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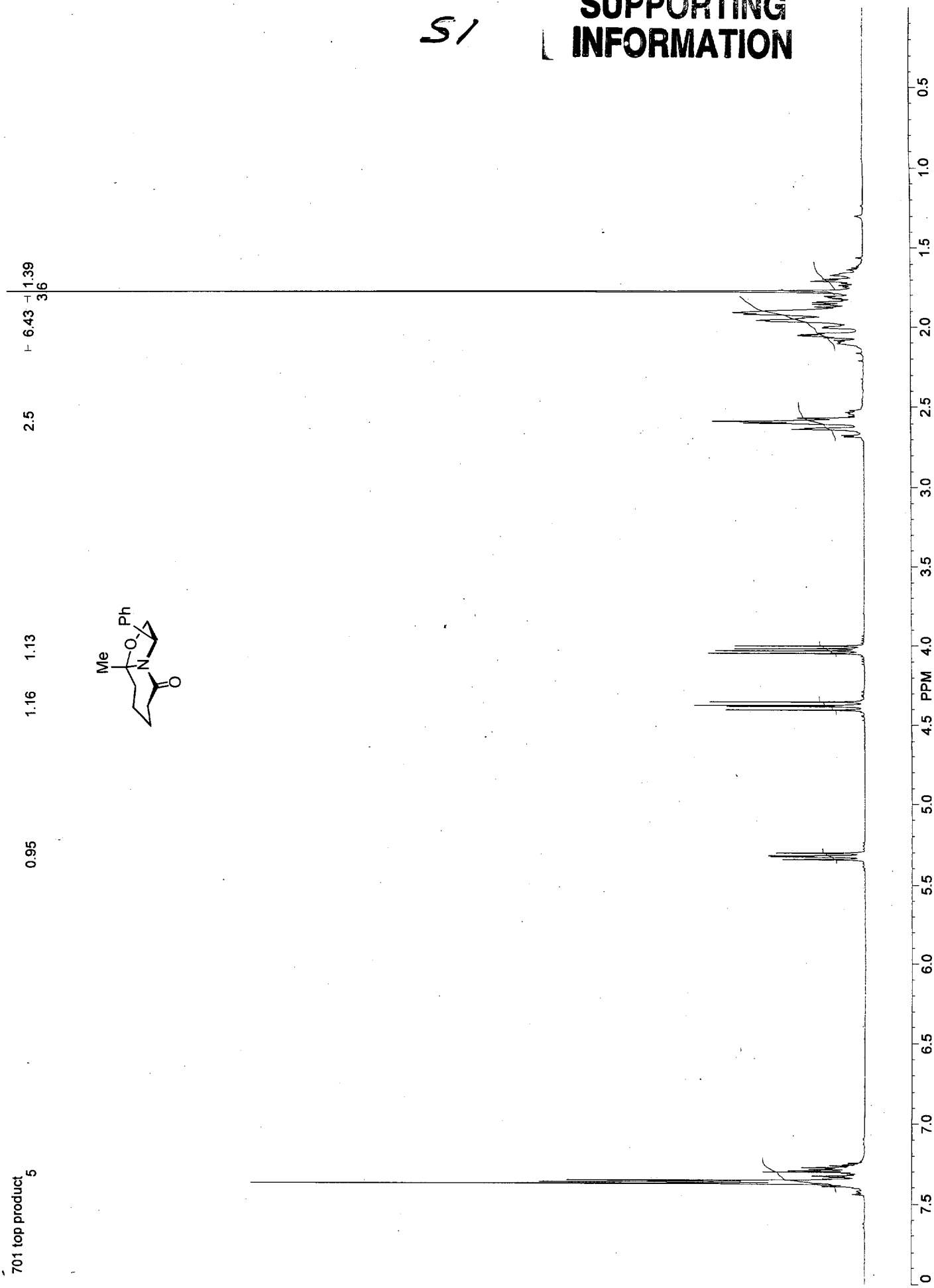
S1

SUPPORTING INFORMATION



701 top product

="Top Diastereomer"

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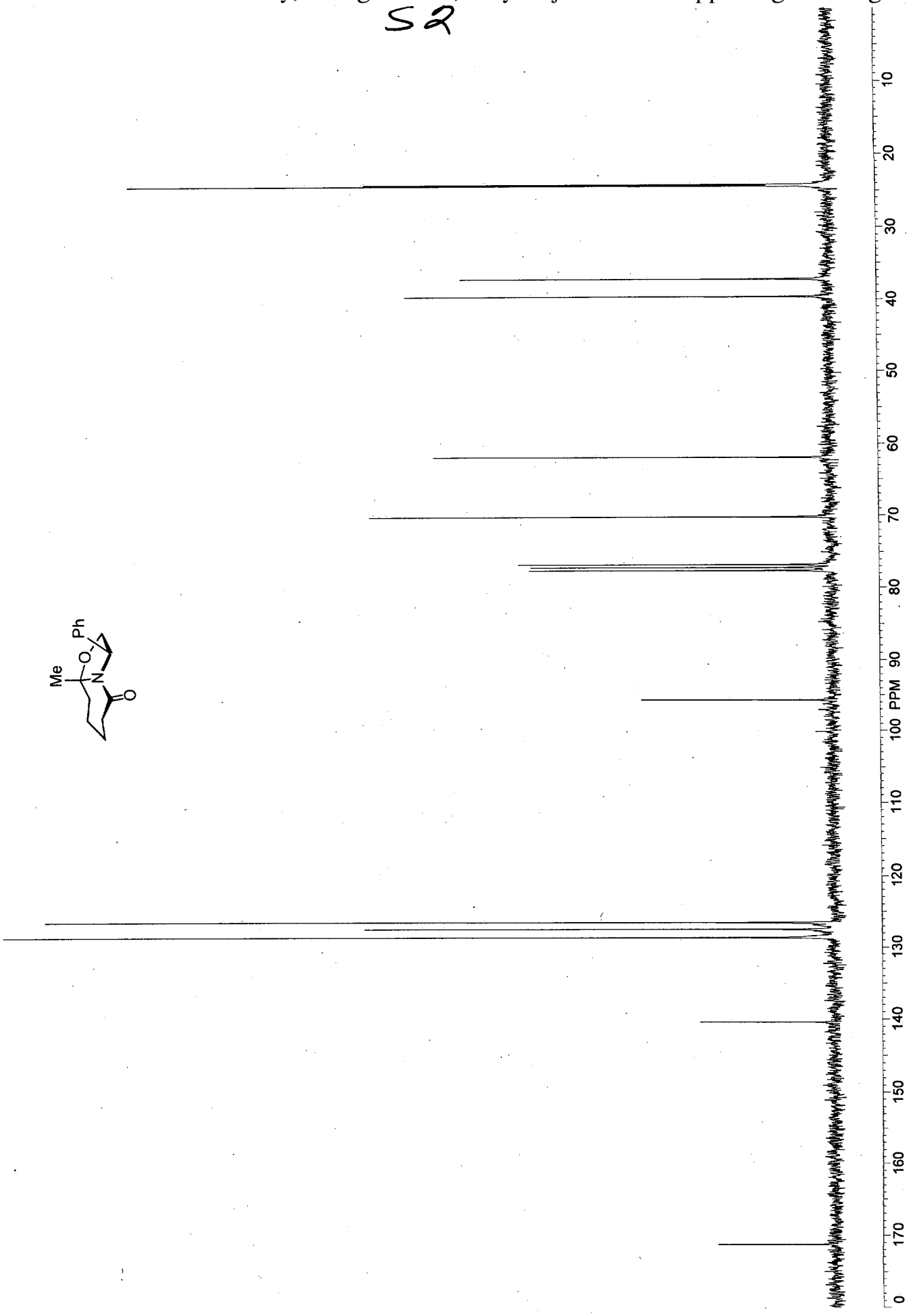
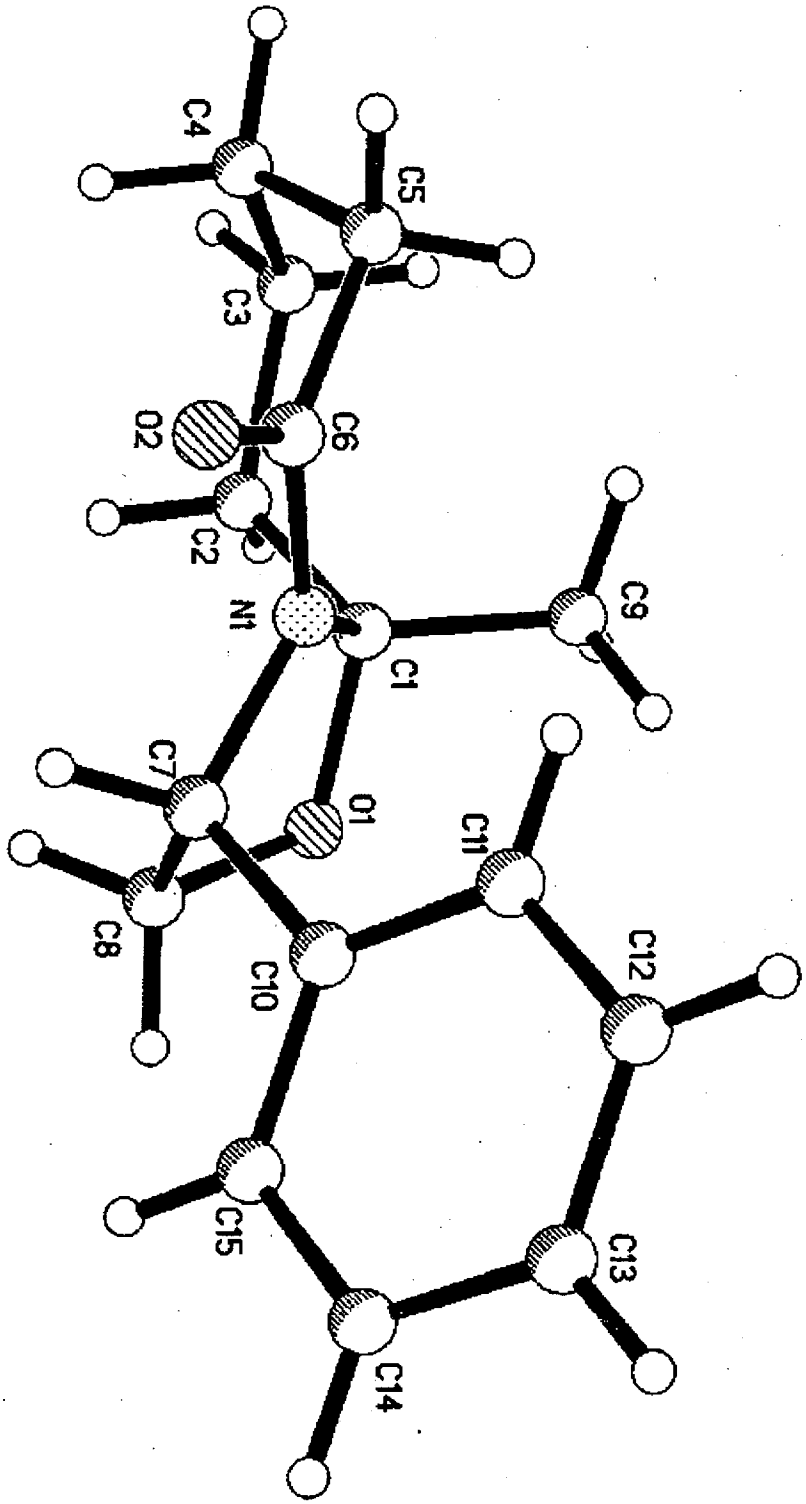
S2

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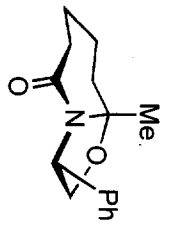
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Me
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Ph

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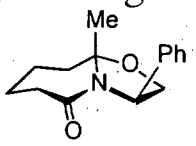

Table 1. Crystal data and structure refinement for 1.

Identification code	amccd22 SVD701TOP Downing/Meyers
Empirical formula	$C_{15}H_{19}NO_2$
Formula weight	245.31
Temperature	167(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 8.0338(2) Å alpha = 90° b = 10.2400(2) Å beta = 90° c = 15.93020(10) Å gamma = 90°
Volume, Z	1310.52(4) Å^3, 4
Density (calculated)	1.243 Mg/m^3
Absorption coefficient	0.082 mm^{-1}
F(000)	528
Crystal size	0.08 x 0.24 x 0.25 mm
θ range for data collection	2.36 to 28.44°
Limiting indices	$-10 \le h \le 10$, $-13 \le k \le 12$, $-13 \le l \le 20$
Reflections collected	8852
Independent reflections	3191 (R_{int} = 0.0427)
Absorption correction	SADABS
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3191 / 0 / 163
Goodness-of-fit on F^2	1.017
Final R indices [$I>2\sigma(I)$]	R1 = 0.0450, wR2 = 0.0881
R indices (all data)	R1 = 0.0717, wR2 = 0.0987
Largest diff. peak and hole	0.143 and -0.203 eÅ^{-3}

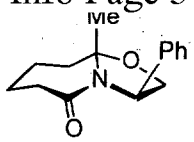

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	8690(1)	5364(1)	8021(1)	31(1)
O(2)	5763(2)	8234(1)	6505(1)	44(1)
N(1)	7557(2)	6978(1)	7227(1)	26(1)
C(1)	9138(2)	6245(2)	7359(1)	27(1)
C(2)	9625(2)	5443(2)	6587(1)	36(1)
C(3)	10328(3)	6190(2)	5837(1)	46(1)
C(4)	9122(3)	7123(2)	5419(1)	45(1)
C(5)	8538(2)	8236(2)	5990(1)	36(1)
C(6)	7197(2)	7825(2)	6591(1)	30(1)
C(7)	6194(2)	6429(2)	7726(1)	27(1)
C(8)	6944(2)	5114(2)	7974(1)	32(1)
C(9)	10542(2)	7056(2)	7711(1)	39(1)
C(10)	5636(2)	7278(2)	8453(1)	26(1)
C(11)	6061(2)	8589(2)	8516(1)	28(1)
C(12)	5459(2)	9363(2)	9167(1)	34(1)
C(13)	4418(2)	8826(2)	9768(1)	41(1)
C(14)	3970(3)	7532(2)	9706(1)	47(1)
C(15)	4567(2)	6764(2)	9059(1)	39(1)

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S6

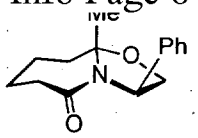

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-C(8)	1.428(2)	O(1)-C(1)	1.434(2)
O(2)-C(6)	1.233(2)	N(1)-C(6)	1.365(2)
N(1)-C(7)	1.464(2)	N(1)-C(1)	1.490(2)
C(1)-C(9)	1.509(2)	C(1)-C(2)	1.529(2)
C(2)-C(3)	1.527(3)	C(3)-C(4)	1.516(3)
C(4)-C(5)	1.532(2)	C(5)-C(6)	1.502(2)
C(7)-C(10)	1.517(2)	C(7)-C(8)	1.528(2)
C(10)-C(11)	1.389(2)	C(10)-C(15)	1.394(2)
C(11)-C(12)	1.392(2)	C(12)-C(13)	1.385(3)
C(13)-C(14)	1.377(3)	C(14)-C(15)	1.383(3)

C(8)-O(1)-C(1)	108.71(12)	C(6)-N(1)-C(7)	119.22(13)
C(6)-N(1)-C(1)	127.19(13)	C(7)-N(1)-C(1)	111.60(12)
O(1)-C(1)-N(1)	101.90(12)	O(1)-C(1)-C(9)	105.09(13)
N(1)-C(1)-C(9)	114.37(13)	O(1)-C(1)-C(2)	108.49(12)
N(1)-C(1)-C(2)	112.07(13)	C(9)-C(1)-C(2)	113.78(14)
C(3)-C(2)-C(1)	117.0(2)	C(4)-C(3)-C(2)	115.0(2)
C(3)-C(4)-C(5)	113.8(2)	C(6)-C(5)-C(4)	112.9(2)
O(2)-C(6)-N(1)	119.7(2)	O(2)-C(6)-C(5)	120.2(2)
N(1)-C(6)-C(5)	120.0(2)	N(1)-C(7)-C(10)	114.54(13)
N(1)-C(7)-C(8)	100.56(13)	C(10)-C(7)-C(8)	115.11(14)
O(1)-C(8)-C(7)	104.07(13)	C(11)-C(10)-C(15)	117.8(2)
C(11)-C(10)-C(7)	122.4(2)	C(15)-C(10)-C(7)	119.6(2)
C(10)-C(11)-C(12)	121.2(2)	C(13)-C(12)-C(11)	119.9(2)
C(14)-C(13)-C(12)	119.3(2)	C(13)-C(14)-C(15)	120.7(2)
C(14)-C(15)-C(10)	121.0(2)		

Symmetry transformations used to generate equivalent atoms:

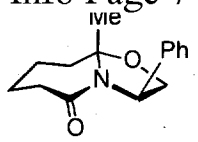

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	30(1)	24(1)	38(1)	7(1)	-5(1)	-2(1)
O(2)	44(1)	57(1)	30(1)	2(1)	-2(1)	26(1)
N(1)	26(1)	26(1)	25(1)	0(1)	0(1)	6(1)
C(1)	26(1)	20(1)	34(1)	4(1)	-4(1)	3(1)
C(2)	34(1)	27(1)	47(1)	-4(1)	3(1)	8(1)
C(3)	51(1)	42(1)	46(1)	-4(1)	16(1)	11(1)
C(4)	58(1)	46(1)	32(1)	0(1)	13(1)	10(1)
C(5)	49(1)	32(1)	27(1)	7(1)	4(1)	9(1)
C(6)	40(1)	28(1)	23(1)	-4(1)	-3(1)	10(1)
C(7)	24(1)	29(1)	28(1)	-2(1)	-4(1)	-2(1)
C(8)	32(1)	26(1)	40(1)	0(1)	1(1)	-5(1)
C(9)	35(1)	30(1)	51(1)	5(1)	-12(1)	-7(1)
C(10)	23(1)	30(1)	24(1)	1(1)	-4(1)	0(1)
C(11)	28(1)	31(1)	26(1)	0(1)	-1(1)	-1(1)
C(12)	39(1)	32(1)	32(1)	-5(1)	-4(1)	4(1)
C(13)	43(1)	50(1)	30(1)	-9(1)	5(1)	6(1)
C(14)	46(1)	58(1)	37(1)	2(1)	15(1)	-5(1)
C(15)	40(1)	39(1)	38(1)	-1(1)	5(1)	-7(1)

S8

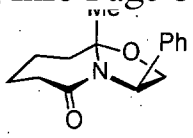

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	10461(2)	4788(2)	6763(1)	43
H(2B)	8628(2)	4958(2)	6396(1)	43
H(3A)	11313(3)	6691(2)	6026(1)	56
H(3B)	10714(3)	5550(2)	5414(1)	56
H(4A)	8137(3)	6625(2)	5227(1)	54
H(4B)	9663(3)	7502(2)	4916(1)	54
H(5A)	9501(2)	8569(2)	6313(1)	43
H(5B)	8115(2)	8960(2)	5637(1)	43
H(7A)	5220(2)	6271(2)	7348(1)	32
H(8A)	6506(2)	4818(2)	8522(1)	39
H(8B)	6698(2)	4440(2)	7545(1)	39
H(9A)	10913(2)	7686(2)	7287(1)	58
H(9B)	11472(2)	6484(2)	7864(1)	58
H(9C)	10154(2)	7525(2)	8210(1)	58
H(11A)	6776(2)	8964(2)	8107(1)	34
H(12A)	5762(2)	10258(2)	9199(1)	41
H(13A)	4018(2)	9345(2)	10219(1)	50
H(14A)	3242(3)	7162(2)	10111(1)	57
H(15A)	4245(2)	5873(2)	9026(1)	47

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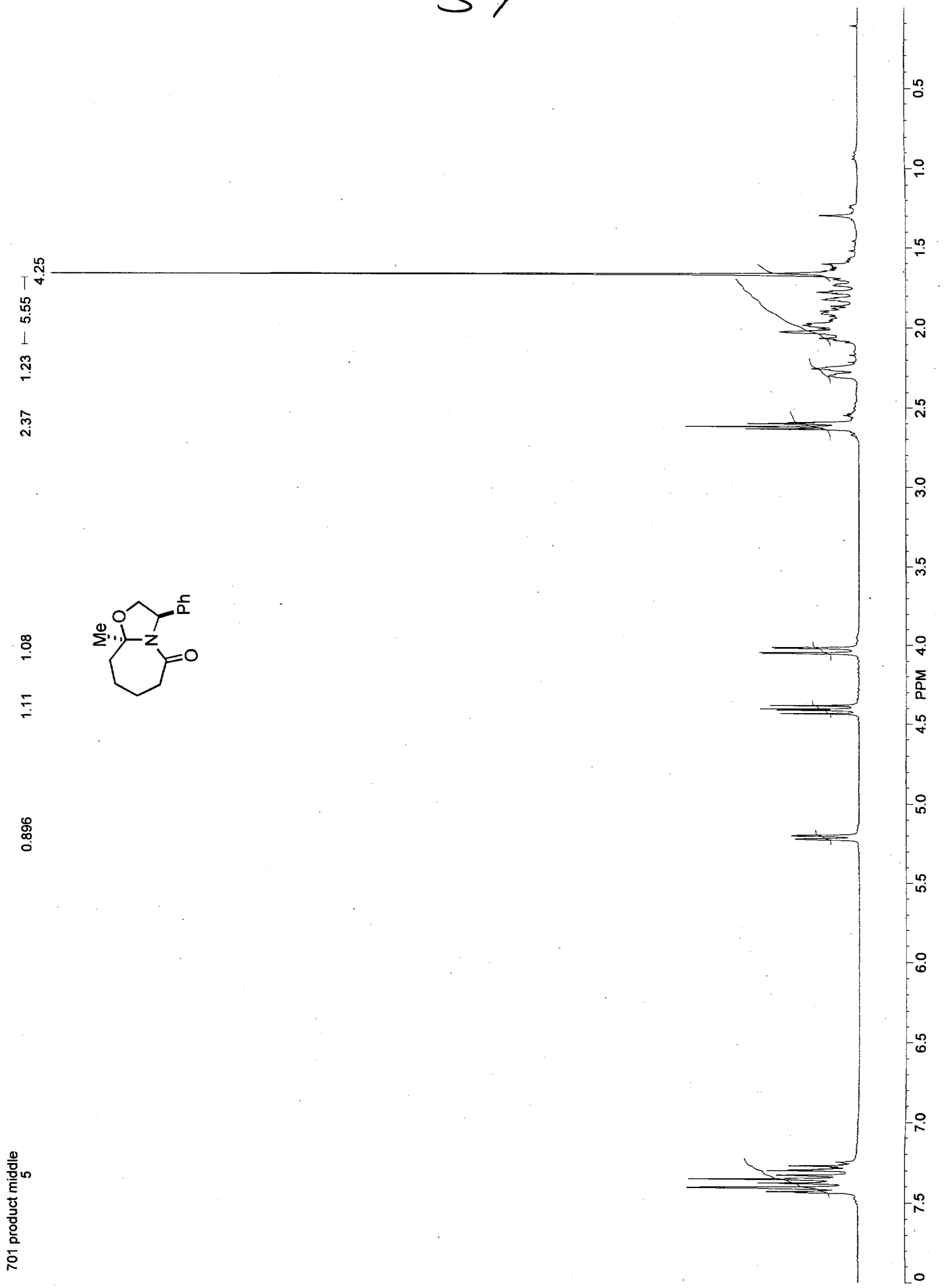
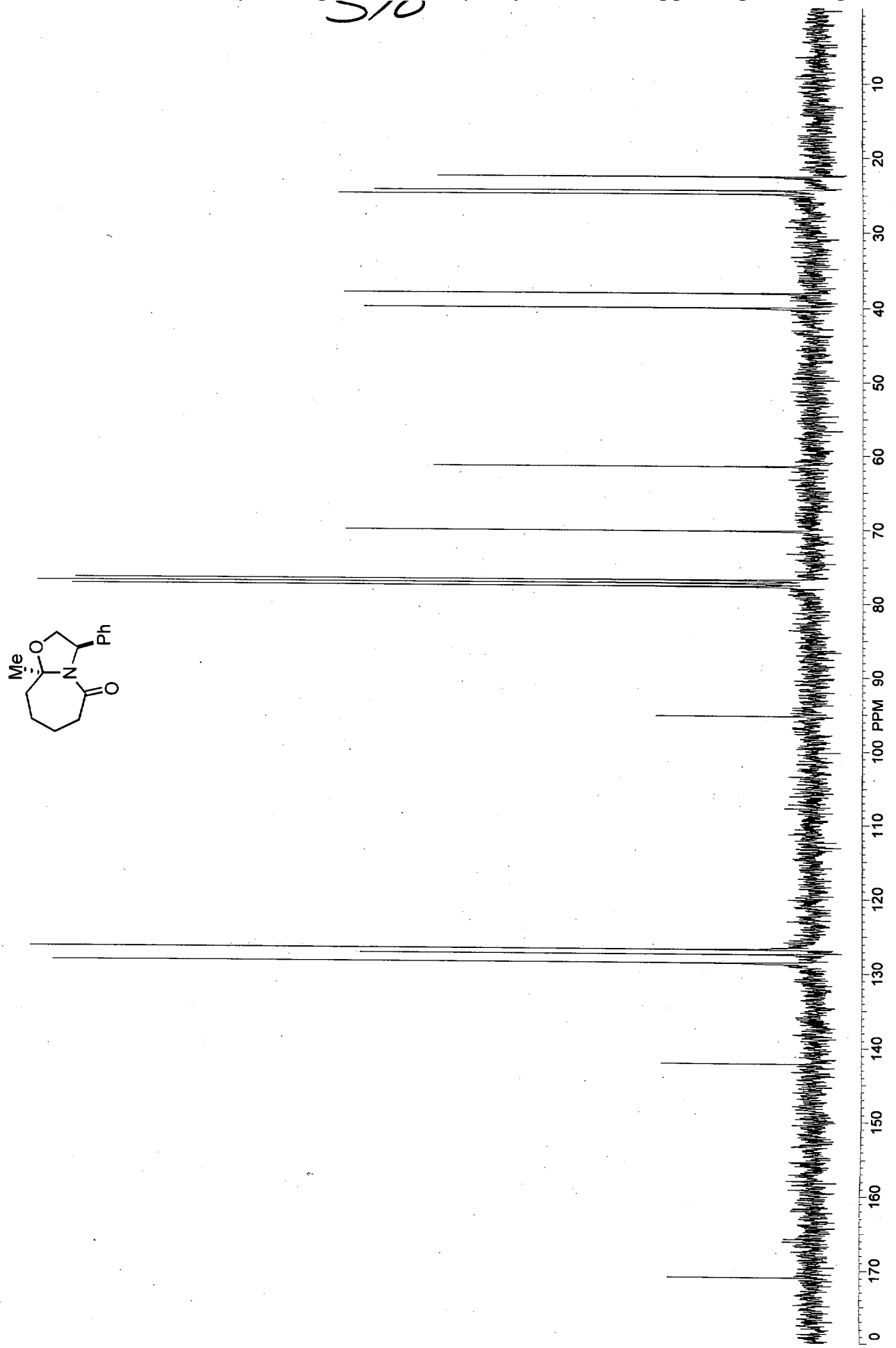


= "Bottom Diastereomer"

S10



701 Bottom Diastereomer

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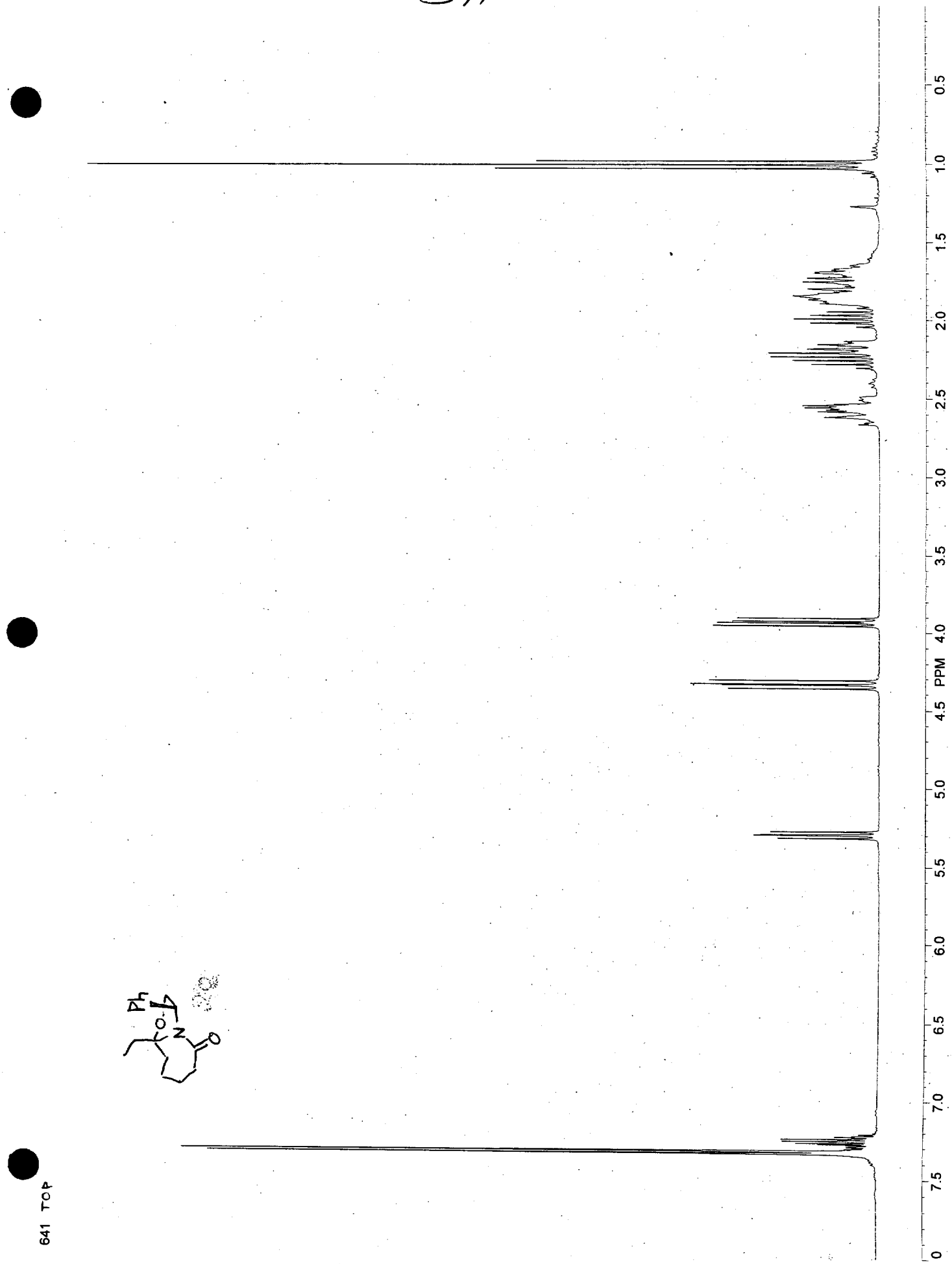

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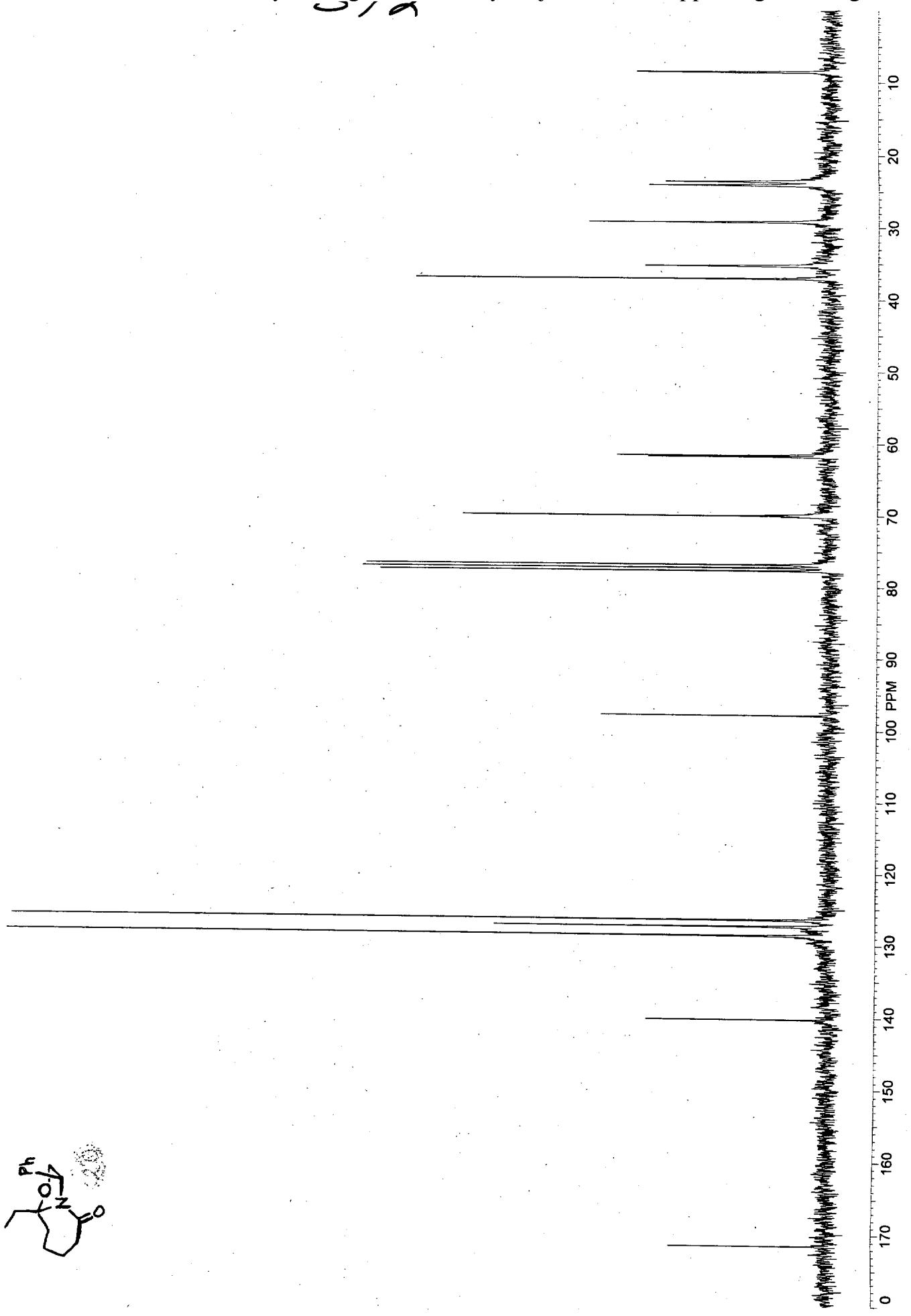

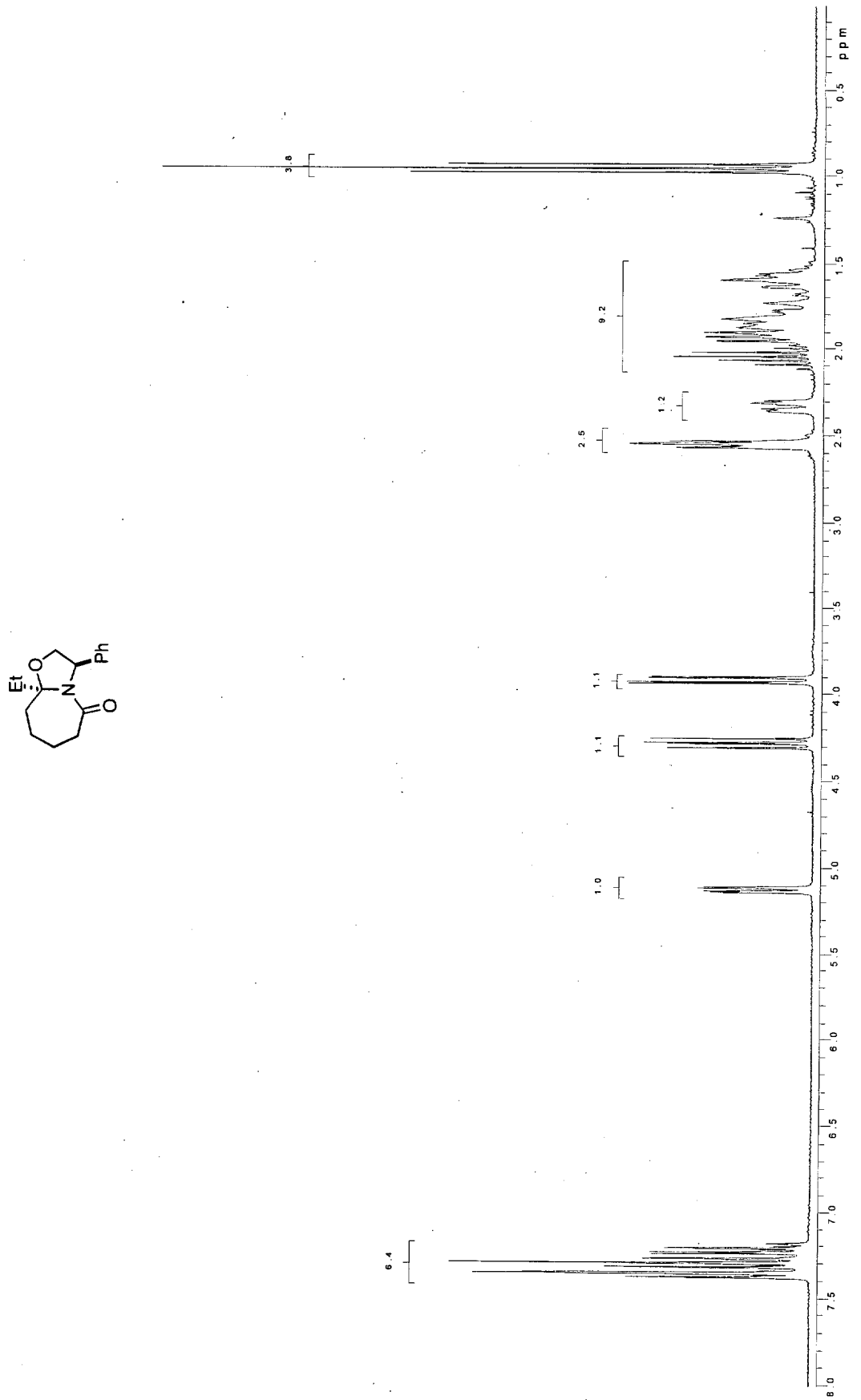
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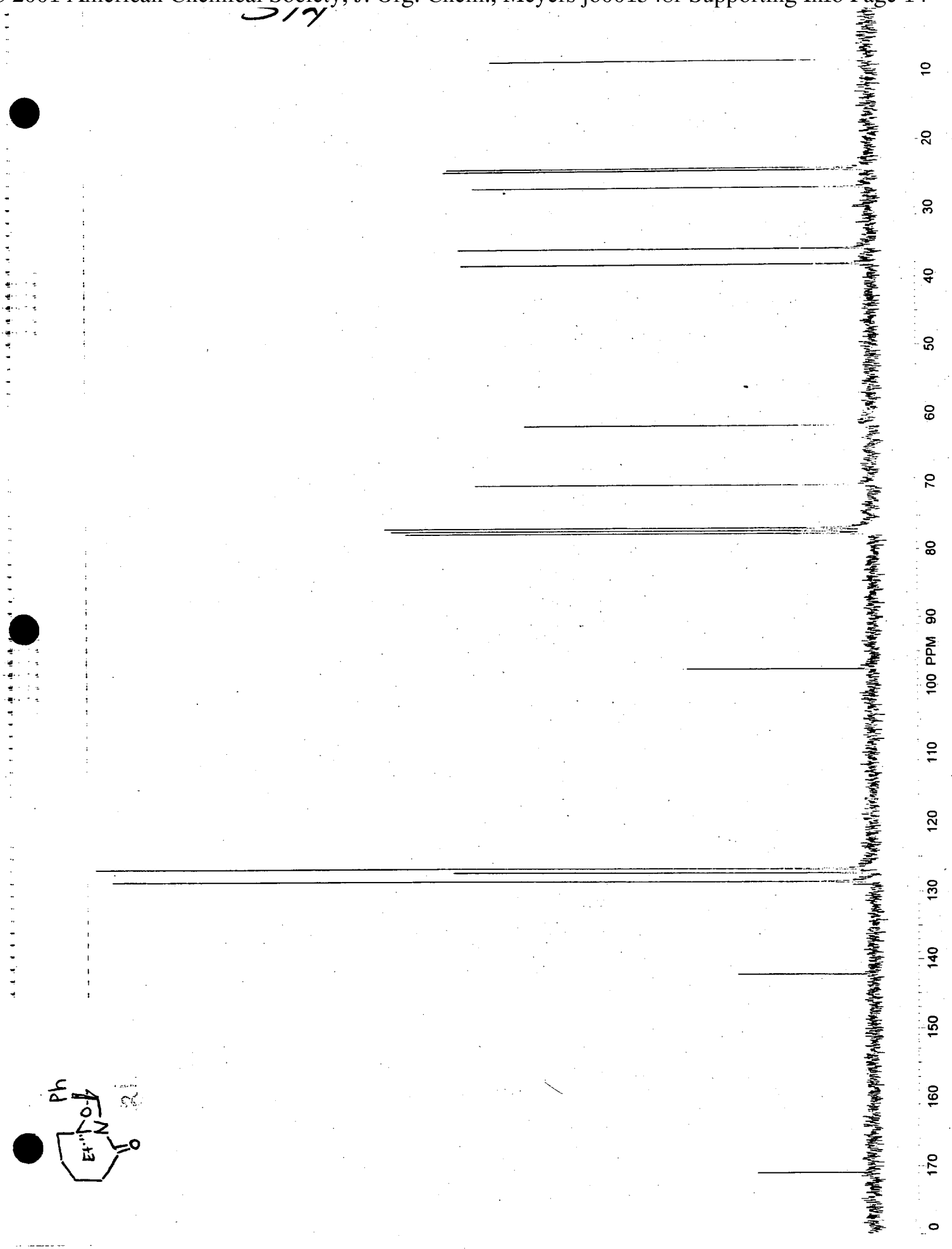

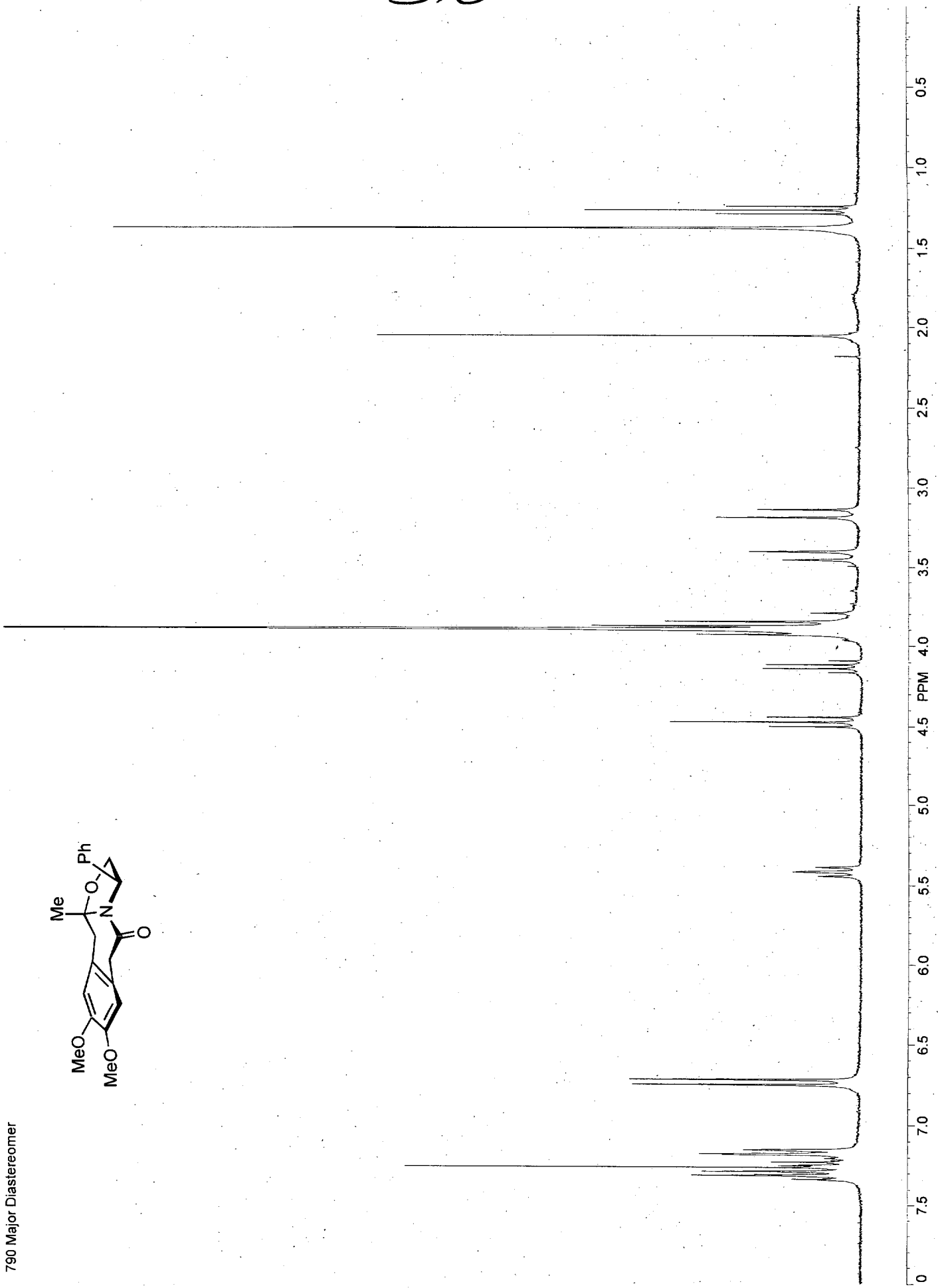

790 Major Diastereomer

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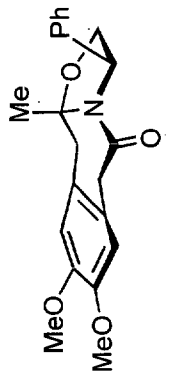

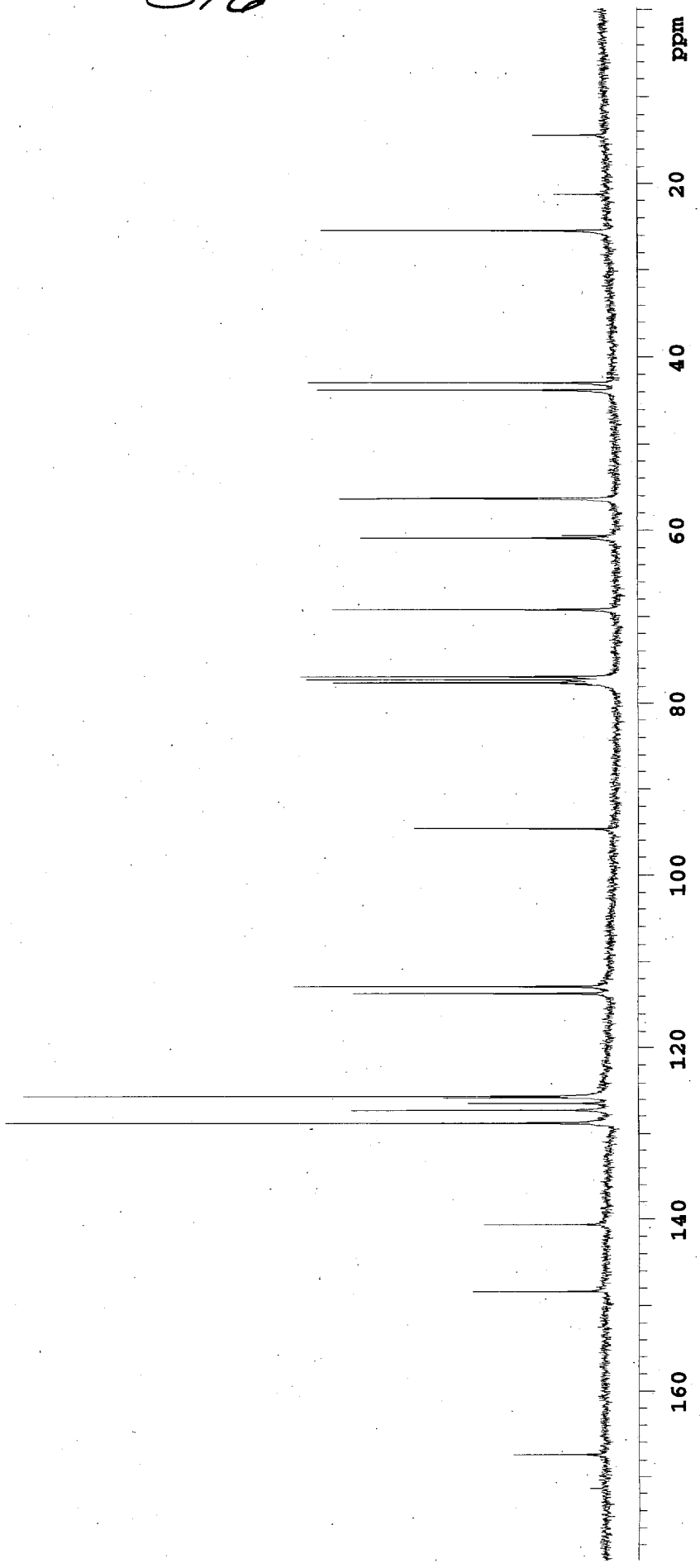

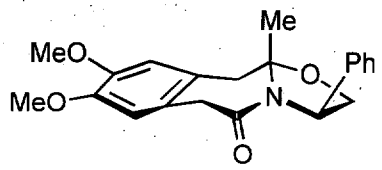

Table 1. Crystal data and structure refinement for 1.

Identification code	amccd21 (Downing/Meyers)
Empirical formula	$C_{23}H_{28}NO_{4.50}$
Formula weight	390.46
Temperature	167(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12$
Unit cell dimensions	*a* = 13.0477(9) Å alpha = 90° *b* = 14.3234(10) Å beta = 90° *c* = 11.1515(8) Å gamma = 90°
Volume, Z	2084.1(3) Å^3, 4
Density (calculated)	1.244 Mg/m^3
Absorption coefficient	0.086 mm^{-1}
F(000)	836
Crystal size	0.04 x 0.26 x 0.38 mm
θ range for data collection	1.83 to 28.41°
Limiting indices	$-17 \le h \le 16$, $-19 \le k \le 15$, $-14 \le l \le 9$
Reflections collected	13826
Independent reflections	5028 (R_{int} = 0.1431)
Absorption correction	SADABS
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5028 / 0 / 258
Goodness-of-fit on F^2	1.004
Final R indices [I>2σ(I)]	R1 = 0.0904, wR2 = 0.1598
R indices (all data)	R1 = 0.2289, wR2 = 0.2173
Largest diff. peak and hole	0.253 and -0.307 eÅ^{-3}

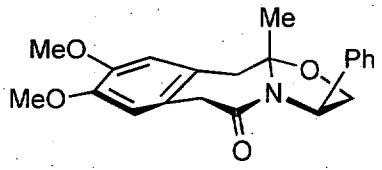

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	6421(3)	2348(2)	1498(4)	30(1)
O(1)	6786(2)	3893(2)	1327(3)	40(1)
O(2)	6635(2)	871(2)	877(3)	38(1)
O(3)	1474(2)	3318(2)	2171(3)	42(1)
O(4)	1478(2)	1523(2)	1964(3)	40(1)
C(1)	5955(4)	3288(3)	1629(5)	34(1)
C(2)	5100(4)	3501(3)	750(5)	36(1)
C(3)	4116(4)	2975(3)	1041(4)	29(1)
C(4)	3246(4)	3431(3)	1458(5)	35(1)
C(5)	2370(4)	2942(4)	1760(5)	35(1)
C(6)	2373(4)	1960(3)	1651(5)	31(1)
C(7)	3241(3)	1510(3)	1236(4)	32(1)
C(8)	4122(4)	2010(3)	933(5)	31(1)
C(9)	5023(4)	1505(3)	394(5)	33(1)
C(10)	6076(4)	1555(4)	963(5)	32(1)
C(11)	7529(3)	2420(3)	1726(5)	33(1)
C(12)	7689(4)	3481(3)	1831(5)	39(1)
C(13)	5622(4)	3462(4)	2935(5)	41(1)
C(14)	1437(4)	4318(3)	2212(5)	45(2)
C(15)	1476(4)	530(3)	1874(6)	46(2)
C(16)	7926(4)	1892(3)	2815(5)	32(1)
C(17)	7280(4)	1546(4)	3680(5)	45(2)
C(18)	7677(5)	1082(5)	4675(6)	61(2)
C(19)	8707(6)	978(4)	4822(6)	64(2)
C(20)	9365(4)	1333(4)	3958(6)	54(2)
C(21)	8973(4)	1783(4)	2963(6)	44(2)
O(5)	5000	0	4563(6)	70(2)
C(23)	4409(5)	631(4)	3855(6)	63(2)
C(22)	3832(7)	1295(5)	4638(8)	105(3)

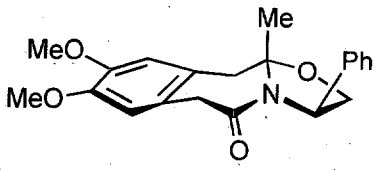

Table 3. Bond lengths [Å] and angles [°] for 1.

N(1)-C(10)	1.360(6)	N(1)-C(11)	1.471(5)
N(1)-C(1)	1.485(6)	O(1)-C(12)	1.432(6)
O(1)-C(1)	1.428(5)	O(2)-C(10)	1.226(5)
O(3)-C(5)	1.366(6)	O(3)-C(14)	1.434(5)
O(4)-C(6)	1.370(5)	O(4)-C(15)	1.427(5)
C(1)-C(2)	1.517(7)	C(1)-C(13)	1.540(7)
C(2)-C(3)	1.524(7)	C(3)-C(4)	1.390(6)
C(3)-C(8)	1.387(6)	C(4)-C(5)	1.382(7)
C(5)-C(6)	1.412(6)	C(6)-C(7)	1.383(6)
C(7)-C(8)	1.396(6)	C(8)-C(9)	1.506(7)
C(9)-C(10)	1.515(7)	C(11)-C(16)	1.522(7)
C(11)-C(12)	1.538(6)	C(16)-C(17)	1.374(7)
C(16)-C(21)	1.386(6)	C(17)-C(18)	1.393(8)
C(18)-C(19)	1.362(8)	C(19)-C(20)	1.388(8)
C(20)-C(21)	1.382(8)	O(5)-C(23)	1.426(7)
O(5)-C(23)#1	1.426(7)	C(23)-C(22)	1.495(9)

C(10)-N(1)-C(11)	117.4(4)	C(10)-N(1)-C(1)	131.7(4)
C(11)-N(1)-C(1)	108.7(3)	C(12)-O(1)-C(1)	106.4(3)
C(5)-O(3)-C(14)	115.7(4)	C(6)-O(4)-C(15)	116.1(4)
O(1)-C(1)-N(1)	102.5(3)	O(1)-C(1)-C(2)	106.5(4)
N(1)-C(1)-C(2)	114.8(4)	O(1)-C(1)-C(13)	109.8(4)
N(1)-C(1)-C(13)	110.8(4)	C(2)-C(1)-C(13)	111.8(4)
C(1)-C(2)-C(3)	112.5(4)	C(4)-C(3)-C(8)	120.2(5)
C(4)-C(3)-C(2)	121.7(4)	C(8)-C(3)-C(2)	118.0(5)
C(5)-C(4)-C(3)	121.2(4)	O(3)-C(5)-C(4)	126.1(4)
O(3)-C(5)-C(6)	115.1(5)	C(4)-C(5)-C(6)	118.8(5)
O(4)-C(6)-C(7)	124.8(4)	O(4)-C(6)-C(5)	115.5(4)
C(7)-C(6)-C(5)	119.7(5)	C(6)-C(7)-C(8)	121.1(4)
C(3)-C(8)-C(7)	119.0(5)	C(3)-C(8)-C(9)	121.2(5)
C(7)-C(8)-C(9)	119.6(4)	C(8)-C(9)-C(10)	121.2(4)
O(2)-C(10)-N(1)	120.3(4)	O(2)-C(10)-C(9)	118.0(4)
N(1)-C(10)-C(9)	121.6(4)	N(1)-C(11)-C(16)	115.9(4)
N(1)-C(11)-C(12)	102.5(4)	C(16)-C(11)-C(12)	112.6(4)
O(1)-C(12)-C(11)	105.4(4)	C(17)-C(16)-C(21)	118.7(5)
C(17)-C(16)-C(11)	122.1(4)	C(21)-C(16)-C(11)	119.1(5)
C(16)-C(17)-C(18)	120.2(5)	C(19)-C(18)-C(17)	121.0(6)
C(18)-C(19)-C(20)	119.2(6)	C(21)-C(20)-C(19)	119.9(5)
C(20)-C(21)-C(16)	120.9(6)	C(23)-O(5)-C(23)#1	112.8(7)
O(5)-C(23)-C(22)	110.6(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,z

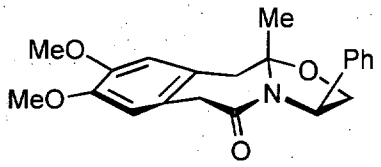

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
N(1)	34(2)	26(2)	30(2)	-4(2)	1(2)	-3(2)
O(1)	37(2)	36(2)	47(2)	5(2)	1(2)	-7(2)
O(2)	40(2)	33(2)	40(2)	-2(2)	0(2)	3(2)
O(3)	43(2)	36(2)	46(2)	-1(2)	4(2)	12(2)
O(4)	34(2)	33(2)	52(2)	9(2)	7(2)	-1(2)
C(1)	35(3)	28(3)	39(3)	0(3)	6(3)	-5(2)
C(2)	38(3)	28(3)	40(3)	1(3)	2(3)	2(2)
C(3)	33(3)	27(3)	28(3)	2(2)	0(3)	-4(2)
C(4)	43(3)	30(3)	32(3)	1(3)	1(3)	4(3)
C(5)	40(3)	36(3)	30(3)	-2(3)	0(3)	6(2)
C(6)	35(3)	34(3)	23(3)	6(3)	-1(3)	2(2)
C(7)	35(3)	25(2)	35(3)	1(2)	-7(3)	4(2)
C(8)	35(3)	30(3)	26(3)	1(2)	-6(3)	-5(2)
C(9)	32(3)	31(3)	34(3)	1(3)	-1(3)	0(2)
C(10)	33(3)	35(3)	26(3)	1(3)	6(3)	-2(3)
C(11)	33(3)	32(3)	33(3)	-3(3)	-2(2)	0(2)
C(12)	37(3)	39(3)	41(4)	2(3)	-3(3)	-7(2)
C(13)	44(3)	43(3)	36(3)	-8(3)	5(3)	5(3)
C(14)	47(3)	40(3)	48(4)	-7(3)	2(3)	14(3)
C(15)	42(3)	33(3)	63(4)	15(3)	6(3)	-4(2)
C(16)	29(3)	31(3)	35(3)	-4(3)	-9(3)	1(2)
C(17)	37(3)	65(4)	35(3)	2(3)	-4(3)	2(3)
C(18)	62(4)	72(5)	48(4)	11(4)	-18(4)	-13(4)
C(19)	90(5)	54(4)	47(4)	7(3)	-38(4)	-4(4)
C(20)	49(4)	49(4)	65(5)	-14(3)	-32(4)	0(3)
C(21)	44(3)	43(3)	44(4)	-13(3)	-12(3)	4(3)
O(5)	114(5)	58(4)	39(4)	0	0	-8(4)
C(23)	80(5)	52(4)	58(5)	2(4)	7(4)	-3(3)
C(22)	168(9)	61(5)	86(6)	-4(5)	26(6)	1(5)

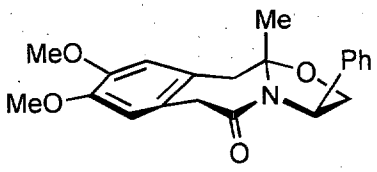

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	5327(4)	3332(3)	-69(5)	43
H(2B)	4959(4)	4180(3)	760(5)	43
H(4A)	3254(4)	4091(3)	1536(5)	42
H(7A)	3237(3)	850(3)	1155(4)	38
H(9A)	5095(4)	1731(3)	-441(5)	39
H(9B)	4835(4)	837(3)	345(5)	39
H(11A)	7903(3)	2193(3)	1000(5)	39
H(12A)	7770(4)	3667(3)	2681(5)	47
H(12B)	8306(4)	3678(3)	1381(5)	47
H(13A)	5051(4)	3046(4)	3136(5)	61
H(13B)	5404(4)	4112(4)	3026(5)	61
H(13C)	6200(4)	3337(4)	3473(5)	61
H(14A)	767(4)	4518(3)	2515(5)	68
H(14B)	1542(4)	4570(3)	1404(5)	68
H(14C)	1977(4)	4549(3)	2746(5)	68
H(15A)	804(4)	289(3)	2118(6)	69
H(15B)	2007(4)	271(3)	2399(6)	69
H(15C)	1614(4)	347(3)	1043(6)	69
H(17A)	6560(4)	1623(4)	3600(5)	55
H(18A)	7223(5)	834(5)	5260(6)	73
H(19A)	8971(6)	667(4)	5508(6)	76
H(20A)	10086(4)	1267(4)	4051(6)	65
H(21A)	9428(4)	2021(4)	2372(6)	53
H(23A)	3921(5)	274(4)	3353(6)	76
H(23B)	4869(5)	985(4)	3315(6)	76
H(22A)	3431(7)	1722(5)	4137(8)	158
H(22B)	4316(7)	1654(5)	5126(8)	158
H(22C)	3370(7)	944(5)	5165(8)	158

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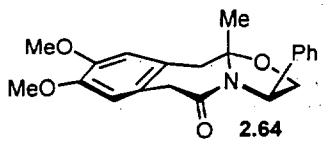
S22



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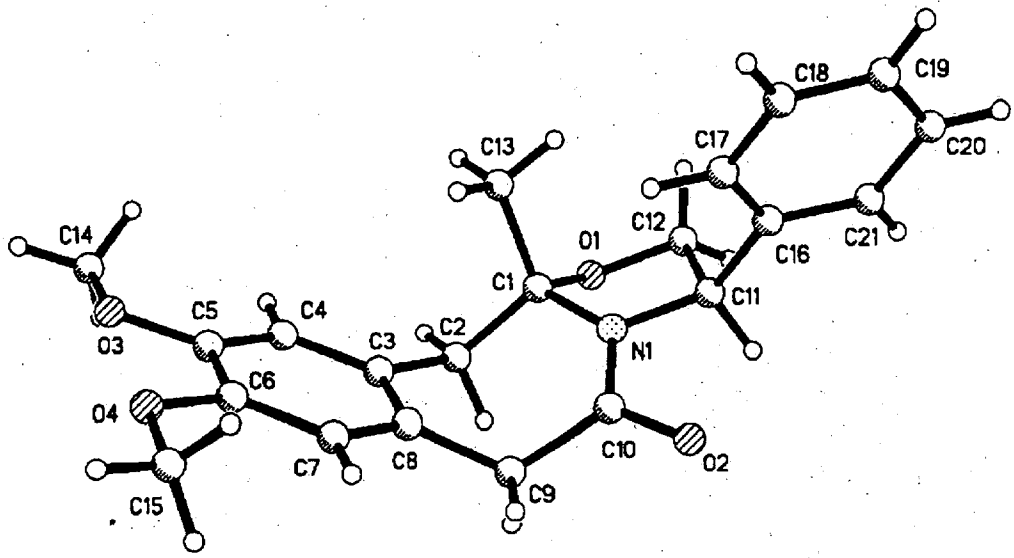

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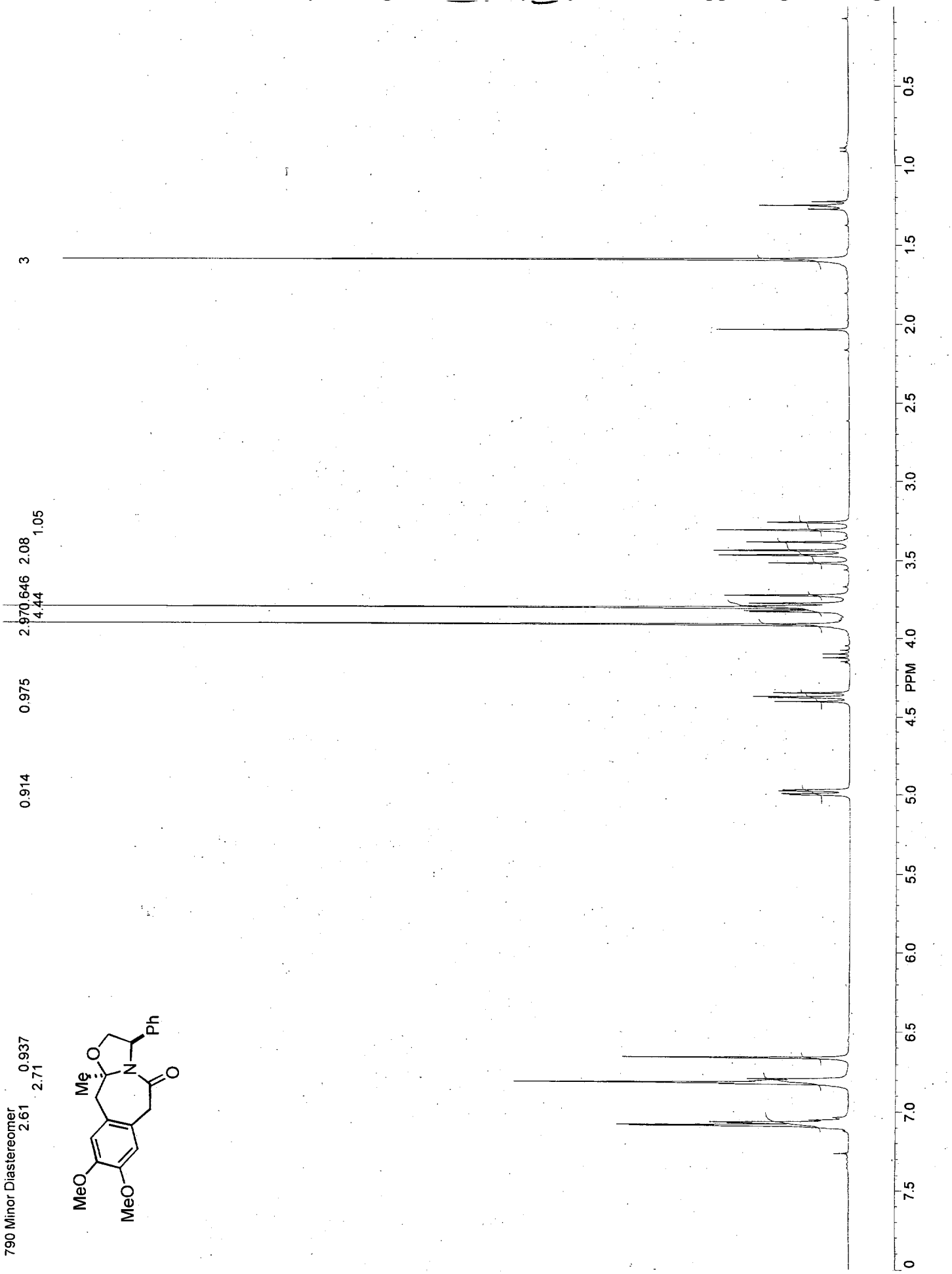

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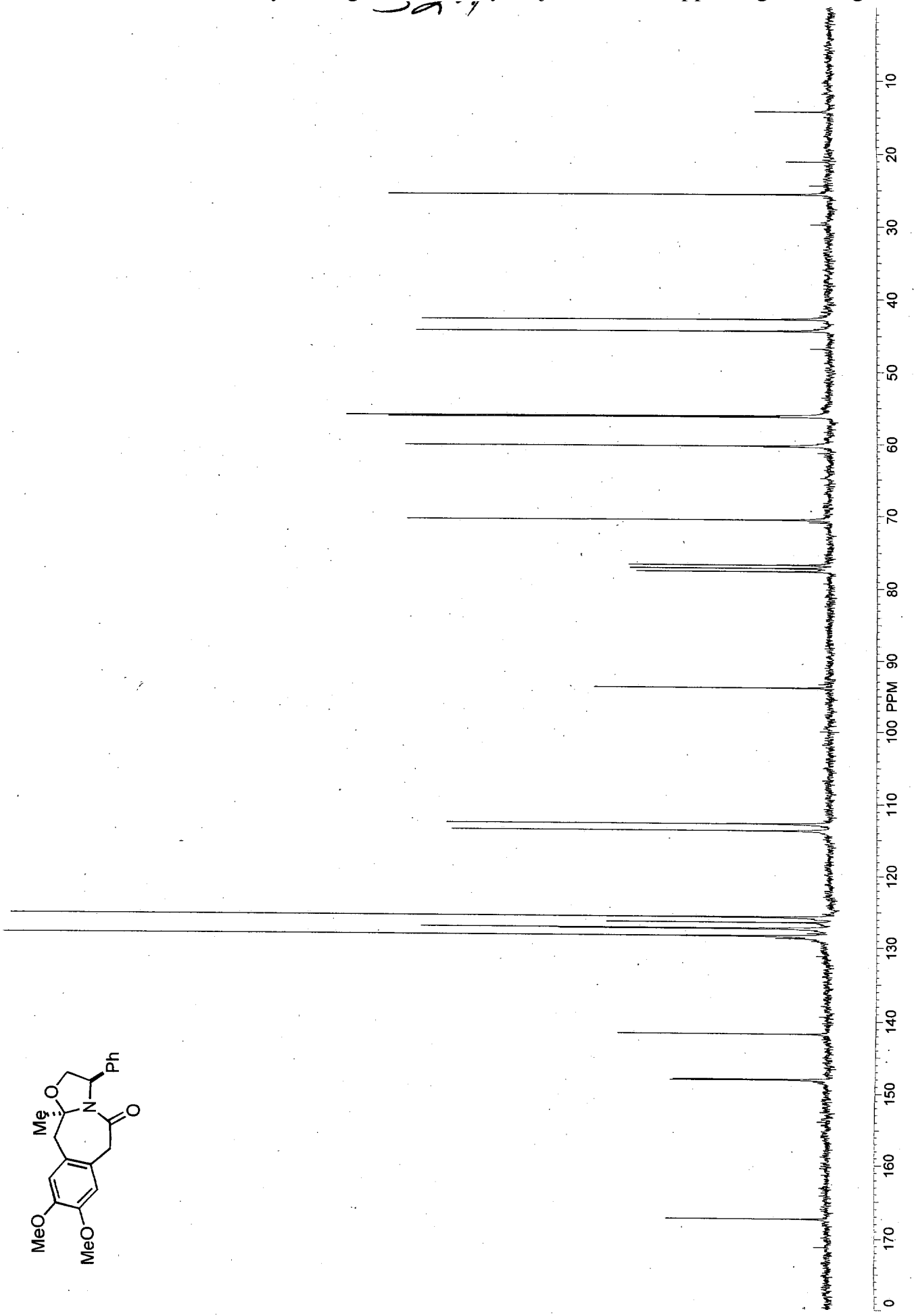

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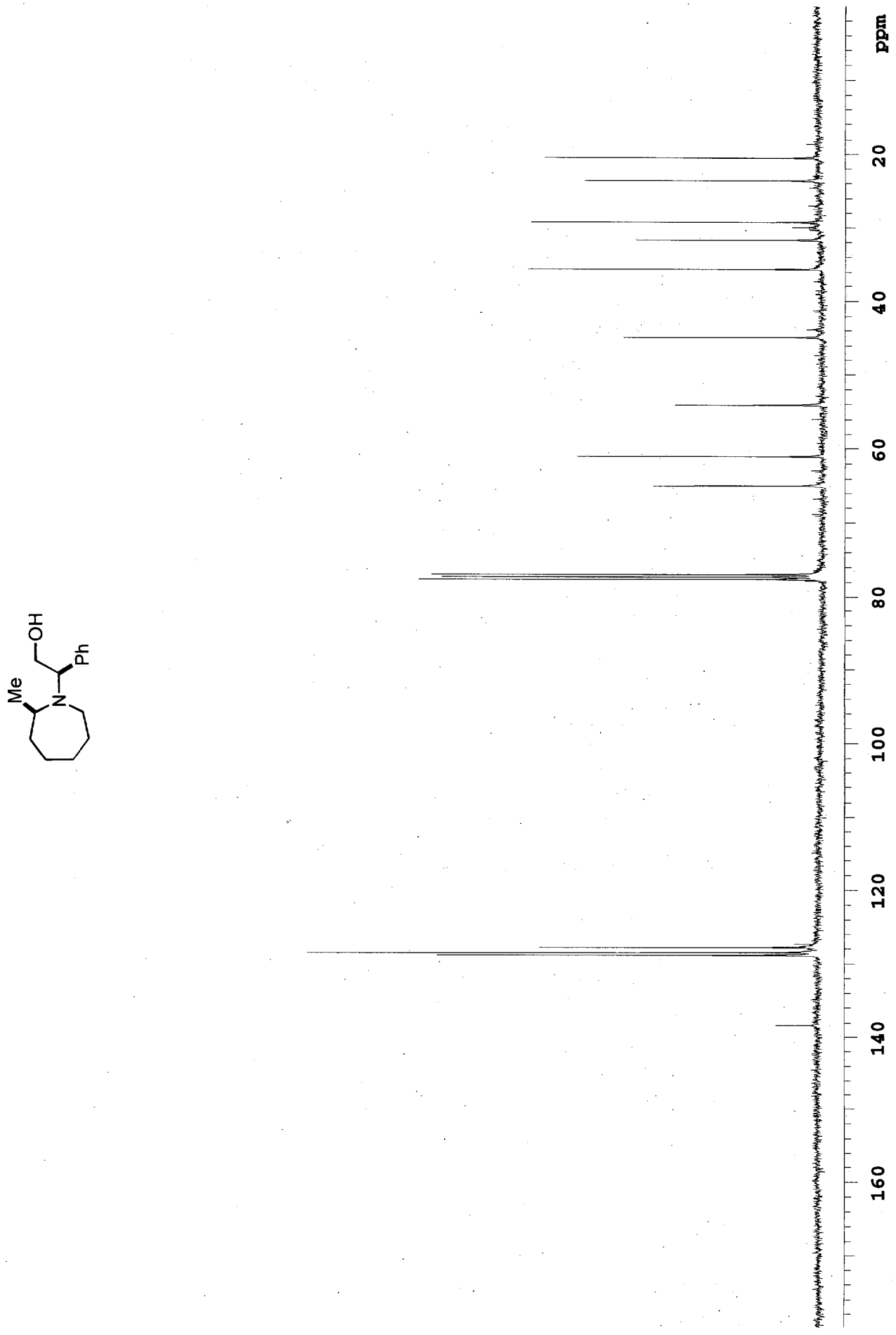

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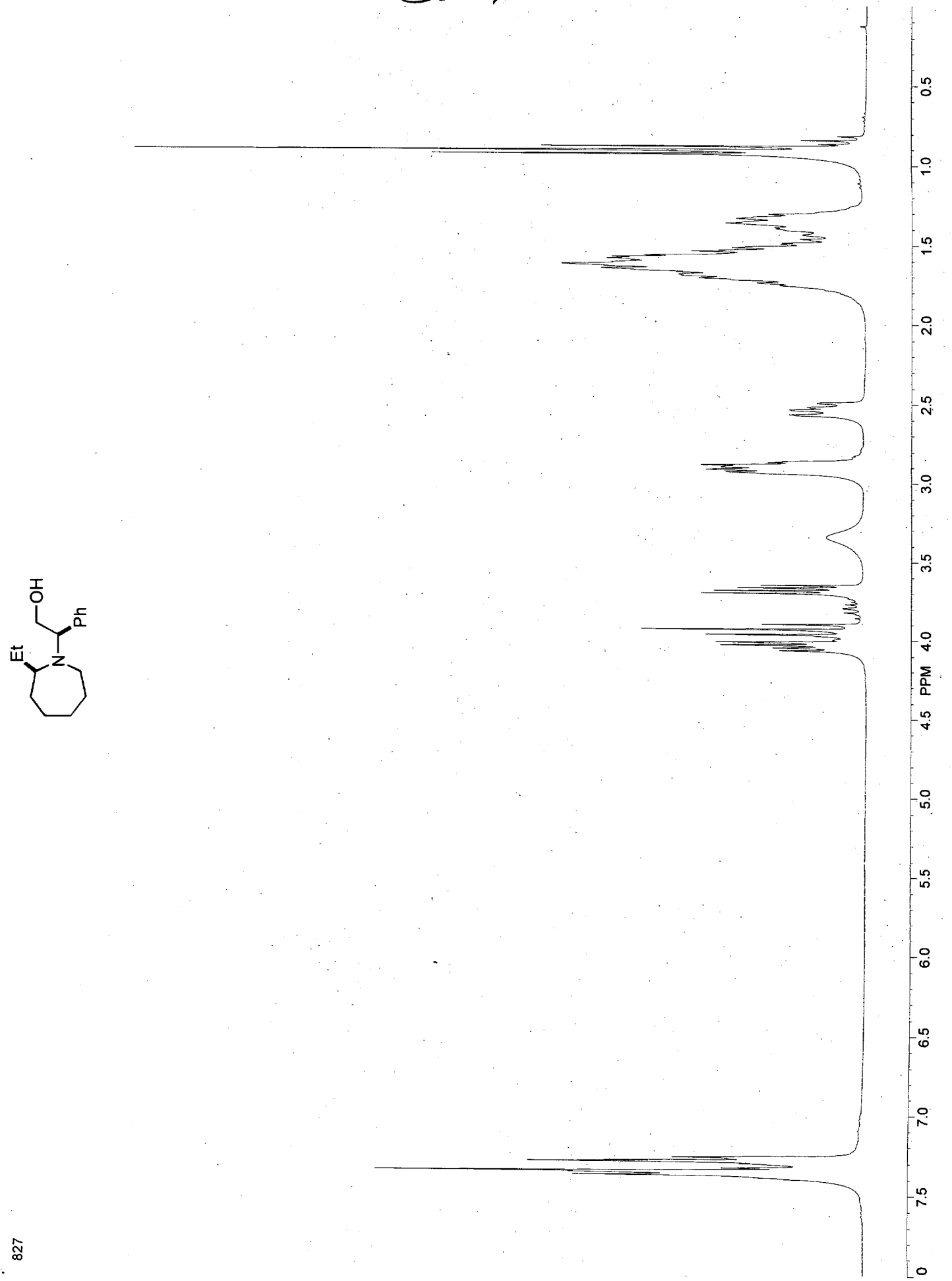

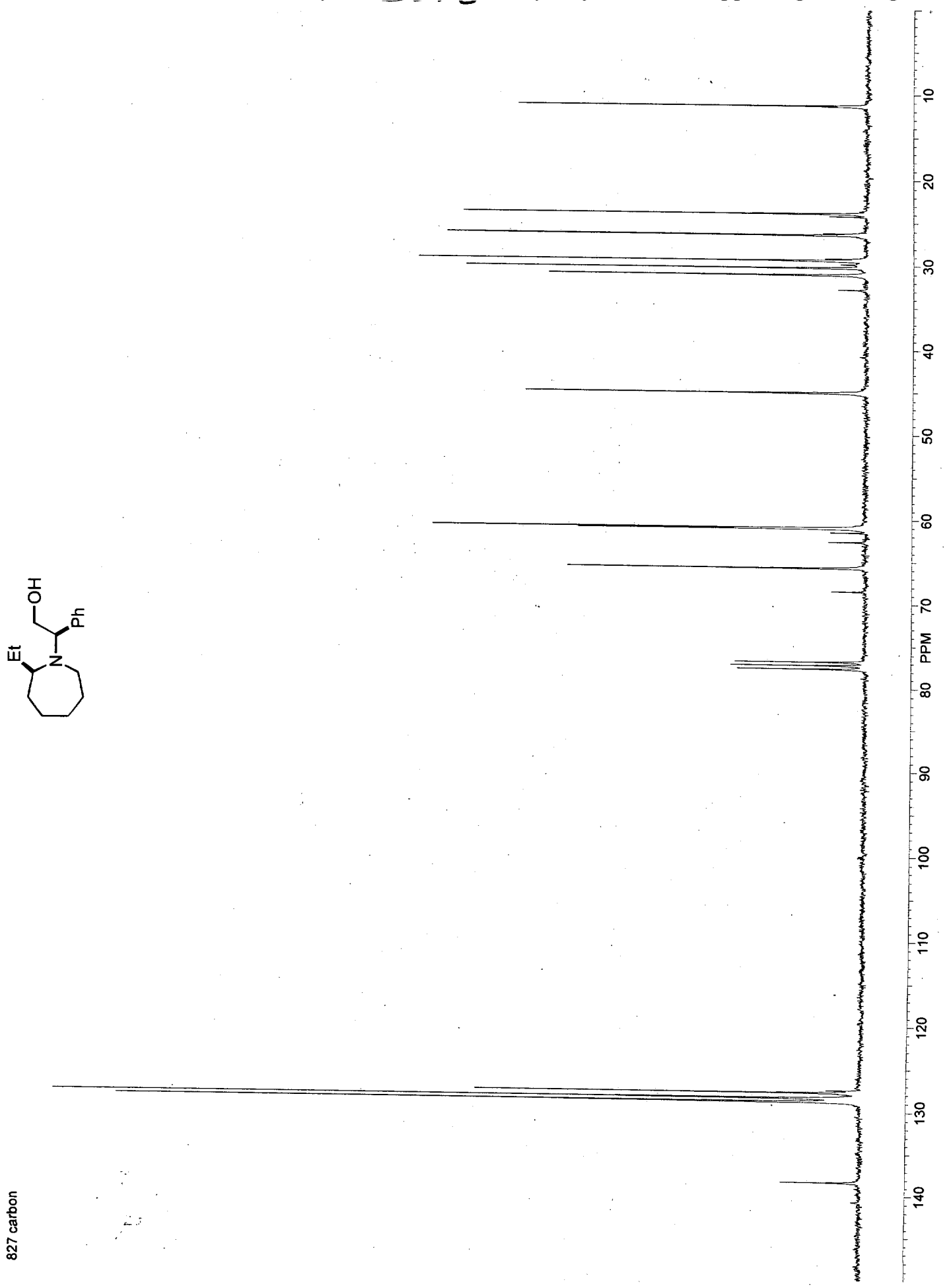
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100
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120
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140
PPM

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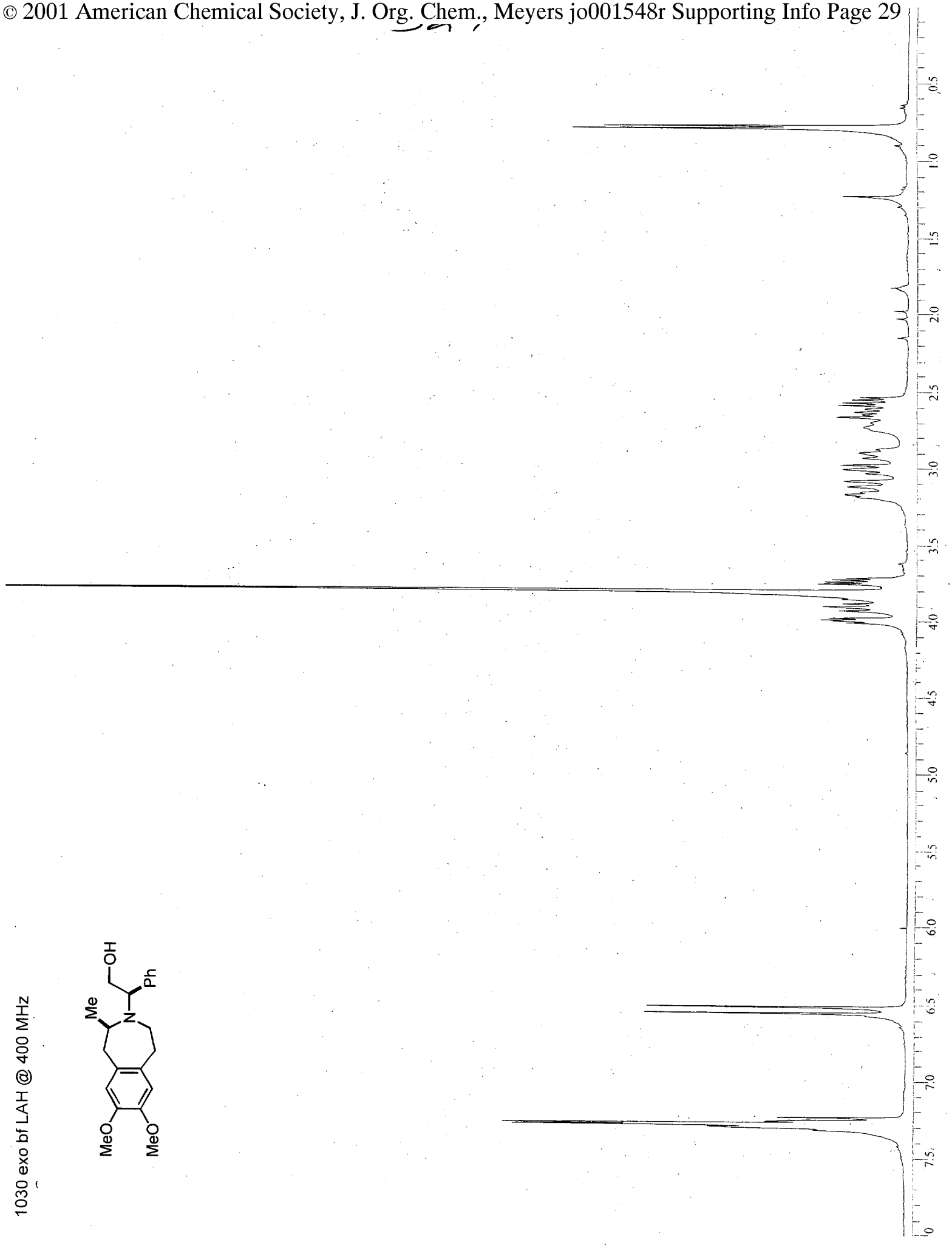

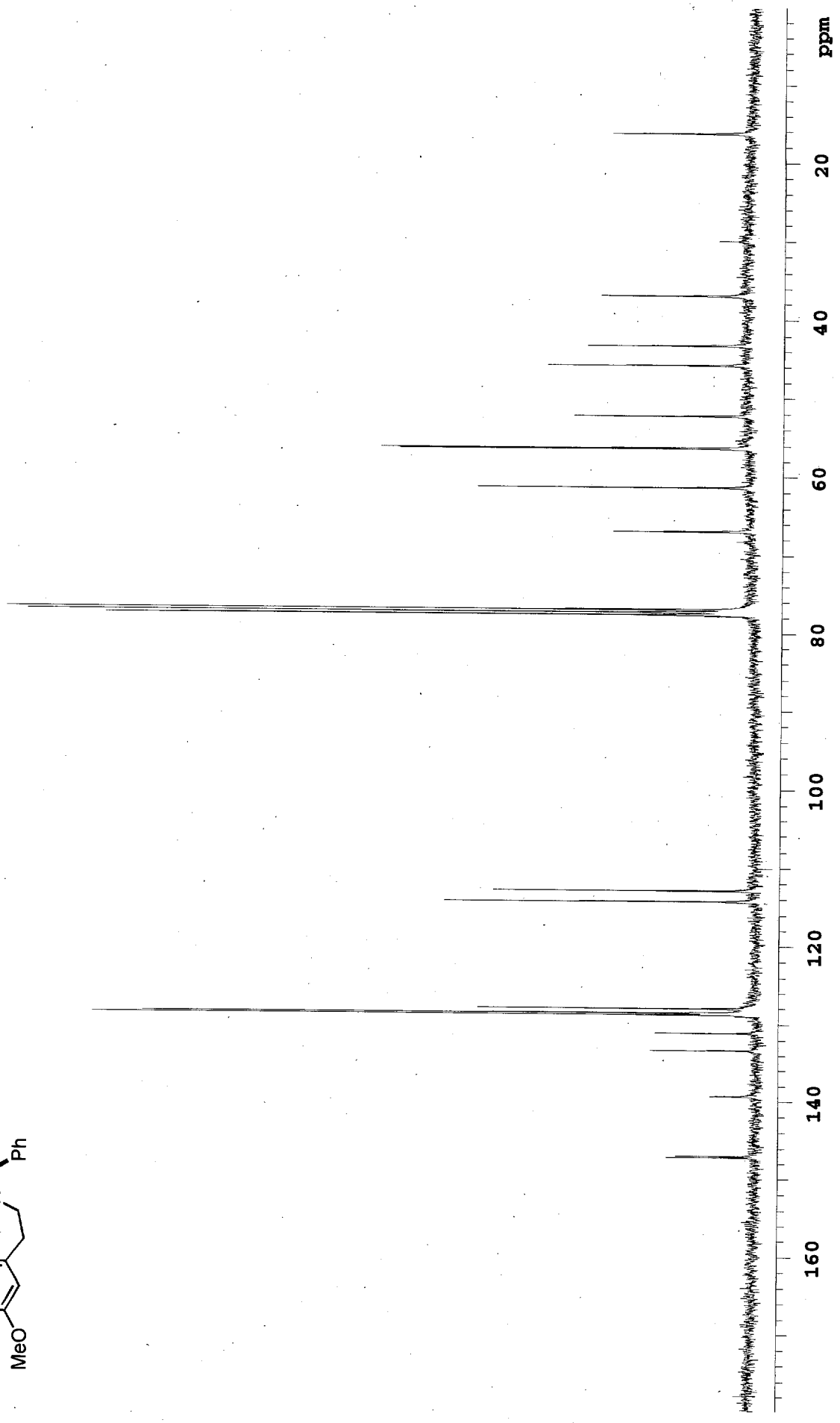
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Ph
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N
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MeO

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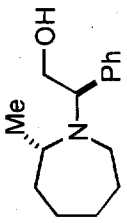

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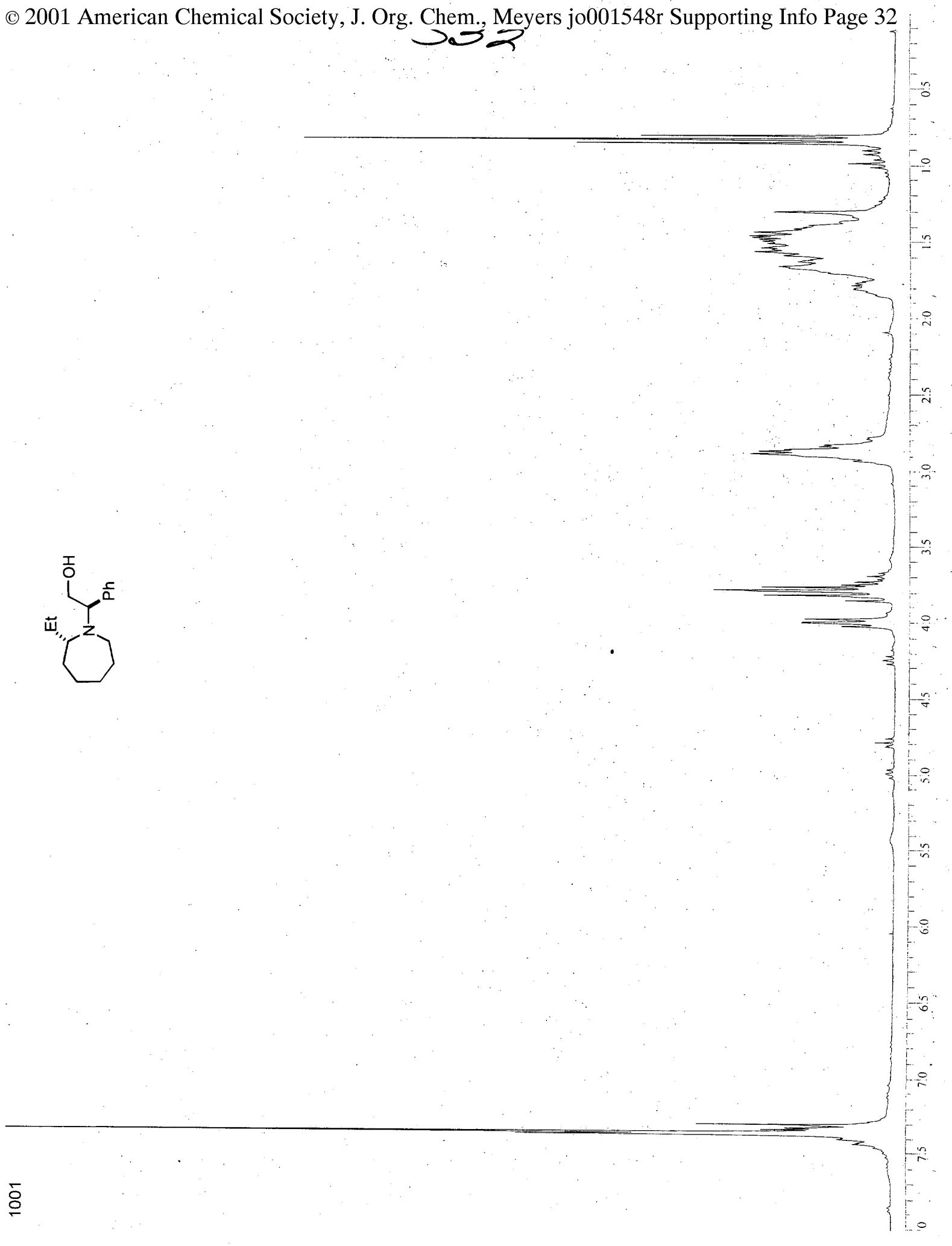

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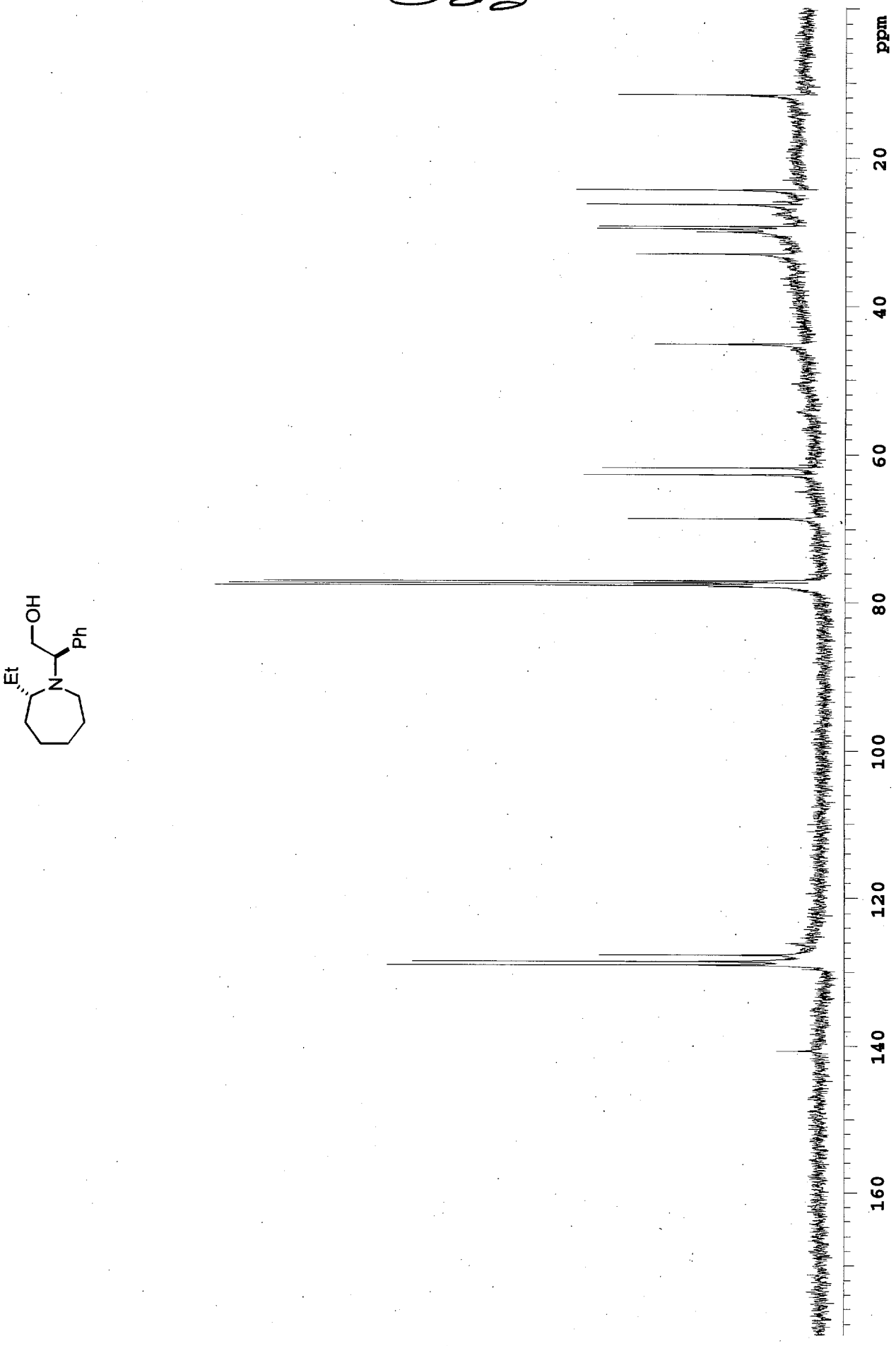

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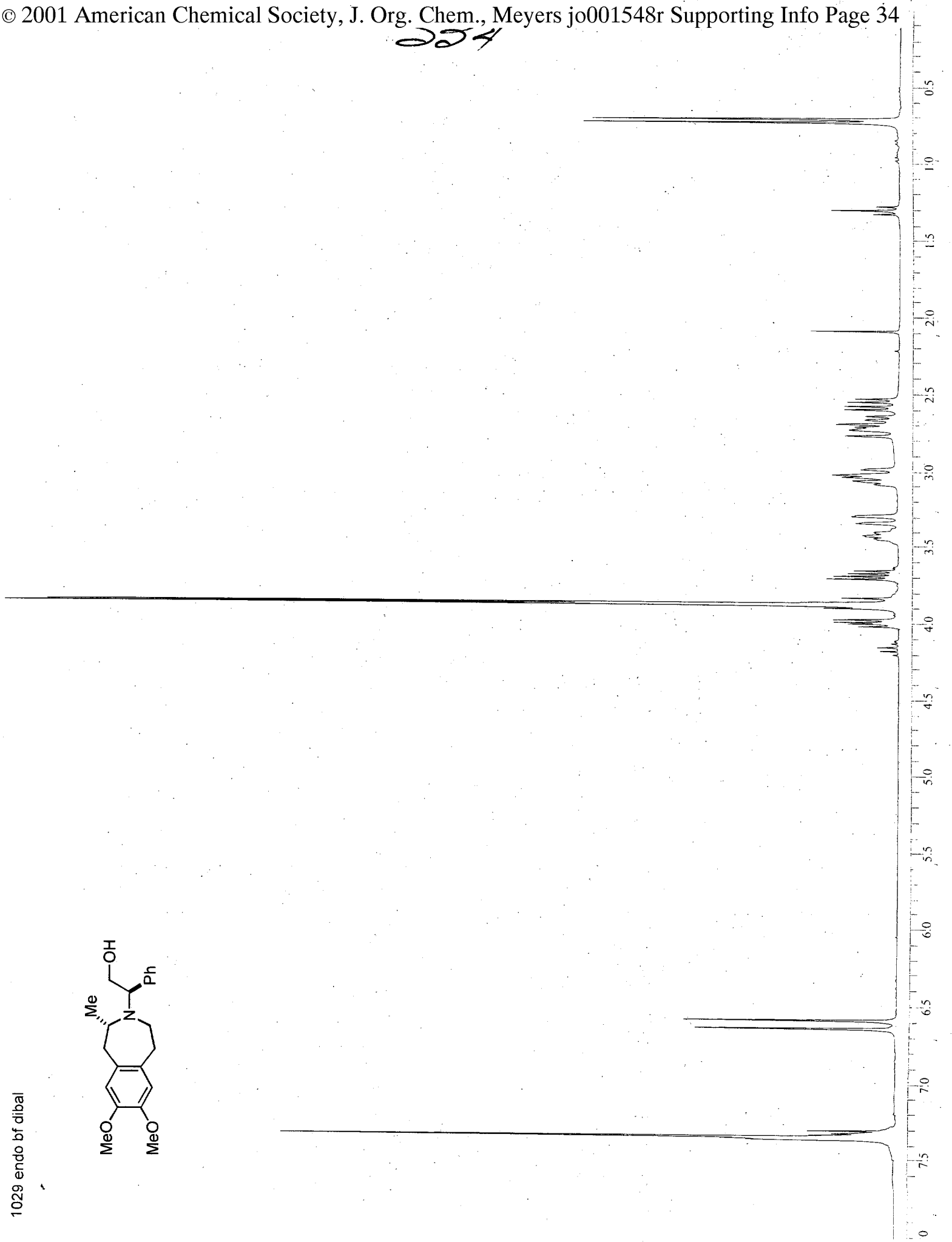

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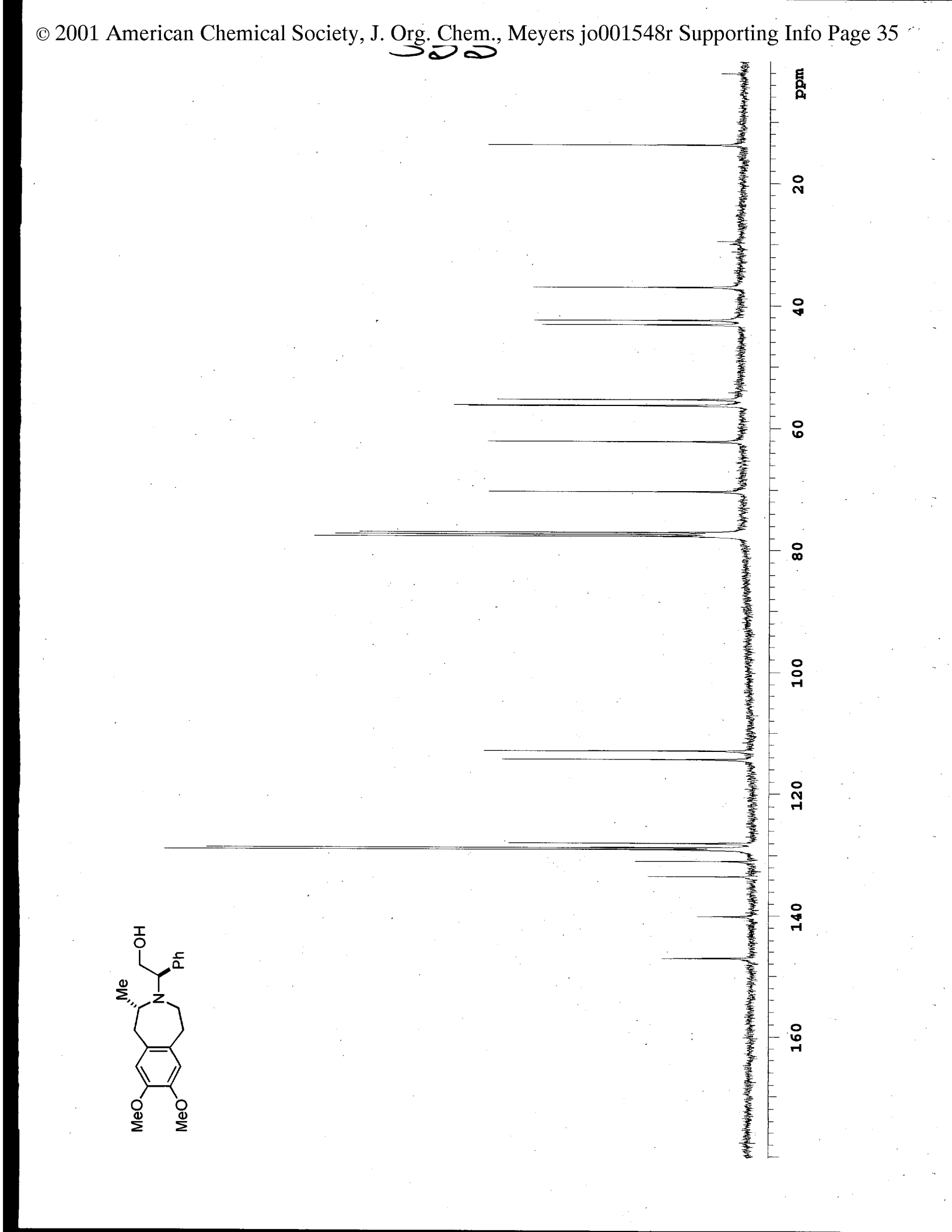

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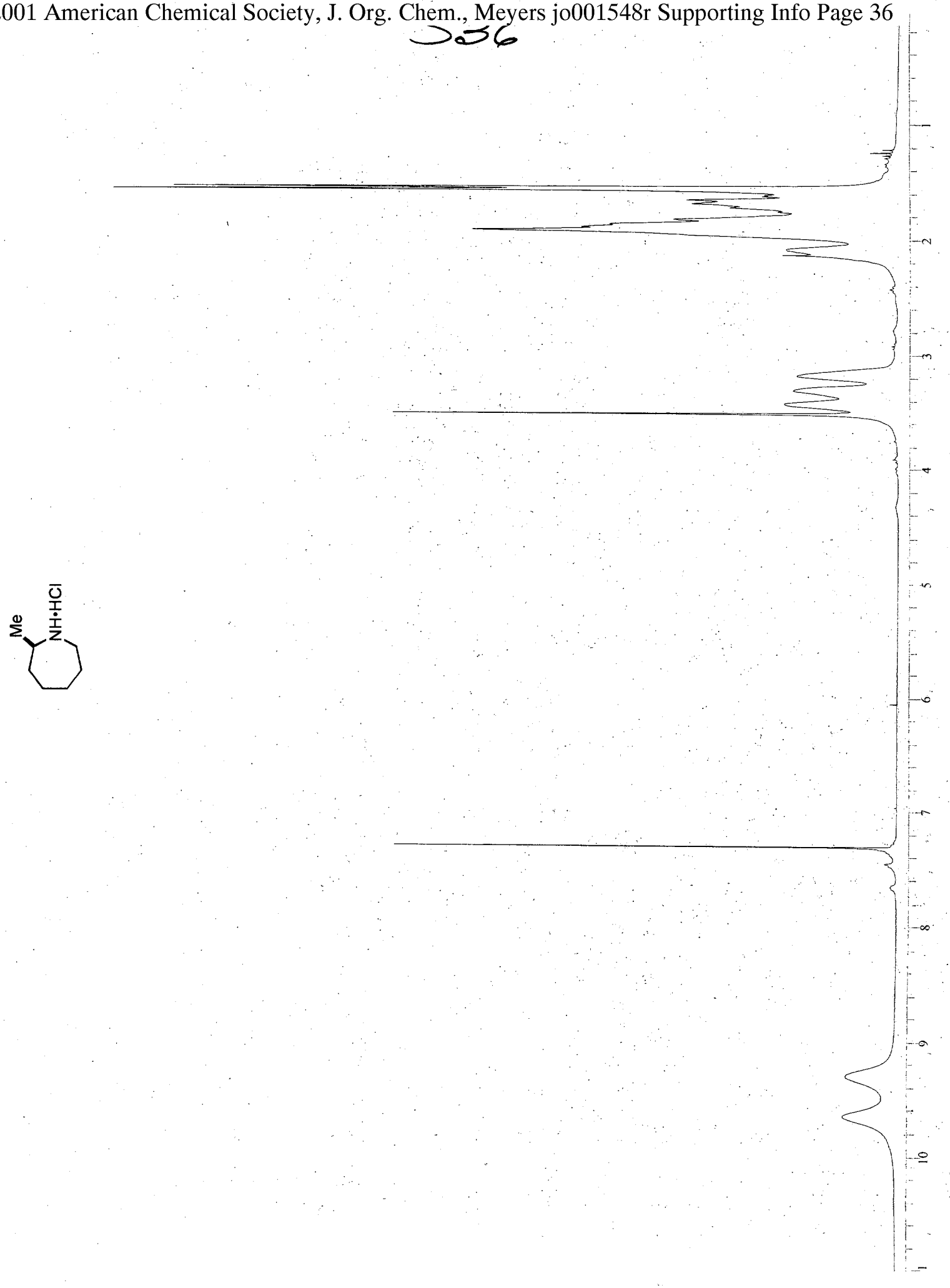

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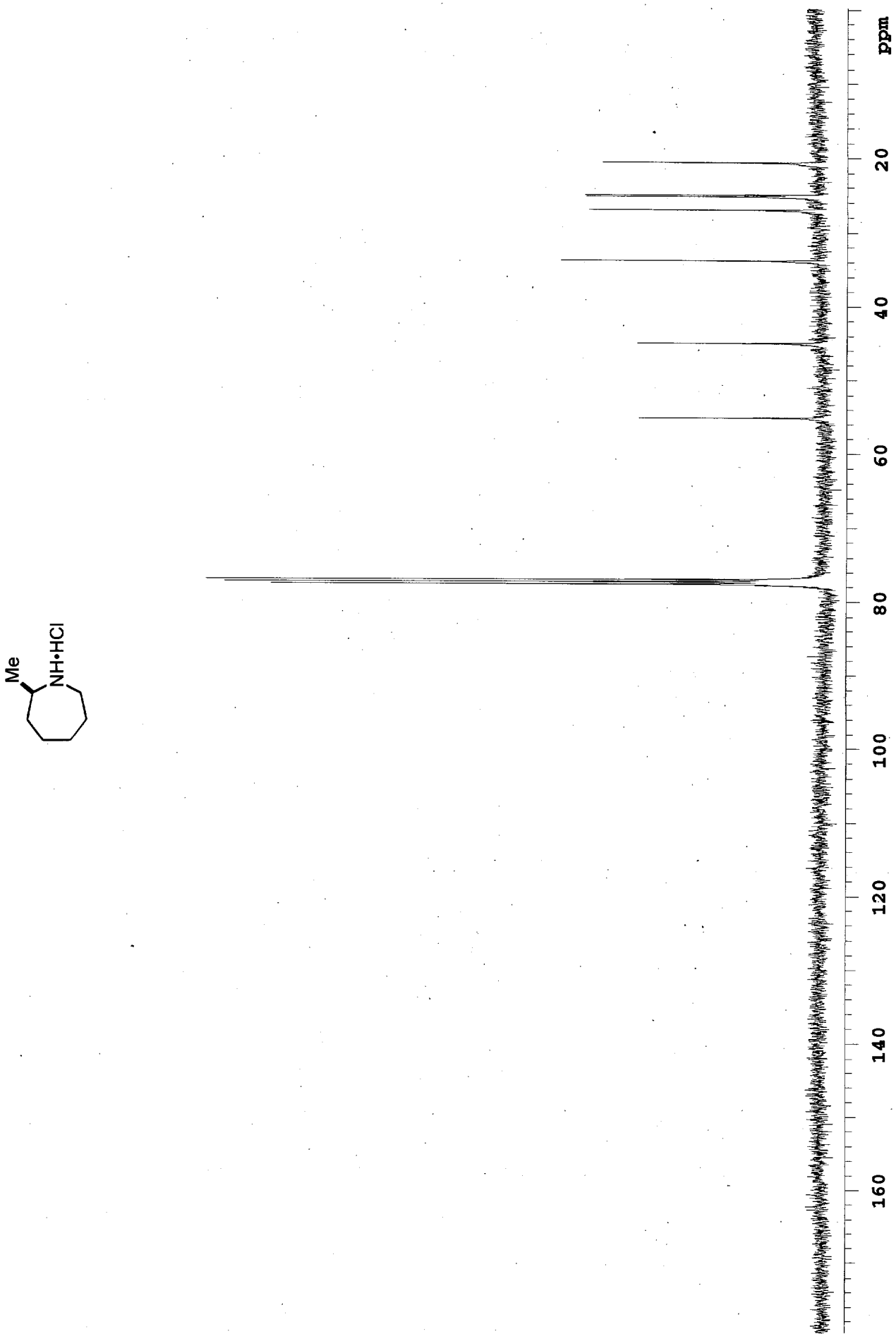

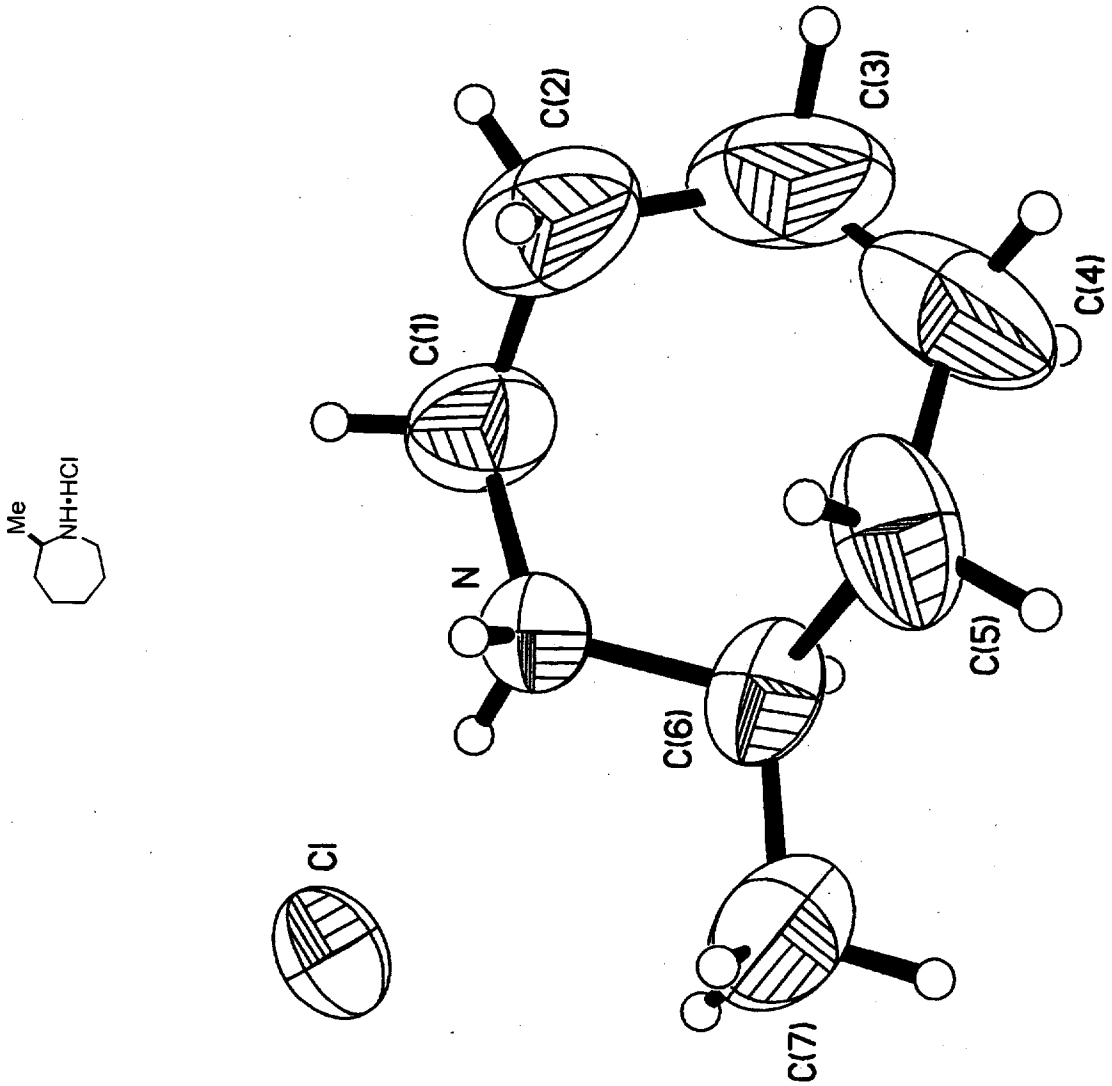
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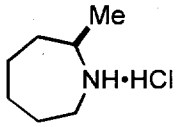
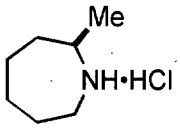
NH·HCl
C(1)
C(2)
C(3)
C(4)
C(5)
C(6)
C(7)
N
Cl

Table 1. Crystal data and structure refinement for 1.



Identification code	sadam23a
Empirical formula	$C_7H_{16}ClN$
Formula weight	149.66
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 7.4172(12) Å alpha = 90.000(4)°
	b = 7.3943(11) Å beta = 93.570(3)°
	c = 8.1849(13) Å gamma = 90.000(3)°
Volume, Z	448.03(12) Å^3, 2
Density (calculated)	1.109 Mg/m^3
Absorption coefficient	0.352 mm^{-1}
Absorption correction	SADABS
Transmission factors	0.809 - 0.978
F(000)	164
Crystal size	0.42 x 0.13 x 0.03 mm
θ range for data collection	2.49 to 28.19°
Limiting indices	$-9 \le h \le 9$, $-8 \le k \le 8$, $-10 \le l \le 6$
Reflections collected	2300
Independent reflections	1814 (R_{int} = 0.0615)
Completeness to θ = 28.19°	91.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1814 / 1 / 84
Goodness-of-fit on F^2	1.011
Final R indices [I>2σ(I)]	R1 = 0.0764, wR2 = 0.1228
R indices (all data)	R1 = 0.2006, wR2 = 0.1488



Absolute structure parameter	**0.00(19)**
Extinction coefficient	**0.030(8)**
Largest diff. peak and hole	**0.199 and -0.170 eÅ^{-3}**