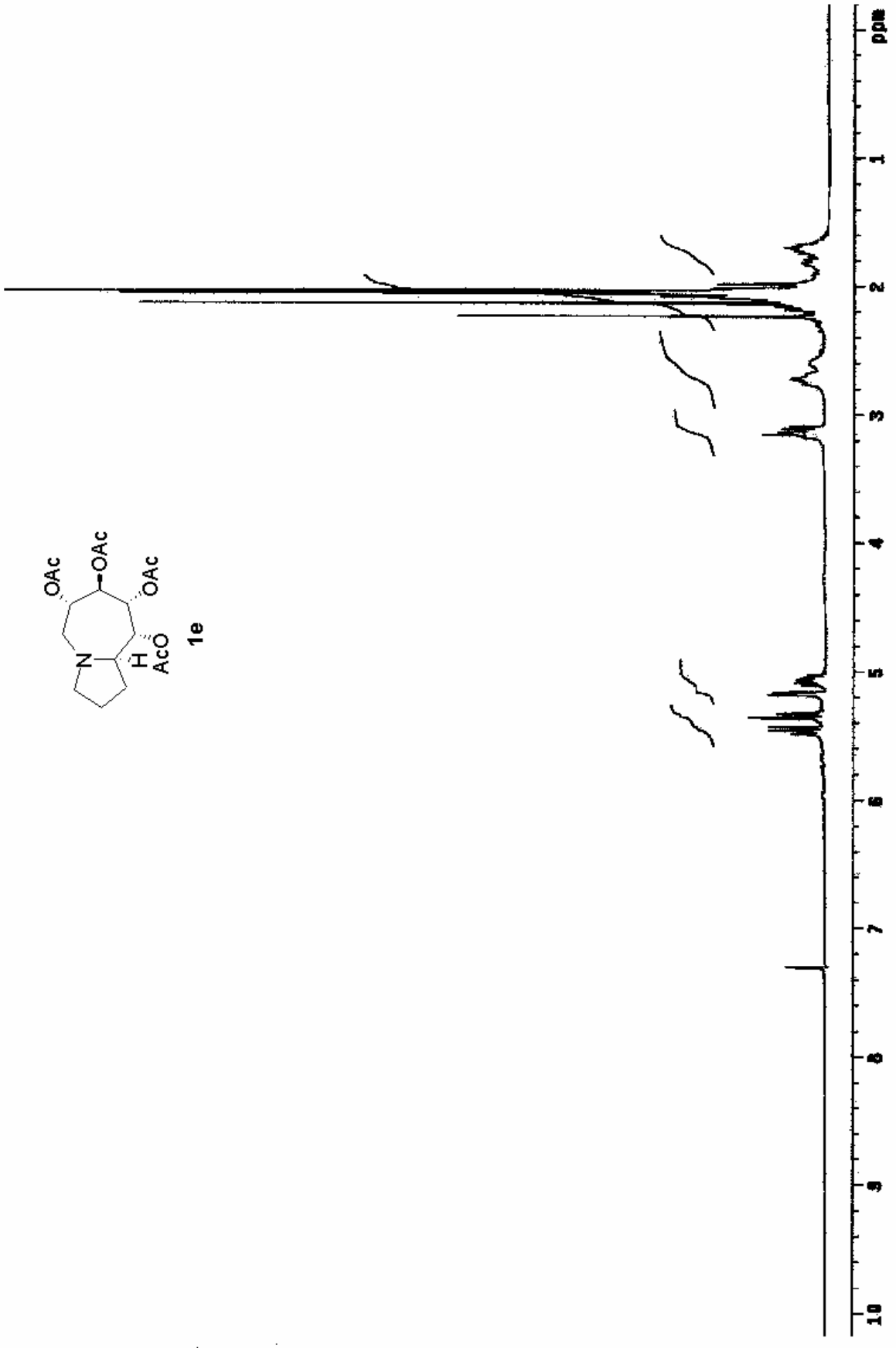

Figure 29: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 1e

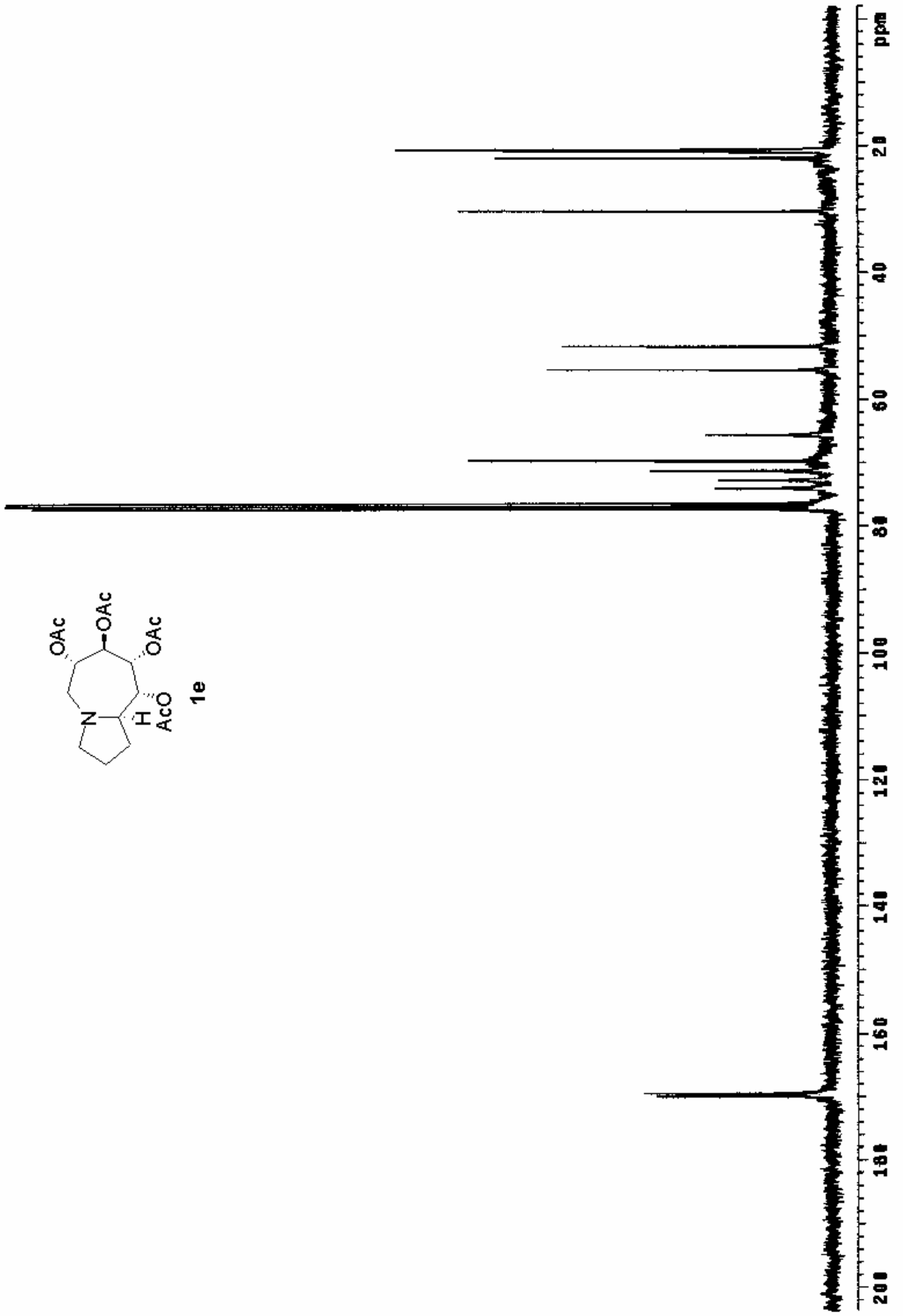

Figure 30: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 1e

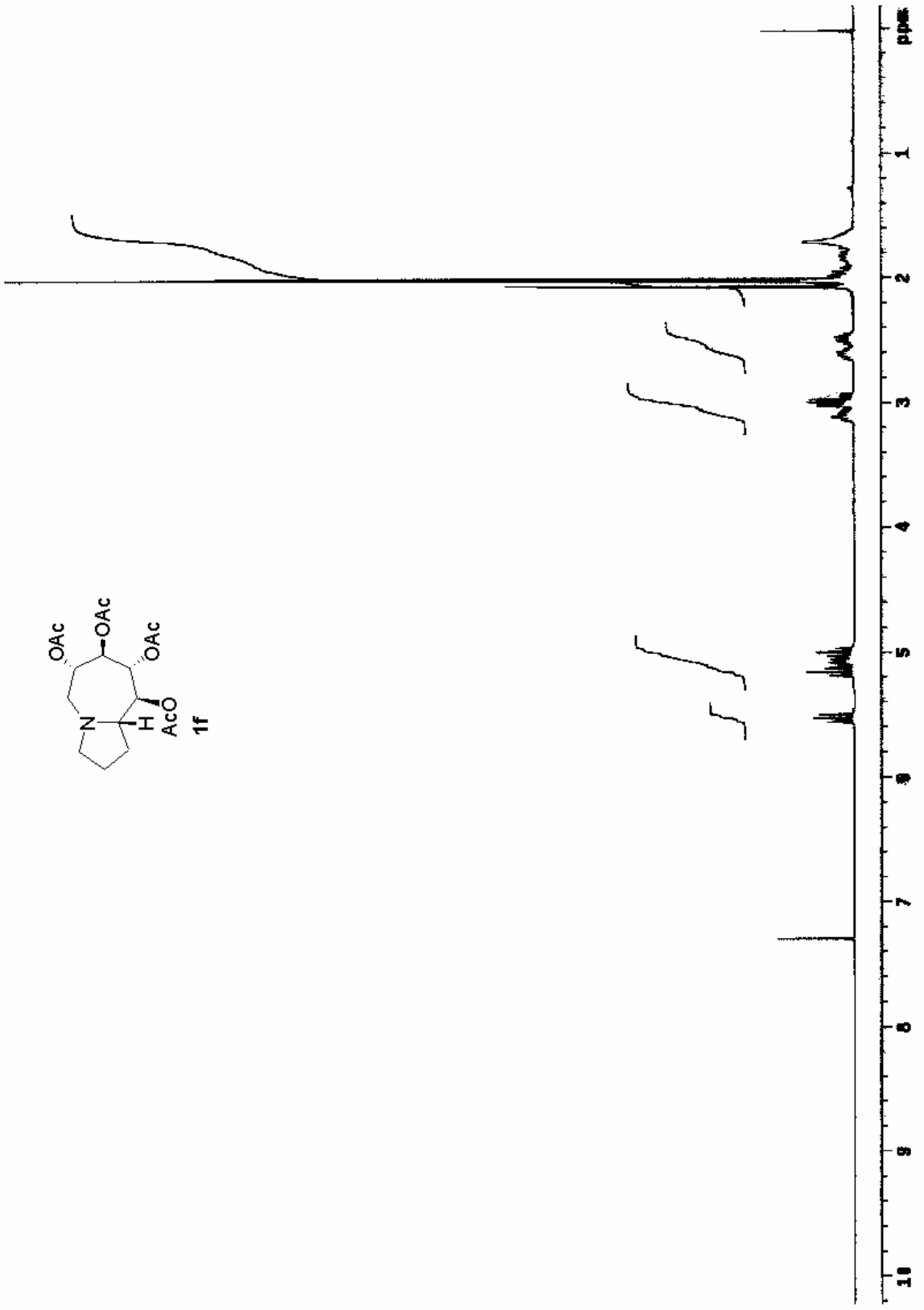

Figure 31: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 1f

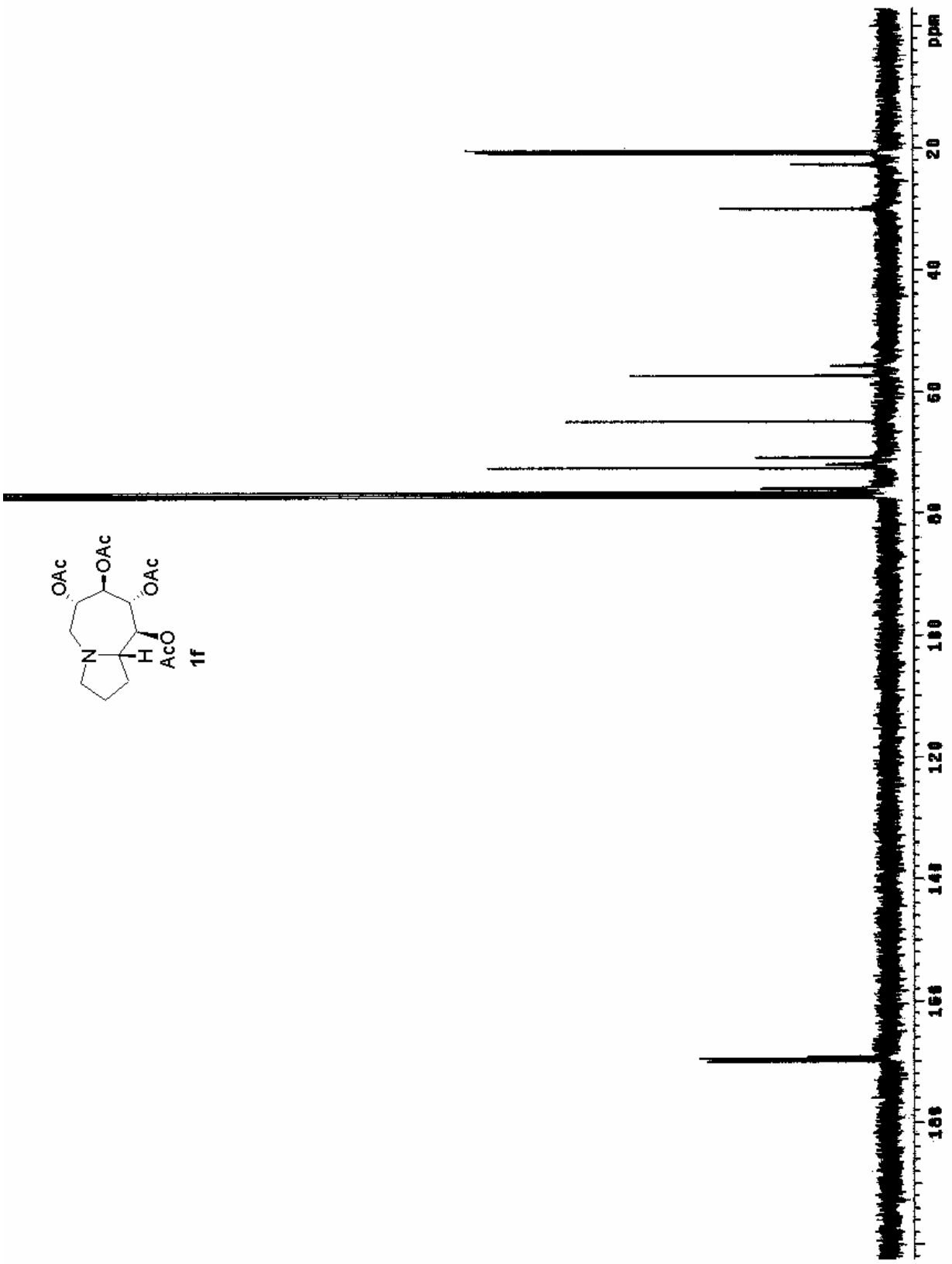

Figure 32: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 1f

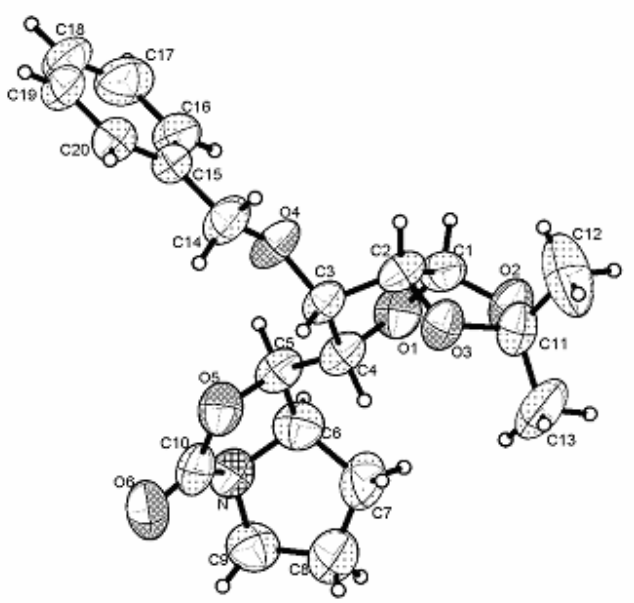

Fig.2 ORTEP drawing of the compound **12a**, the ellipsoids are drawn at 50% probability

Table 1. Crystal data and structure refinement for 3-*O*-benzyl-(6-*N*,5-*O*-carbonyl)-6,7,8,9-tetradeoxy-1,2-*O*-isopropylidene-α-D-*glycero*-D-*gluco*-nonofuranose **12a**.

Empirical formula	C20 H25 N O6
Formula weight	375.41
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P212121
Unit cell dimensions	a = 5.5259(4) A b = 10.0212(7) A c = 34.600(2) A
Volume	1916.0(2) A^3
Z, Calculated density	4, 1.301 Mg/m^3
Absorption coefficient	0.096 mm^-1
F(000)	800
Crystal size	0.54 x 0.17 x 0.13 mm
Theta range for data collection	2.12 to 25.00 deg.
Limiting indices	-6<=h<=6, -11<=k<=9, -32<=l<=41
Reflections collected / unique	9697 / 3372 [R(int) = 0.0270]

Completeness to theta = 25.00	100.0 %
Max. and min. transmission	0.9872 and 0.9499
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters 3372 / 0 / 246

Goodness-of-fit on F^2 1.178

Final R indices [I>2sigma(I)] R1 = 0.0622, wR2 = 0.1473

R indices (all data) R1 = 0.0694, wR2 = 0.1516

Absolute structure parameter 0.6(19)

Largest diff. peak and hole 0.191 and -0.154 e.A^-3

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

	x	y	z	U(eq)
O(1)	11724(4)	6034(2)	8413(1)	67(1)
O(2)	11780(5)	3741(2)	8484(1)	74(1)
O(3)	8849(4)	4052(2)	8930(1)	62(1)
O(4)	10877(5)	7406(2)	9146(1)	68(1)
O(5)	7154(5)	8611(2)	8511(1)	71(1)
O(6)	4213(5)	9856(3)	8251(1)	85(1)
N	7499(6)	9200(3)	7892(1)	63(1)
C(1)	12291(6)	4959(4)	8656(1)	60(1)
C(2)	10591(6)	5058(4)	9004(1)	60(1)
C(3)	9432(6)	6426(3)	8967(1)	55(1)
C(4)	9453(6)	6593(3)	8530(1)	58(1)
C(5)	9382(6)	8001(3)	8381(1)	61(1)
C(6)	9265(8)	8128(4)	7940(1)	71(1)
C(7)	8298(11)	7003(4)	7692(1)	106(2)
C(8)	6461(10)	7595(4)	7430(1)	99(1)
C(9)	6326(8)	9039(4)	7516(1)	76(1)
C(10)	6098(7)	9285(3)	8212(1)	64(1)
C(11)	9919(7)	3068(3)	8687(1)	65(1)
C(12)	11032(13)	1979(5)	8922(2)	135(2)
C(13)	8036(9)	2610(5)	8409(2)	119(2)
C(14)	10084(7)	7792(4)	9505(1)	74(1)
C(15)	11563(6)	8922(3)	9662(1)	58(1)
C(16)	13603(7)	9389(4)	9478(1)	70(1)
C(17)	14892(9)	10434(4)	9647(2)	92(1)
C(18)	14122(11)	11012(4)	9987(1)	91(2)
C(19)	12141(10)	10549(4)	10159(1)	87(1)
C(20)	10840(8)	9517(4)	10002(1)	74(1)

Table 3. Bond lengths [A] and angles [deg] for 3-*O*-benzyl-(6-*N*,5-*O*-carbonyl)-6,7,8,9-tetradeoxy-1,2-*O*-isopropylidene-α-D-*glycero*-D-*gluco*-nonofuranose **12a**..

O(1)-C(1)	1.402(4)
O(1)-C(4)	1.433(4)
O(2)-C(1)	1.386(4)
O(2)-C(11)	1.416(4)
O(3)-C(2)	1.417(4)

O(3)-C(11)	1.423(4)
O(4)-C(14)	1.372(4)
O(4)-C(3)	1.410(4)
O(5)-C(10)	1.367(4)
O(5)-C(5)	1.446(4)

O(6)-C(10)	1.196(5)
N-C(10)	1.353(5)
N-C(6)	1.461(5)
N-C(9)	1.463(4)
C(1)-C(2)	1.531(5)
C(1)-H(1)	0.9800
C(2)-C(3)	1.519(5)
C(2)-H(2)	0.9800
C(3)-C(4)	1.519(4)
C(3)-H(3)	0.9800
C(4)-C(5)	1.503(5)
C(4)-H(4)	0.9800
C(5)-C(6)	1.535(5)
C(5)-H(5)	0.9800
C(6)-C(7)	1.514(6)
C(6)-H(6)	0.9800
C(7)-C(8)	1.484(6)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-C(9)	1.480(6)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(11)-C(12)	1.494(6)
C(11)-C(13)	1.491(6)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.498(5)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.376(5)
C(15)-C(20)	1.378(5)
C(16)-C(17)	1.395(5)
C(16)-H(16)	0.9300
C(17)-C(18)	1.378(7)
C(17)-H(17)	0.9300
C(18)-C(19)	1.330(7)
C(18)-H(18)	0.9300
C(19)-C(20)	1.371(6)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300

C(1)-O(1)-C(4)	109.0(2)
C(1)-O(2)-C(11)	110.8(3)
C(2)-O(3)-C(11)	108.5(2)
C(14)-O(4)-C(3)	114.4(3)
C(10)-O(5)-C(5)	109.7(3)
C(10)-N-C(6)	109.6(3)
C(10)-N-C(9)	118.7(3)
C(6)-N-C(9)	108.4(3)
O(2)-C(1)-O(1)	112.0(2)
O(2)-C(1)-C(2)	105.6(3)
O(1)-C(1)-C(2)	106.6(3)
O(2)-C(1)-H(1)	110.8
O(1)-C(1)-H(1)	110.8
C(2)-C(1)-H(1)	110.8

O(3)-C(2)-C(3)	109.9(3)
O(3)-C(2)-C(1)	103.2(2)
C(3)-C(2)-C(1)	104.5(3)
O(3)-C(2)-H(2)	112.8
C(3)-C(2)-H(2)	112.8
C(1)-C(2)-H(2)	112.8

O(4)-C(3)-C(2)	110.7(3)
O(4)-C(3)-C(4)	110.8(3)
C(2)-C(3)-C(4)	100.4(2)
O(4)-C(3)-H(3)	111.5
C(2)-C(3)-H(3)	111.5
C(4)-C(3)-H(3)	111.5
O(1)-C(4)-C(5)	107.0(3)
O(1)-C(4)-C(3)	104.2(3)
C(5)-C(4)-C(3)	116.4(3)
O(1)-C(4)-H(4)	109.6
C(5)-C(4)-H(4)	109.6
C(3)-C(4)-H(4)	109.6
O(5)-C(5)-C(4)	108.2(3)
O(5)-C(5)-C(6)	103.8(3)
C(4)-C(5)-C(6)	114.9(3)
O(5)-C(5)-H(5)	109.9
C(4)-C(5)-H(5)	109.9
C(6)-C(5)-H(5)	109.9
N-C(6)-C(7)	104.3(3)
N-C(6)-C(5)	101.6(3)
C(7)-C(6)-C(5)	121.1(3)
N-C(6)-H(6)	109.6
C(7)-C(6)-H(6)	109.6
C(5)-C(6)-H(6)	109.6
C(8)-C(7)-C(6)	106.8(4)
C(8)-C(7)-H(7A)	110.4
C(6)-C(7)-H(7A)	110.4
C(8)-C(7)-H(7B)	110.4
C(6)-C(7)-H(7B)	110.4
H(7A)-C(7)-H(7B)	108.6
C(9)-C(8)-C(7)	107.6(4)
C(9)-C(8)-H(8A)	110.2
C(7)-C(8)-H(8A)	110.2
C(9)-C(8)-H(8B)	110.2
C(7)-C(8)-H(8B)	110.2
H(8A)-C(8)-H(8B)	108.5
N-C(9)-C(8)	105.3(3)
N-C(9)-H(9A)	110.7
C(8)-C(9)-H(9A)	110.7
N-C(9)-H(9B)	110.7
C(8)-C(9)-H(9B)	110.7
H(9A)-C(9)-H(9B)	108.8
O(6)-C(10)-N	128.4(4)
O(6)-C(10)-O(5)	121.4(3)
N-C(10)-O(5)	110.1(3)
O(2)-C(11)-O(3)	105.3(3)
O(2)-C(11)-C(12)	108.6(4)
O(3)-C(11)-C(12)	110.9(3)
O(2)-C(11)-C(13)	109.4(3)
O(3)-C(11)-C(13)	107.7(3)
C(12)-C(11)-C(13)	114.5(4)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5

C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(4)-C(14)-C(15)	111.5(3)
O(4)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14A)	109.3
O(4)-C(14)-H(14B)	109.3

C(15)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
C(16)-C(15)-C(20)	119.0(3)
C(16)-C(15)-C(14)	122.5(3)
C(20)-C(15)-C(14)	118.6(3)
C(15)-C(16)-C(17)	118.7(4)
C(15)-C(16)-H(16)	120.7
C(17)-C(16)-H(16)	120.7
C(18)-C(17)-C(16)	121.0(5)
C(18)-C(17)-H(17)	119.5
C(16)-C(17)-H(17)	119.5
C(19)-C(18)-C(17)	119.3(4)
C(19)-C(18)-H(18)	120.3
C(17)-C(18)-H(18)	120.3
C(18)-C(19)-C(20)	121.1(4)
C(18)-C(19)-H(19)	119.4
C(20)-C(19)-H(19)	119.4
C(19)-C(20)-C(15)	120.9(4)
C(19)-C(20)-H(20)	119.6
C(15)-C(20)-H(20)	119.6

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 3-*O*-benzyl-(6-*N*,5-*O*-carbonyl)-6,7,8,9-tetradeoxy-1,2-*O*-isopropylidene-α-D-*glycero*-D-*gluco*-nonofuranose **12a**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	75(2)	73(2)	54(1)	-2(1)	14(1)	0(1)
O(2)	78(2)	71(2)	72(2)	-20(1)	20(1)	-8(1)
O(3)	67(1)	58(1)	62(1)	-12(1)	13(1)	-6(1)
O(4)	75(2)	78(2)	52(1)	-24(1)	8(1)	-27(1)
O(5)	83(2)	68(1)	61(1)	-9(1)	12(1)	3(1)
O(6)	81(2)	61(2)	113(2)	-10(2)	15(2)	9(2)
N	70(2)	55(2)	63(2)	3(1)	5(2)	-11(2)
C(1)	51(2)	71(2)	57(2)	-8(2)	-4(2)	-4(2)
C(2)	70(2)	70(2)	40(2)	-10(2)	-8(2)	-10(2)
C(3)	57(2)	60(2)	49(2)	-16(2)	2(2)	-8(2)
C(4)	63(2)	65(2)	47(2)	-10(2)	1(2)	-12(2)
C(5)	60(2)	66(2)	57(2)	-9(2)	1(2)	-15(2)
C(6)	74(2)	84(3)	55(2)	1(2)	5(2)	0(2)
C(7)	175(5)	83(3)	61(2)	-19(2)	-31(3)	35(3)
C(8)	122(4)	85(3)	91(3)	-16(2)	-19(3)	8(3)
C(9)	86(3)	77(2)	65(2)	15(2)	-6(2)	0(2)
C(10)	76(3)	38(2)	76(2)	-7(2)	6(2)	-12(2)
C(11)	73(2)	54(2)	67(2)	-11(2)	18(2)	-4(2)
C(12)	197(6)	96(3)	112(4)	30(3)	52(4)	62(4)
C(13)	91(3)	120(4)	146(4)	-81(4)	3(3)	-22(3)
C(14)	71(2)	83(2)	69(2)	-31(2)	3(2)	-9(2)
C(15)	63(2)	53(2)	59(2)	-11(2)	-16(2)	6(2)
C(16)	70(2)	67(2)	72(2)	-5(2)	-15(2)	-5(2)
C(17)	91(3)	81(3)	105(3)	13(3)	-24(3)	-26(3)
C(18)	123(4)	54(2)	96(3)	-7(2)	-55(3)	-13(3)
C(19)	121(4)	64(3)	76(3)	-20(2)	-43(3)	15(3)
C(20)	76(2)	75(2)	70(2)	-19(2)	-13(2)	9(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 3-*O*-benzyl-(6-*N*,5-*O*-carbonyl)-6,7,8,9-tetradeoxy-1,2-*O*-isopropylidene-α-D-*glycero*-D-*gluco*-nonofuranose **12a**.

	x	y	z	U(eq)
H(1)	13987	5000	8738	72
H(2)	11429	4933	9251	72
H(3)	7779	6430	9069	66
H(4)	8124	6079	8416	70
H(5)	10771	8503	8481	73
H(6)	10841	8418	7840	85
H(7A)	9597	6602	7543	127
H(7B)	7569	6320	7852	127
H(8A)	6923	7455	7163	119
H(8B)	4898	7179	7472	119
H(9A)	7166	9551	7319	91
H(9B)	4655	9333	7527	91
H(12A)	11977	2362	9127	202
H(12B)	12055	1443	8760	202
H(12C)	9778	1431	9031	202
H(13A)	6755	2173	8547	179
H(13B)	8745	1997	8228	179
H(13C)	7396	3365	8272	179
H(14A)	10181	7039	9681	89
H(14B)	8403	8064	9488	89
H(16)	14111	9015	9246	84
H(17)	16294	10745	9528	111
H(18)	14979	11719	10095	109
H(19)	11629	10930	10390	105
H(20)	9452	9216	10126	88

Table 6. Torsion angles [deg] for 3-*O*-benzyl-(6-*N*,5-*O*-carbonyl)-6,7,8,9-tetradeoxy-1,2-*O*-isopropylidene-α-D-*glycero*-D-*gluco*-nonofuranose **12a**.

C(11)-O(2)-C(1)-O(1)	-115.1(3)
C(11)-O(2)-C(1)-C(2)	0.4(4)
C(4)-O(1)-C(1)-O(2)	100.9(3)
C(4)-O(1)-C(1)-C(2)	-14.1(3)
C(11)-O(3)-C(2)-C(3)	136.1(3)
C(11)-O(3)-C(2)-C(1)	25.1(3)
O(2)-C(1)-C(2)-O(3)	-15.5(3)
O(1)-C(1)-C(2)-O(3)	103.7(3)
O(2)-C(1)-C(2)-C(3)	-130.5(3)
O(1)-C(1)-C(2)-C(3)	-11.3(3)
C(14)-O(4)-C(3)-C(2)	-101.3(4)
C(14)-O(4)-C(3)-C(4)	148.3(3)
O(3)-C(2)-C(3)-O(4)	162.7(2)
C(1)-C(2)-C(3)-O(4)	-87.1(3)
O(3)-C(2)-C(3)-C(4)	-80.2(3)
C(1)-C(2)-C(3)-C(4)	30.0(3)
C(1)-O(1)-C(4)-C(5)	157.9(2)
C(1)-O(1)-C(4)-C(3)	34.1(3)
O(4)-C(3)-C(4)-O(1)	78.1(3)
C(2)-C(3)-C(4)-O(1)	-38.8(3)
O(4)-C(3)-C(4)-C(5)	-39.4(4)
C(2)-C(3)-C(4)-C(5)	-156.4(3)
C(10)-O(5)-C(5)-C(4)	-134.7(3)
C(10)-O(5)-C(5)-C(6)	-12.2(3)
O(1)-C(4)-C(5)-O(5)	-177.4(2)
C(3)-C(4)-C(5)-O(5)	-61.4(4)

O(1)-C(4)-C(5)-C(6)	67.2(4)
C(3)-C(4)-C(5)-C(6)	-176.8(3)
C(10)-N-C(6)-C(7)	104.2(4)
C(9)-N-C(6)-C(7)	-26.8(4)
C(10)-N-C(6)-C(5)	-22.4(4)
C(9)-N-C(6)-C(5)	-153.5(3)

O(5)-C(5)-C(6)-N	20.2(3)
C(4)-C(5)-C(6)-N	138.1(3)
O(5)-C(5)-C(6)-C(7)	-94.6(4)
C(4)-C(5)-C(6)-C(7)	23.3(6)
N-C(6)-C(7)-C(8)	16.0(5)
C(5)-C(6)-C(7)-C(8)	129.4(4)
C(6)-C(7)-C(8)-C(9)	0.2(6)
C(10)-N-C(9)-C(8)	-98.6(4)
C(6)-N-C(9)-C(8)	27.3(4)
C(7)-C(8)-C(9)-N	-16.4(5)
C(6)-N-C(10)-O(6)	-164.8(3)
C(9)-N-C(10)-O(6)	-39.5(5)
C(6)-N-C(10)-O(5)	16.1(4)
C(9)-N-C(10)-O(5)	141.4(3)
C(5)-O(5)-C(10)-O(6)	179.1(3)
C(5)-O(5)-C(10)-N	-1.7(4)
C(1)-O(2)-C(11)-O(3)	14.9(4)
C(1)-O(2)-C(11)-C(12)	-103.9(4)
C(1)-O(2)-C(11)-C(13)	130.5(3)
C(2)-O(3)-C(11)-O(2)	-25.5(4)
C(2)-O(3)-C(11)-C(12)	91.9(4)
C(2)-O(3)-C(11)-C(13)	-142.2(3)
C(3)-O(4)-C(14)-C(15)	-174.6(3)
O(4)-C(14)-C(15)-C(16)	-6.4(5)
O(4)-C(14)-C(15)-C(20)	173.3(3)
C(20)-C(15)-C(16)-C(17)	1.2(5)
C(14)-C(15)-C(16)-C(17)	-179.1(4)
C(15)-C(16)-C(17)-C(18)	-1.4(6)
C(16)-C(17)-C(18)-C(19)	1.2(7)
C(17)-C(18)-C(19)-C(20)	-0.8(6)
C(18)-C(19)-C(20)-C(15)	0.6(6)
C(16)-C(15)-C(20)-C(19)	-0.8(5)
C(14)-C(15)-C(20)-C(19)	179.5(3)