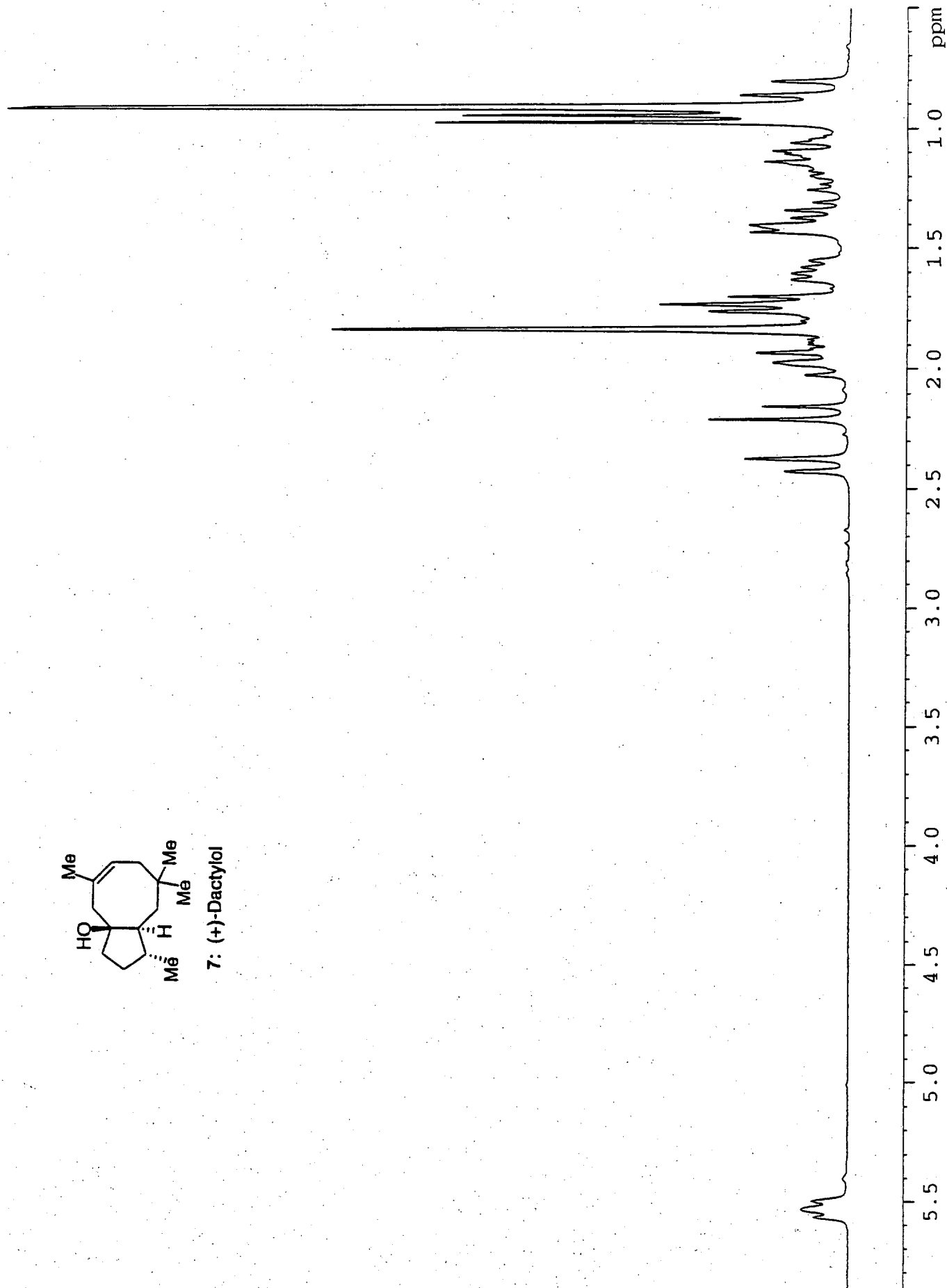
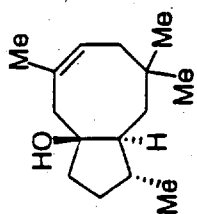
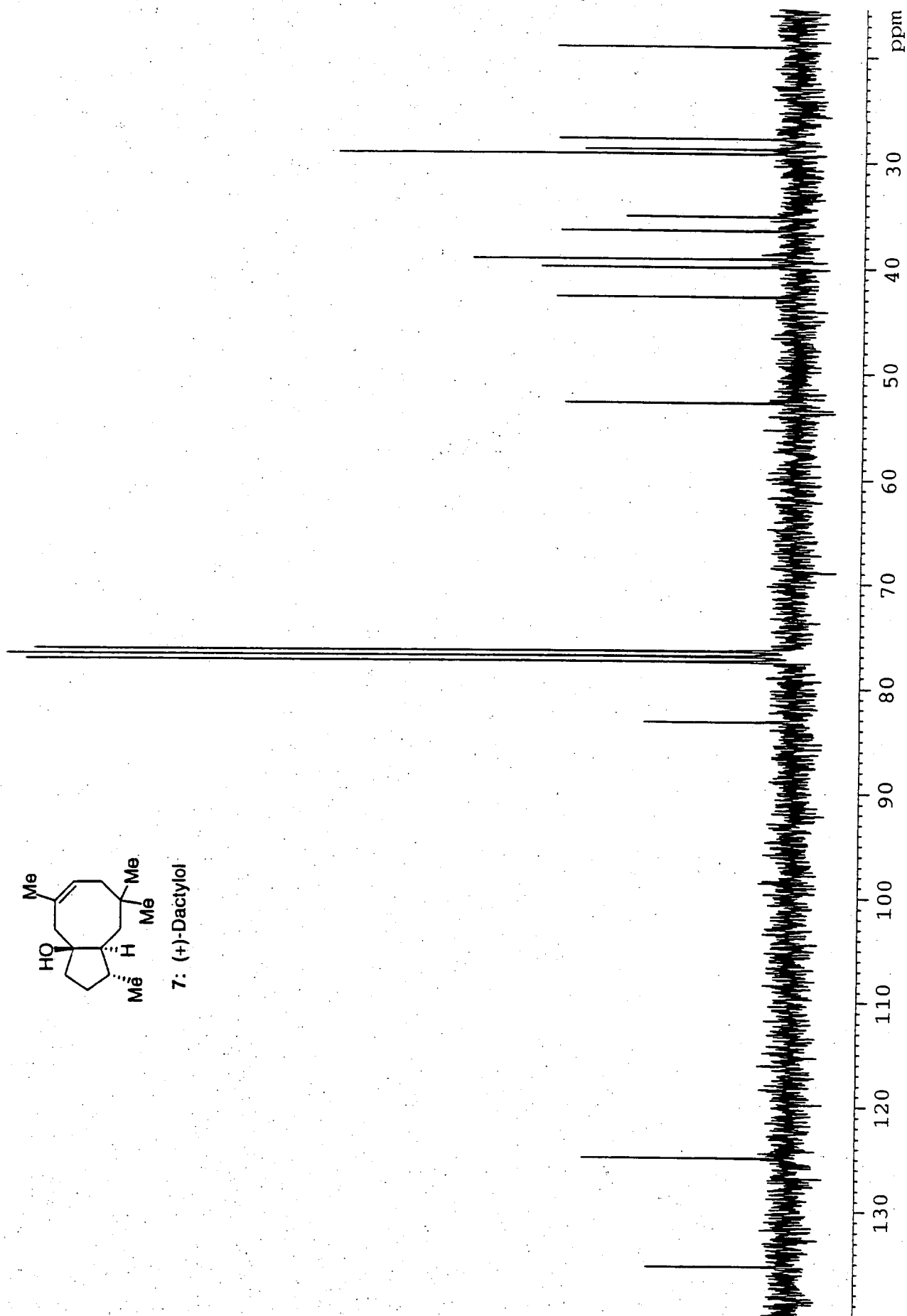


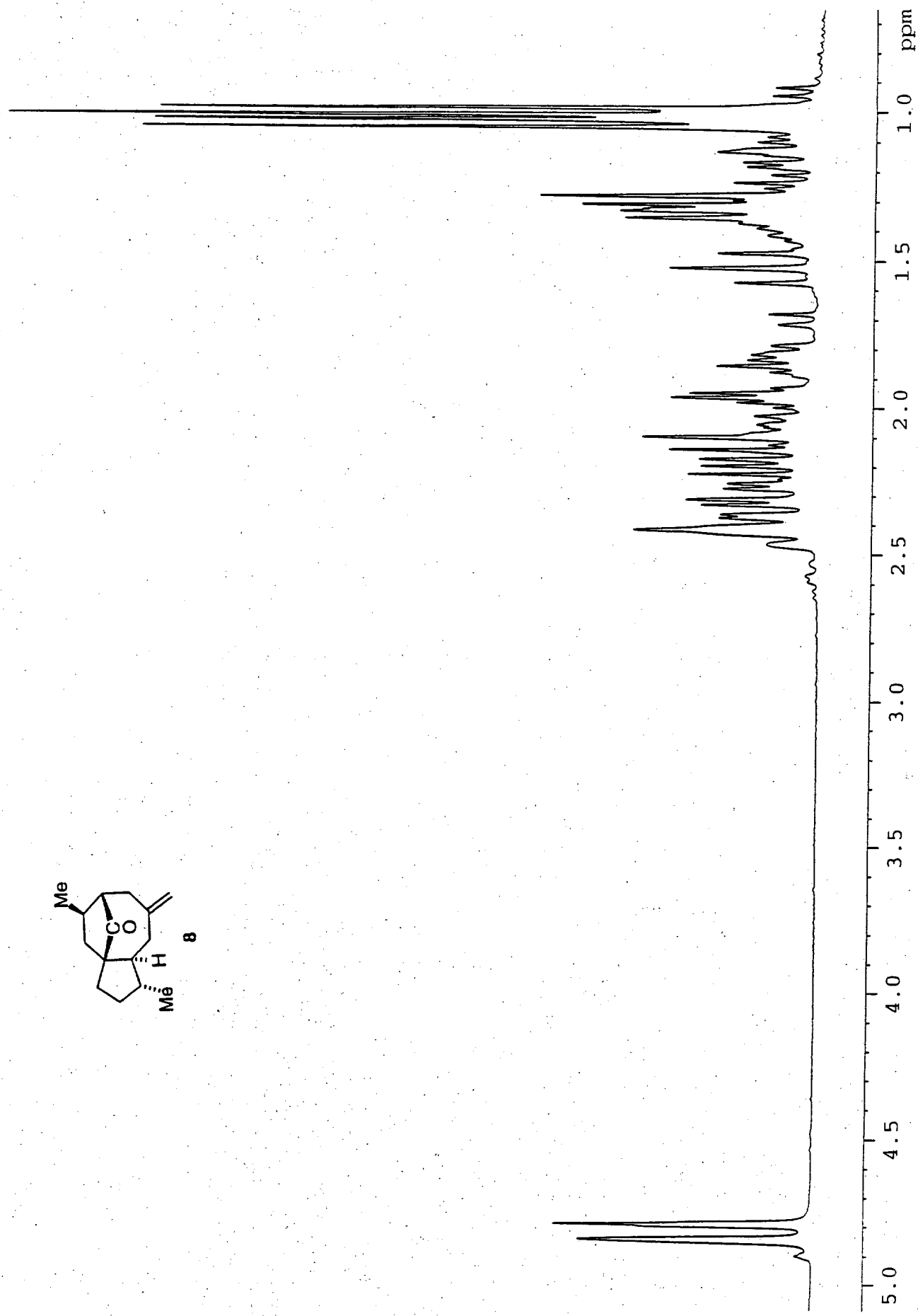
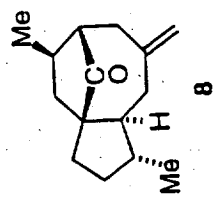
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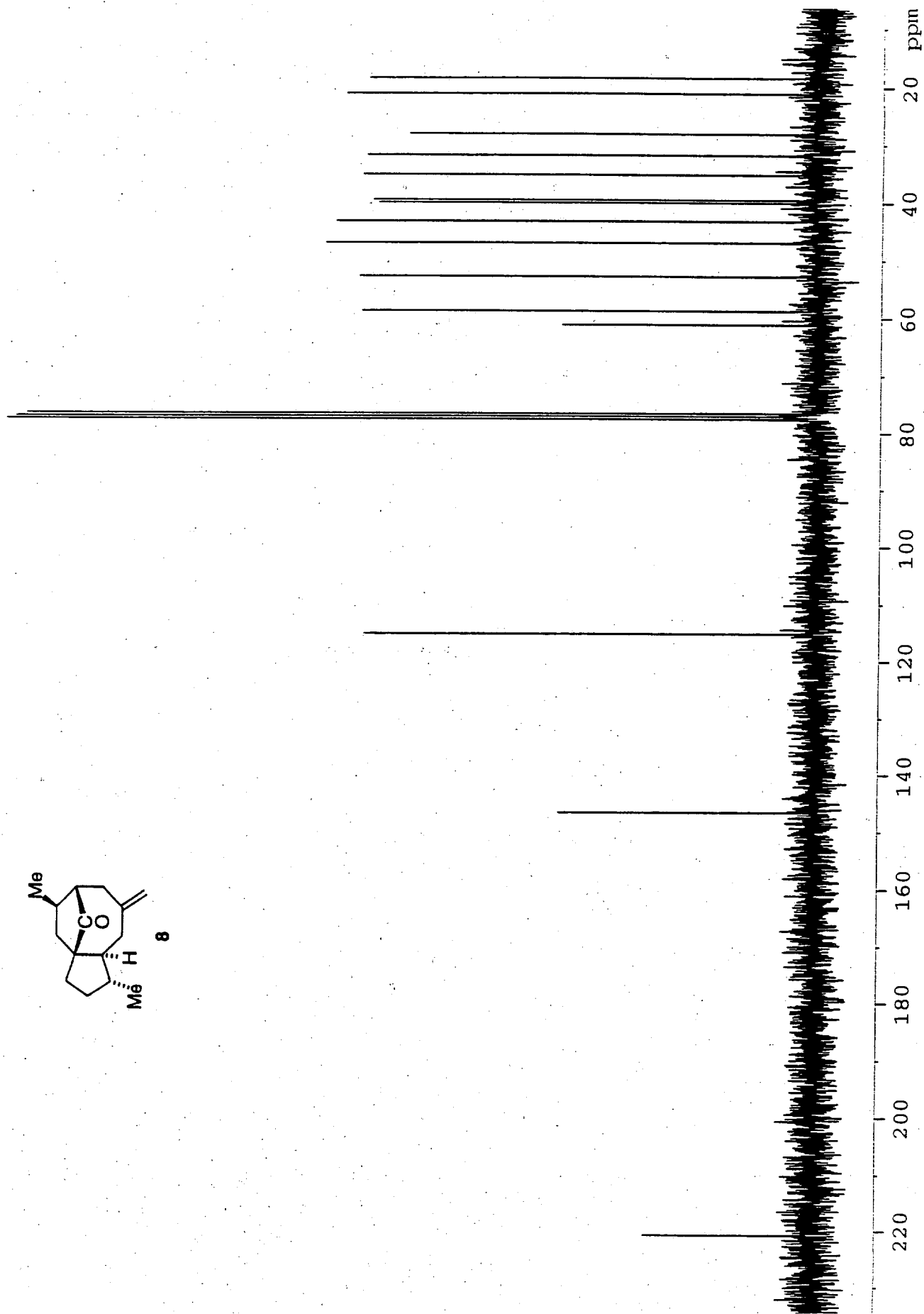
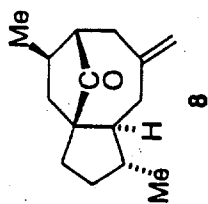


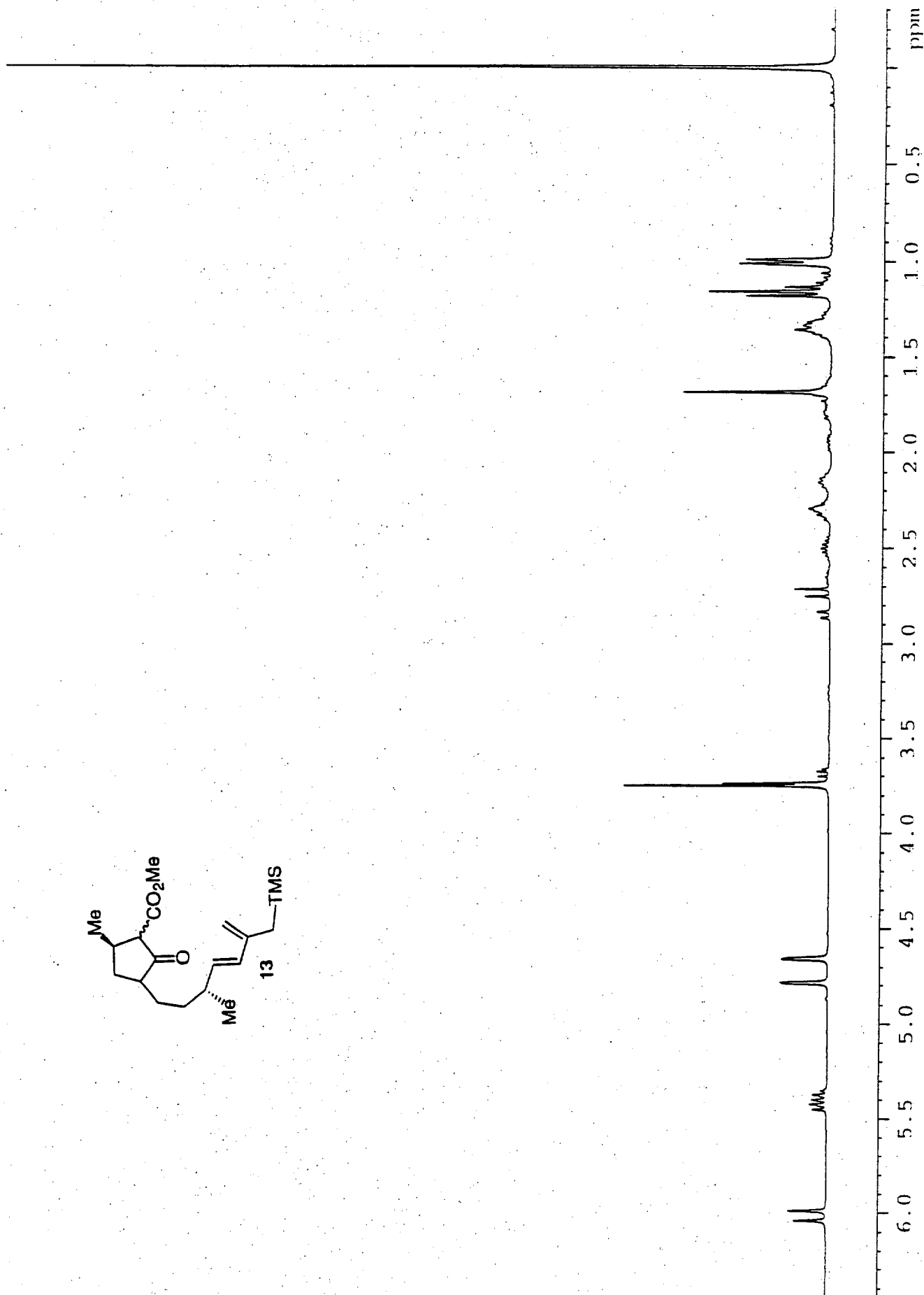
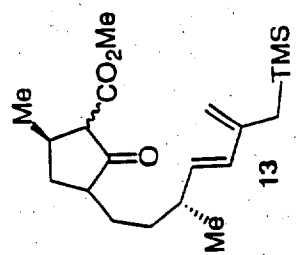


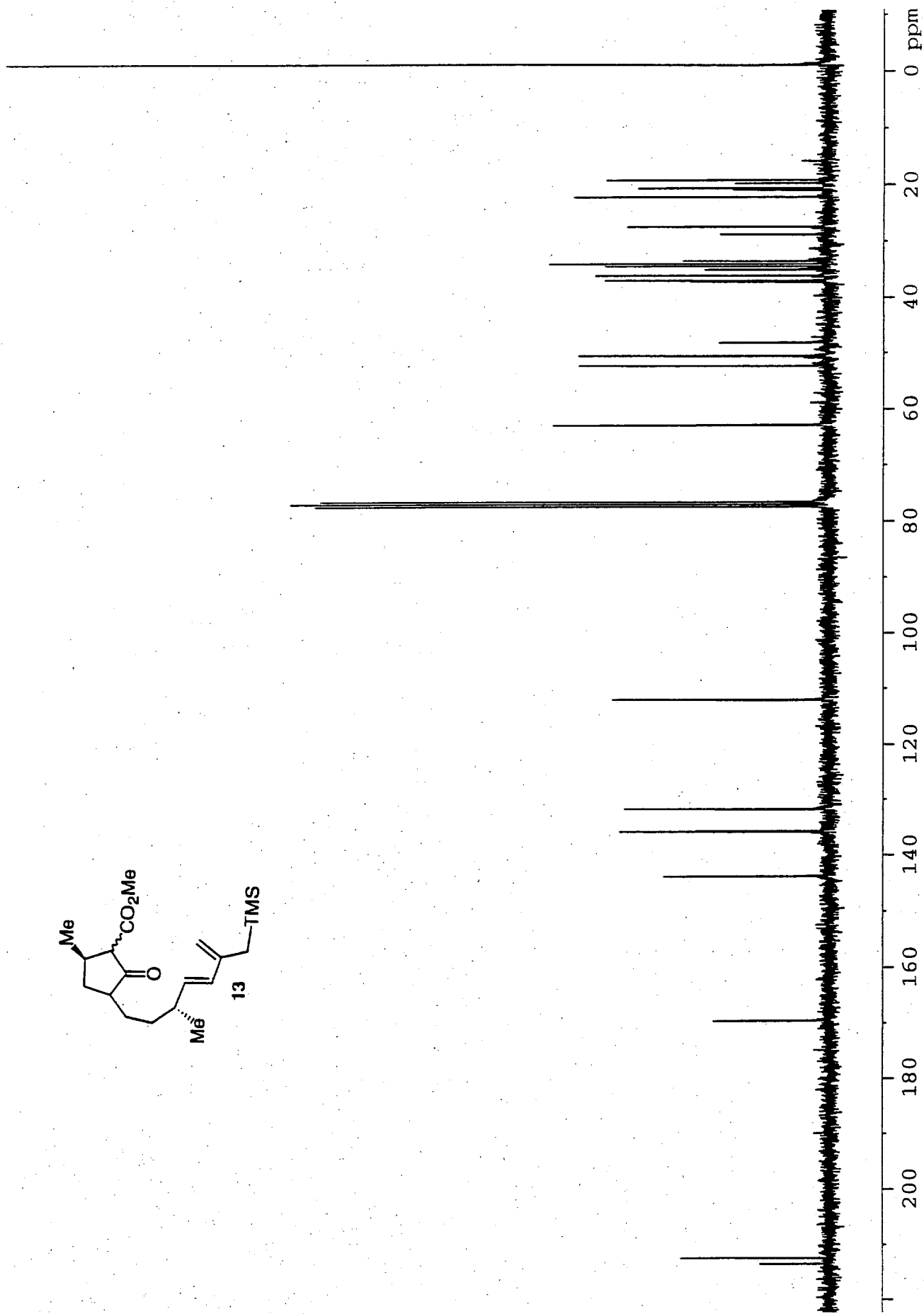
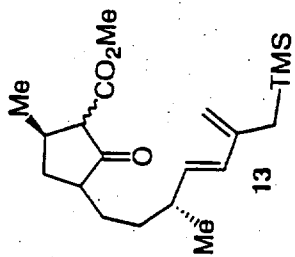
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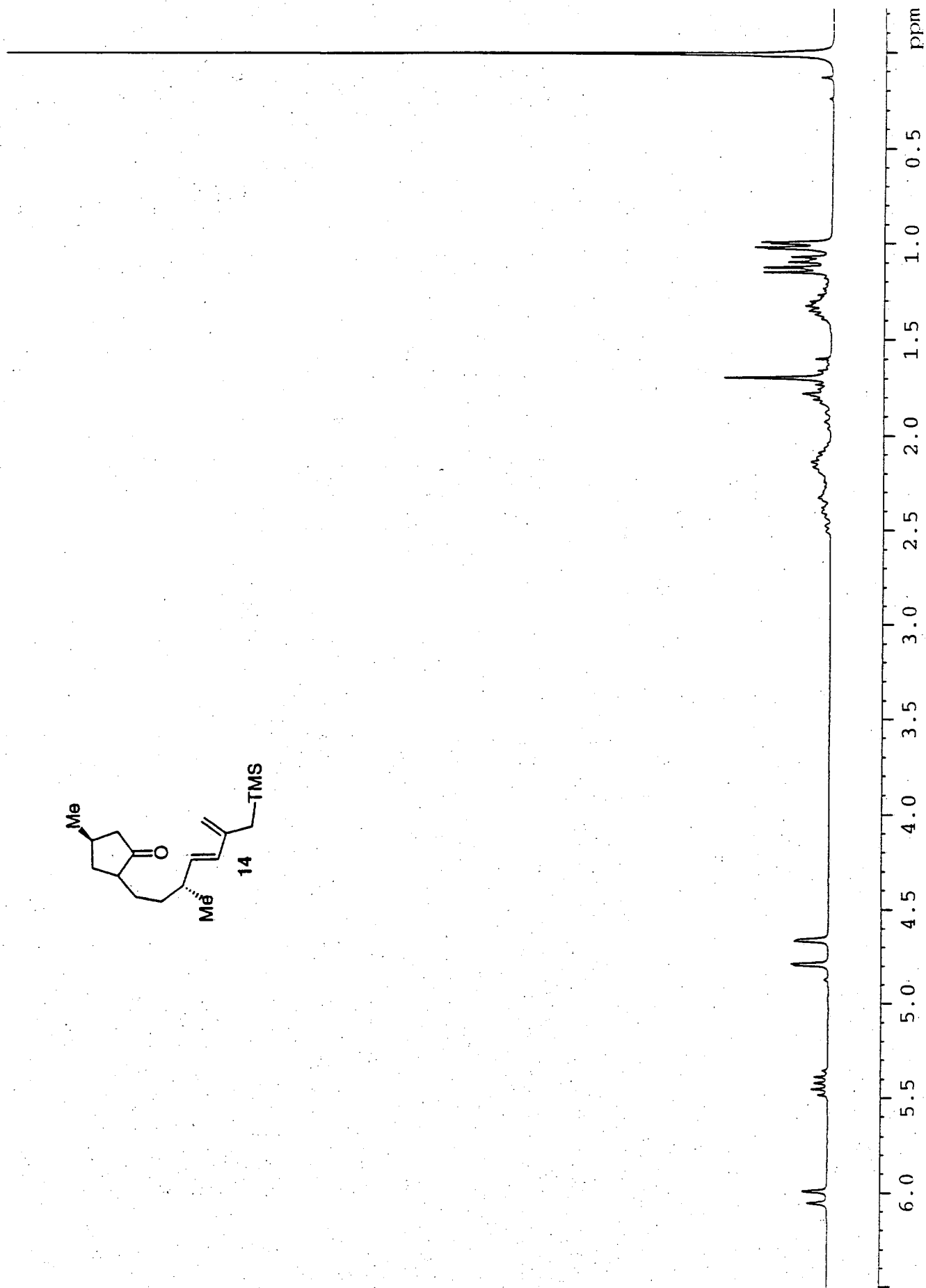
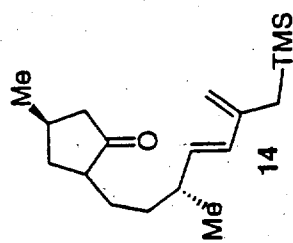


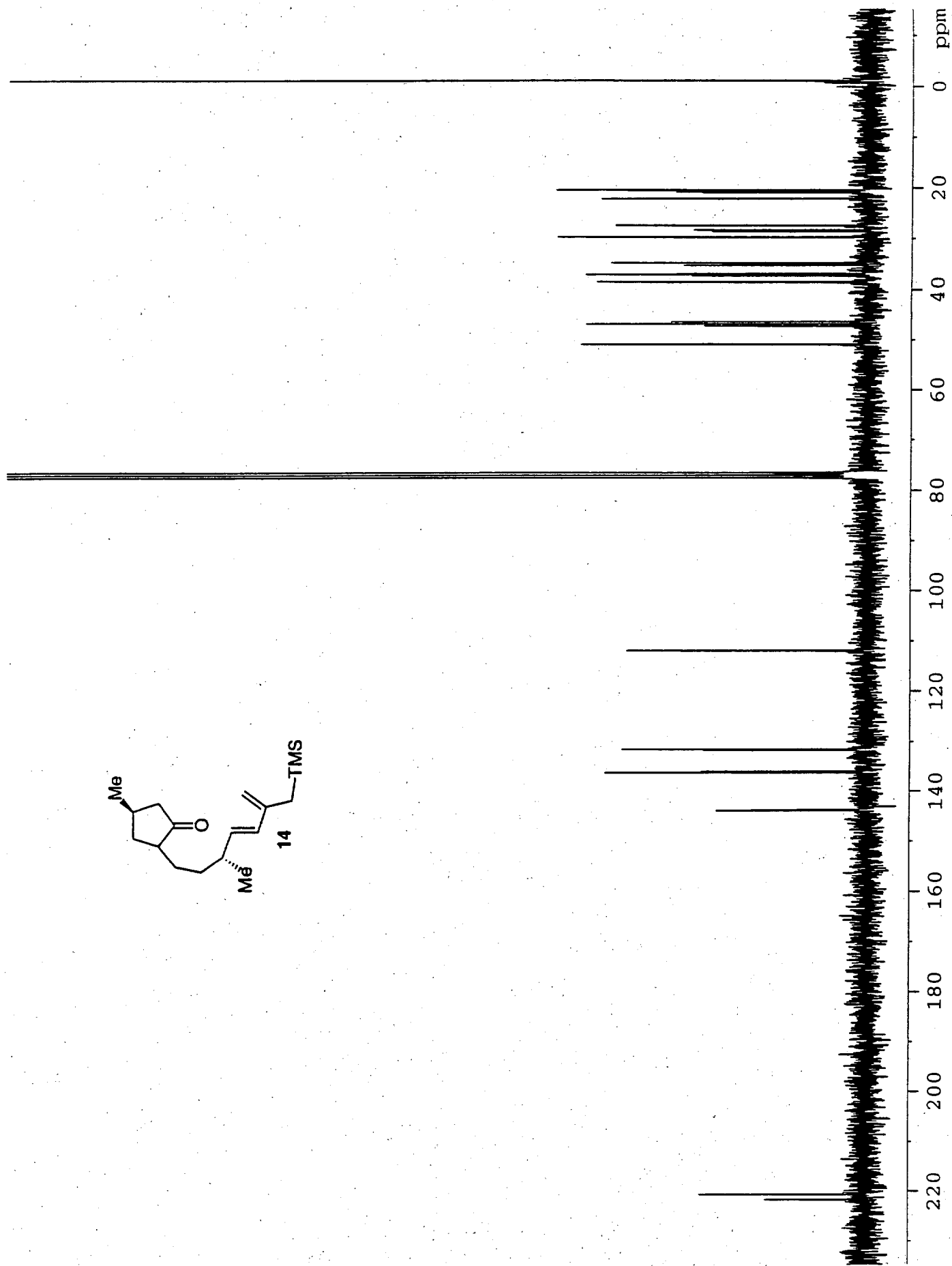


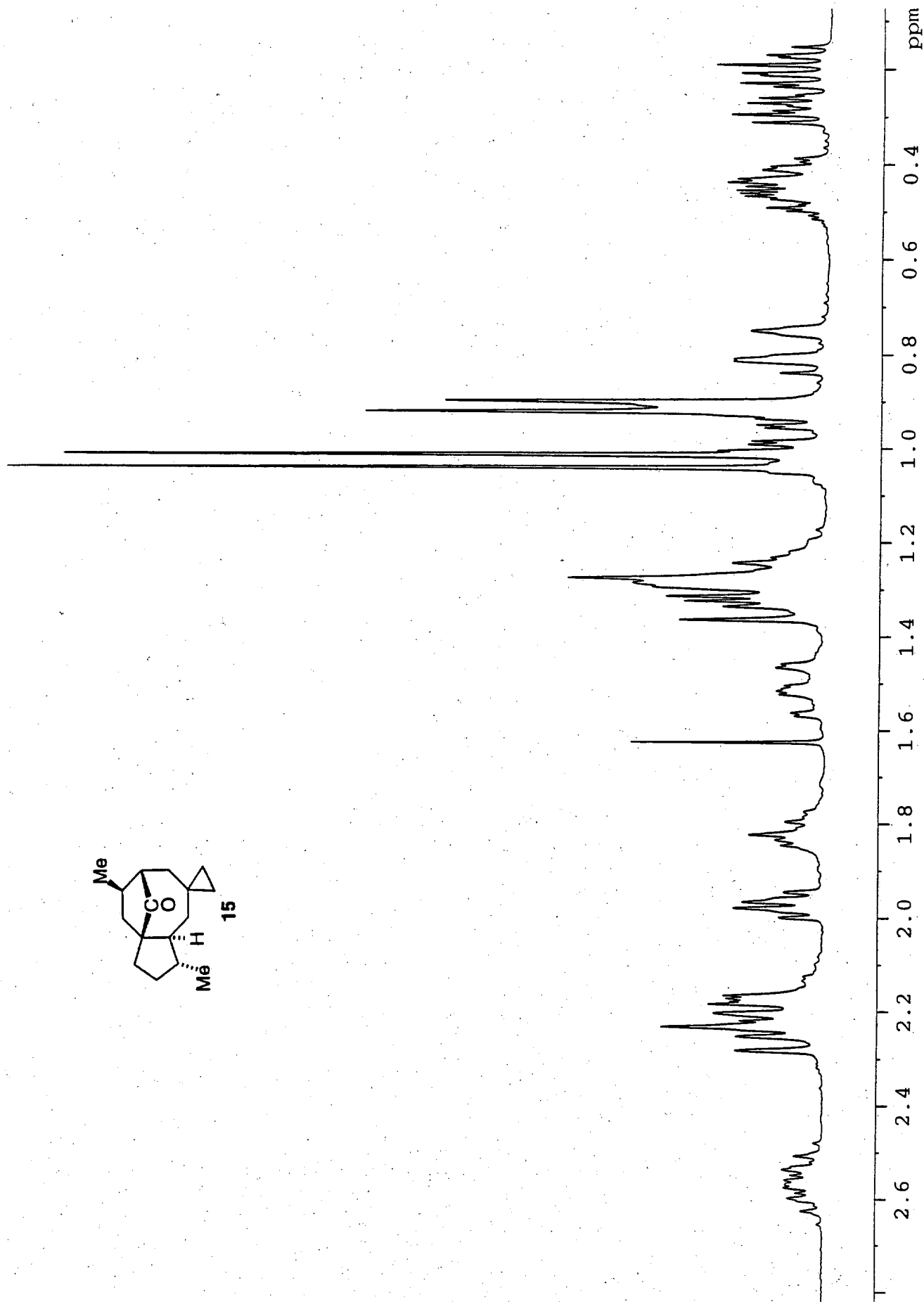
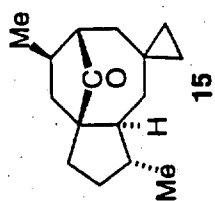


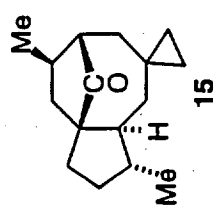
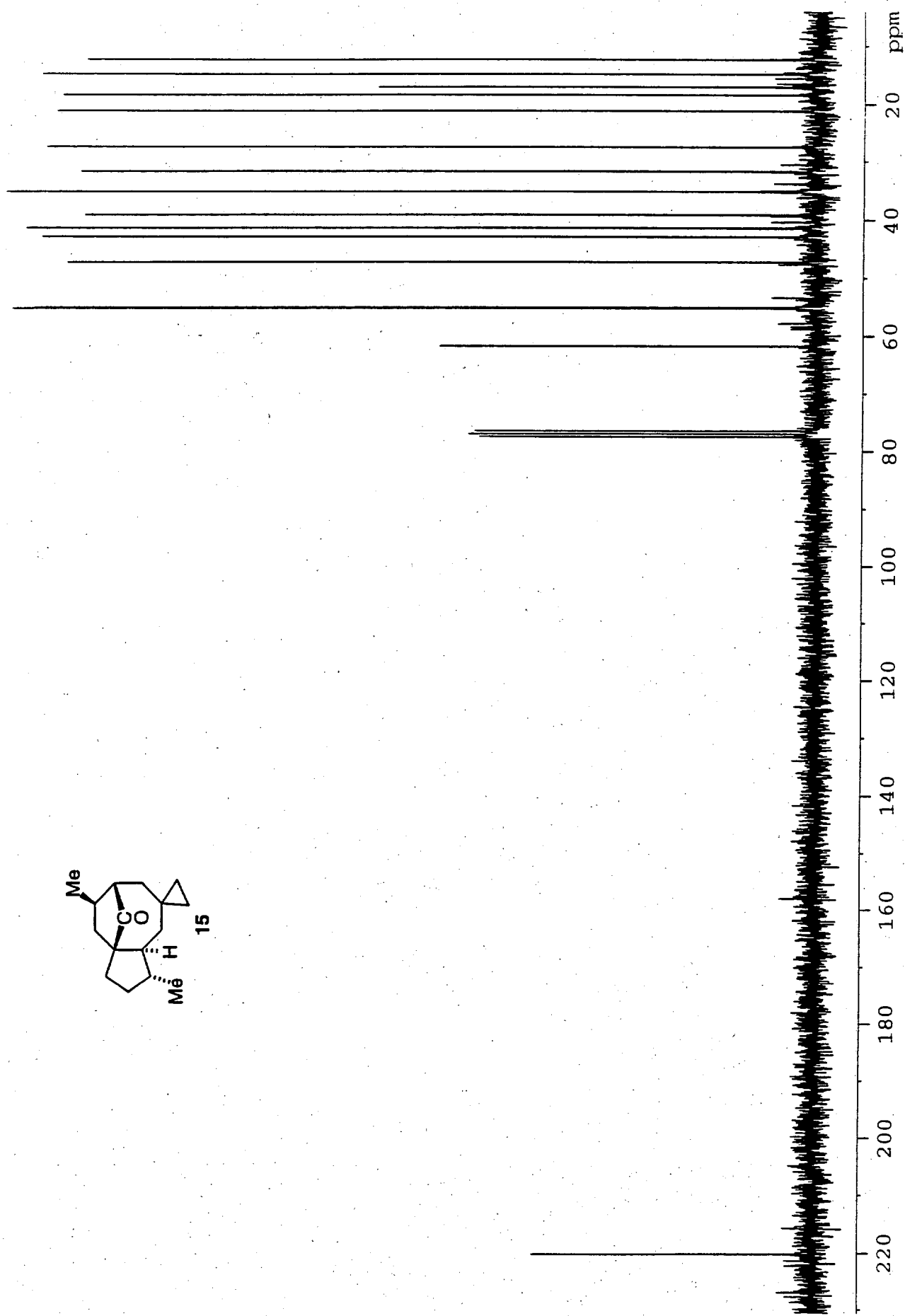


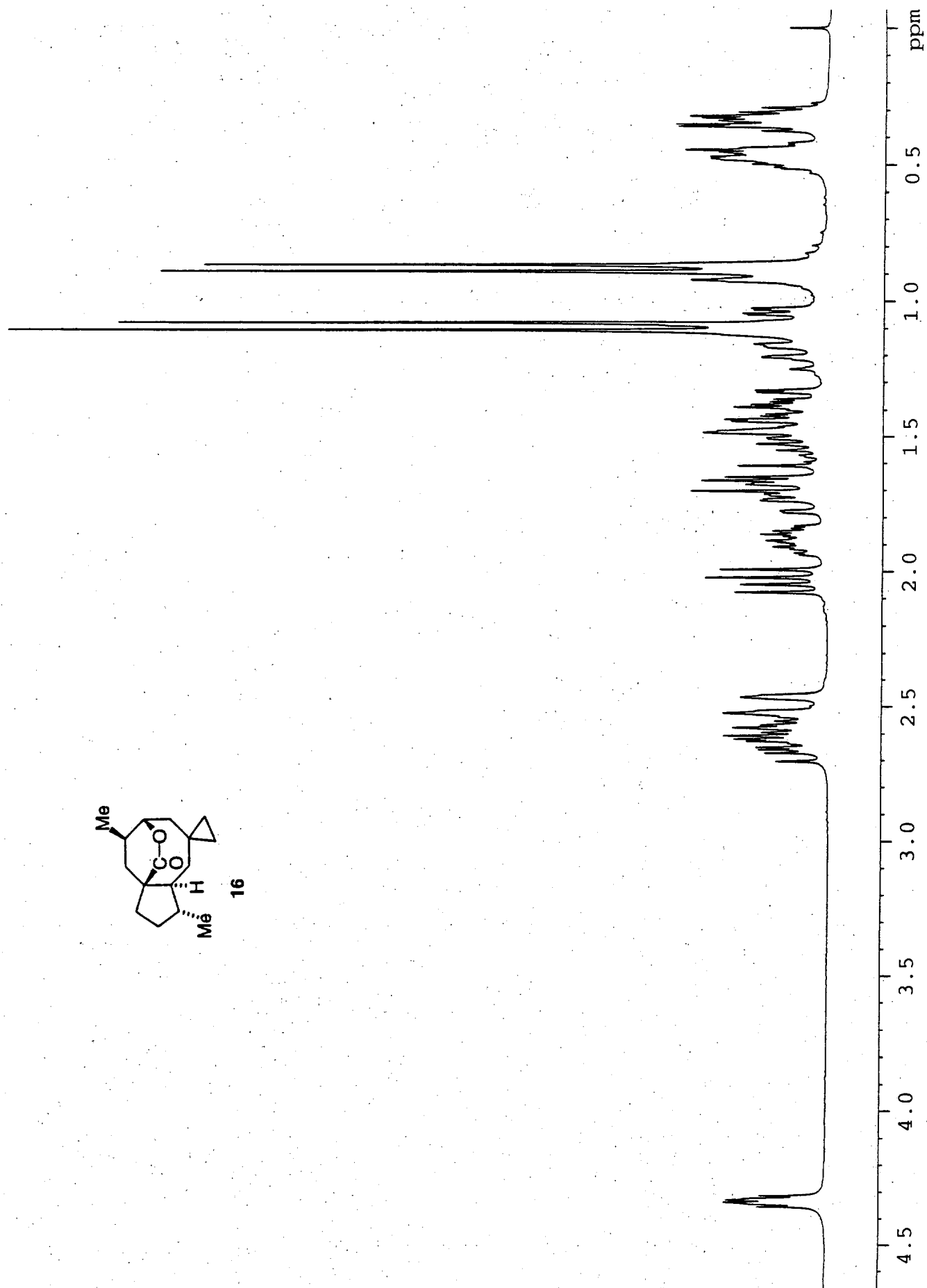
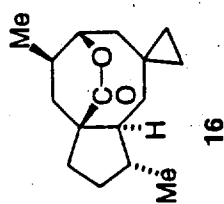


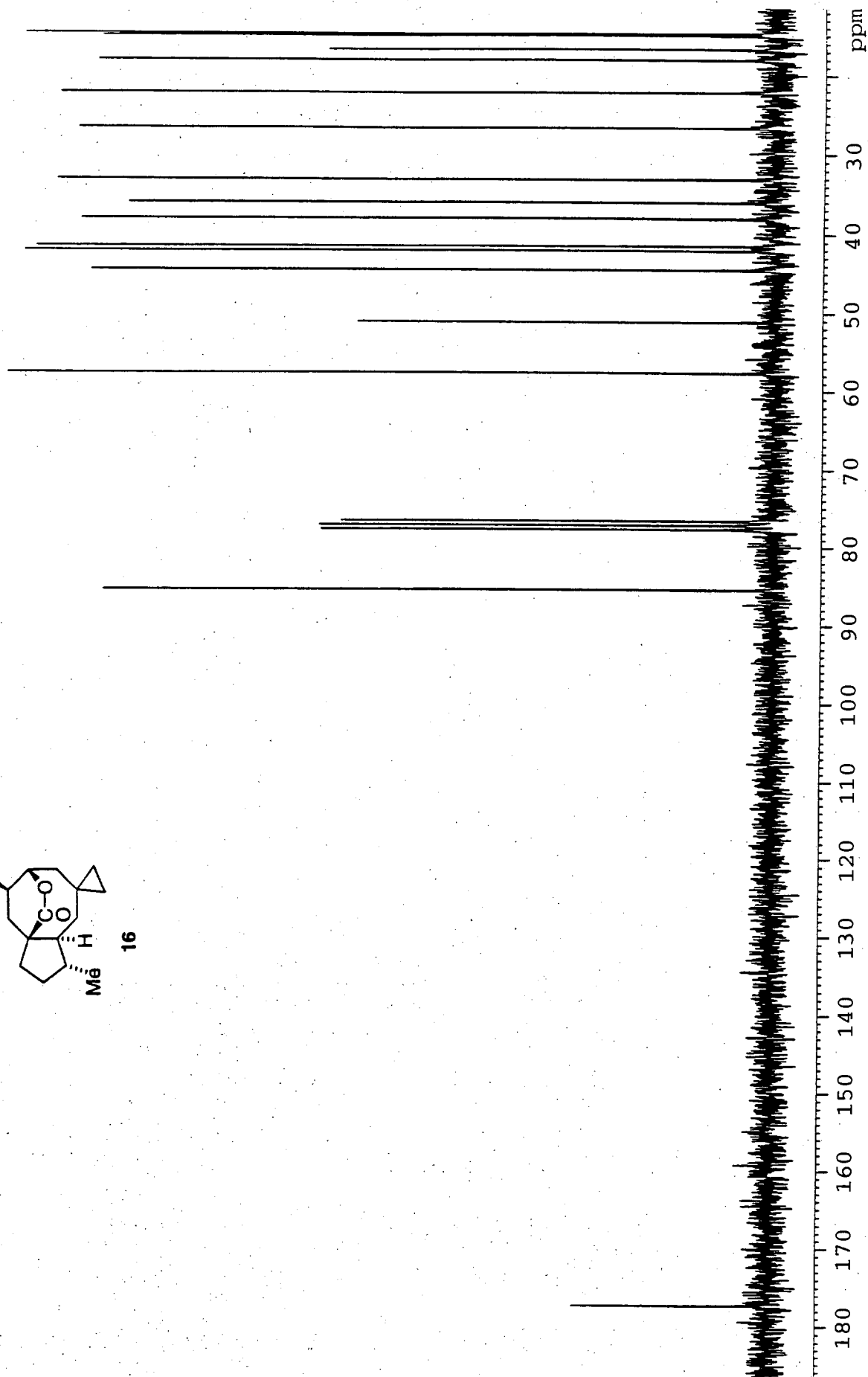
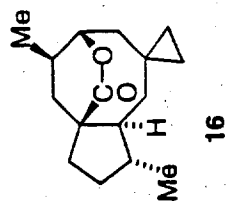


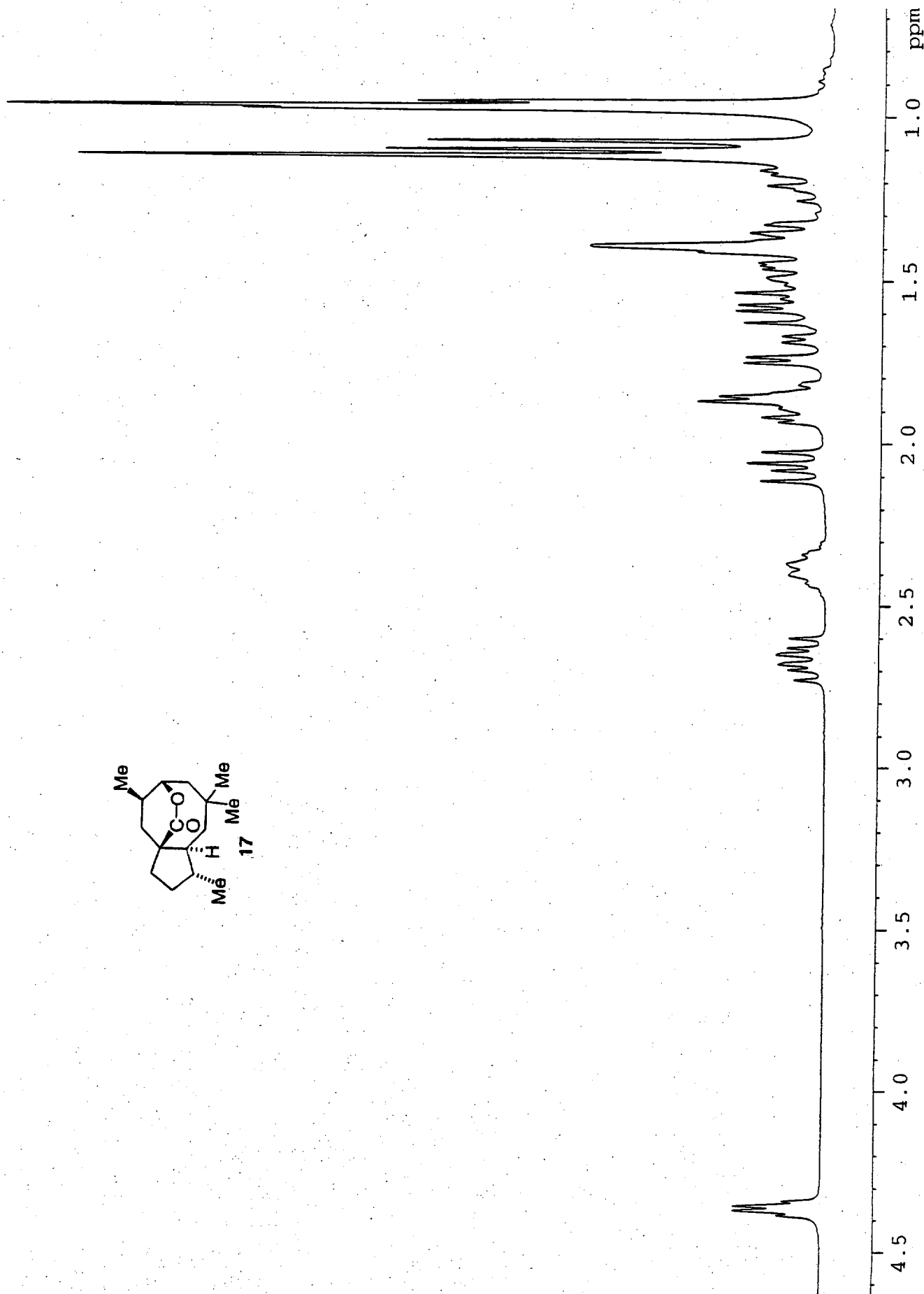
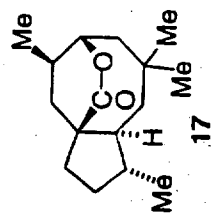


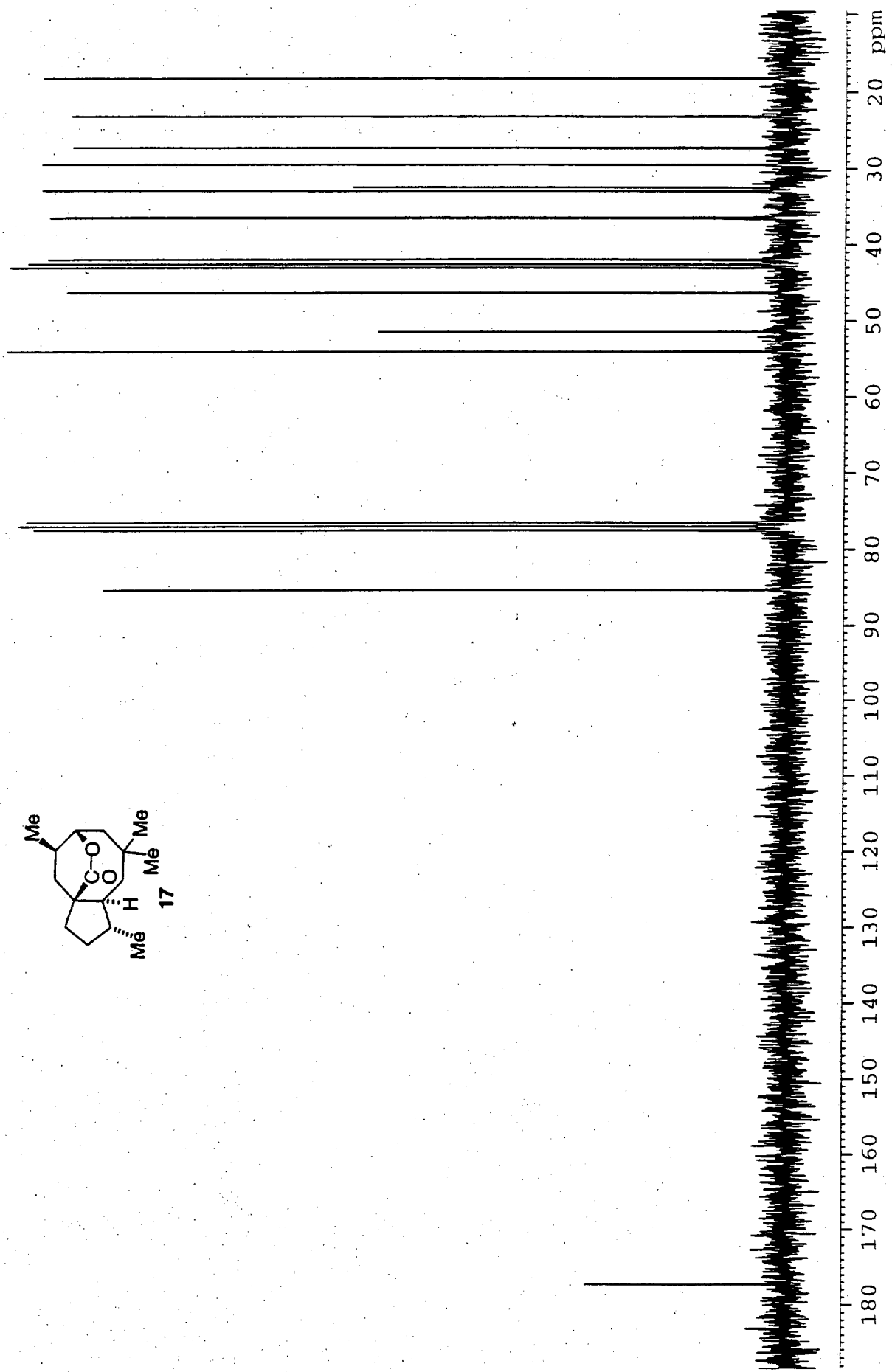
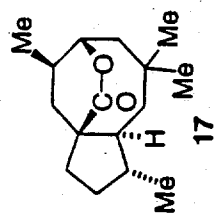


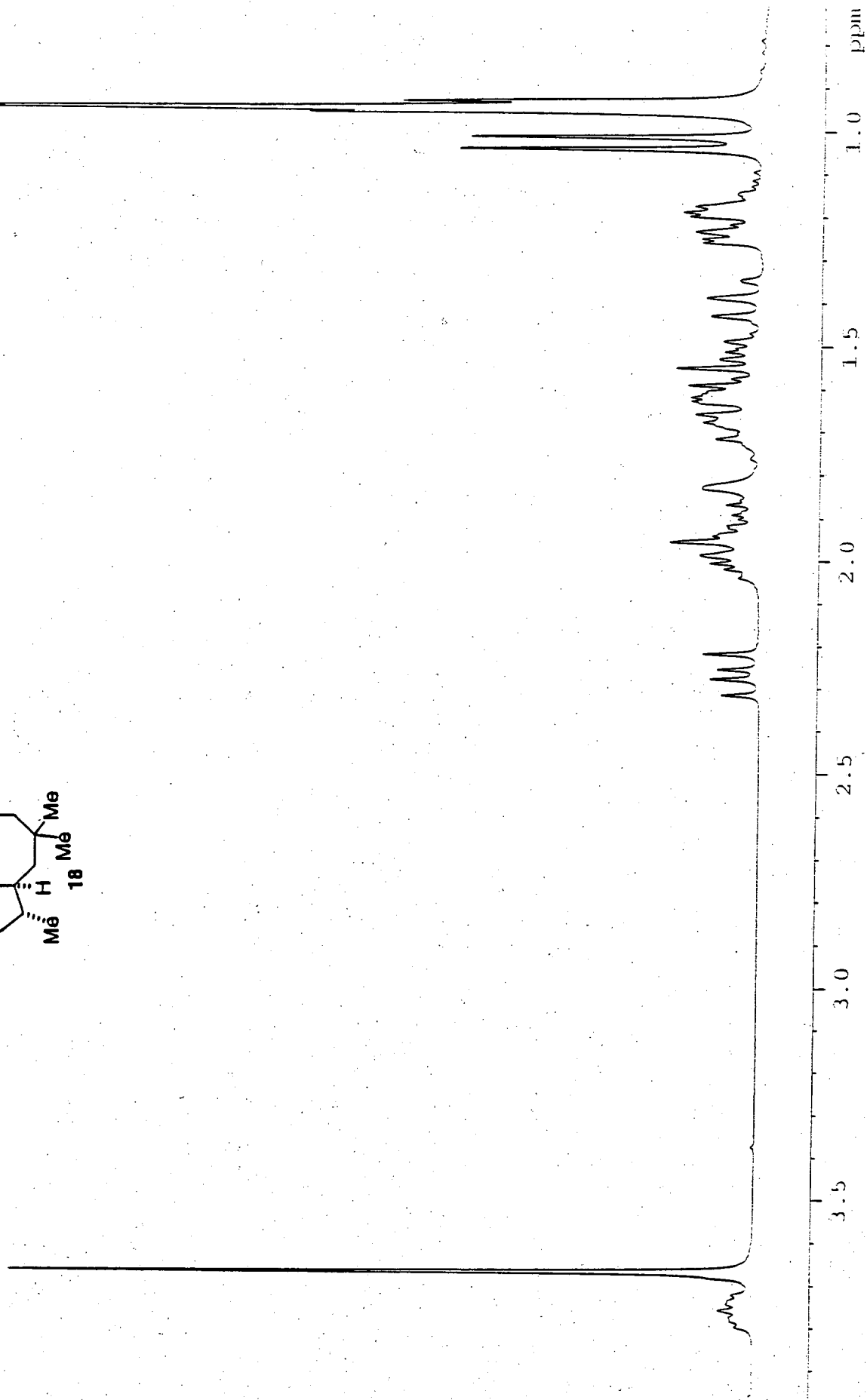
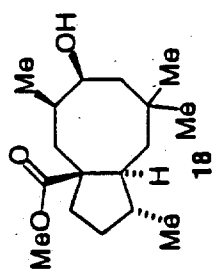


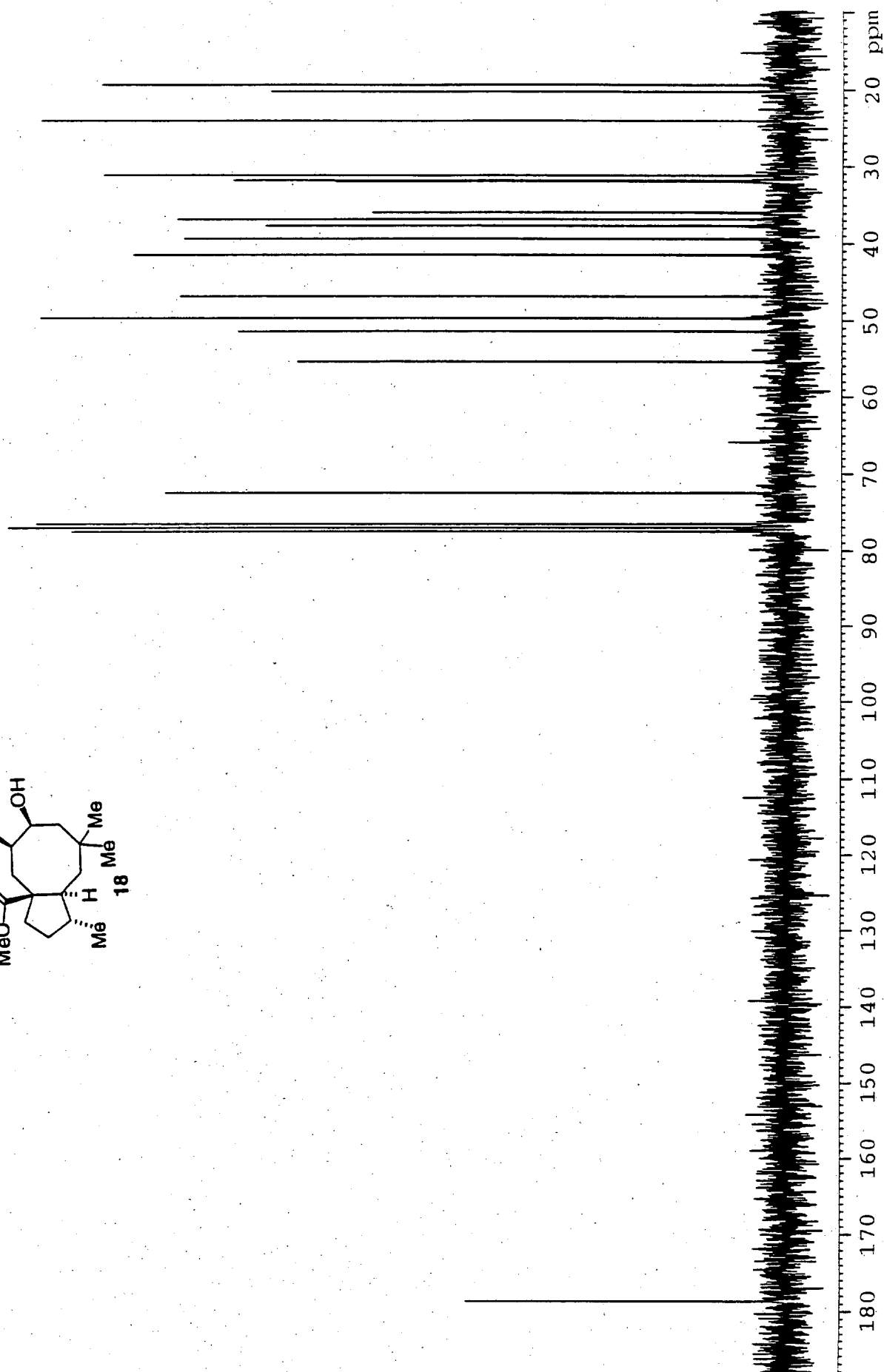
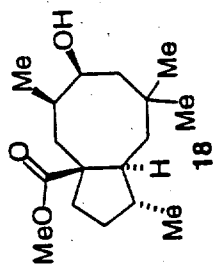


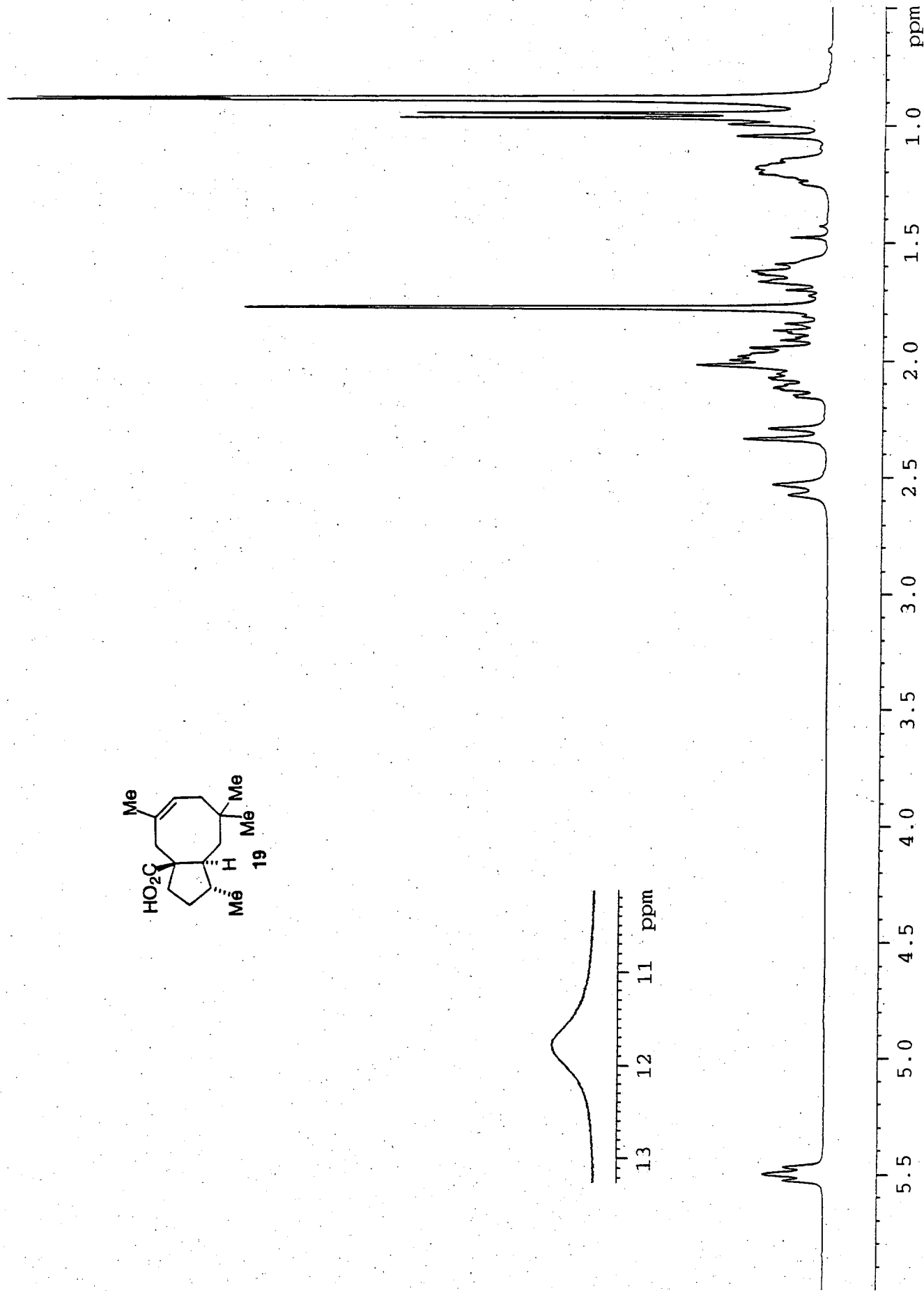
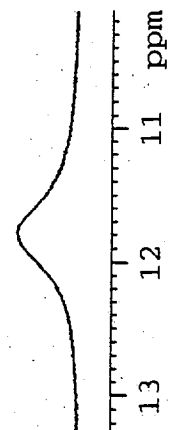
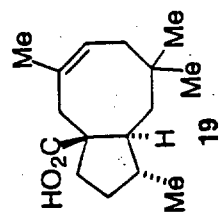


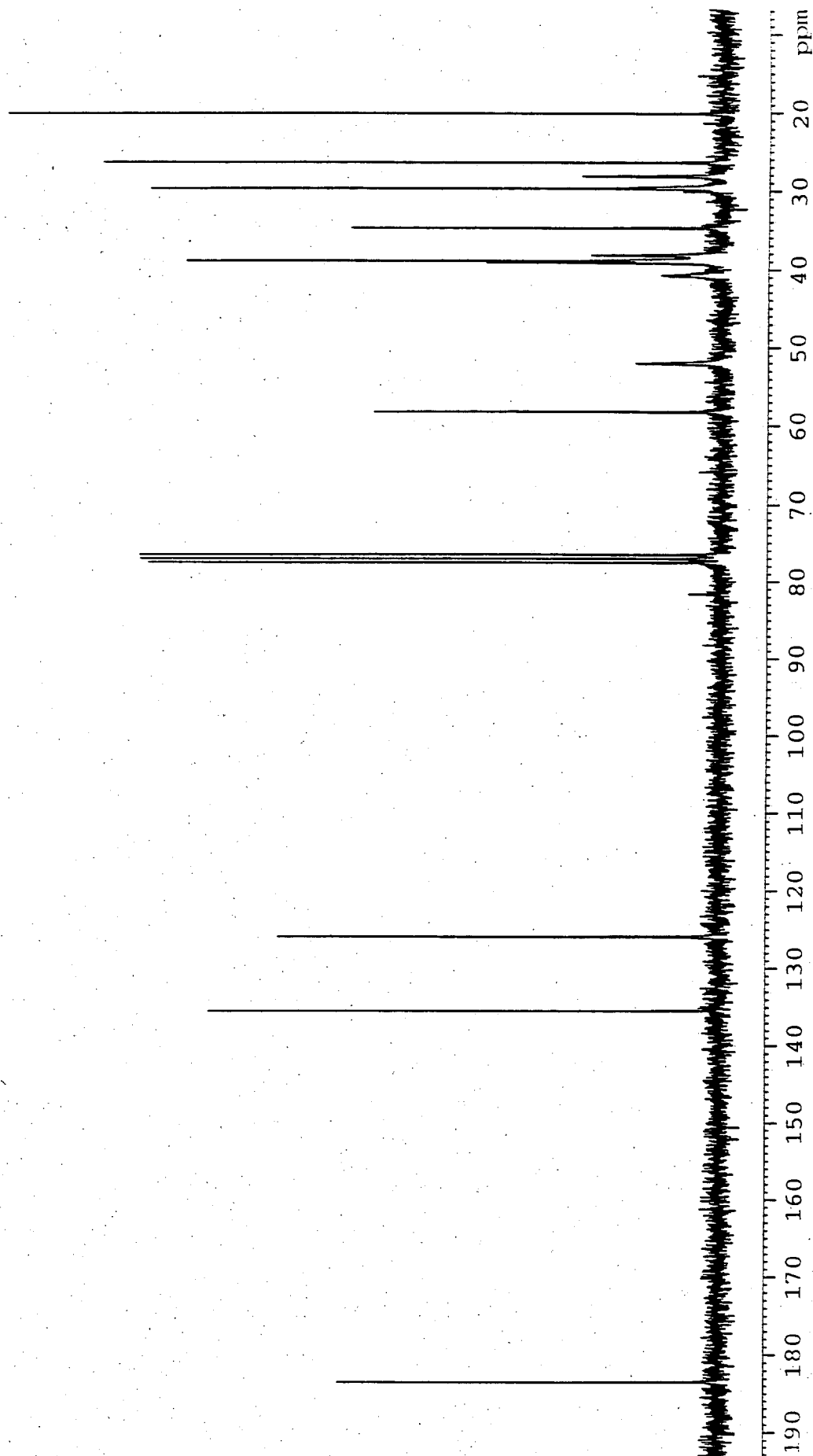
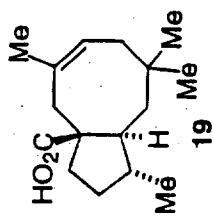












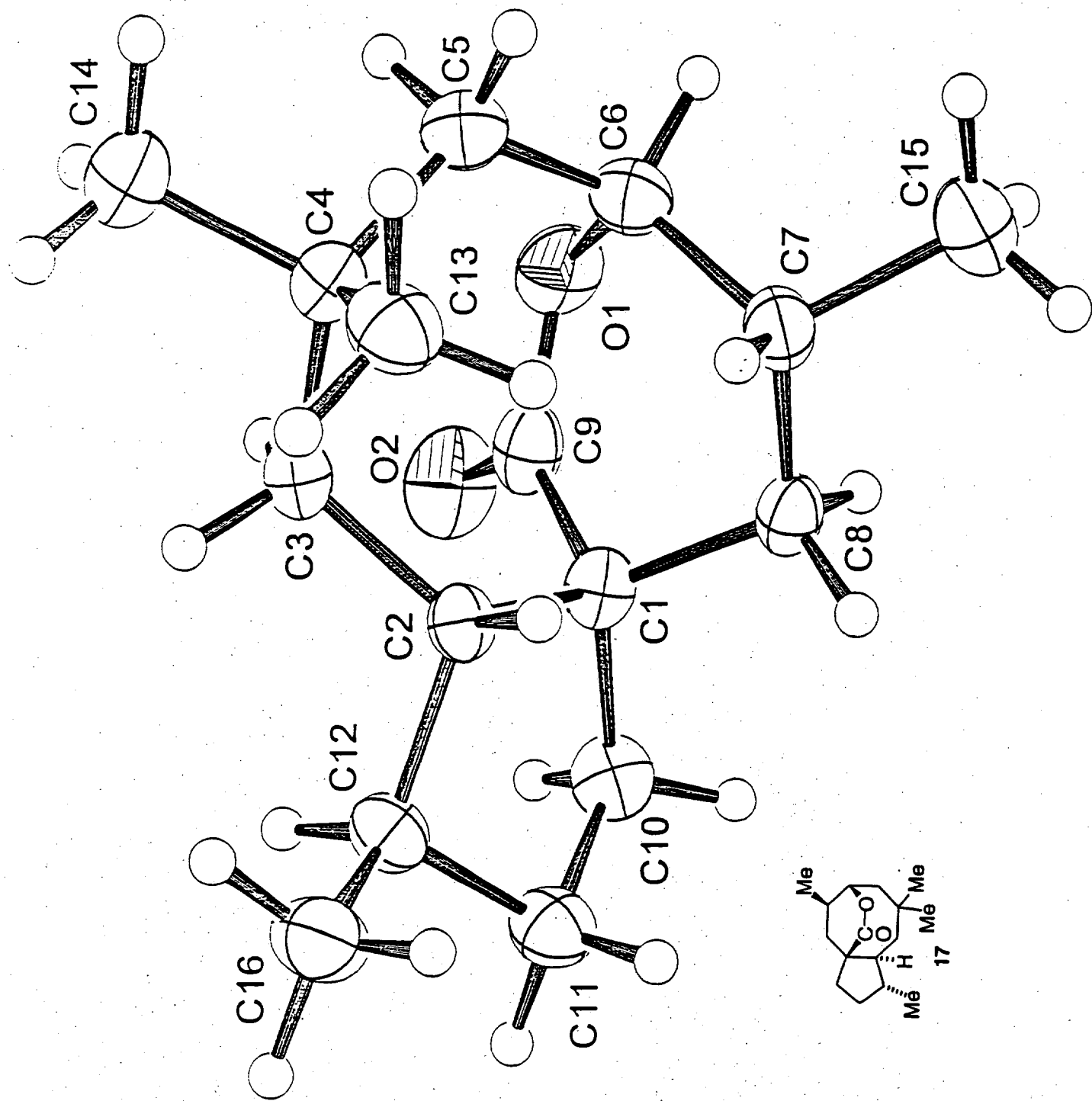


Table 1. Crystal data and structure refinement for pait1.

Identification code	PAIT1
Empirical formula	C ₁₆ H ₂₆ O ₂
Formula weight	250.37
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 6.1721(6) Å alpha = 90 deg. b = 12.8720(12) Å beta = 90 deg. c = 18.3198(17) Å gamma = 90 deg.
Volume	1455.5(2) Å ³
Z, Calculated density	4, 1.143 Mg/m ³
Absorption coefficient	0.073 mm ⁻¹
F(000)	552
Crystal size	0.45 x 0.20 x 0.10 mm
Theta range for data collection	1.93 to 27.11 deg.
Limiting indices	-7<=h<=7, -12<=k<=16, -23<=l<=22
Reflections collected / unique	9135 / 3201 [R(int) = 0.0394]
Completeness to theta = 27.11	99.9 %
Absorption correction	Multiscan
Max. and min. transmission	0.9927 and 0.9679
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3201 / 0 / 167
Goodness-of-fit on F ²	0.915
Final R indices [I>2sigma(I)]	R1 = 0.0437, wR2 = 0.0791
R indices (all data)	R1 = 0.0728, wR2 = 0.0860
Absolute structure parameter	-0.7(13)
Largest diff. peak and hole	0.150 and -0.155 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for paitl. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	9556(2)	4794(1)	7327(1)	43(1)
O(2)	8080(2)	5916(1)	6585(1)	55(1)
C(2)	13030(3)	5190(1)	6038(1)	27(1)
C(12)	13301(3)	5889(1)	5363(1)	32(1)
C(8)	13277(3)	5893(1)	7356(1)	31(1)
C(1)	11986(3)	5915(1)	6642(1)	29(1)
C(9)	9744(3)	5559(1)	6831(1)	37(1)
C(3)	11856(3)	4167(1)	5861(1)	31(1)
C(7)	13543(3)	4798(1)	7649(1)	34(1)
C(6)	11440(3)	4176(1)	7568(1)	37(1)
C(11)	13632(3)	6966(1)	5687(1)	37(1)
C(5)	11526(3)	3188(1)	7109(1)	39(1)
C(10)	11960(3)	7005(1)	6297(1)	38(1)
C(15)	14373(4)	4793(2)	8439(1)	51(1)
C(4)	12389(3)	3188(1)	6312(1)	33(1)
C(13)	14837(3)	2972(1)	6279(1)	39(1)
C(14)	11274(3)	2266(1)	5934(1)	48(1)
C(16)	15135(3)	5534(1)	4865(1)	44(1)

Table 3. Bond lengths [Å] and angles [deg] for pait1.

O(1)-C(9)	1.346(2)
O(1)-C(6)	1.476(2)
O(2)-C(9)	1.211(2)
C(2)-C(3)	1.537(2)
C(2)-C(12)	1.540(2)
C(2)-C(1)	1.584(2)
C(12)-C(11)	1.522(2)
C(12)-C(16)	1.524(2)
C(8)-C(7)	1.517(2)
C(8)-C(1)	1.532(2)
C(1)-C(9)	1.498(3)
C(1)-C(10)	1.539(2)
C(3)-C(4)	1.543(2)
C(7)-C(6)	1.533(2)
C(7)-C(15)	1.535(2)
C(6)-C(5)	1.526(2)
C(11)-C(10)	1.521(3)
C(5)-C(4)	1.554(2)
C(4)-C(14)	1.536(2)
C(4)-C(13)	1.538(3)
C(9)-O(1)-C(6)	121.92(14)
C(3)-C(2)-C(12)	112.41(13)
C(3)-C(2)-C(1)	117.41(14)
C(12)-C(2)-C(1)	105.12(13)
C(11)-C(12)-C(16)	114.02(16)
C(11)-C(12)-C(2)	103.48(13)
C(16)-C(12)-C(2)	112.70(14)
C(7)-C(8)-C(1)	112.01(13)
C(9)-C(1)-C(8)	106.14(14)
C(9)-C(1)-C(10)	111.30(15)
C(8)-C(1)-C(10)	111.88(14)
C(9)-C(1)-C(2)	110.93(14)
C(8)-C(1)-C(2)	111.96(14)
C(10)-C(1)-C(2)	104.75(13)
O(2)-C(9)-O(1)	117.04(17)
O(2)-C(9)-C(1)	125.61(17)
O(1)-C(9)-C(1)	117.32(16)
C(2)-C(3)-C(4)	119.03(13)
C(8)-C(7)-C(6)	111.08(14)
C(8)-C(7)-C(15)	111.93(14)
C(6)-C(7)-C(15)	111.78(14)
O(1)-C(6)-C(5)	108.19(14)
O(1)-C(6)-C(7)	114.48(14)
C(5)-C(6)-C(7)	117.31(15)
C(10)-C(11)-C(12)	103.01(14)
C(6)-C(5)-C(4)	121.98(14)
C(11)-C(10)-C(1)	105.35(14)
C(14)-C(4)-C(13)	106.43(15)
C(14)-C(4)-C(3)	107.11(13)
C(13)-C(4)-C(3)	109.66(14)
C(14)-C(4)-C(5)	105.64(14)
C(13)-C(4)-C(5)	111.90(14)
C(3)-C(4)-C(5)	115.51(14)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pait1.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	29(1)	52(1)	48(1)	-3(1)	9(1)	-7(1)
O(2)	26(1)	70(1)	68(1)	-8(1)	-4(1)	9(1)
C(2)	23(1)	29(1)	27(1)	-1(1)	-4(1)	3(1)
C(12)	33(1)	35(1)	29(1)	4(1)	-1(1)	5(1)
C(8)	25(1)	37(1)	30(1)	-7(1)	1(1)	-4(1)
C(1)	23(1)	32(1)	33(1)	-4(1)	1(1)	3(1)
C(9)	30(1)	43(1)	38(1)	-12(1)	1(1)	0(1)
C(3)	30(1)	35(1)	27(1)	-4(1)	-3(1)	0(1)
C(7)	33(1)	41(1)	27(1)	-3(1)	-1(1)	-4(1)
C(6)	38(1)	43(1)	30(1)	3(1)	6(1)	-6(1)
C(11)	44(1)	31(1)	37(1)	6(1)	-1(1)	5(1)
C(5)	40(1)	40(1)	37(1)	4(1)	3(1)	-7(1)
C(10)	37(1)	36(1)	41(1)	0(1)	-1(1)	7(1)
C(15)	66(2)	54(1)	33(1)	0(1)	-8(1)	-4(1)
C(4)	36(1)	29(1)	32(1)	-1(1)	-2(1)	-4(1)
C(13)	45(1)	36(1)	37(1)	4(1)	-2(1)	8(1)
C(14)	59(1)	38(1)	46(1)	-5(1)	-7(1)	-8(1)
C(16)	53(1)	41(1)	36(1)	4(1)	9(1)	-2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pait1.

	x	y	z	U(eq)
H(2)	14518	5003	6211	32
H(12)	11916	5885	5079	39
H(8A)	14726	6201	7271	37
H(8B)	12524	6323	7725	37
H(3A)	12144	4003	5342	37
H(3B)	10280	4296	5906	37
H(7)	14666	4447	7342	40
H(6)	11072	3939	8073	44
H(11A)	15119	7047	5882	45
H(11B)	13360	7515	5319	45
H(5A)	10035	2906	7092	47
H(5B)	12411	2680	7384	47
H(10A)	10506	7168	6099	45
H(10B)	12353	7539	6662	45
H(15A)	15808	5117	8458	76
H(15B)	14474	4075	8613	76
H(15C)	13367	5183	8749	76
H(13A)	15319	2980	5770	59
H(13B)	15139	2290	6494	59
H(13C)	15614	3509	6554	59
H(14A)	11917	2160	5451	72
H(14B)	9723	2412	5882	72
H(14C)	11470	1638	6229	72
H(16A)	15211	5990	4438	66
H(16B)	14864	4819	4706	66
H(16C)	16510	5564	5132	66

Table 6. Torsion angles [deg] for pait1.

C(3)-C(2)-C(12)-C(11)	158.56(14)
C(1)-C(2)-C(12)-C(11)	29.71(17)
C(3)-C(2)-C(12)-C(16)	-77.79(19)
C(1)-C(2)-C(12)-C(16)	153.36(14)
C(7)-C(8)-C(1)-C(9)	65.50(18)
C(7)-C(8)-C(1)-C(10)	-172.92(14)
C(7)-C(8)-C(1)-C(2)	-55.68(18)
C(3)-C(2)-C(1)-C(9)	-11.5(2)
C(12)-C(2)-C(1)-C(9)	114.29(15)
C(3)-C(2)-C(1)-C(8)	106.86(16)
C(12)-C(2)-C(1)-C(8)	-127.34(14)
C(3)-C(2)-C(1)-C(10)	-131.70(15)
C(12)-C(2)-C(1)-C(10)	-5.90(17)
C(6)-O(1)-C(9)-O(2)	169.09(15)
C(6)-O(1)-C(9)-C(1)	-12.3(2)
C(8)-C(1)-C(9)-O(2)	140.51(18)
C(10)-C(1)-C(9)-O(2)	18.6(2)
C(2)-C(1)-C(9)-O(2)	-97.7(2)
C(8)-C(1)-C(9)-O(1)	-37.9(2)
C(10)-C(1)-C(9)-O(1)	-159.90(14)
C(2)-C(1)-C(9)-O(1)	83.89(18)
C(12)-C(2)-C(3)-C(4)	150.05(14)
C(1)-C(2)-C(3)-C(4)	-87.83(18)
C(1)-C(8)-C(7)-C(6)	-41.45(18)
C(1)-C(8)-C(7)-C(15)	-167.18(15)
C(9)-O(1)-C(6)-C(5)	-94.95(16)
C(9)-O(1)-C(6)-C(7)	37.9(2)
C(8)-C(7)-C(6)-O(1)	-8.1(2)
C(15)-C(7)-C(6)-O(1)	117.72(16)
C(8)-C(7)-C(6)-C(5)	120.33(16)
C(15)-C(7)-C(6)-C(5)	-113.87(17)
C(16)-C(12)-C(11)-C(10)	-165.41(15)
C(2)-C(12)-C(11)-C(10)	-42.63(17)
O(1)-C(6)-C(5)-C(4)	77.3(2)
C(7)-C(6)-C(5)-C(4)	-54.0(2)
C(12)-C(11)-C(10)-C(1)	39.20(17)
C(9)-C(1)-C(10)-C(11)	-140.18(15)
C(8)-C(1)-C(10)-C(11)	101.26(16)
C(2)-C(1)-C(10)-C(11)	-20.23(18)
C(2)-C(3)-C(4)-C(14)	-170.84(16)
C(2)-C(3)-C(4)-C(13)	-55.7(2)
C(2)-C(3)-C(4)-C(5)	71.8(2)
C(6)-C(5)-C(4)-C(14)	-153.91(17)
C(6)-C(5)-C(4)-C(13)	90.7(2)
C(6)-C(5)-C(4)-C(3)	-35.7(2)

Symmetry transformations used to generate equivalent atoms: