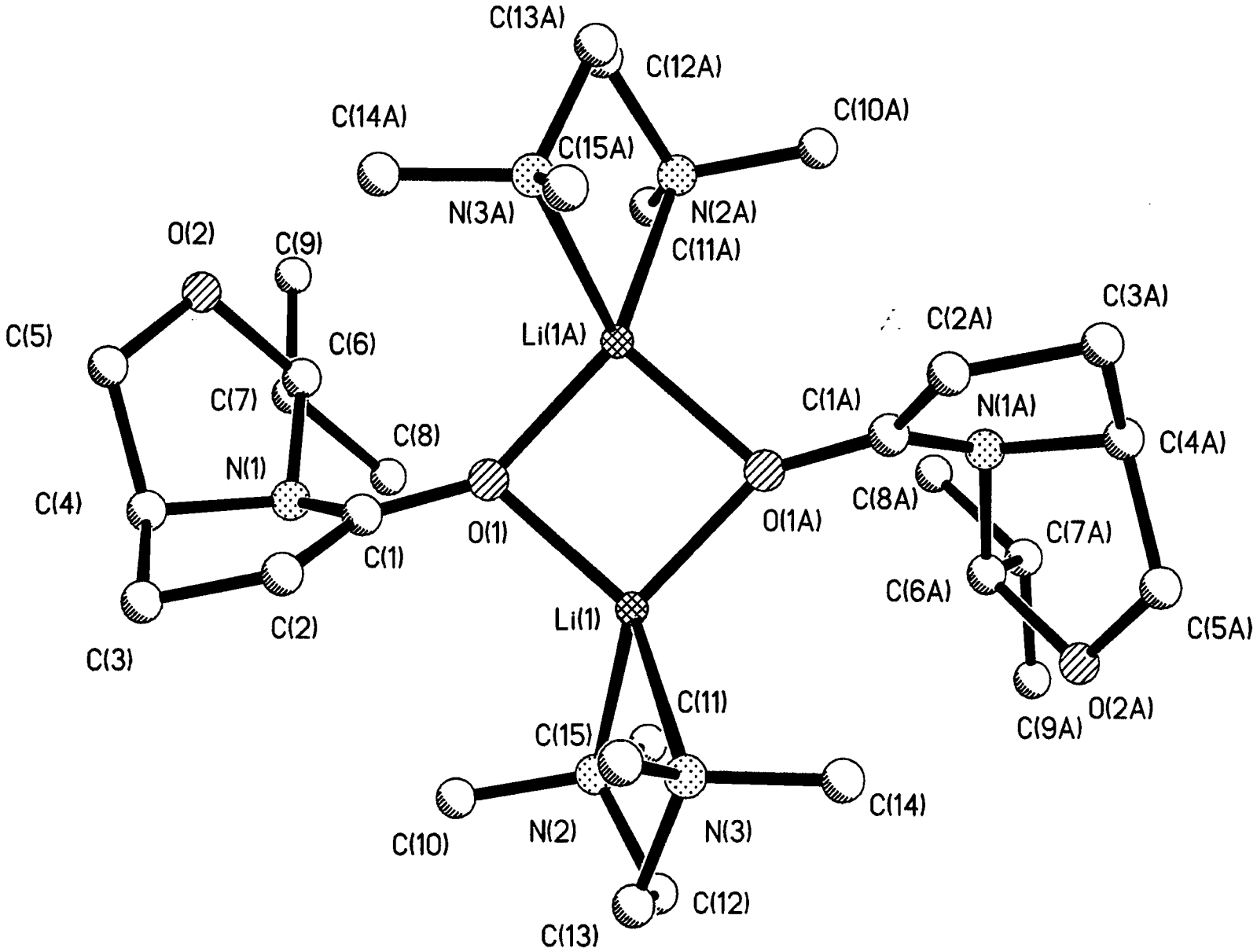
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(30), 7429-7438, DOI:10.1021/ja980614s



Material for footnote:

X-ray diffraction data were recorded at approx. -35° C on a Siemens P4 diffractometer. The structure solved routinely with SHELX direct methods and was refined utilizing full matrix lest squares on F^2. Crystallographic parameters are summarized as follows: crystallization from ?? solution in the non-centrosymmetric, monoclinic space group C2 with unit cell parameters a=18.849(4) A, b=8.893(3) A, c=11.076(3) A and β=105.54°. Of the 1330 reflections recorded, a total of 1260 independent reflections with Rint=0.0146 were utilized in refinement of 190 parameters. The final model resulted in the following statistical parameters: GOOF=1.156, R(all data) 0.0485 and wR2 (all data) 0.1382.

Table 1. Crystal data and structure refinement for 1.

Identification code	csu1
Empirical formula	$C_{15}H_{30}LiN_3O_2$
Formula weight	291.36
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	C2
Unit cell dimensions	a = 18.849(4) Å alpha = 90° b = 8.893(3) Å beta = 105.54(3)° c = 11.076(3) Å gamma = 90°
Volume, Z	1788.7(9) $Å^3$, 4
Density (calculated)	1.082 Mg/m^3
Absorption coefficient	0.071 mm^{-1}
F(000)	640
Crystal size	? x ? x ? mm
θ range for data collection	2.24 to 22.53°
Limiting indices	$-20 \le h \le 19$, $0 \le k \le 9$, $0 \le l \le 11$
Reflections collected	1330
Independent reflections	1260 (R_{int} = 0.0146)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1260 / 1 / 190
Goodness-of-fit on F^2	1.156
Final R indices [I>2σ(I)]	R1 = 0.0438, wR2 = 0.1332
R indices (all data)	R1 = 0.0485, wR2 = 0.1382
Absolute structure parameter	1(3)
Largest diff. peak and hole	0.172 and -0.192 $eÅ^{-3}$

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)	578(1)	196(4)	6066(2)	31(1)
O(2)	1154(2)	-735(5)	9497(3)	45(1)
N(1)	1548(2)	-732(5)	7691(3)	30(1)
N(2)	1285(2)	-970(5)	3819(3)	35(1)
N(3)	725(2)	2000(5)	3044(4)	34(1)
C(1)	1206(2)	475(6)	6867(4)	30(1)
C(2)	1640(3)	1689(6)	7045(4)	39(1)
C(3)	2331(3)	1405(8)	8049(5)	52(2)
C(4)	2132(2)	8(7)	8703(4)	41(1)
C(5)	1742(2)	296(8)	9684(4)	47(1)
C(6)	1097(2)	-1529(6)	8349(4)	32(1)
C(7)	1321(3)	-3141(6)	8625(5)	44(1)
C(8)	1258(4)	-4006(8)	7415(6)	64(2)
C(9)	877(3)	-3901(8)	9389(6)	63(2)
C(10)	1969(3)	-996(9)	4834(5)	54(2)
C(11)	1046(3)	-2530(7)	3583(6)	56(2)
C(12)	1407(3)	-257(7)	2711(5)	48(2)
C(13)	1412(3)	1429(7)	2835(6)	48(1)
C(14)	134(3)	2021(7)	1871(5)	53(2)
C(15)	828(4)	3518(7)	3544(6)	60(2)
Li(1)	448(4)	361(9)	4291(6)	30(2)

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

O(1)-C(1)	1.300(5)	O(1)-Li(1)#1	1.873(7)
O(1)-Li(1)	1.920(7)	O(2)-C(5)	1.411(6)
O(2)-C(6)	1.434(6)	N(1)-C(6)	1.445(6)
N(1)-C(1)	1.443(6)	N(1)-C(4)	1.497(6)
N(2)-C(12)	1.453(7)	N(2)-C(11)	1.460(8)
N(2)-C(10)	1.466(6)	N(2)-Li(1)	2.146(8)
N(3)-C(15)	1.452(7)	N(3)-C(13)	1.465(7)
N(3)-C(14)	1.468(6)	N(3)-Li(1)	2.166(8)
C(1)-C(2)	1.337(7)	C(2)-C(3)	1.490(7)
C(3)-C(4)	1.534(8)	C(4)-C(5)	1.488(7)
C(6)-C(7)	1.503(7)	C(7)-C(9)	1.501(8)
C(7)-C(8)	1.523(8)	C(12)-C(13)	1.505(9)
Li(1)-O(1)#1	1.873(7)	Li(1)-Li(1)#1	2.597(13)

C(1)-O(1)-Li(1)#1	146.0(3)	C(1)-O(1)-Li(1)	121.9(3)
Li(1)#1-O(1)-Li(1)	86.4(3)	C(5)-O(2)-C(6)	108.6(3)
C(6)-N(1)-C(1)	117.5(3)	C(6)-N(1)-C(4)	104.6(3)
C(1)-N(1)-C(4)	105.1(4)	C(12)-N(2)-C(11)	112.0(4)
C(12)-N(2)-C(10)	110.4(4)	C(11)-N(2)-C(10)	106.8(5)
C(12)-N(2)-Li(1)	104.9(4)	C(11)-N(2)-Li(1)	110.8(4)
C(10)-N(2)-Li(1)	112.0(3)	C(15)-N(3)-C(13)	110.4(5)
C(15)-N(3)-C(14)	108.5(4)	C(13)-N(3)-C(14)	111.0(4)
C(15)-N(3)-Li(1)	114.4(4)	C(13)-N(3)-Li(1)	104.0(4)
C(14)-N(3)-Li(1)	108.5(4)	O(1)-C(1)-C(2)	131.6(5)
O(1)-C(1)-N(1)	117.4(4)	C(2)-C(1)-N(1)	110.9(4)
C(1)-C(2)-C(3)	110.5(5)	C(2)-C(3)-C(4)	102.4(4)
N(1)-C(4)-C(5)	102.4(3)	N(1)-C(4)-C(3)	103.1(3)
C(5)-C(4)-C(3)	115.8(5)	O(2)-C(5)-C(4)	107.7(4)
O(2)-C(6)-N(1)	107.0(4)	O(2)-C(6)-C(7)	109.8(4)
N(1)-C(6)-C(7)	113.6(4)	C(6)-C(7)-C(9)	112.1(5)
C(6)-C(7)-C(8)	110.6(4)	C(9)-C(7)-C(8)	110.2(5)
N(2)-C(12)-C(13)	110.9(5)	N(3)-C(13)-C(12)	112.1(5)
O(1)#1-Li(1)-O(1)	92.9(3)	O(1)#1-Li(1)-N(2)	133.7(4)
O(1)-Li(1)-N(2)	107.9(3)	O(1)#1-Li(1)-N(3)	109.3(3)
O(1)-Li(1)-N(3)	135.9(4)	N(2)-Li(1)-N(3)	84.1(3)
O(1)#1-Li(1)-Li(1)#1	47.6(2)	O(1)-Li(1)-Li(1)#1	46.0(2)
N(2)-Li(1)-Li(1)#1	141.9(3)	N(3)-Li(1)-Li(1)#1	133.8(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1

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)	22(2)	48(2)	17(1)	-2(2)	-2(1)	2(2)
O(2)	39(2)	59(3)	39(2)	-6(2)	13(2)	-15(2)
N(1)	22(2)	48(3)	13(2)	3(2)	-3(2)	-3(2)
N(2)	36(2)	40(3)	31(2)	-4(2)	13(2)	4(2)
N(3)	34(2)	34(2)	33(2)	2(2)	6(2)	-2(2)
C(1)	31(2)	41(3)	19(2)	-1(2)	8(2)	1(2)
C(2)	47(3)	45(3)	24(2)	1(2)	8(2)	-10(3)
C(3)	48(3)	74(4)	30(3)	-1(3)	5(2)	-29(3)
C(4)	25(2)	67(4)	25(2)	6(3)	-3(2)	-11(3)
C(5)	36(3)	63(4)	35(3)	2(3)	-1(2)	-18(3)
C(6)	23(2)	43(3)	29(2)	1(2)	2(2)	-4(2)
C(7)	35(3)	46(3)	44(3)	13(3)	0(2)	0(2)
C(8)	81(4)	44(4)	62(4)	-3(3)	10(3)	5(3)
C(9)	46(3)	55(4)	77(4)	27(3)	-3(3)	-9(3)
C(10)	40(3)	76(4)	45(3)	-1(3)	8(2)	15(3)
C(11)	49(4)	50(4)	74(4)	1(3)	24(3)	3(3)
C(12)	55(3)	57(4)	41(3)	4(3)	27(3)	12(3)
C(13)	47(3)	52(4)	53(3)	12(3)	26(3)	0(3)
C(14)	51(3)	65(4)	36(3)	13(3)	2(3)	-5(3)
C(15)	66(4)	45(4)	62(4)	0(3)	7(3)	6(3)
Li(1)	27(3)	33(4)	29(4)	1(4)	6(3)	2(4)

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

	x	y	z	U(eq)
H(2)	1526(3)	2586(6)	6604(4)	44
H(3A)	2452(3)	2249(8)	8622(5)	67
H(3B)	2741(3)	1207(8)	7699(5)	67
H(4)	2559(2)	-653(7)	9011(4)	53
H(5A)	2077(2)	161(8)	10511(4)	61
H(5B)	1557(2)	1319(8)	9618(4)	61
H(6)	584(2)	-1500(6)	7843(4)	45
H(7)	1839(3)	-3155(6)	9111(5)	52
H(8A)	1402(4)	-5032(8)	7608(6)	80
H(8B)	1574(4)	-3556(8)	6965(6)	80
H(8C)	757(4)	-3975(8)	6908(6)	80
H(9A)	1036(3)	-4925(8)	9544(6)	80
H(9B)	366(3)	-3880(8)	8939(6)	80
H(9C)	946(3)	-3384(8)	10173(6)	80
H(10A)	1881(3)	-1471(9)	5558(5)	75
H(10B)	2137(3)	15(9)	5040(5)	75
H(10C)	2338(3)	-1548(9)	4568(5)	75
H(11A)	971(3)	-2960(7)	4335(6)	73
H(11B)	1416(3)	-3093(7)	3329(6)	73
H(11C)	593(3)	-2562(7)	2931(6)	73
H(12A)	1021(3)	-555(7)	1980(5)	63
H(12B)	1874(3)	-590(7)	2595(5)	63
H(13A)	1821(3)	1727(7)	3531(6)	59
H(13B)	1484(3)	1876(7)	2079(6)	59
H(14A)	59(3)	1024(7)	1529(5)	70
H(14B)	268(3)	2681(7)	1282(5)	70
H(14C)	-313(3)	2373(7)	2035(5)	70
H(15A)	374(4)	3876(7)	3675(6)	73
H(15B)	975(4)	4164(7)	2960(6)	73
H(15C)	1203(4)	3516(7)	4326(6)	73

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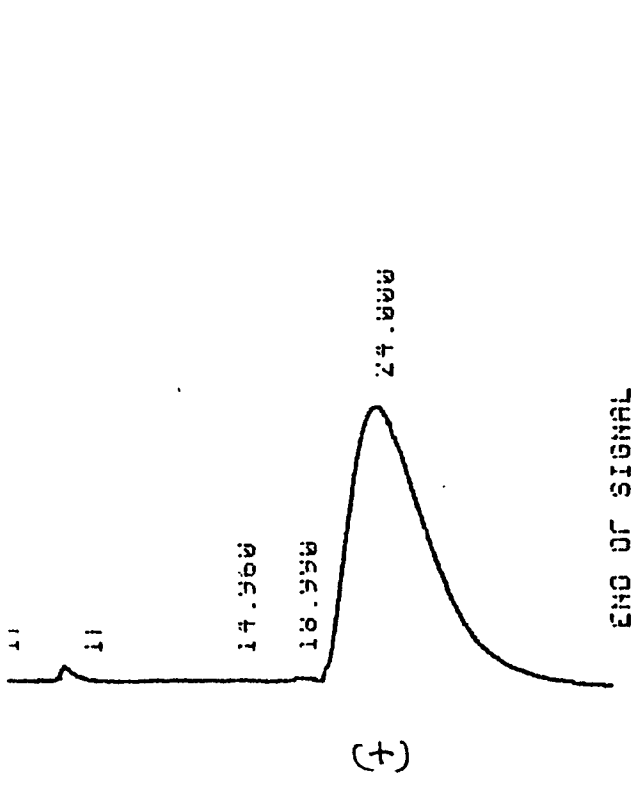

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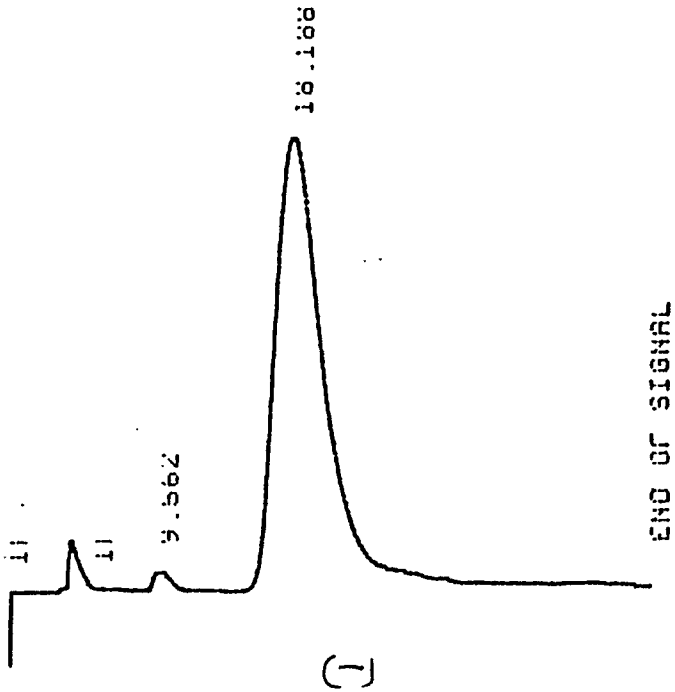

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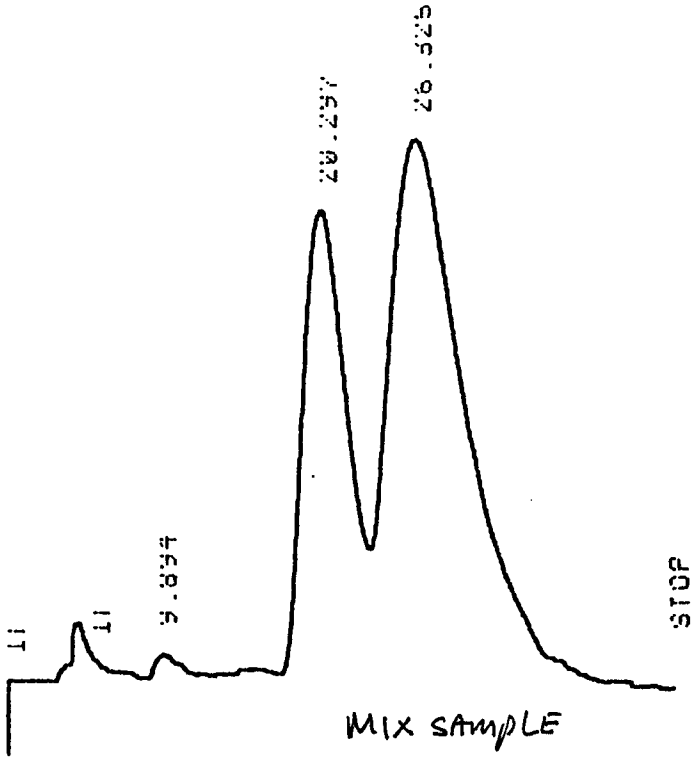

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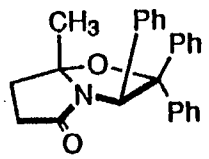

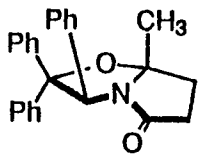

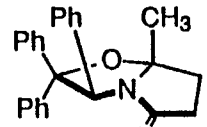

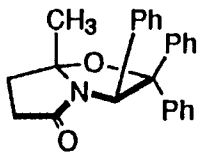

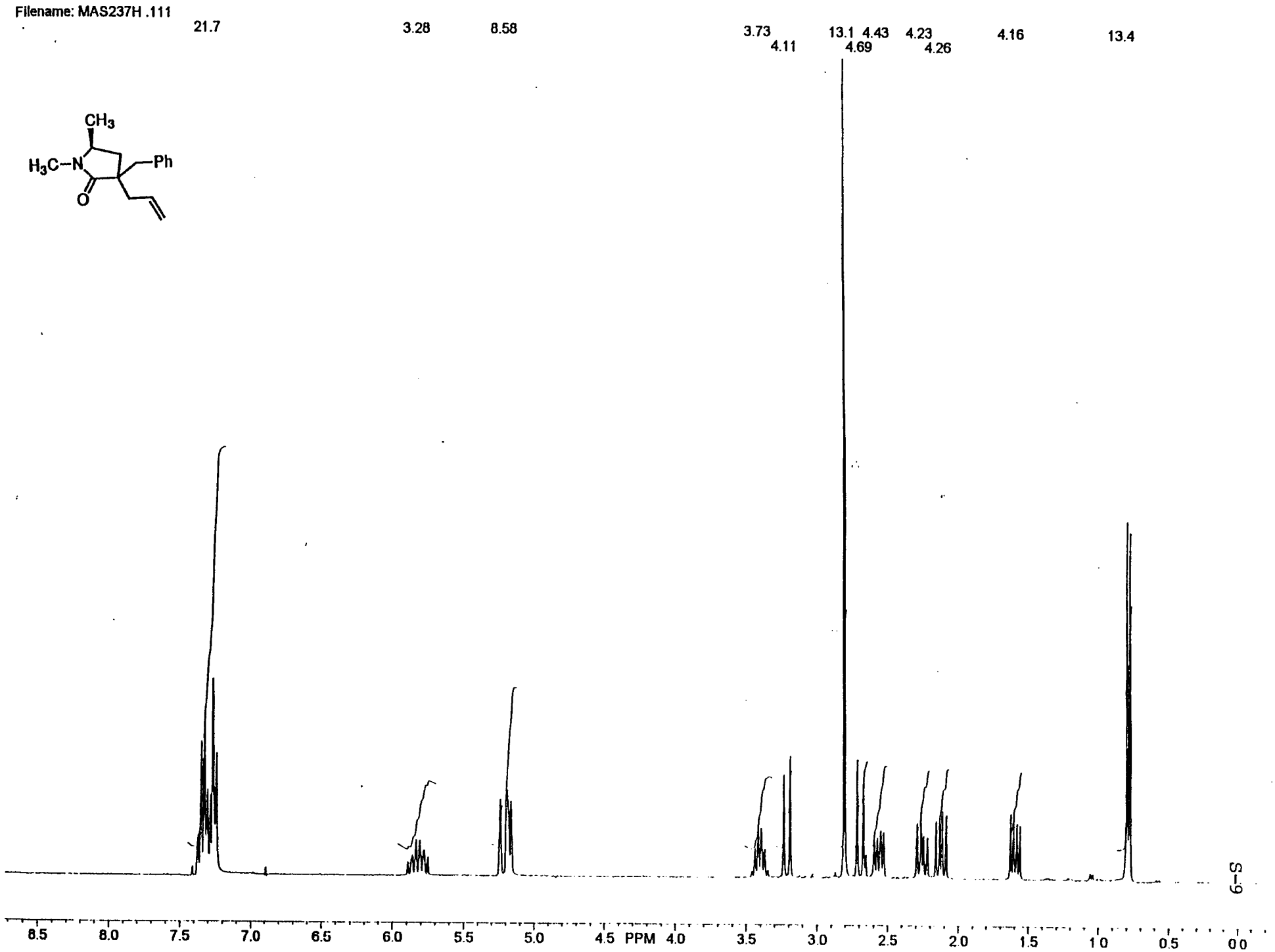

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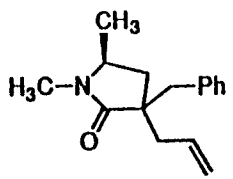

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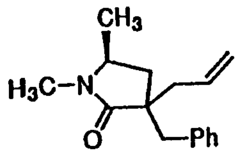

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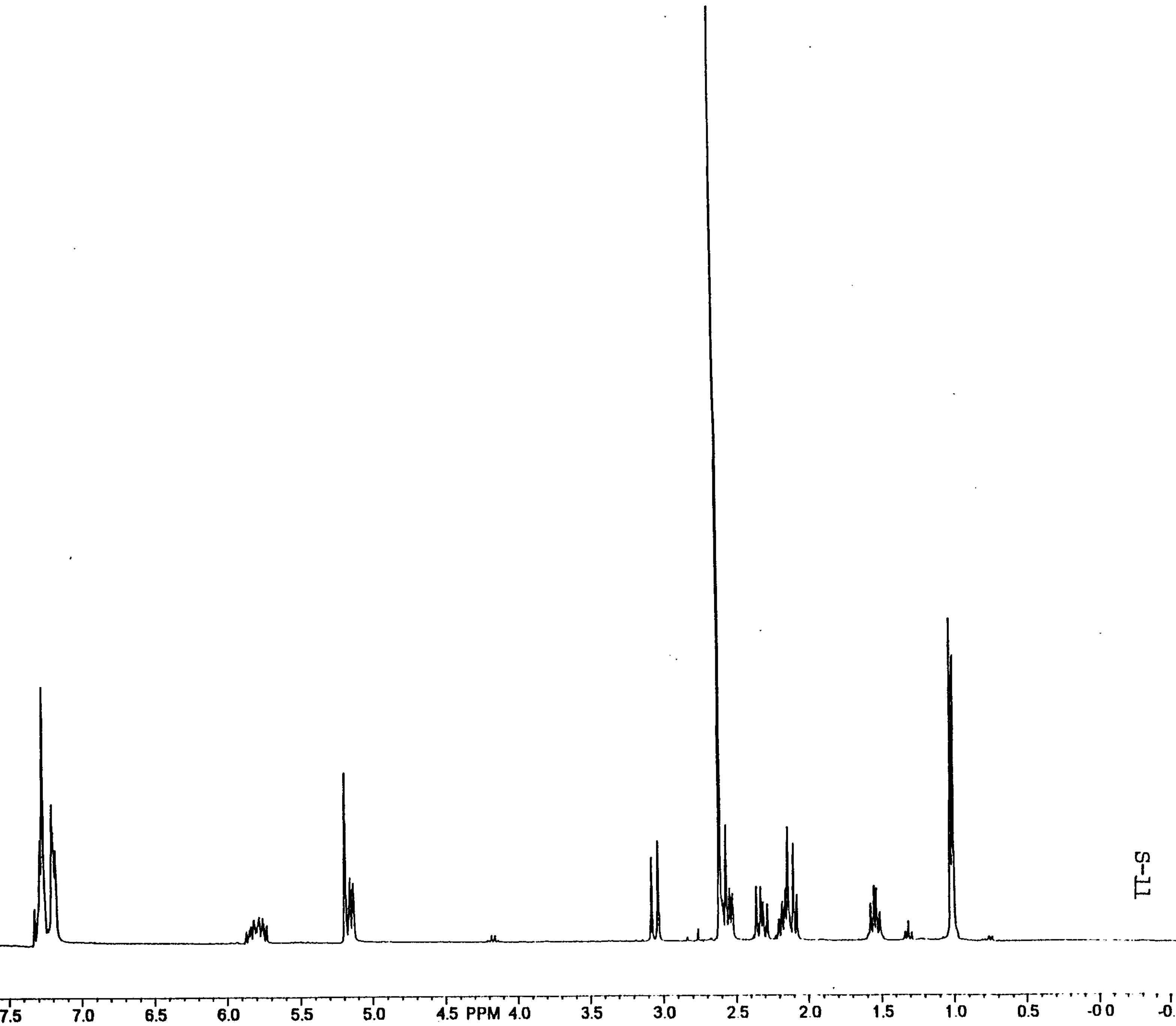

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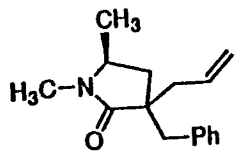

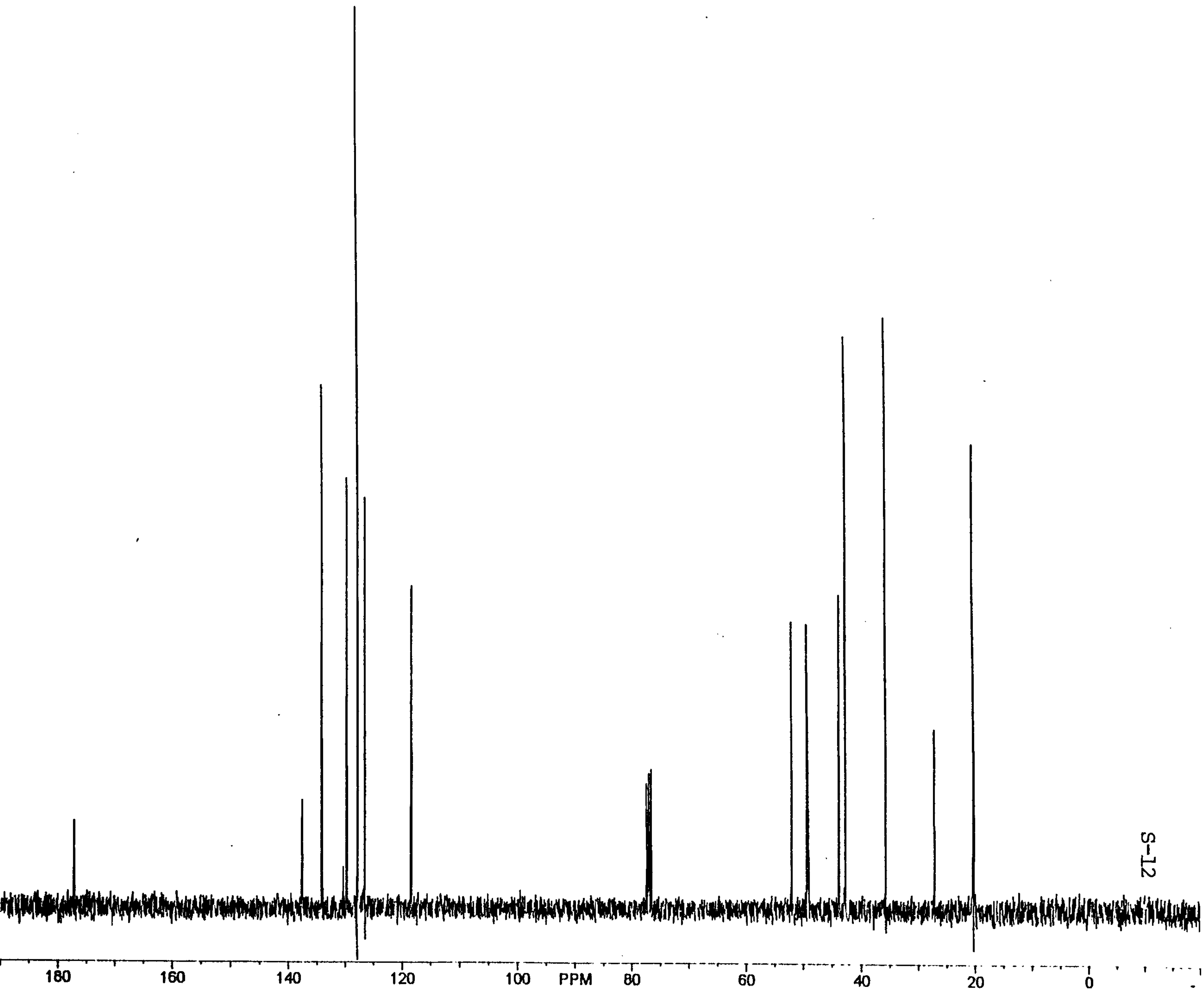

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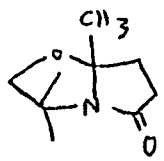

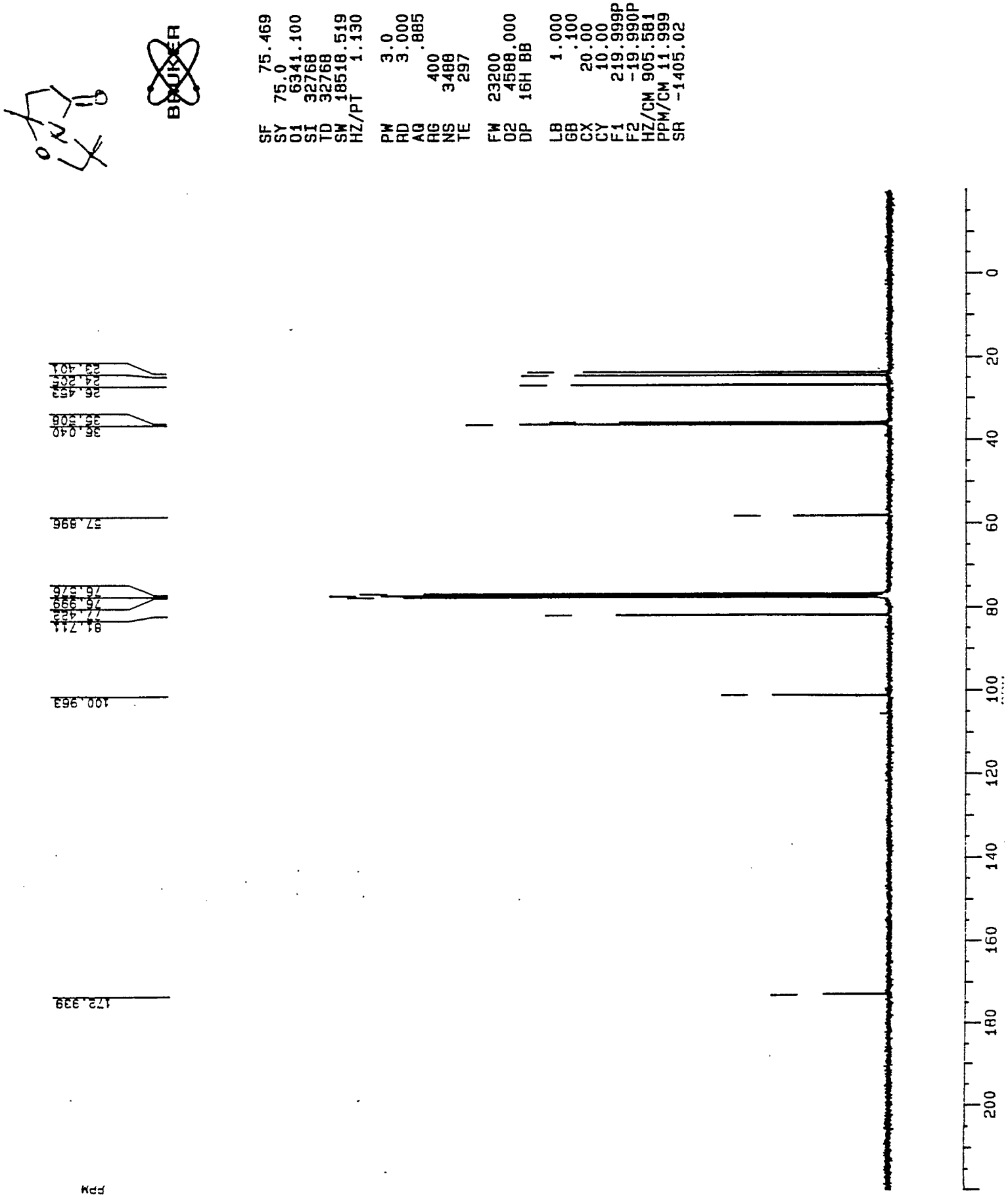
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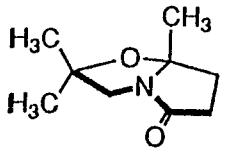

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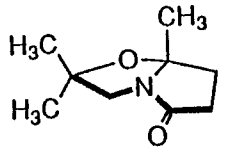

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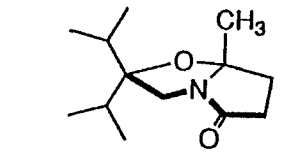

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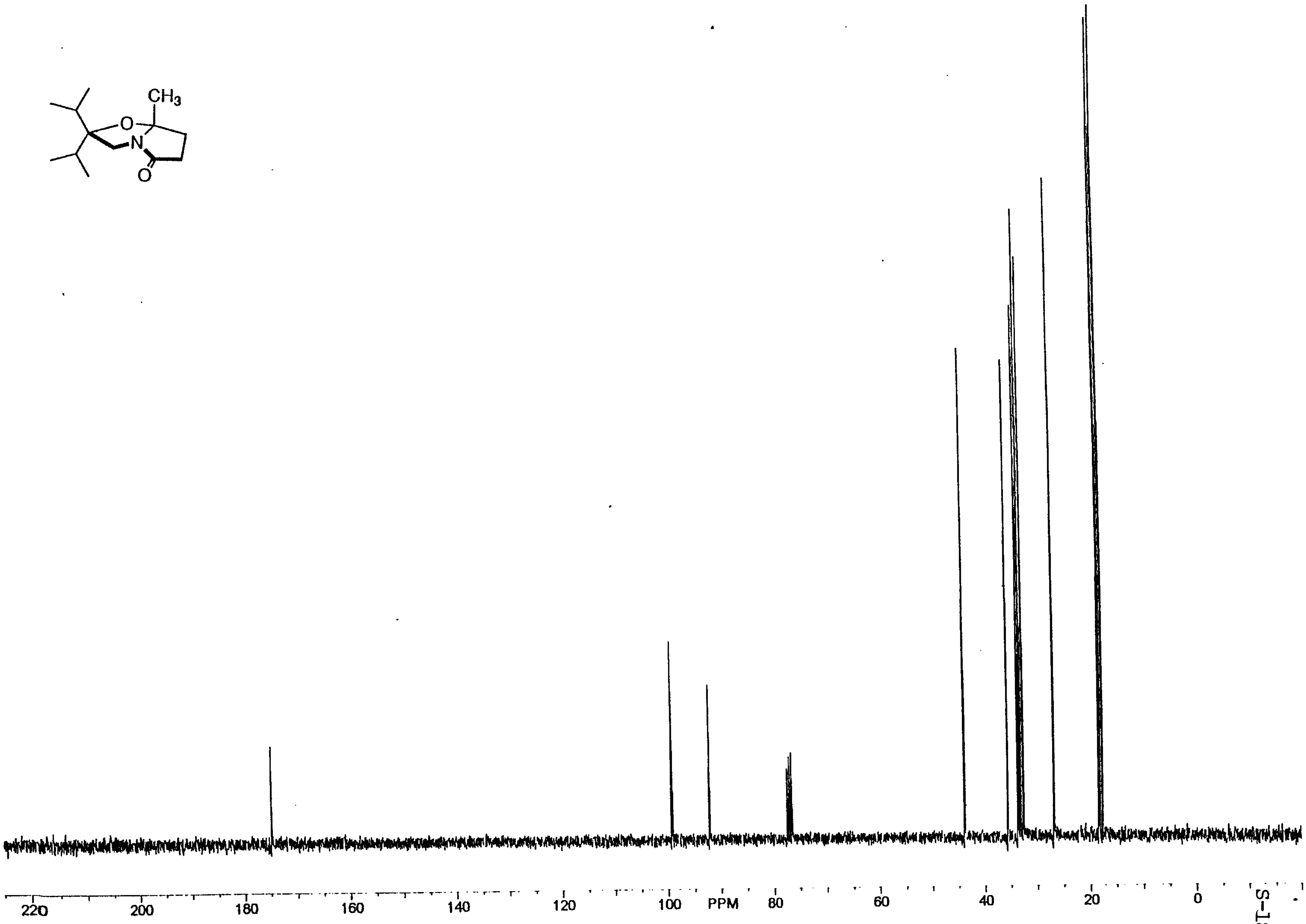

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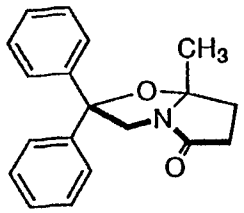

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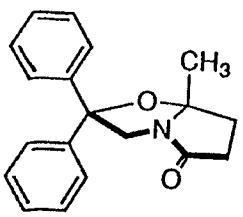

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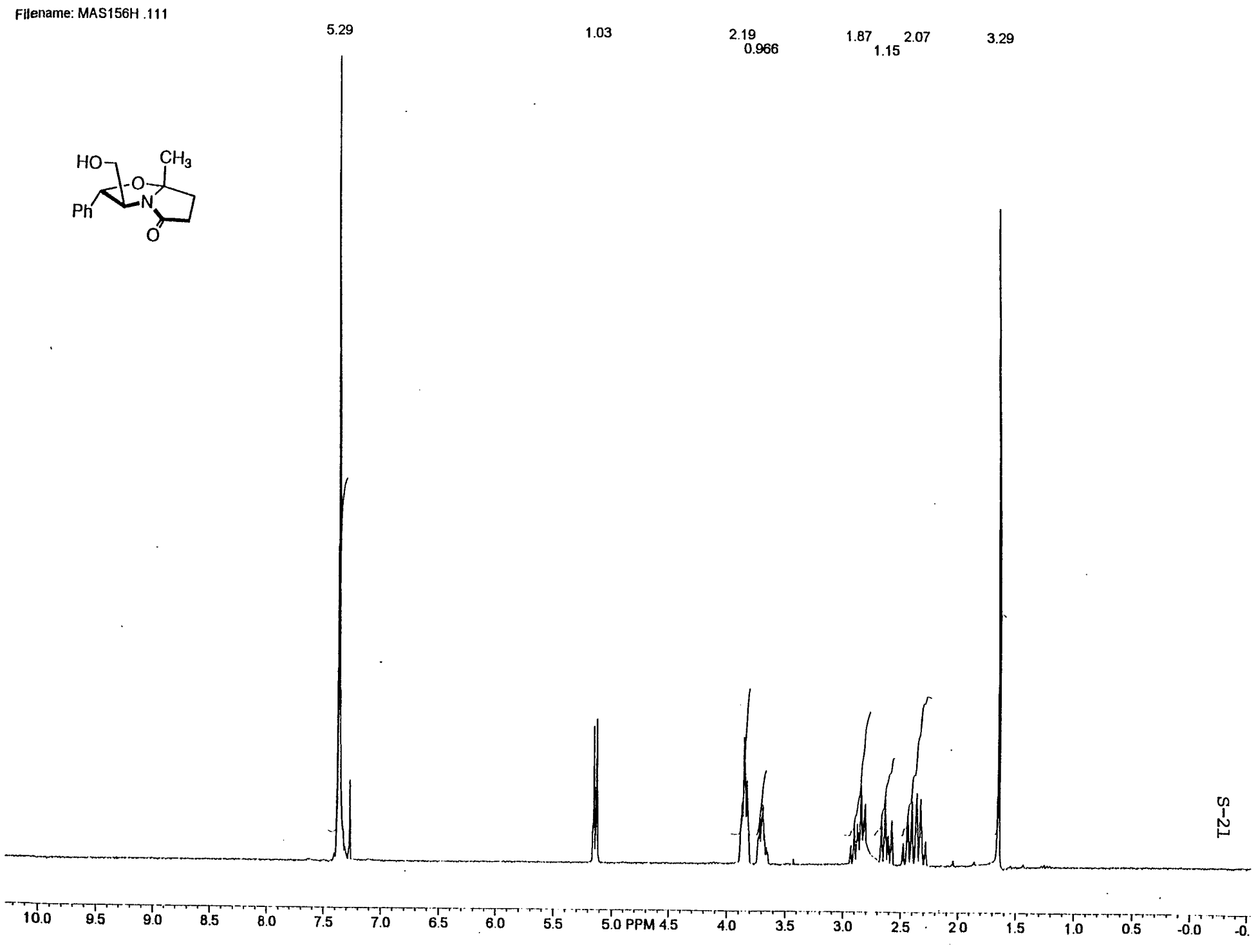

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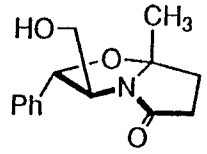

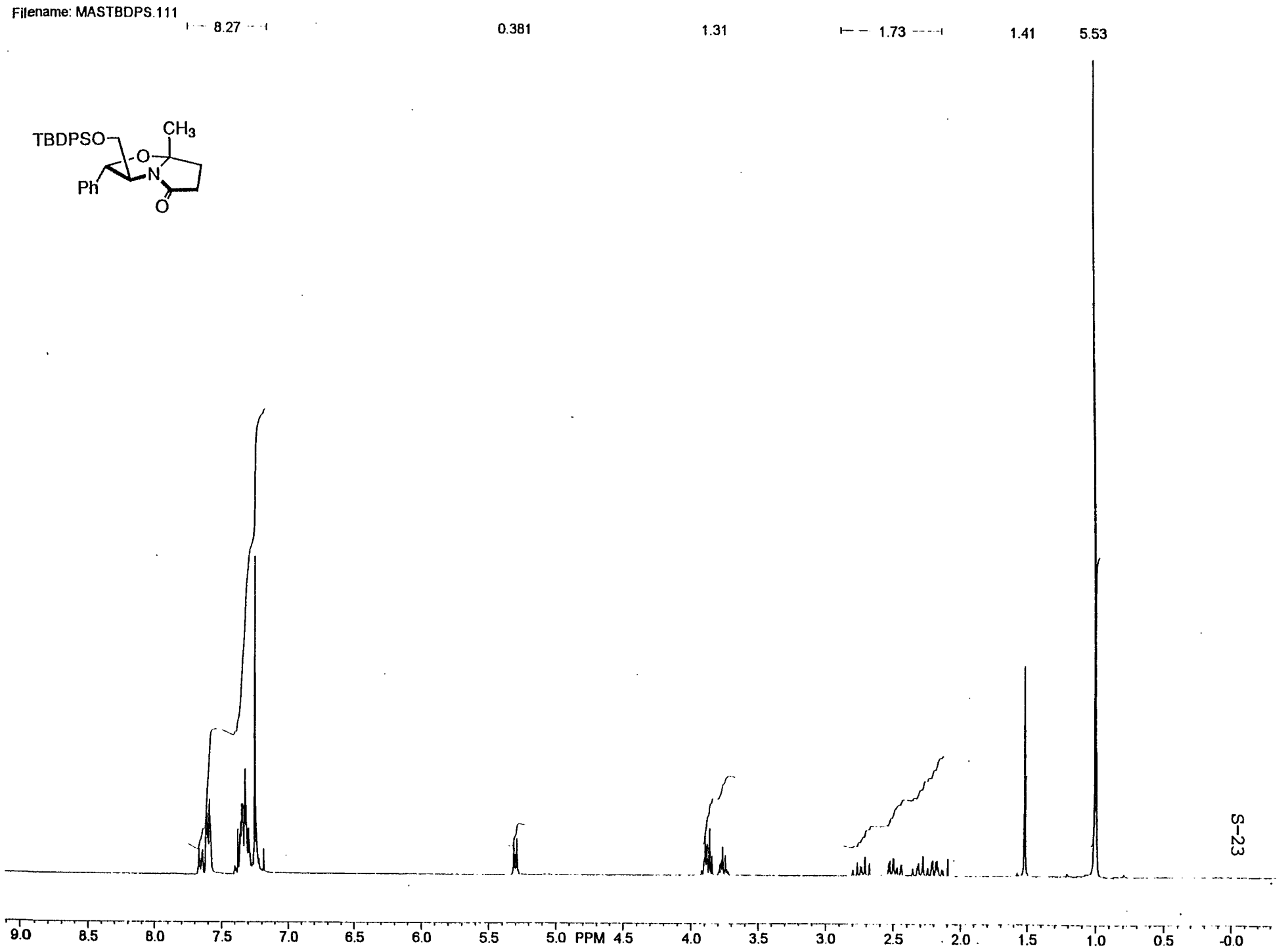

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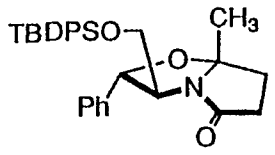

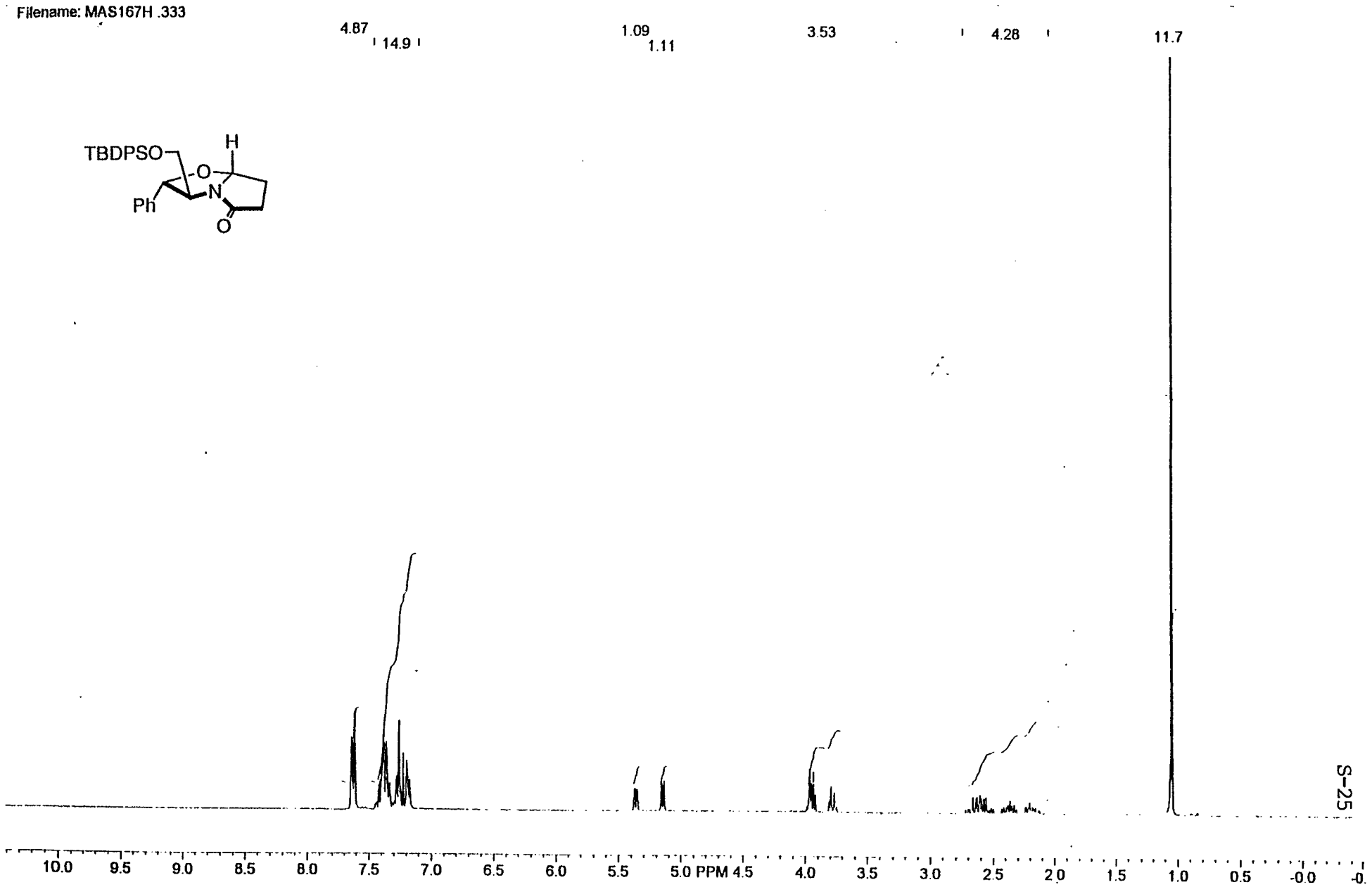

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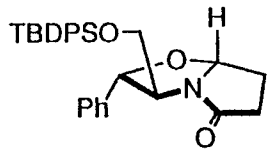

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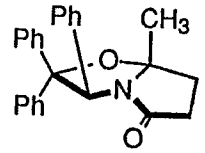

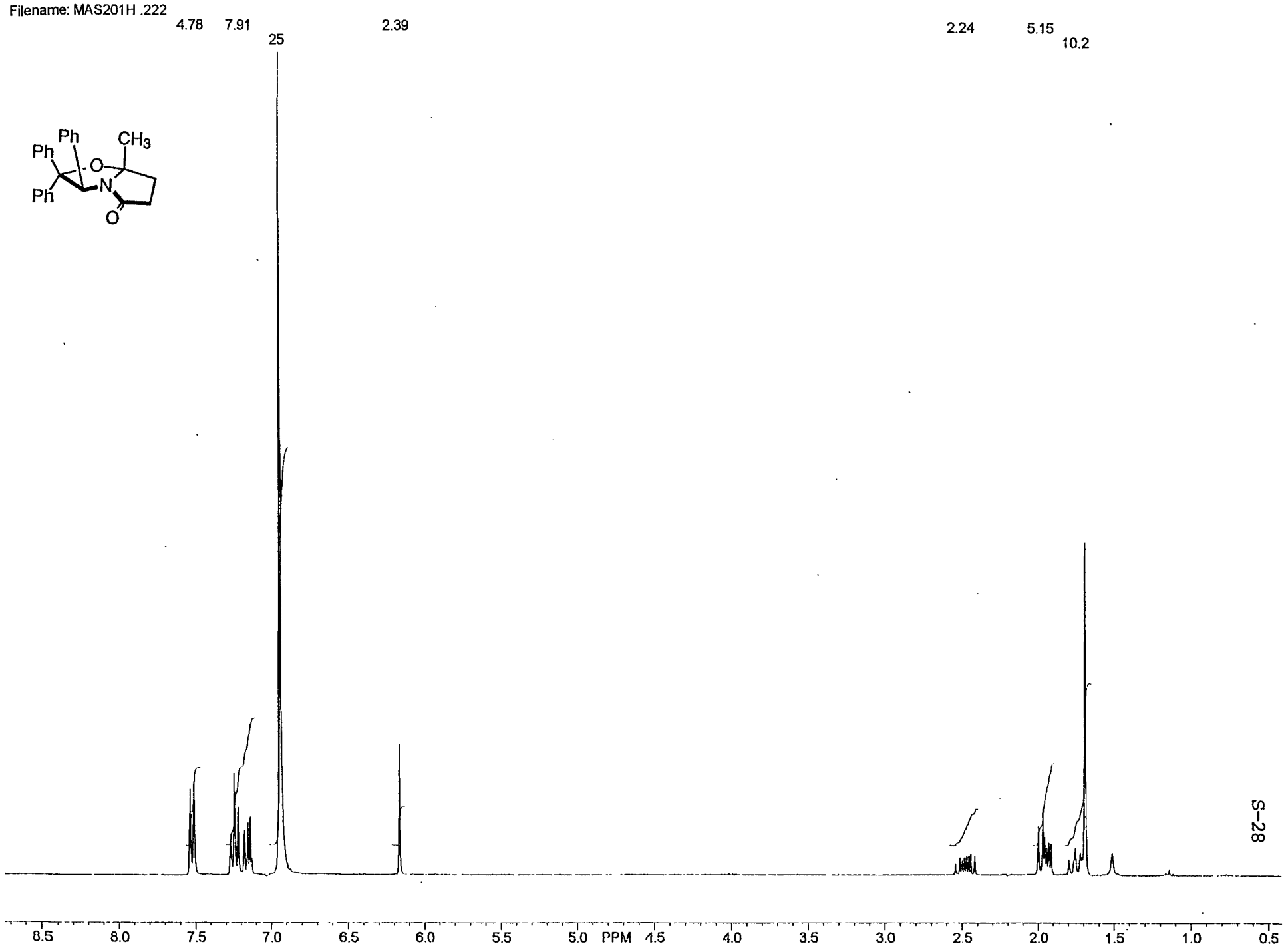

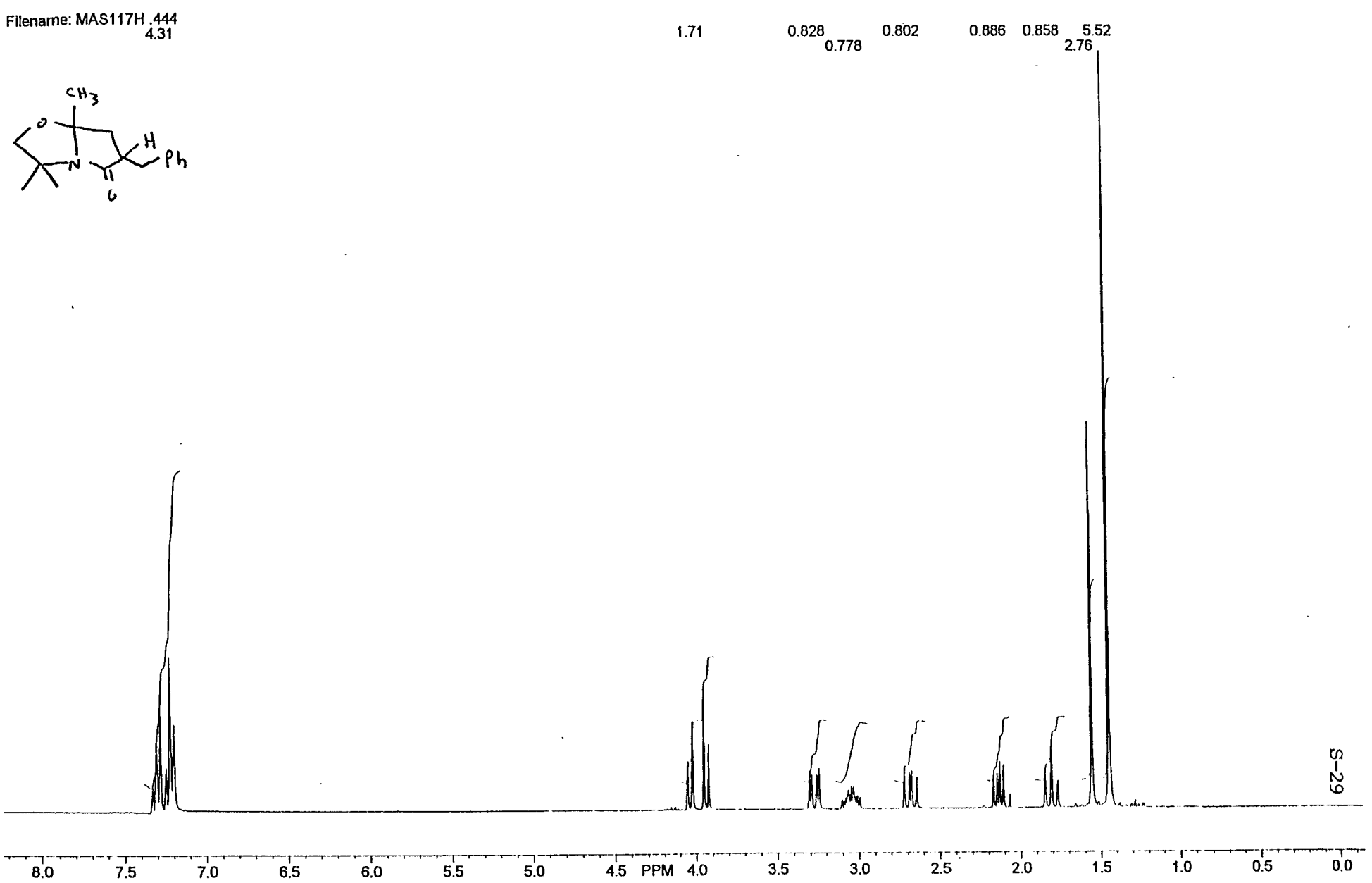

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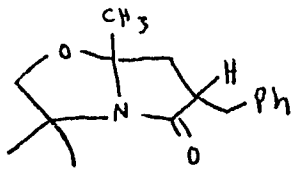

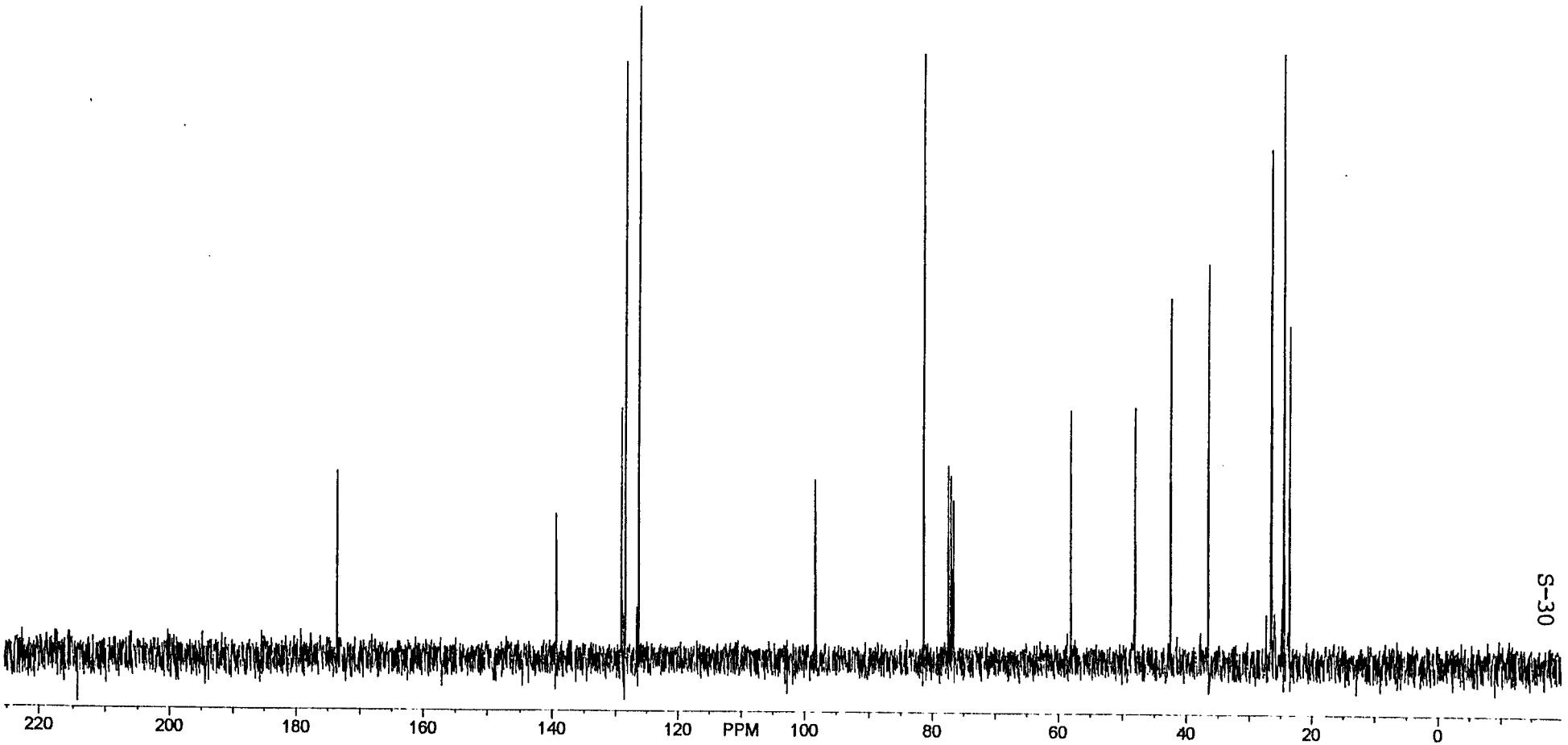

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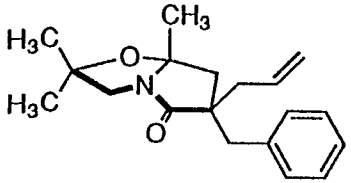
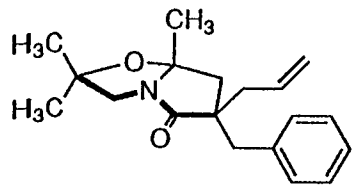
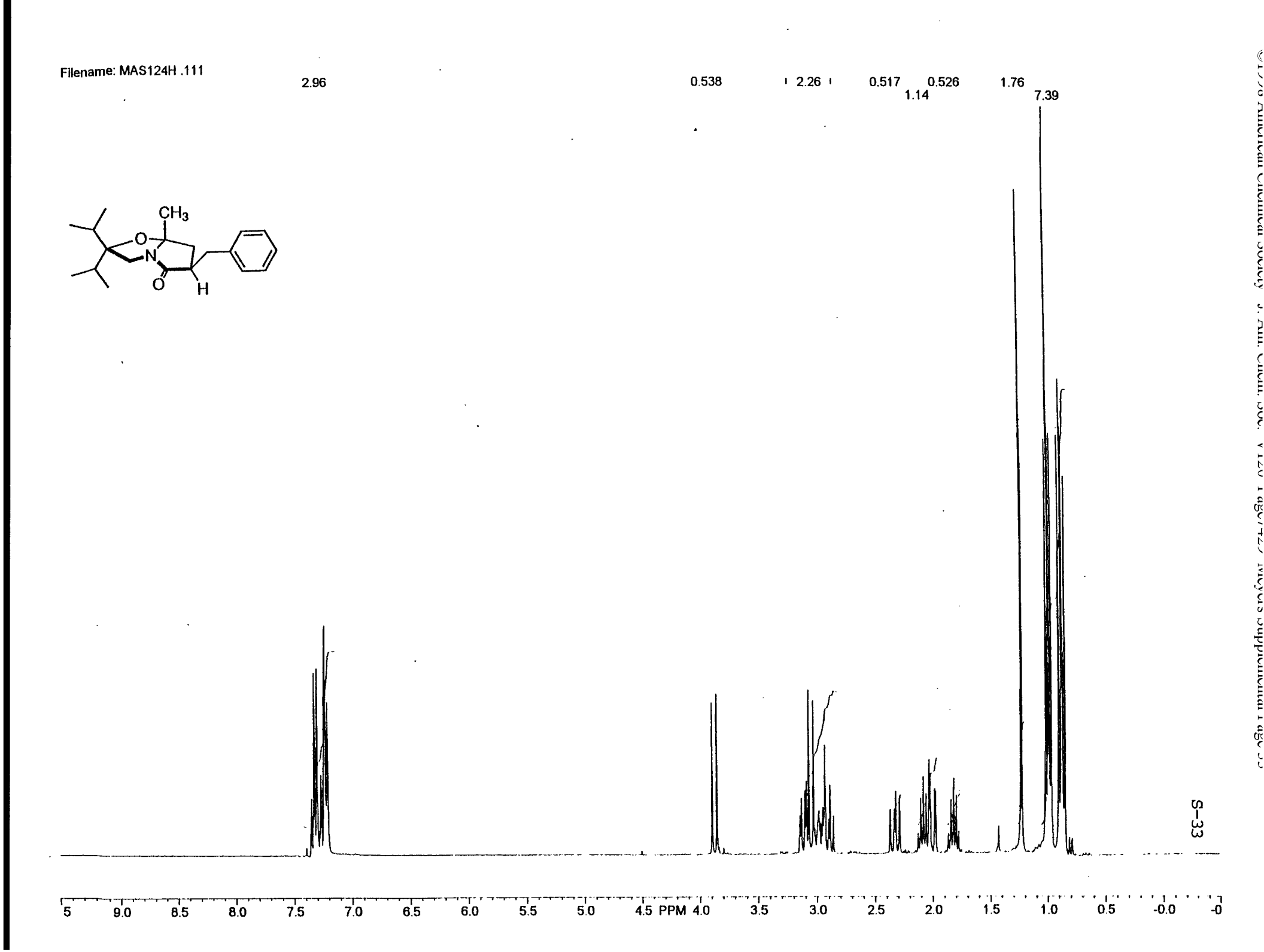


Filename: MAS155C 333

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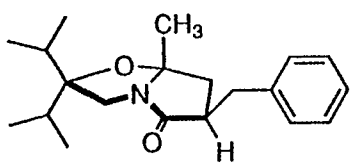

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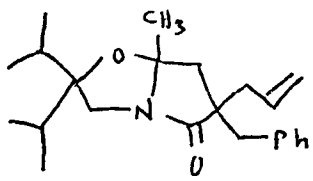

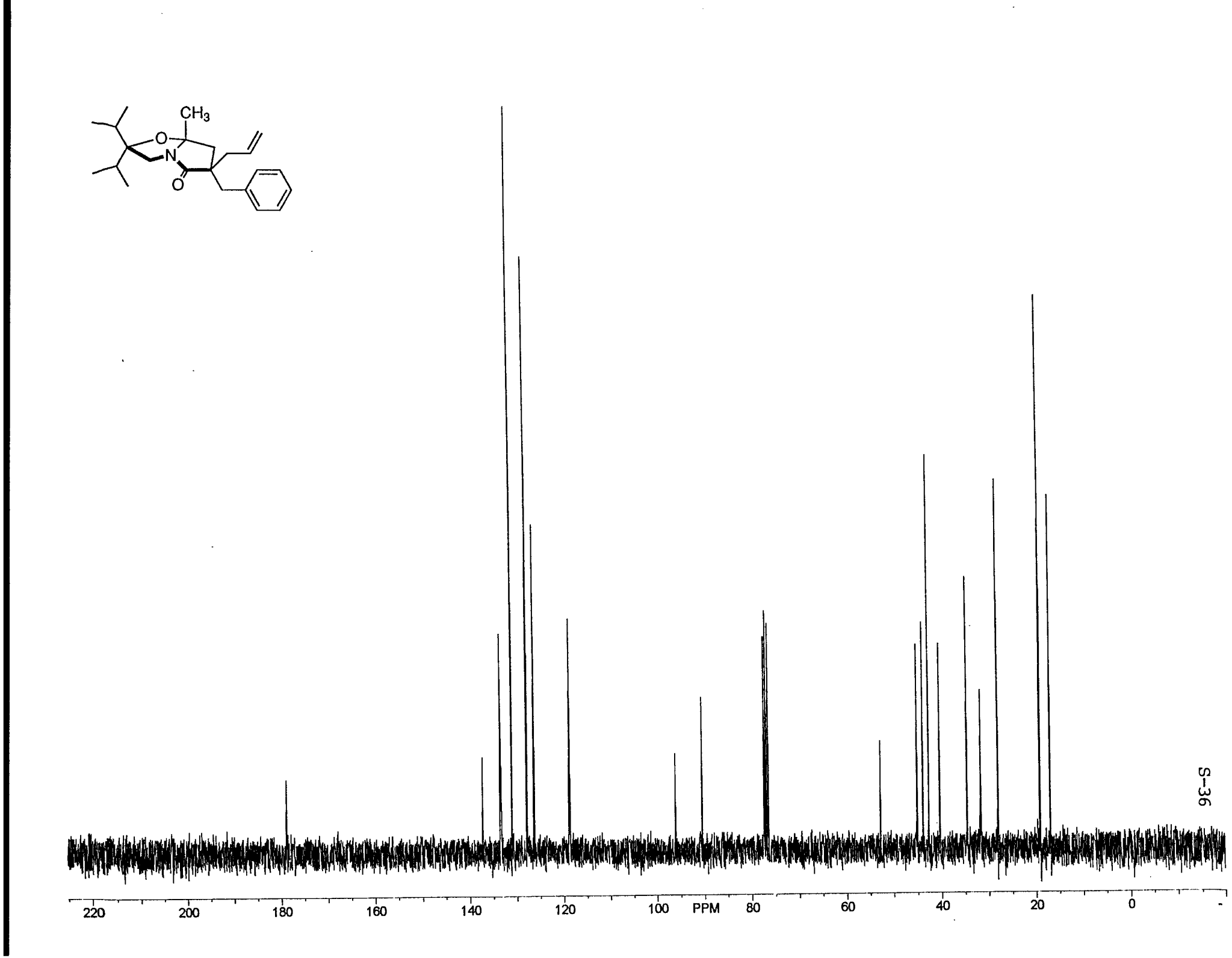

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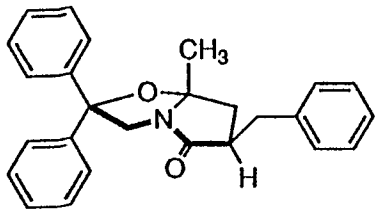

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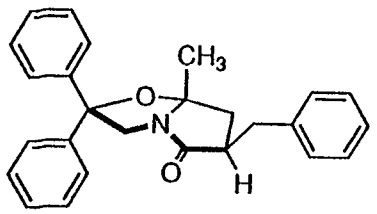

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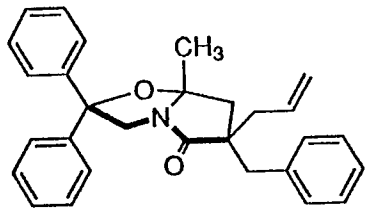
Filename: MAS152H .007



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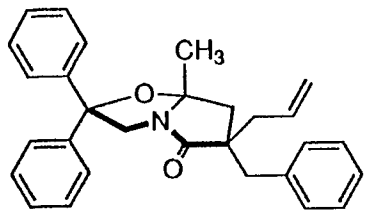

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