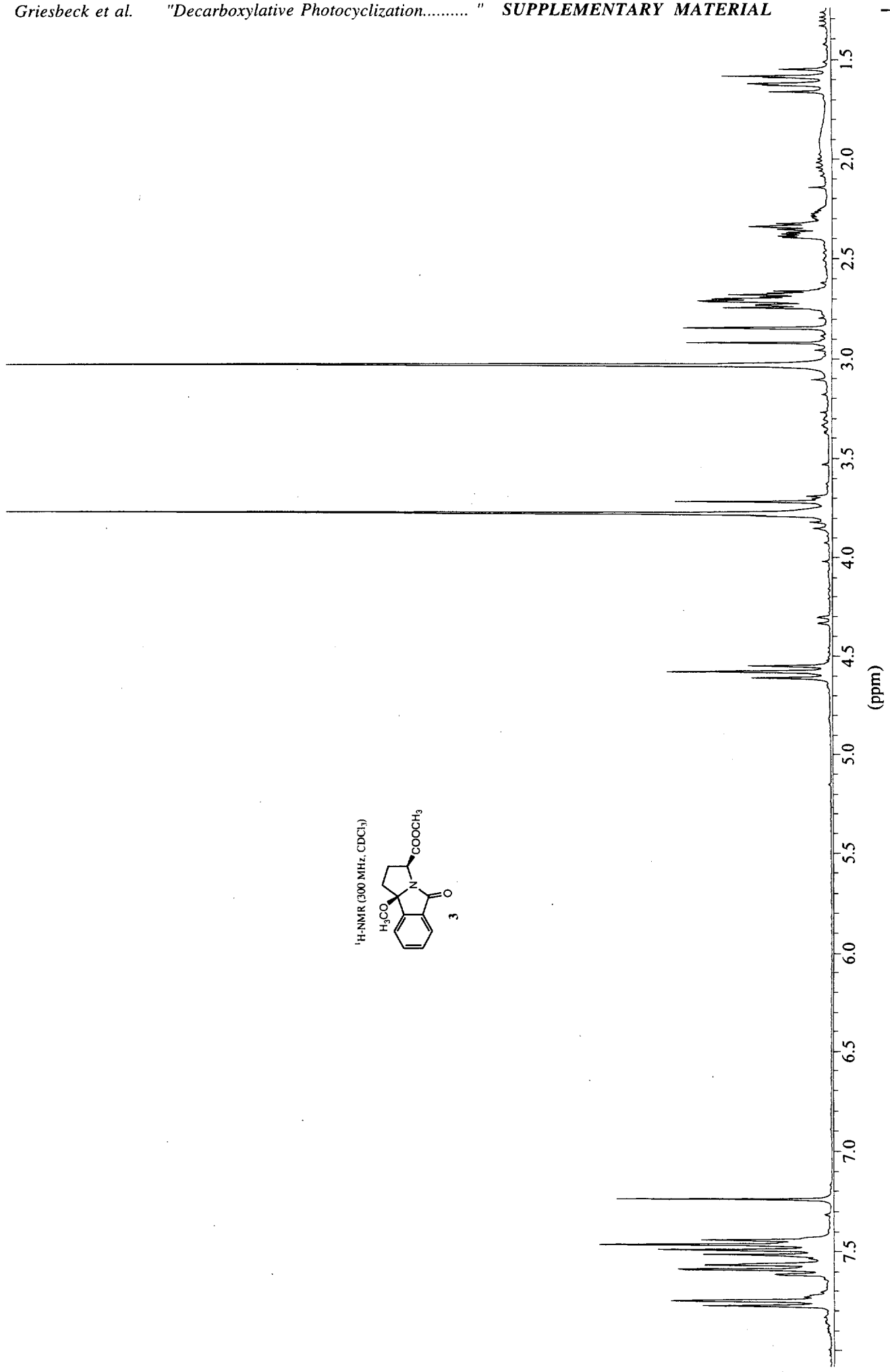
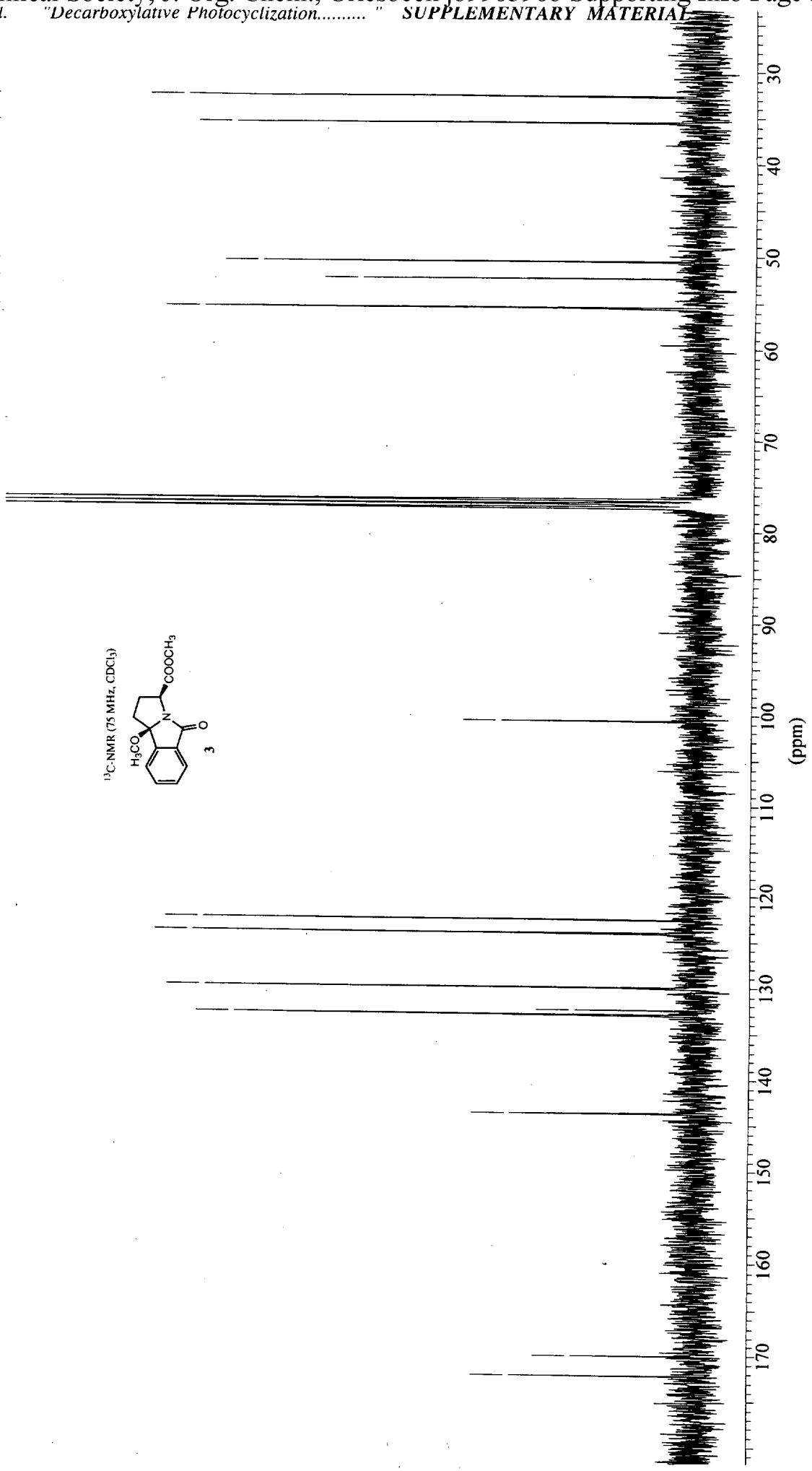
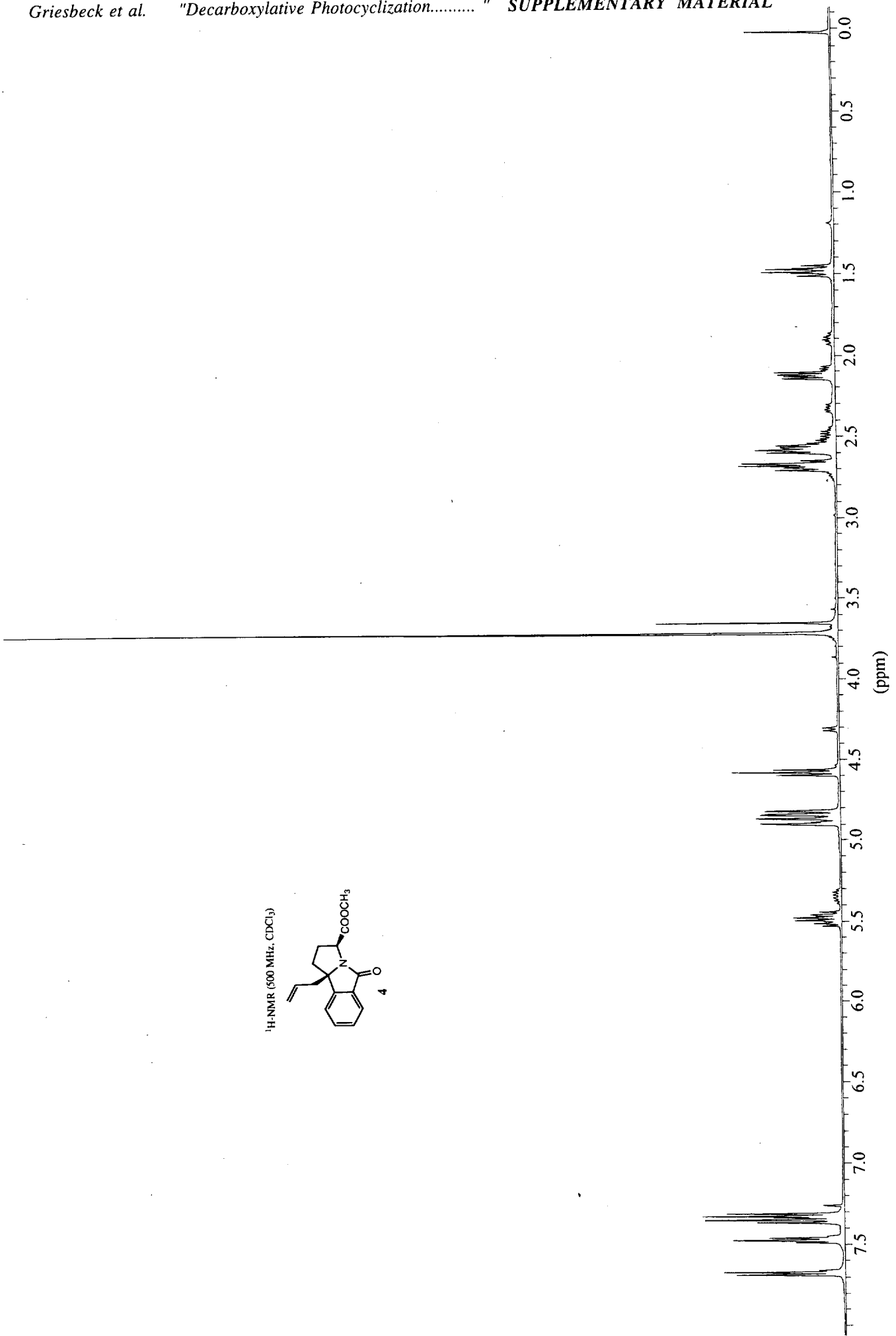
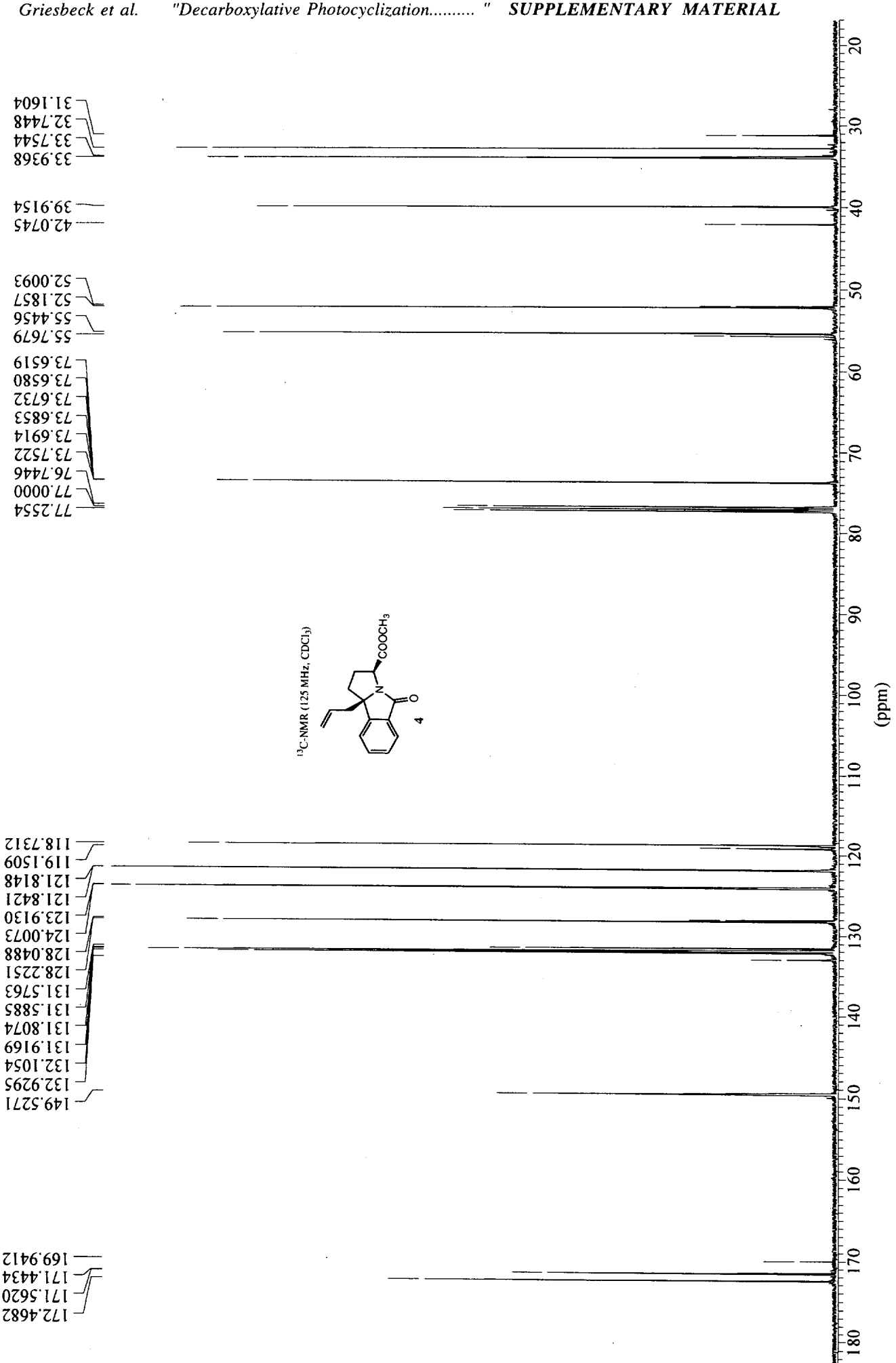


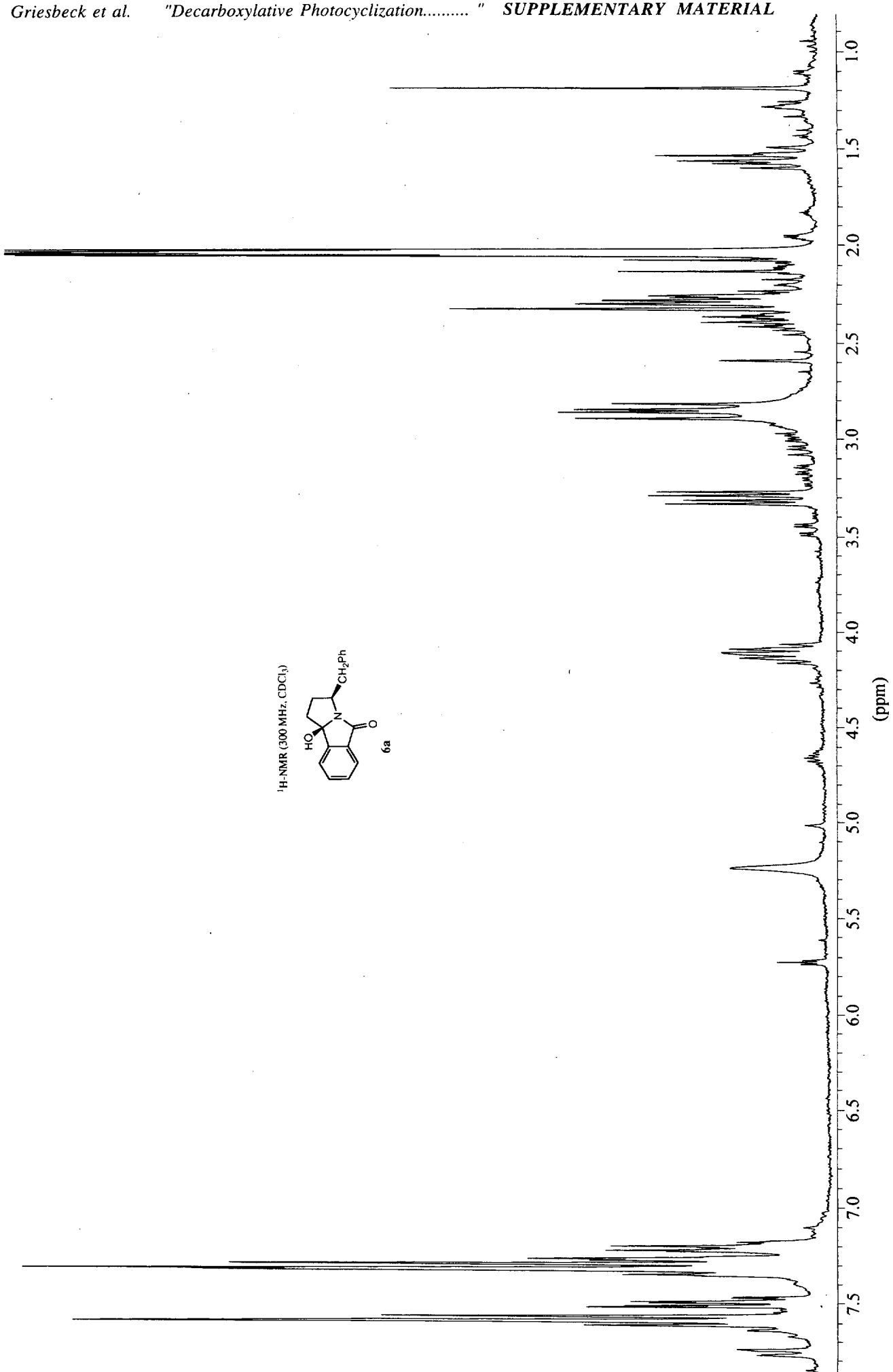




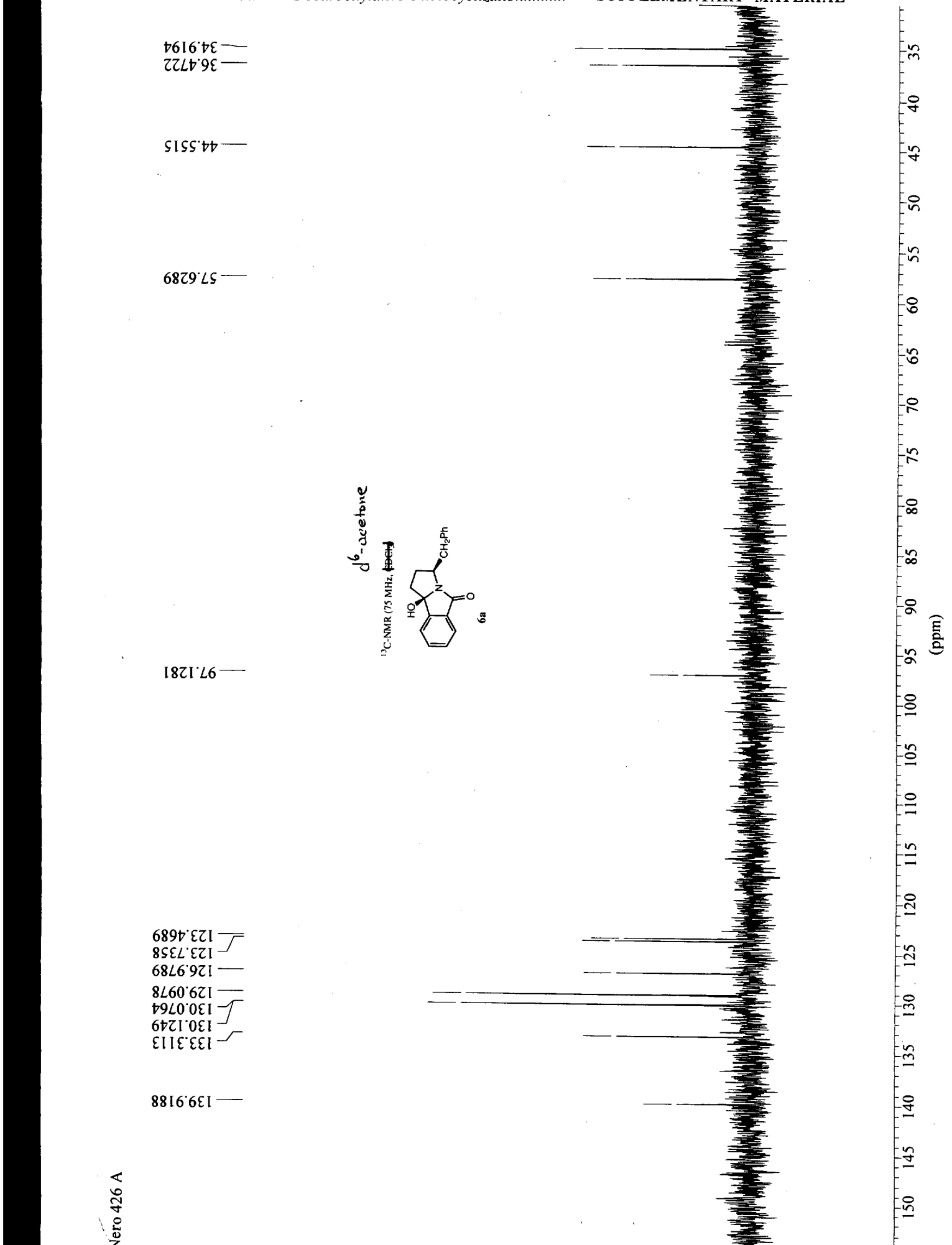
^{1}H-NMR (500 MHz, $CDCl_3$)

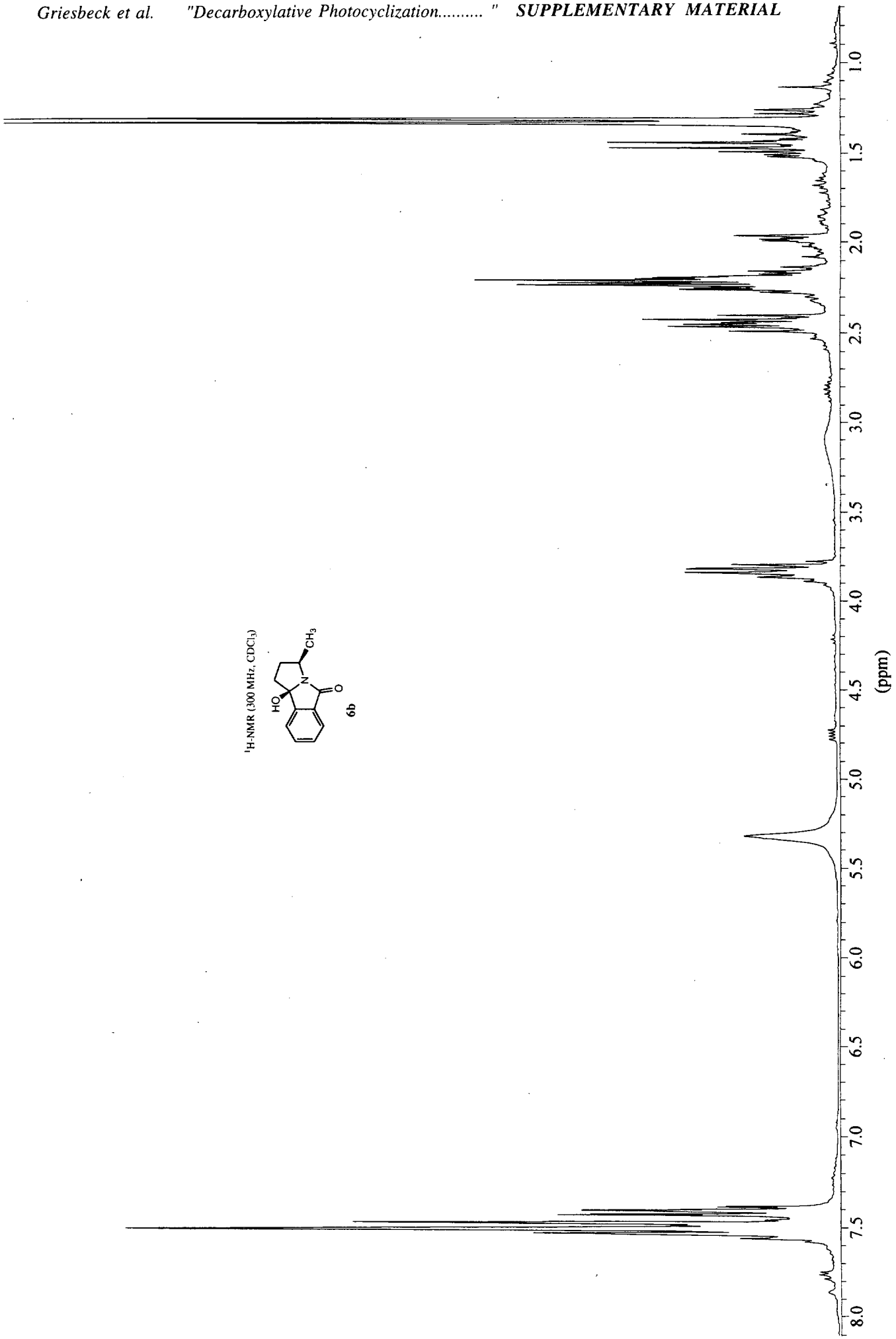
4

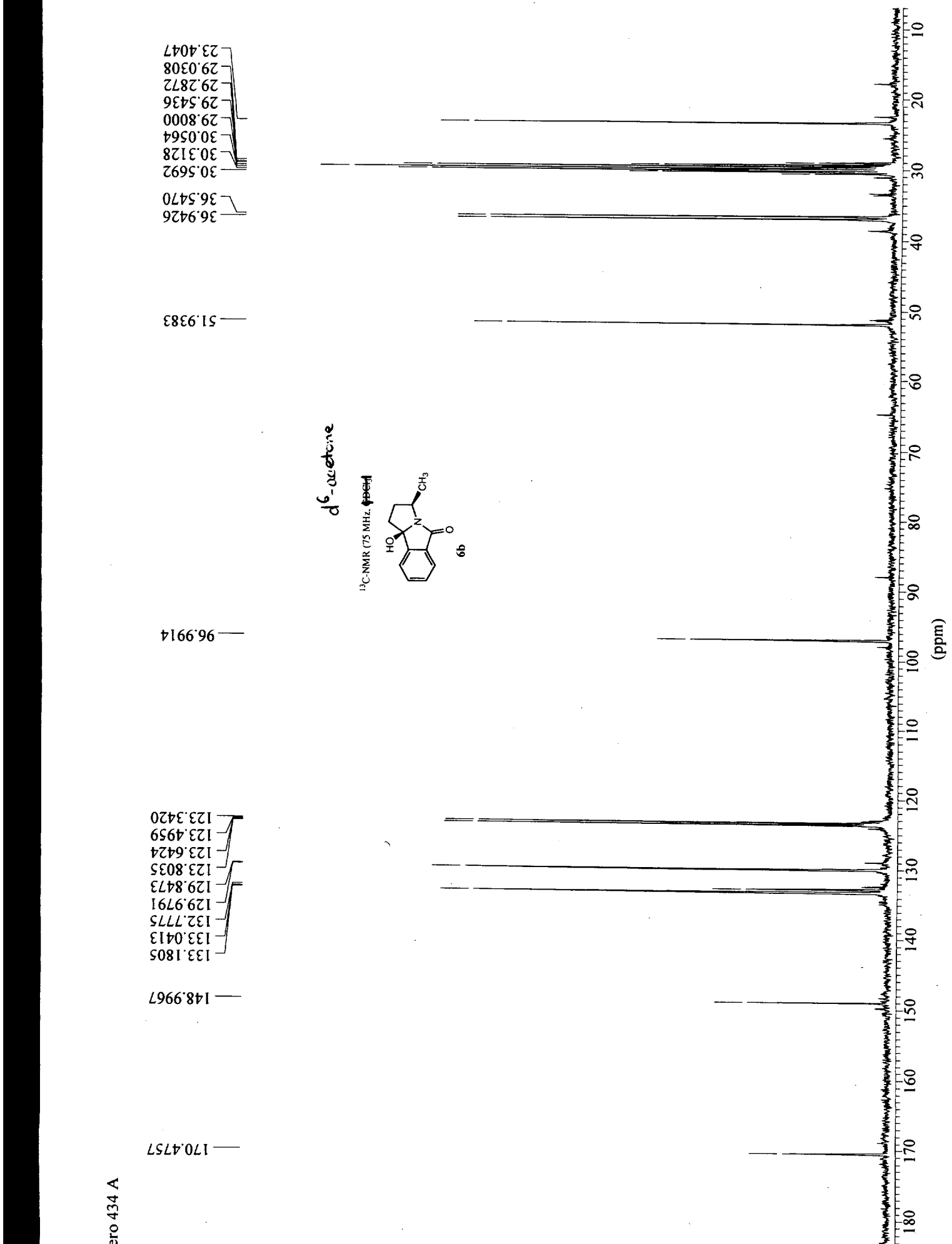


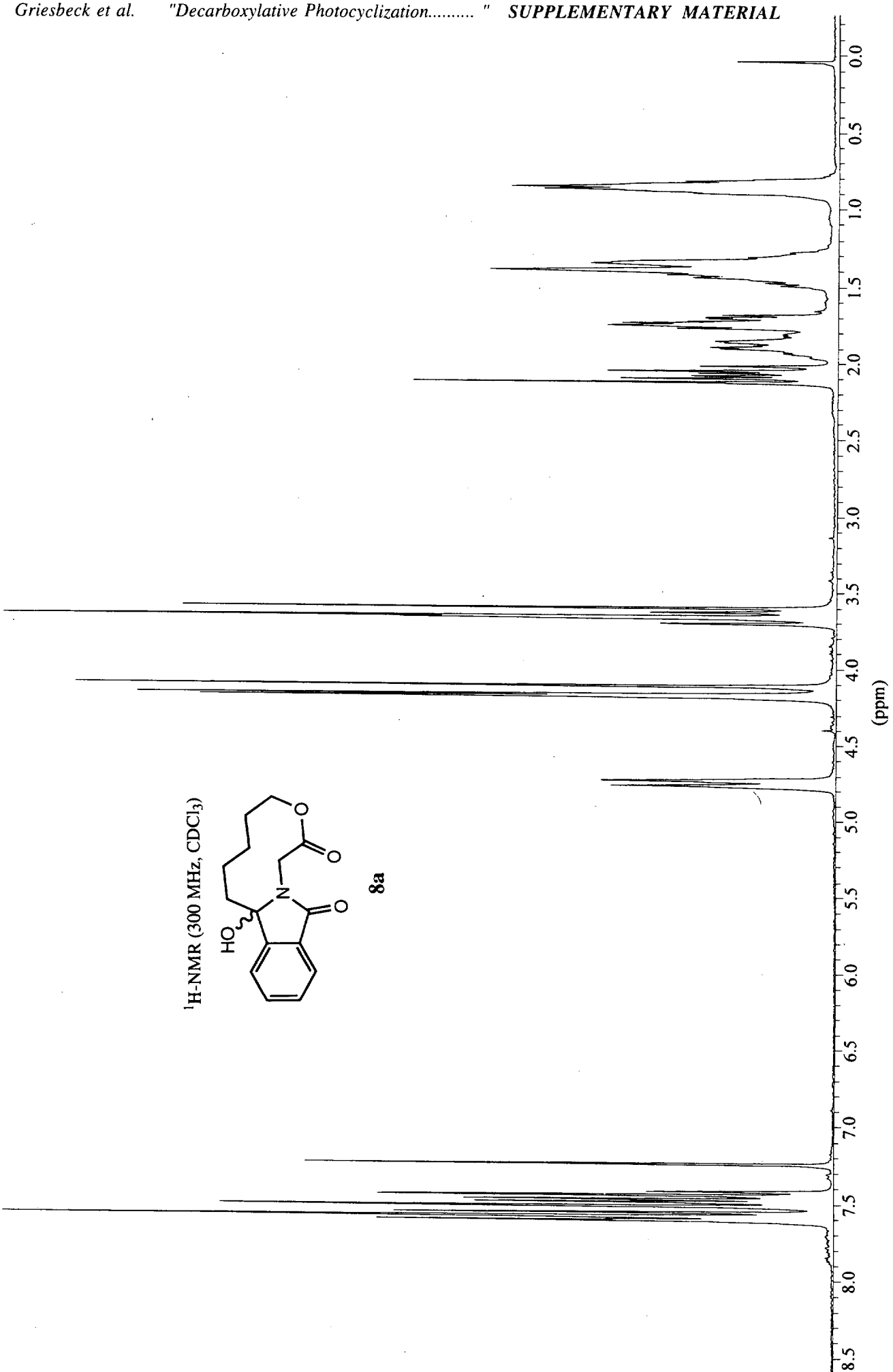


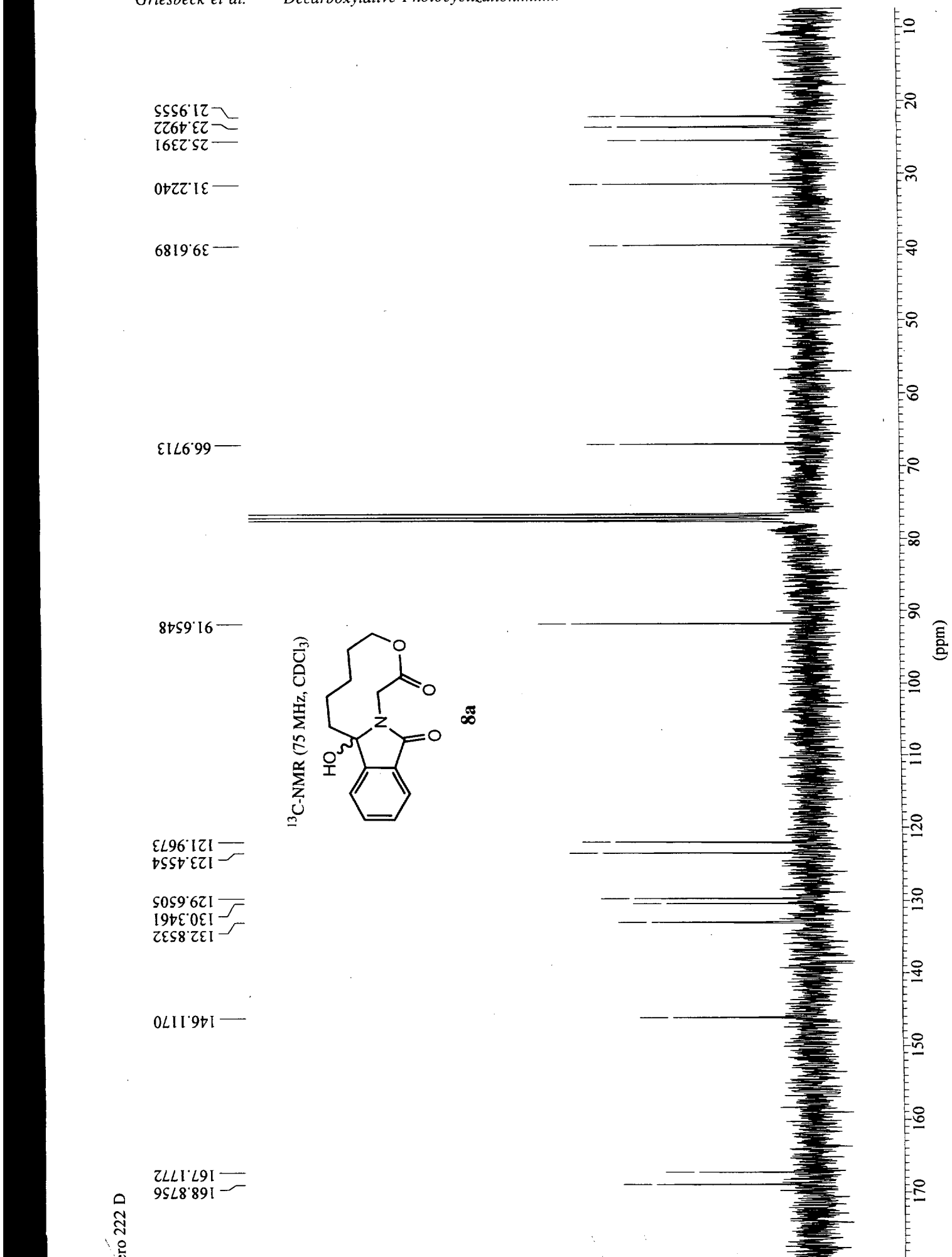
1+-

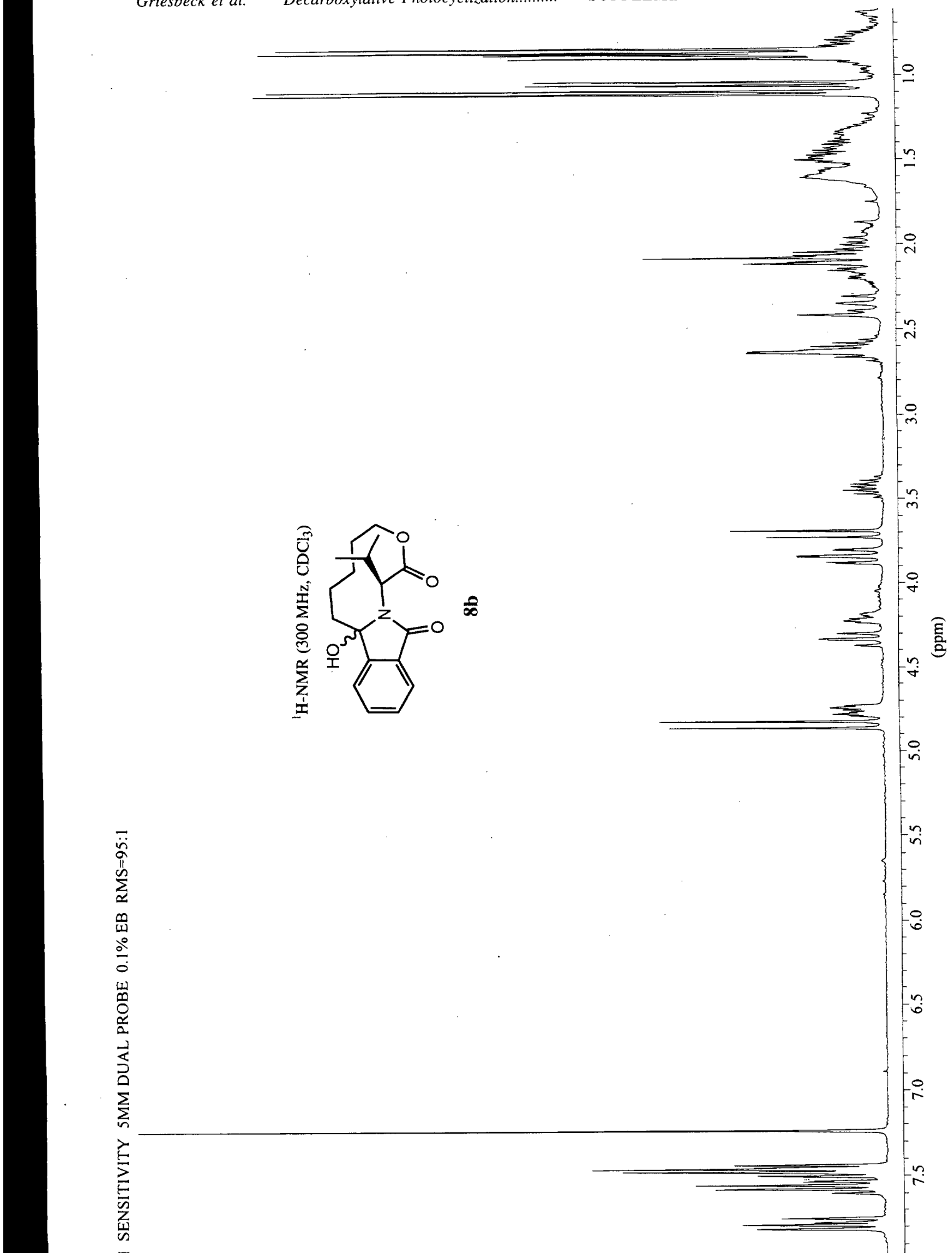


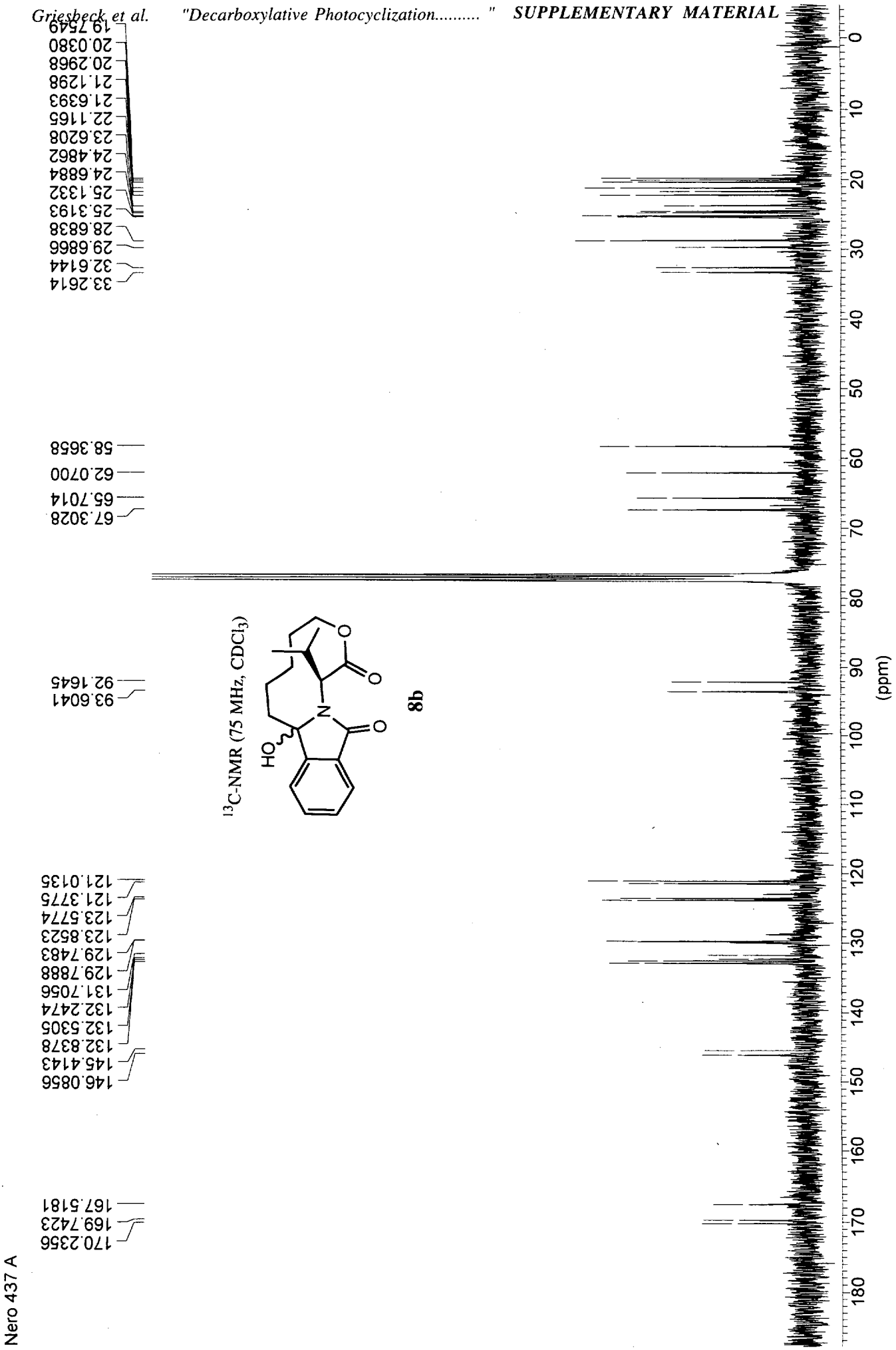


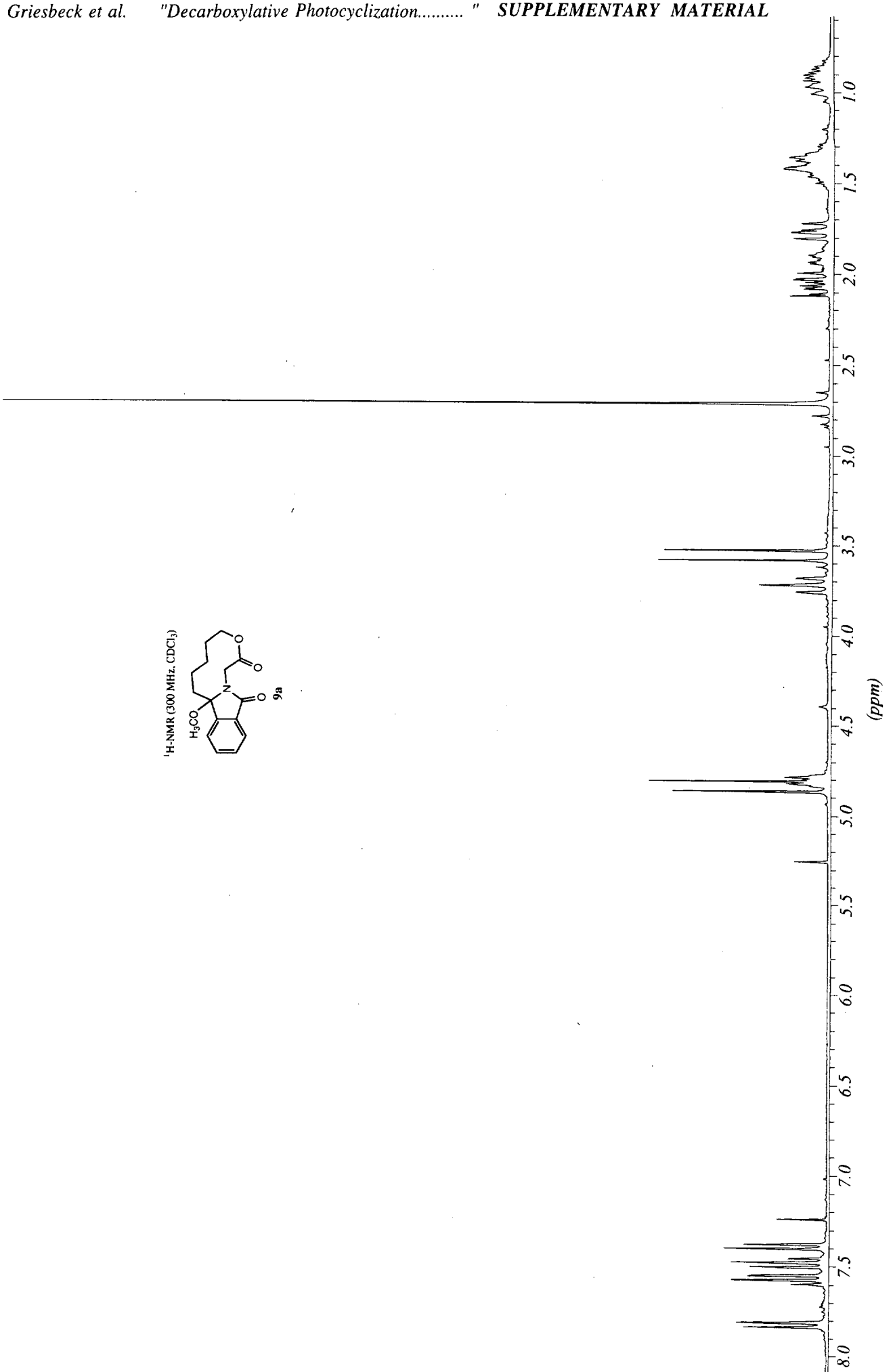


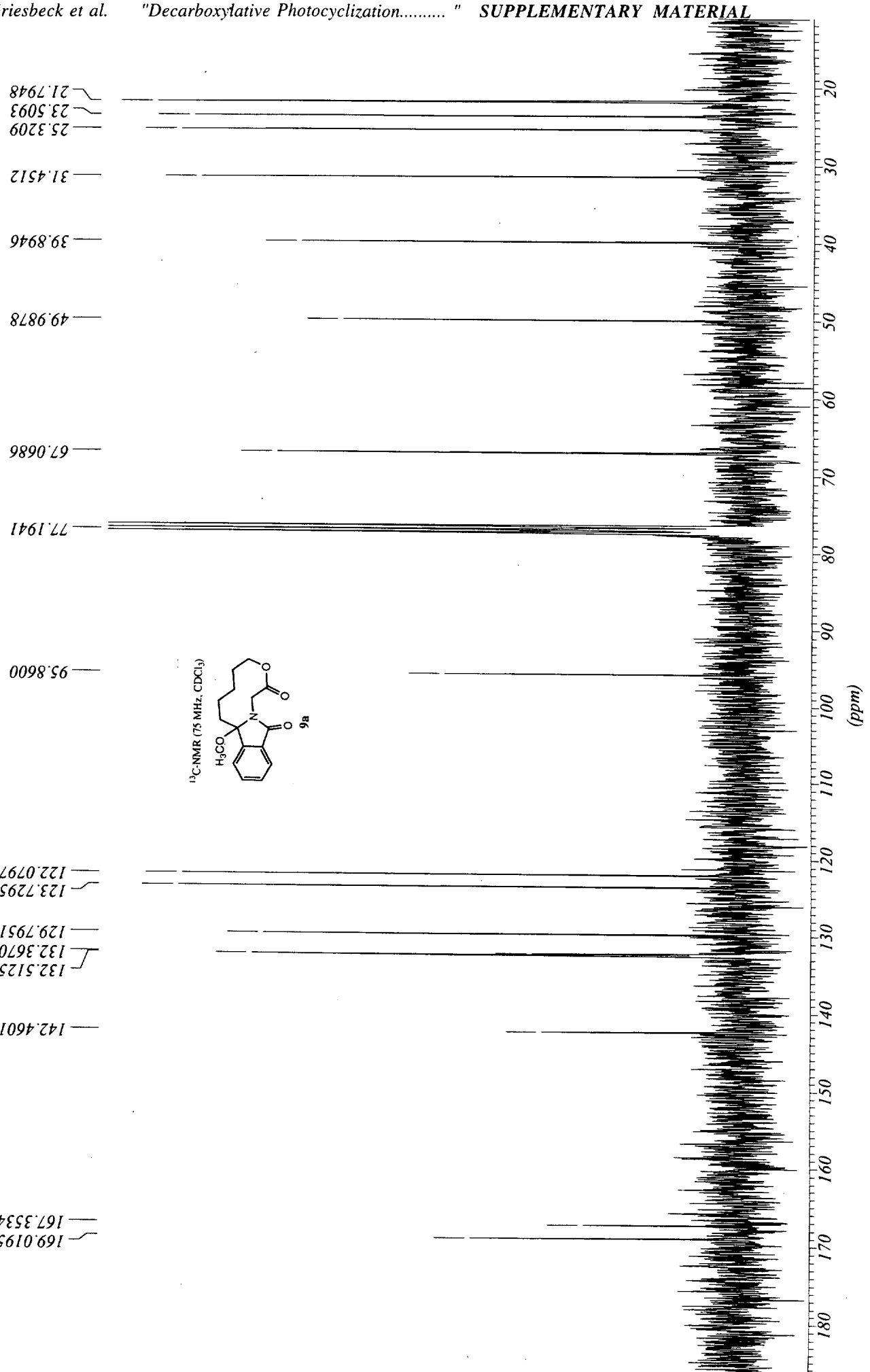












X-ray data of compound **(rac)-3**

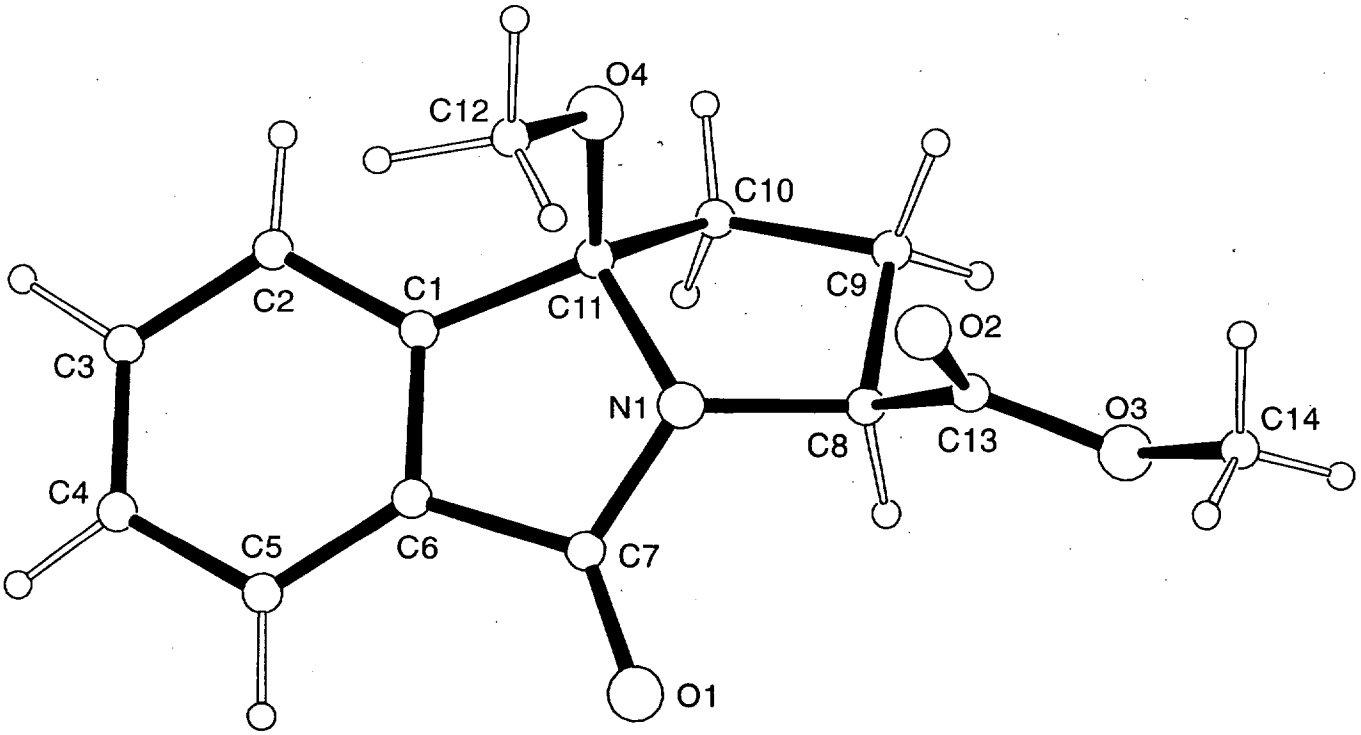


Table 1. Crystal data and structure refinement for 1.

Identification code	neromet
Empirical formula	C14 H15 N O4
Formula weight	261.27
Temperature	293(2) K
Wavelength	.71069 A
Crystal system	monoclinic
Space group	P21/n
Unit cell dimensions	a = 10.684(3) A alpha = 90 deg. b = 13.237(4) A beta = 106.84(2) deg c = 9.659(2) A gamma = 90 deg.
Volume	1307.4(6) A^3
Z	4
Density (calculated)	1.327 Mg/m^3
Absorption coefficient	0.098 mm^-1
F(000)	552
Crystal size	0.25 x 0.15 x 0.10 mm
Theta range for data collection	2.51 to 26.97 deg.
Index ranges	0<=h<=13, 0<=k<=16, -12<=l<=11
Reflections collected	2916
Independent reflections	2844
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2752 / 0 / 233
Goodness-of-fit on F^2	1.064
Weighting scheme calc w=	1/[s^2^(Fo^2^)+(0.0680P)^2^+0.3368P] where P=(Fo^2^+2Fc^2^)/3
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1169
Reflection observed [I>2sigma(I)]	2187
R indices (all data)	R1 = 0.0645, wR2 = 0.1409
Largest diff. peak and hole	.211 and -.218 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	10910(2)	4132(1)	3225(2)	38(1)
C(2)	11610(2)	5023(1)	3293(2)	50(1)
C(3)	10926(2)	5928(2)	3168(2)	57(1)
C(4)	9593(2)	5948(2)	2997(2)	54(1)
C(5)	8903(2)	5059(1)	2972(2)	46(1)
C(6)	9580(2)	4155(1)	3075(2)	37(1)
C(7)	9109(2)	3099(1)	3094(2)	36(1)
C(8)	10349(2)	1488(1)	3666(2)	39(1)
C(9)	11824(2)	1476(2)	4498(2)	50(1)
C(10)	12223(2)	2589(1)	4633(2)	46(1)
C(11)	11362(2)	3052(1)	3238(2)	37(1)
C(12)	11266(3)	3107(2)	716(2)	61(1)
C(13)	9980(2)	665(1)	2531(2)	43(1)
C(14)	9890(3)	-1104(2)	2190(4)	68(1)
N(1)	10132(1)	2492(1)	3023(1)	36(1)
O(1)	8064(1)	2802(1)	3194(2)	49(1)
O(2)	9597(2)	792(1)	1267(2)	90(1)
O(3)	10162(2)	-236(1)	3151(2)	64(1)
O(4)	11982(1)	2838(1)	2157(1)	46(1)

Table 3. Bond lengths [A] and angles [deg] for 1.

C(1)-C(6)	1.386(2)
C(1)-C(2)	1.387(2)
C(1)-C(11)	1.508(2)
C(2)-C(3)	1.390(3)
C(3)-C(4)	1.386(3)
C(4)-C(5)	1.385(3)
C(5)-C(6)	1.387(2)
C(6)-C(7)	1.488(2)
C(7)-O(1)	1.214(2)
C(7)-N(1)	1.373(2)
C(8)-N(1)	1.457(2)
C(8)-C(13)	1.514(2)
C(8)-C(9)	1.547(3)
C(9)-C(10)	1.529(3)
C(10)-C(11)	1.524(2)
C(11)-O(4)	1.418(2)
C(11)-N(1)	1.471(2)
C(12)-O(4)	1.425(3)
C(13)-O(2)	1.182(2)
C(13)-O(3)	1.324(2)
C(14)-O(3)	1.452(3)

C(6)-C(1)-C(2)	120.6(2)
C(6)-C(1)-C(11)	109.71(13)
C(2)-C(1)-C(11)	129.7(2)
C(1)-C(2)-C(3)	117.8(2)
C(4)-C(3)-C(2)	121.5(2)
C(3)-C(4)-C(5)	120.7(2)
C(4)-C(5)-C(6)	117.9(2)
C(1)-C(6)-C(5)	121.6(2)
C(1)-C(6)-C(7)	108.57(13)
C(5)-C(6)-C(7)	129.8(2)
O(1)-C(7)-N(1)	125.3(2)
O(1)-C(7)-C(6)	128.9(2)
N(1)-C(7)-C(6)	105.80(13)
N(1)-C(8)-C(13)	111.82(14)
N(1)-C(8)-C(9)	104.13(13)
C(13)-C(8)-C(9)	112.40(14)
C(10)-C(9)-C(8)	104.54(14)
C(11)-C(10)-C(9)	103.31(14)
O(4)-C(11)-N(1)	112.61(13)
O(4)-C(11)-C(1)	113.61(13)
N(1)-C(11)-C(1)	101.90(12)
O(4)-C(11)-C(10)	106.25(13)
N(1)-C(11)-C(10)	101.98(13)
C(1)-C(11)-C(10)	119.91(14)
O(2)-C(13)-O(3)	123.8(2)
O(2)-C(13)-C(8)	125.8(2)
O(3)-C(13)-C(8)	110.4(2)
C(7)-N(1)-C(8)	122.92(13)
C(7)-N(1)-C(11)	112.91(13)
C(8)-N(1)-C(11)	111.97(12)
C(13)-O(3)-C(14)	116.6(2)
C(11)-O(4)-C(12)	115.83(14)

Table 4. Torsion angles [deg] for 1.

C(6)-C(1)-C(2)-C(3)	-1.6(3)
C(11)-C(1)-C(2)-C(3)	176.0(2)
C(1)-C(2)-C(3)-C(4)	.6(3)
C(2)-C(3)-C(4)-C(5)	1.3(3)
C(3)-C(4)-C(5)-C(6)	-2.2(3)
C(2)-C(1)-C(6)-C(5)	.7(3)
C(11)-C(1)-C(6)-C(5)	-177.3(2)
C(2)-C(1)-C(6)-C(7)	-177.7(2)
C(11)-C(1)-C(6)-C(7)	4.2(2)
C(4)-C(5)-C(6)-C(1)	1.2(3)
C(4)-C(5)-C(6)-C(7)	179.3(2)
C(1)-C(6)-C(7)-O(1)	168.7(2)
C(5)-C(6)-C(7)-O(1)	-9.6(3)
C(1)-C(6)-C(7)-N(1)	-9.3(2)
C(5)-C(6)-C(7)-N(1)	172.4(2)
N(1)-C(8)-C(9)-C(10)	17.0(2)
C(13)-C(8)-C(9)-C(10)	138.2(2)
C(8)-C(9)-C(10)-C(11)	-33.6(2)
C(6)-C(1)-C(11)-O(4)	123.48(14)
C(2)-C(1)-C(11)-O(4)	-54.3(2)
C(6)-C(1)-C(11)-N(1)	2.1(2)
C(2)-C(1)-C(11)-N(1)	-175.7(2)
C(6)-C(1)-C(11)-C(10)	-109.4(2)
C(2)-C(1)-C(11)-C(10)	72.8(2)
C(9)-C(10)-C(11)-O(4)	-81.3(2)
C(9)-C(10)-C(11)-N(1)	36.8(2)
C(9)-C(10)-C(11)-C(1)	148.3(2)
N(1)-C(8)-C(13)-O(2)	2.2(3)
C(9)-C(8)-C(13)-O(2)	-114.5(2)
N(1)-C(8)-C(13)-O(3)	-178.65(14)
C(9)-C(8)-C(13)-O(3)	64.6(2)
O(1)-C(7)-N(1)-C(8)	-27.8(2)
C(6)-C(7)-N(1)-C(8)	150.31(14)
O(1)-C(7)-N(1)-C(11)	-167.0(2)
C(6)-C(7)-N(1)-C(11)	11.1(2)
C(13)-C(8)-N(1)-C(7)	105.7(2)
C(9)-C(8)-N(1)-C(7)	-132.7(2)
C(13)-C(8)-N(1)-C(11)	-114.8(2)
C(9)-C(8)-N(1)-C(11)	6.9(2)
O(4)-C(11)-N(1)-C(7)	-130.49(14)
C(1)-C(11)-N(1)-C(7)	-8.4(2)
C(10)-C(11)-N(1)-C(7)	116.04(14)
O(4)-C(11)-N(1)-C(8)	85.7(2)
C(1)-C(11)-N(1)-C(8)	-152.19(13)
C(10)-C(11)-N(1)-C(8)	-27.7(2)
O(2)-C(13)-O(3)-C(14)	1.2(3)
C(8)-C(13)-O(3)-C(14)	-177.9(2)
N(1)-C(11)-O(4)-C(12)	62.5(2)
C(1)-C(11)-O(4)-C(12)	-52.7(2)
C(10)-C(11)-O(4)-C(12)	173.3(2)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for 1. 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
C(1)	42(1)	36(1)	37(1)	-1(1)	16(1)	-1(1)
C(2)	51(1)	42(1)	63(1)	-3(1)	25(1)	-8(1)
C(3)	75(1)	35(1)	70(1)	-2(1)	35(1)	-10(1)
C(4)	73(1)	35(1)	61(1)	1(1)	31(1)	7(1)
C(5)	50(1)	40(1)	51(1)	1(1)	20(1)	8(1)
C(6)	41(1)	36(1)	35(1)	-1(1)	14(1)	1(1)
C(7)	35(1)	37(1)	35(1)	-2(1)	10(1)	0(1)
C(8)	46(1)	32(1)	42(1)	3(1)	16(1)	2(1)
C(9)	55(1)	42(1)	46(1)	3(1)	3(1)	8(1)
C(10)	44(1)	45(1)	44(1)	-3(1)	5(1)	2(1)
C(11)	34(1)	36(1)	42(1)	-3(1)	14(1)	0(1)
C(12)	70(1)	72(2)	46(1)	-1(1)	26(1)	7(1)
C(13)	44(1)	33(1)	52(1)	-1(1)	13(1)	2(1)
C(14)	71(2)	34(1)	103(2)	-13(1)	34(2)	-8(1)
N(1)	36(1)	31(1)	40(1)	-1(1)	11(1)	0(1)
O(1)	39(1)	47(1)	66(1)	-1(1)	20(1)	-3(1)
O(2)	150(2)	47(1)	52(1)	-7(1)	-4(1)	16(1)
O(3)	97(1)	30(1)	68(1)	0(1)	28(1)	-6(1)
O(4)	44(1)	53(1)	49(1)	-1(1)	23(1)	7(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2)	12509(20)	4990(16)	3419(22)	56(6)
H(3)	11376(23)	6526(20)	3185(28)	75(7)
H(4)	9132(24)	6600(21)	2862(28)	83(8)
H(5)	7992(19)	5065(15)	2845(21)	51(5)
H(8)	9791(18)	1392(15)	4305(21)	48(5)
H(9A)	12008(21)	1150(18)	5417(26)	67(6)
H(9B)	12336(21)	1100(17)	3970(24)	63(6)
H(10A)	12002(18)	2914(15)	5444(22)	48(5)
H(10B)	13147(22)	2672(16)	4741(23)	56(6)
H(12A)	11780(24)	2877(18)	91(28)	75(7)
H(12B)	11162(31)	3873(28)	605(37)	123(11)
H(12C)	10412(28)	2761(21)	451(31)	94(9)
H(14A)	8994(29)	-1234(23)	1842(33)	98(9)
H(14B)	10372(33)	-1654(33)	2766(40)	133(13)
H(14C)	10295(37)	-1018(28)	1427(44)	136(13)

X-ray data of compound (+)-3

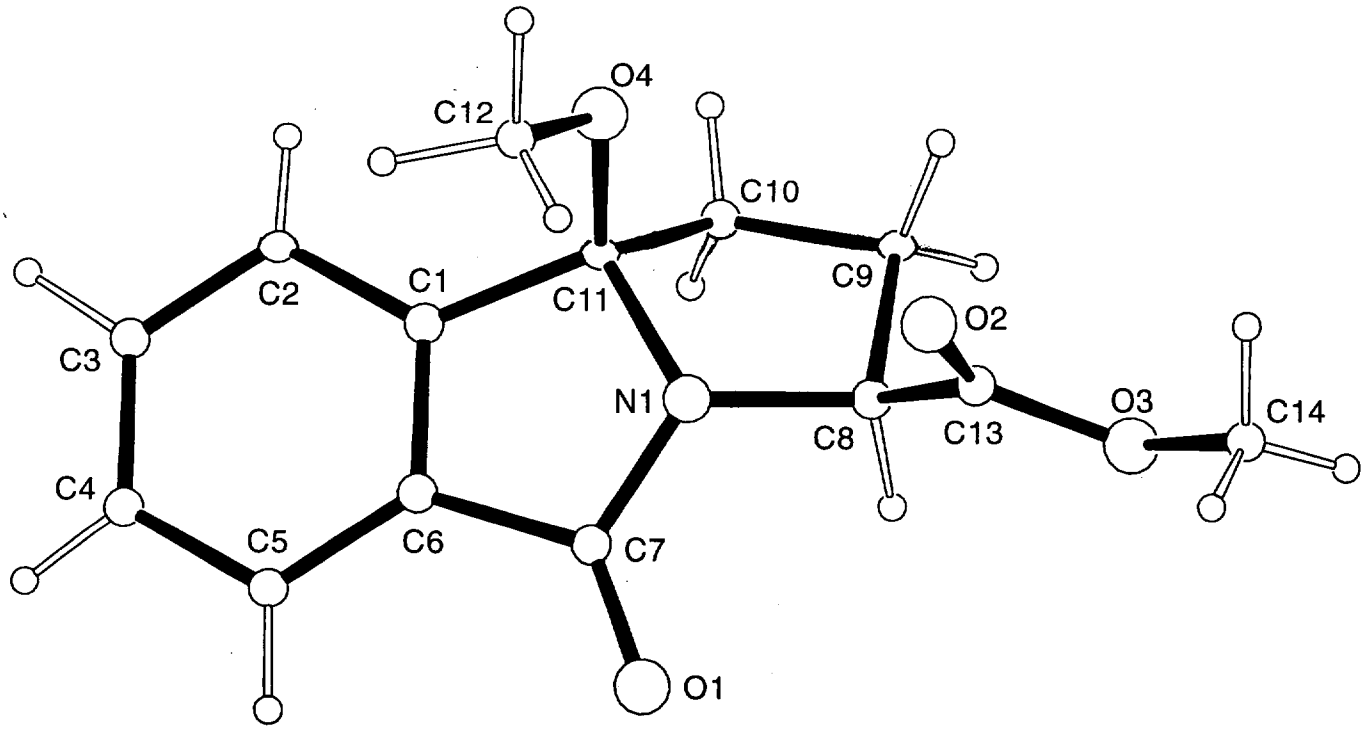


Table 1. Crystal data and structure refinement for 1.

Identification code	neromet3
Empirical formula	C14 H15 N O4
Formula weight	261.27
Temperature	293(2) K
Wavelength	.71069 A
Crystal system	orthorhombic
Space group	P212121
Unit cell dimensions	a = 7.023(1) A alpha = 90 deg. b = 11.237(2) A beta = 90 deg. c = 16.733(2) A gamma = 90 deg.
Volume	1320.5(3) A^3
Z	4
Density (calculated)	1.314 Mg/m^3
Absorption coefficient	0.097 mm^-1
F(000)	552
Crystal size	0.25 x 0.20 x 0.18 mm
Theta range for data collection	2.18 to 26.96 deg.
Index ranges	0<=h<=8, 0<=k<=14, 0<=l<=21
Reflections collected	1664
Independent reflections	1664
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1625 / 0 / 234
Goodness-of-fit on F^2	1.103
Weighting scheme calc w=	1/[s^2^(Fo^2^)+(0.0540P)^2^+0.2280P] where P=(Fo^2^+2Fc^2^)/3
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1045
Reflection observed [I>2sigma(I)]	1146
R indices (all data)	R1 = 0.0792, wR2 = 0.1266
Absolute structure parameter	0(3)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8138(5)	8430(3)	3799(2)	49(1)
C(2)	8111(7)	8437(4)	4630(2)	60(1)
C(3)	6834(7)	9182(4)	5006(3)	68(1)
C(4)	5605(7)	9884(4)	4584(3)	69(1)
C(5)	5612(6)	9879(4)	3747(3)	62(1)
C(6)	6893(5)	9135(3)	3375(2)	51(1)
C(7)	7249(5)	8956(3)	2504(2)	52(1)
C(8)	9945(5)	7978(3)	1814(2)	50(1)
C(9)	11791(6)	7612(4)	2262(2)	58(1)
C(10)	11422(5)	7964(4)	3127(2)	58(1)
C(11)	9313(5)	7688(3)	3236(2)	48(1)
C(12)	7237(8)	6005(4)	3349(4)	74(1)
C(13)	9405(5)	7114(3)	1174(2)	57(1)
C(14)	9889(9)	6603(6)	-175(3)	81(2)
N(1)	8526(4)	8049(3)	2453(2)	48(1)
O(1)	6603(4)	9517(3)	1947(2)	72(1)
O(2)	8369(6)	6287(3)	1253(2)	108(1)
O(3)	10282(4)	7364(3)	502(1)	66(1)
O(4)	9145(4)	6453(2)	3365(2)	58(1)

Table 3. Bond lengths [A] and angles [deg] for 1.

C(1)-C(6)	1.376(5)
C(1)-C(2)	1.391(5)
C(1)-C(11)	1.504(5)
C(2)-C(3)	1.379(6)
C(3)-C(4)	1.367(6)
C(4)-C(5)	1.401(6)
C(5)-C(6)	1.377(6)
C(6)-C(7)	1.492(5)
C(7)-O(1)	1.214(4)
C(7)-N(1)	1.360(4)
C(8)-N(1)	1.465(4)
C(8)-C(13)	1.494(5)
C(8)-C(9)	1.553(5)
C(9)-C(10)	1.523(6)
C(10)-C(11)	1.524(5)
C(11)-O(4)	1.410(4)
C(11)-N(1)	1.478(4)
C(12)-O(4)	1.432(6)
C(13)-O(2)	1.188(5)
C(13)-O(3)	1.313(4)
C(14)-O(3)	1.445(5)
C(6)-C(1)-C(2)	120.2(4)
C(6)-C(1)-C(11)	110.2(3)
C(2)-C(1)-C(11)	129.5(4)
C(3)-C(2)-C(1)	118.0(4)
C(4)-C(3)-C(2)	121.7(4)
C(3)-C(4)-C(5)	120.8(4)
C(6)-C(5)-C(4)	117.2(4)
C(1)-C(6)-C(5)	122.2(4)
C(1)-C(6)-C(7)	108.6(3)
C(5)-C(6)-C(7)	129.2(4)
O(1)-C(7)-N(1)	126.0(3)
O(1)-C(7)-C(6)	128.2(3)
N(1)-C(7)-C(6)	105.8(3)
N(1)-C(8)-C(13)	112.7(3)
N(1)-C(8)-C(9)	103.3(3)
C(13)-C(8)-C(9)	112.7(3)
C(10)-C(9)-C(8)	104.4(3)
C(11)-C(10)-C(9)	103.1(3)
O(4)-C(11)-N(1)	112.0(3)
O(4)-C(11)-C(1)	113.8(3)
N(1)-C(11)-C(1)	101.4(3)
O(4)-C(11)-C(10)	107.5(3)
N(1)-C(11)-C(10)	101.6(3)
C(1)-C(11)-C(10)	119.7(3)
O(2)-C(13)-O(3)	123.4(4)
O(2)-C(13)-C(8)	125.8(4)
O(3)-C(13)-C(8)	110.9(3)
C(7)-N(1)-C(8)	122.3(3)
C(7)-N(1)-C(11)	113.4(3)
C(8)-N(1)-C(11)	112.2(3)
C(13)-O(3)-C(14)	117.1(4)
C(11)-O(4)-C(12)	114.9(3)

Table 4. Torsion angles [deg] for 1.

C(6)-C(1)-C(2)-C(3)	-1.2(6)
C(11)-C(1)-C(2)-C(3)	-177.7(4)
C(1)-C(2)-C(3)-C(4)	.9(7)
C(2)-C(3)-C(4)-C(5)	-.6(7)
C(3)-C(4)-C(5)-C(6)	.4(7)
C(2)-C(1)-C(6)-C(5)	1.1(6)
C(11)-C(1)-C(6)-C(5)	178.2(3)
C(2)-C(1)-C(6)-C(7)	179.5(4)
C(11)-C(1)-C(6)-C(7)	-3.4(4)
C(4)-C(5)-C(6)-C(1)	-.7(6)
C(4)-C(5)-C(6)-C(7)	-178.8(4)
C(1)-C(6)-C(7)-O(1)	-170.5(4)
C(5)-C(6)-C(7)-O(1)	7.8(7)
C(1)-C(6)-C(7)-N(1)	7.2(4)
C(5)-C(6)-C(7)-N(1)	-174.5(4)
N(1)-C(8)-C(9)-C(10)	-20.8(4)
C(13)-C(8)-C(9)-C(10)	-142.7(4)
C(8)-C(9)-C(10)-C(11)	36.8(4)
C(6)-C(1)-C(11)-O(4)	-121.8(3)
C(2)-C(1)-C(11)-O(4)	54.9(5)
C(6)-C(1)-C(11)-N(1)	-1.4(4)
C(2)-C(1)-C(11)-N(1)	175.3(4)
C(6)-C(1)-C(11)-C(10)	109.1(4)
C(2)-C(1)-C(11)-C(10)	-74.1(5)
C(9)-C(10)-C(11)-O(4)	79.8(4)
C(9)-C(10)-C(11)-N(1)	-37.9(4)
C(9)-C(10)-C(11)-C(1)	-148.4(3)
N(1)-C(8)-C(13)-O(2)	-24.4(6)
C(9)-C(8)-C(13)-O(2)	91.9(5)
N(1)-C(8)-C(13)-O(3)	157.5(3)
C(9)-C(8)-C(13)-O(3)	-86.2(4)
O(1)-C(7)-N(1)-C(8)	29.8(5)
C(6)-C(7)-N(1)-C(8)	-148.0(3)
O(1)-C(7)-N(1)-C(11)	169.4(4)
C(6)-C(7)-N(1)-C(11)	-8.4(4)
C(13)-C(8)-N(1)-C(7)	-101.7(4)
C(9)-C(8)-N(1)-C(7)	136.4(3)
C(13)-C(8)-N(1)-C(11)	118.3(3)
C(9)-C(8)-N(1)-C(11)	-3.6(4)
O(4)-C(11)-N(1)-C(7)	128.0(3)
C(1)-C(11)-N(1)-C(7)	6.3(4)
C(10)-C(11)-N(1)-C(7)	-117.5(3)
O(4)-C(11)-N(1)-C(8)	-88.2(4)
C(1)-C(11)-N(1)-C(8)	150.1(3)
C(10)-C(11)-N(1)-C(8)	26.2(4)
O(2)-C(13)-O(3)-C(14)	2.2(6)
C(8)-C(13)-O(3)-C(14)	-179.6(4)
N(1)-C(11)-O(4)-C(12)	-59.4(5)
C(1)-C(11)-O(4)-C(12)	54.8(5)
C(10)-C(11)-O(4)-C(12)	-170.2(4)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for 1. 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
C(1)	47(2)	55(2)	46(2)	1(2)	-1(2)	-4(2)
C(2)	67(3)	65(2)	49(2)	3(2)	-3(2)	-3(2)
C(3)	85(3)	70(3)	49(2)	-5(2)	13(2)	-8(3)
C(4)	77(3)	64(3)	66(3)	-13(2)	21(3)	-1(3)
C(5)	56(2)	63(2)	67(3)	1(2)	5(2)	3(2)
C(6)	43(2)	57(2)	52(2)	-4(2)	1(2)	-3(2)
C(7)	45(2)	62(2)	49(2)	-2(2)	-6(2)	7(2)
C(8)	48(2)	53(2)	50(2)	-1(2)	6(2)	-2(2)
C(9)	43(2)	71(3)	61(2)	-1(2)	5(2)	0(2)
C(10)	44(2)	76(3)	55(2)	3(2)	-5(2)	-5(2)
C(11)	43(2)	54(2)	47(2)	3(2)	-1(2)	1(2)
C(12)	65(3)	65(3)	91(4)	1(3)	10(3)	-12(2)
C(13)	49(2)	62(2)	59(2)	-3(2)	9(2)	-6(2)
C(14)	75(3)	110(5)	57(3)	-19(3)	4(3)	12(3)
N(1)	42(2)	60(2)	42(2)	-3(1)	1(1)	4(2)
O(1)	67(2)	96(2)	54(2)	10(2)	-7(2)	24(2)
O(2)	128(3)	120(3)	77(2)	-31(2)	34(2)	-69(3)
O(3)	68(2)	83(2)	47(1)	-5(1)	11(1)	-6(2)
O(4)	53(2)	57(2)	64(2)	4(1)	2(1)	5(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2)	8888(59)	7898(31)	4882(23)	66(13)
H(3)	6901(61)	9160(35)	5619(25)	78(13)
H(4)	4777(68)	10480(39)	4831(27)	79(14)
H(5)	4794(56)	10417(33)	3437(22)	64(12)
H(8)	10029(45)	8785(28)	1608(17)	37(8)
H(9A)	12897(55)	8007(32)	2028(21)	54(10)
H(9B)	12108(62)	6732(39)	2228(21)	69(12)
H(10A)	11764(54)	8877(34)	3272(22)	62(10)
H(10B)	12197(59)	7518(35)	3481(23)	72(13)
H(12A)	7361(76)	5115(46)	3493(28)	97(15)
H(12B)	6419(83)	6354(51)	3827(37)	132(21)
H(12C)	6648(121)	6142(66)	2914(46)	189(36)
H(14A)	8563(100)	6571(54)	-362(36)	129(23)
H(14B)	10742(93)	6813(59)	-539(36)	135(25)
H(14C)	10076(89)	5781(56)	-16(32)	118(23)

X-ray data of compound (+)-4

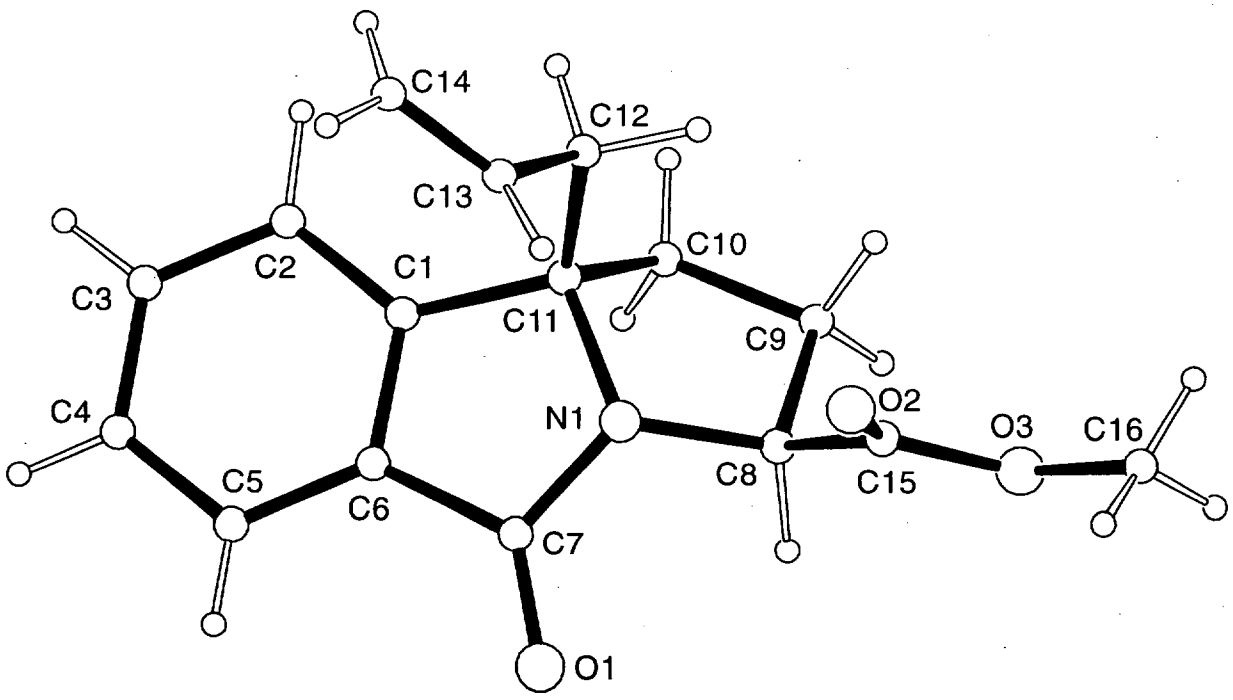


Table 1. Crystal data and structure refinement for 1.

Identification code	nerolen
Empirical formula	C32 H34 N2 O6
Formula weight	542.61
Temperature	293(2) K
Wavelength	.71069 A
Crystal system	monoclinic
Space group	Pc
Unit cell dimensions	a = 6.894(2) A alpha = 90 deg. b = 12.480(3) A beta = 90.68(2) deg. c = 16.762(5) A gamma = 90 deg.
Volume	1442.1(7) A^3
Z	2
Density (calculated)	1.250 Mg/m^3
Absorption coefficient	0.086 mm^-1
F(000)	576
Crystal size	0.20 x 0.18 x 0.15 mm
Theta range for data collection	2.03 to 26.96 deg.
Index ranges	0<=h<=8, 0<=k<=15, -21<=l<=21
Reflections collected	3219
Independent reflections	3135
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3079 / 2 / 498
Goodness-of-fit on F^2	1.139
Weighting scheme calc w=	1/[s^2^(Fo^2^)+(0.0495P)^2^+0.1587P] where P=(Fo^2^+2Fc^2^)/3
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.0940
Reflection observed [I>2sigma(I)]	2398
R indices (all data)	R1 = 0.0699, wR2 = 0.1123

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1A)	2247(5)	4331(3)	-767(2)	42(1)
C(2A)	2317(6)	4164(3)	-1589(2)	51(1)
C(3A)	3599(6)	4754(4)	-2019(2)	56(1)
C(4A)	4831(6)	5495(4)	-1666(2)	56(1)
C(5A)	4781(6)	5658(3)	-843(2)	48(1)
C(6A)	3481(5)	5073(3)	-412(2)	39(1)
C(7A)	3026(5)	5120(3)	456(2)	40(1)
C(8A)	248(5)	4362(3)	1199(2)	43(1)
C(9A)	-1657(6)	4047(4)	756(2)	52(1)
C(10A)	-1129(6)	4080(3)	-133(2)	48(1)
C(11A)	1016(5)	3797(3)	-148(2)	40(1)
C(12A)	1377(6)	2577(3)	-124(3)	49(1)
C(13A)	3426(7)	2264(3)	33(3)	59(1)
C(14A)	4480(10)	1671(5)	-423(4)	86(2)
C(15A)	683(6)	3608(3)	1894(2)	45(1)
C(16A)	-218(9)	3179(5)	3205(3)	74(1)
N(1A)	1727(4)	4315(2)	595(2)	39(1)
O(1A)	3650(4)	5757(2)	954(2)	52(1)
O(2A)	1894(5)	2928(3)	1903(2)	68(1)
O(3A)	-518(4)	3810(3)	2493(2)	62(1)
C(1B)	-18(5)	8432(3)	1881(2)	43(1)
C(2B)	-391(6)	8743(3)	2658(2)	53(1)
C(3B)	-1785(6)	8170(4)	3074(2)	59(1)
C(4B)	-2768(6)	7319(4)	2731(3)	57(1)
C(5B)	-2419(6)	7021(3)	1952(3)	51(1)
C(6B)	-1052(5)	7587(3)	1535(2)	42(1)
C(7B)	-361(5)	7448(3)	705(2)	44(1)
C(8B)	2602(6)	8132(3)	69(2)	46(1)
C(9B)	4307(6)	8559(5)	586(3)	60(1)
C(10B)	3502(6)	8641(4)	1425(2)	54(1)
C(11B)	1360(5)	8908(3)	1292(2)	43(1)
C(12B)	991(6)	10101(3)	1148(3)	52(1)
C(13B)	-1058(7)	10359(3)	925(3)	58(1)
C(14B)	-2234(9)	10937(5)	1357(4)	78(2)
C(15B)	2505(6)	8722(3)	-715(2)	51(1)
C(16B)	4285(15)	9002(8)	-1904(4)	99(2)
N(1B)	910(4)	8268(2)	565(2)	42(1)
O(1B)	-762(4)	6727(2)	236(2)	58(1)
O(2B)	1249(5)	9302(3)	-946(2)	77(1)
O(3B)	4066(5)	8486(3)	-1129(2)	77(1)

Table 3. Bond lengths [A] and angles [deg] for 1.

C(1A)-C(6A)	1.386(5)
C(1A)-C(2A)	1.395(5)
C(1A)-C(11A)	1.504(5)
C(2A)-C(3A)	1.364(6)
C(3A)-C(4A)	1.384(7)
C(4A)-C(5A)	1.396(6)
C(5A)-C(6A)	1.368(5)
C(6A)-C(7A)	1.493(5)
C(7A)-O(1A)	1.227(4)
C(7A)-N(1A)	1.368(4)
C(8A)-N(1A)	1.447(4)
C(8A)-C(15A)	1.524(5)
C(8A)-C(9A)	1.552(6)
C(9A)-C(10A)	1.538(6)
C(10A)-C(11A)	1.521(5)
C(11A)-N(1A)	1.481(4)
C(11A)-C(12A)	1.544(5)
C(12A)-C(13A)	1.486(6)
C(13A)-C(14A)	1.293(7)
C(15A)-O(2A)	1.191(5)
C(15A)-O(3A)	1.334(5)
C(16A)-O(3A)	1.443(5)
C(1B)-C(2B)	1.385(5)
C(1B)-C(6B)	1.395(5)
C(1B)-C(11B)	1.501(5)
C(2B)-C(3B)	1.392(6)
C(3B)-C(4B)	1.382(7)
C(4B)-C(5B)	1.382(6)
C(5B)-C(6B)	1.375(5)
C(6B)-C(7B)	1.486(5)
C(7B)-O(1B)	1.225(4)
C(7B)-N(1B)	1.370(5)
C(8B)-N(1B)	1.450(5)
C(8B)-C(15B)	1.507(5)
C(8B)-C(9B)	1.547(6)
C(9B)-C(10B)	1.522(6)
C(10B)-C(11B)	1.527(6)
C(11B)-N(1B)	1.486(4)
C(11B)-C(12B)	1.530(5)
C(12B)-C(13B)	1.492(6)
C(13B)-C(14B)	1.311(7)
C(15B)-O(2B)	1.190(5)
C(15B)-O(3B)	1.320(5)
C(16B)-O(3B)	1.460(6)

C(6A)-C(1A)-C(2A)	119.7(3)
C(6A)-C(1A)-C(11A)	110.4(3)
C(2A)-C(1A)-C(11A)	129.9(3)
C(3A)-C(2A)-C(1A)	118.1(4)
C(2A)-C(3A)-C(4A)	122.2(4)
C(3A)-C(4A)-C(5A)	119.9(4)
C(6A)-C(5A)-C(4A)	117.9(4)
C(5A)-C(6A)-C(1A)	122.2(3)
C(5A)-C(6A)-C(7A)	129.7(3)
C(1A)-C(6A)-C(7A)	108.0(3)
O(1A)-C(7A)-N(1A)	125.8(3)

C(15A)-C(8A)-C(9A)	111.5(3)
C(10A)-C(9A)-C(8A)	104.4(3)
C(11A)-C(10A)-C(9A)	104.5(3)
N(1A)-C(11A)-C(1A)	101.7(3)
N(1A)-C(11A)-C(10A)	101.4(3)
C(1A)-C(11A)-C(10A)	117.7(3)
N(1A)-C(11A)-C(12A)	110.9(3)
C(1A)-C(11A)-C(12A)	111.3(3)
C(10A)-C(11A)-C(12A)	112.6(3)
C(13A)-C(12A)-C(11A)	114.6(3)
C(14A)-C(13A)-C(12A)	125.9(6)
O(2A)-C(15A)-O(3A)	124.5(3)
O(2A)-C(15A)-C(8A)	125.5(3)
O(3A)-C(15A)-C(8A)	109.9(3)
C(7A)-N(1A)-C(8A)	123.9(3)
C(7A)-N(1A)-C(11A)	112.8(3)
C(8A)-N(1A)-C(11A)	112.2(3)
C(15A)-O(3A)-C(16A)	115.8(4)
C(2B)-C(1B)-C(6B)	120.2(4)
C(2B)-C(1B)-C(11B)	129.3(3)
C(6B)-C(1B)-C(11B)	110.5(3)
C(1B)-C(2B)-C(3B)	117.7(4)
C(4B)-C(3B)-C(2B)	121.6(4)
C(3B)-C(4B)-C(5B)	120.7(4)
C(6B)-C(5B)-C(4B)	118.0(4)
C(5B)-C(6B)-C(1B)	121.8(4)
C(5B)-C(6B)-C(7B)	130.1(3)
C(1B)-C(6B)-C(7B)	108.1(3)
O(1B)-C(7B)-N(1B)	125.4(3)
O(1B)-C(7B)-C(6B)	127.9(3)
N(1B)-C(7B)-C(6B)	106.6(3)
N(1B)-C(8B)-C(15B)	114.5(3)
N(1B)-C(8B)-C(9B)	104.5(3)
C(15B)-C(8B)-C(9B)	110.2(3)
C(10B)-C(9B)-C(8B)	104.9(3)
C(9B)-C(10B)-C(11B)	104.0(3)
N(1B)-C(11B)-C(1B)	101.5(3)
N(1B)-C(11B)-C(10B)	101.2(3)
C(1B)-C(11B)-C(10B)	115.8(3)
N(1B)-C(11B)-C(12B)	111.1(3)
C(1B)-C(11B)-C(12B)	112.6(3)
C(10B)-C(11B)-C(12B)	113.2(3)
C(13B)-C(12B)-C(11B)	113.8(3)
C(14B)-C(13B)-C(12B)	124.7(5)
O(2B)-C(15B)-O(3B)	124.0(4)
O(2B)-C(15B)-C(8B)	127.3(4)
O(3B)-C(15B)-C(8B)	108.7(4)
C(7B)-N(1B)-C(8B)	122.1(3)
C(7B)-N(1B)-C(11B)	112.8(3)
C(8B)-N(1B)-C(11B)	111.8(3)
C(15B)-O(3B)-C(16B)	117.6(5)

Table 4. Torsion angles [deg] for 1.

C(6A)-C(1A)-C(2A)-C(3A)	-.8(5)
C(11A)-C(1A)-C(2A)-C(3A)	-179.2(4)
C(1A)-C(2A)-C(3A)-C(4A)	.8(6)
C(2A)-C(3A)-C(4A)-C(5A)	-.2(6)
C(3A)-C(4A)-C(5A)-C(6A)	-.5(6)
C(4A)-C(5A)-C(6A)-C(1A)	.5(5)
C(4A)-C(5A)-C(6A)-C(7A)	-176.1(3)
C(2A)-C(1A)-C(6A)-C(5A)	.2(5)
C(11A)-C(1A)-C(6A)-C(5A)	178.8(3)
C(2A)-C(1A)-C(6A)-C(7A)	177.4(3)
C(11A)-C(1A)-C(6A)-C(7A)	-3.9(4)
C(5A)-C(6A)-C(7A)-O(1A)	5.5(6)
C(1A)-C(6A)-C(7A)-O(1A)	-171.5(3)
C(5A)-C(6A)-C(7A)-N(1A)	-175.5(4)
C(1A)-C(6A)-C(7A)-N(1A)	7.5(4)
N(1A)-C(8A)-C(9A)-C(10A)	-12.0(4)
C(15A)-C(8A)-C(9A)-C(10A)	-133.4(3)
C(8A)-C(9A)-C(10A)-C(11A)	29.9(4)
C(6A)-C(1A)-C(11A)-N(1A)	-.8(3)
C(2A)-C(1A)-C(11A)-N(1A)	177.7(4)
C(6A)-C(1A)-C(11A)-C(10A)	108.8(3)
C(2A)-C(1A)-C(11A)-C(10A)	-72.7(5)
C(6A)-C(1A)-C(11A)-C(12A)	-119.0(3)
C(2A)-C(1A)-C(11A)-C(12A)	59.5(5)
C(9A)-C(10A)-C(11A)-N(1A)	-35.5(4)
C(9A)-C(10A)-C(11A)-C(1A)	-145.4(3)
C(9A)-C(10A)-C(11A)-C(12A)	83.0(4)
N(1A)-C(11A)-C(12A)-C(13A)	-55.0(5)
C(1A)-C(11A)-C(12A)-C(13A)	57.5(4)
C(10A)-C(11A)-C(12A)-C(13A)	-167.9(4)
C(11A)-C(12A)-C(13A)-C(14A)	-122.6(5)
N(1A)-C(8A)-C(15A)-O(2A)	-11.6(5)
C(9A)-C(8A)-C(15A)-O(2A)	105.4(5)
N(1A)-C(8A)-C(15A)-O(3A)	169.3(3)
C(9A)-C(8A)-C(15A)-O(3A)	-73.7(4)
O(1A)-C(7A)-N(1A)-C(8A)	29.8(5)
C(6A)-C(7A)-N(1A)-C(8A)	-149.2(3)
O(1A)-C(7A)-N(1A)-C(11A)	170.7(3)
C(6A)-C(7A)-N(1A)-C(11A)	-8.3(4)
C(15A)-C(8A)-N(1A)-C(7A)	-109.1(4)
C(9A)-C(8A)-N(1A)-C(7A)	129.9(3)
C(15A)-C(8A)-N(1A)-C(11A)	109.9(3)
C(9A)-C(8A)-N(1A)-C(11A)	-11.2(4)
C(1A)-C(11A)-N(1A)-C(7A)	5.9(3)
C(10A)-C(11A)-N(1A)-C(7A)	-115.8(3)
C(12A)-C(11A)-N(1A)-C(7A)	124.3(3)
C(1A)-C(11A)-N(1A)-C(8A)	151.4(3)
C(10A)-C(11A)-N(1A)-C(8A)	29.7(3)
C(12A)-C(11A)-N(1A)-C(8A)	-90.2(3)
O(2A)-C(15A)-O(3A)-C(16A)	3.1(6)
C(8A)-C(15A)-O(3A)-C(16A)	-177.8(4)
C(6B)-C(1B)-C(2B)-C(3B)	1.4(6)
C(11B)-C(1B)-C(2B)-C(3B)	178.7(4)
C(1B)-C(2B)-C(3B)-C(4B)	.0(6)
C(2B)-C(3B)-C(4B)-C(5B)	-1.1(7)
C(3B)-C(4B)-C(5B)-C(6B)	.8(6)

C(2B)-C(1B)-C(6B)-C(7B)	179.3(3)
C(11B)-C(1B)-C(6B)-C(7B)	1.5(4)
C(5B)-C(6B)-C(7B)-O(1B)	-7.0(6)
C(1B)-C(6B)-C(7B)-O(1B)	171.8(4)
C(5B)-C(6B)-C(7B)-N(1B)	175.7(4)
C(1B)-C(6B)-C(7B)-N(1B)	-5.5(4)
N(1B)-C(8B)-C(9B)-C(10B)	14.3(5)
C(15B)-C(8B)-C(9B)-C(10B)	137.8(4)
C(8B)-C(9B)-C(10B)-C(11B)	-31.9(5)
C(2B)-C(1B)-C(11B)-N(1B)	-174.8(4)
C(6B)-C(1B)-C(11B)-N(1B)	2.7(4)
C(2B)-C(1B)-C(11B)-C(10B)	76.5(5)
C(6B)-C(1B)-C(11B)-C(10B)	-106.0(4)
C(2B)-C(1B)-C(11B)-C(12B)	-55.9(5)
C(6B)-C(1B)-C(11B)-C(12B)	121.6(3)
C(9B)-C(10B)-C(11B)-N(1B)	36.4(4)
C(9B)-C(10B)-C(11B)-C(1B)	145.2(4)
C(9B)-C(10B)-C(11B)-C(12B)	-82.7(4)
N(1B)-C(11B)-C(12B)-C(13B)	60.2(5)
C(1B)-C(11B)-C(12B)-C(13B)	-52.9(5)
C(10B)-C(11B)-C(12B)-C(13B)	173.4(4)
C(11B)-C(12B)-C(13B)-C(14B)	115.3(5)
N(1B)-C(8B)-C(15B)-O(2B)	2.9(6)
C(9B)-C(8B)-C(15B)-O(2B)	-114.5(5)
N(1B)-C(8B)-C(15B)-O(3B)	-176.4(3)
C(9B)-C(8B)-C(15B)-O(3B)	66.2(4)
O(1B)-C(7B)-N(1B)-C(8B)	-32.2(5)
C(6B)-C(7B)-N(1B)-C(8B)	145.2(3)
O(1B)-C(7B)-N(1B)-C(11B)	-169.8(3)
C(6B)-C(7B)-N(1B)-C(11B)	7.6(4)
C(15B)-C(8B)-N(1B)-C(7B)	110.8(4)
C(9B)-C(8B)-N(1B)-C(7B)	-128.7(4)
C(15B)-C(8B)-N(1B)-C(11B)	-111.2(4)
C(9B)-C(8B)-N(1B)-C(11B)	9.4(4)
C(1B)-C(11B)-N(1B)-C(7B)	-6.4(4)
C(10B)-C(11B)-N(1B)-C(7B)	113.2(3)
C(12B)-C(11B)-N(1B)-C(7B)	-126.3(3)
C(1B)-C(11B)-N(1B)-C(8B)	-148.5(3)
C(10B)-C(11B)-N(1B)-C(8B)	-28.9(4)
C(12B)-C(11B)-N(1B)-C(8B)	91.6(4)
O(2B)-C(15B)-O(3B)-C(16B)	2.3(7)
C(8B)-C(15B)-O(3B)-C(16B)	-178.4(5)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for 1.
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
C(1A)	51(2)	39(2)	35(2)	3(1)	-2(2)	7(2)
C(2A)	64(3)	51(2)	37(2)	-3(2)	-1(2)	7(2)
C(3A)	71(3)	66(3)	32(2)	4(2)	4(2)	18(2)
C(4A)	57(3)	67(3)	44(2)	12(2)	10(2)	11(2)
C(5A)	47(2)	49(2)	47(2)	8(2)	1(2)	3(2)
C(6A)	43(2)	37(2)	38(2)	4(1)	-2(1)	6(2)
C(7A)	46(2)	40(2)	34(2)	8(1)	-6(1)	0(2)
C(8A)	50(2)	39(2)	39(2)	0(2)	1(2)	2(2)
C(9A)	48(2)	59(3)	50(2)	4(2)	-2(2)	0(2)
C(10A)	51(2)	48(2)	44(2)	0(2)	-7(2)	-6(2)
C(11A)	52(2)	34(2)	33(2)	1(1)	-7(1)	1(2)
C(12A)	56(3)	41(2)	51(2)	0(2)	2(2)	-6(2)
C(13A)	76(3)	41(2)	61(3)	6(2)	7(2)	3(2)
C(14A)	91(4)	84(4)	85(4)	15(3)	26(3)	21(3)
C(15A)	53(2)	44(2)	37(2)	3(2)	-1(2)	-4(2)
C(16A)	79(4)	102(4)	40(2)	22(2)	3(2)	-6(3)
N(1A)	47(2)	39(2)	30(1)	4(1)	-3(1)	-3(1)
O(1A)	61(2)	56(2)	38(1)	-3(1)	-8(1)	-15(1)
O(2A)	90(2)	66(2)	47(2)	14(1)	7(2)	23(2)
O(3A)	65(2)	79(2)	41(1)	16(1)	10(1)	6(2)
C(1B)	50(2)	40(2)	39(2)	5(2)	-5(2)	-3(2)
C(2B)	62(2)	60(2)	38(2)	-2(2)	-1(2)	-6(2)
C(3B)	60(3)	81(3)	38(2)	2(2)	4(2)	4(2)
C(4B)	51(2)	67(3)	54(2)	19(2)	6(2)	-4(2)
C(5B)	48(2)	49(2)	57(2)	9(2)	-4(2)	-7(2)
C(6B)	44(2)	36(2)	45(2)	6(2)	-4(2)	1(2)
C(7B)	48(2)	36(2)	47(2)	3(2)	-9(2)	2(2)
C(8B)	53(2)	44(2)	42(2)	6(2)	2(2)	3(2)
C(9B)	45(2)	80(3)	54(2)	9(2)	0(2)	-1(2)
C(10B)	53(2)	66(3)	44(2)	5(2)	-9(2)	-3(2)
C(11B)	49(2)	43(2)	37(2)	-1(1)	-3(2)	-9(2)
C(12B)	68(3)	35(2)	53(2)	0(2)	-1(2)	-10(2)
C(13B)	68(3)	40(2)	64(3)	11(2)	1(2)	0(2)
C(14B)	75(4)	73(4)	86(4)	10(3)	9(3)	3(3)
C(15B)	63(3)	49(2)	40(2)	2(2)	1(2)	-3(2)
C(16B)	107(6)	141(7)	51(3)	26(4)	20(4)	-28(6)
N(1B)	52(2)	37(2)	36(2)	0(1)	0(1)	-2(1)
O(1B)	71(2)	51(2)	53(2)	-13(1)	-4(1)	-13(1)
O(2B)	93(2)	82(2)	55(2)	24(2)	-2(2)	16(2)
O(3B)	84(2)	98(2)	50(2)	16(2)	17(2)	7(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	1455(59)	3665(33)	-1808(22)	49(10)
H(3A)	3654(60)	4666(34)	-2527(28)	57(12)
H(4A)	5810(69)	5869(40)	-1994(28)	72(13)
H(5A)	5673(66)	6103(37)	-576(27)	66(13)
H(8A)	154(59)	5036(39)	1421(26)	61(12)
H(9A1)	-2046(57)	3306(36)	929(25)	53(11)
H(9A2)	-2793(69)	4520(41)	908(27)	76(14)
H(10A)	-1866(53)	3587(32)	-418(22)	41(10)
H(10B)	-1222(58)	4875(38)	-326(25)	61(12)
H(12A)	597(56)	2312(32)	282(26)	48(11)
H(12B)	938(53)	2289(32)	-650(25)	47(10)
H(13A)	4183(94)	2559(56)	467(42)	118(22)
H(14A)	5935(106)	1530(52)	-240(40)	112(20)
H(14B)	3774(125)	1272(75)	-923(55)	168(34)
H(16A)	-1288(86)	3237(47)	3557(36)	84(17)
H(16B)	905(94)	3324(51)	3462(39)	98(20)
H(16C)	-781(91)	2432(56)	3138(40)	107(20)
H(2B)	341(66)	9341(37)	2966(28)	67(13)
H(3B)	-2096(58)	8384(36)	3606(27)	58(12)
H(4B)	-3727(63)	6922(35)	3030(25)	55(11)
H(5B)	-3105(60)	6464(33)	1709(23)	49(11)
H(8B)	2748(56)	7330(36)	-50(23)	50(10)
H(9B1)	5460(67)	8078(36)	520(26)	63(12)
H(9B2)	4730(60)	9255(38)	414(25)	59(12)
H(10C)	3586(52)	7960(32)	1700(23)	43(10)
H(10D)	4142(64)	9158(37)	1759(27)	60(12)
H(12C)	1318(66)	10497(40)	1561(30)	71(14)
H(12D)	1951(58)	10417(32)	721(25)	56(11)
H(13B)	-1448(72)	10162(41)	392(33)	77(15)
H(14C)	-3637(95)	10976(45)	1218(33)	94(17)
H(14D)	-1613(89)	11119(50)	1838(40)	100(20)
H(16D)	5250(134)	8645(76)	-2108(55)	144(38)
H(16E)	5330(121)	9493(73)	-1800(47)	146(32)
H(16F)	3194(128)	8832(69)	-2118(47)	125(34)

X-ray data of compound **cis-6a**

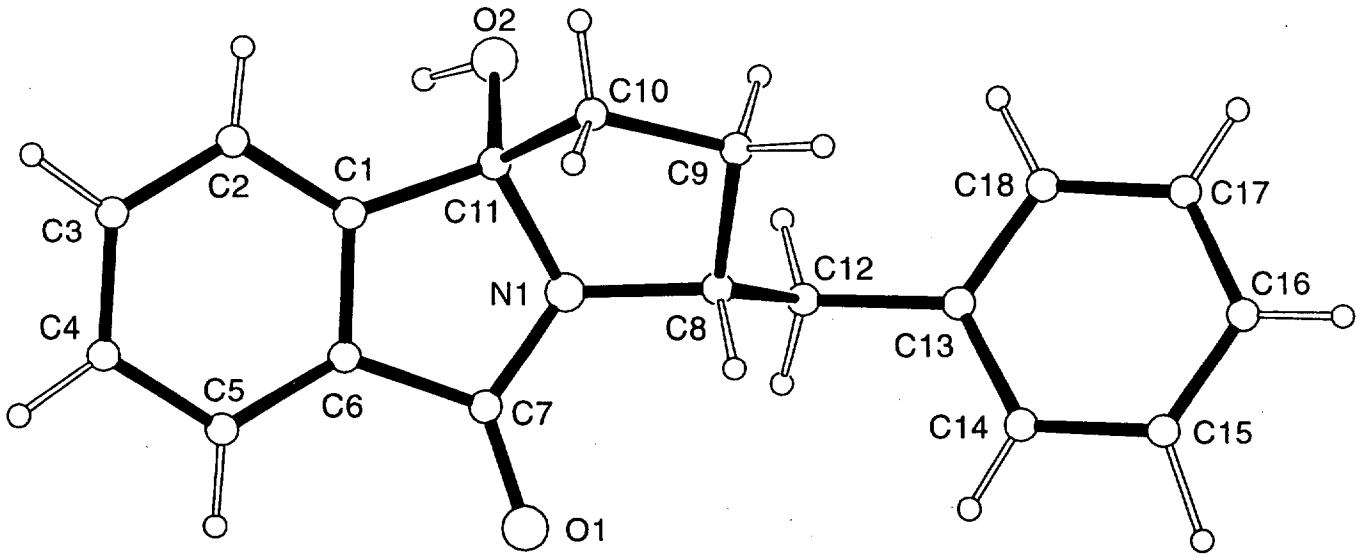


Table 1. Crystal data and structure refinement for 1.

Identification code	nero04
Empirical formula	C18 H17 N O2
Formula weight	279.33
Temperature	293(2) K
Wavelength	.71069 A
Crystal system	monoclinic
Space group	P21
Unit cell dimensions	a = 7.431(1) A alpha = 90 deg. b = 7.903(1) A beta = 94.91(1) deg. c = 12.492(1) A gamma = 90 deg.
Volume	730.9(2) A^3
Z	2
Density (calculated)	1.269 Mg/m^3
Absorption coefficient	0.083 mm^-1
F(000)	296
Crystal size	0.20 x 0.10 x 0.10 mm
Theta range for data collection	3.05 to 27.11 deg.
Index ranges	-9<=h<=9, -10<=k<=8, -16<=l<=16
Reflections collected	5170
Independent reflections	2935
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2819 / 1 / 260
Goodness-of-fit on F^2	1.004
Weighting scheme calc w=	1/[s^2^(Fo^2^)+(0.0232P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3
Final R indices [I>2sigma(I)]	R1 = 0.0679, wR2 = 0.0800
Reflection observed [I>2sigma(I)]	1361
R indices (all data)	R1 = 0.1959, wR2 = 0.1046

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	7495(5)	6784(4)	10230(3)	52(1)
C(2)	9049(6)	6905(6)	10874(4)	76(1)
C(3)	8989(8)	6774(6)	11947(5)	82(1)
C(4)	7445(8)	6494(5)	12406(4)	80(1)
C(5)	5849(7)	6350(4)	11754(4)	66(1)
C(6)	5913(5)	6518(4)	10665(3)	52(1)
C(7)	4477(5)	6363(4)	9789(3)	53(1)
C(8)	4605(6)	5981(5)	7838(3)	59(1)
C(9)	6369(7)	5460(6)	7405(4)	77(1)
C(10)	7715(8)	5439(6)	8371(5)	76(2)
C(11)	7156(5)	6878(5)	9043(3)	58(1)
C(12)	3458(8)	7143(6)	7117(3)	68(1)
C(13)	2775(6)	6285(4)	6093(3)	63(1)
C(14)	1333(8)	5229(6)	6069(4)	80(2)
C(15)	701(10)	4378(7)	5152(6)	102(2)
C(16)	1530(11)	4570(8)	4256(5)	102(2)
C(17)	2959(11)	5613(10)	4249(5)	109(2)
C(18)	3595(7)	6473(7)	5163(4)	89(2)
N(1)	5205(4)	6757(4)	8873(2)	51(1)
O(1)	2929(3)	5927(3)	9862(2)	67(1)
O(2)	7801(4)	8389(3)	8614(2)	74(1)

Table 3. Bond lengths [A] and angles [deg] for 1.

C(1)-C(6)	1.353(4)
C(1)-C(2)	1.353(5)
C(1)-C(11)	1.484(4)
C(2)-C(3)	1.349(5)
C(3)-C(4)	1.344(6)
C(4)-C(5)	1.385(5)
C(5)-C(6)	1.371(4)
C(6)-C(7)	1.467(4)
C(7)-O(1)	1.212(4)
C(7)-N(1)	1.343(4)
C(8)-N(1)	1.465(4)
C(8)-C(9)	1.517(5)
C(8)-C(12)	1.500(5)
C(9)-C(10)	1.499(6)
C(10)-C(11)	1.494(5)
C(11)-O(2)	1.410(4)
C(11)-N(1)	1.451(4)
C(12)-C(13)	1.498(5)
C(13)-C(14)	1.357(5)
C(13)-C(18)	1.365(5)
C(14)-C(15)	1.375(7)
C(15)-C(16)	1.332(8)
C(16)-C(17)	1.345(7)
C(17)-C(18)	1.377(8)

C(6)-C(1)-C(2)	119.9(4)
C(6)-C(1)-C(11)	109.3(3)
C(2)-C(1)-C(11)	130.8(4)
C(3)-C(2)-C(1)	119.1(5)
C(4)-C(3)-C(2)	122.6(5)
C(3)-C(4)-C(5)	118.8(5)
C(4)-C(5)-C(6)	118.3(4)
C(1)-C(6)-C(5)	121.3(4)
C(1)-C(6)-C(7)	108.3(3)
C(5)-C(6)-C(7)	130.3(4)
O(1)-C(7)-N(1)	125.8(3)
O(1)-C(7)-C(6)	127.0(4)
N(1)-C(7)-C(6)	107.3(3)
N(1)-C(8)-C(9)	102.8(3)
N(1)-C(8)-C(12)	112.8(3)
C(9)-C(8)-C(12)	114.6(4)
C(10)-C(9)-C(8)	104.7(4)
C(11)-C(10)-C(9)	104.2(4)
O(2)-C(11)-N(1)	111.7(3)
O(2)-C(11)-C(1)	112.8(3)
N(1)-C(11)-C(1)	103.0(3)
O(2)-C(11)-C(10)	108.1(3)
N(1)-C(11)-C(10)	100.9(3)
C(1)-C(11)-C(10)	119.5(4)
C(8)-C(12)-C(13)	111.7(3)
C(14)-C(13)-C(18)	117.2(4)
C(14)-C(13)-C(12)	120.4(4)
C(18)-C(13)-C(12)	122.4(5)
C(13)-C(14)-C(15)	122.2(5)
C(16)-C(15)-C(14)	119.6(6)

Table 4. Torsion angles [deg] for 1.

C(6)-C(1)-C(2)-C(3)	-.7(6)
C(11)-C(1)-C(2)-C(3)	-180.0(4)
C(1)-C(2)-C(3)-C(4)	1.4(7)
C(2)-C(3)-C(4)-C(5)	-.6(7)
C(3)-C(4)-C(5)-C(6)	-.7(5)
C(2)-C(1)-C(6)-C(5)	-.6(5)
C(11)-C(1)-C(6)-C(5)	178.8(3)
C(2)-C(1)-C(6)-C(7)	-177.4(3)
C(11)-C(1)-C(6)-C(7)	2.0(4)
C(4)-C(5)-C(6)-C(1)	1.3(5)
C(4)-C(5)-C(6)-C(7)	177.3(3)
C(1)-C(6)-C(7)-O(1)	170.7(3)
C(5)-C(6)-C(7)-O(1)	-5.7(5)
C(1)-C(6)-C(7)-N(1)	-7.7(3)
C(5)-C(6)-C(7)-N(1)	175.8(3)
N(1)-C(8)-C(9)-C(10)	18.9(4)
C(12)-C(8)-C(9)-C(10)	141.7(4)
C(8)-C(9)-C(10)-C(11)	-35.9(5)
C(6)-C(1)-C(11)-O(2)	124.5(3)
C(2)-C(1)-C(11)-O(2)	-56.2(5)
C(6)-C(1)-C(11)-N(1)	3.9(4)
C(2)-C(1)-C(11)-N(1)	-176.8(4)
C(6)-C(1)-C(11)-C(10)	-106.8(4)
C(2)-C(1)-C(11)-C(10)	72.5(6)
C(9)-C(10)-C(11)-O(2)	-79.6(4)
C(9)-C(10)-C(11)-N(1)	37.7(4)
C(9)-C(10)-C(11)-C(1)	149.5(4)
N(1)-C(8)-C(12)-C(13)	-176.7(4)
C(9)-C(8)-C(12)-C(13)	66.2(5)
C(8)-C(12)-C(13)-C(14)	79.7(5)
C(8)-C(12)-C(13)-C(18)	-97.9(5)
C(18)-C(13)-C(14)-C(15)	-.3(6)
C(12)-C(13)-C(14)-C(15)	-178.0(4)
C(13)-C(14)-C(15)-C(16)	.8(8)
C(14)-C(15)-C(16)-C(17)	-1.1(9)
C(15)-C(16)-C(17)-C(18)	.9(9)
C(14)-C(13)-C(18)-C(17)	.1(6)
C(12)-C(13)-C(18)-C(17)	177.7(5)
C(16)-C(17)-C(18)-C(13)	-.4(8)
O(1)-C(7)-N(1)-C(11)	-168.0(3)
C(6)-C(7)-N(1)-C(11)	10.5(3)
O(1)-C(7)-N(1)-C(8)	-30.7(5)
C(6)-C(7)-N(1)-C(8)	147.8(3)
O(2)-C(11)-N(1)-C(7)	-130.4(3)
C(1)-C(11)-N(1)-C(7)	-9.0(4)
C(10)-C(11)-N(1)-C(7)	114.9(4)
O(2)-C(11)-N(1)-C(8)	87.8(4)
C(1)-C(11)-N(1)-C(8)	-150.9(3)
C(10)-C(11)-N(1)-C(8)	-26.9(4)
C(9)-C(8)-N(1)-C(7)	-131.6(4)
C(12)-C(8)-N(1)-C(7)	104.5(4)
C(9)-C(8)-N(1)-C(11)	5.2(4)
C(12)-C(8)-N(1)-C(11)	-118.7(4)