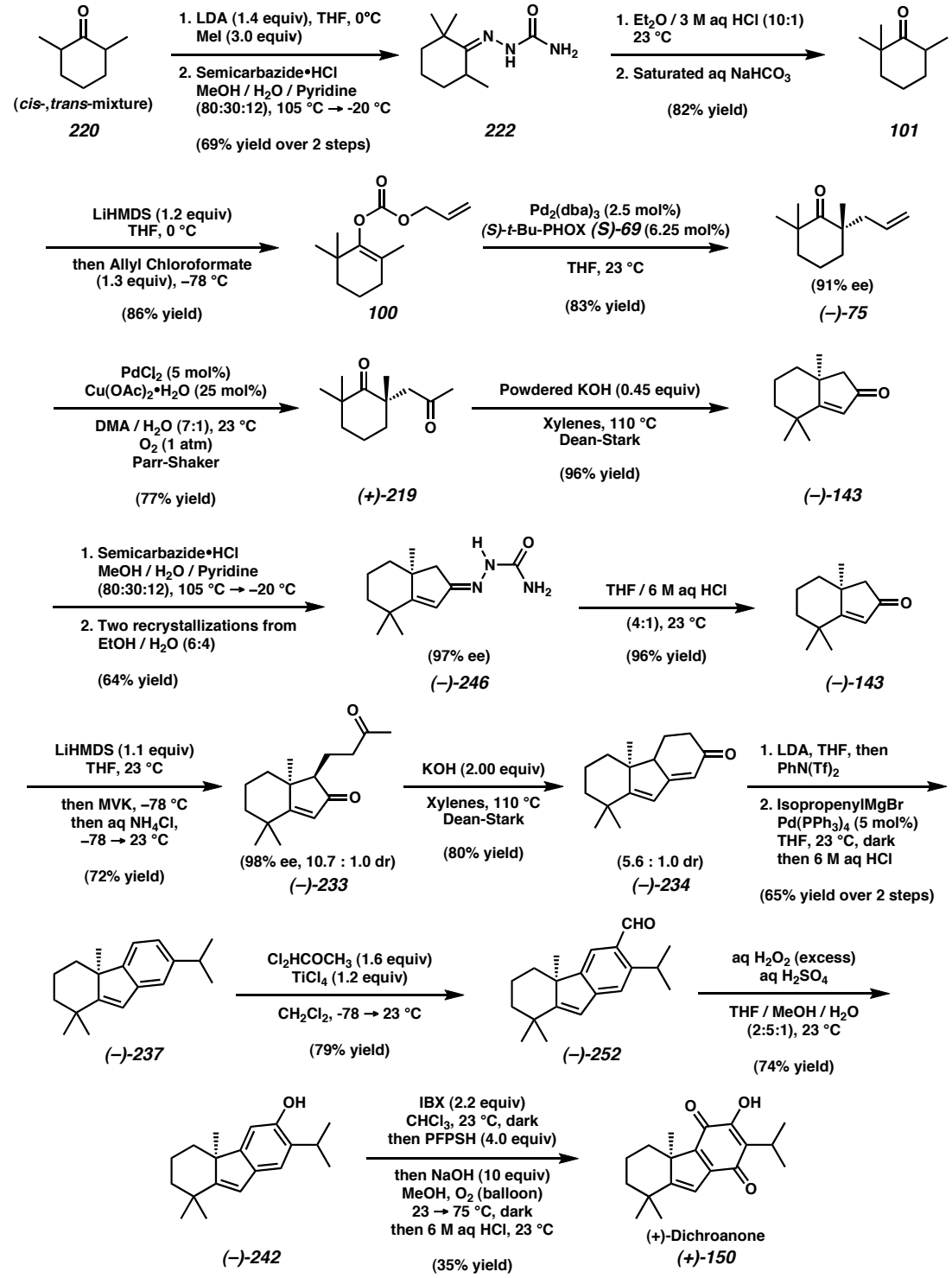
Appendix THREE

Synthetic Summary of the Enantioselective Total Synthesis of (+)-Dichroanone

Scheme A3.1 Enantioselective Total Synthesis of (+)-Dichroanone



Appendix FOUR

Spectra of Compounds Relevant to Chapter 3

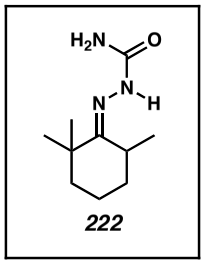


Figure A4.1 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **222**.

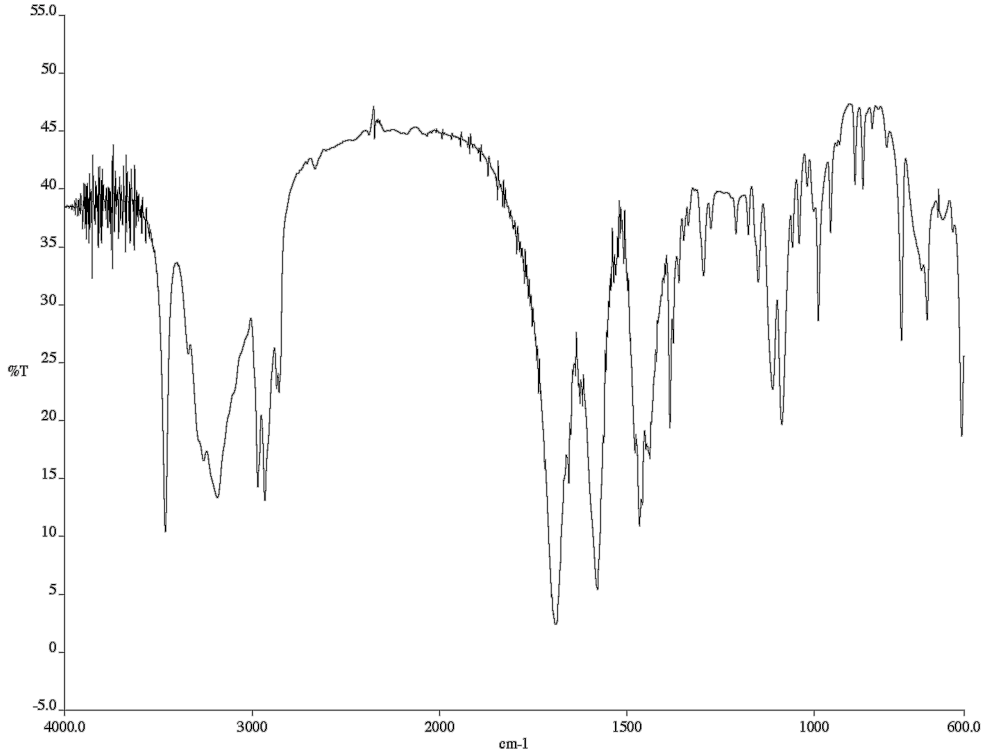


Figure A4.2 Infrared spectrum (KBr) of compound **222**.

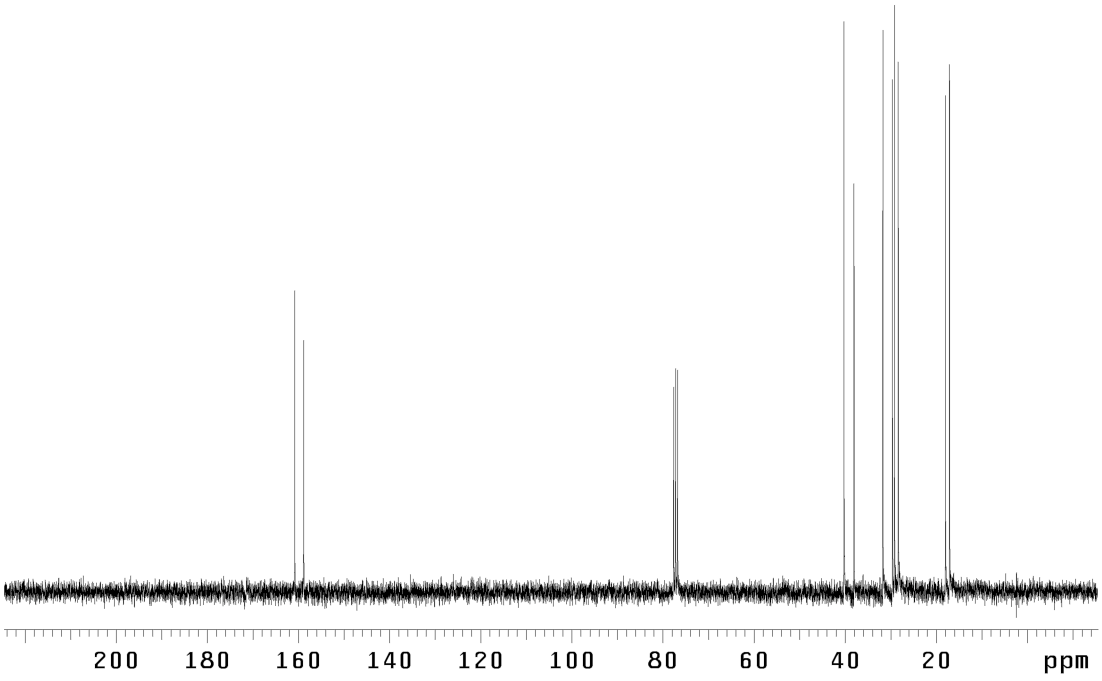


Figure A4.3 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **222**.

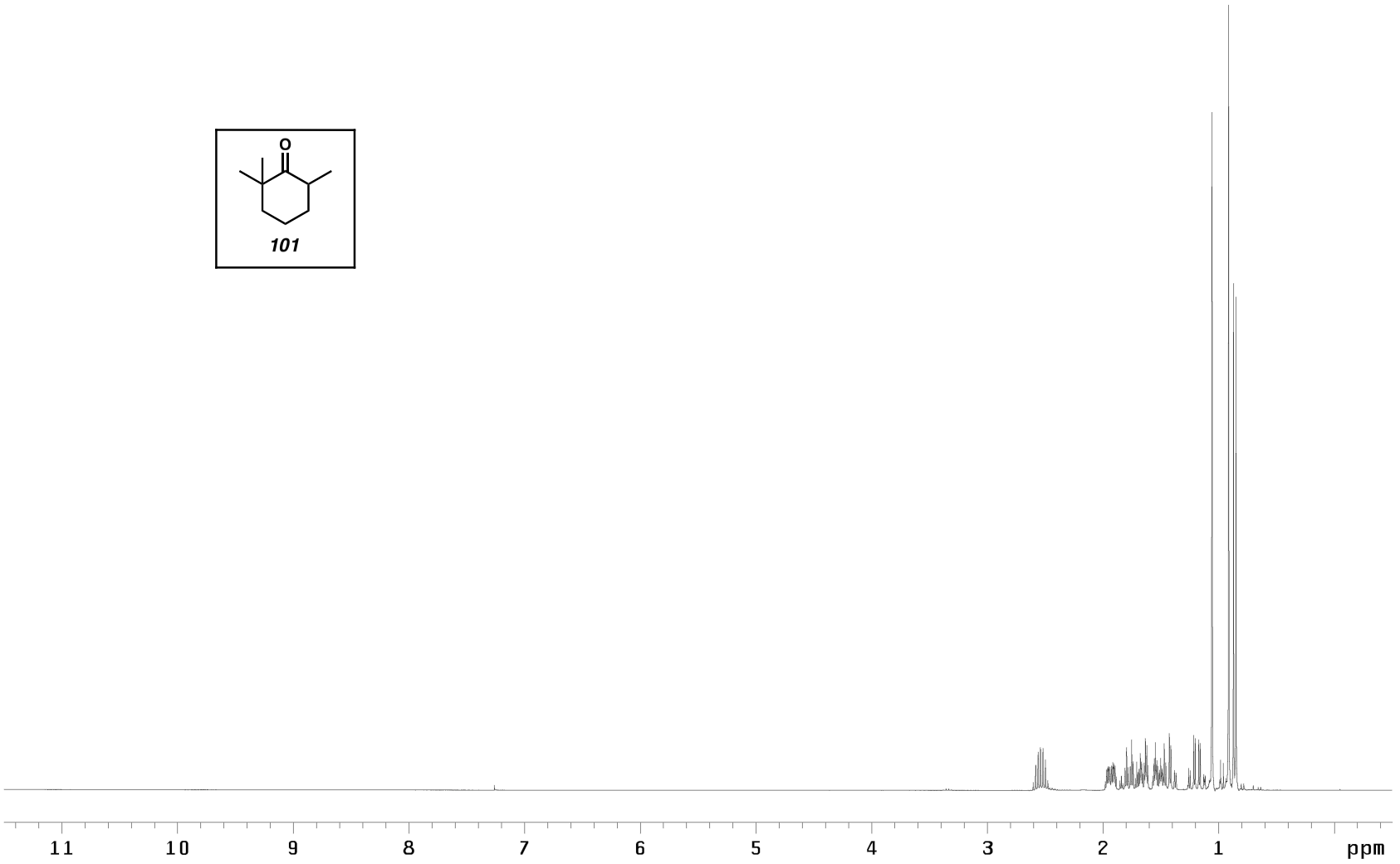


Figure A4.4 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **101**.

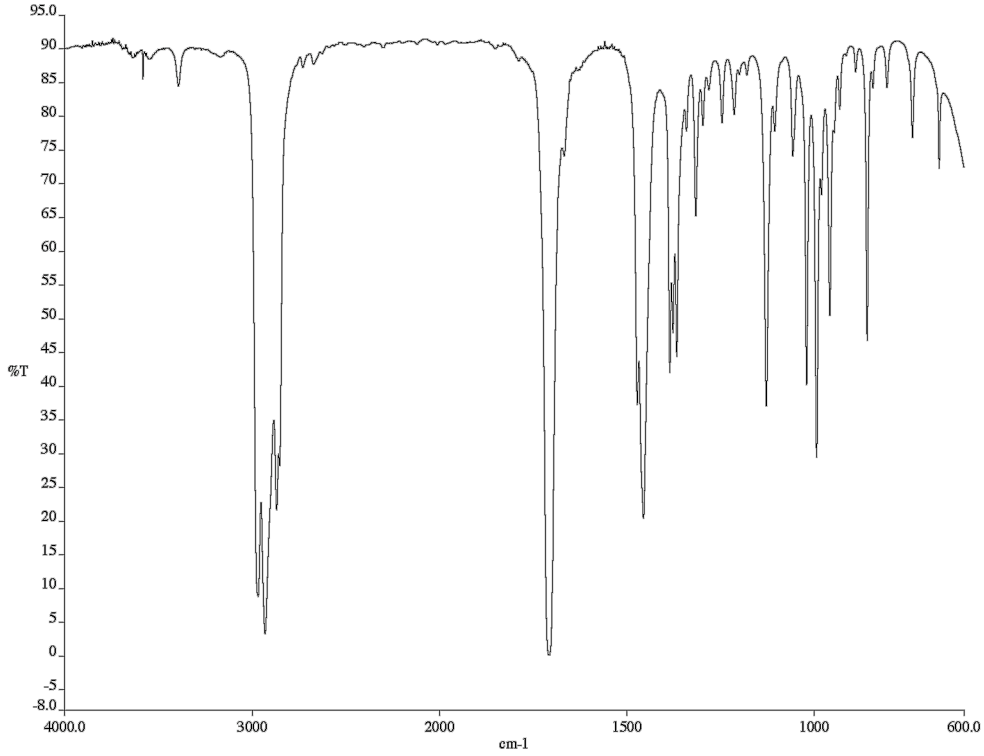


Figure A4.5 Infrared spectrum ($NaCl/CDCl_3$) of compound **101**.

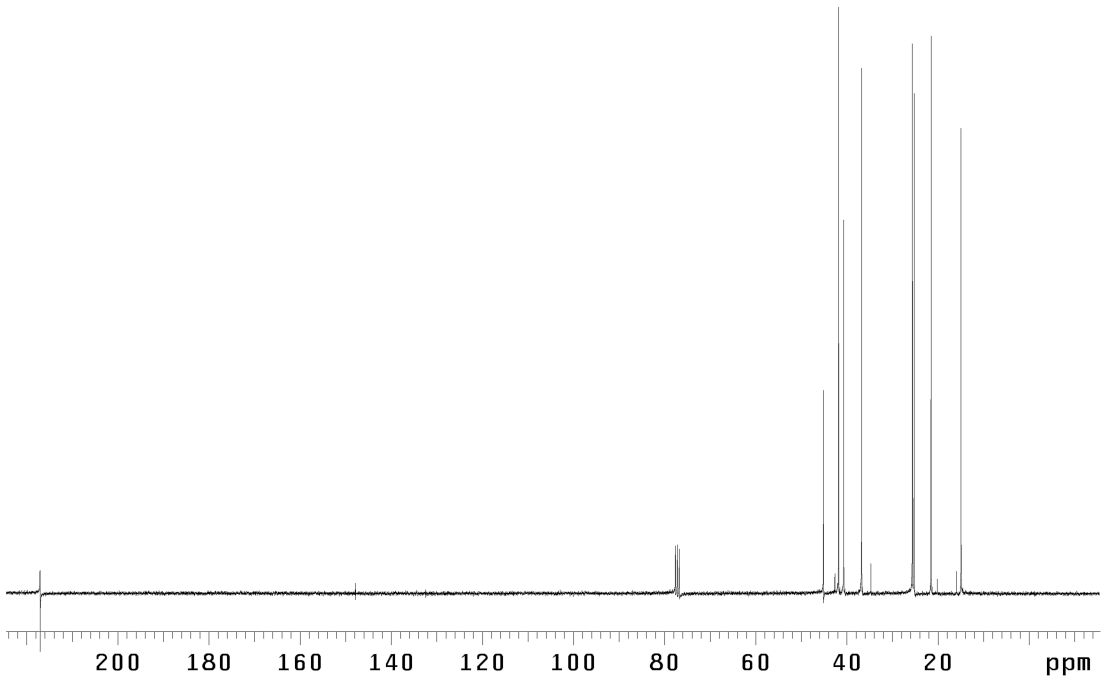


Figure A4.6 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **101**.

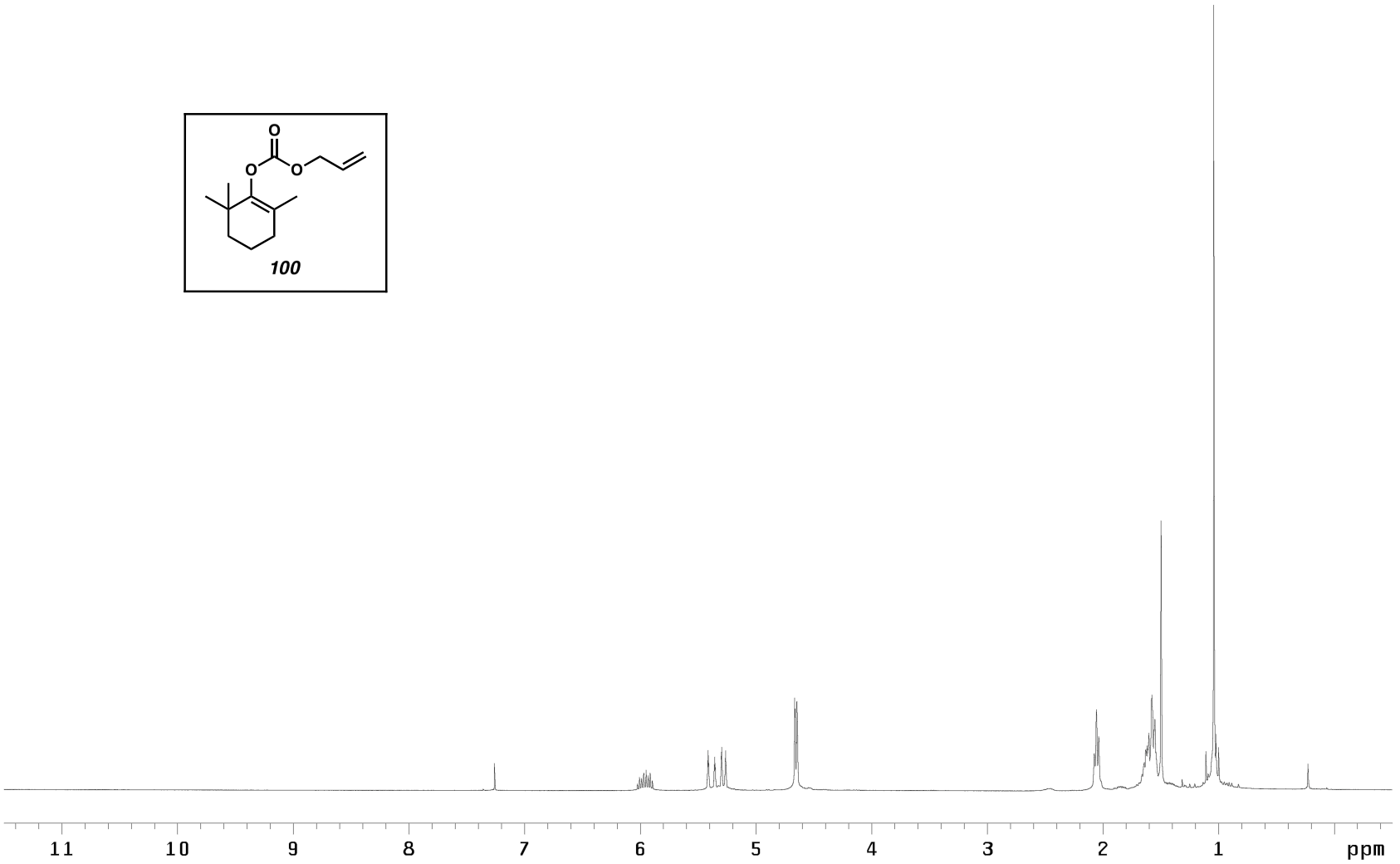


Figure A4.7 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **100**.

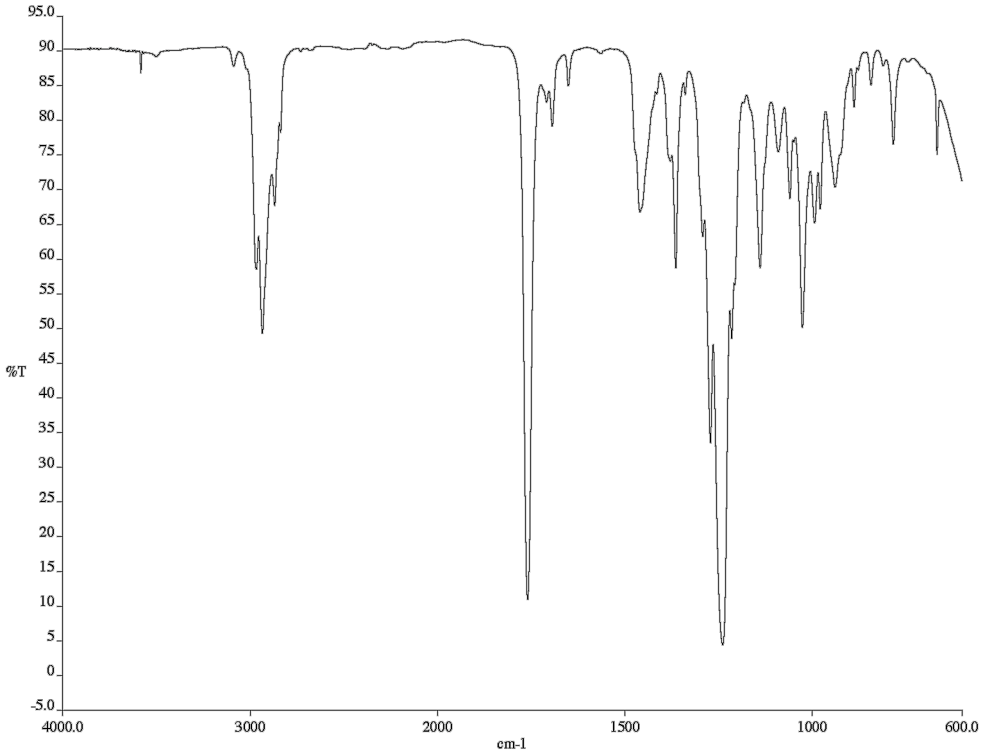


Figure A4.8 Infrared spectrum ($NaCl/CDCl_3$) of compound **100**.

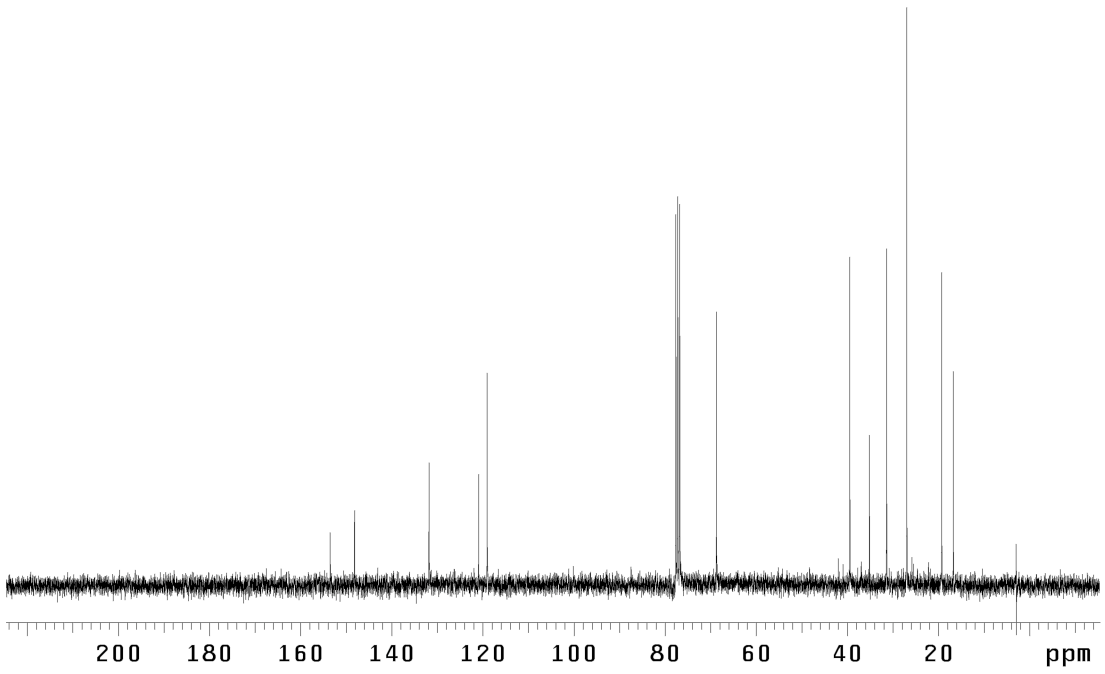


Figure A4.9 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **100**.

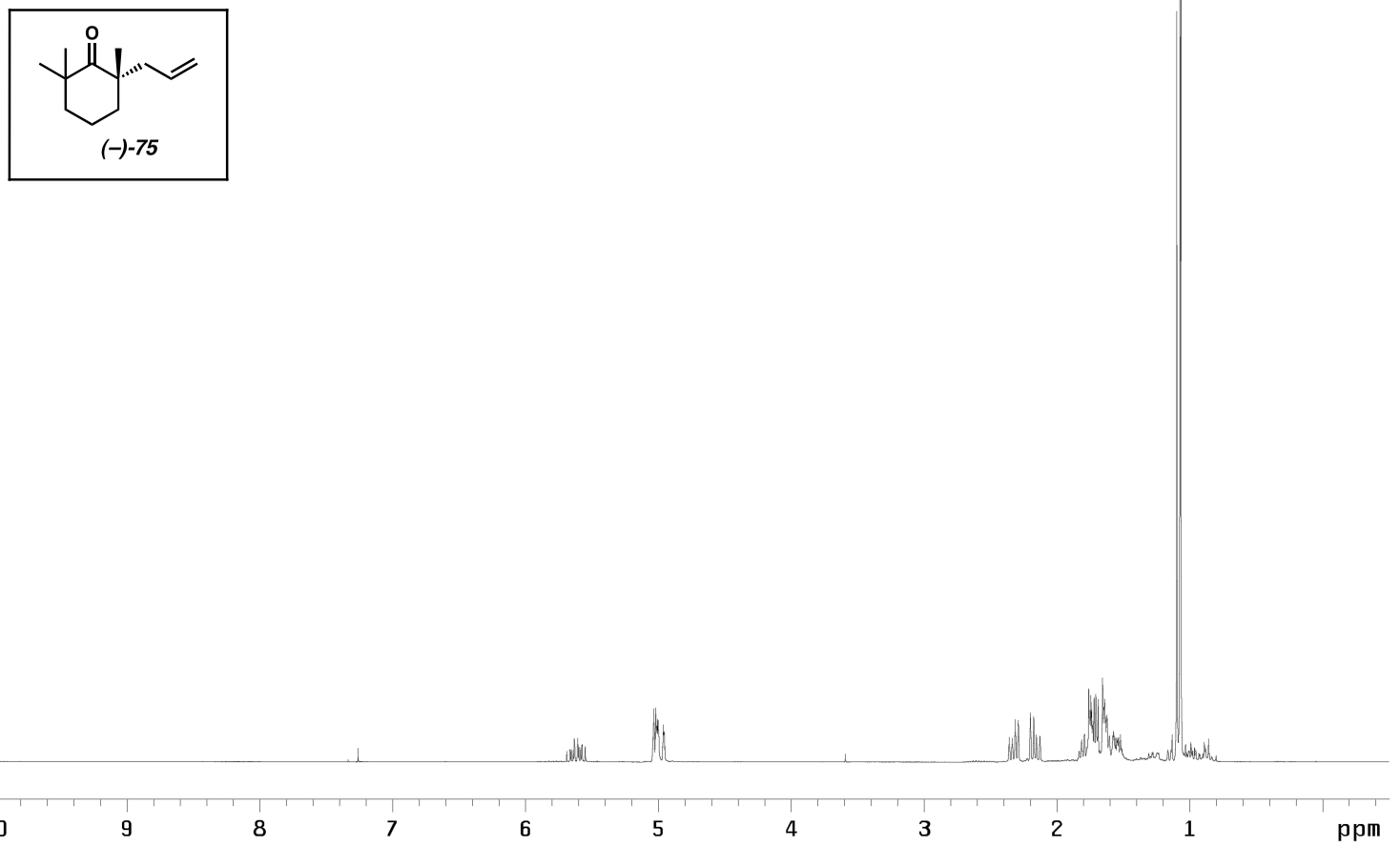


Figure A4.10 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **75**.

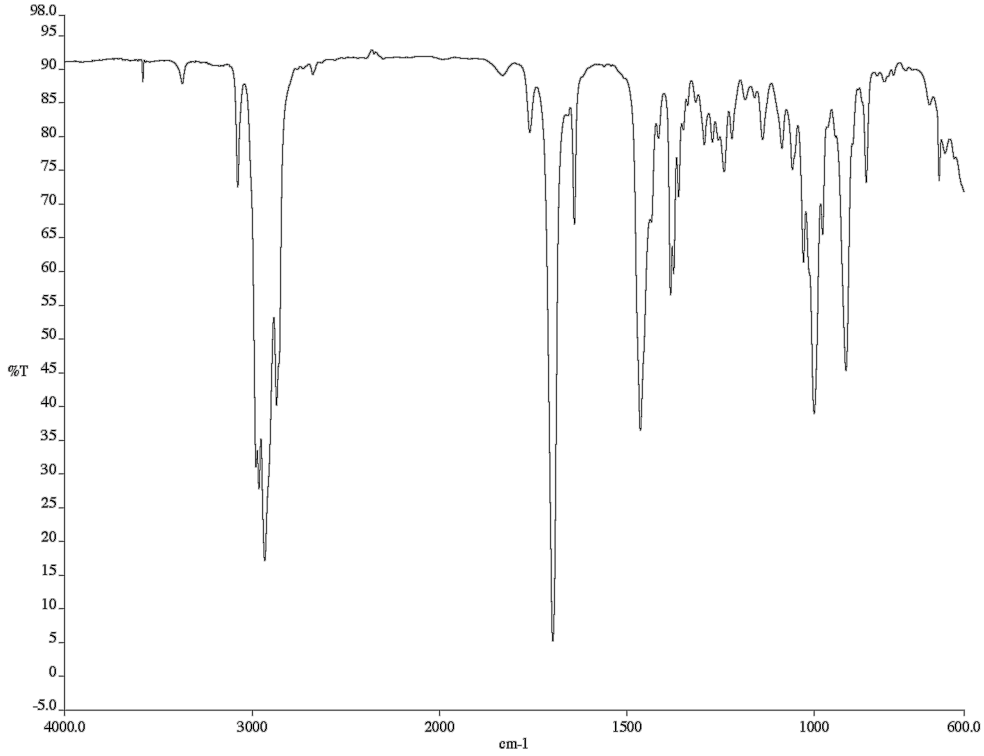


Figure A4.11 Infrared spectrum ($NaCl/CDCl_3$) of compound **75**.

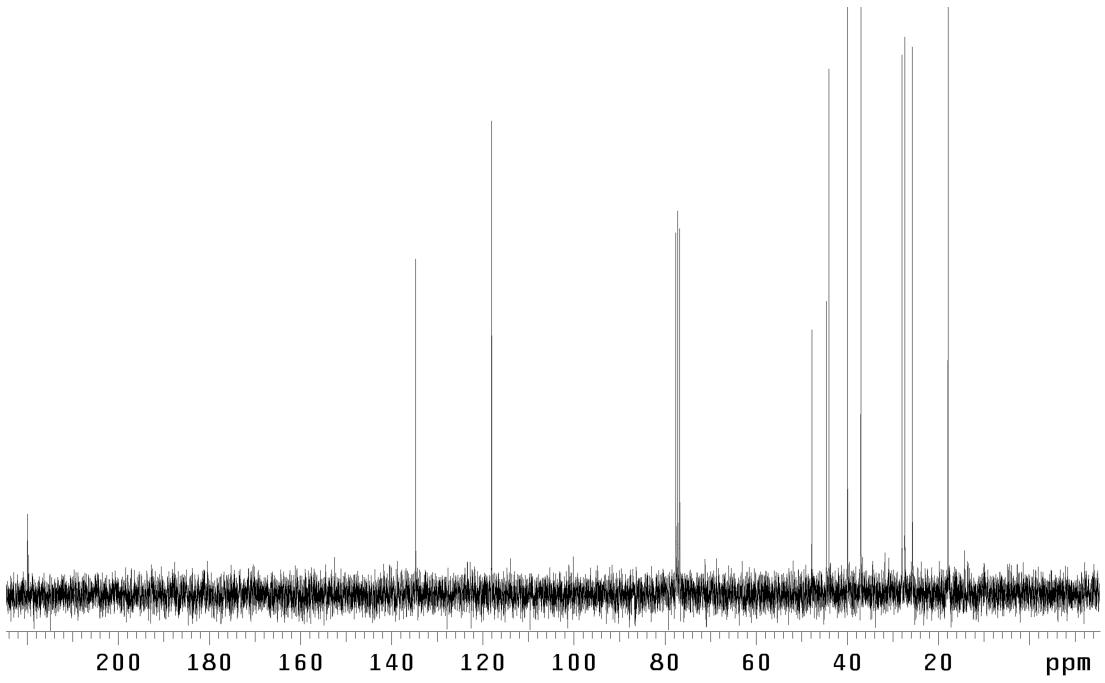


Figure A4.12 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **75**.

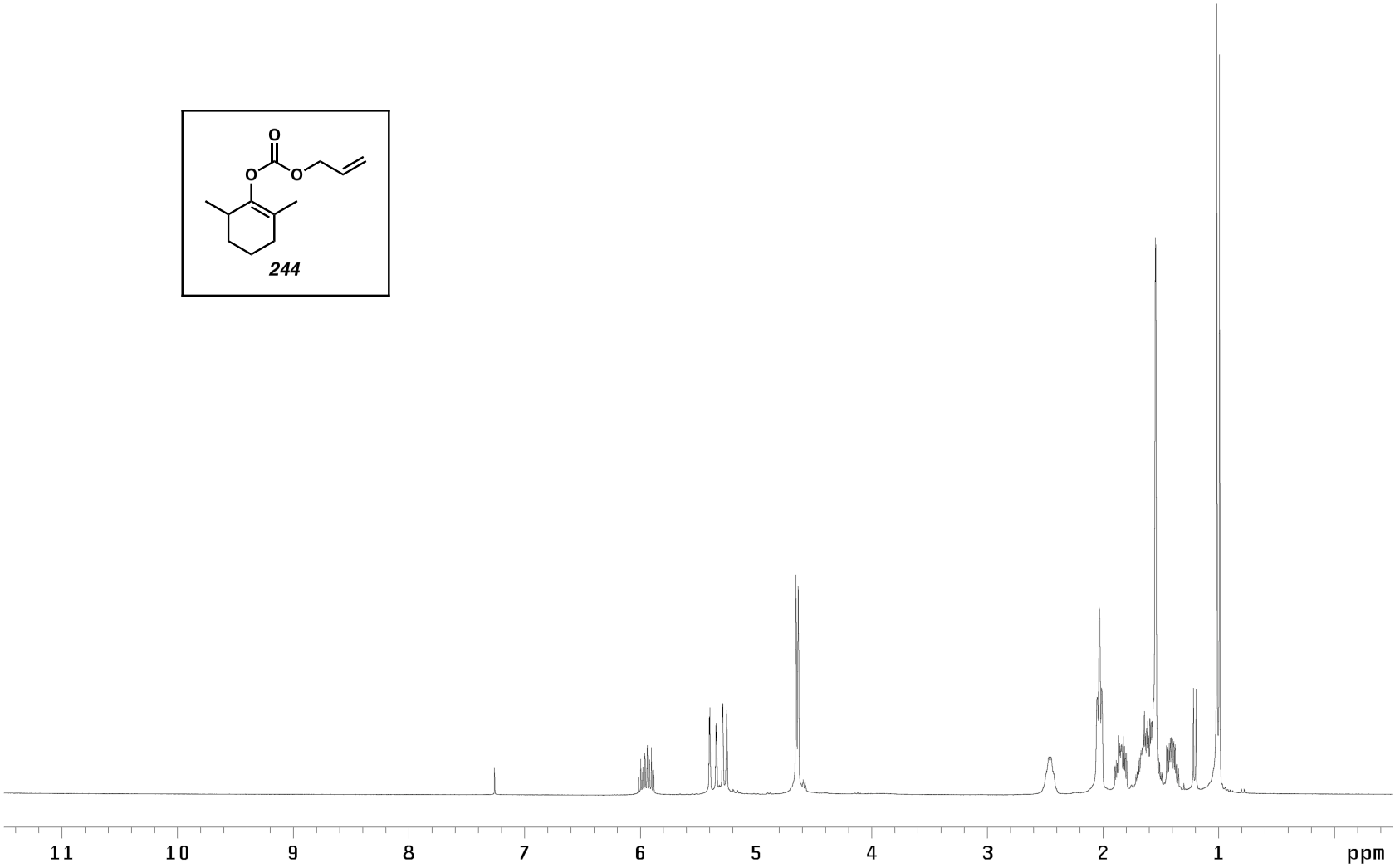


Figure A4.13 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **244**.

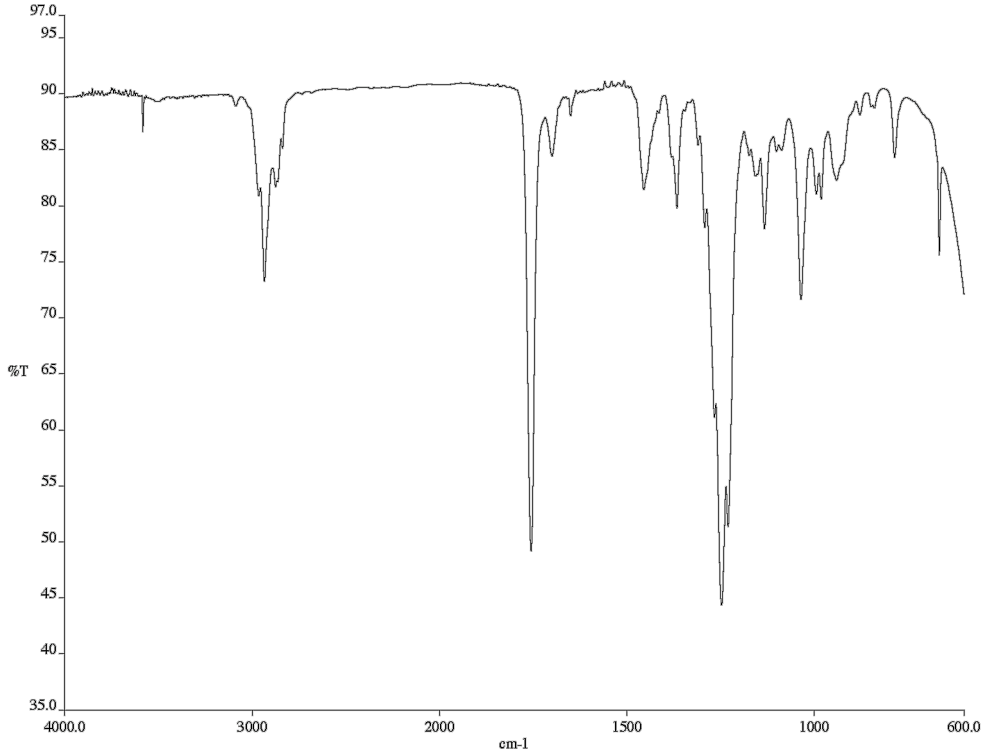


Figure A4.14 Infrared spectrum ($NaCl/CDCl_3$) of compound **244**.

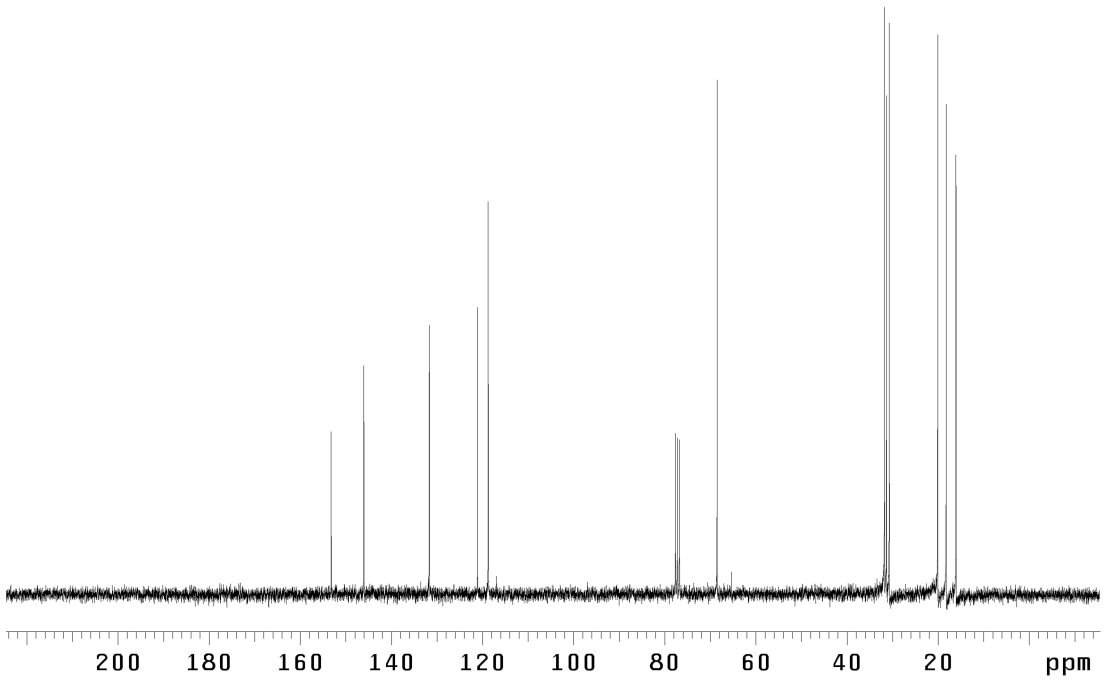


Figure A4.15 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **244**.

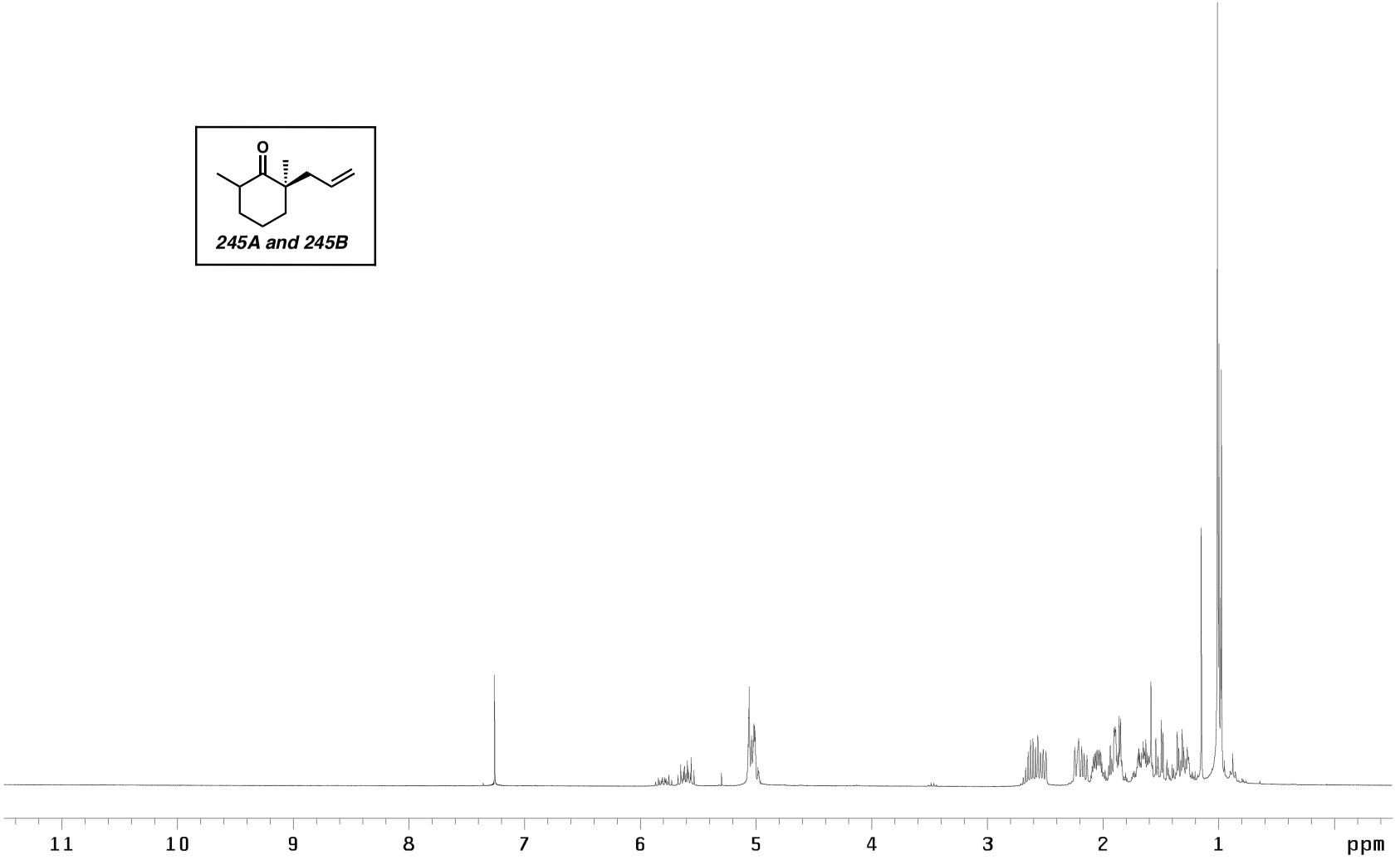


Figure A4.16 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **245A** and **245B**.

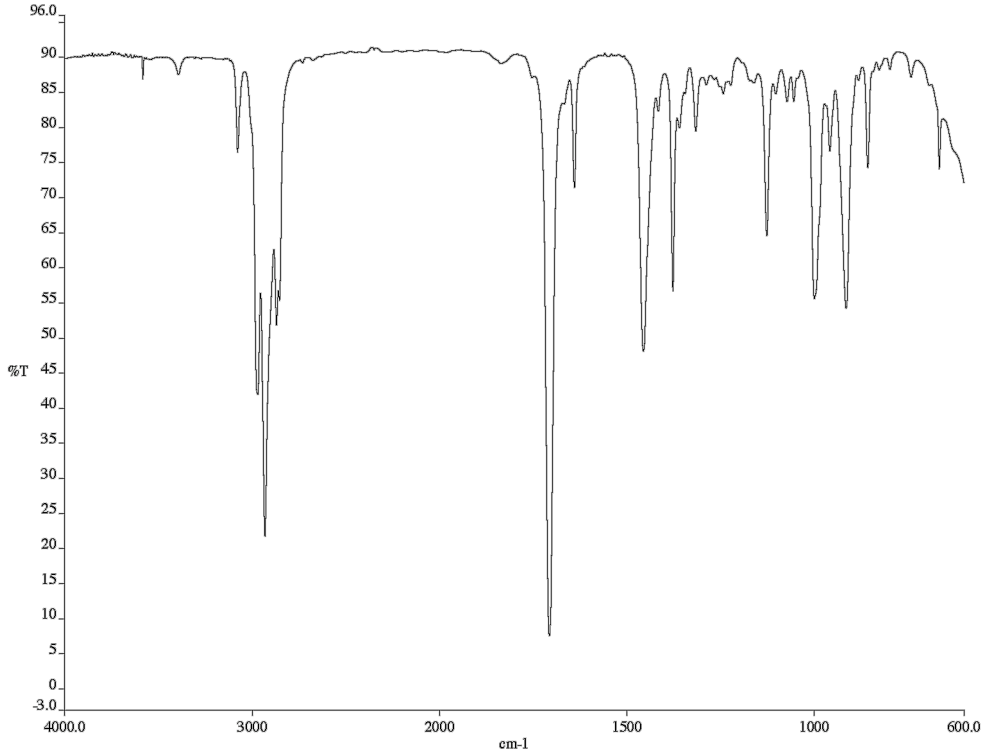


Figure A4.17 Infrared spectrum ($NaCl/CDCl_3$) of compound **245A** and **245B**.

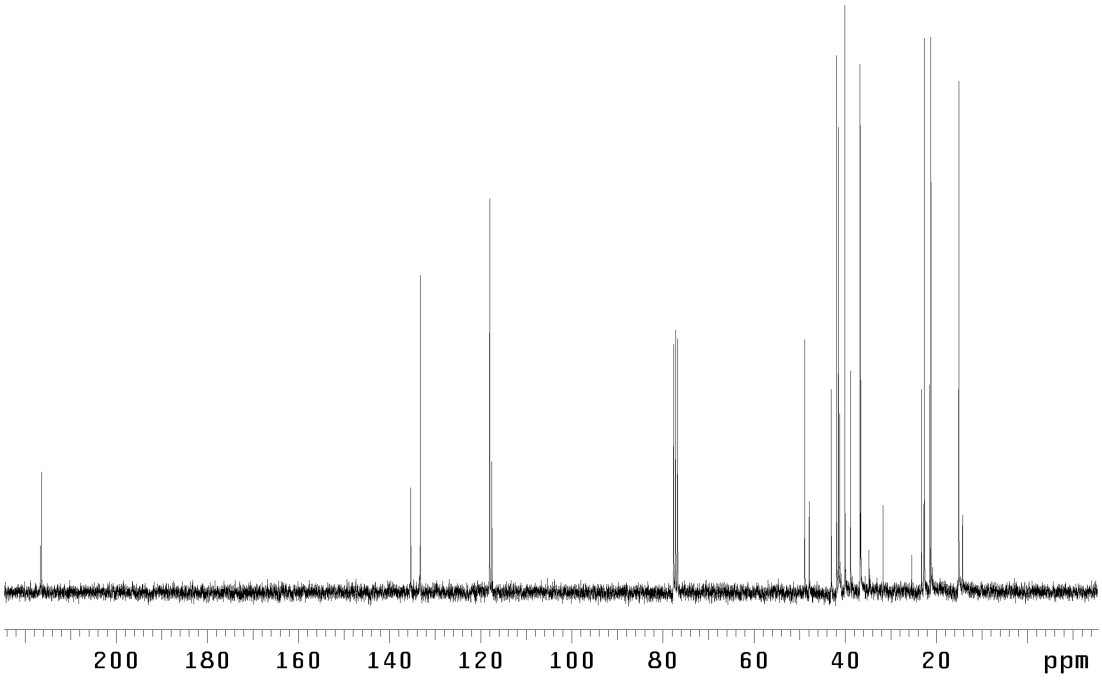


Figure A4.18 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **245A** and **245B**.

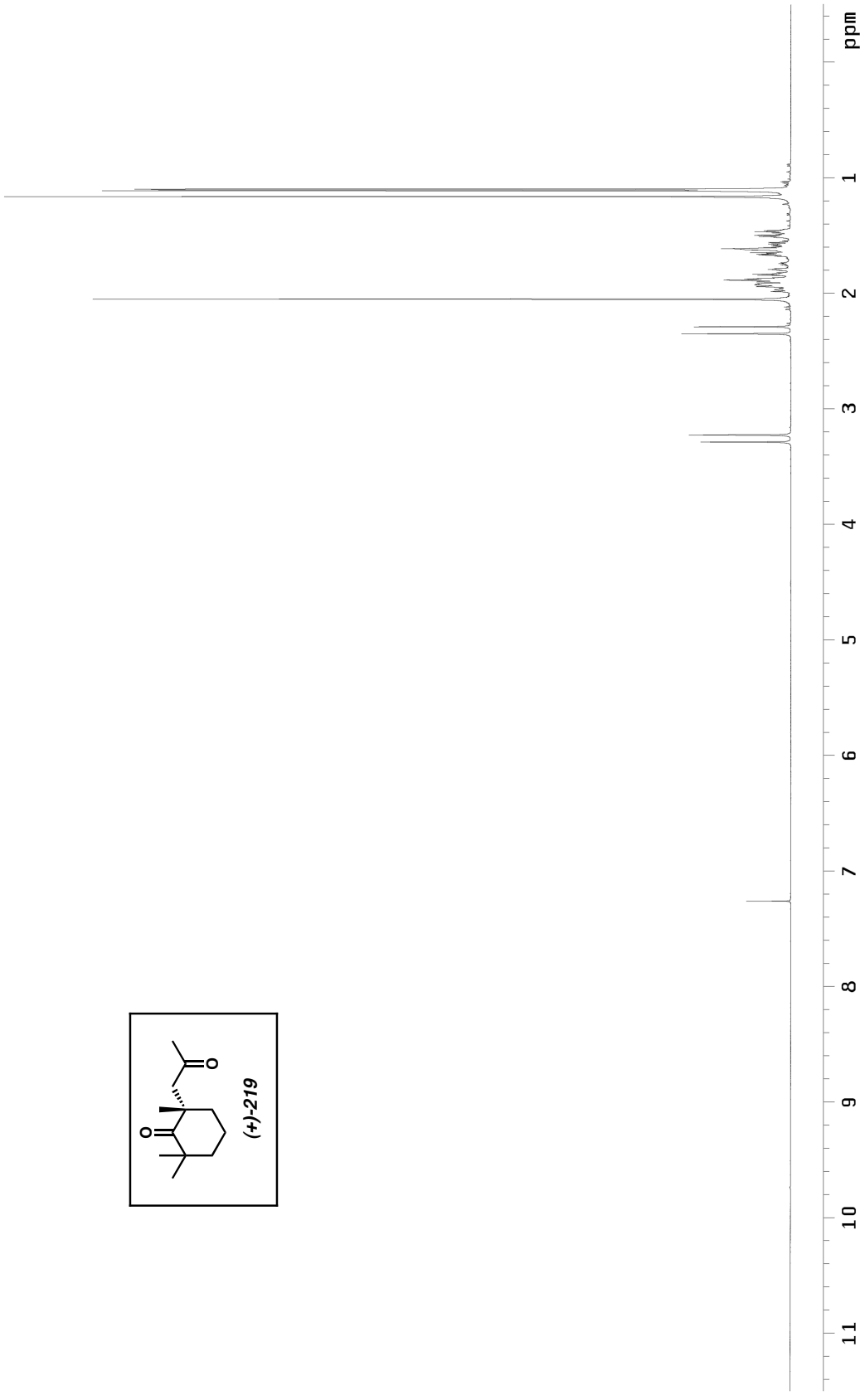


Figure A4.19 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **219**.

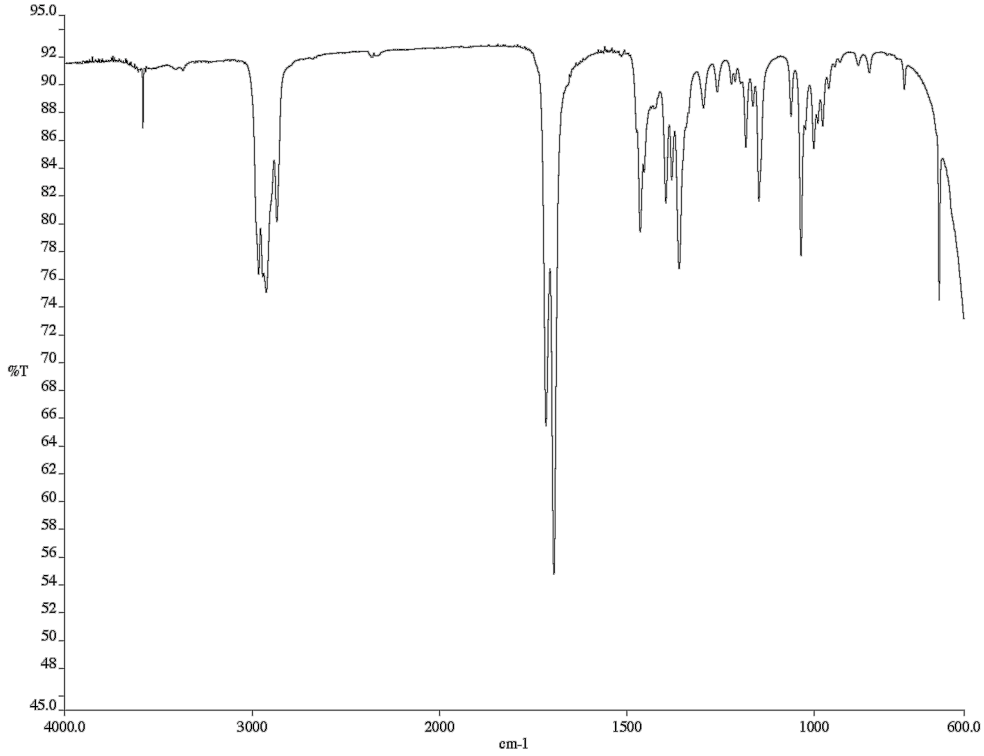


Figure A4.20 Infrared spectrum (NaCl/$CDCl_3$) of compound **219**.

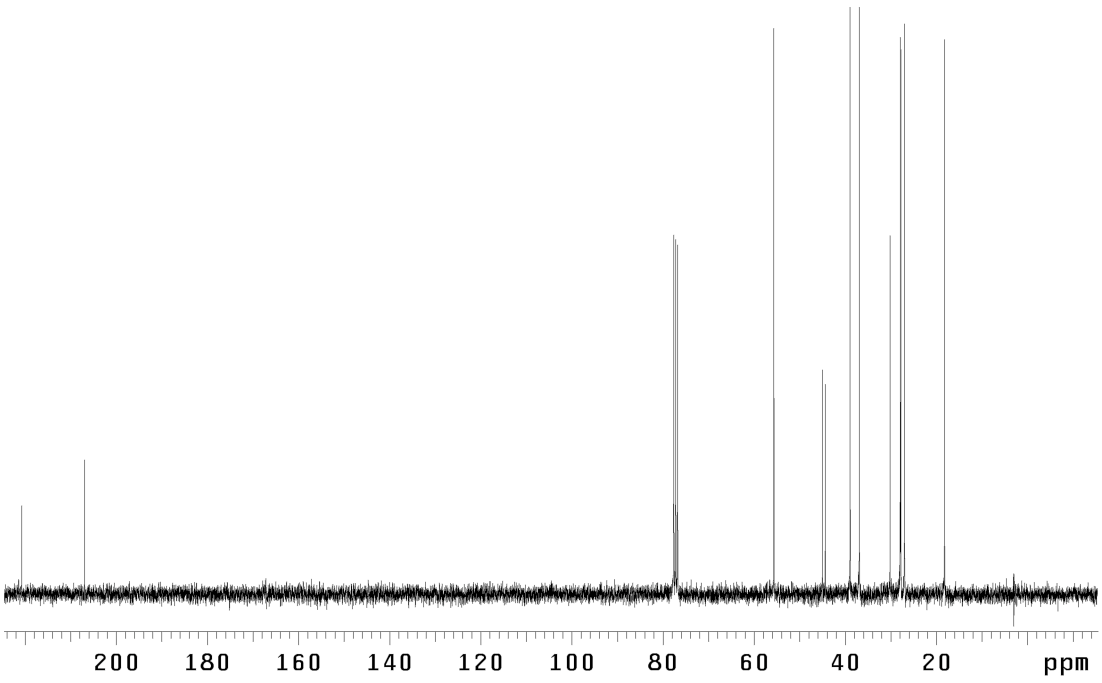


Figure A4.21 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **219**.

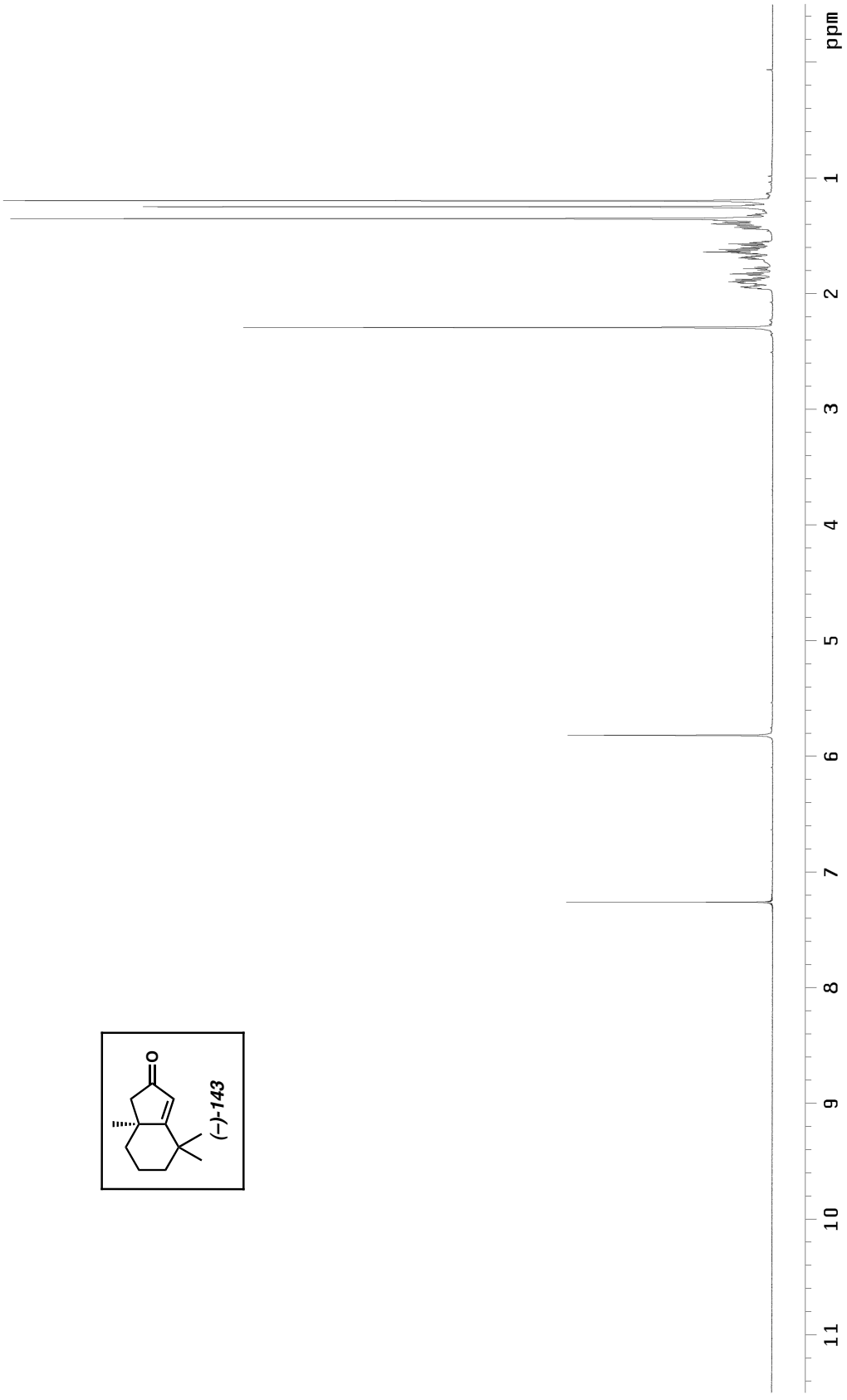


Figure A4.22 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **143**.

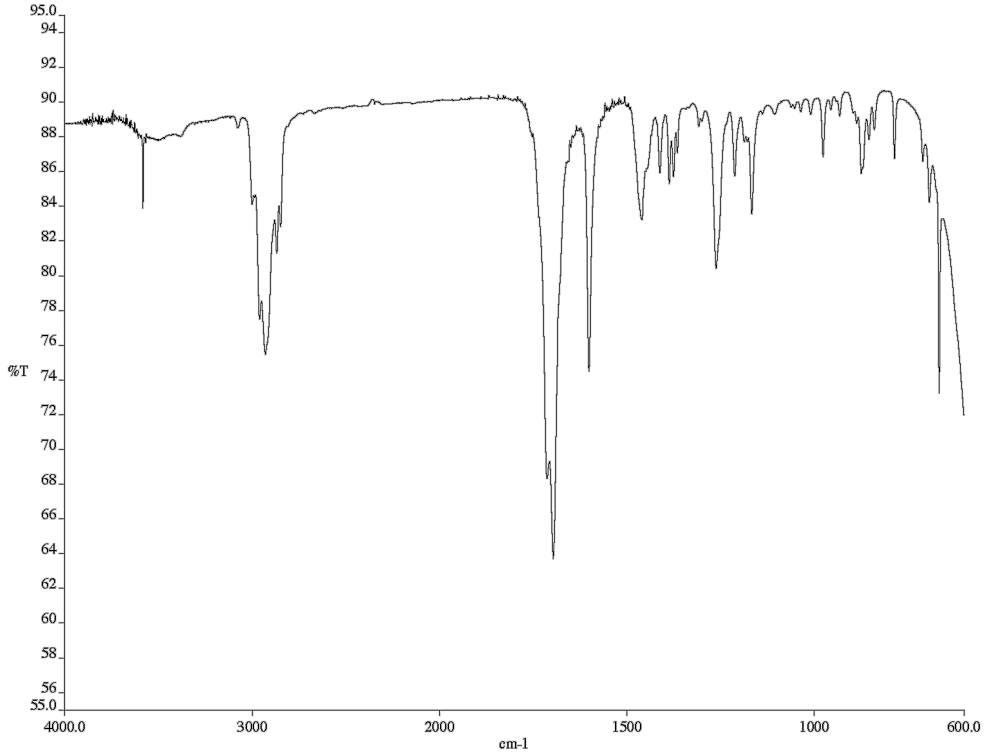


Figure A4.23 Infrared spectrum ($NaCl/CDCl_3$) of compound **143**.

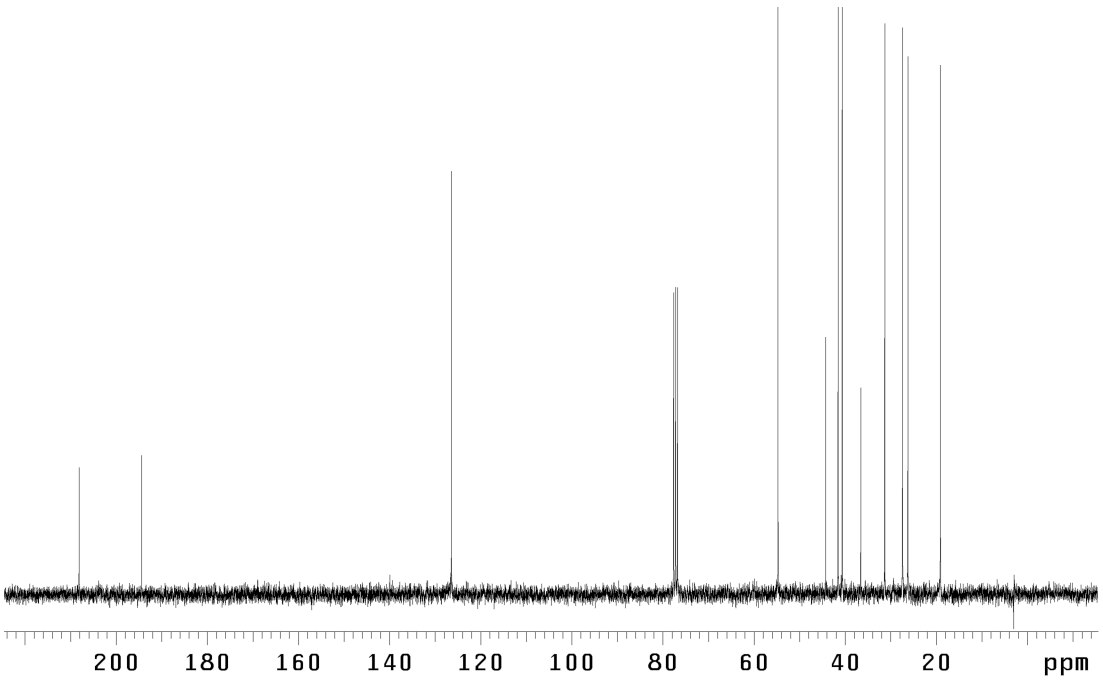


Figure A4.24 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **143**.

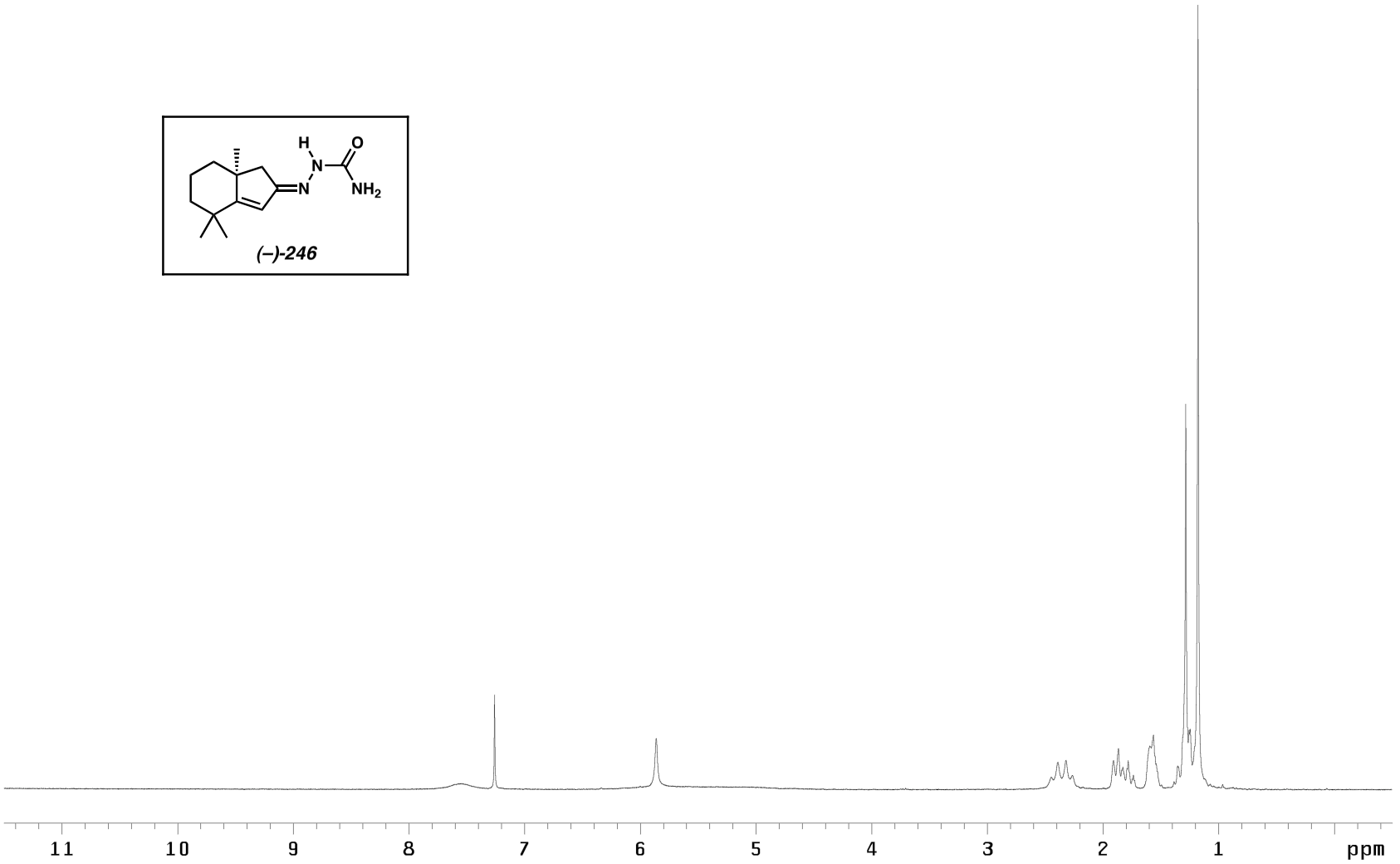


Figure A4.25 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **246**.

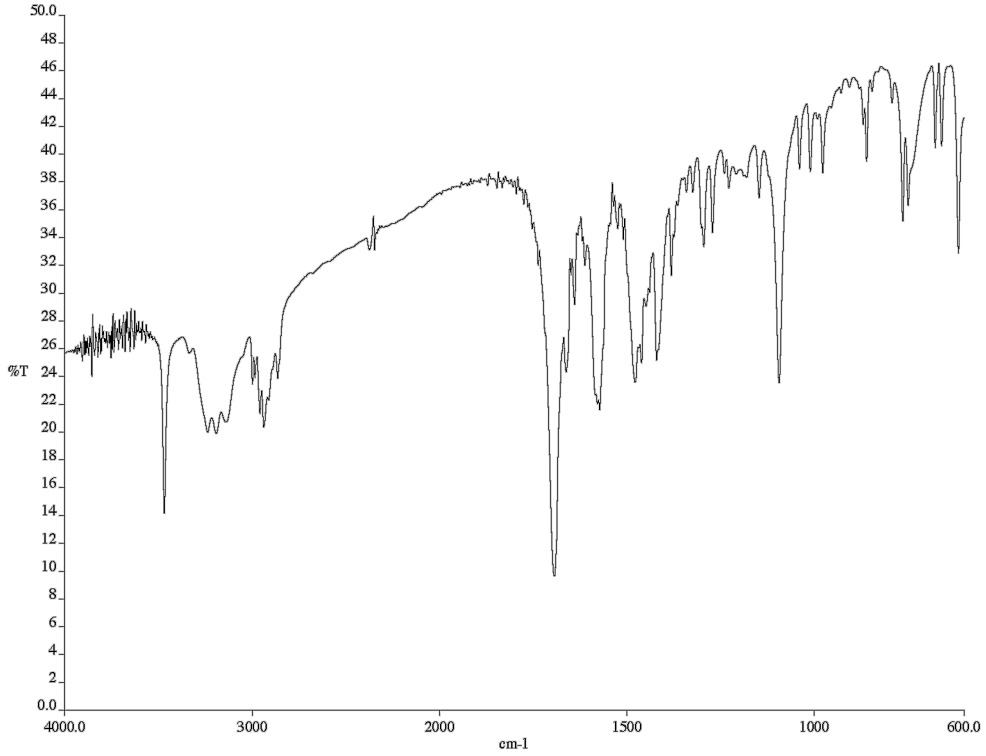


Figure A4.26 Infrared spectrum (KBr) of compound **246**.

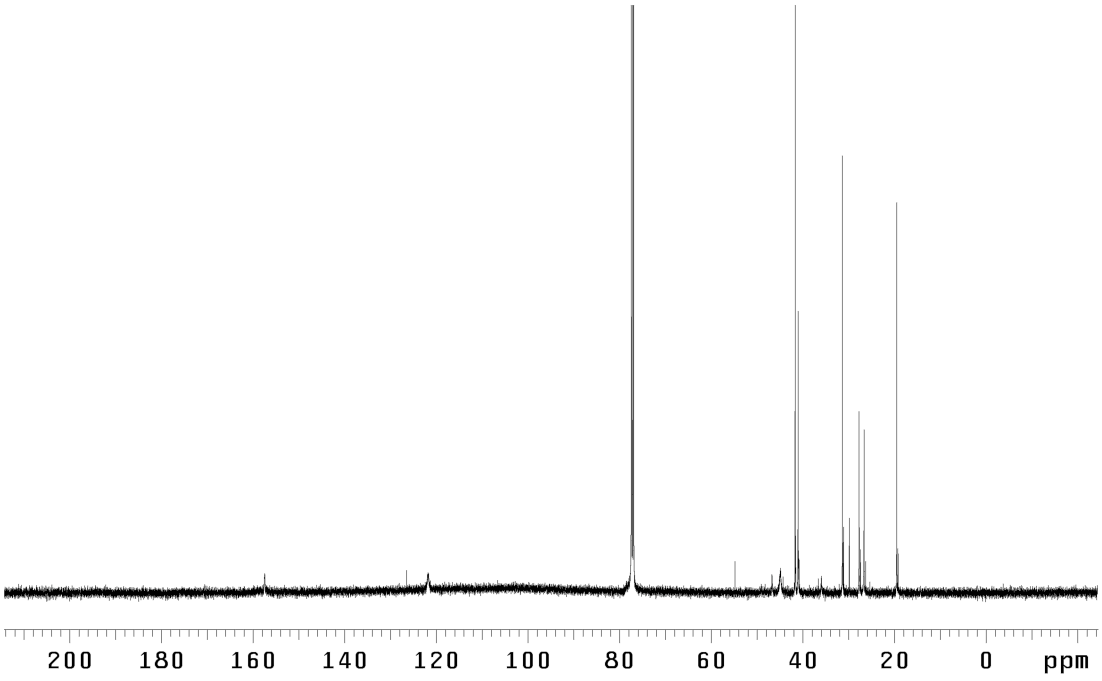


Figure A4.27 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **246**.

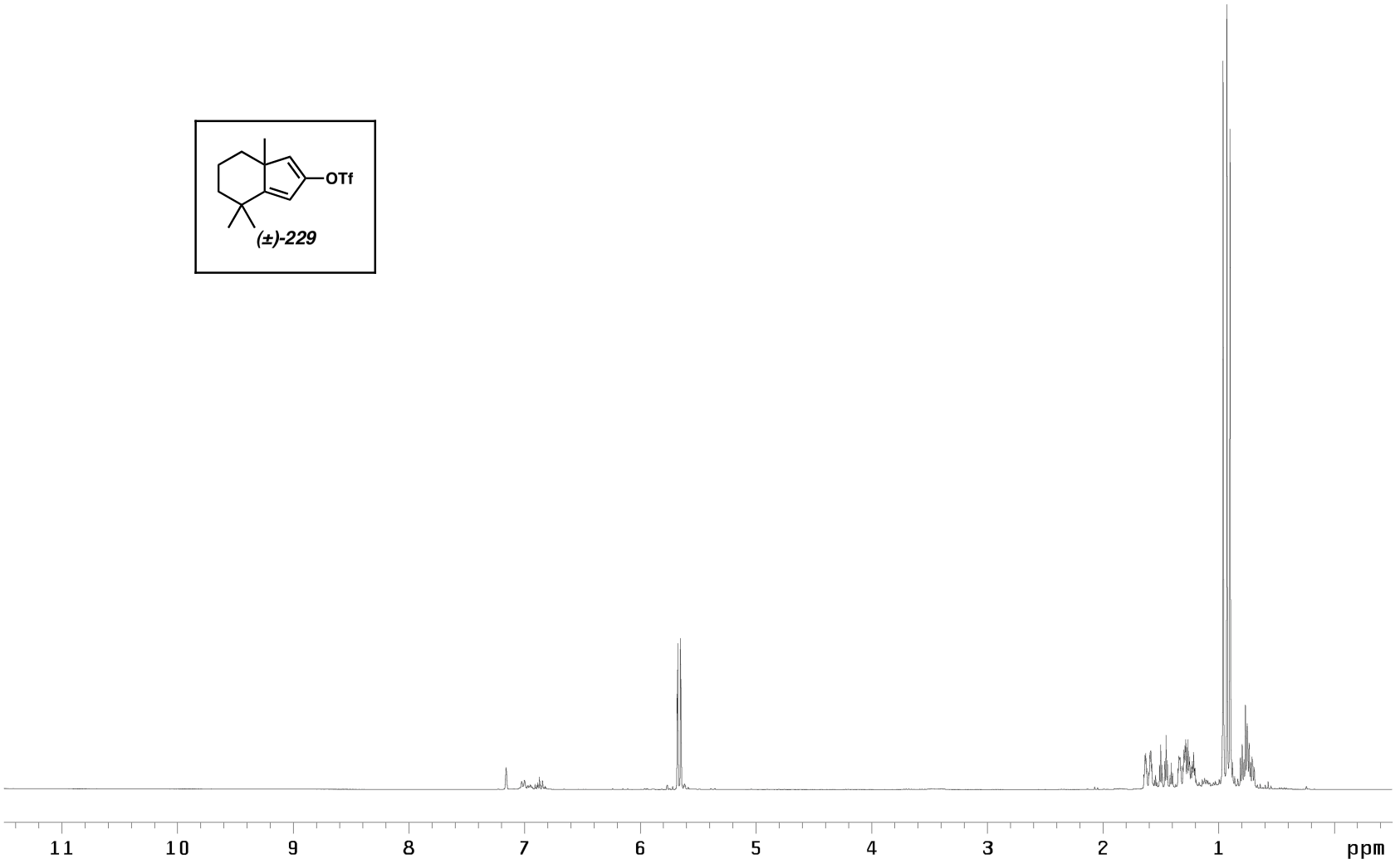


Figure A4.28 ^{1}H NMR (300 MHz, C_6D_6) of compound **229**.

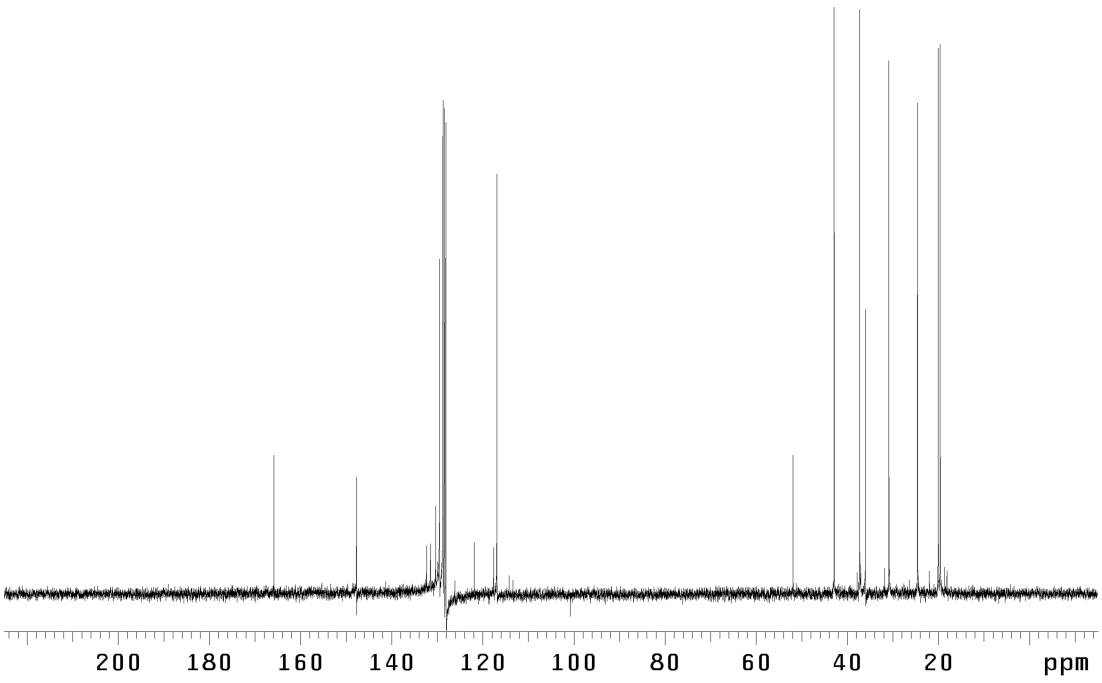


Figure A4.29 ^{13}C NMR (75 MHz, C_6D_6) of compound **229**.

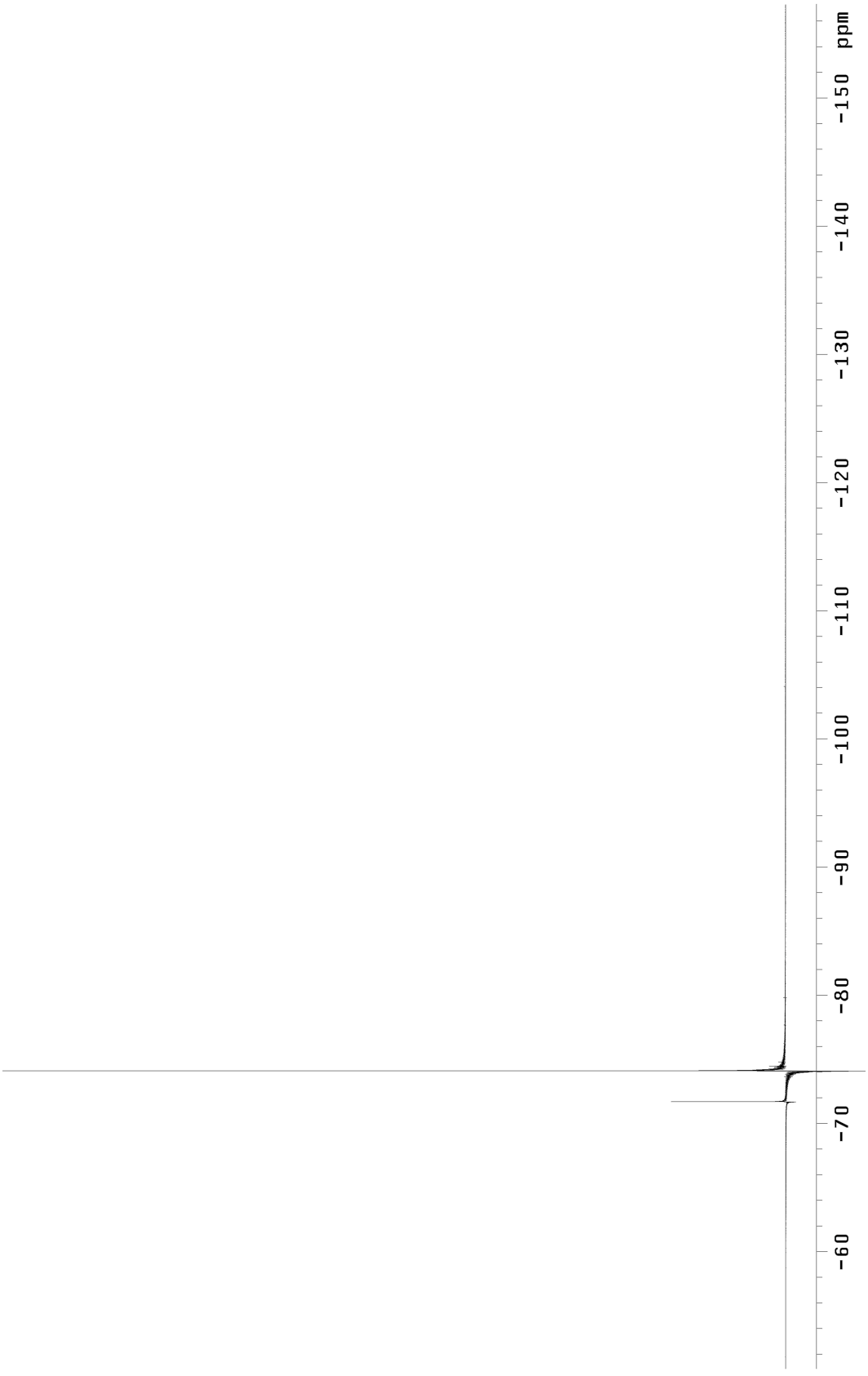


Figure A4.30 ^{19}F NMR (282 MHz, C_6D_6) of compound **229**.

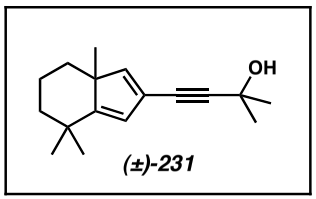


Figure A4.31 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **231**.

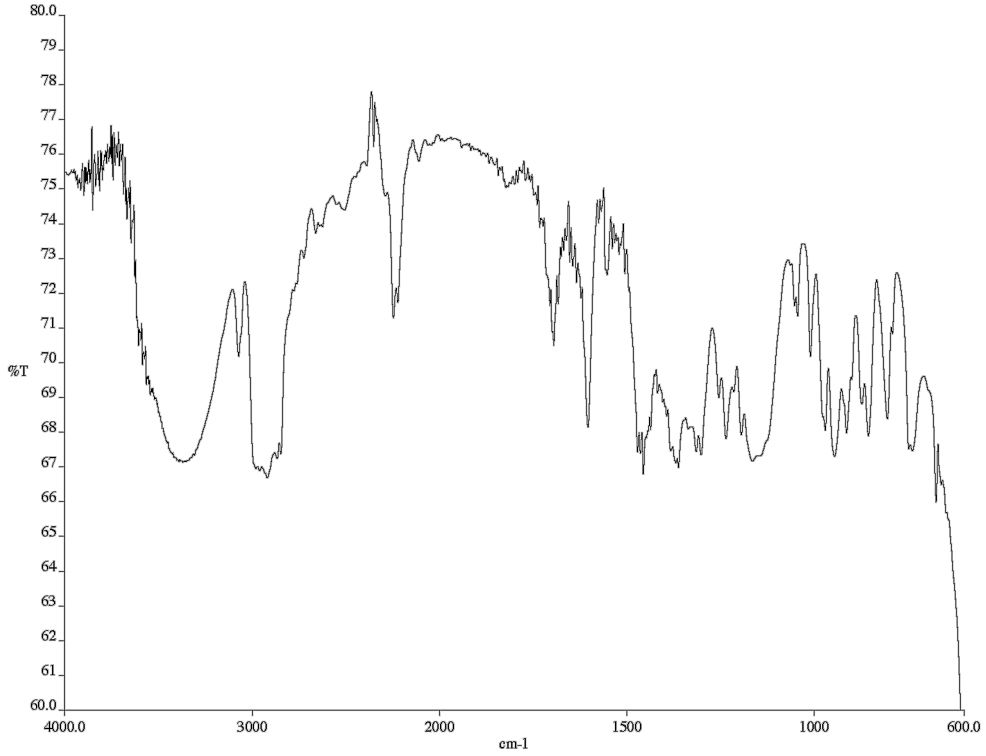


Figure A4.32 Infrared spectrum ($NaCl/CDCl_3$) of compound **231**.

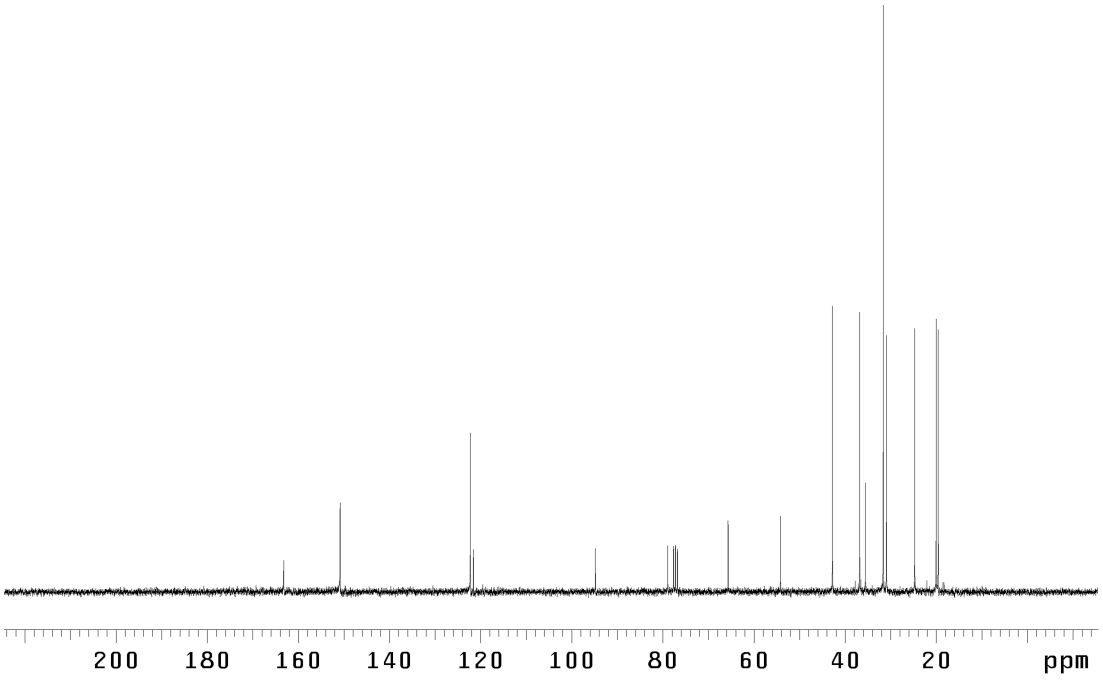


Figure A4.33 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **231**.

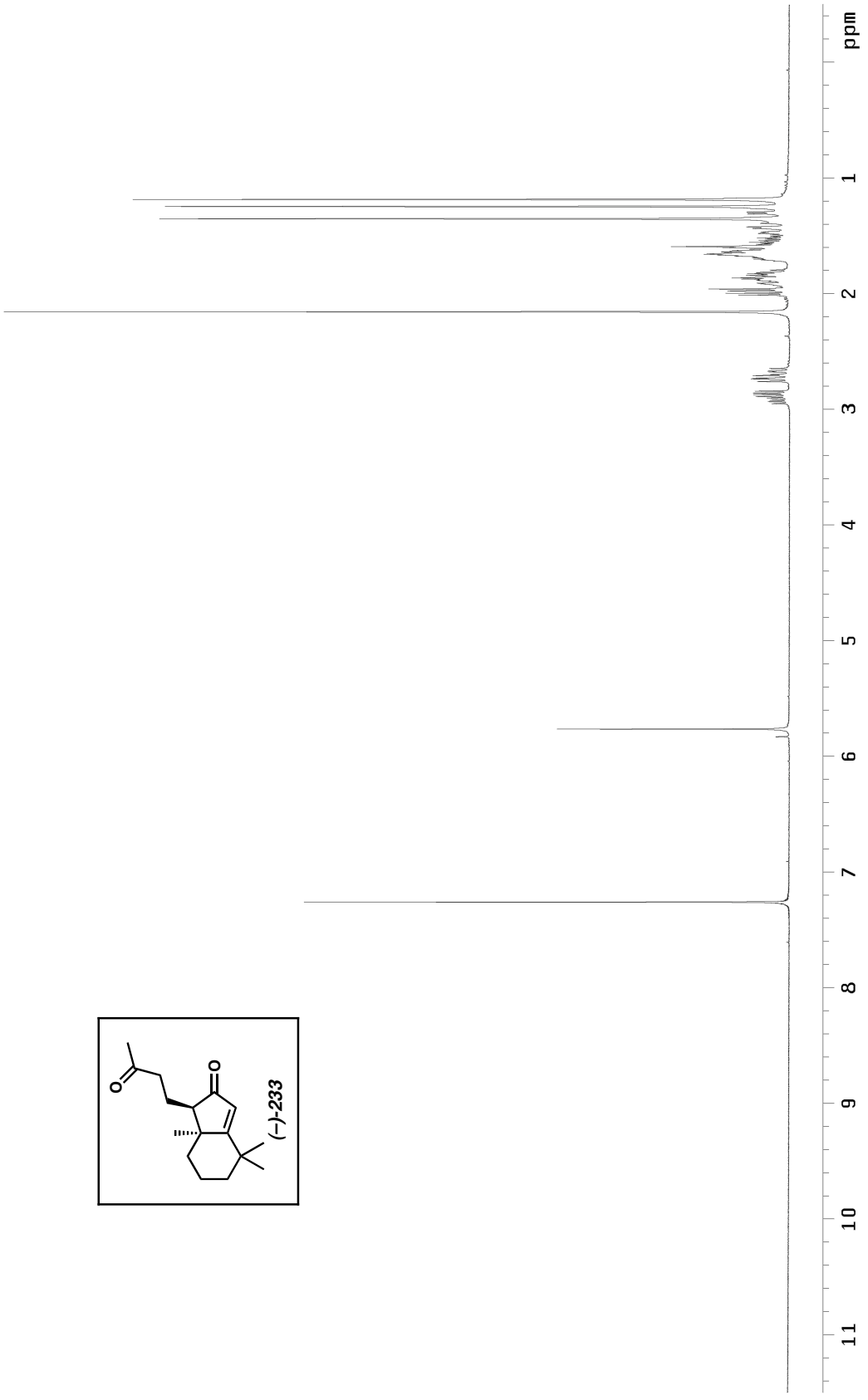


Figure A4.34 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **233**.

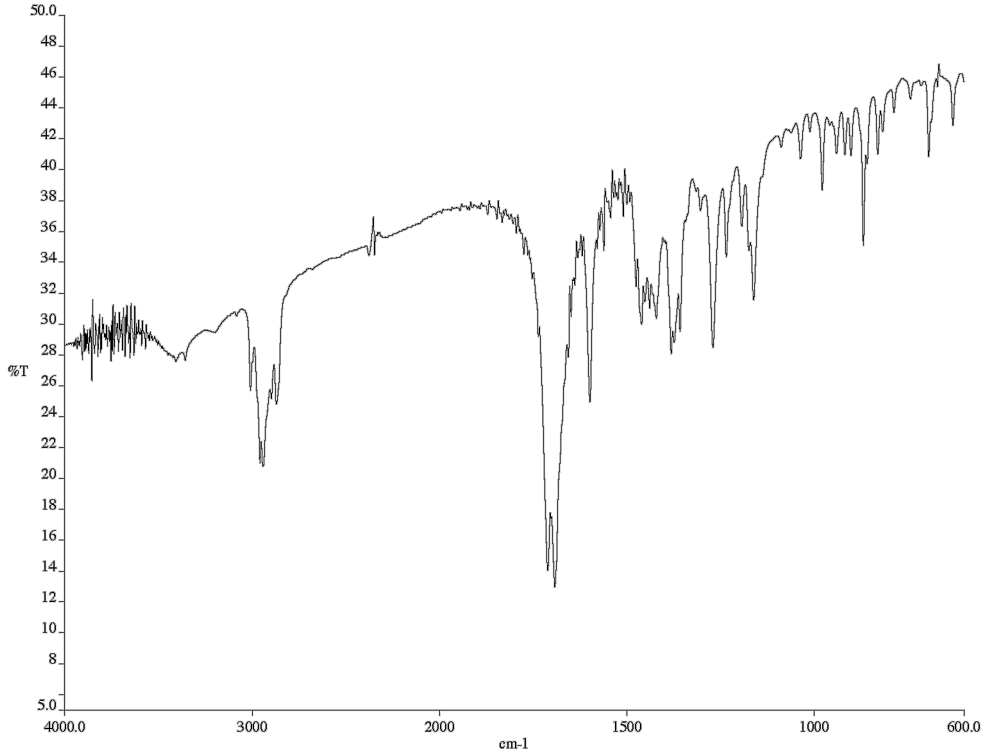


Figure A4.35 Infrared spectrum (KBr) of compound **233**.

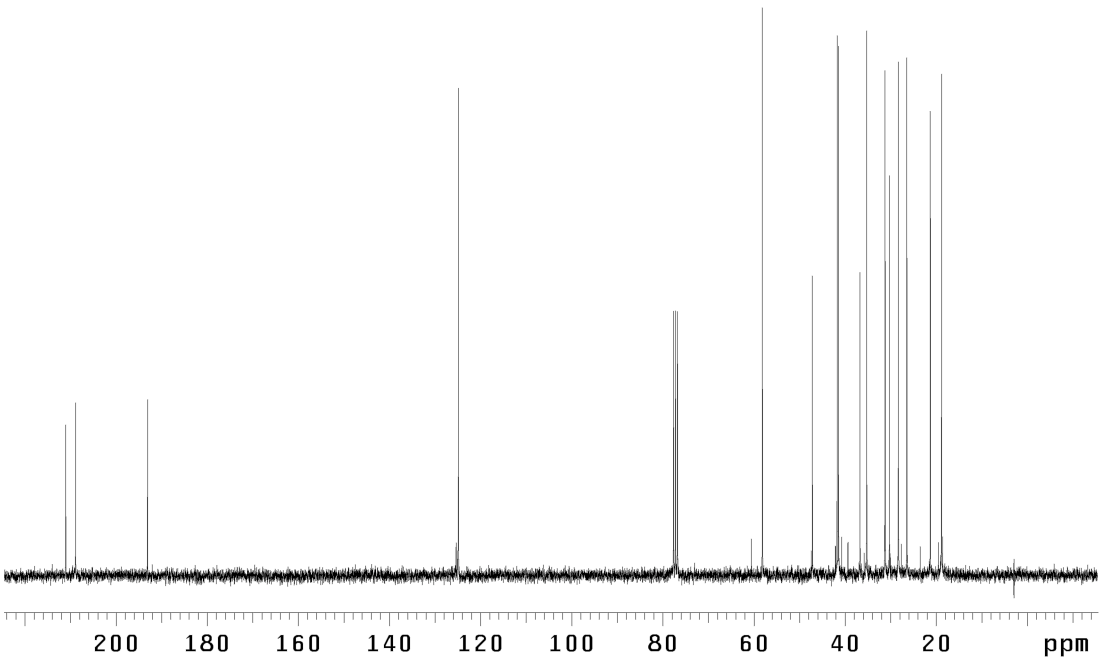


Figure A4.36 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **233**.

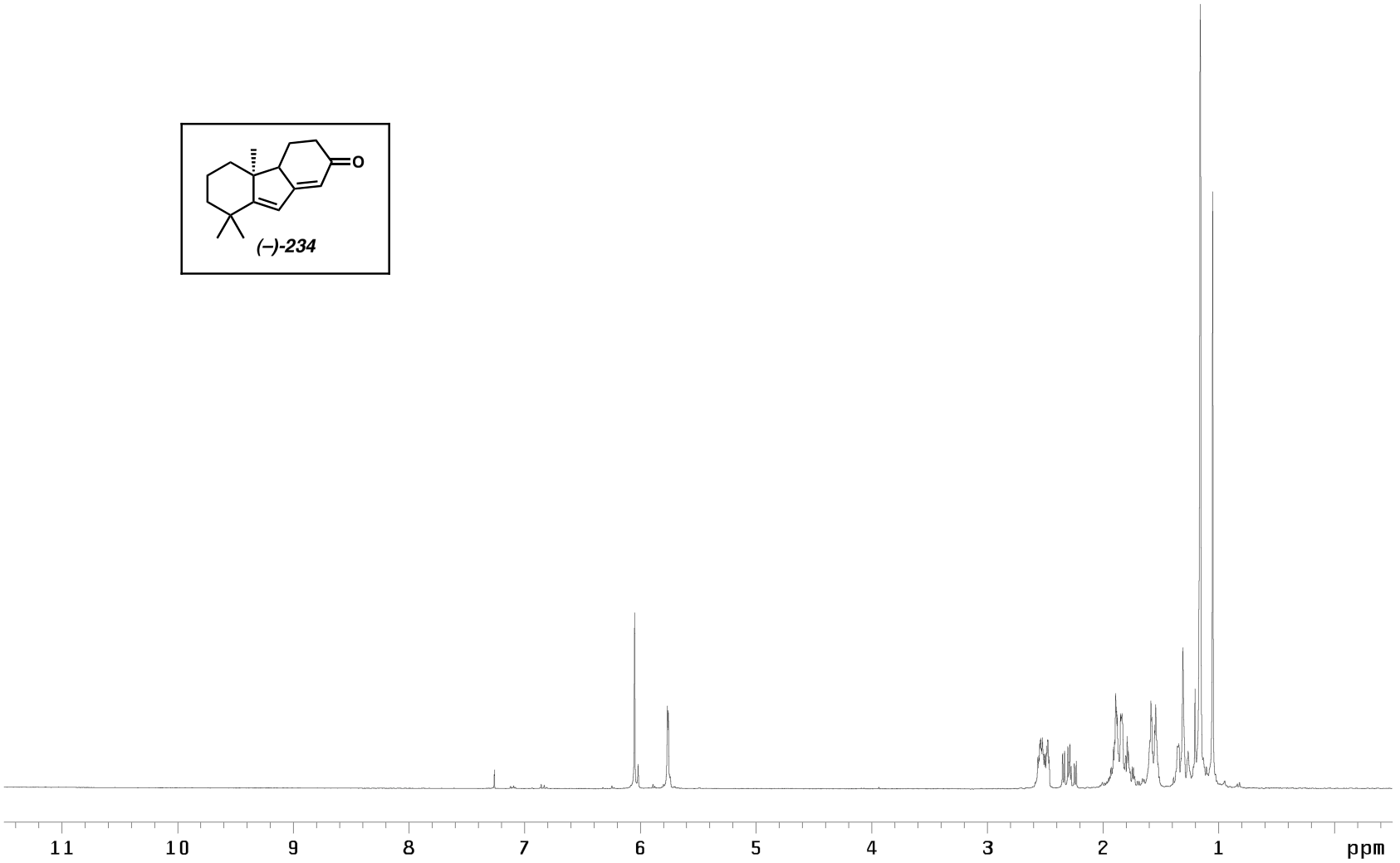


Figure A4.37 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **234**.

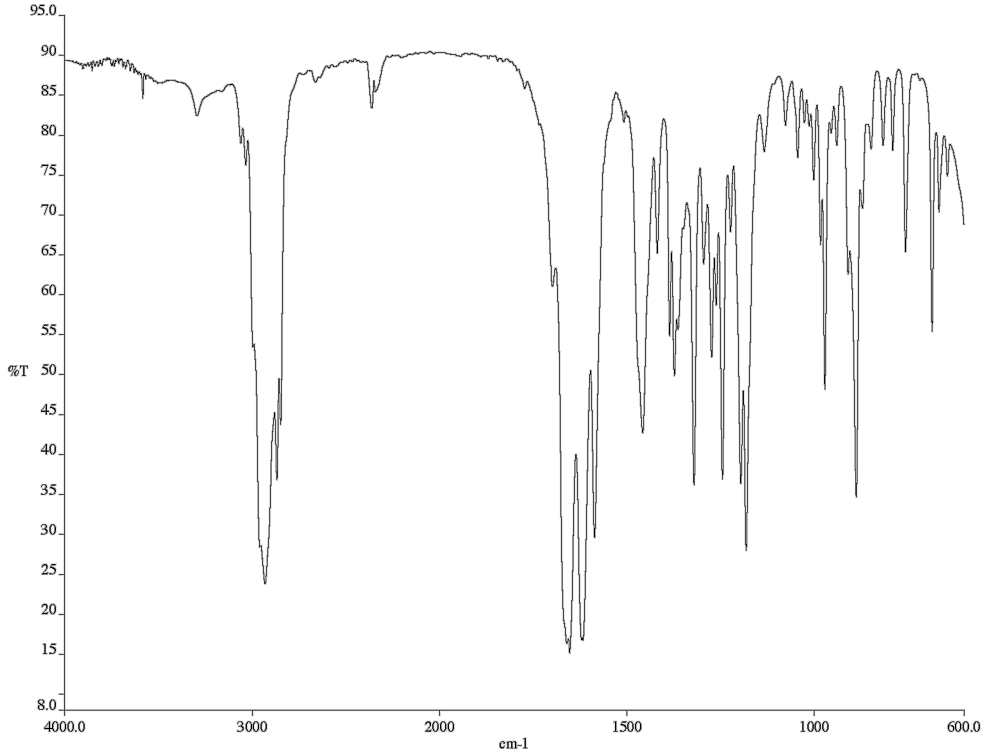


Figure A4.38 Infrared spectrum ($NaCl/CDCl_3$) of compound **234**.

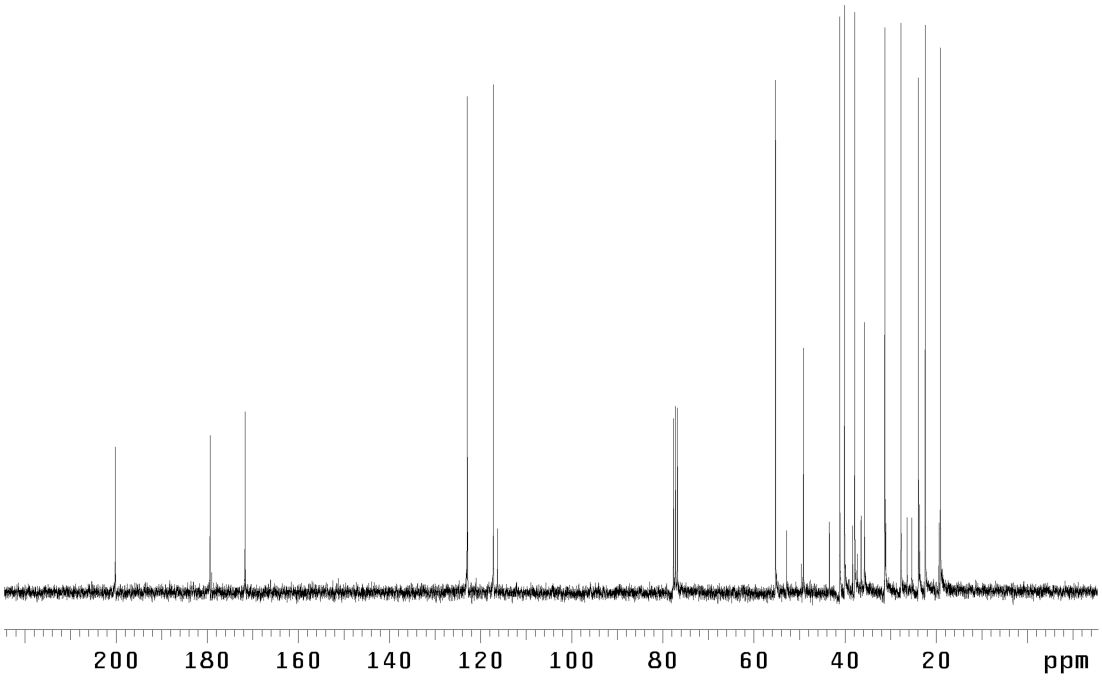


Figure A4.39 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **234**.

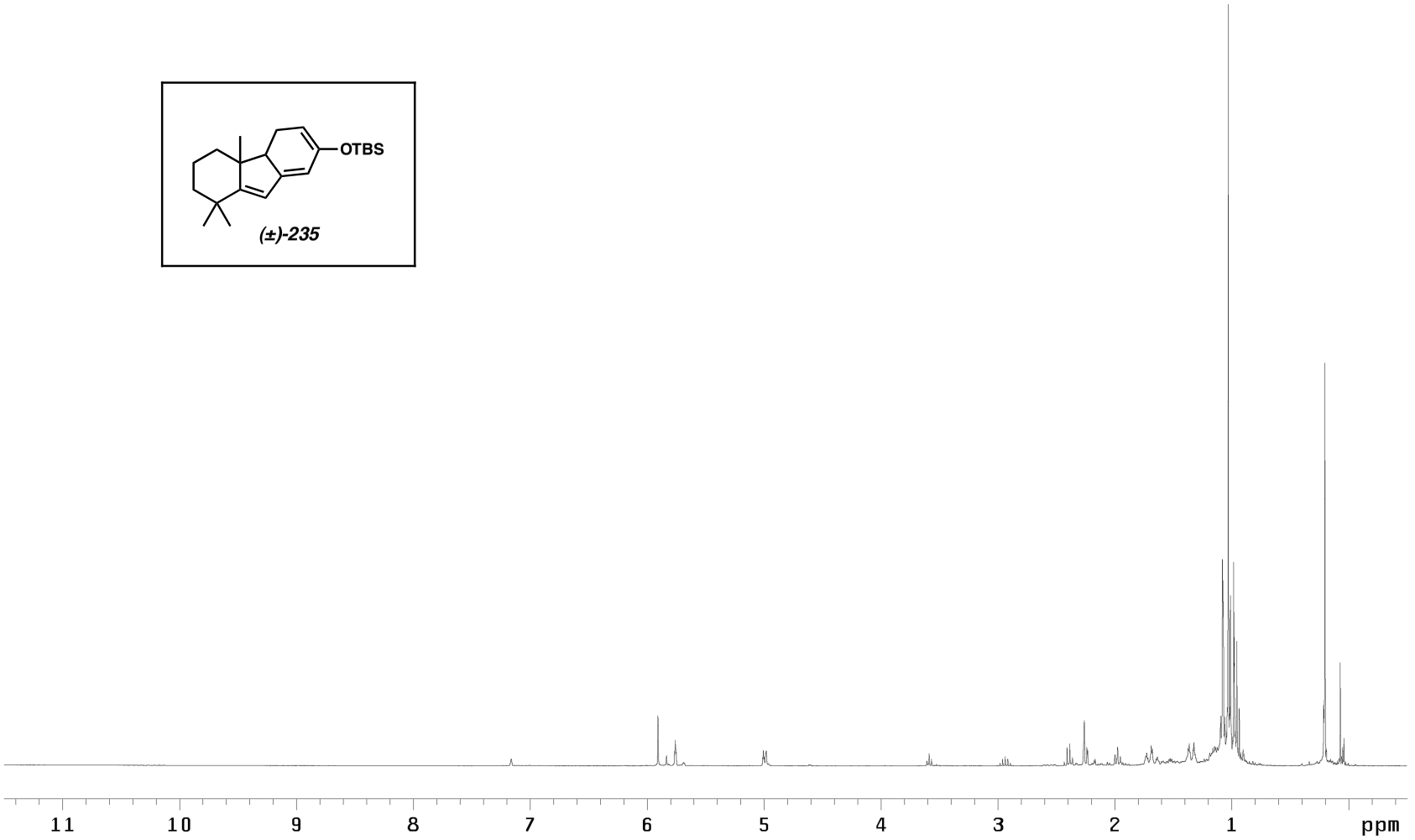


Figure A4.40 ^{1}H NMR (300 MHz, C_6D_6) of compound **235**.

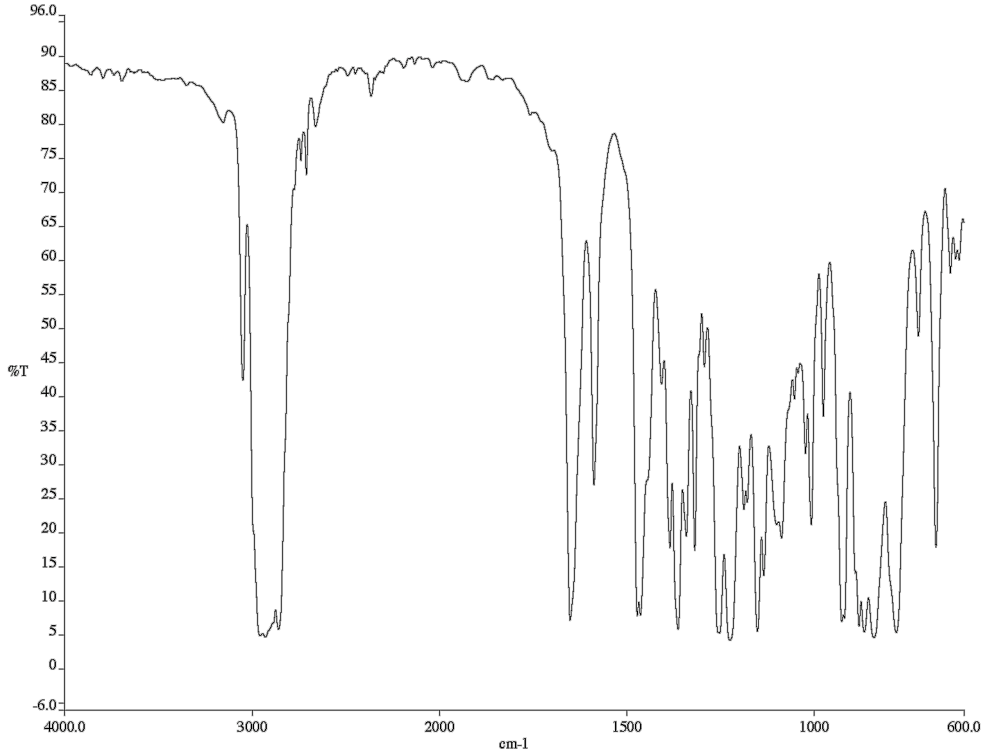


Figure A4.41 Infrared spectrum (NaCl/neat) of compound **235**.

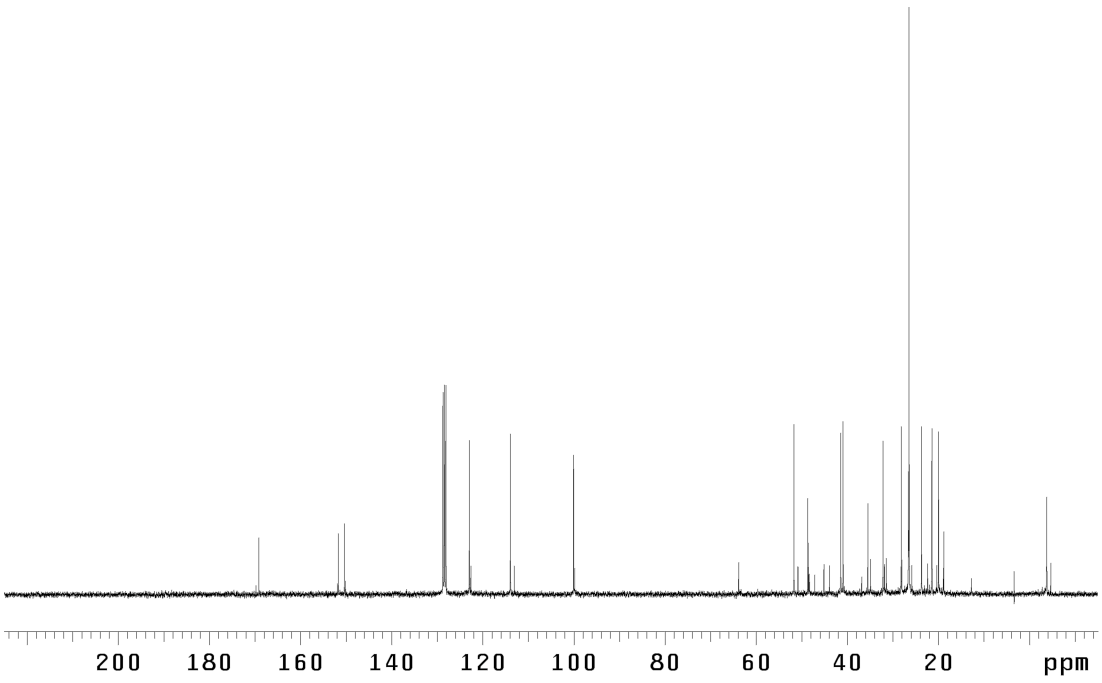


Figure A4.42 ^{13}C NMR (75 MHz, C_6D_6) of compound **235**.

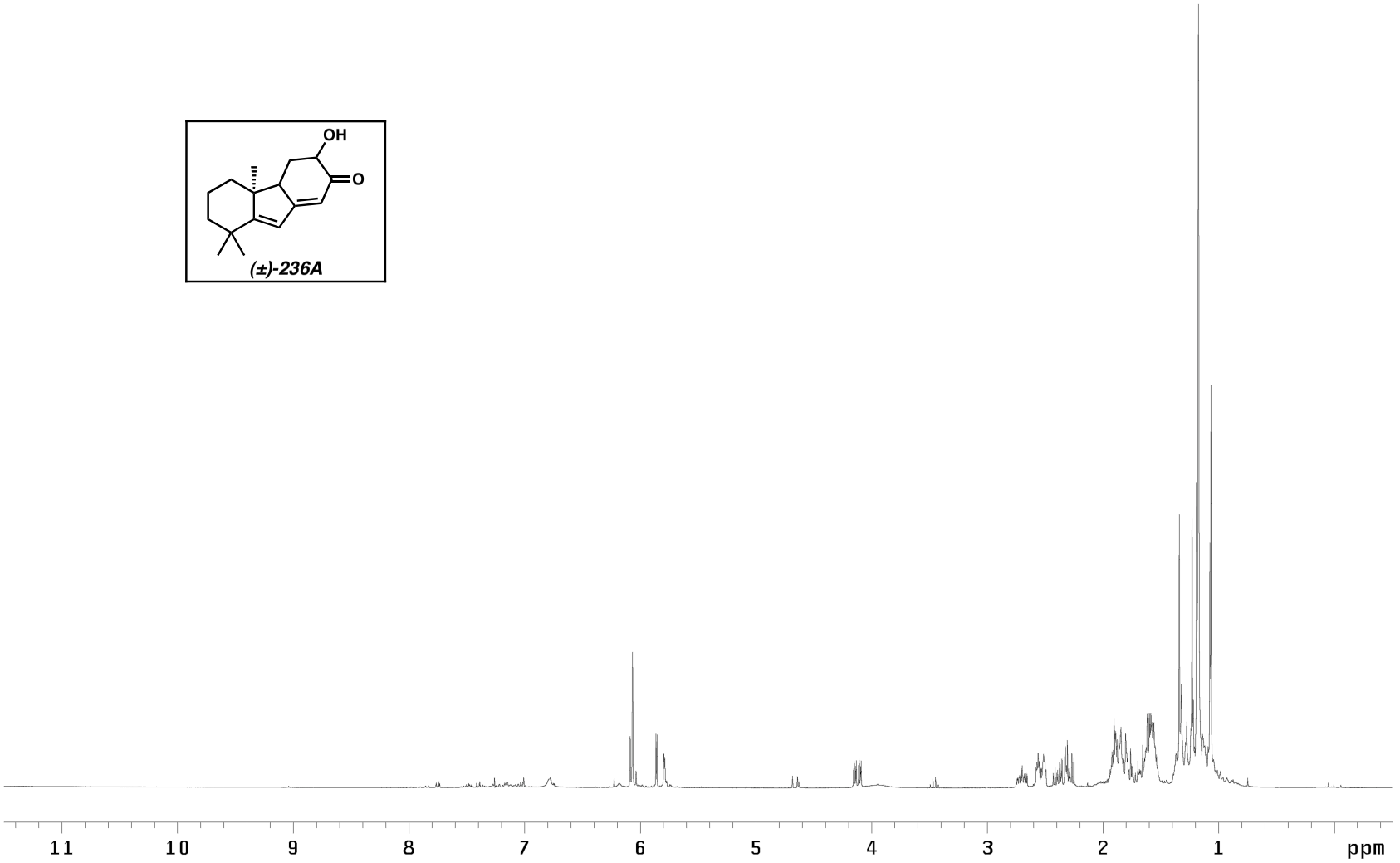


Figure A4.43 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **236A**.

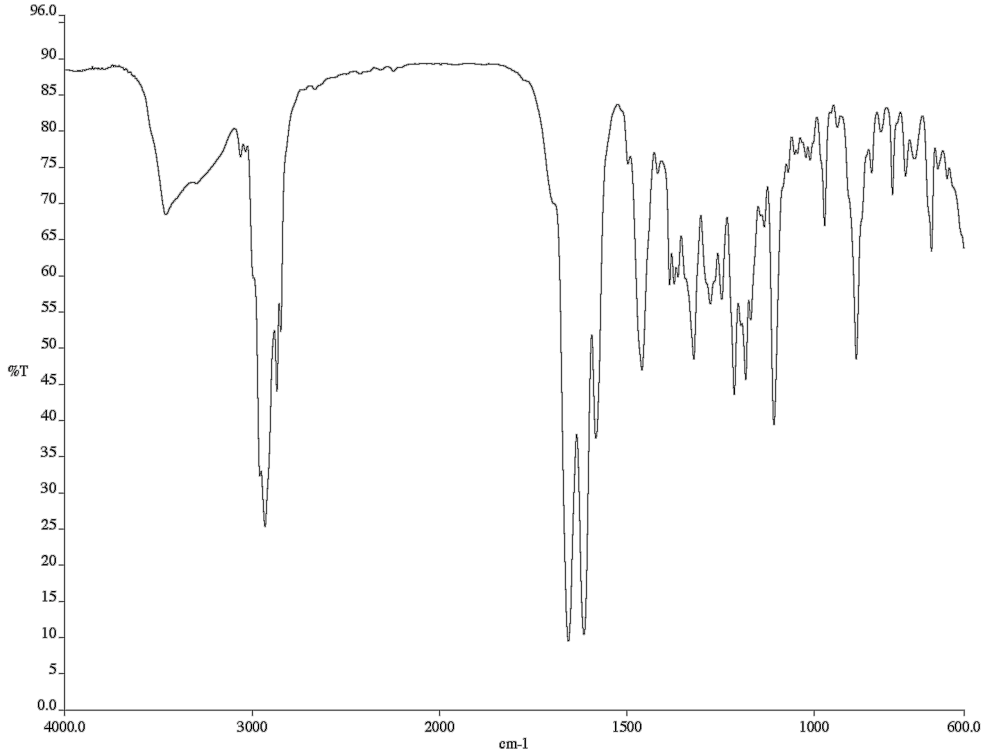


Figure A4.44 Infrared spectrum ($NaCl/CDCl_3$) of compound **236A**.

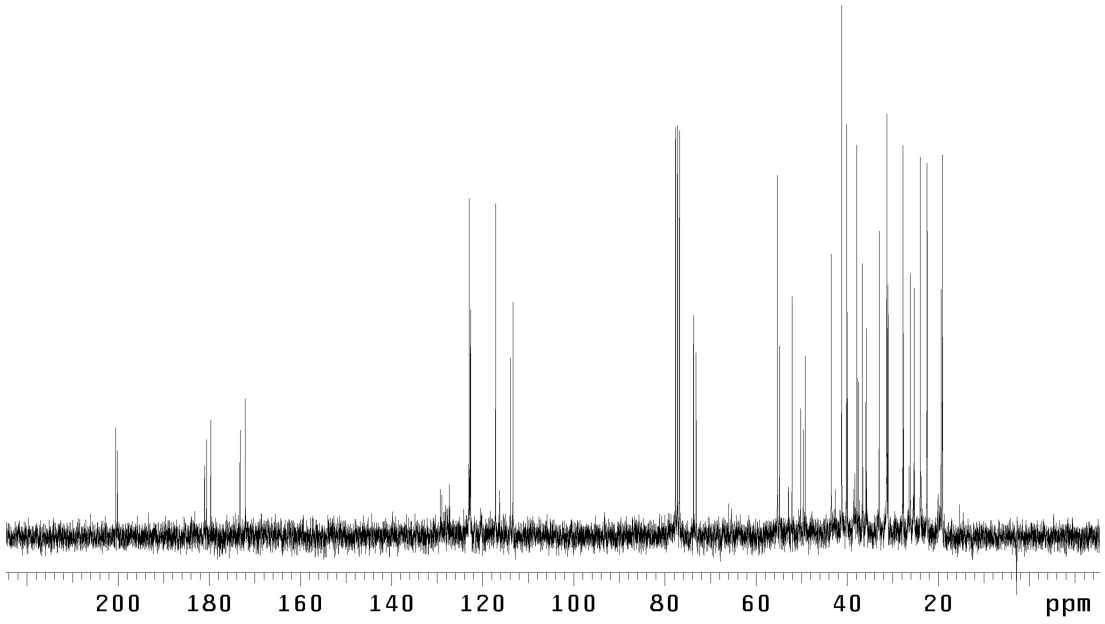


Figure A4.45 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **236A**.

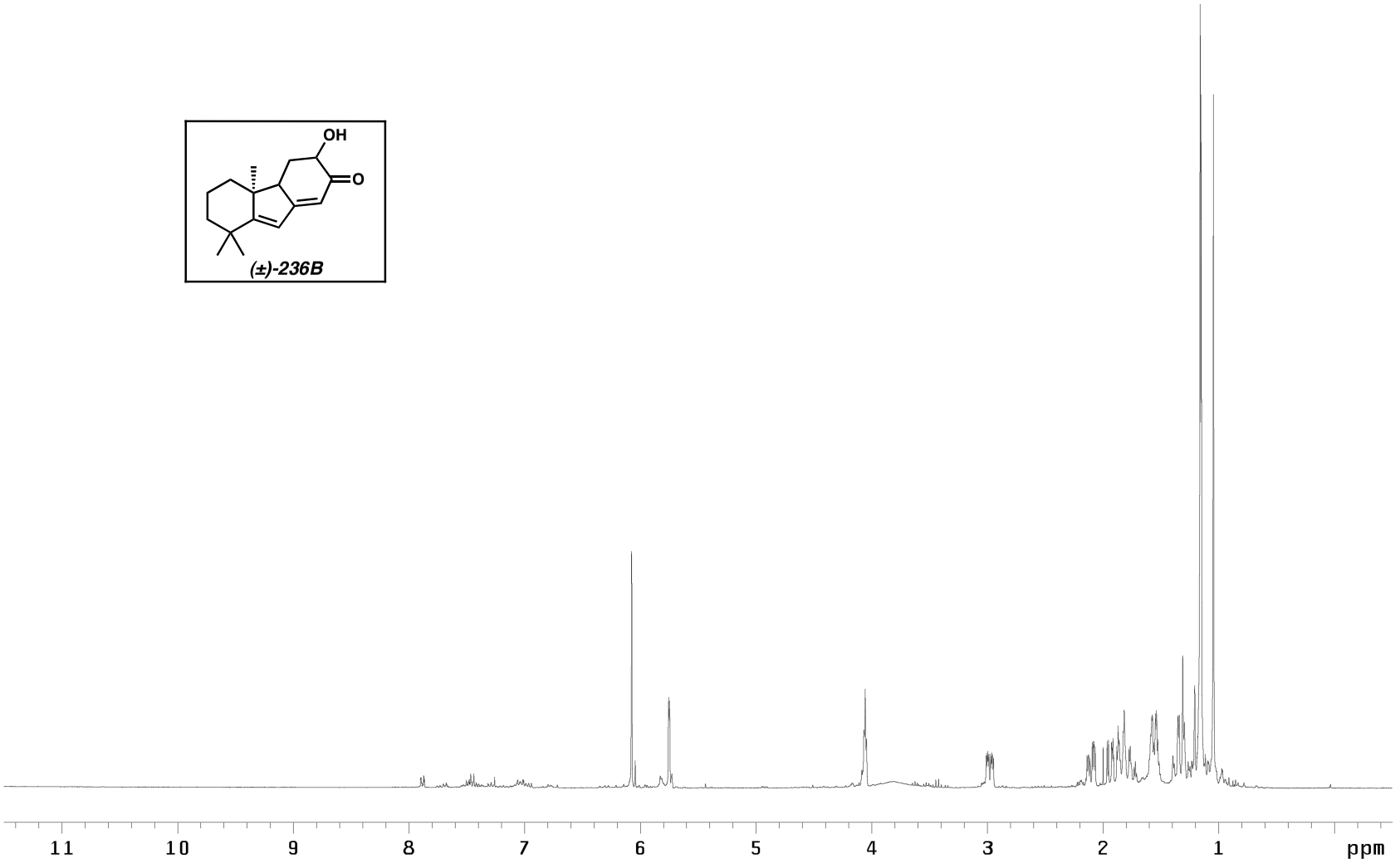


Figure A4.46 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **236B**.

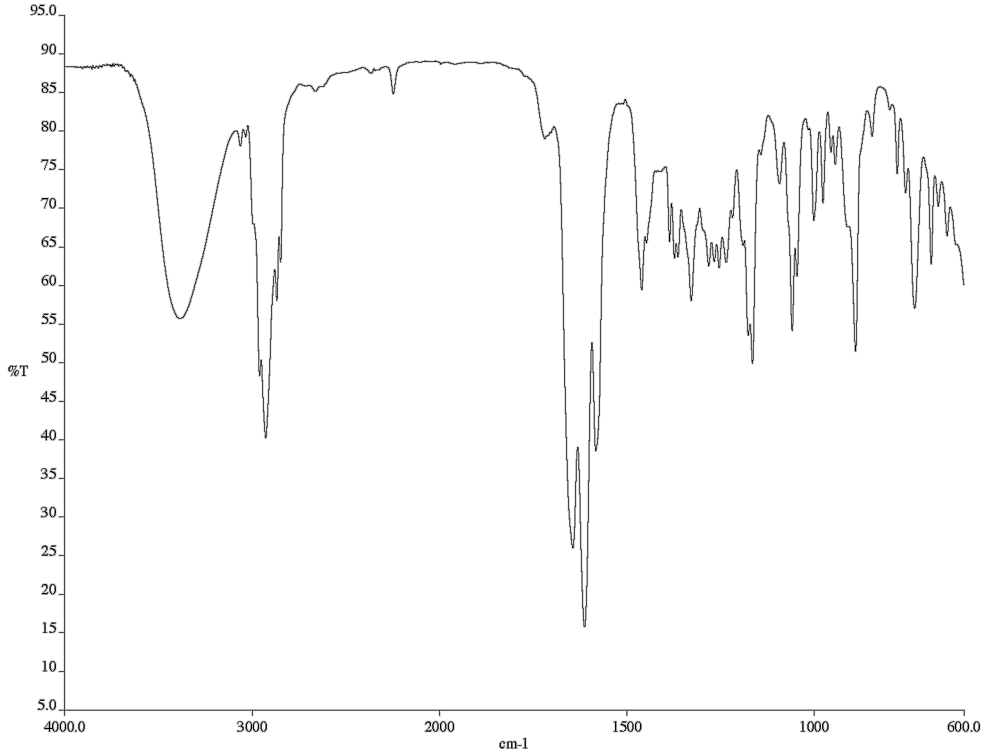


Figure A4.47 Infrared spectrum ($NaCl/CDCl_3$) of compound **236B**.

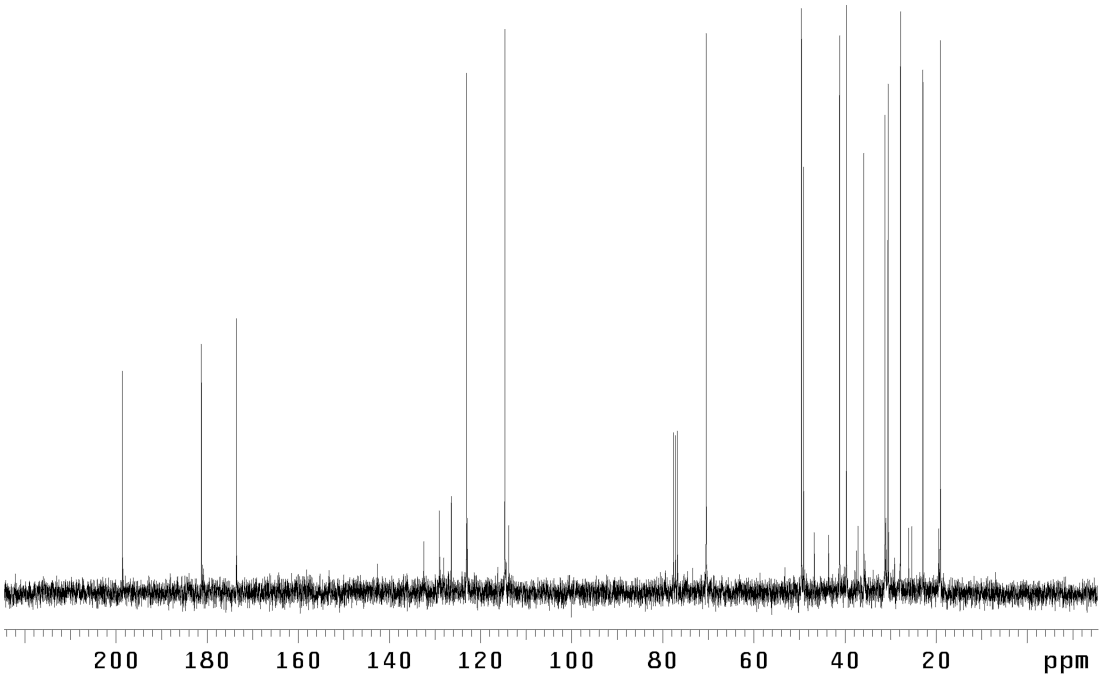


Figure A4.48 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **236B**.

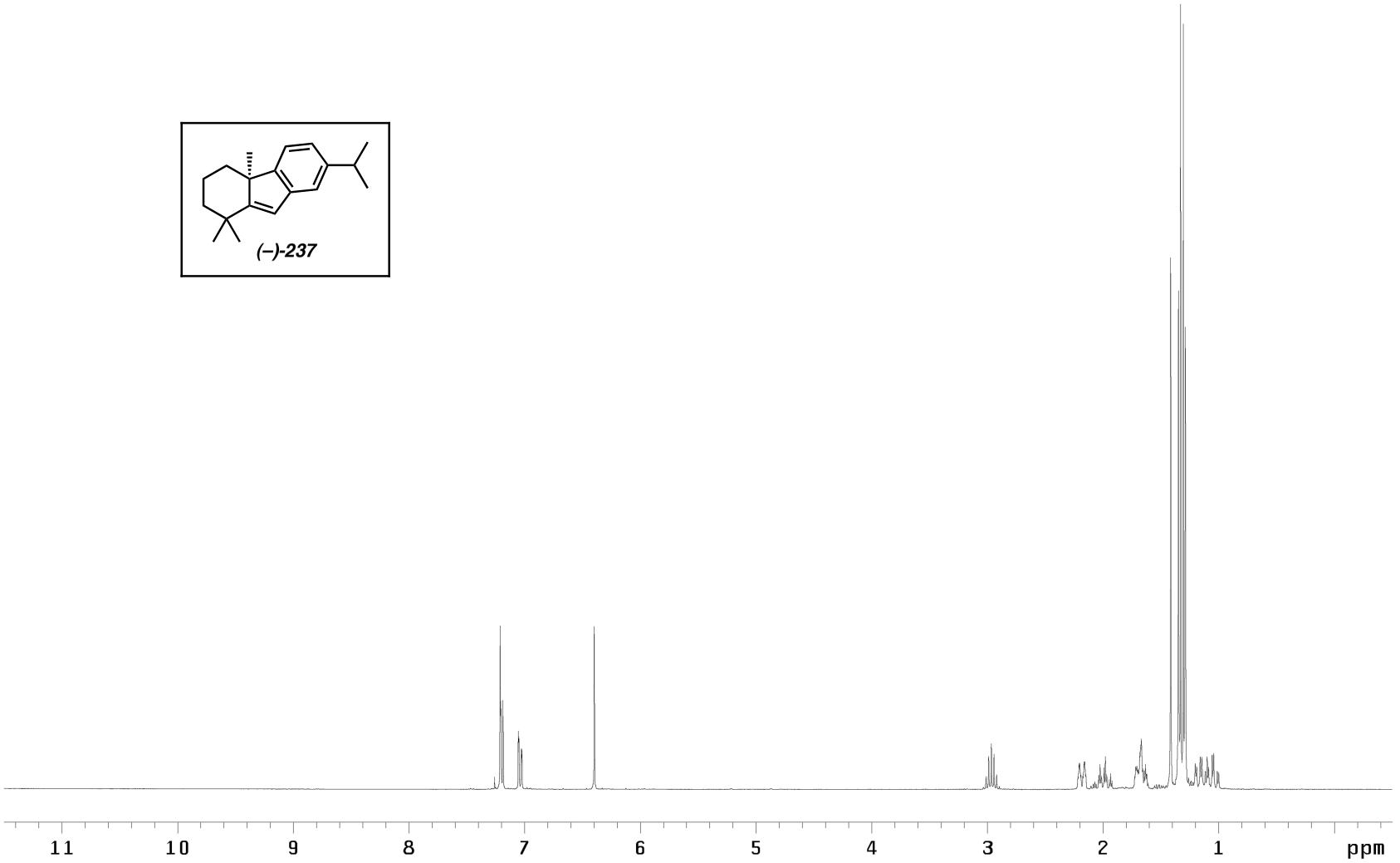


Figure A4.49 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **237**.

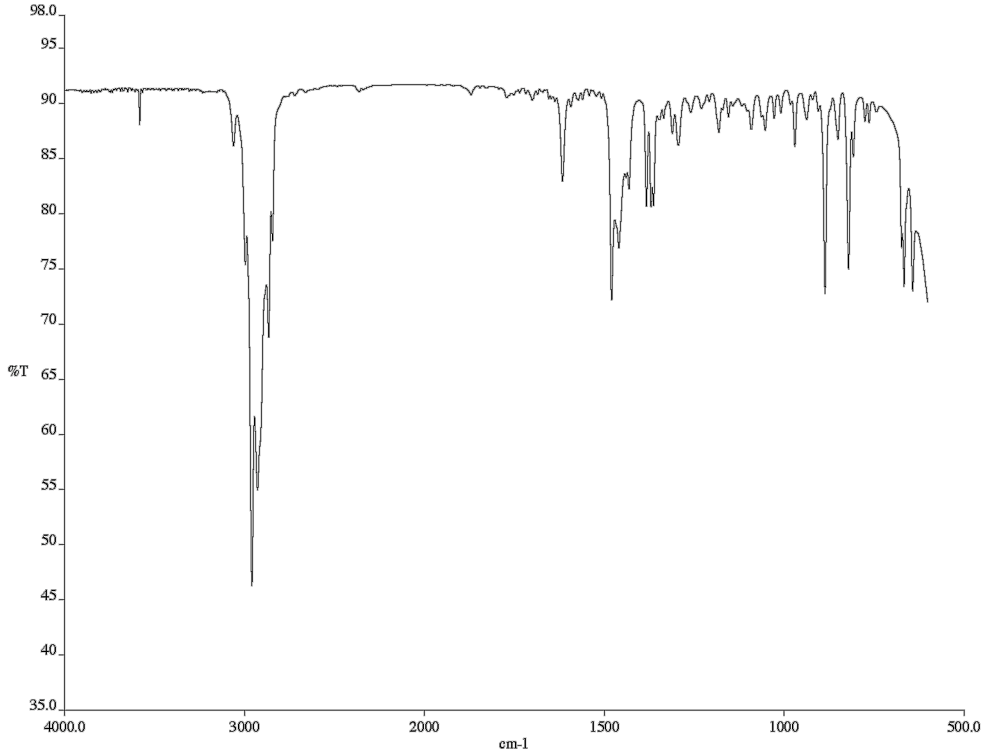


Figure A4.50 Infrared spectrum ($NaCl/CDCl_3$) of compound **237**.

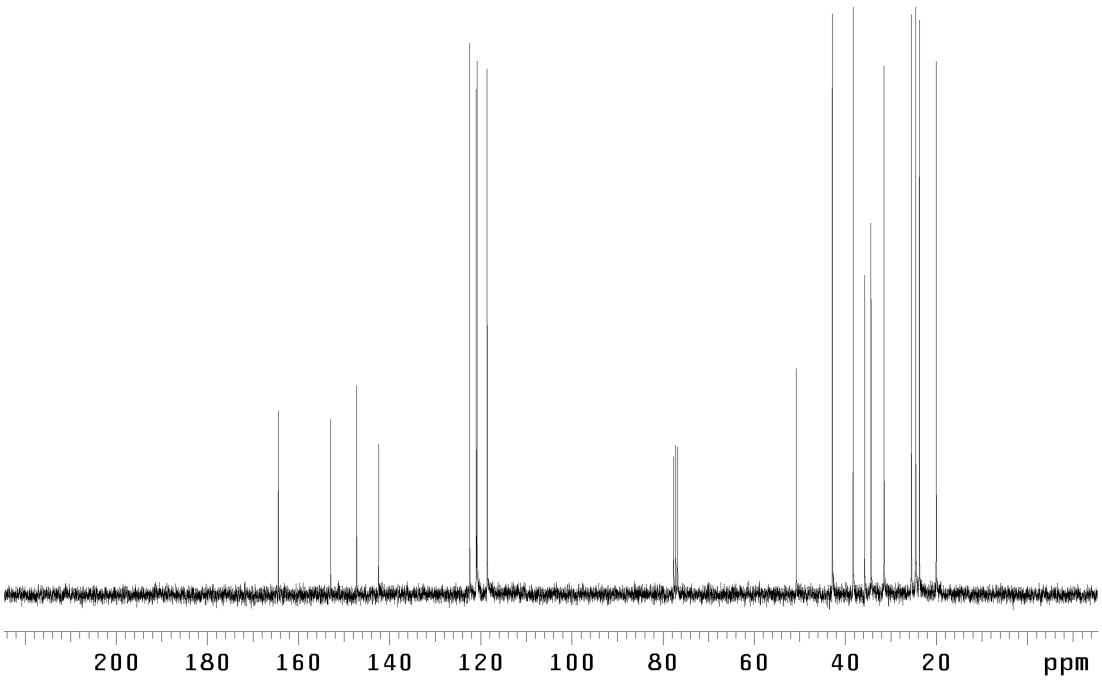


Figure A4.51 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **237**.

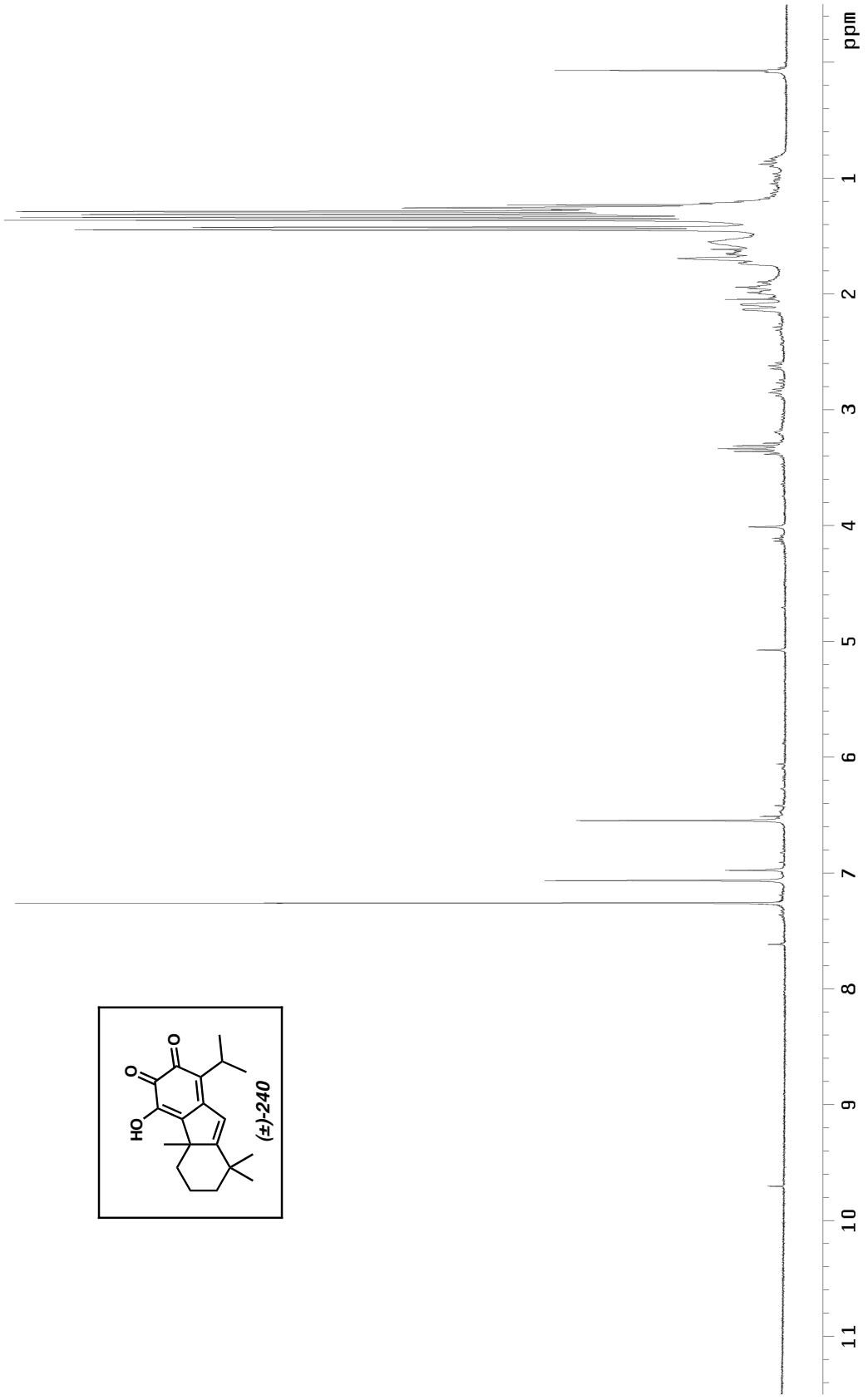


Figure A4.52 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **240**.

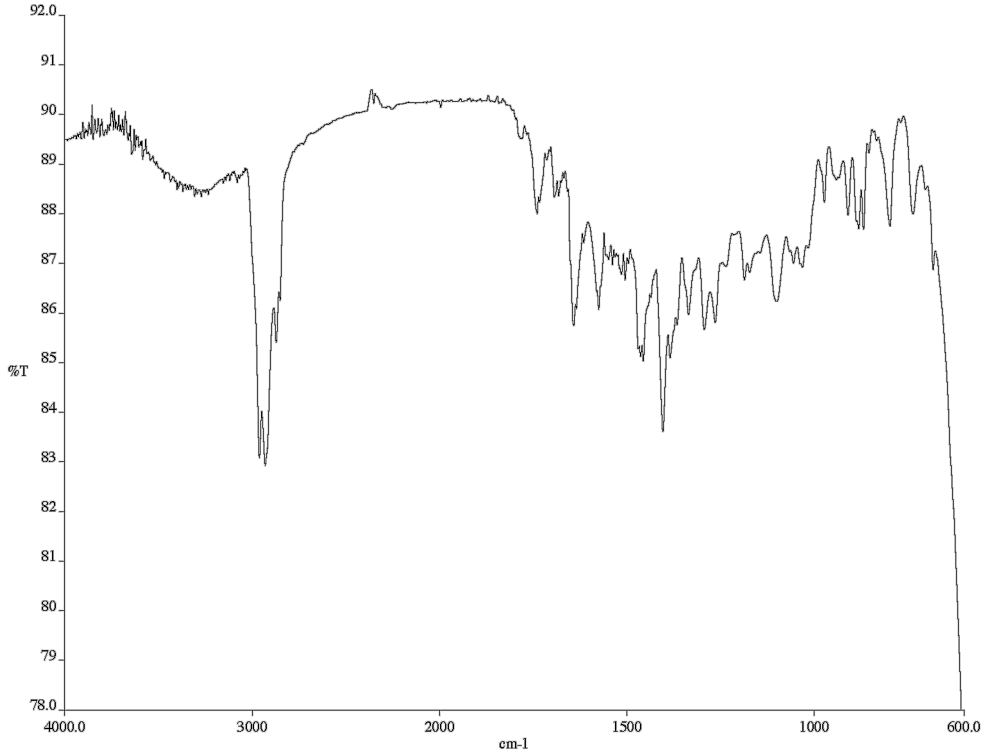


Figure A4.53 Infrared spectrum ($NaCl/CDCl_3$) of compound **240**.

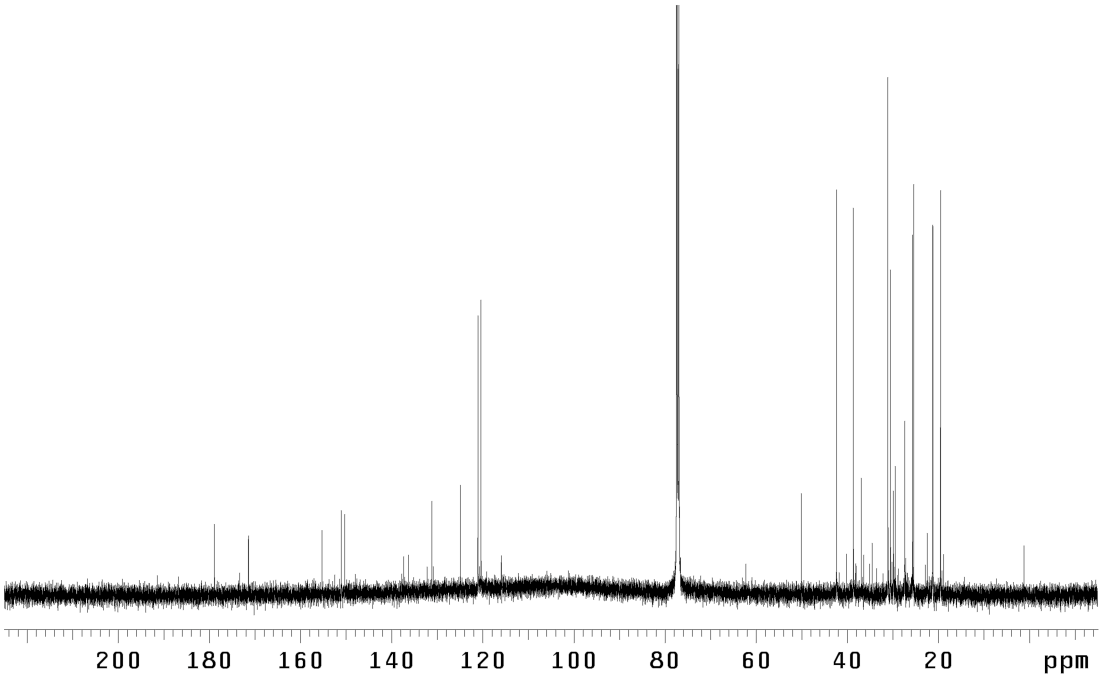


Figure A4.54 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **240**.

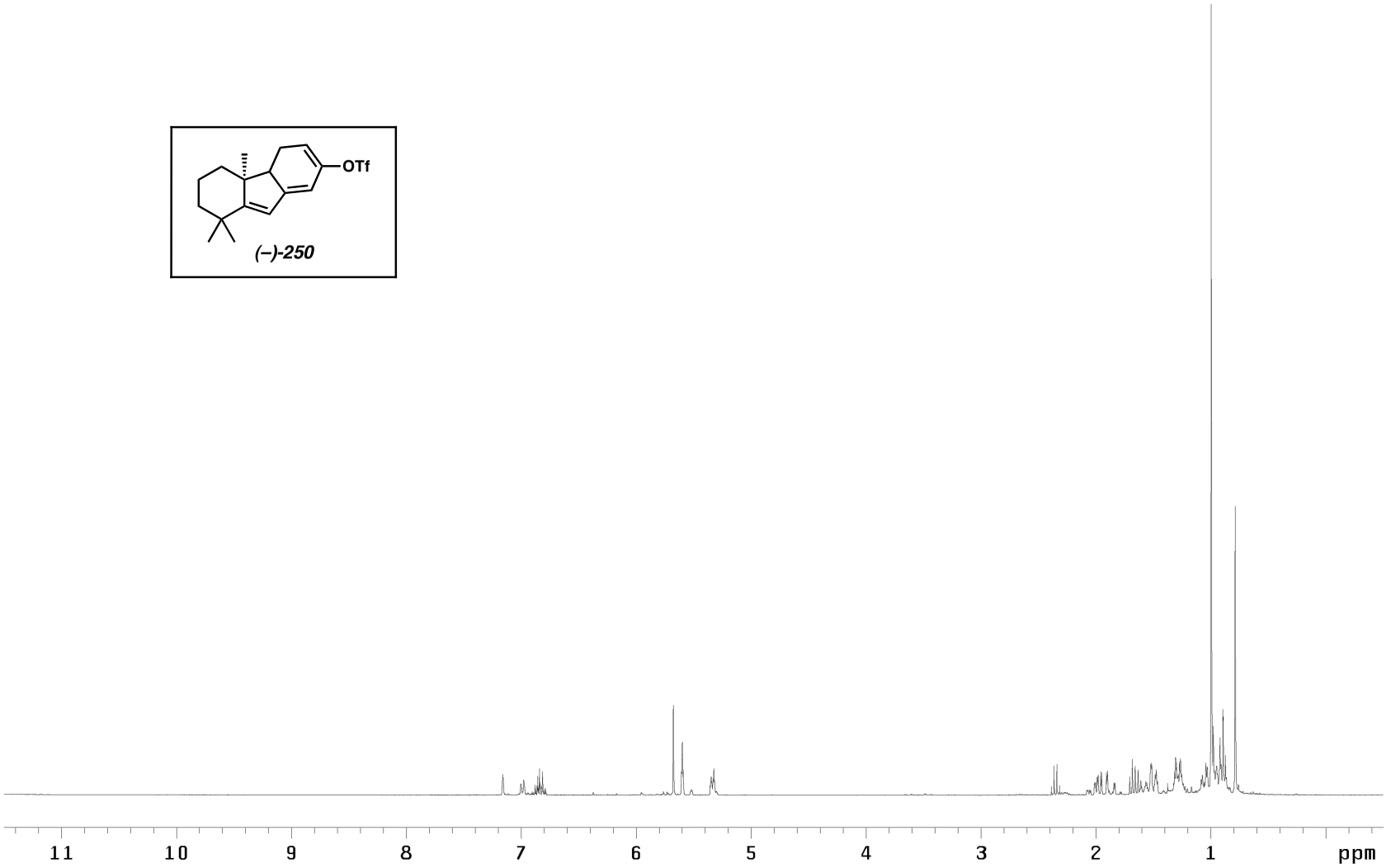


Figure A4.55 ^{1}H NMR (300 MHz, C_6D_6) of compound **250**.

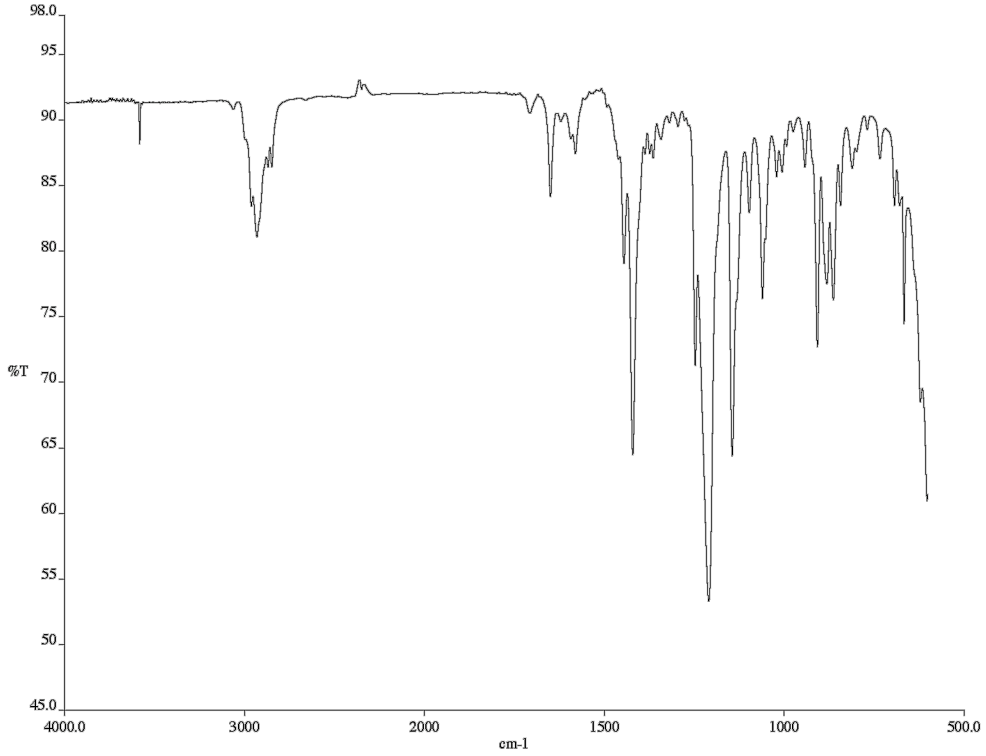


Figure A4.56 Infrared spectrum (NaCl/hexane) of compound **250**.

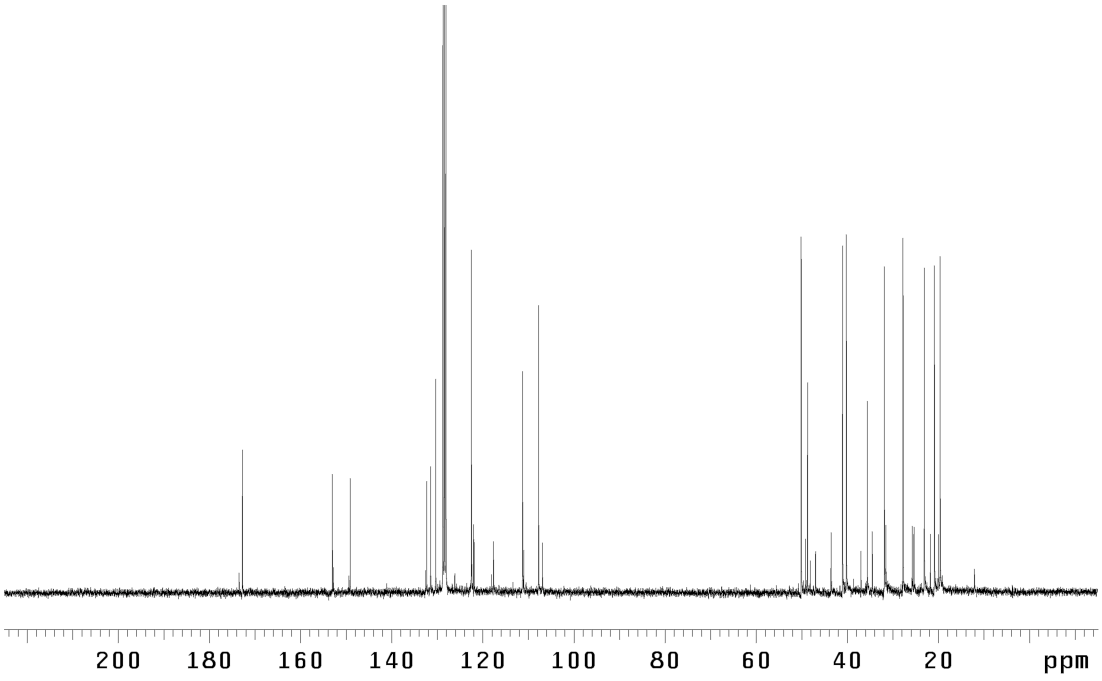


Figure A4.57 ^{13}C NMR (75 MHz, C_6D_6) of compound **250**.

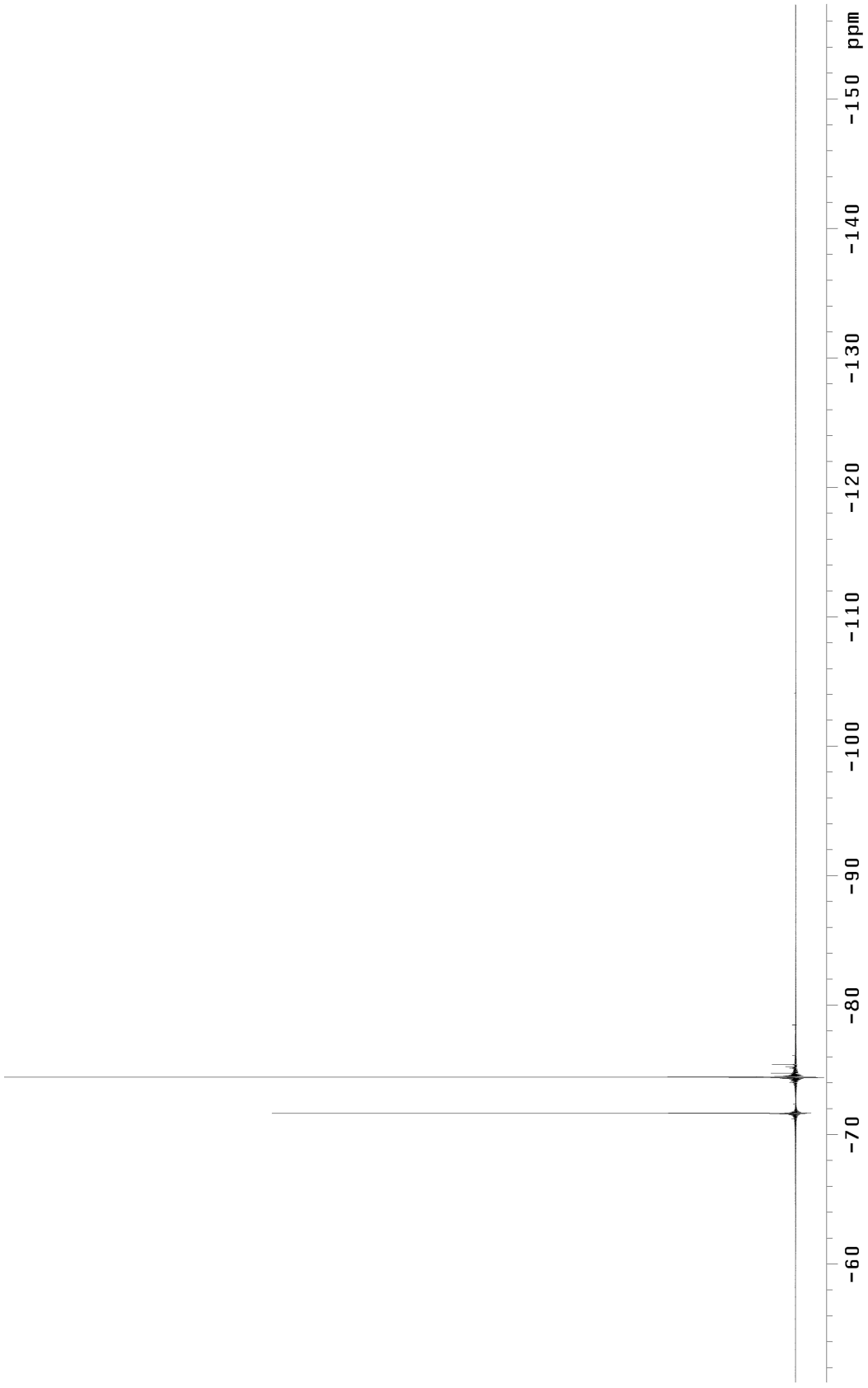


Figure A4.58 ^{19}F NMR (282 MHz, C_6D_6) of compound **250**.

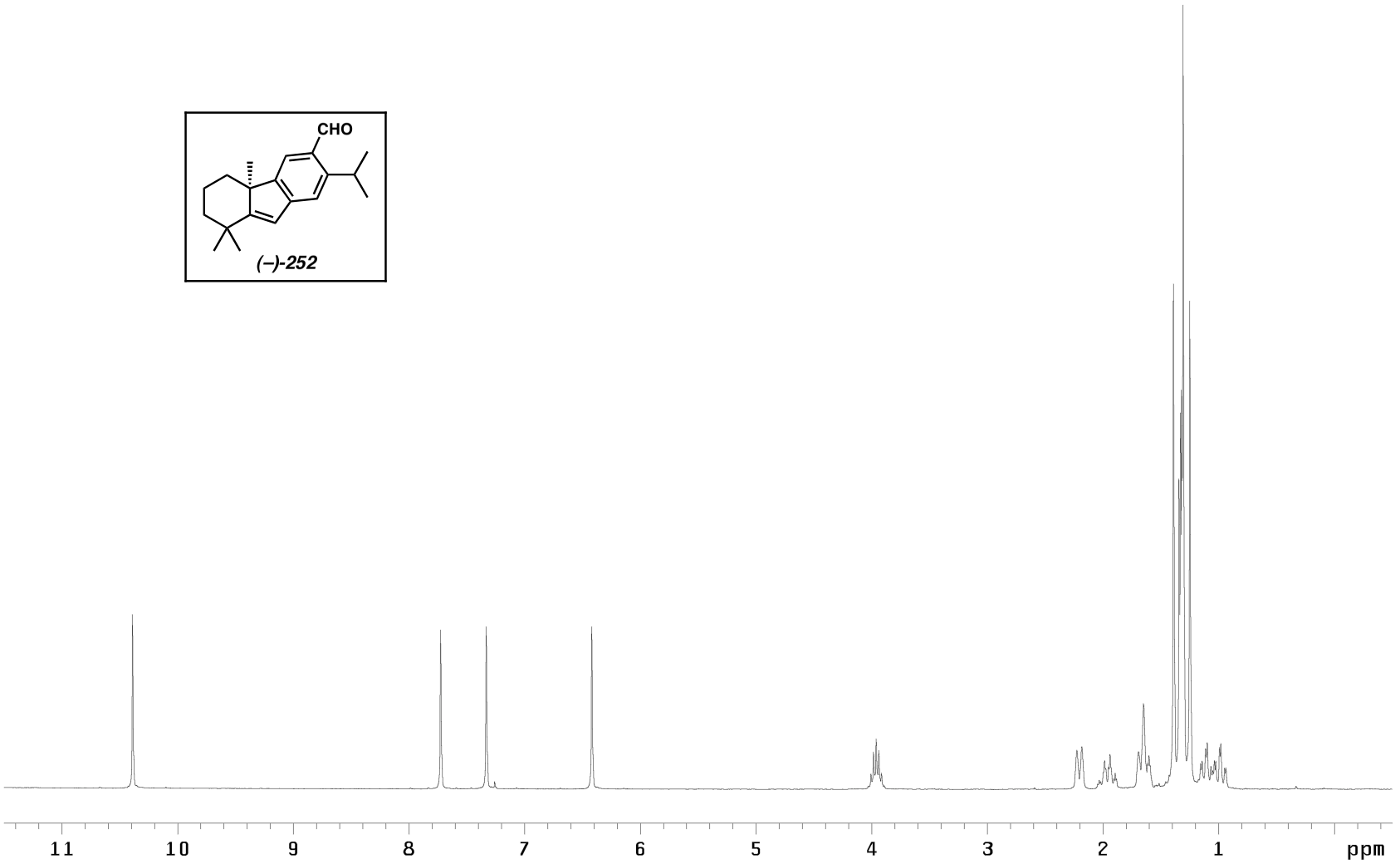


Figure A4.59 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **252**.

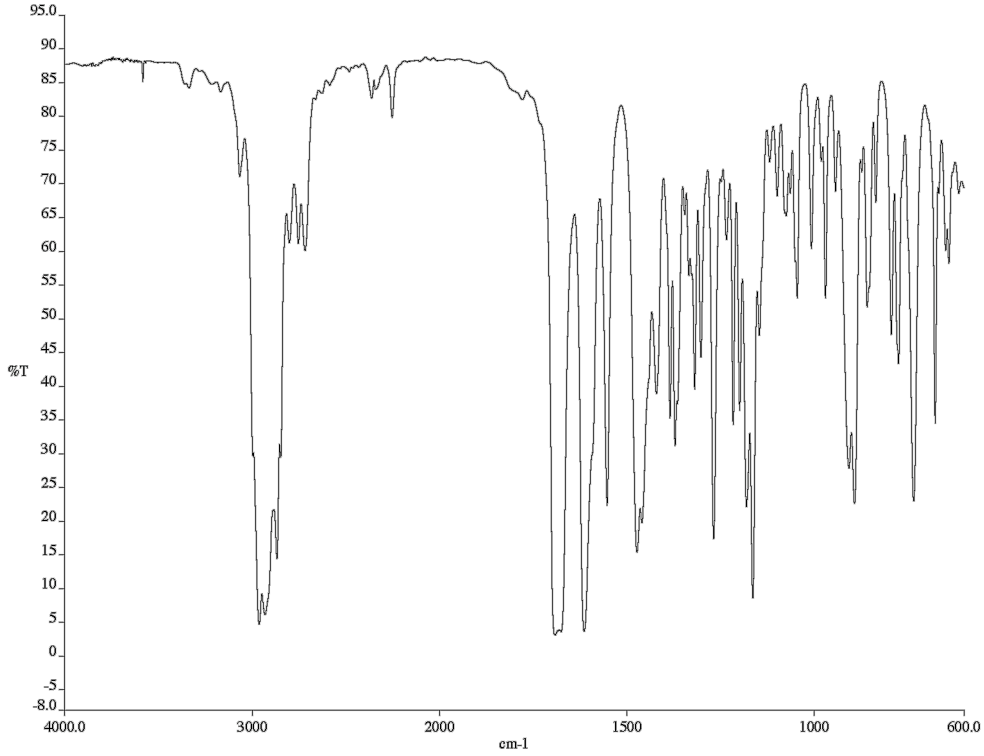


Figure A4.60 Infrared spectrum ($NaCl/CDCl_3$) of compound **252**.

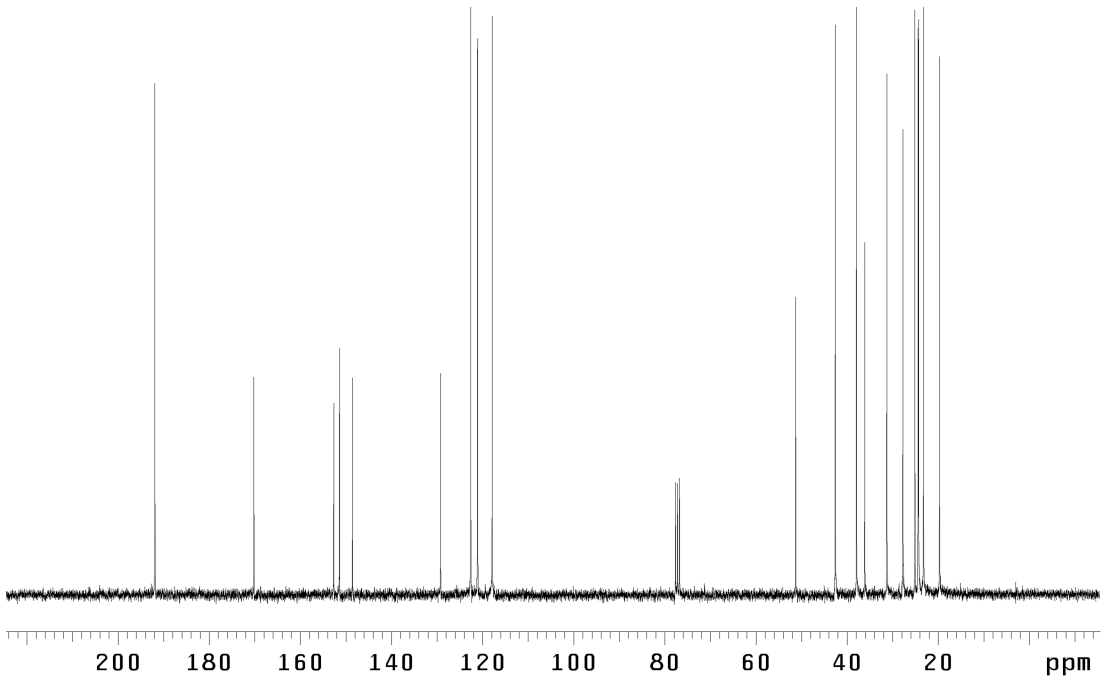


Figure A4.61 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **252**.

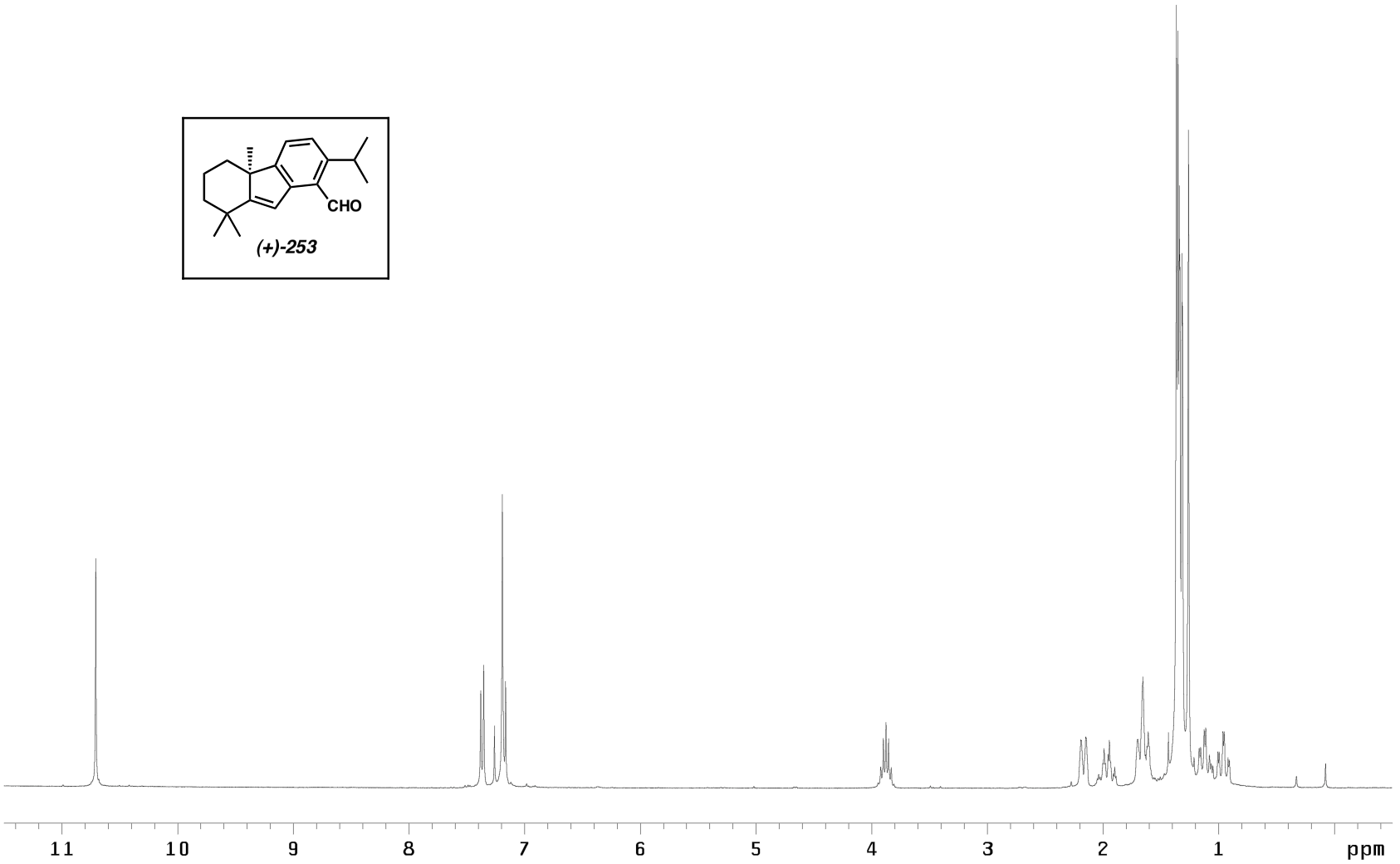


Figure A4.62 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **253**.

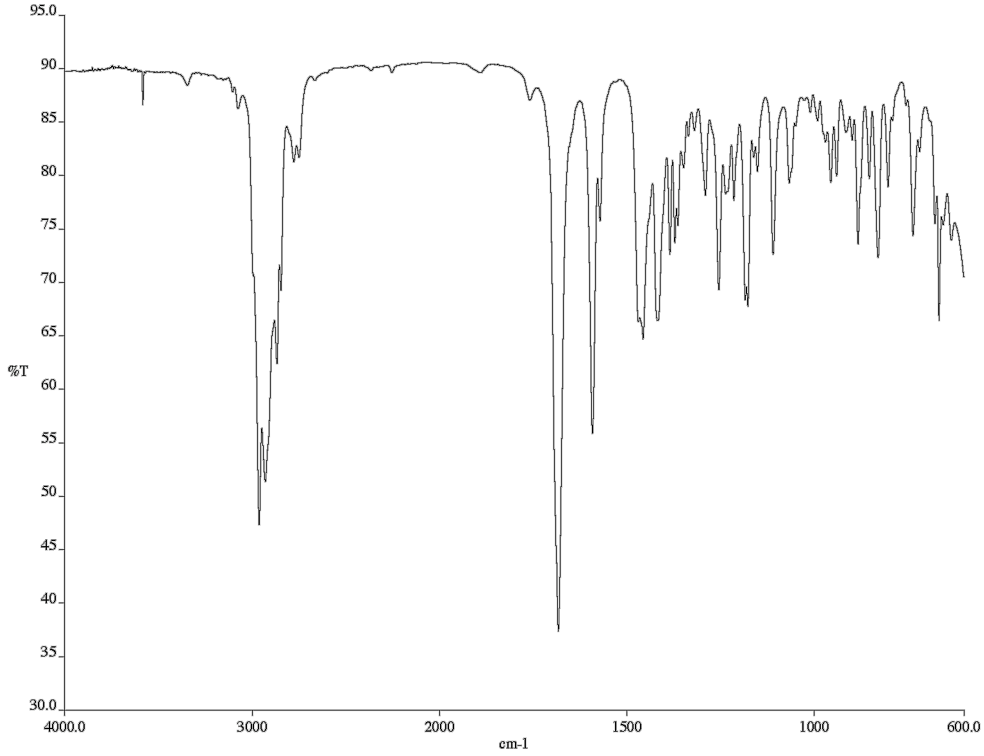


Figure A4.63 Infrared spectrum ($NaCl/CDCl_3$) of compound **253**.

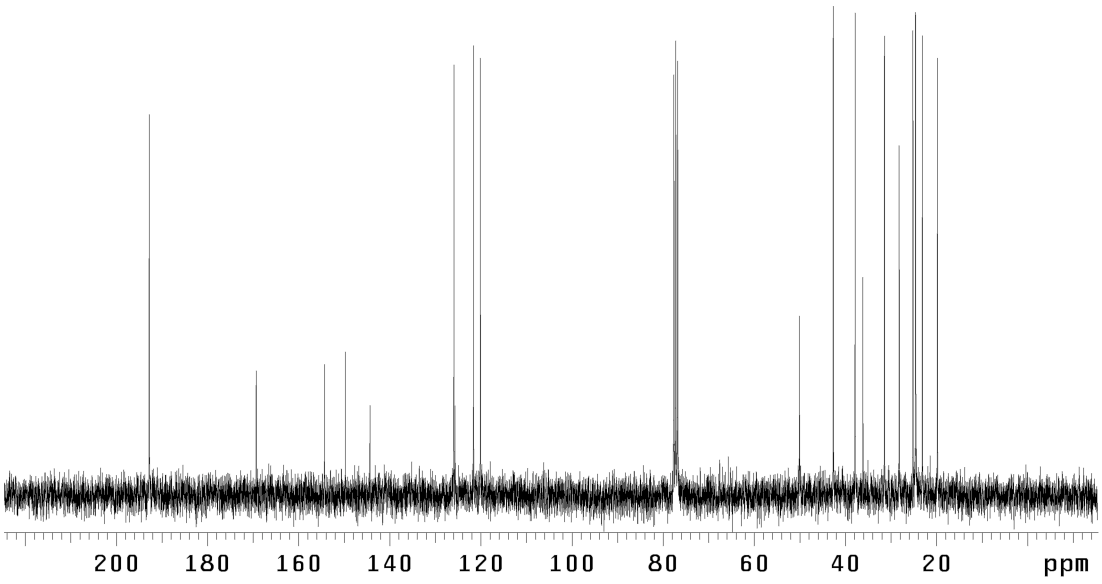


Figure A4.64 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **253**.

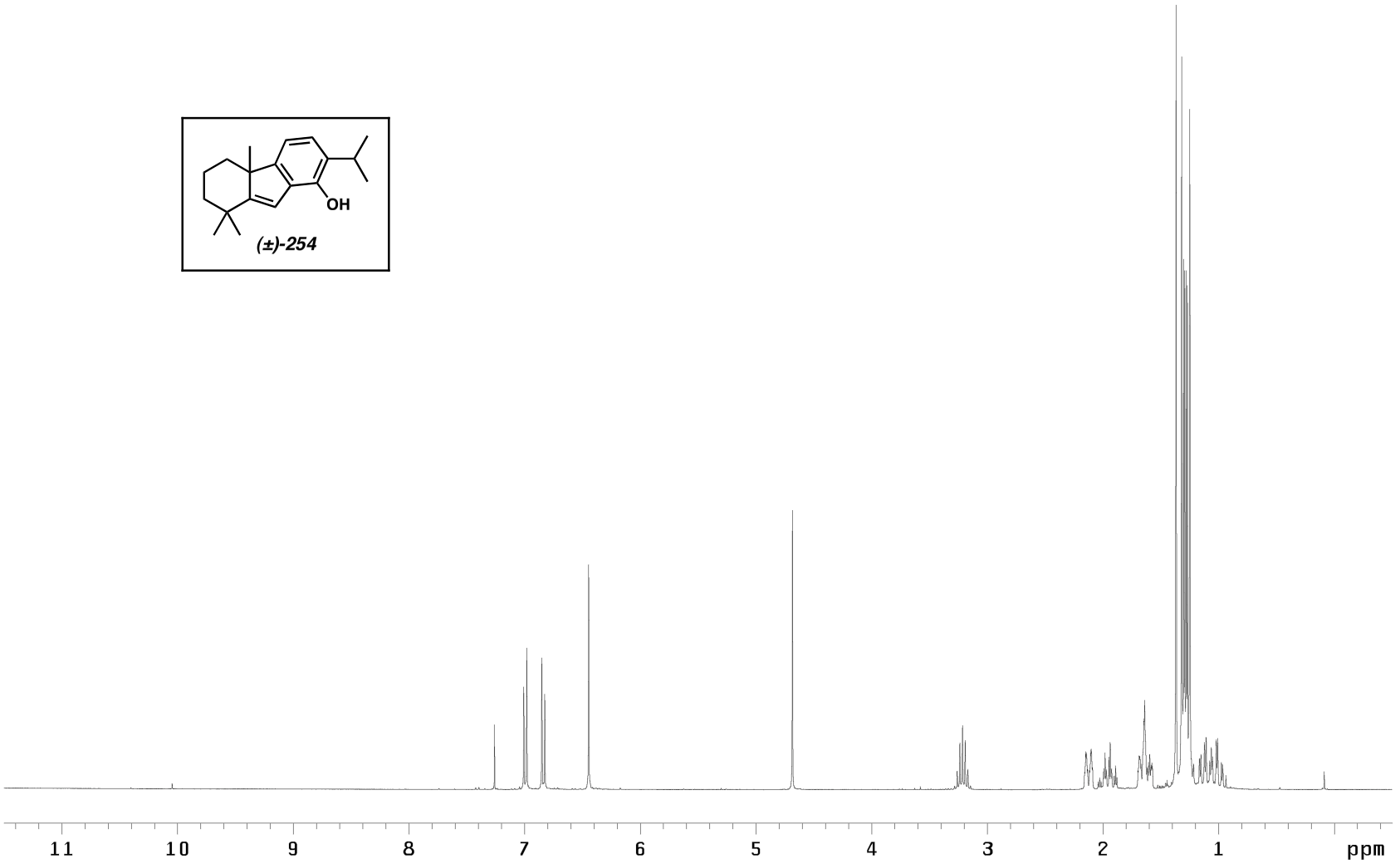


Figure A4.65 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **254**.

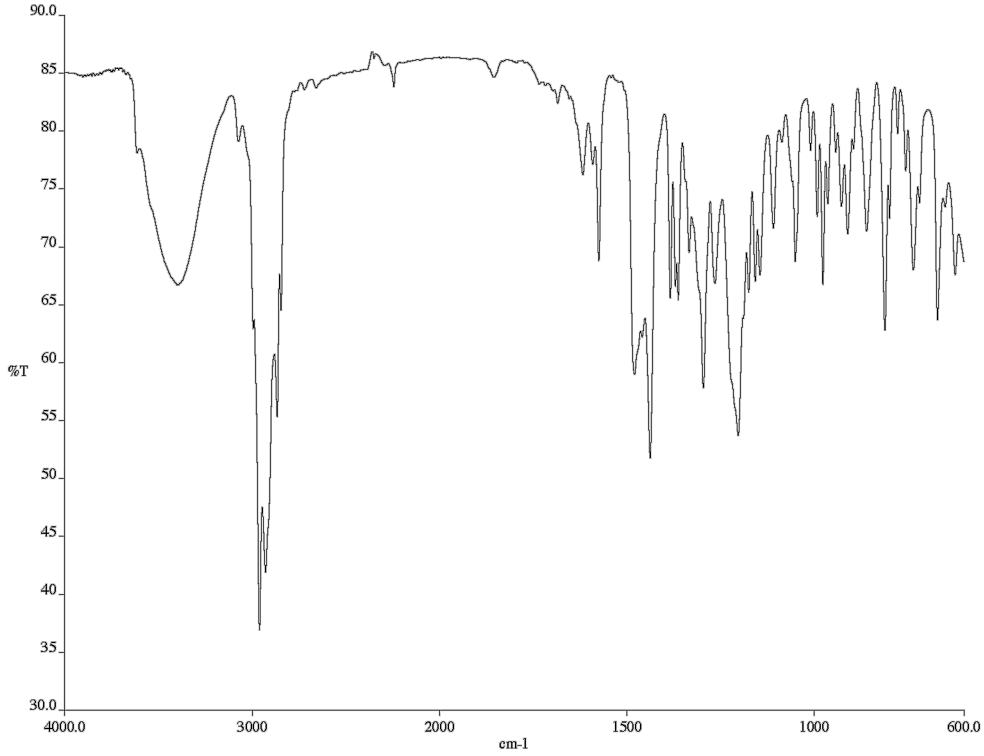


Figure A4.66 Infrared spectrum ($NaCl/CDCl_3$) of compound **254**.

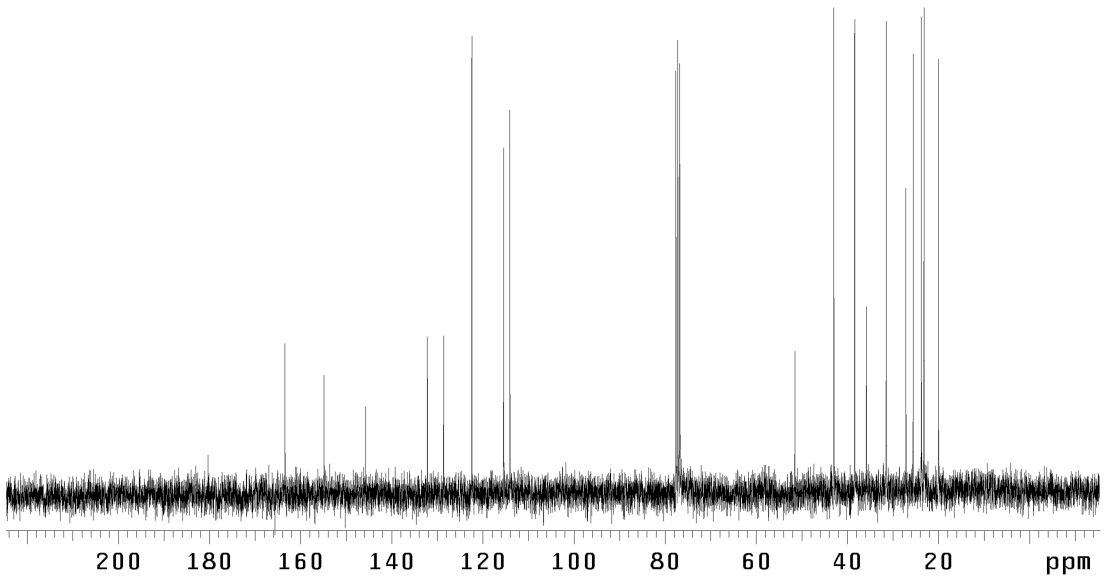


Figure A4.67 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **254**.

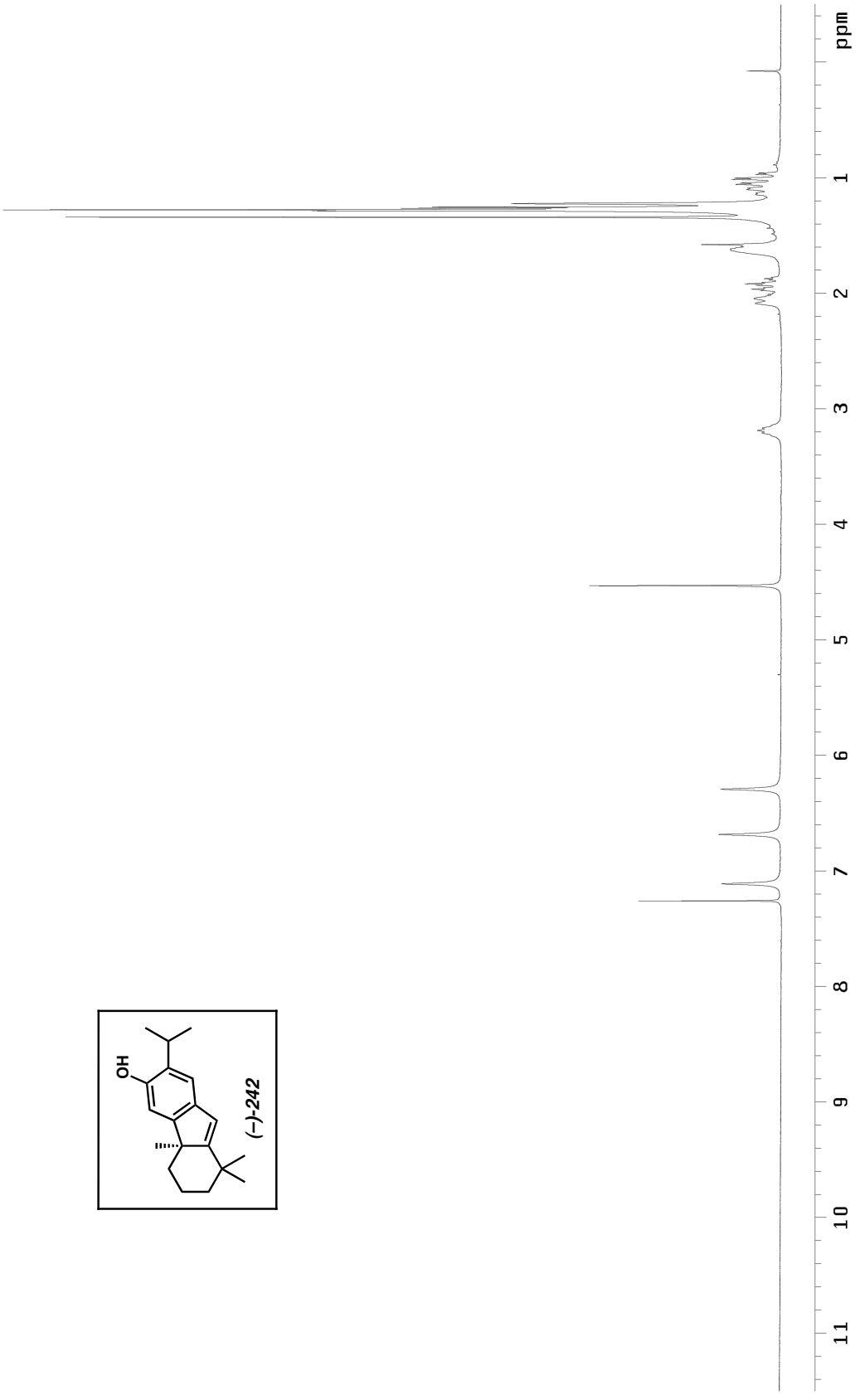


Figure A4.68 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **242**.

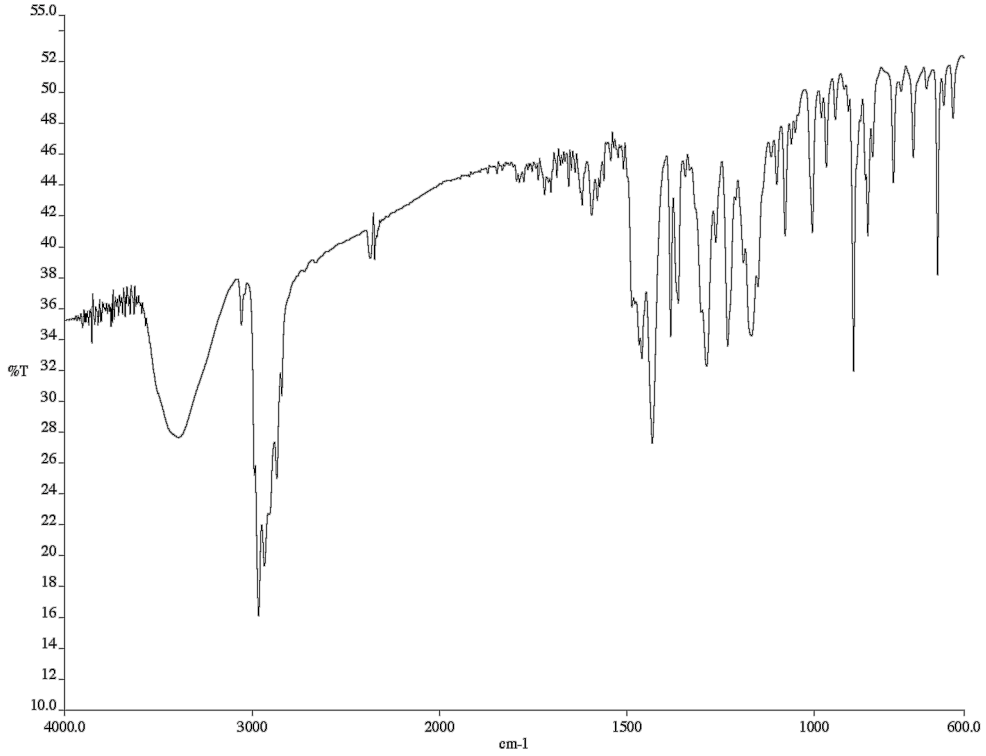


Figure A4.69 Infrared spectrum (KBr) of compound **242**.

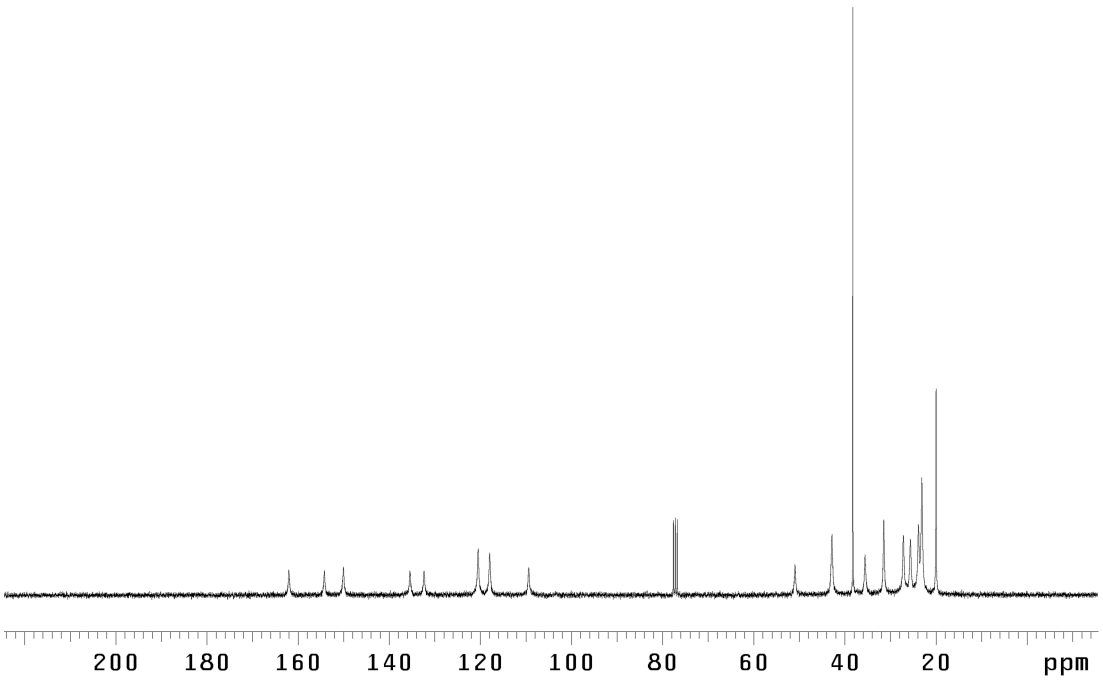


Figure A4.70 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **242**.

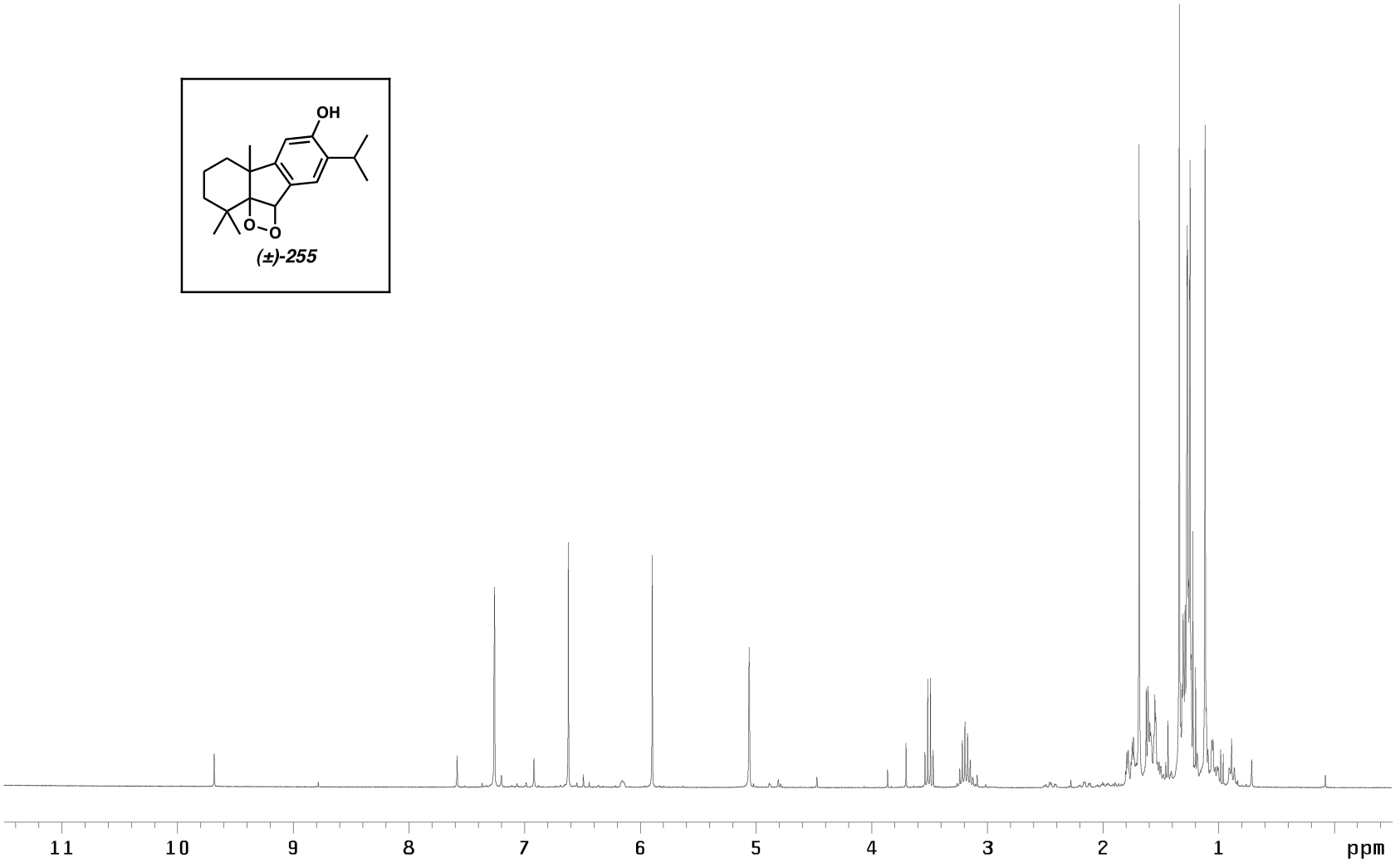


Figure A4.71 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **255**.

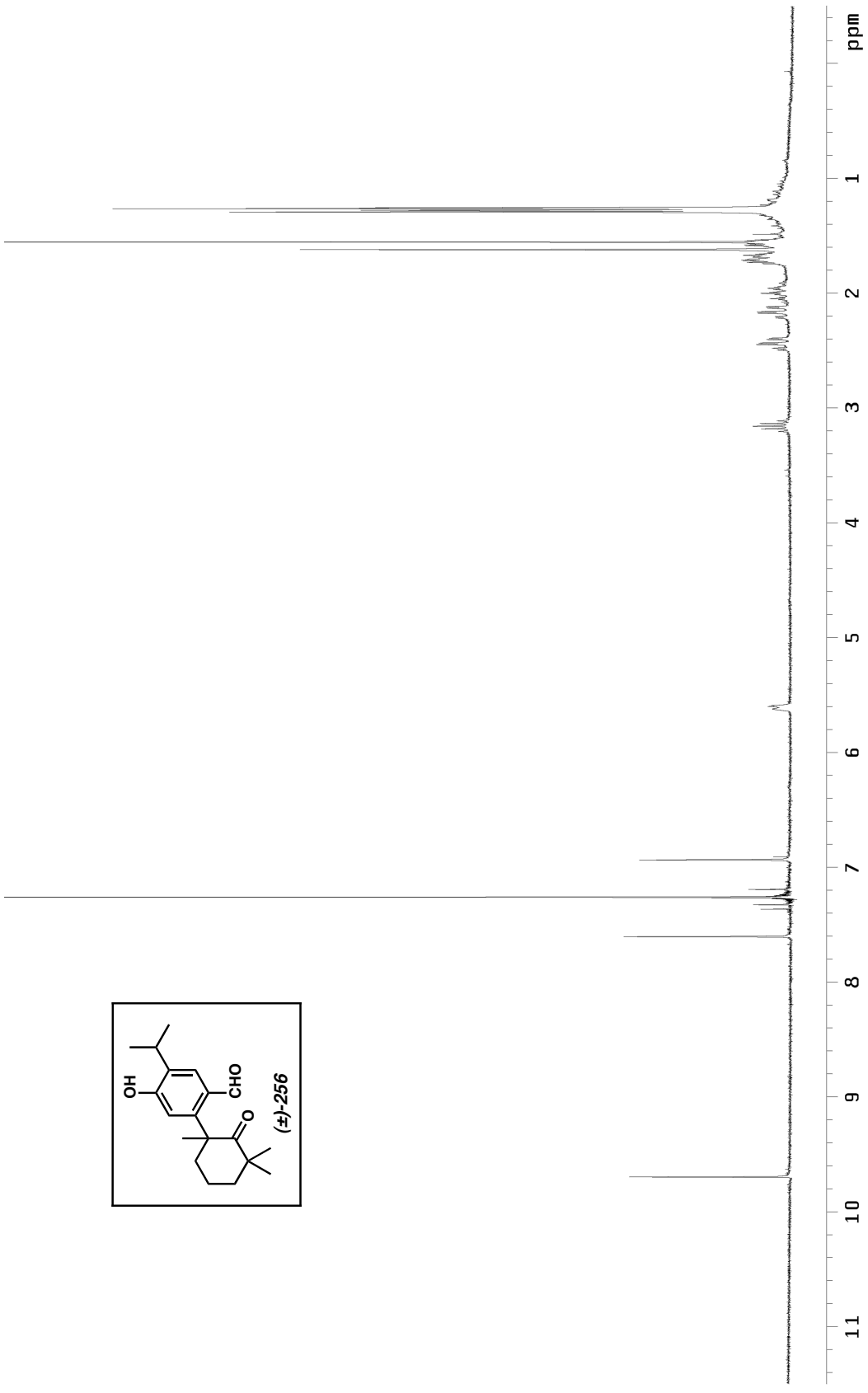


Figure A4.72 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **256**.

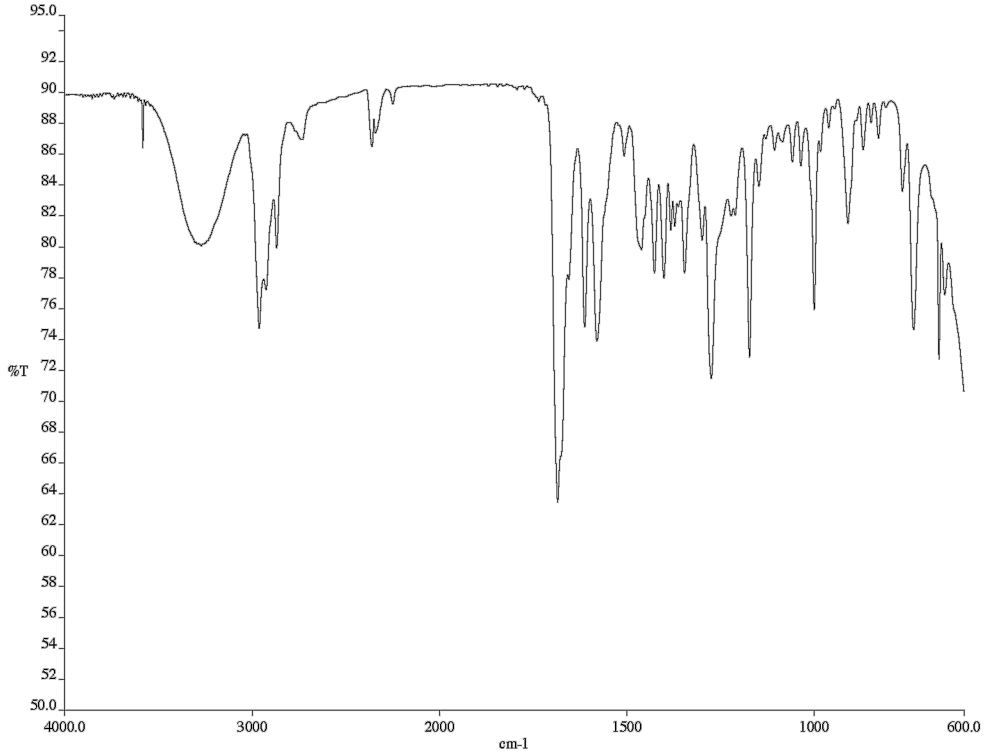


Figure A4.73 Infrared spectrum ($NaCl/CDCl_3$) of compound **256**.

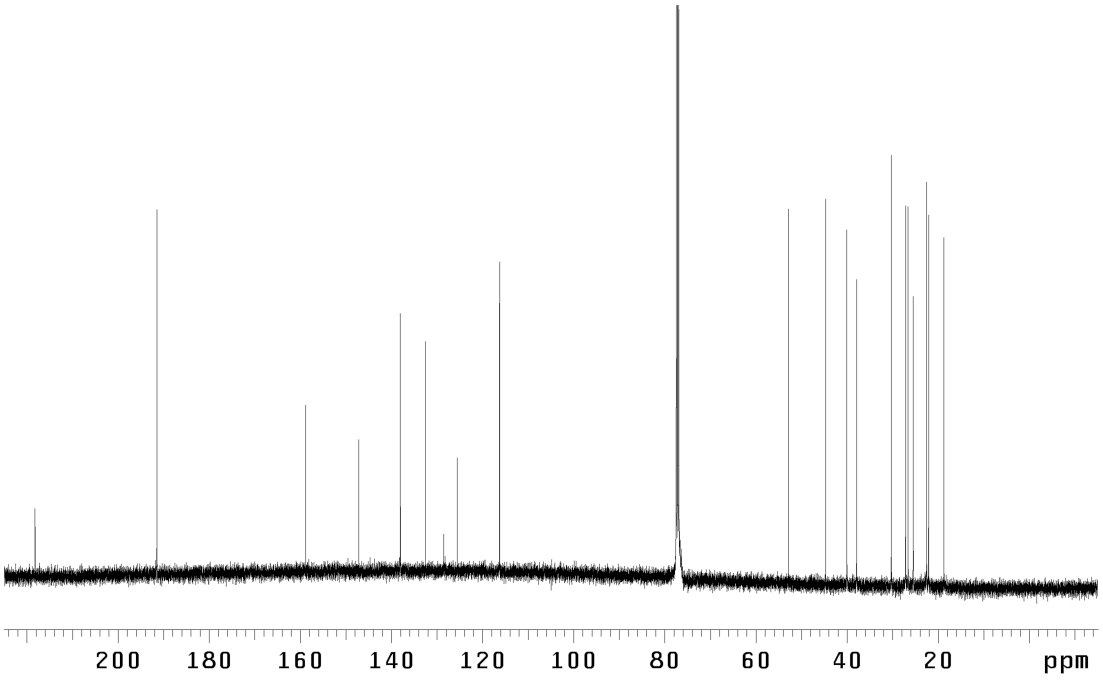


Figure A4.74 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **256**.

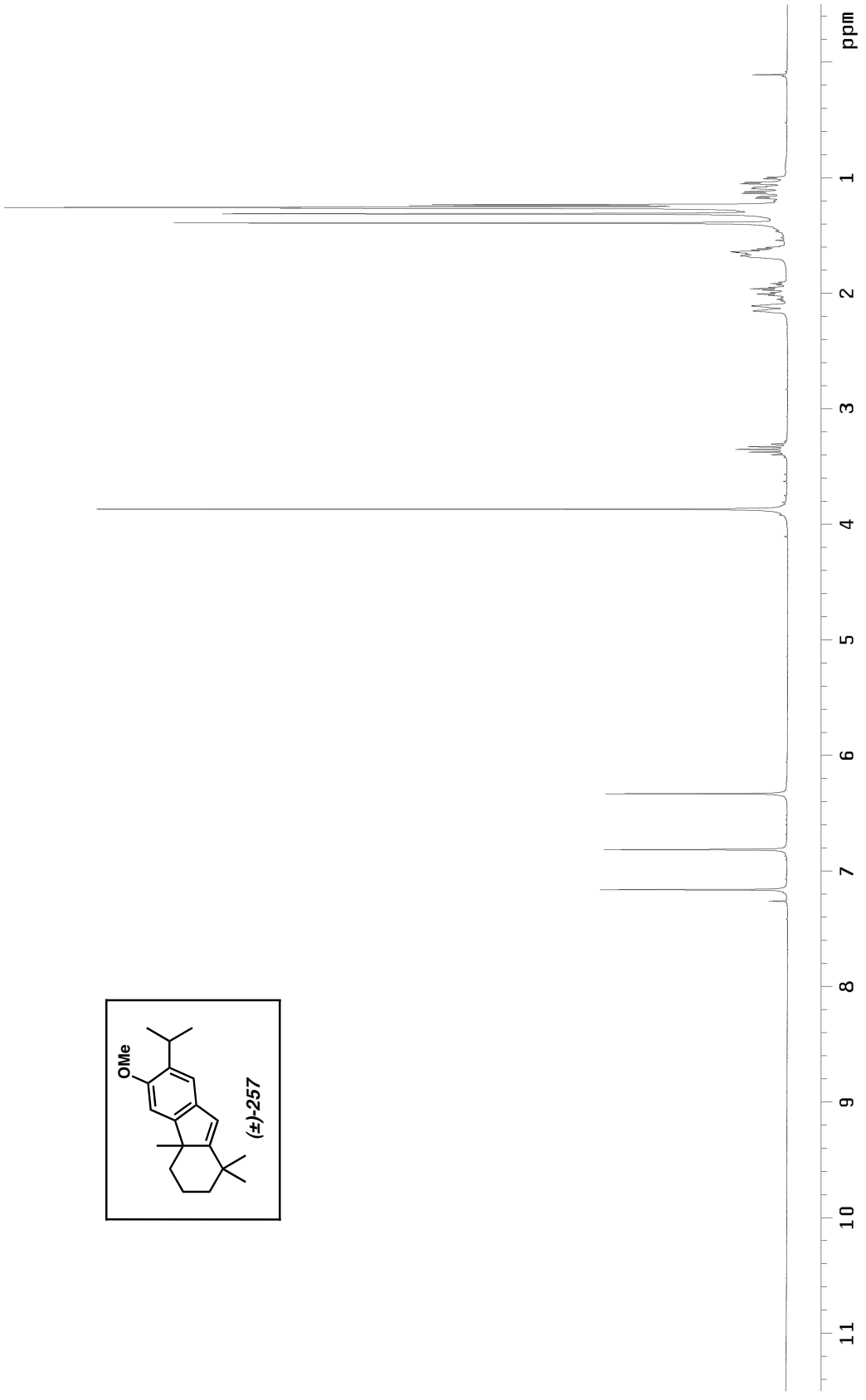


Figure A4.75 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **257**.

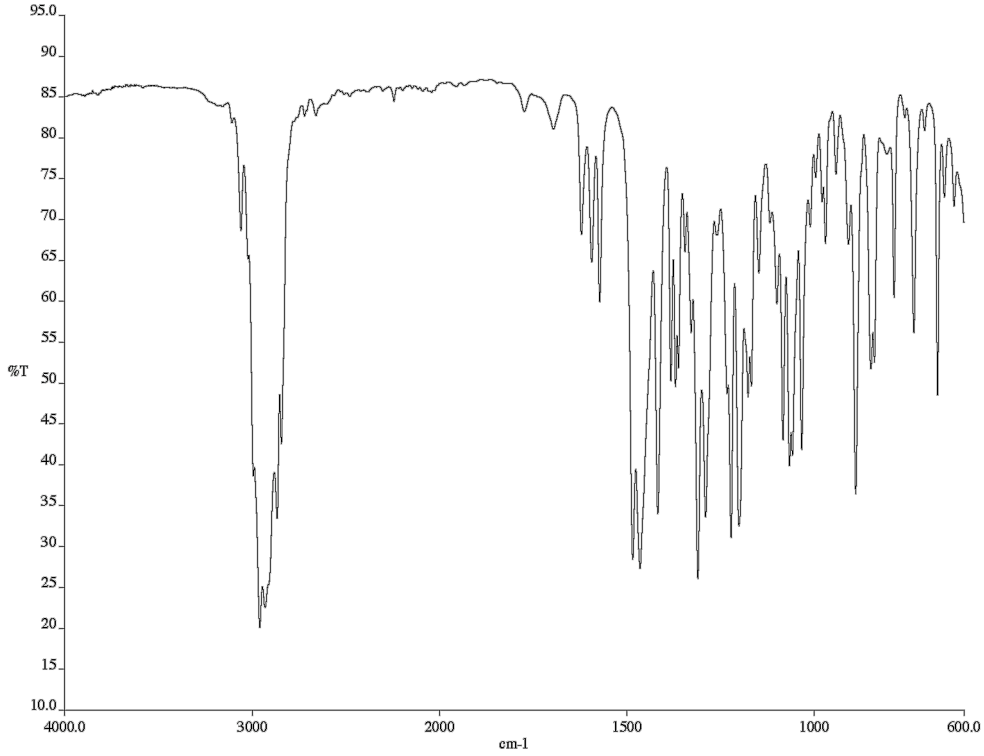


Figure A4.76 Infrared spectrum ($NaCl/CDCl_3$) of compound **257**.

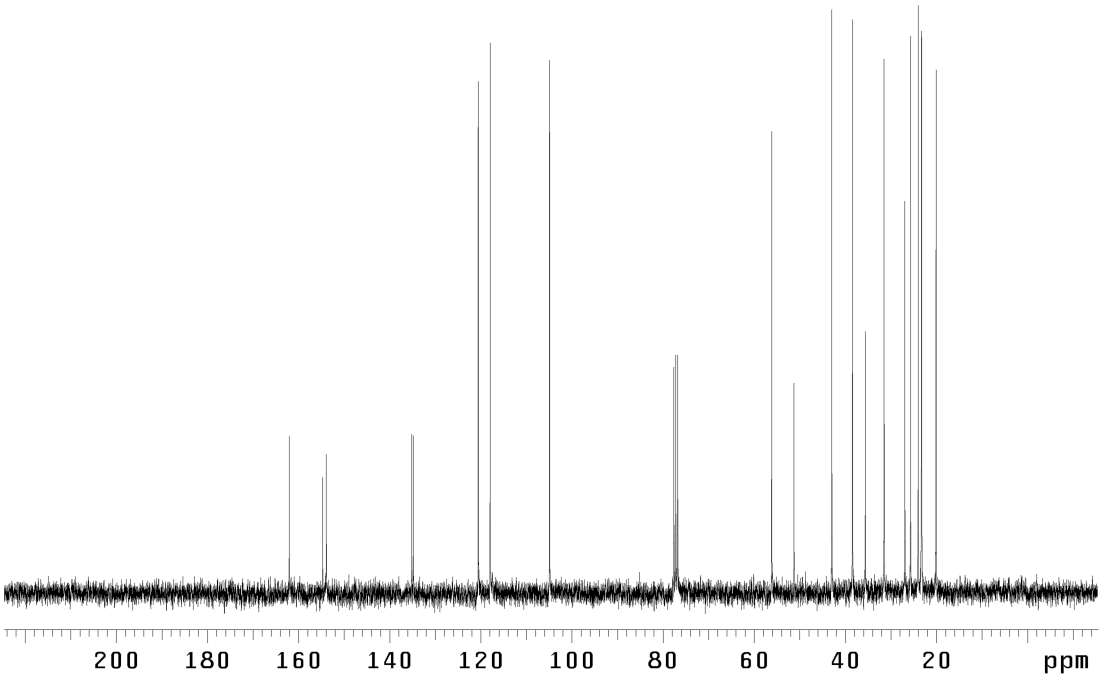


Figure A4.77 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **257**.

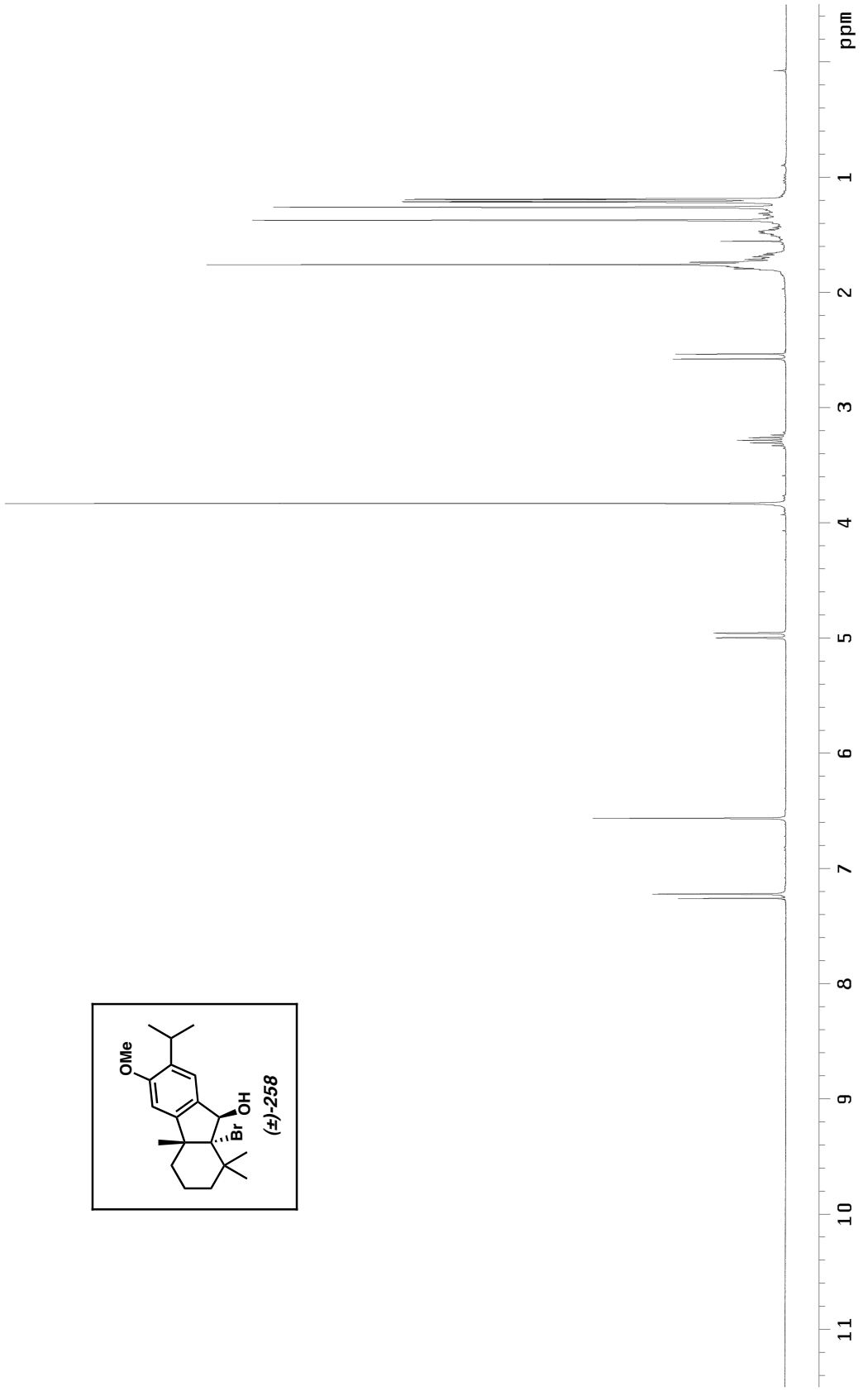


Figure A4.78 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **258**.

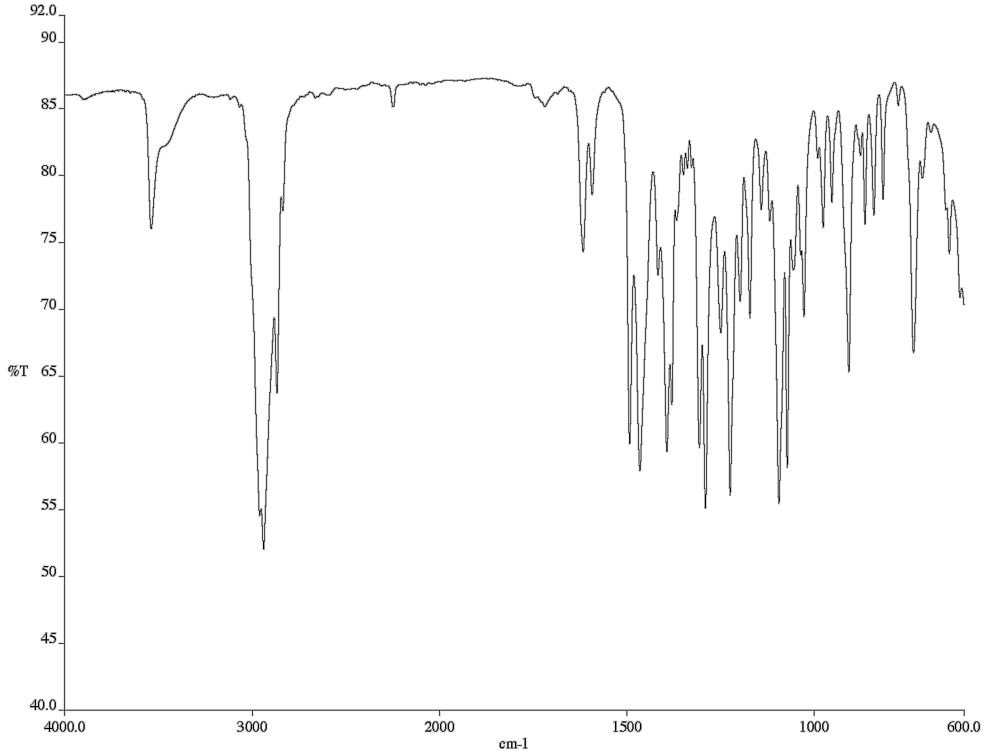


Figure A4.79 Infrared spectrum ($NaCl/CDCl_3$) of compound **258**.

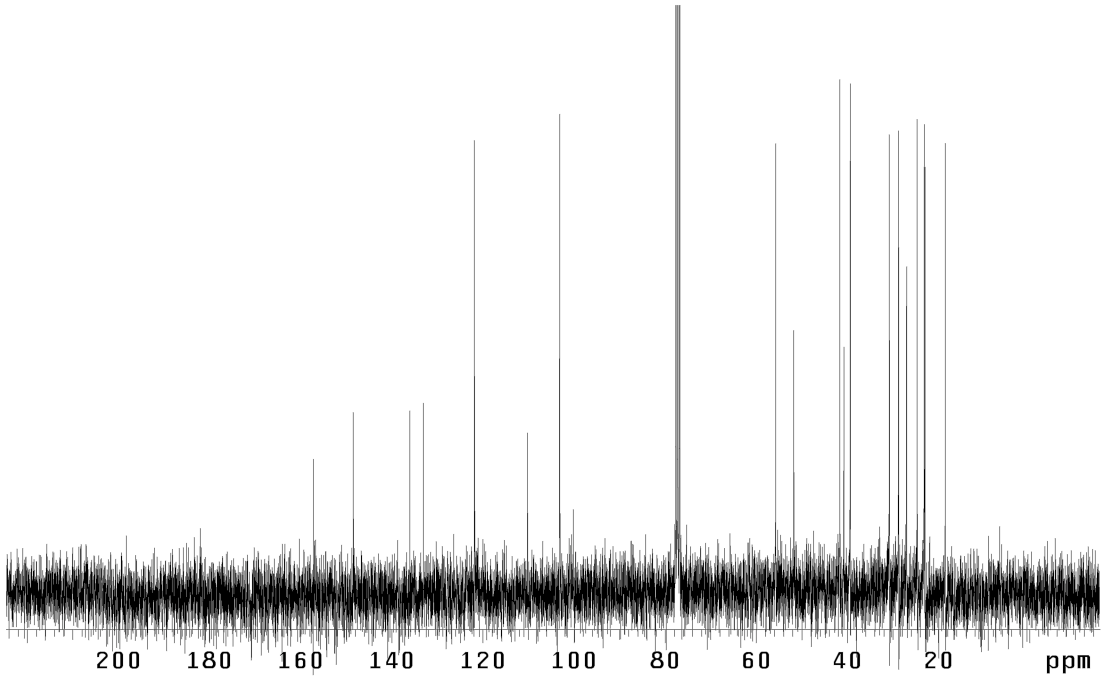


Figure A4.80 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **258**.

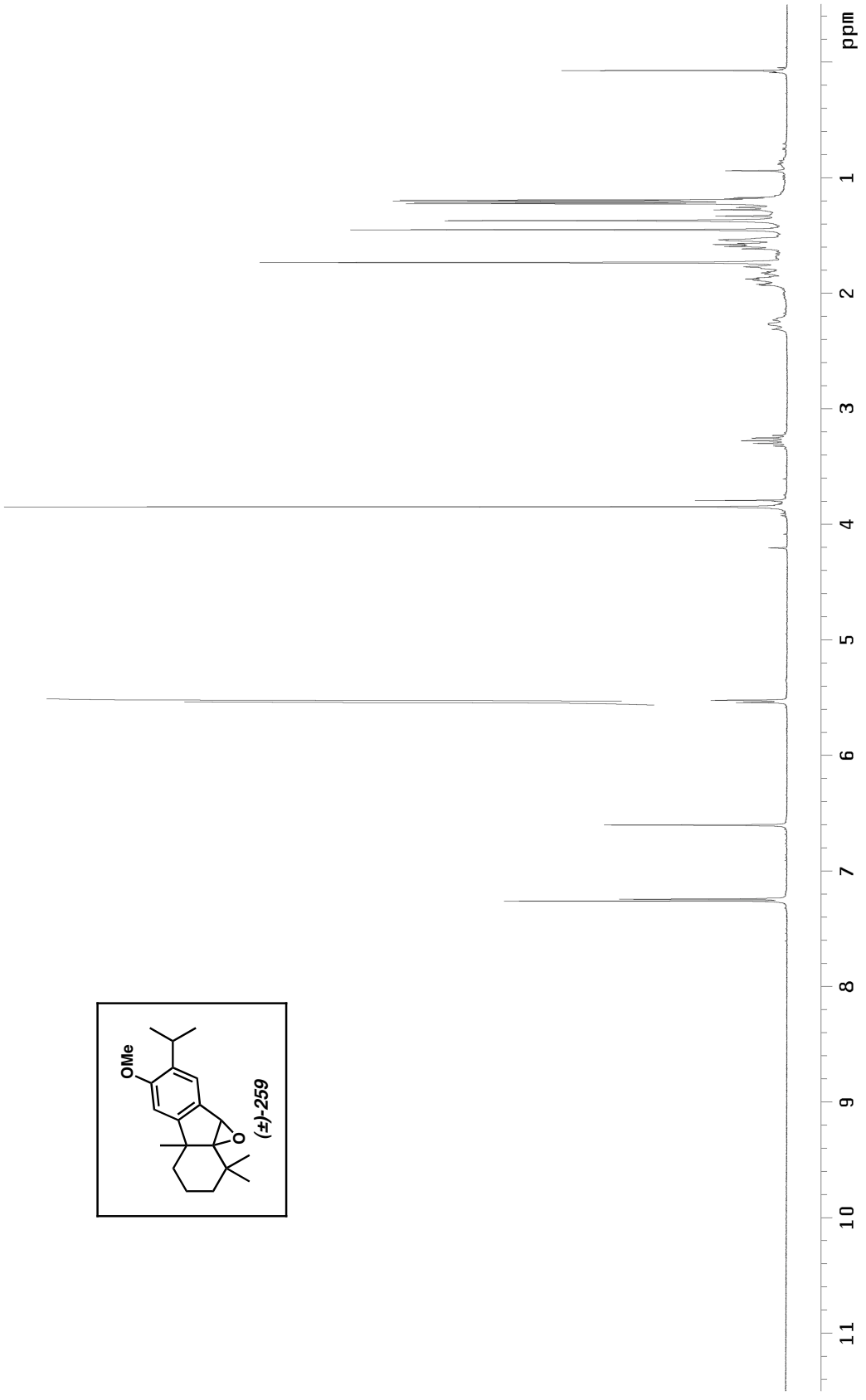


Figure A4.81 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **259**.

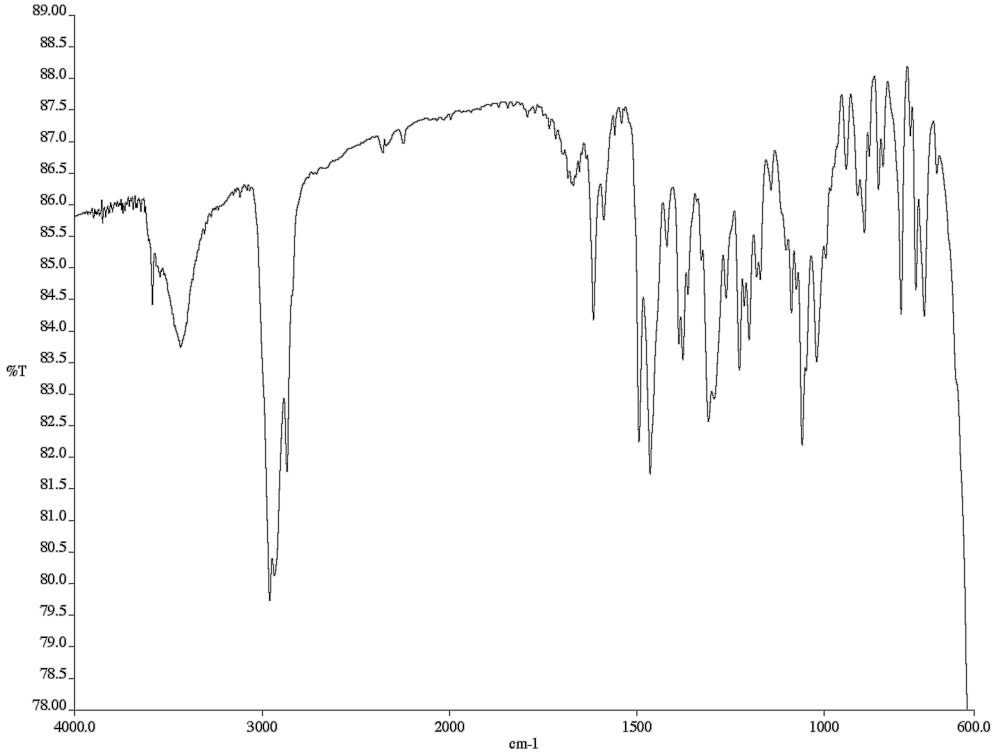


Figure A4.82 Infrared spectrum ($NaCl/CDCl_3/D_2O$) of compound **259**.

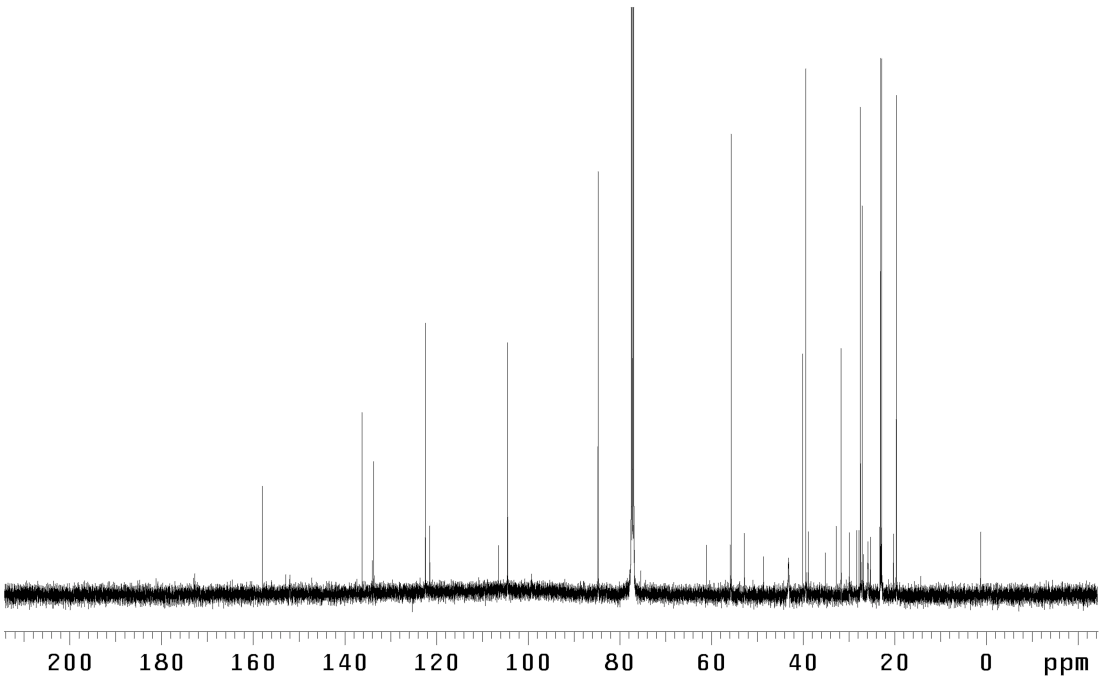


Figure A4.83 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **259**.

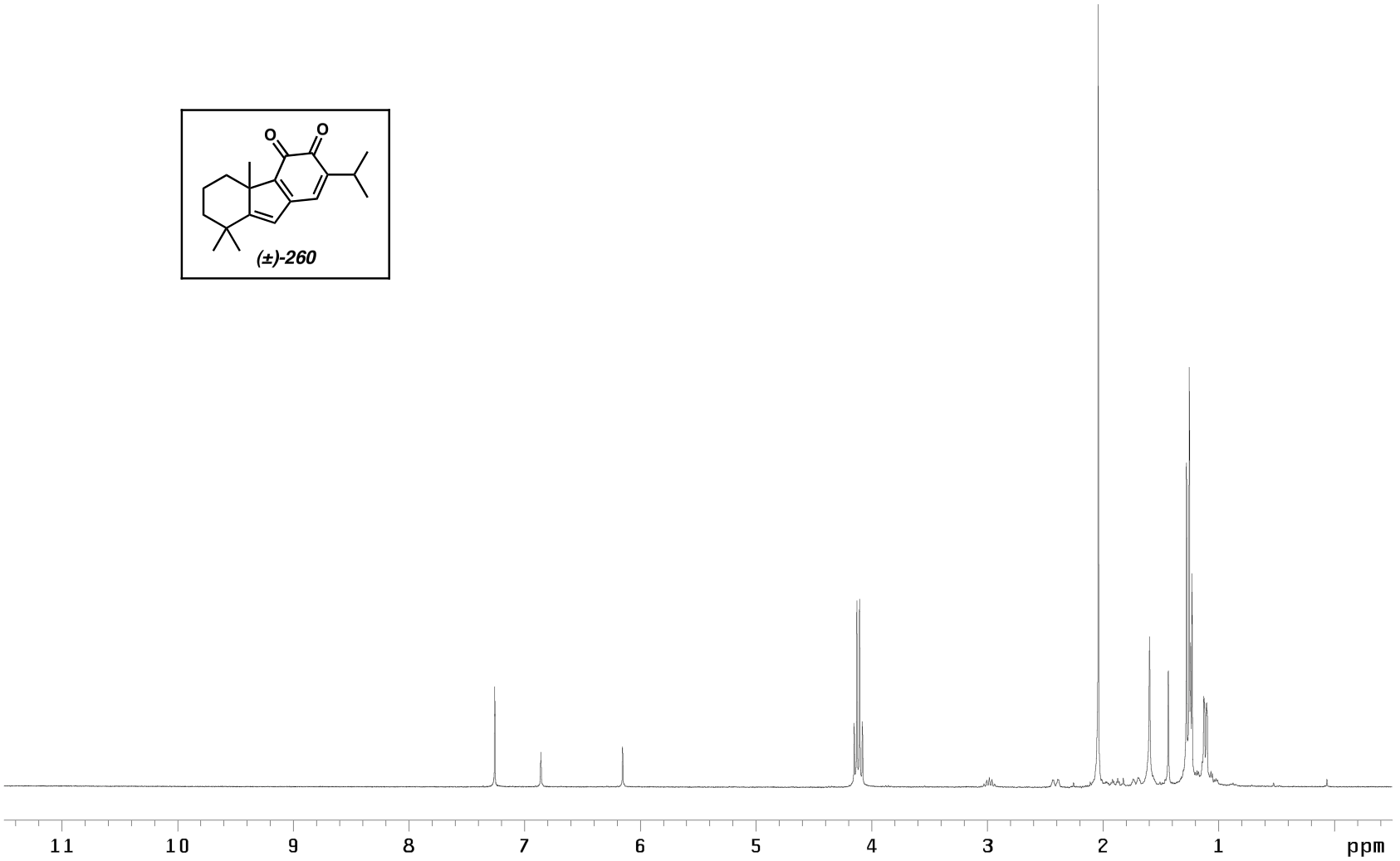


Figure A4.84 ^{1}H NMR (300 MHz, C_6D_6) of compound **260**.

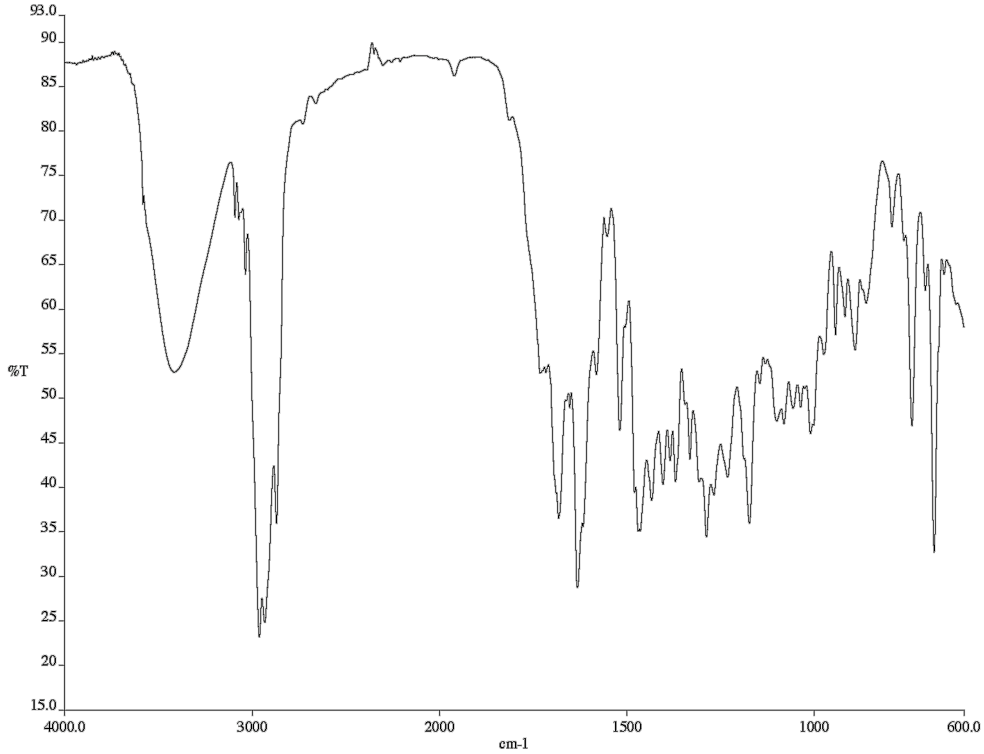


Figure A4.85 Infrared spectrum (NaCl/neat) of compound **260**.

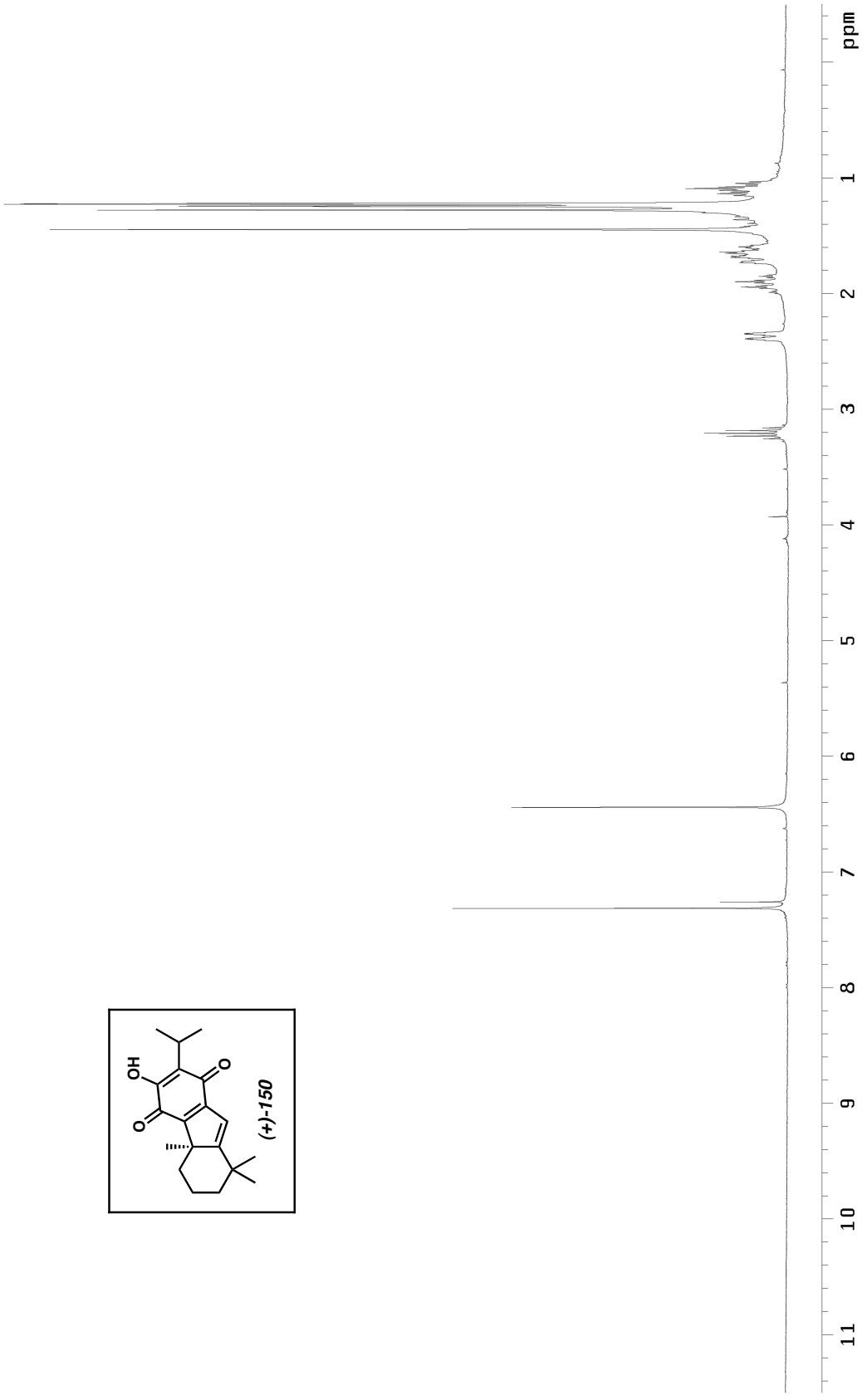


Figure A4.86 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **150**.

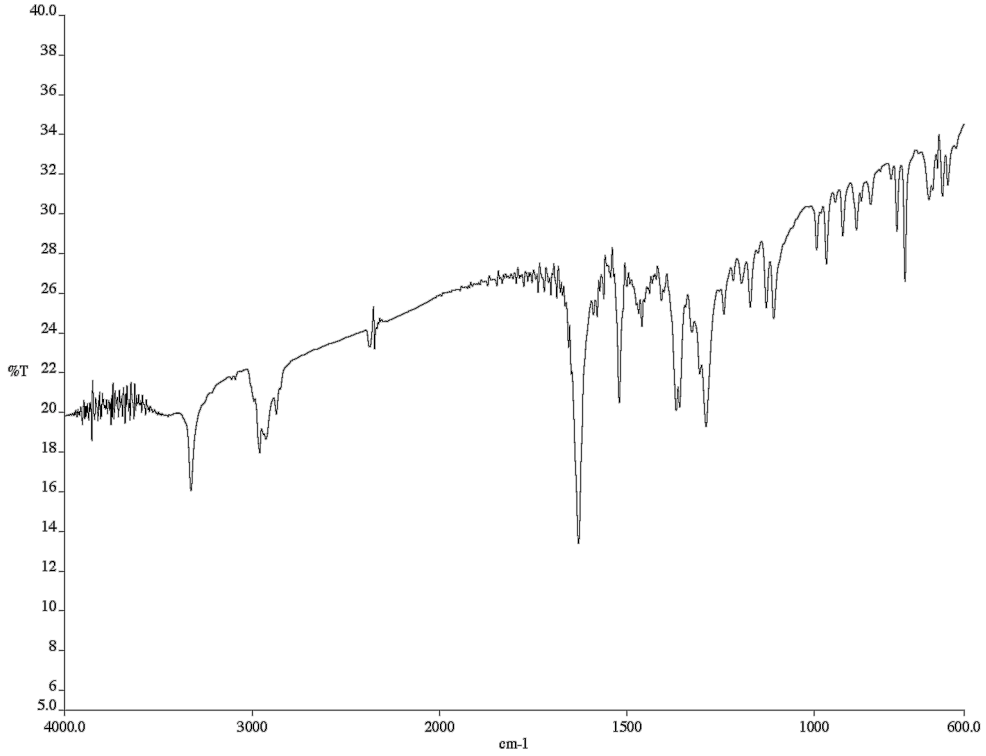


Figure A4.87 Infrared spectrum (KBr) of compound **150**.

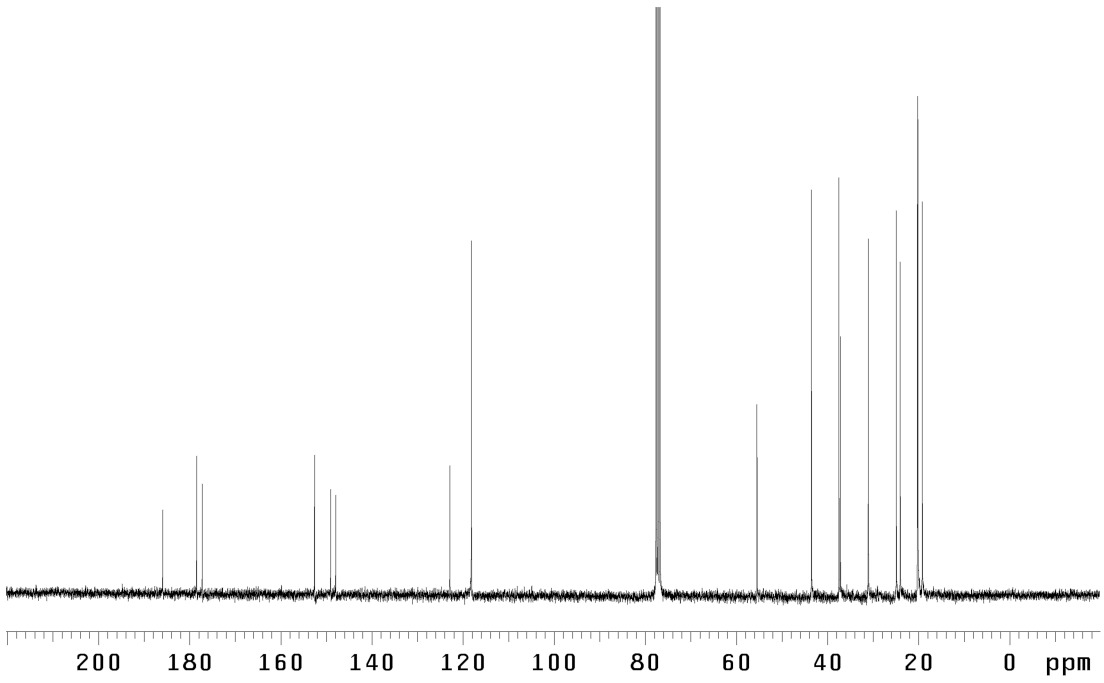


Figure A4.88 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **150**.

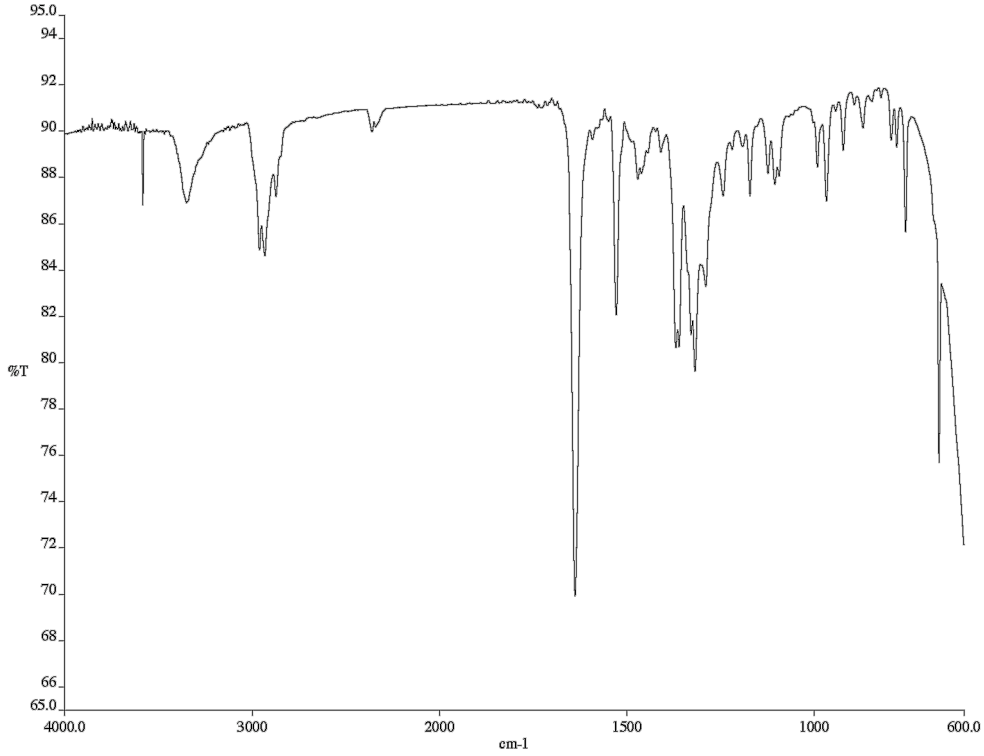


Figure A4.89 Infrared spectrum ($NaCl/CHCl_3$) of compound **150**.

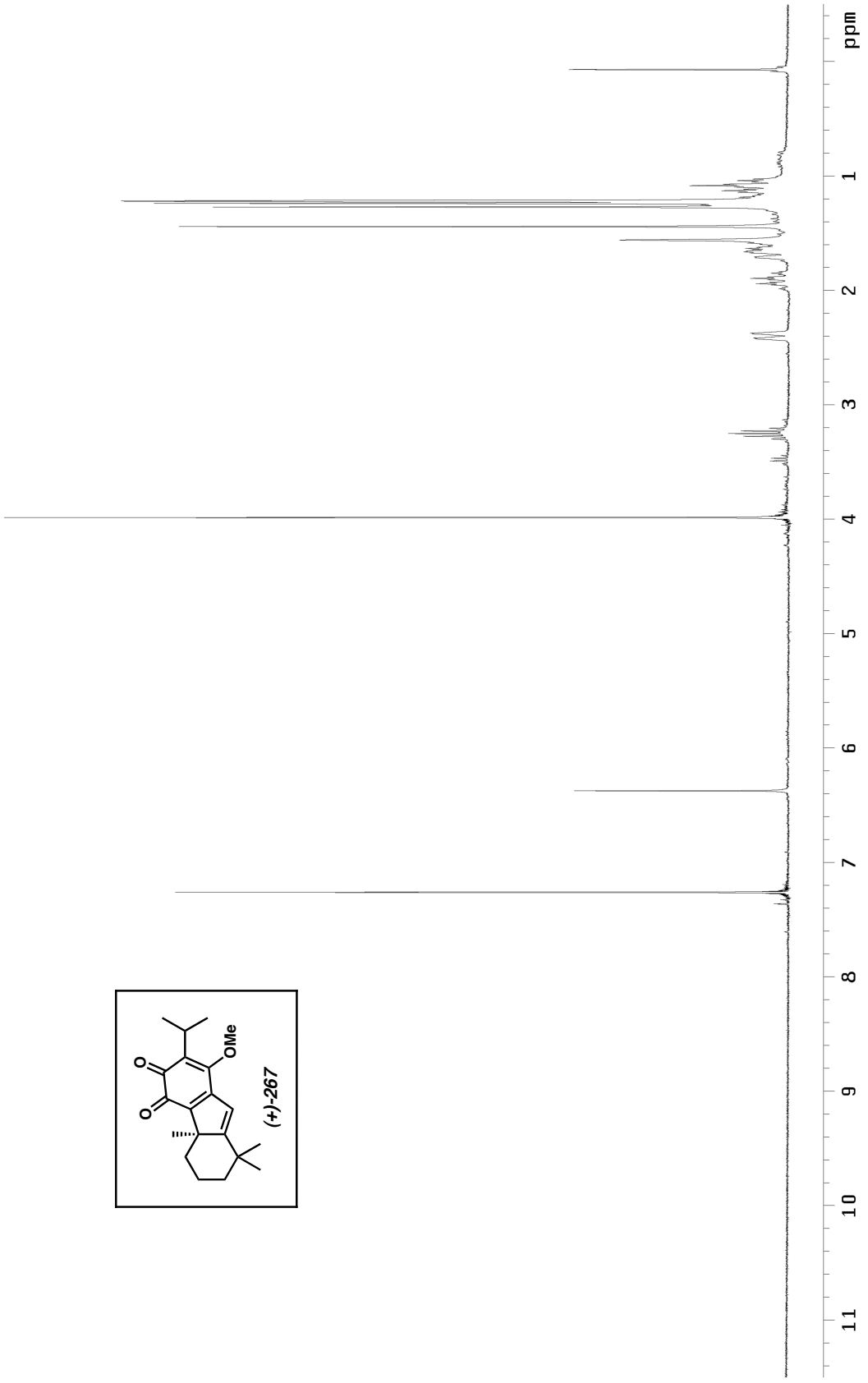


Figure A4.90 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **267**.

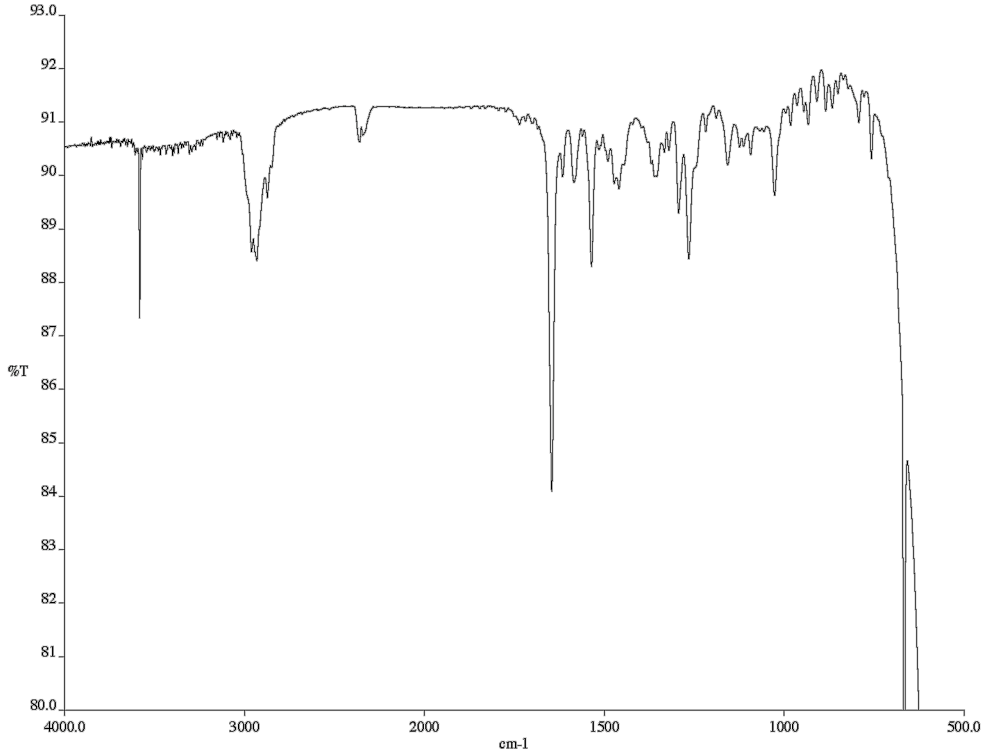


Figure A4.91 Infrared spectrum ($NaCl/CHCl_3$) of compound **267**.

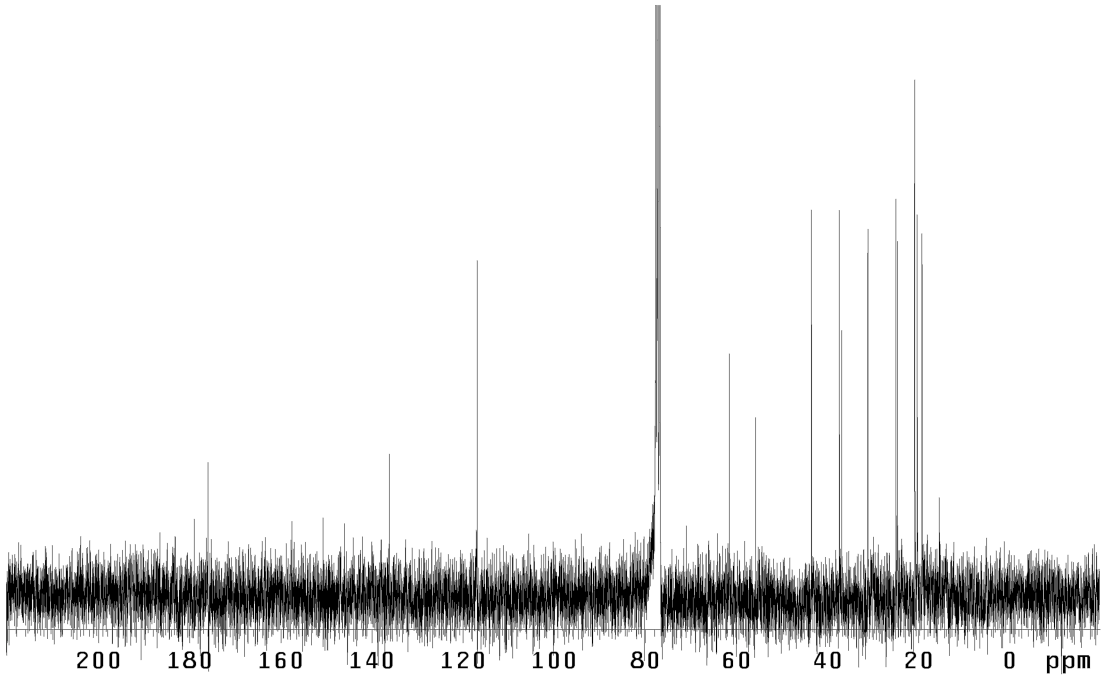


Figure A4.92 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **267**.

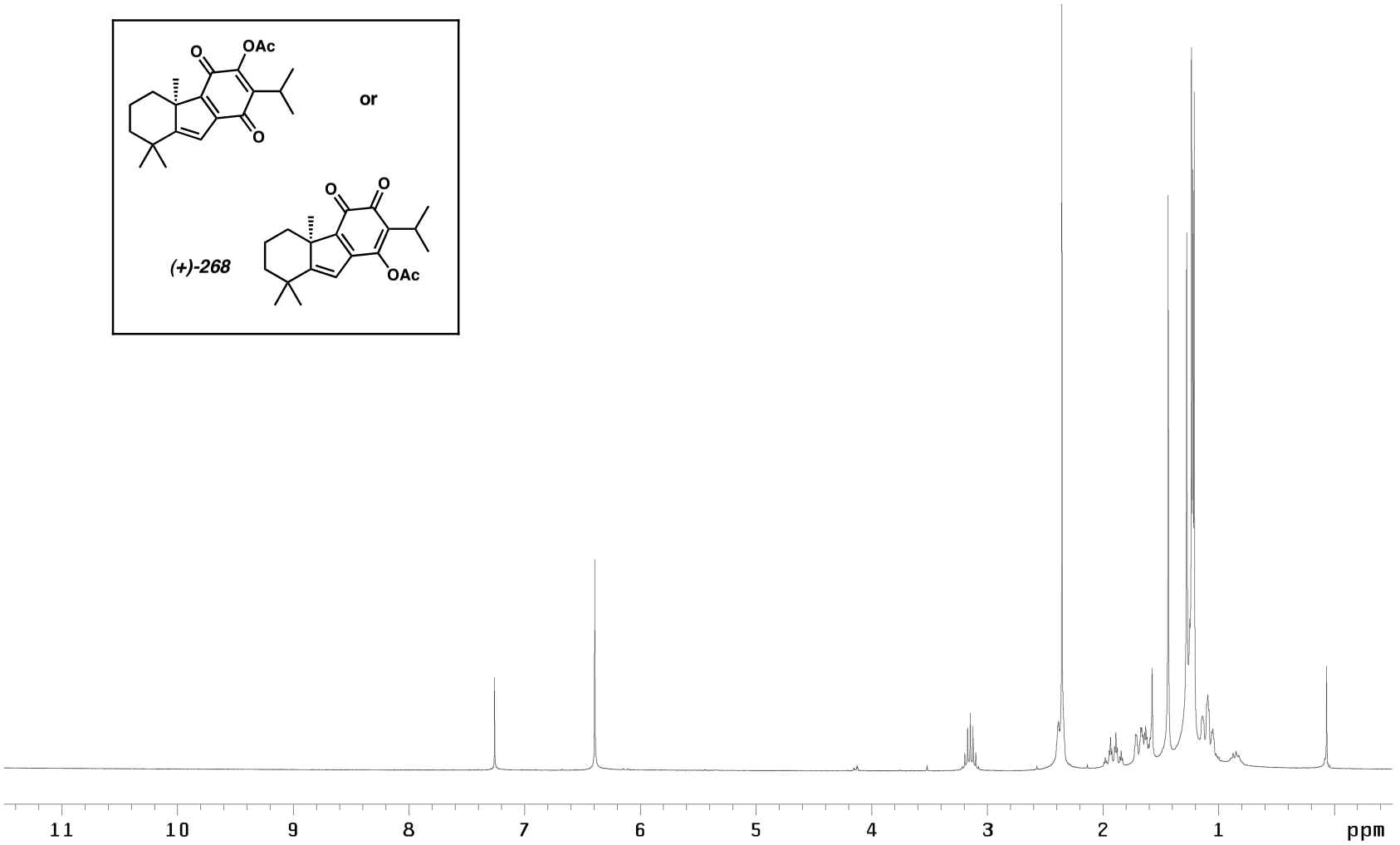


Figure A4.93 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **268**.

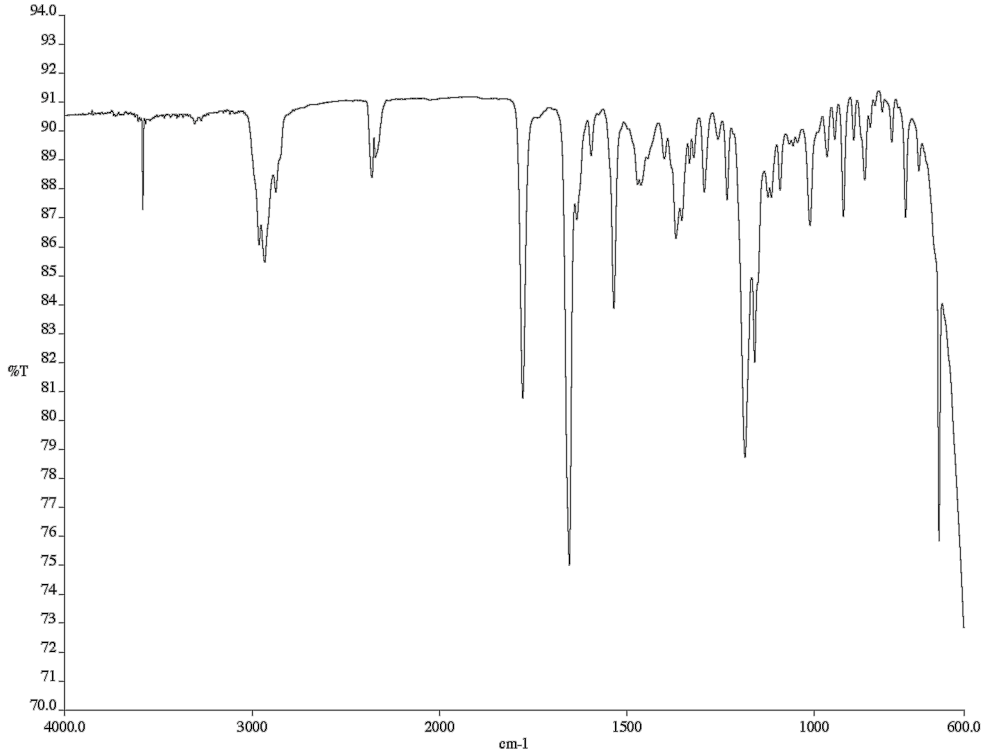


Figure A4.94 Infrared spectrum ($NaCl/CHCl_3$) of compound **268**.

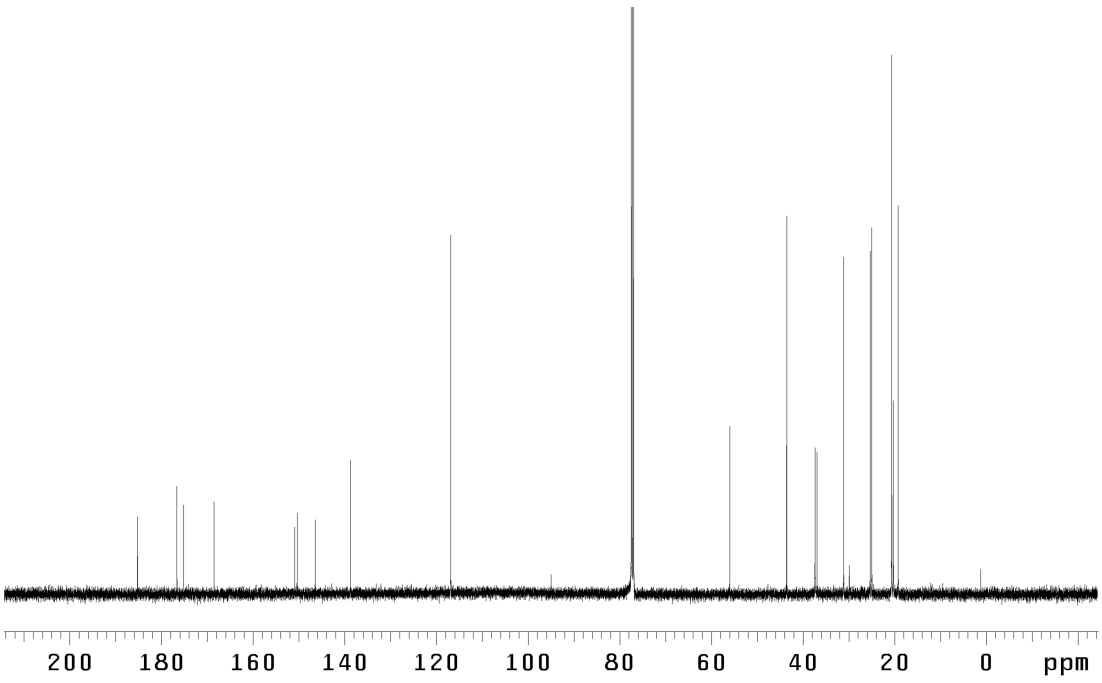


Figure A4.95 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **268**.

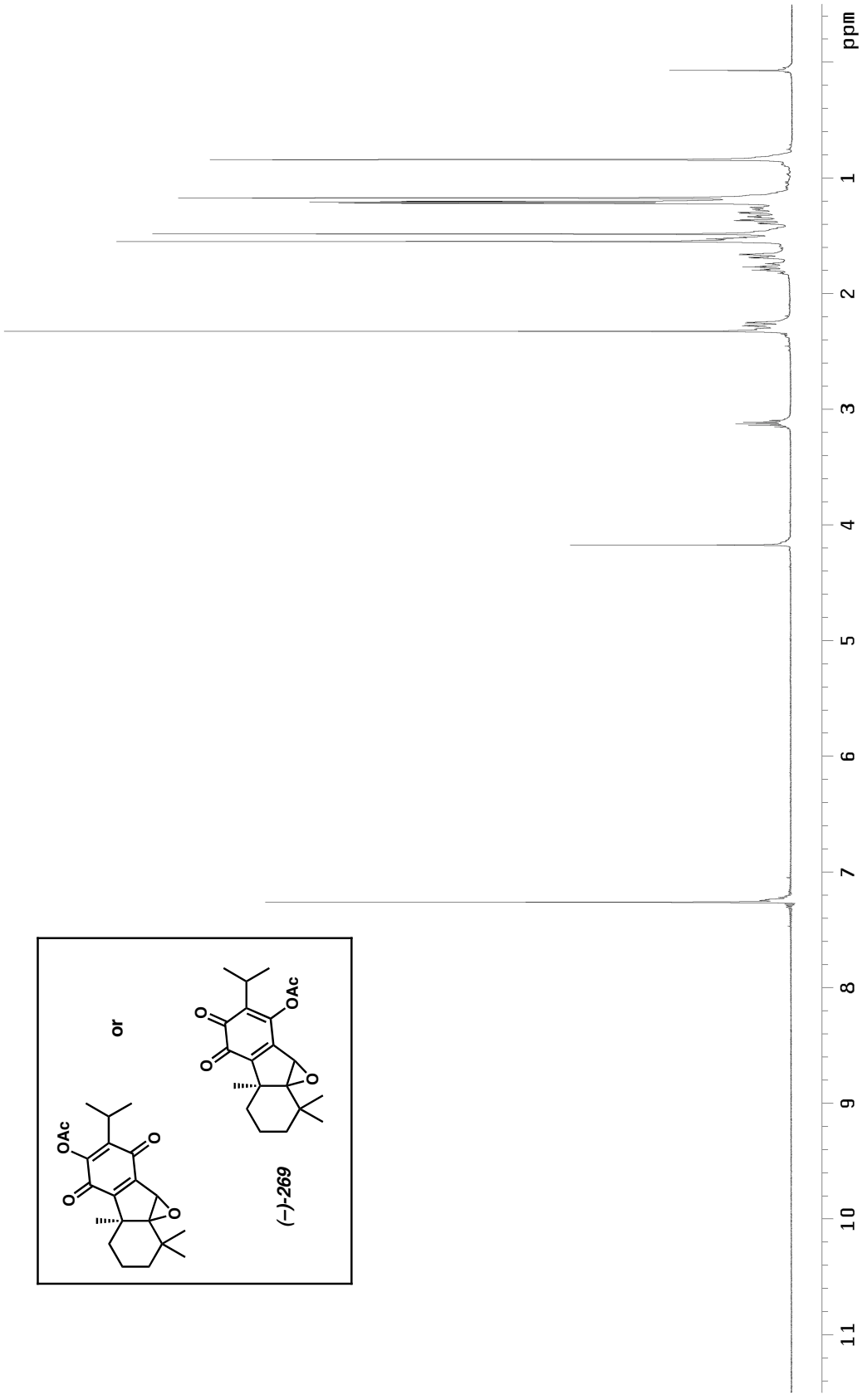


Figure A4.96 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **269**.

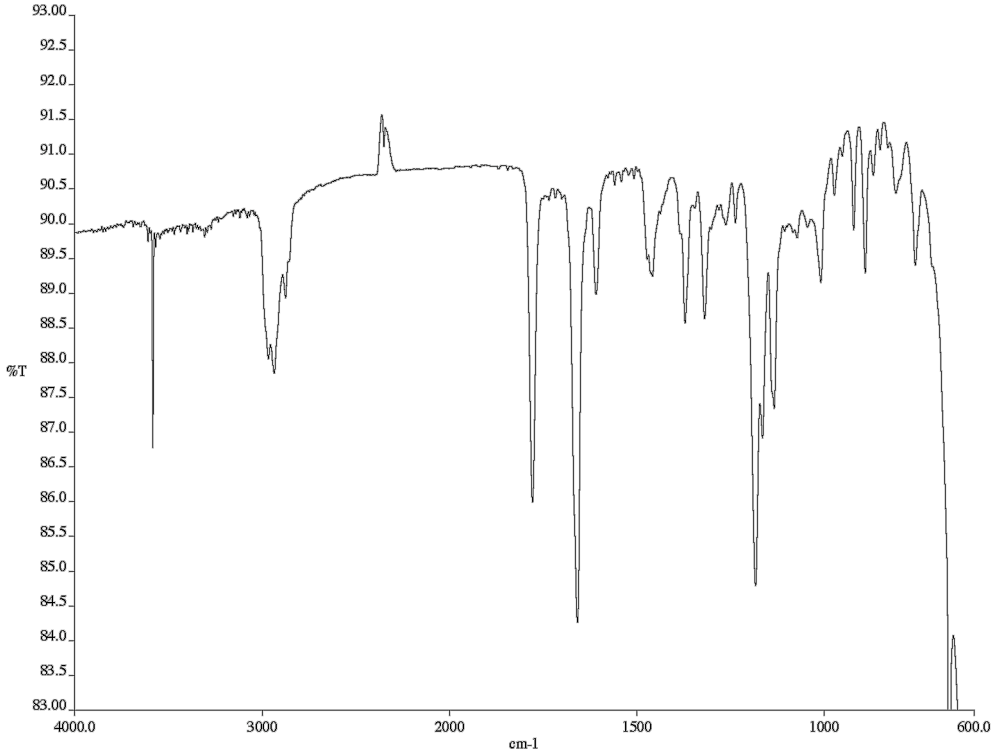


Figure A4.97 Infrared spectrum (NaCl/$CHCl_3$) of compound **269**.

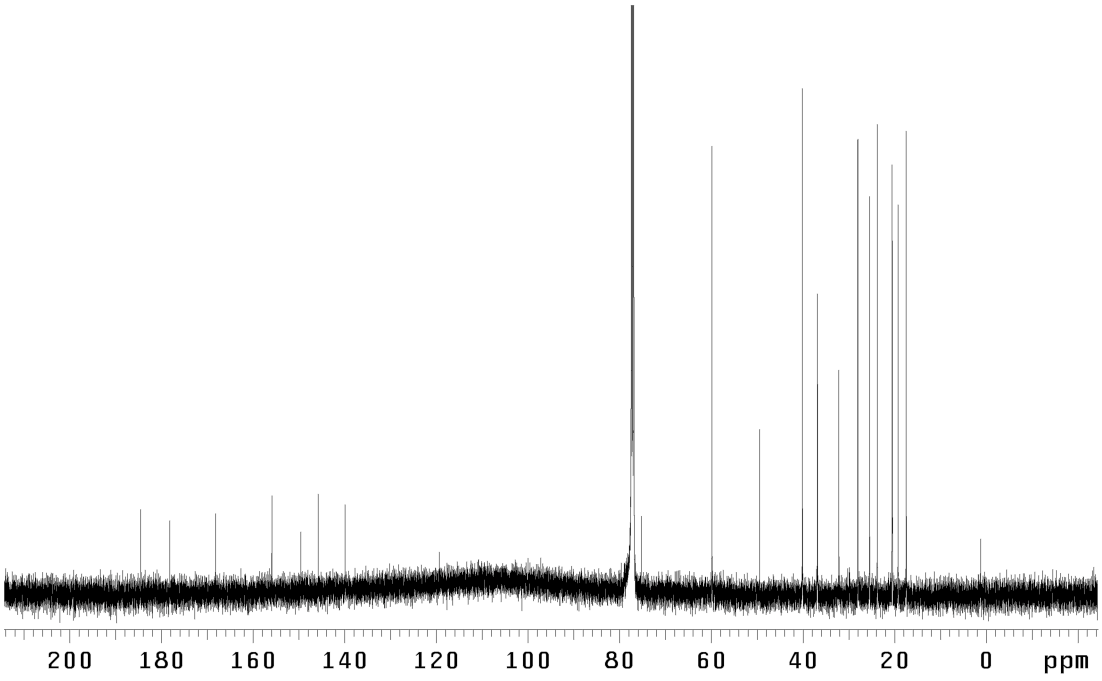


Figure A4.98 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **269**.

Appendix FIVE

X-Ray Crystallographic Data Relevant to Chapter 3

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 22 December 2005

Crystal Structure Analysis of:

233

(shown below)

For Investigator: Ryan McFadden ext. 6131

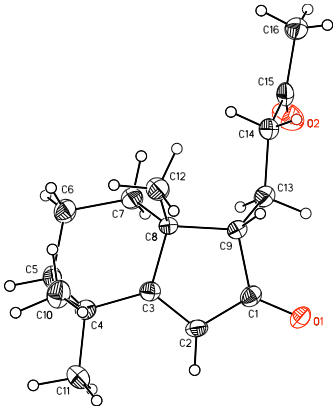
Advisor: B. M. Stoltz ext. 6064

Account Number: BMS1.SQUIBB-2.22-GRANT.SQUIBB1

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents



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Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and have been placed on hold pending further instructions from me. The deposition number is 293604. Ideally, the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 293604."

Table 1. Crystal data and structure refinement for 233 (CCDC 293604).

Empirical formula	$C_{16}H_{24}O_2$
Formula weight	248.35
Crystallization Solvent	From melt
Crystal Habit	Plate
Crystal size	0.36 x 0.27 x 0.03 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 3103 reflections used in lattice determination	2.82 to 27.84°
Unit cell dimensions	a = 7.2276(13) Å b = 9.3724(17) Å β= 92.231(3)° c = 10.3744(18) Å
Volume	702.2(2) $Å^3$
Z	2
Crystal system	Monoclinic
Space group	$P2_1$
Density (calculated)	1.175 Mg/m^3
F(000)	272
Data collection program	Bruker SMART v5.630
θ range for data collection	1.96 to 27.87°
Completeness to θ = 27.87°	93.6 %
Index ranges	$-9 \le h \le 9, -11 \le k \le 12, -13 \le l \le 13$
Data collection scan type	ω scans at 3 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	6194
Independent reflections	2968 [R_{int}= 0.0422]
Absorption coefficient	0.075 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9977 and 0.9734

Table 1 (cont.)

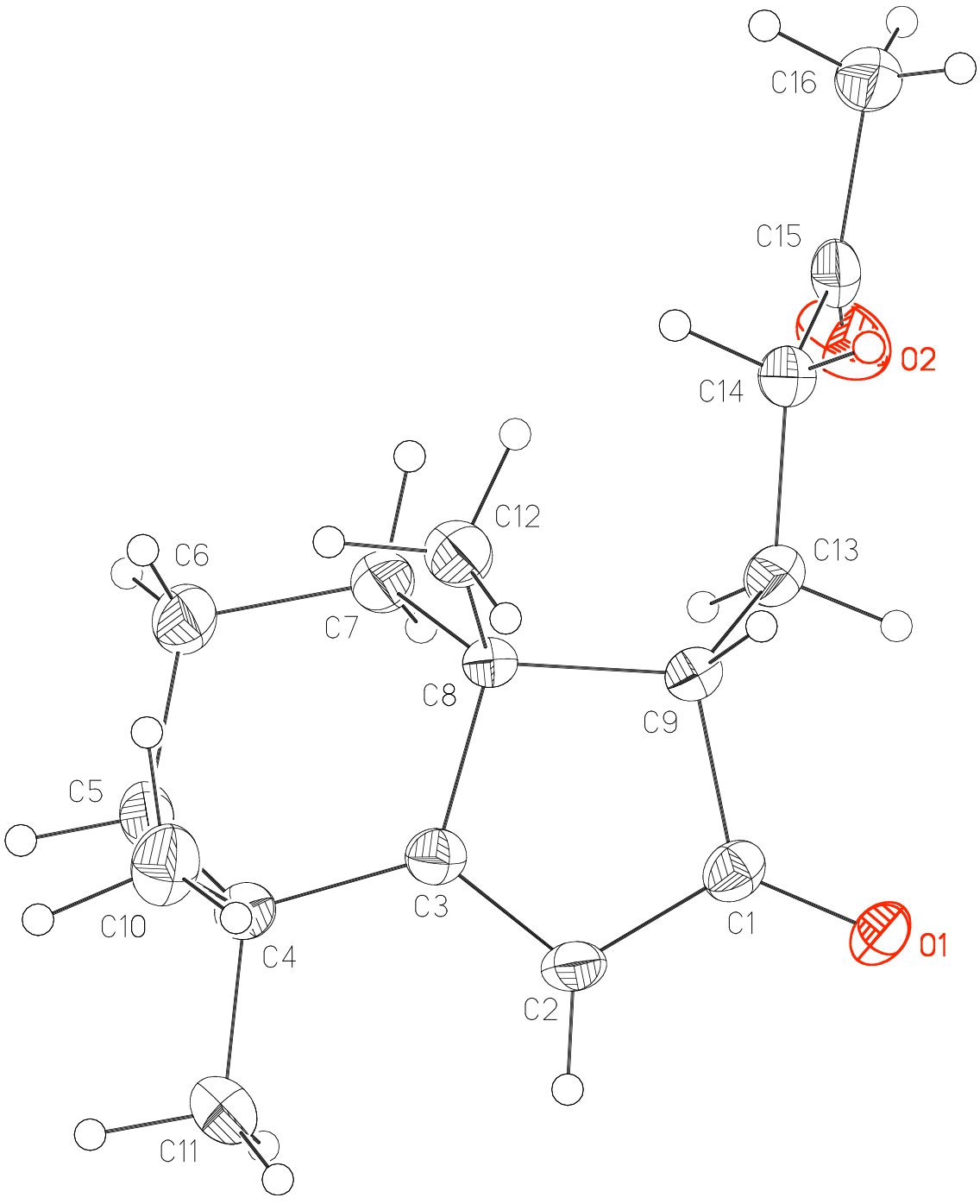
Structure solution and Refinement

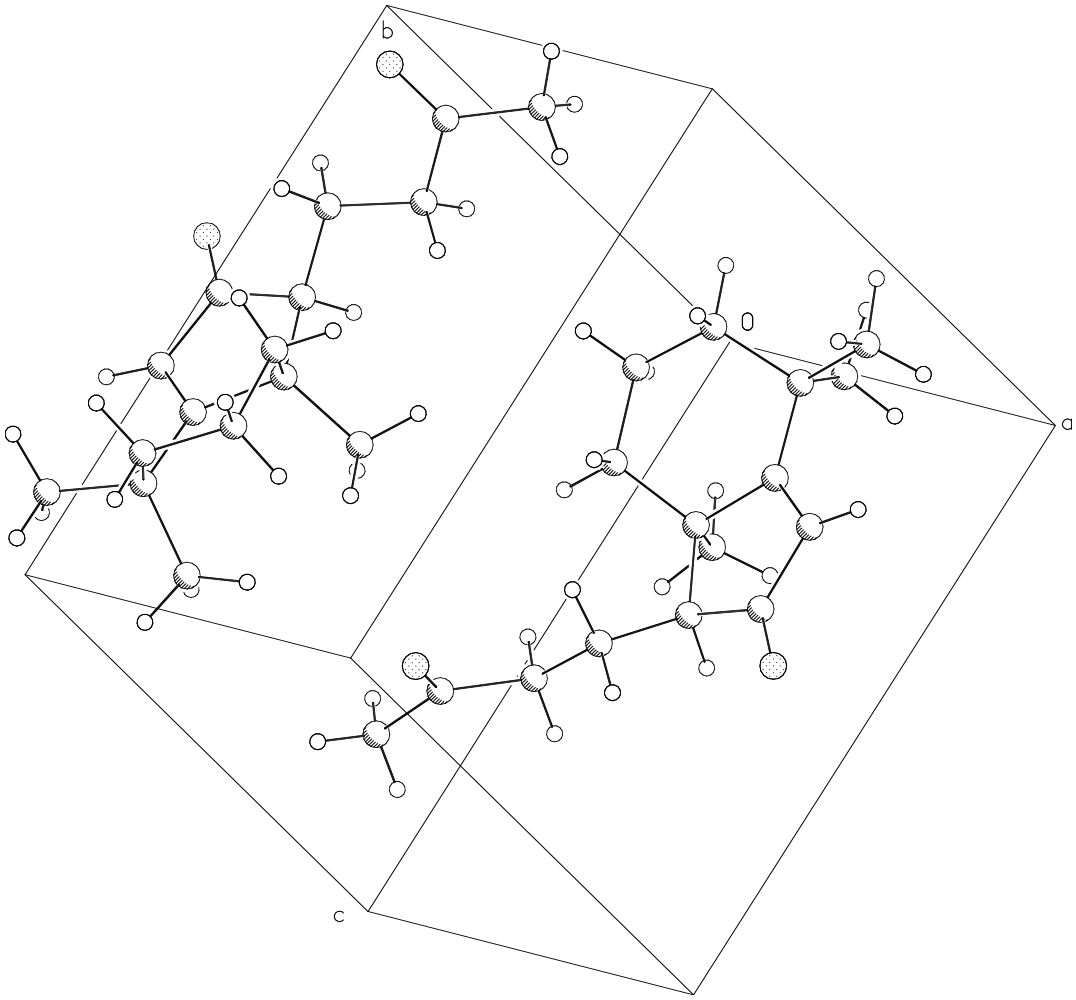
Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	2968 / 1 / 259
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.379
Final R indices [I>2σ(I), 2464 reflections]	R1 = 0.0417, *w*R2 = 0.0708
R indices (all data)	R1 = 0.0528, *w*R2 = 0.0729
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.000
Average shift/error	0.000
Absolute structure determination	Not able to determine
Absolute structure parameter	-0.5(12)
Largest diff. peak and hole	0.279 and -0.197 e.Å^{-3}

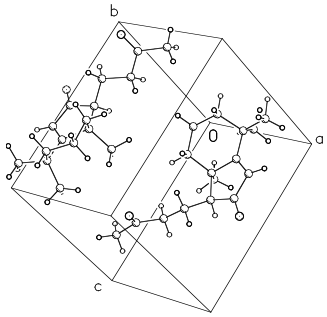
Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2. Conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt), etc., and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C16
C15
O2
C14
C12
C6
C13
C7
C8
C9
C5
C10
C3
C1
O1
C4
C2
C11


b
a
c


b
a
c

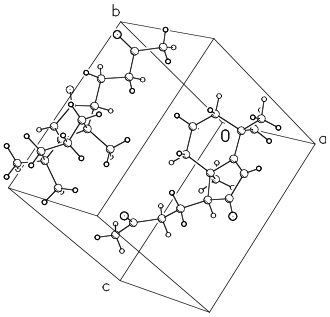

b
a
c

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 233 (CCDC 293604). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	-2410(2)	8958(1)	3790(1)	26(1)
O(2)	3287(2)	11505(2)	1446(1)	43(1)
C(1)	-1126(2)	8961(2)	4599(2)	22(1)
C(2)	-1246(2)	9098(2)	5978(2)	24(1)
C(3)	438(2)	9136(2)	6569(2)	21(1)
C(4)	845(2)	9489(2)	7970(2)	24(1)
C(5)	2195(3)	10768(2)	7999(2)	25(1)
C(6)	3847(3)	10570(2)	7160(2)	30(1)
C(7)	3246(3)	10291(2)	5743(2)	25(1)
C(8)	1987(2)	8962(2)	5616(2)	19(1)
C(9)	904(2)	8804(2)	4288(2)	22(1)
C(10)	1666(3)	8214(2)	8718(2)	33(1)
C(11)	-912(3)	9929(3)	8641(2)	37(1)
C(12)	3162(3)	7620(2)	5848(2)	28(1)
C(13)	1425(3)	9737(2)	3163(2)	25(1)
C(14)	3226(3)	9280(2)	2556(2)	26(1)
C(15)	3946(3)	10329(2)	1605(2)	27(1)
C(16)	5601(3)	9861(3)	880(2)	32(1)

Table 3. Bond lengths [Å] and angles [°] for 233 (CCDC 293604).

O(1)-C(1)	1.2264(18)	C(2)-C(3)-C(8)	112.01(14)
O(2)-C(15)	1.209(2)	C(4)-C(3)-C(8)	121.71(14)
C(1)-C(2)	1.442(2)	C(3)-C(4)-C(11)	111.34(16)
C(1)-C(9)	1.522(2)	C(3)-C(4)-C(10)	111.95(16)
C(2)-C(3)	1.342(2)	C(11)-C(4)-C(10)	106.99(18)
C(2)-H(2)	0.934(16)	C(3)-C(4)-C(5)	106.74(15)
C(3)-C(4)	1.508(2)	C(11)-C(4)-C(5)	108.48(17)
C(3)-C(8)	1.531(2)	C(10)-C(4)-C(5)	111.33(16)
C(4)-C(11)	1.528(3)	C(6)-C(5)-C(4)	113.88(17)
C(4)-C(10)	1.532(3)	C(6)-C(5)-H(5B)	111.9(11)
C(4)-C(5)	1.546(3)	C(4)-C(5)-H(5B)	108.7(11)
C(5)-C(6)	1.516(3)	C(6)-C(5)-H(5A)	112.0(10)
C(5)-H(5B)	1.02(2)	C(4)-C(5)-H(5A)	109.7(10)
C(5)-H(5A)	0.975(18)	H(5B)-C(5)-H(5A)	99.7(14)
C(6)-C(7)	1.539(3)	C(5)-C(6)-C(7)	111.68(17)
C(6)-H(6B)	1.01(2)	C(5)-C(6)-H(6B)	114.1(11)
C(6)-H(6A)	0.98(2)	C(7)-C(6)-H(6B)	107.2(11)
C(7)-C(8)	1.545(3)	C(5)-C(6)-H(6A)	107.9(11)
C(7)-H(7A)	0.974(19)	C(7)-C(6)-H(6A)	106.5(12)
C(7)-H(7B)	0.939(19)	H(6B)-C(6)-H(6A)	109.3(16)
C(8)-C(12)	1.532(3)	C(6)-C(7)-C(8)	111.21(16)
C(8)-C(9)	1.565(2)	C(6)-C(7)-H(7A)	113.1(11)
C(9)-C(13)	1.518(3)	C(8)-C(7)-H(7A)	108.5(11)
C(9)-H(9)	1.02(2)	C(6)-C(7)-H(7B)	109.4(11)
C(10)-H(10A)	1.03(2)	C(8)-C(7)-H(7B)	110.4(11)
C(10)-H(10B)	0.96(2)	H(7A)-C(7)-H(7B)	104.0(15)
C(10)-H(10C)	1.05(2)	C(3)-C(8)-C(12)	113.62(16)
C(11)-H(11A)	0.96(2)	C(3)-C(8)-C(7)	107.62(16)
C(11)-H(11C)	1.03(2)	C(12)-C(8)-C(7)	109.11(14)
C(11)-H(11B)	1.02(2)	C(3)-C(8)-C(9)	103.04(12)
C(12)-H(12C)	1.00(2)	C(12)-C(8)-C(9)	108.39(16)
C(12)-H(12B)	0.97(2)	C(7)-C(8)-C(9)	115.09(15)
C(12)-H(12A)	1.009(19)	C(13)-C(9)-C(1)	112.16(15)
C(13)-C(14)	1.529(3)	C(13)-C(9)-C(8)	119.48(16)
C(13)-H(13A)	1.04(2)	C(1)-C(9)-C(8)	104.92(14)
C(13)-H(13B)	1.006(19)	C(13)-C(9)-H(9)	103.6(11)
C(14)-C(15)	1.500(3)	C(1)-C(9)-H(9)	105.4(10)
C(14)-H(14B)	0.975(18)	C(8)-C(9)-H(9)	110.6(11)
C(14)-H(14A)	0.967(17)	C(4)-C(10)-H(10A)	114.3(12)
C(15)-C(16)	1.503(3)	C(4)-C(10)-H(10B)	108.7(14)
C(16)-H(16B)	0.90(3)	H(10A)-C(10)-H(10B)	112.0(18)
C(16)-H(16C)	0.96(2)	C(4)-C(10)-H(10C)	107.4(12)
C(16)-H(16A)	0.97(2)	H(10A)-C(10)-H(10C)	104.8(18)
		H(10B)-C(10)-H(10C)	109.3(19)
O(1)-C(1)-C(2)	127.29(15)	C(4)-C(11)-H(11A)	113.8(14)
O(1)-C(1)-C(9)	124.39(15)	C(4)-C(11)-H(11C)	106.3(11)
C(2)-C(1)-C(9)	108.32(14)	H(11A)-C(11)-H(11C)	108.7(18)
C(3)-C(2)-C(1)	111.57(15)	C(4)-C(11)-H(11B)	110.4(12)
C(3)-C(2)-H(2)	124.9(10)	H(11A)-C(11)-H(11B)	112.6(19)
C(1)-C(2)-H(2)	123.5(10)	H(11C)-C(11)-H(11B)	104.5(17)
C(2)-C(3)-C(4)	125.86(16)	C(8)-C(12)-H(12C)	110.1(10)

H(12C)-C(12)-H(12B)	106.1(17)
C(8)-C(12)-H(12A)	108.9(11)
H(12C)-C(12)-H(12A)	110.9(15)
H(12B)-C(12)-H(12A)	112.3(18)
C(9)-C(13)-C(14)	113.31(16)
C(9)-C(13)-H(13A)	108.5(10)
C(14)-C(13)-H(13A)	112.1(10)
C(9)-C(13)-H(13B)	105.7(11)
C(14)-C(13)-H(13B)	109.2(11)
H(13A)-C(13)-H(13B)	107.7(14)
C(15)-C(14)-C(13)	114.19(17)
C(15)-C(14)-H(14B)	104.2(11)
C(13)-C(14)-H(14B)	112.2(10)
C(15)-C(14)-H(14A)	108.8(11)
C(13)-C(14)-H(14A)	111.8(11)
H(14B)-C(14)-H(14A)	104.9(16)
O(2)-C(15)-C(14)	122.82(18)
O(2)-C(15)-C(16)	120.97(19)
C(14)-C(15)-C(16)	116.17(19)
C(15)-C(16)-H(16B)	107.5(13)
C(15)-C(16)-H(16C)	109.2(12)
H(16B)-C(16)-H(16C)	111(2)
C(15)-C(16)-H(16A)	111.7(14)
H(16B)-C(16)-H(16A)	107.1(19)
H(16C)-C(16)-H(16A)	110.2(18)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^4$) for 233 (CCDC 293604). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}]

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)180(6)	311(7)	286(7)	-27(7)	-40(5)	-6(6)
O(2)528(10)	395(9)	366(9)	77(7)	117(7)	126(8)
C(1)197(9)	186(9)	286(10)	-22(10)	-10(7)	-15(9)
C(2)158(9)	286(11)	280(10)	-46(9)	48(8)	-18(9)
C(3)198(8)	187(10)	235(9)	-13(8)	25(7)	-10(8)
C(4)194(9)	276(11)	245(11)	-31(8)	19(8)	-18(8)
C(5)275(11)	285(12)	188(11)	-24(9)	-14(9)	-29(9)
C(6)274(12)	334(13)	283(12)	-24(10)	12(9)	-113(10)
C(7)229(11)	262(11)	253(11)	-14(9)	23(10)	-34(9)
C(8)155(8)	232(9)	182(9)	-7(9)	19(6)	-2(9)
C(9)165(9)	281(11)	216(10)	-13(9)	3(7)	10(9)
C(10)356(14)	334(13)	304(13)	45(10)	-32(11)	-83(11)
C(11)333(13)	531(16)	245(12)	-85(11)	59(10)	-24(12)
C(12)284(13)	285(12)	257(12)	15(10)	6(11)	65(10)
C(13)204(10)	305(12)	242(11)	9(9)	-16(8)	13(9)
C(14)220(10)	350(13)	197(10)	-4(9)	-5(8)	19(9)
C(15)263(11)	354(13)	181(10)	-50(9)	-51(8)	21(9)
C(16)247(12)	456(14)	253(12)	20(12)	25(10)	-38(11)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 233 (CCDC 293604).

	x	y	z	U_{iso}
H(12C)	3900(30)	7703(19)	6684(19)	18(5)
H(14B)	4240(20)	9170(20)	3197(17)	24(5)
H(2)	-2360(20)	9190(20)	6393(15)	17(4)
H(16B)	5270(30)	9080(30)	420(20)	55(7)
H(5B)	1470(30)	11670(20)	7763(19)	31(6)
H(14A)	3110(20)	8356(19)	2145(16)	11(4)
H(5A)	2570(20)	10993(18)	8889(18)	17(5)
H(6B)	4700(30)	9760(20)	7443(19)	31(5)
H(9)	1030(20)	7790(20)	3938(18)	26(5)
H(13A)	1470(20)	10800(20)	3472(16)	20(5)
H(7A)	4290(30)	10165(18)	5186(17)	21(5)
H(16C)	6600(30)	9650(20)	1480(20)	35(6)
H(6A)	4550(30)	11460(20)	7172(18)	25(5)
H(7B)	2630(20)	11100(20)	5405(17)	20(5)
H(10A)	2990(30)	7960(20)	8490(20)	44(6)
H(11A)	-1810(30)	9180(30)	8690(20)	55(7)
H(12B)	2340(30)	6820(30)	5940(20)	45(7)
H(12A)	4000(30)	7490(20)	5104(19)	28(6)
H(11C)	-500(30)	10220(20)	9560(20)	33(5)
H(11B)	-1450(30)	10830(30)	8240(20)	44(6)
H(16A)	5970(30)	10580(20)	270(20)	42(6)
H(10B)	840(30)	7420(30)	8610(20)	46(7)
H(13B)	370(30)	9650(20)	2503(19)	26(5)
H(10C)	1770(30)	8500(20)	9690(20)	54(7)