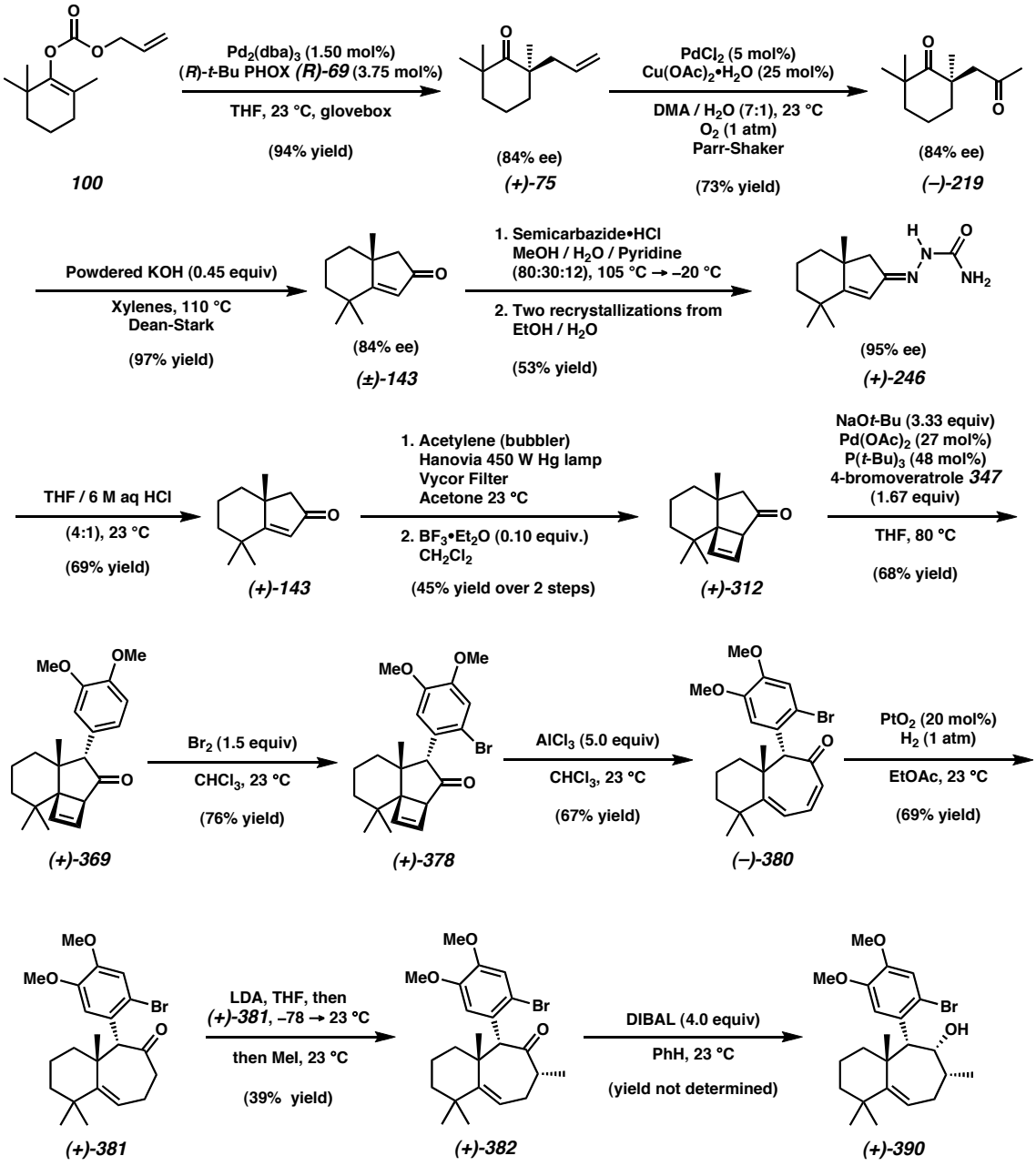
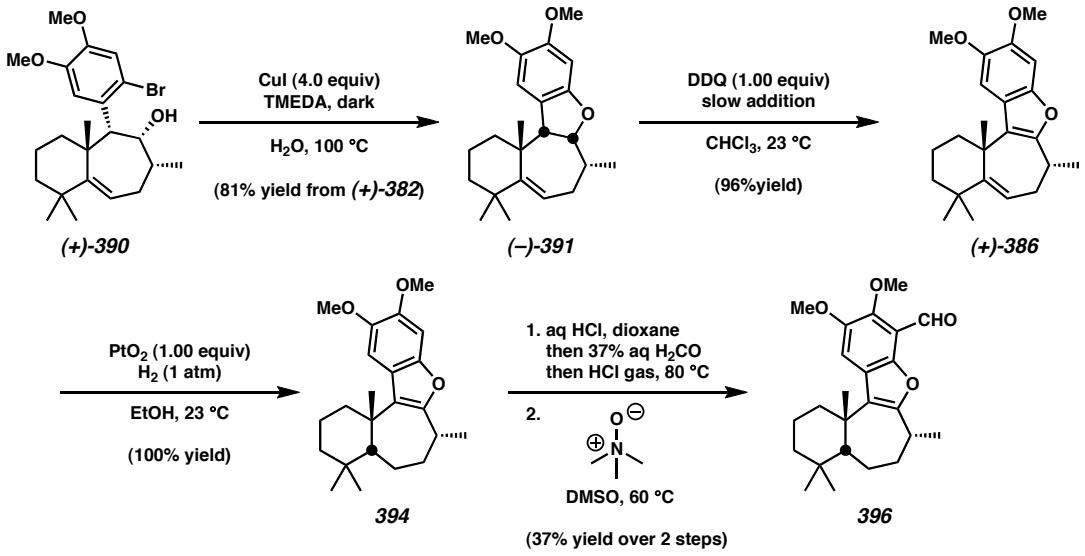
Appendix SIX

Synthetic Summary of Progress Toward the Enantioselective Total Syntheses of Liphagal

Scheme A6.1 Toward the Enantioselective Total Synthesis of Liphagal: Part 1



Scheme A6.2 Toward the Enantioselective Total Synthesis of Liphagal: Part 2



Appendix SEVEN

Spectra of Compounds Relevant to Chapter 4

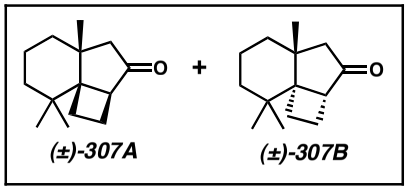


Figure A7.1 ^{1}H NMR (300 MHz, $CDCl_3$) of compounds **307A** and **307B**.

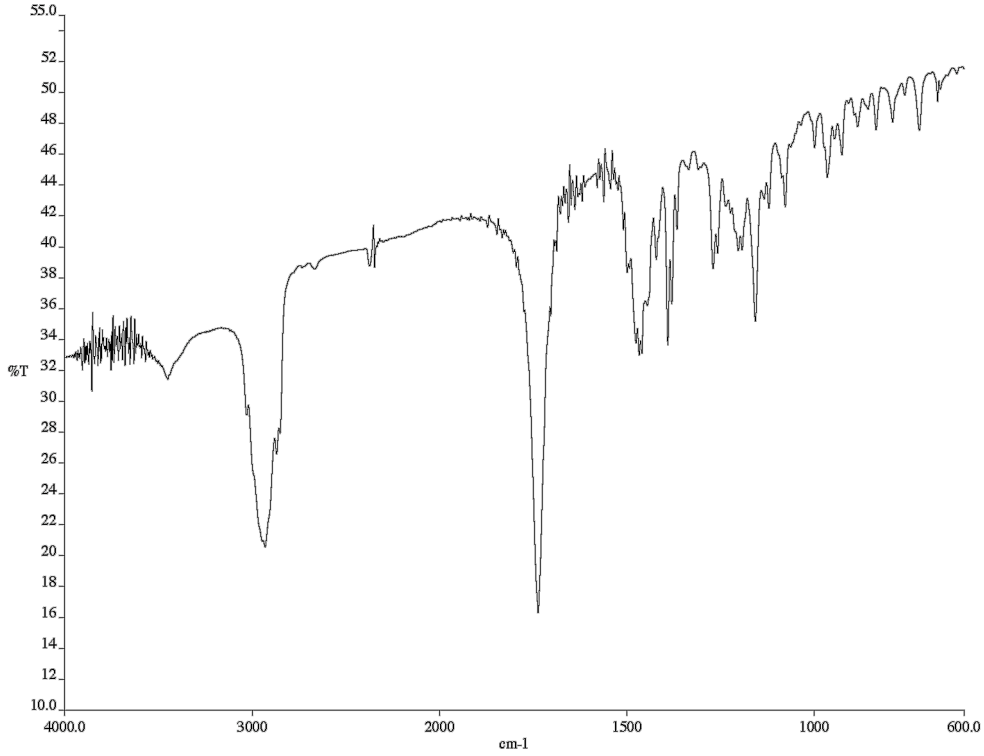


Figure A7.2 Infrared spectrum (KBr) of compounds **307A** and **307B**.

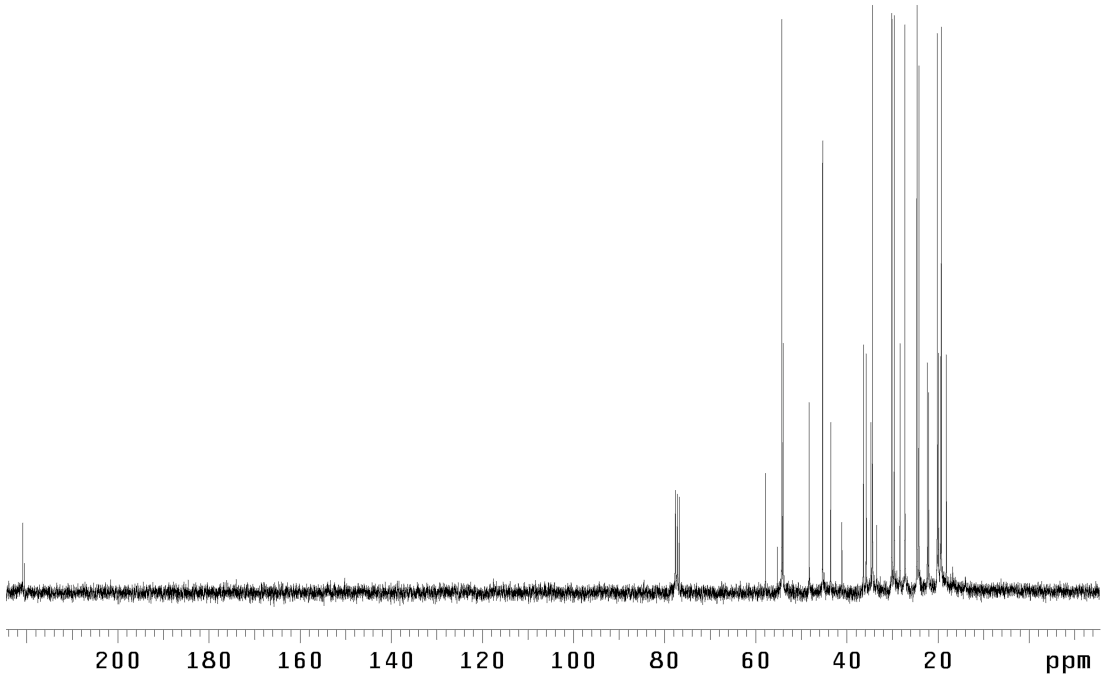


Figure A7.3 ^{13}C NMR (75 MHz, $CDCl_3$) of compounds **307A** and **307B**.

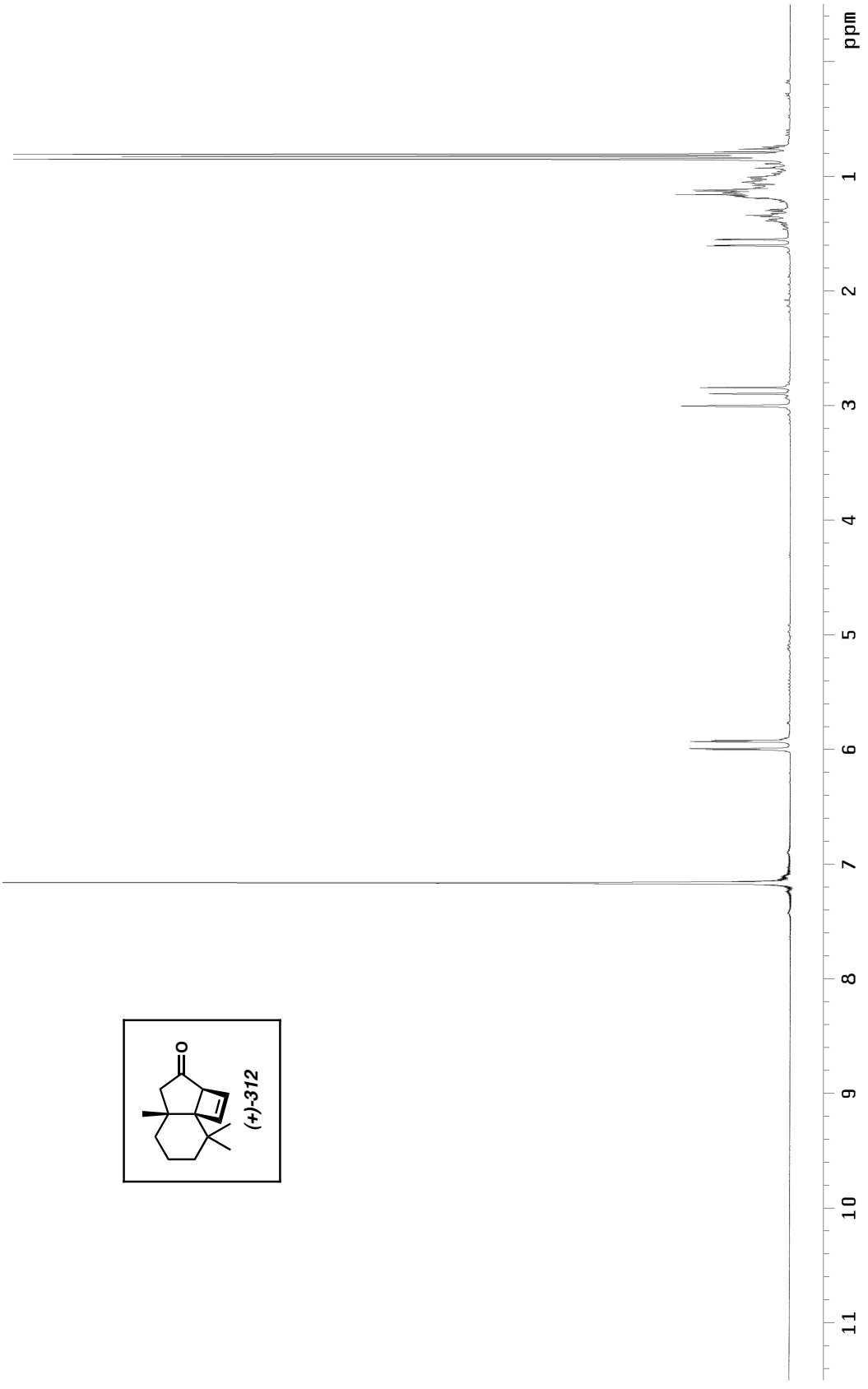


Figure A7.4 ^{1}H NMR (300 MHz, C_6D_6) of compound **312**.

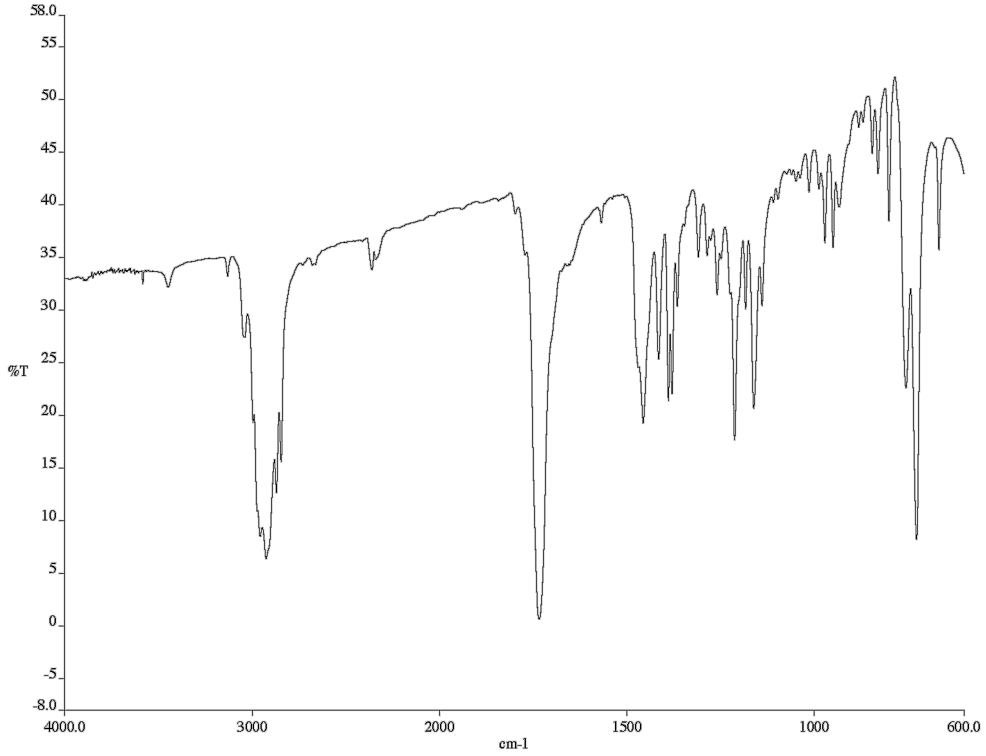


Figure A7.5 Infrared spectrum (NaCl/$CHCl_3$) of compound **312**.

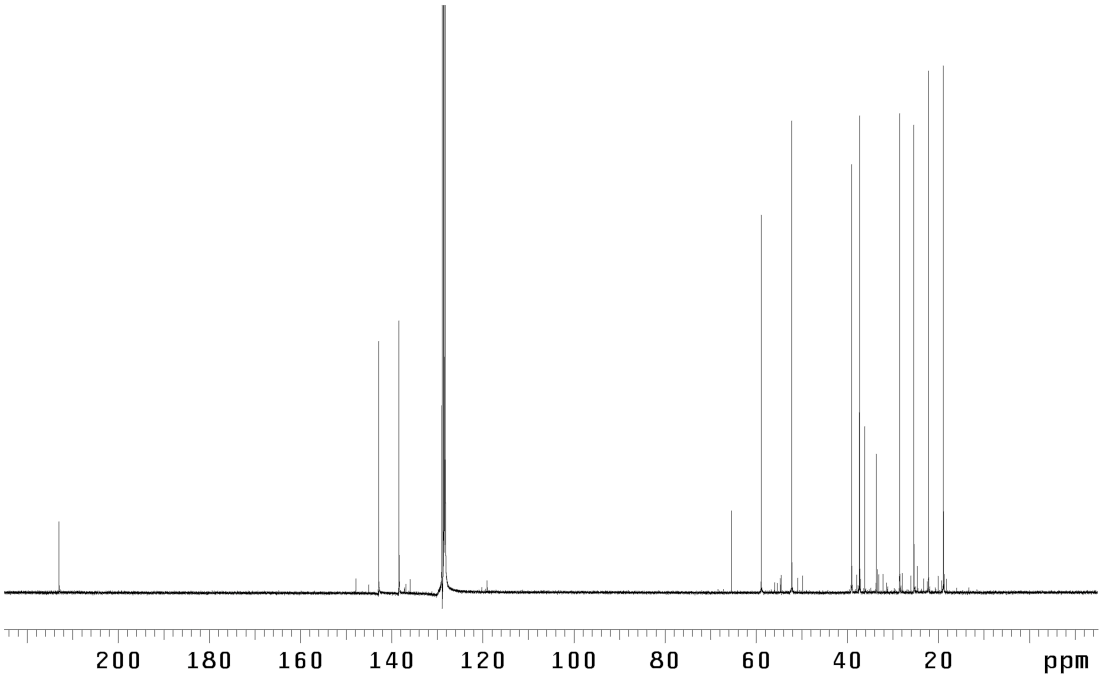


Figure A7.6 ^{13}C NMR (125 MHz, C_6D_6) of compound **312**.

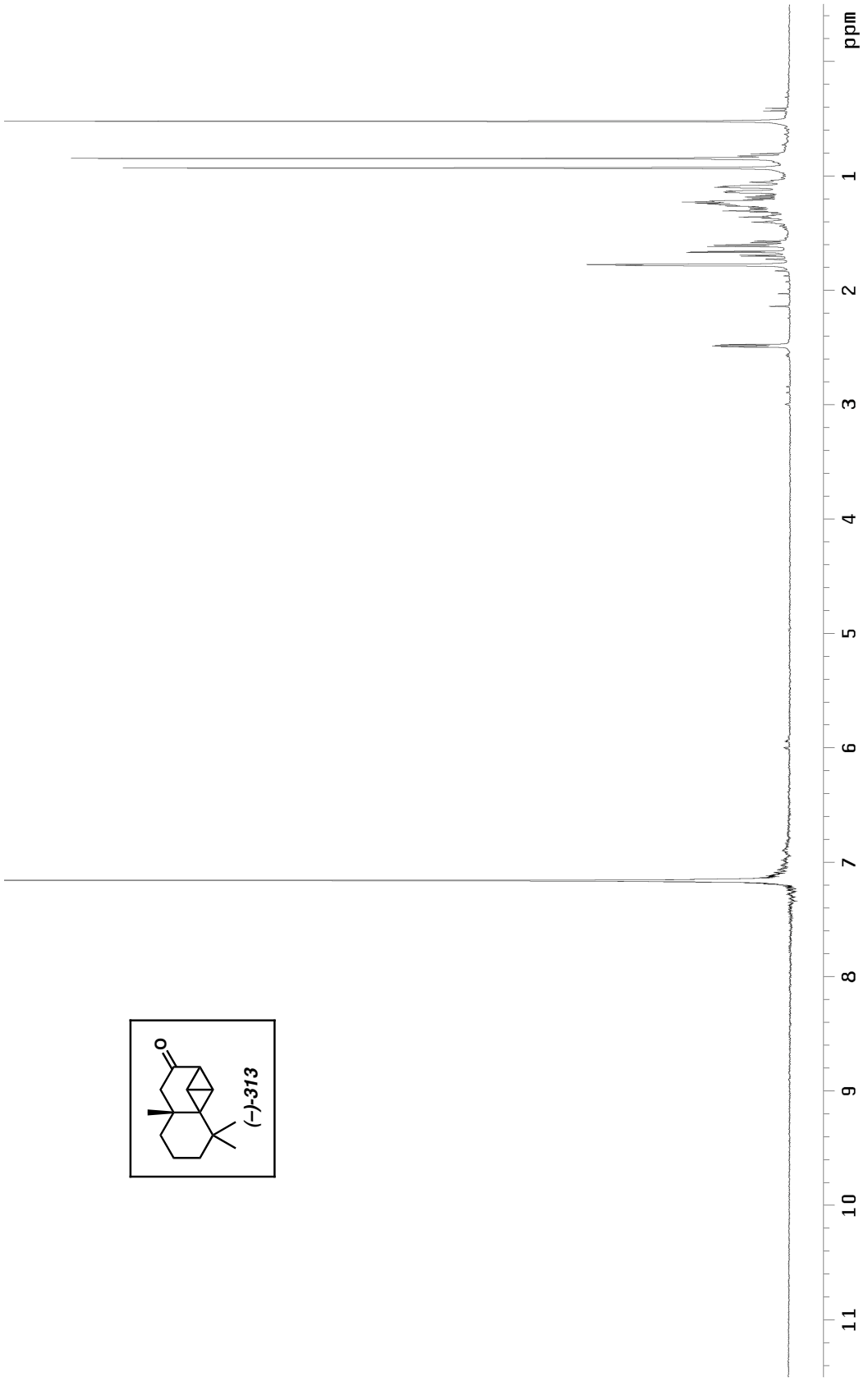


Figure A7.7 ^{1}H NMR (300 MHz, C_6D_6) of compound **313**.

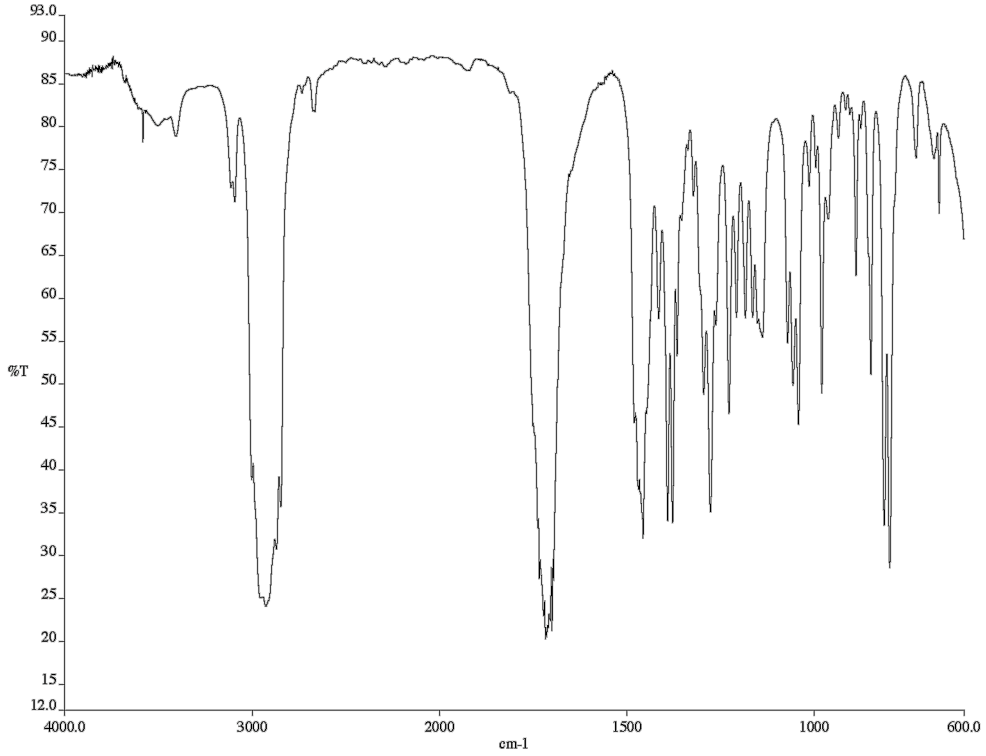


Figure A7.8 Infrared spectrum (NaCl/neat) of compound **313**.

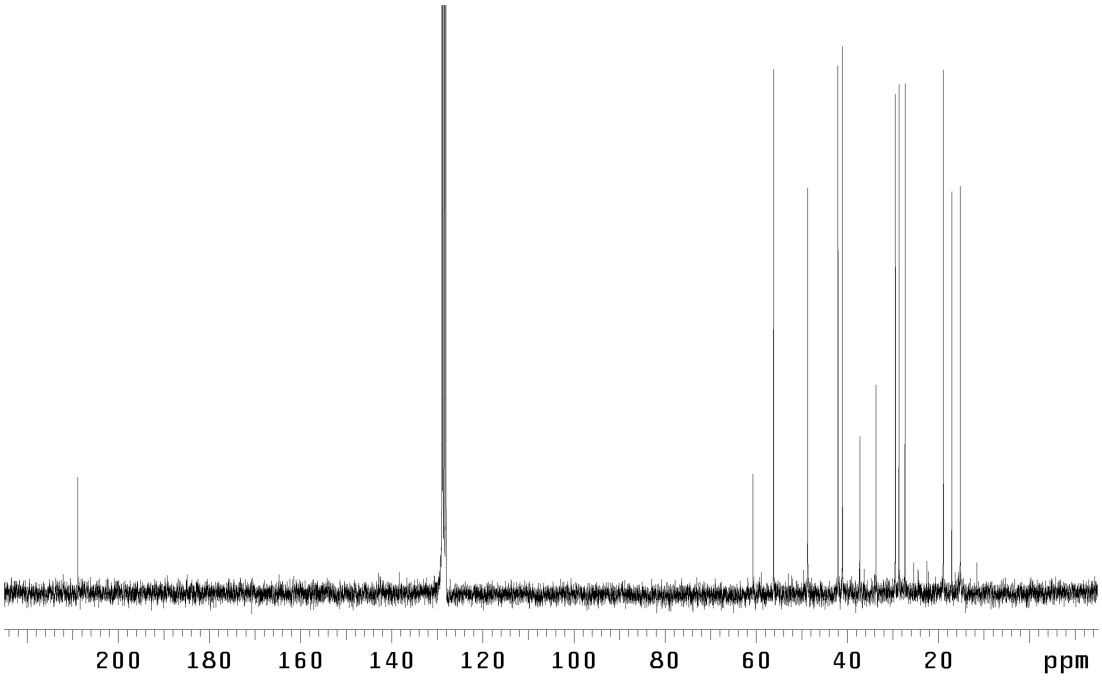


Figure A7.9 ^{13}C NMR (75 MHz, C_6D_6) of compound **313**.

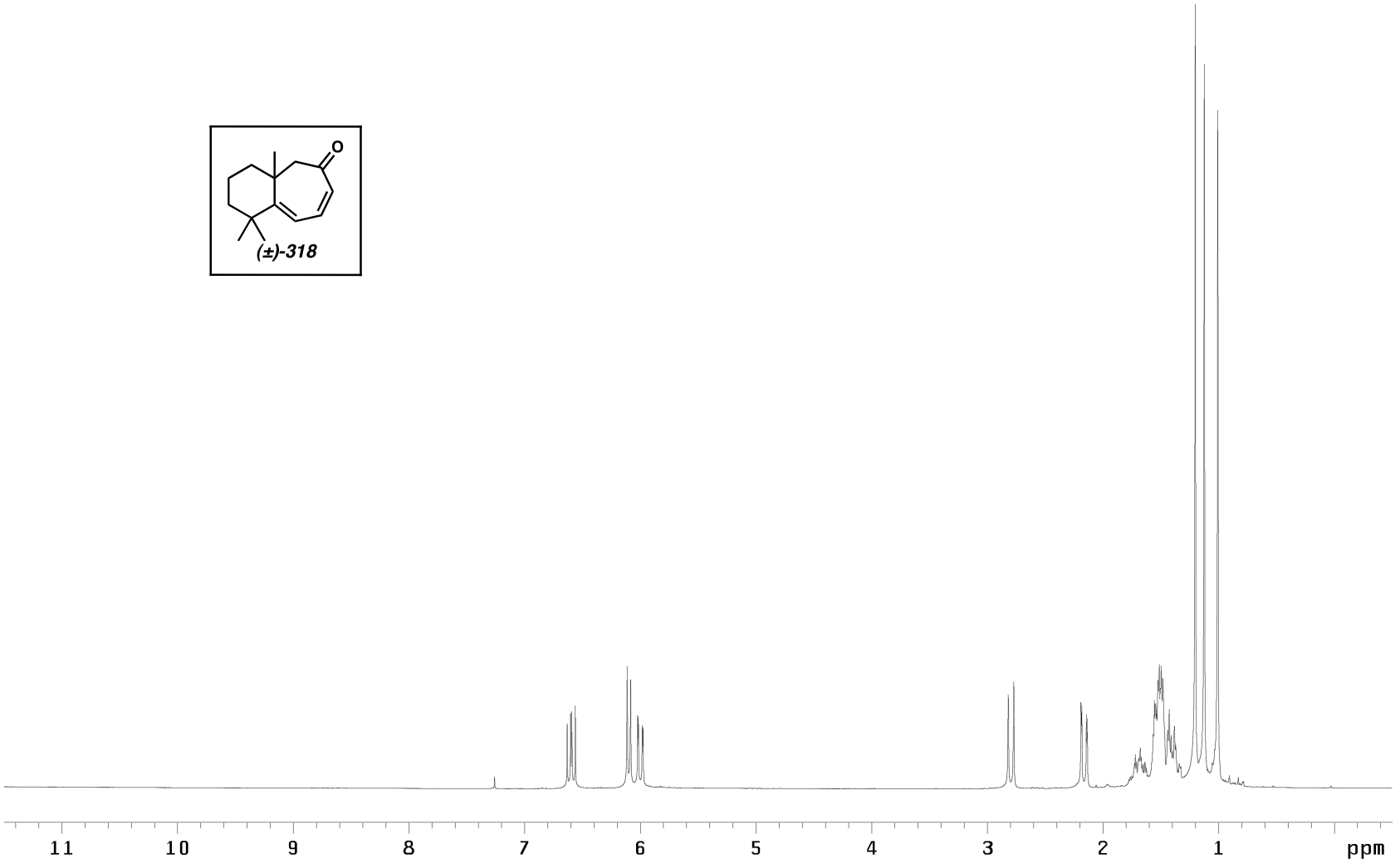


Figure A7.10 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **318**.

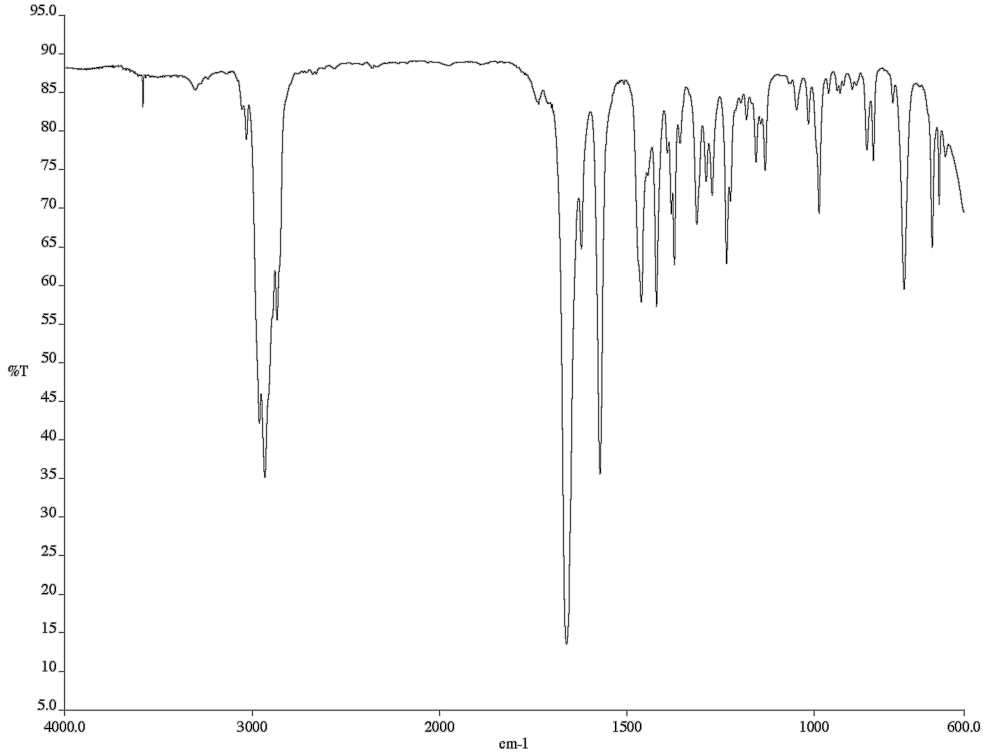


Figure A7.11 Infrared spectrum ($NaCl/CDCl_3$) of compound **318**.

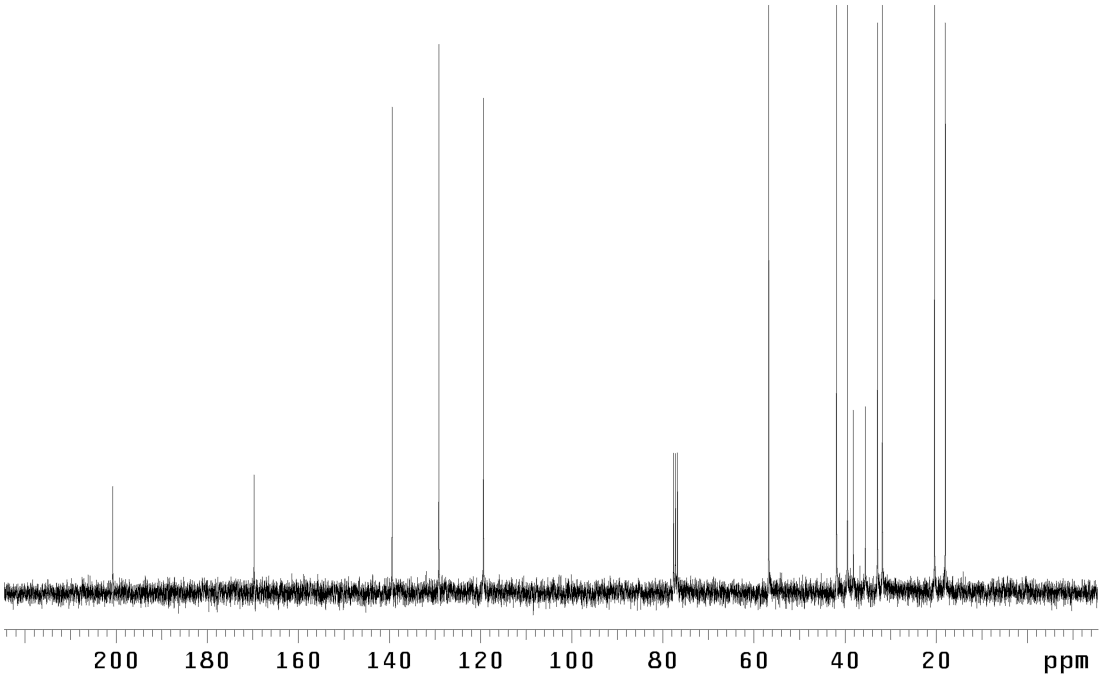


Figure A7.12 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **318**.

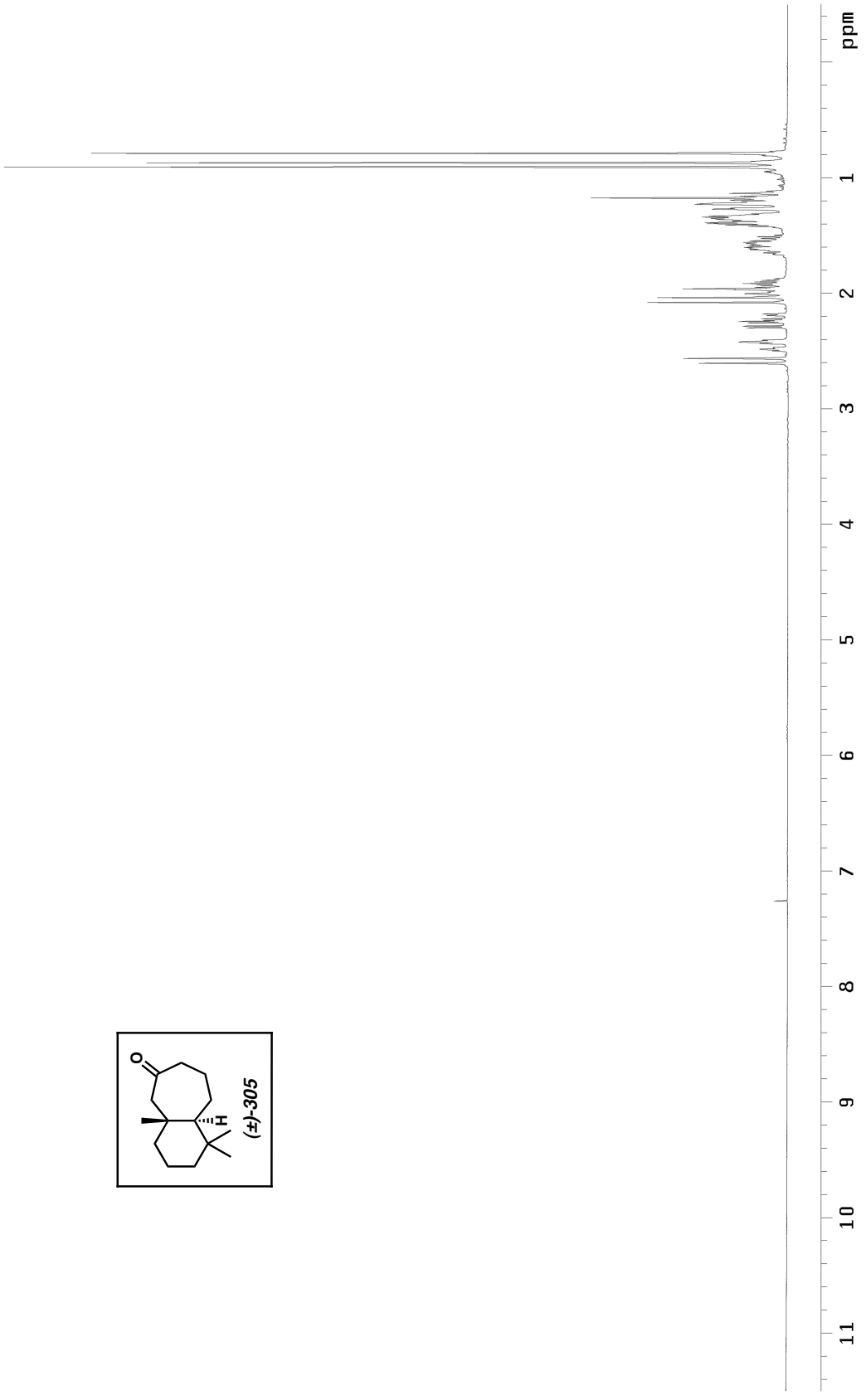


Figure A7.13 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **305**.

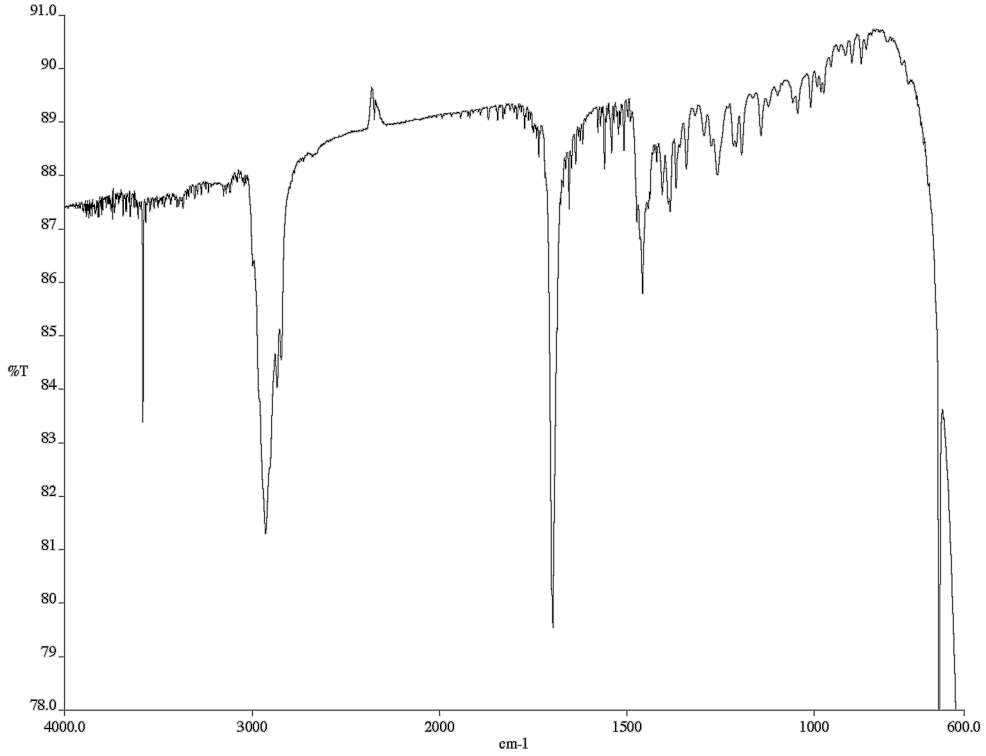


Figure A7.14 Infrared spectrum ($NaCl/CDCl_3$) of compound **305**.

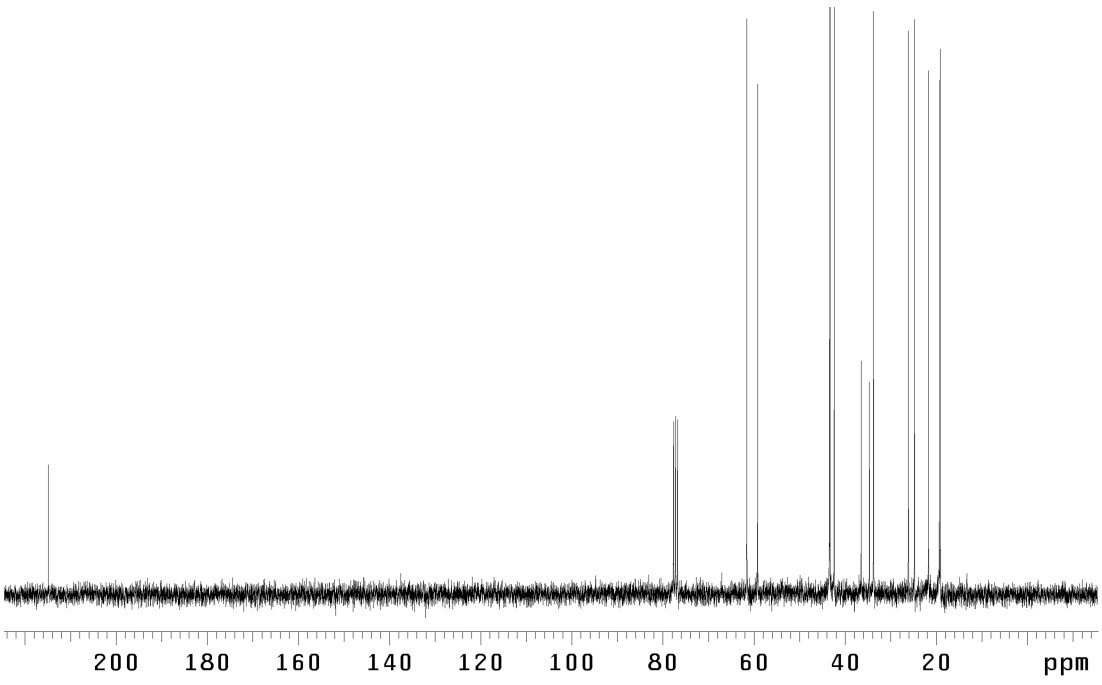


Figure A7.15 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **305**.

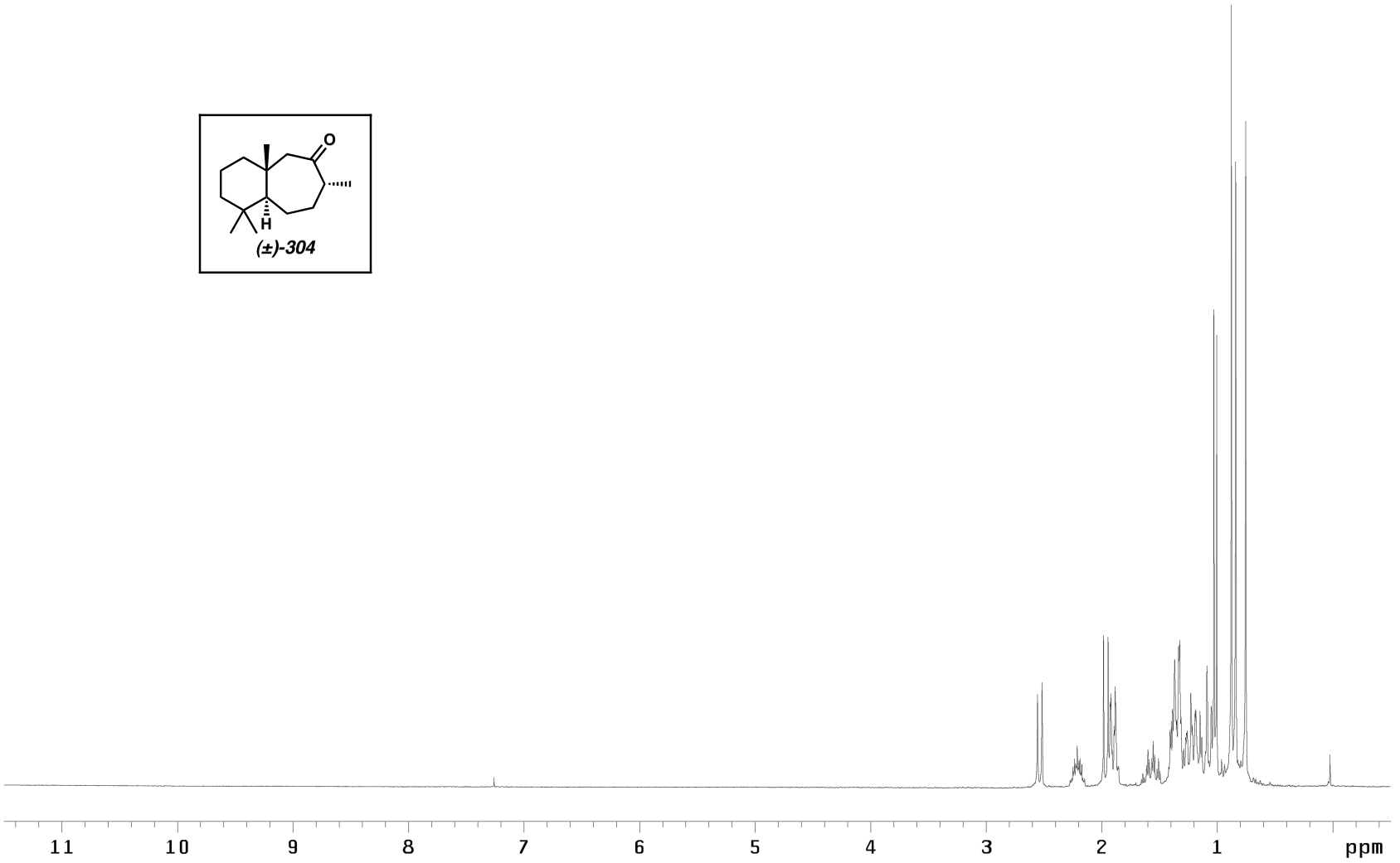


Figure A7.16 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **304**.

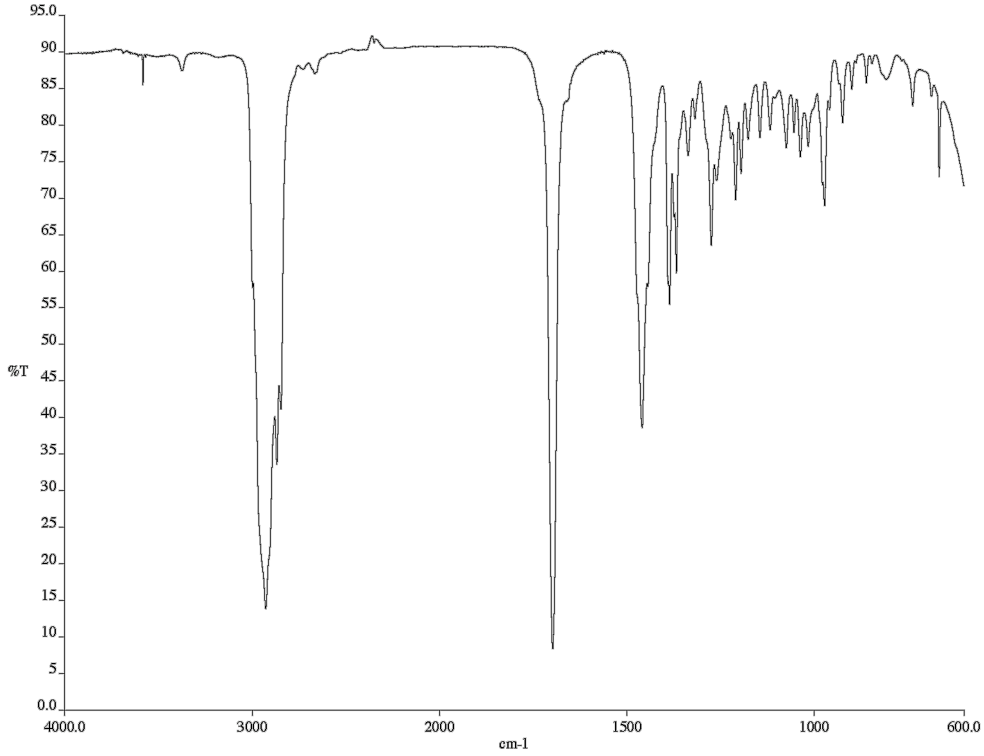


Figure A7.17 Infrared spectrum ($NaCl/CDCl_3$) of compound **304**.

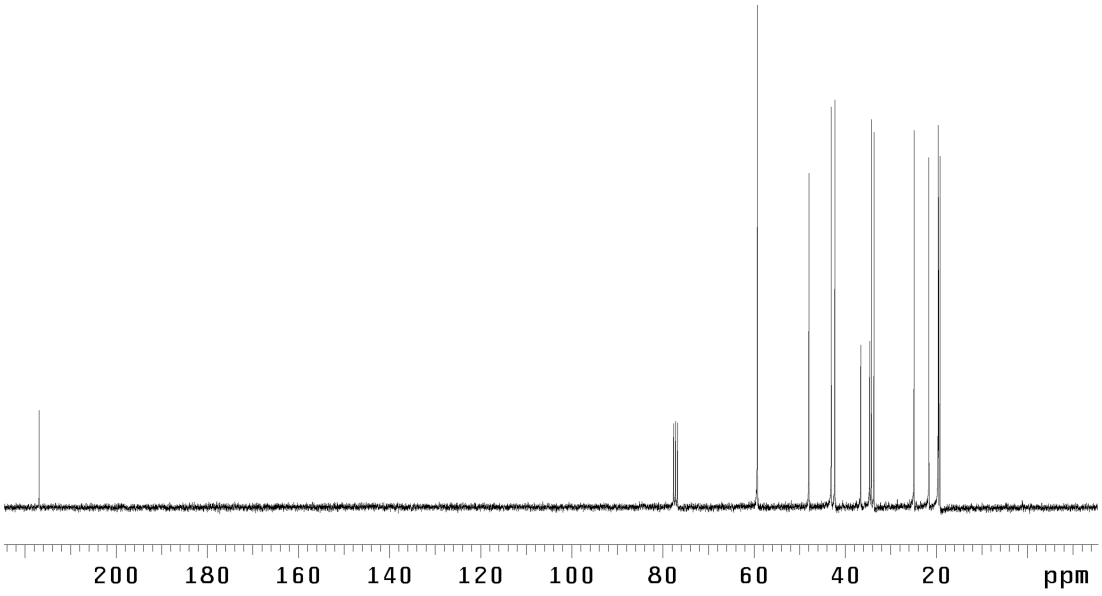


Figure A7.18 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **304**.

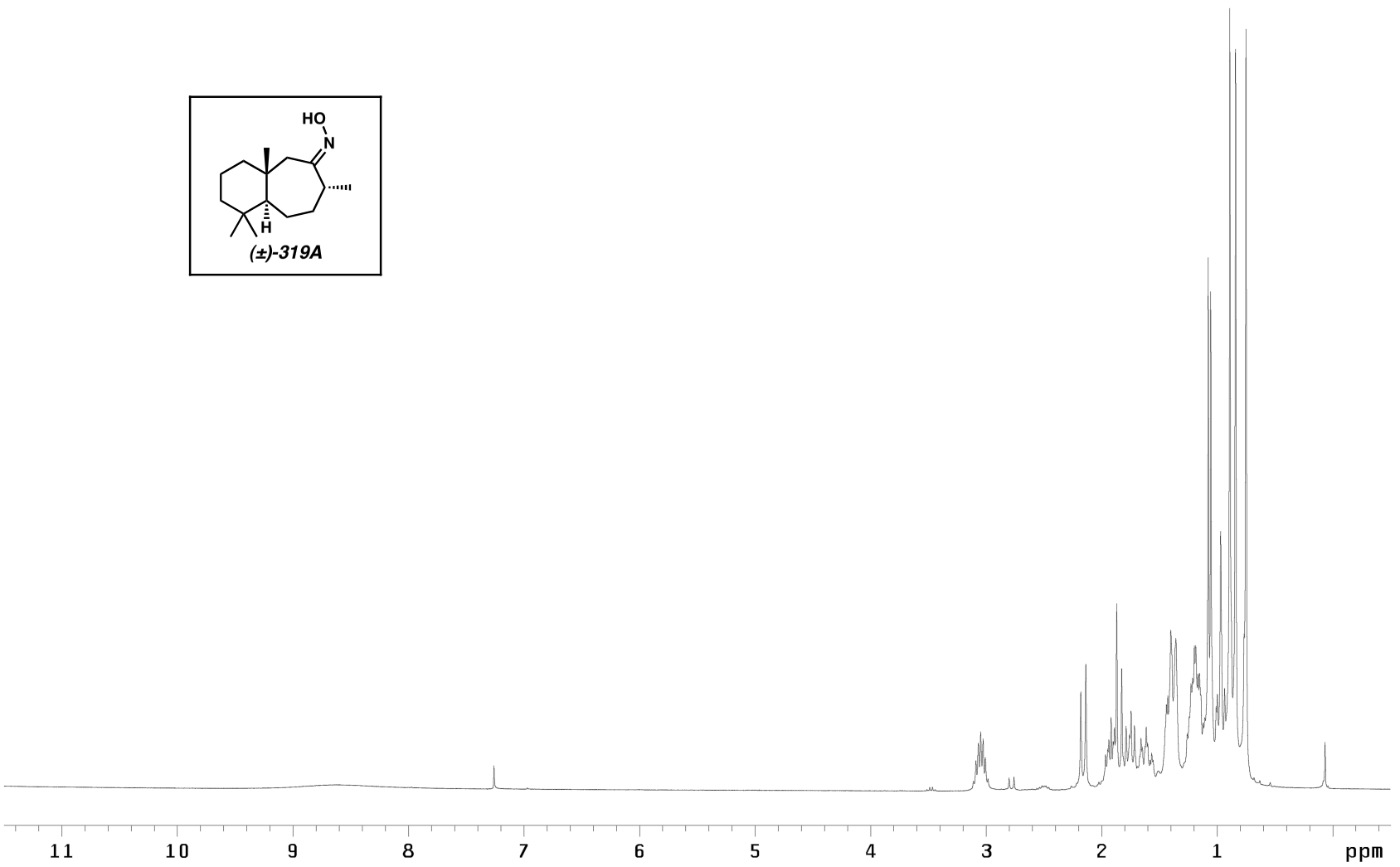


Figure A7.19 ^{1}H NMR (300 MHz, $CDCl_3$) of compounds **319A**.

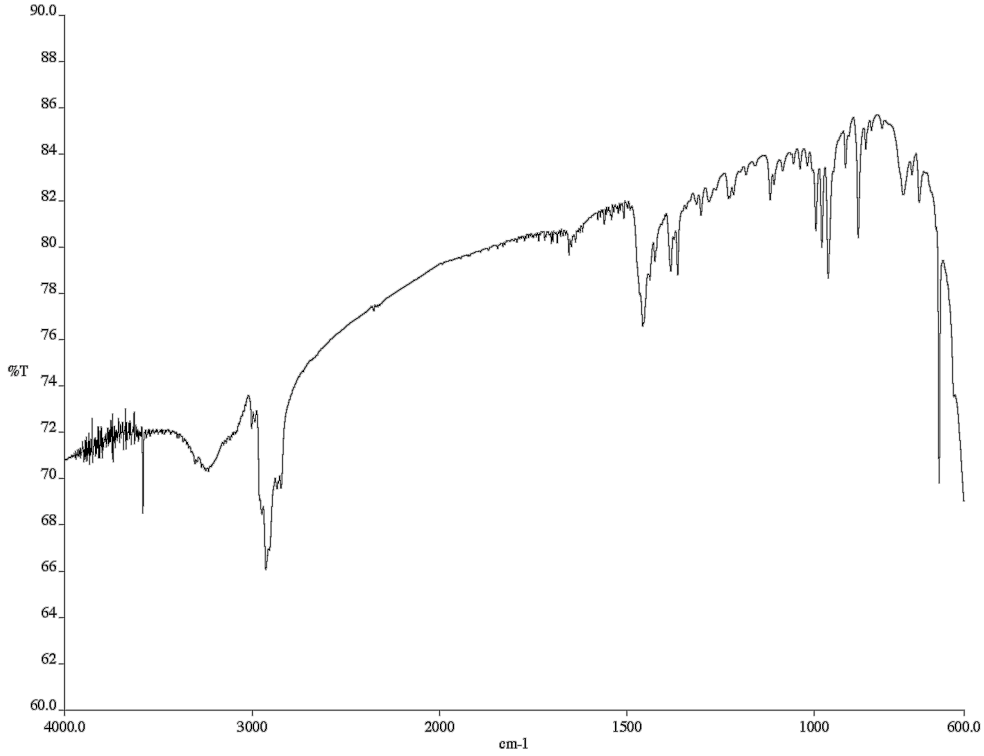


Figure A7.20 Infrared spectrum ($NaCl/CDCl_3$) of compounds **319A**.

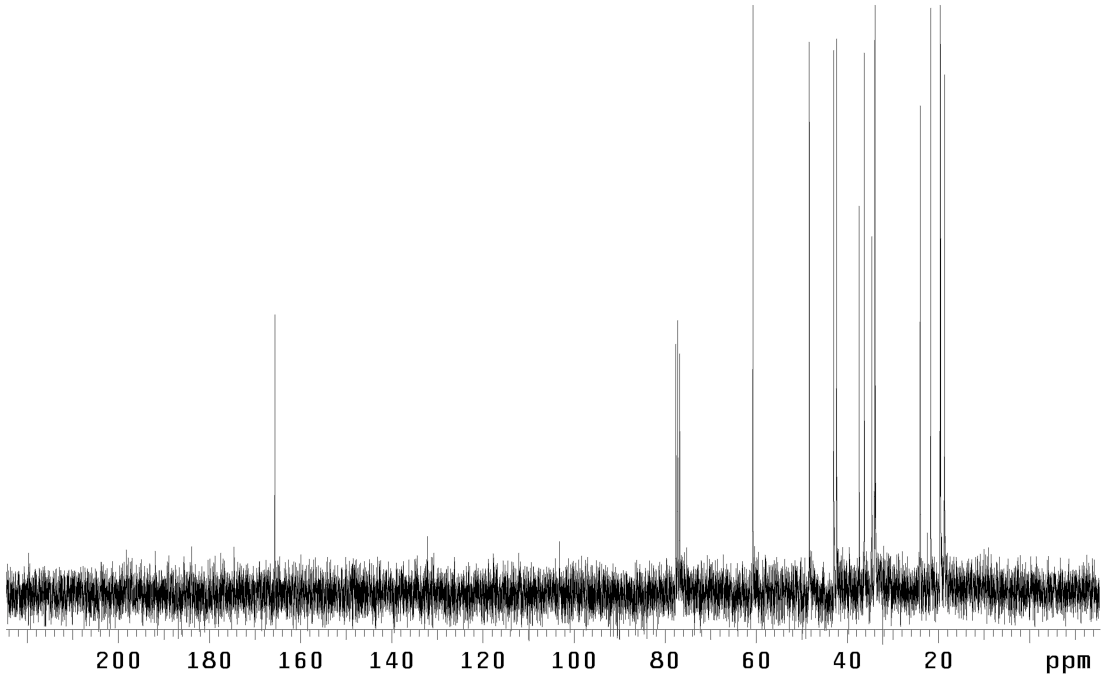


Figure A7.21 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **319A**.

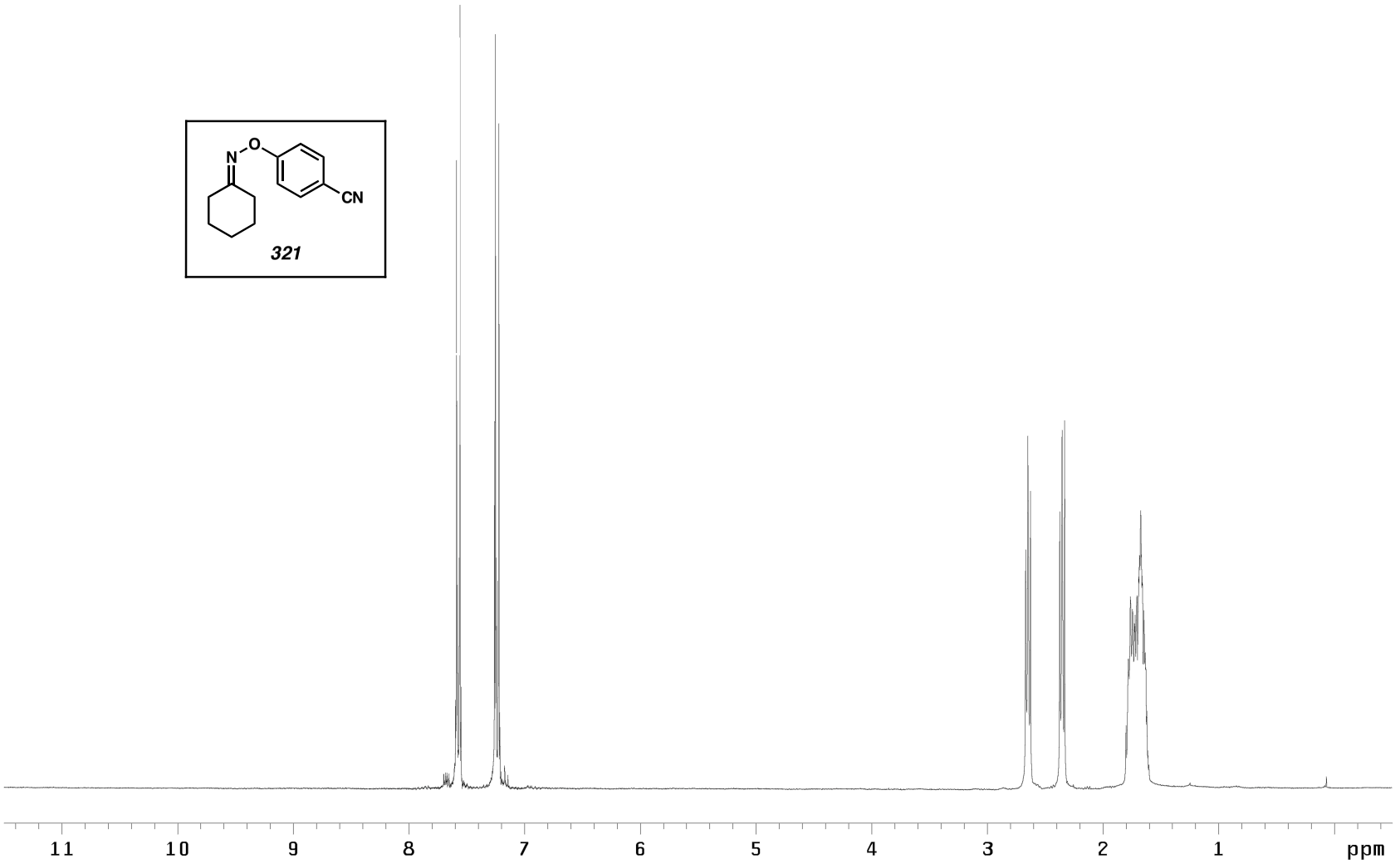


Figure A7.22 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **321**.

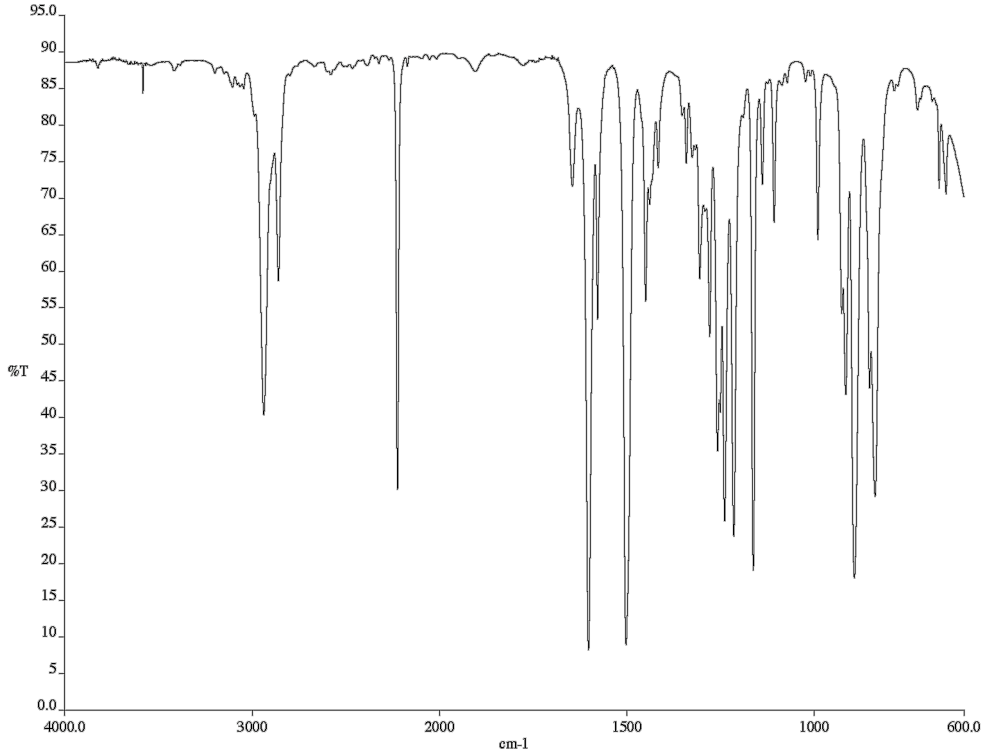


Figure A7.23 Infrared spectrum ($NaCl/CDCl_3$) of compound **321**.

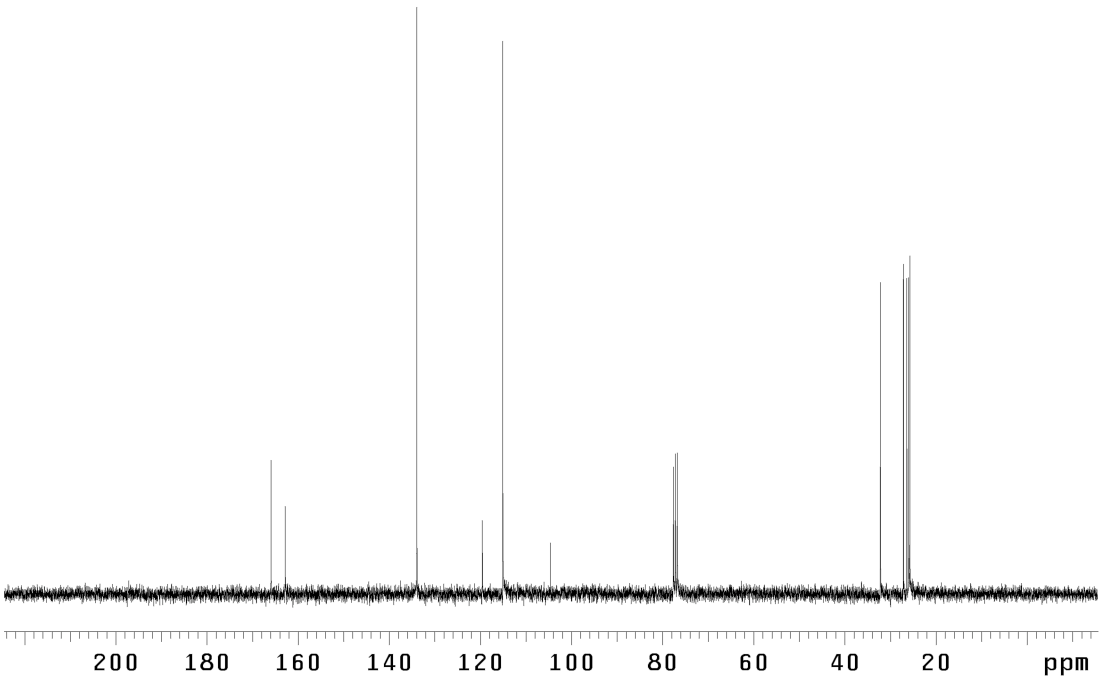


Figure A7.24 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **321**.

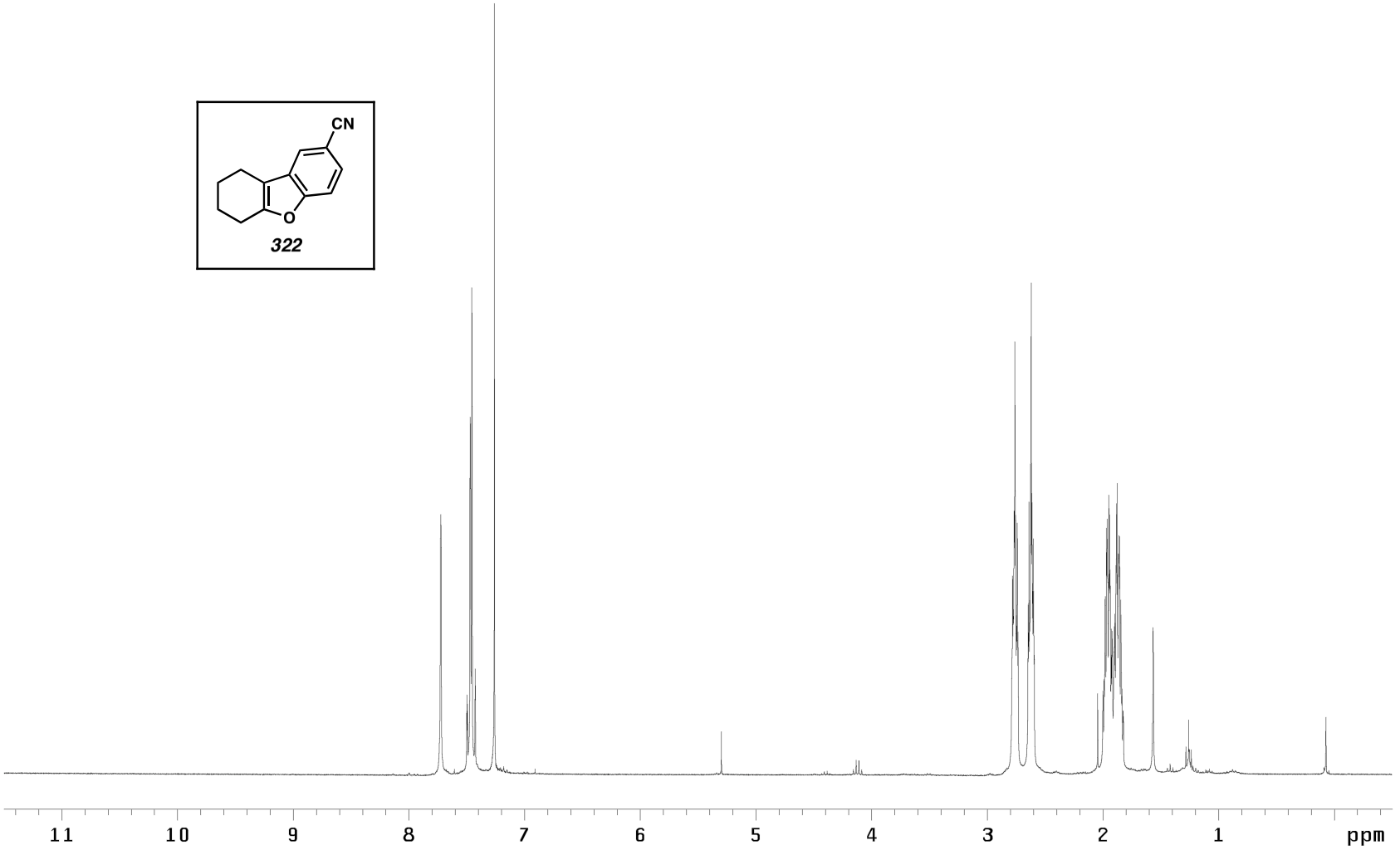


Figure A7.25 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **322**.

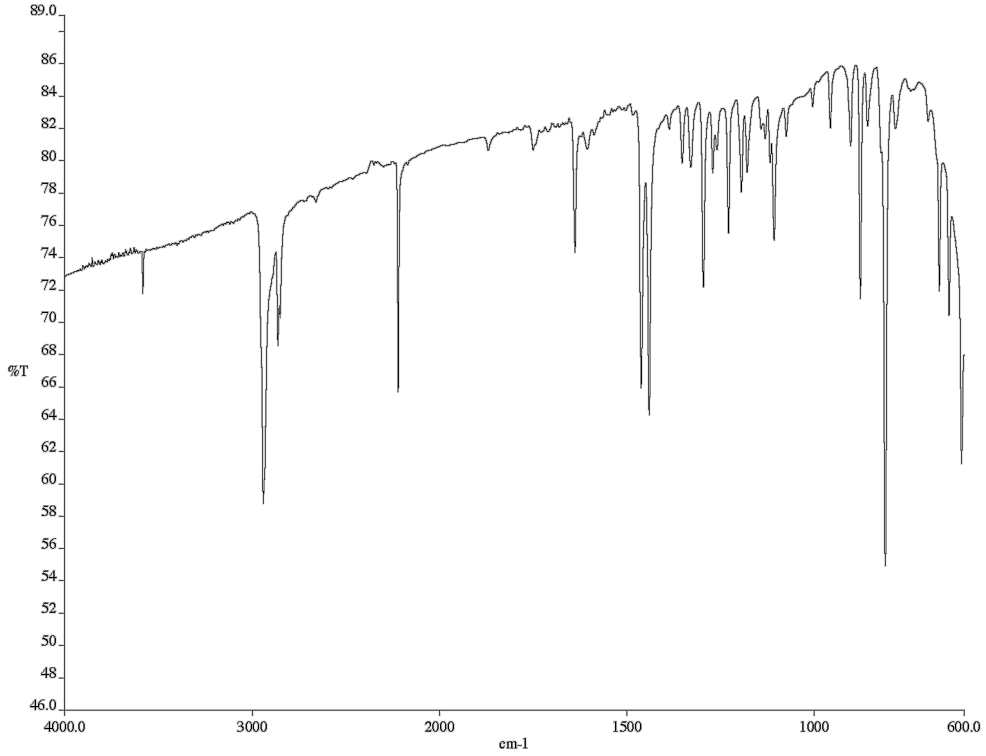


Figure A7.26 Infrared spectrum ($NaCl/CDCl_3$) of compound **322**.

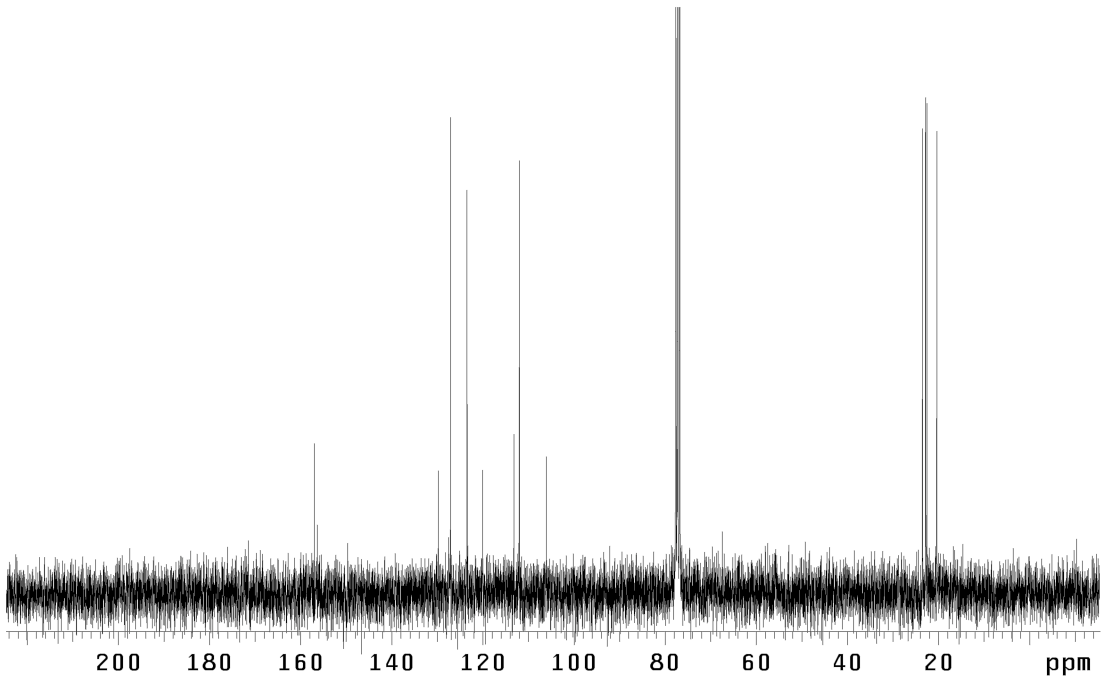


Figure A7.27 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **322**.

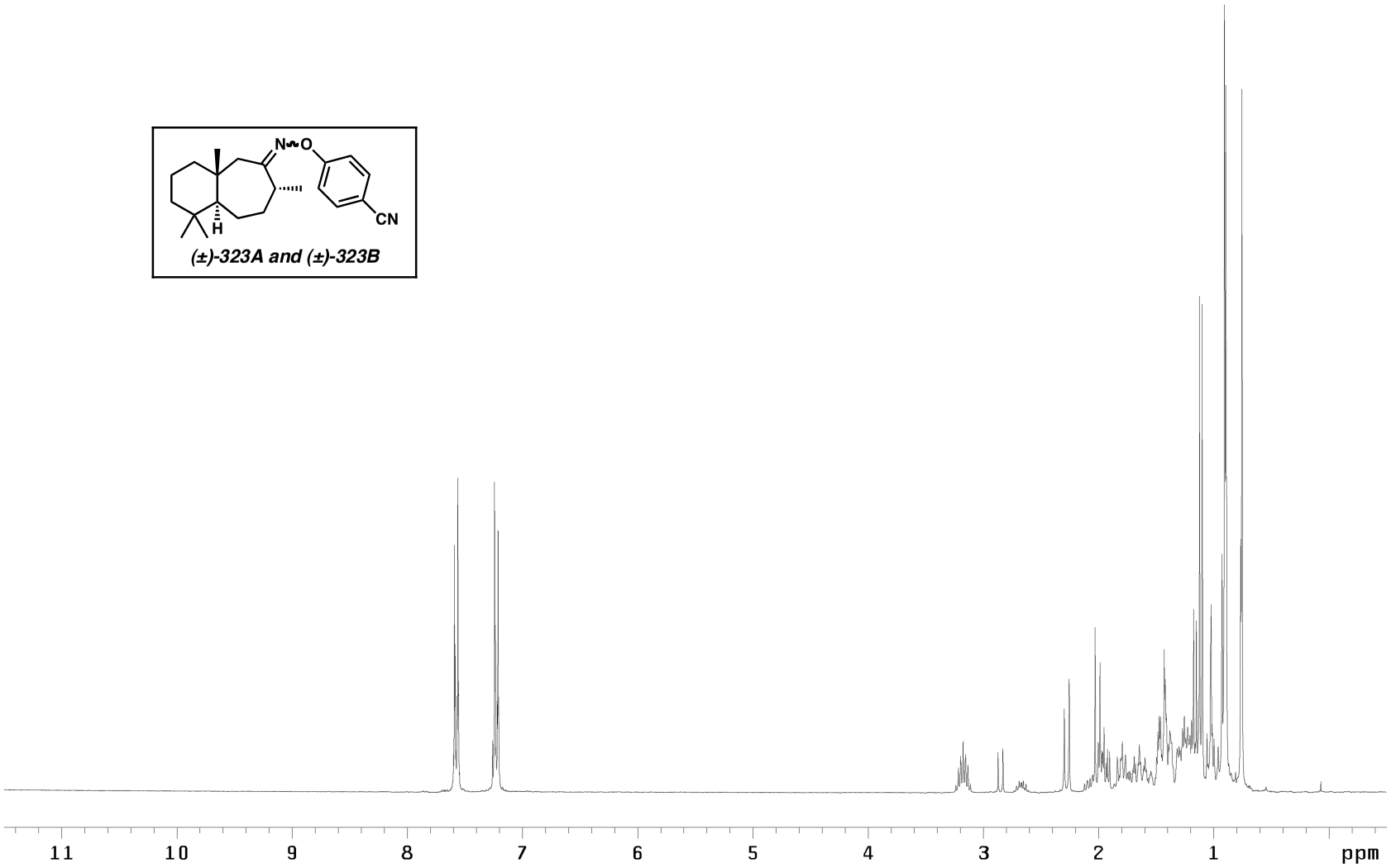


Figure A7.28 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **323A** and **323B**.

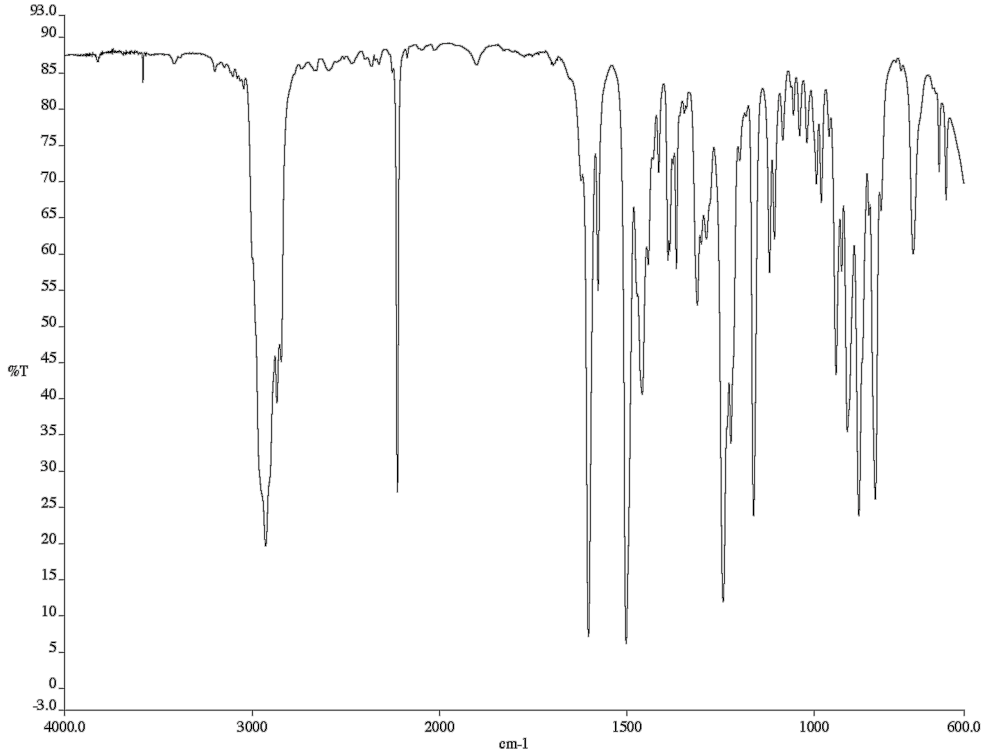


Figure A7.29 Infrared spectrum ($NaCl/CDCl_3$) of compound **323A** and **323B**.

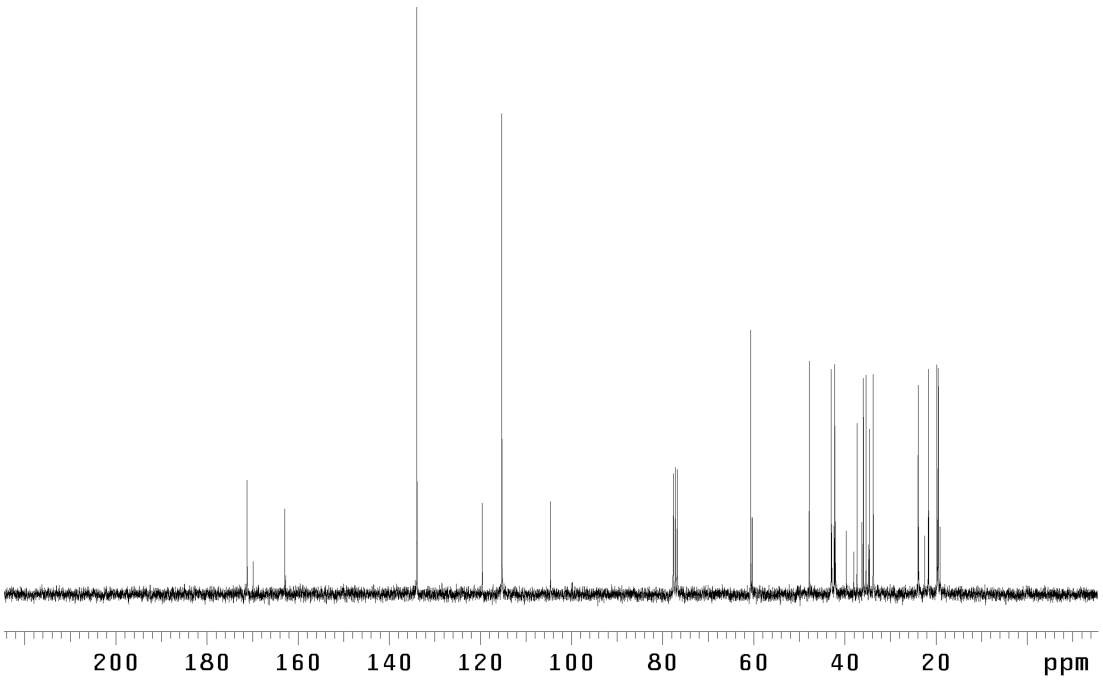


Figure A7.30 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **323A** and **323B**.

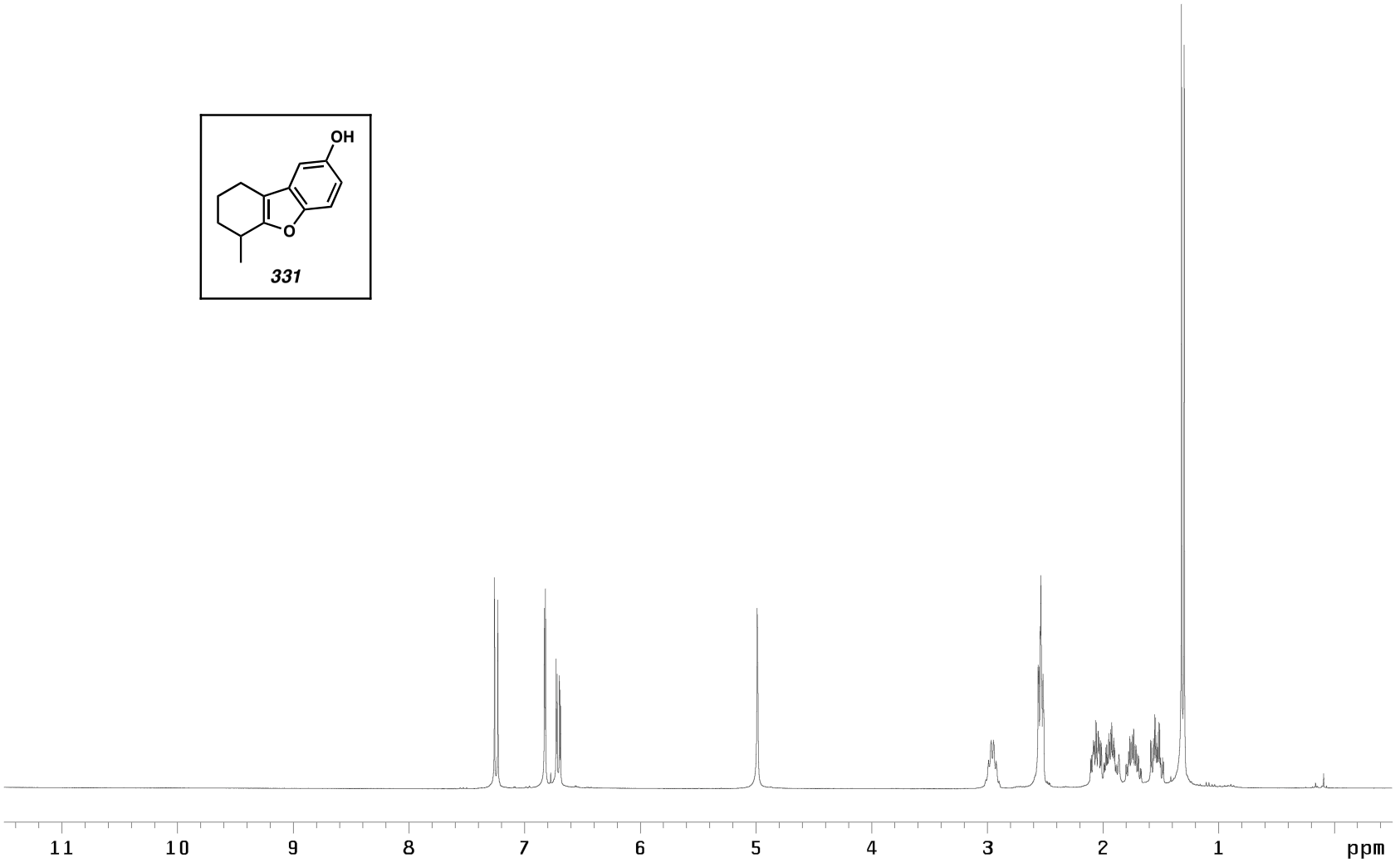


Figure A7.31 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **331**.

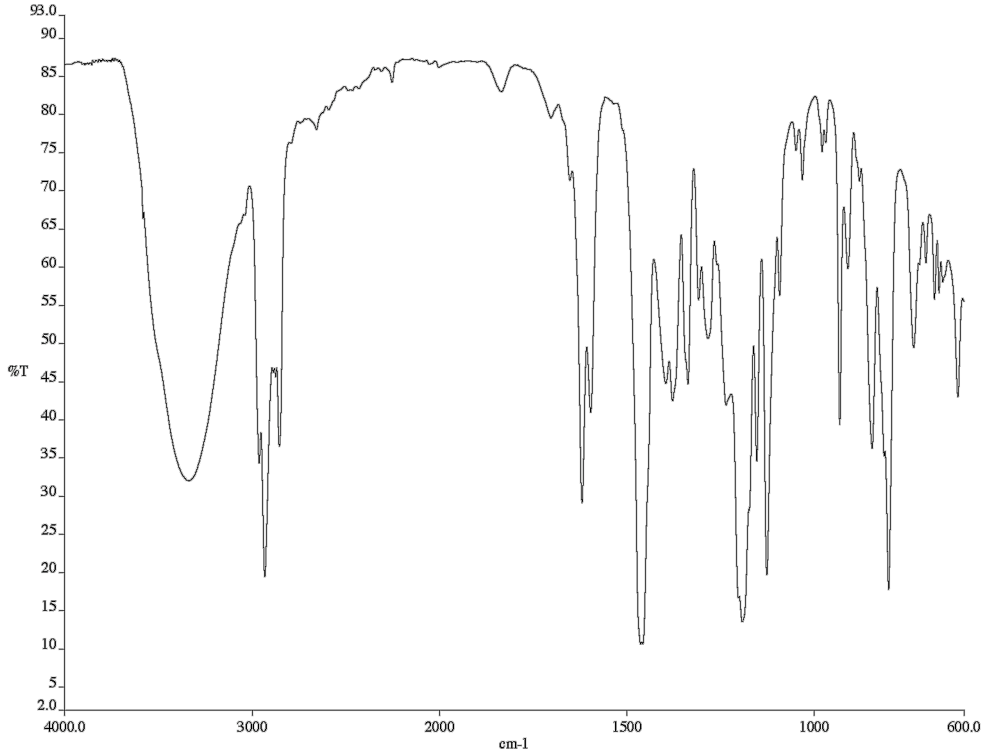


Figure A7.32 Infrared spectrum ($NaCl/CDCl_3$) of compound **331**.

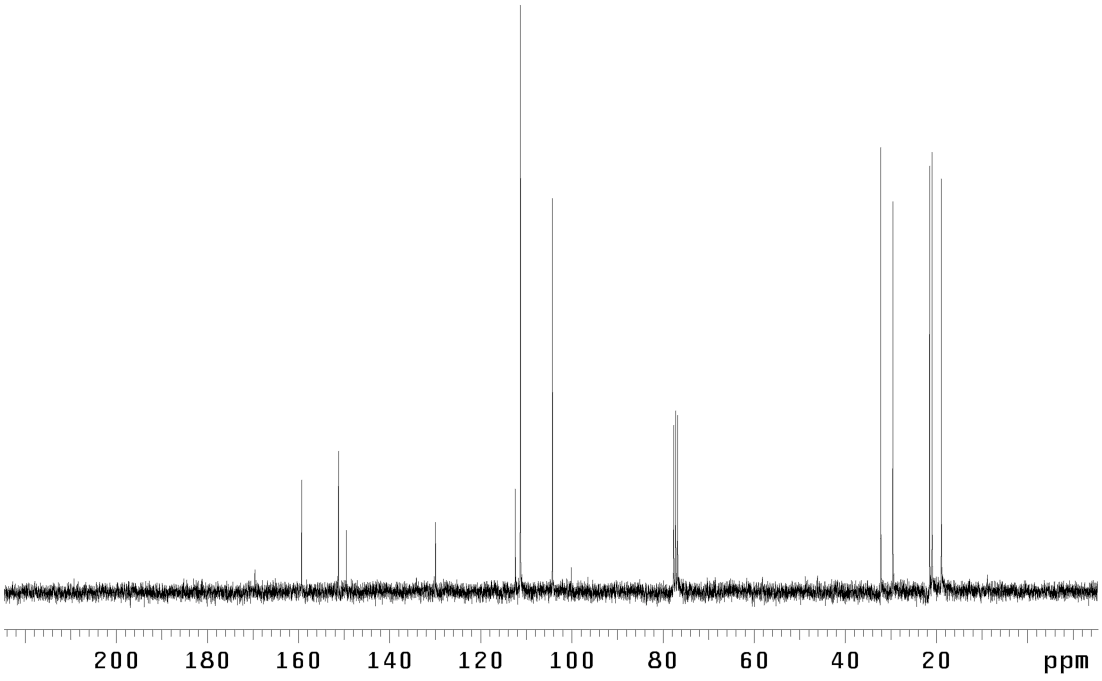


Figure A7.33 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **331**.

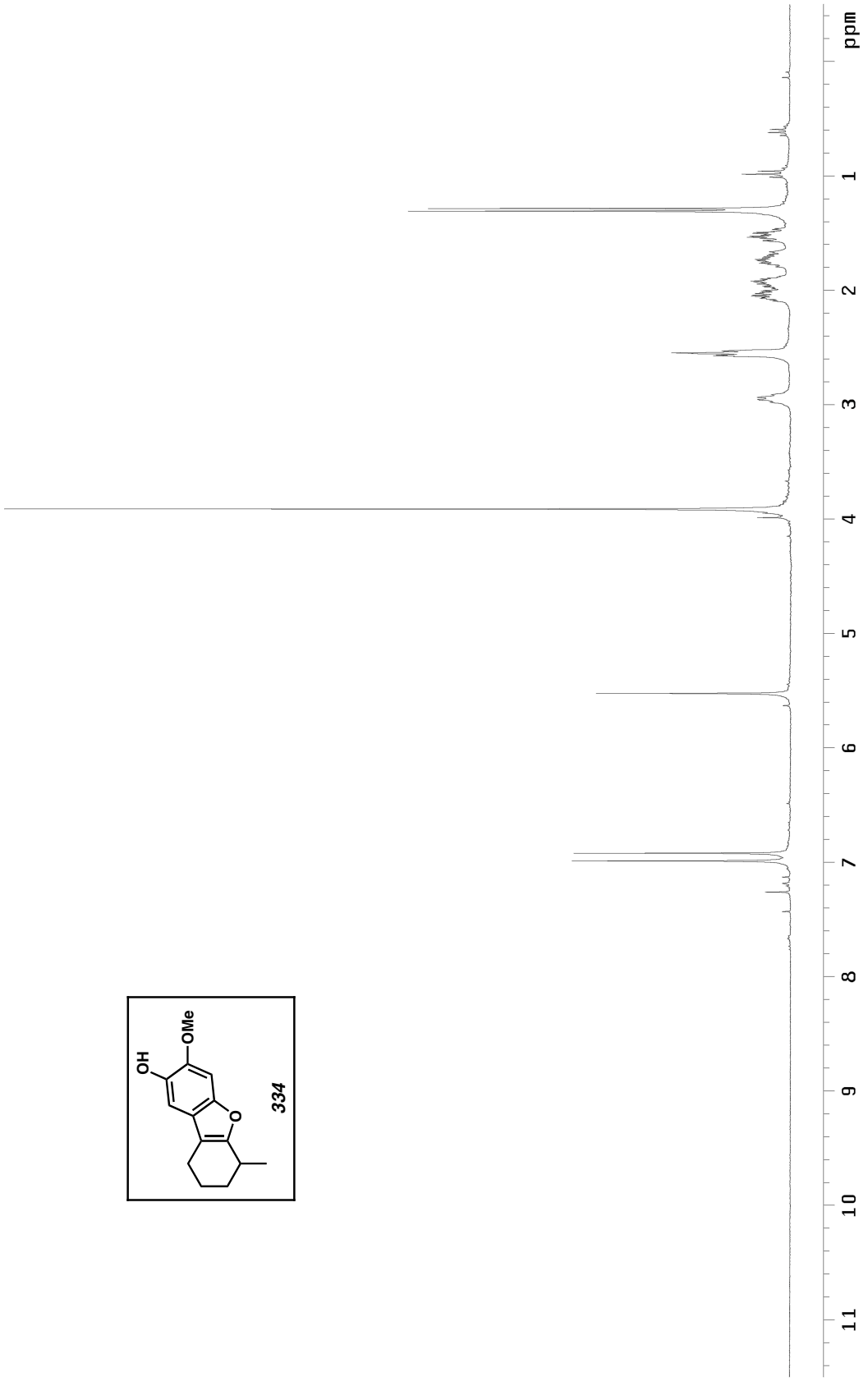


Figure A7.34 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **334**.

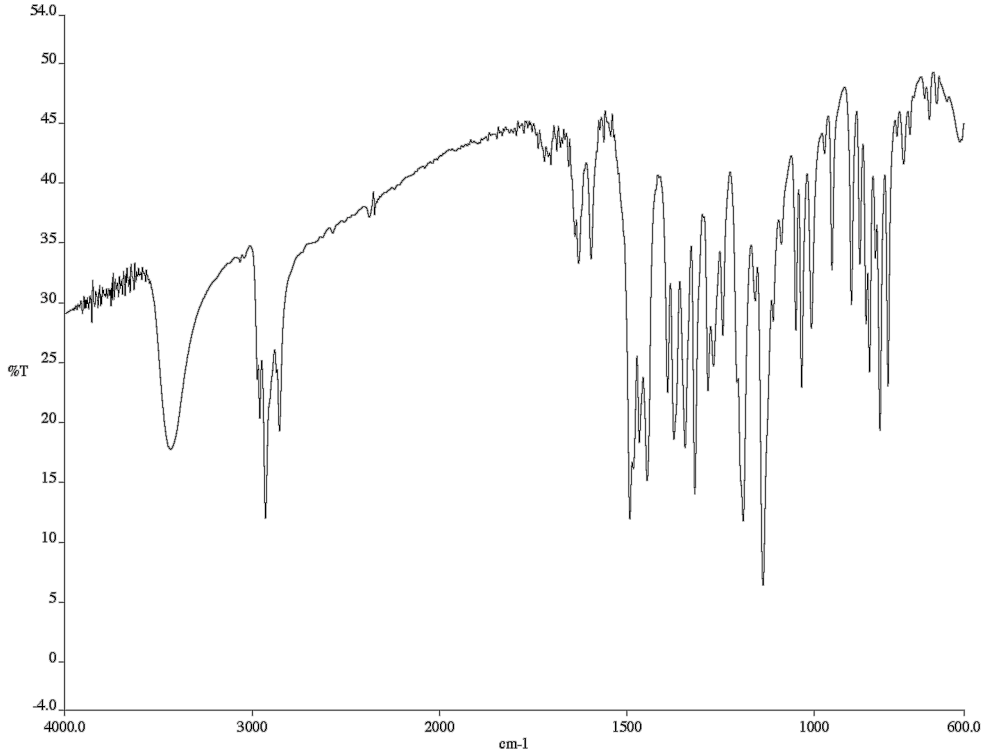


Figure A7.35 Infrared spectrum (KBr) of compound **334**.

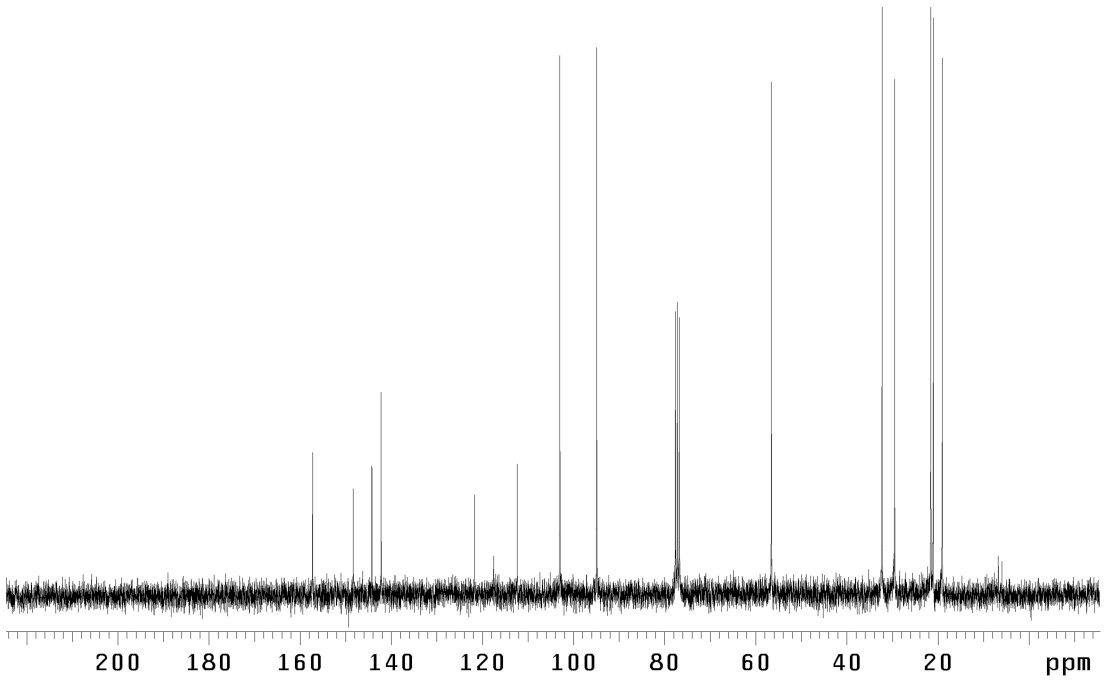


Figure A7.36 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **334**.

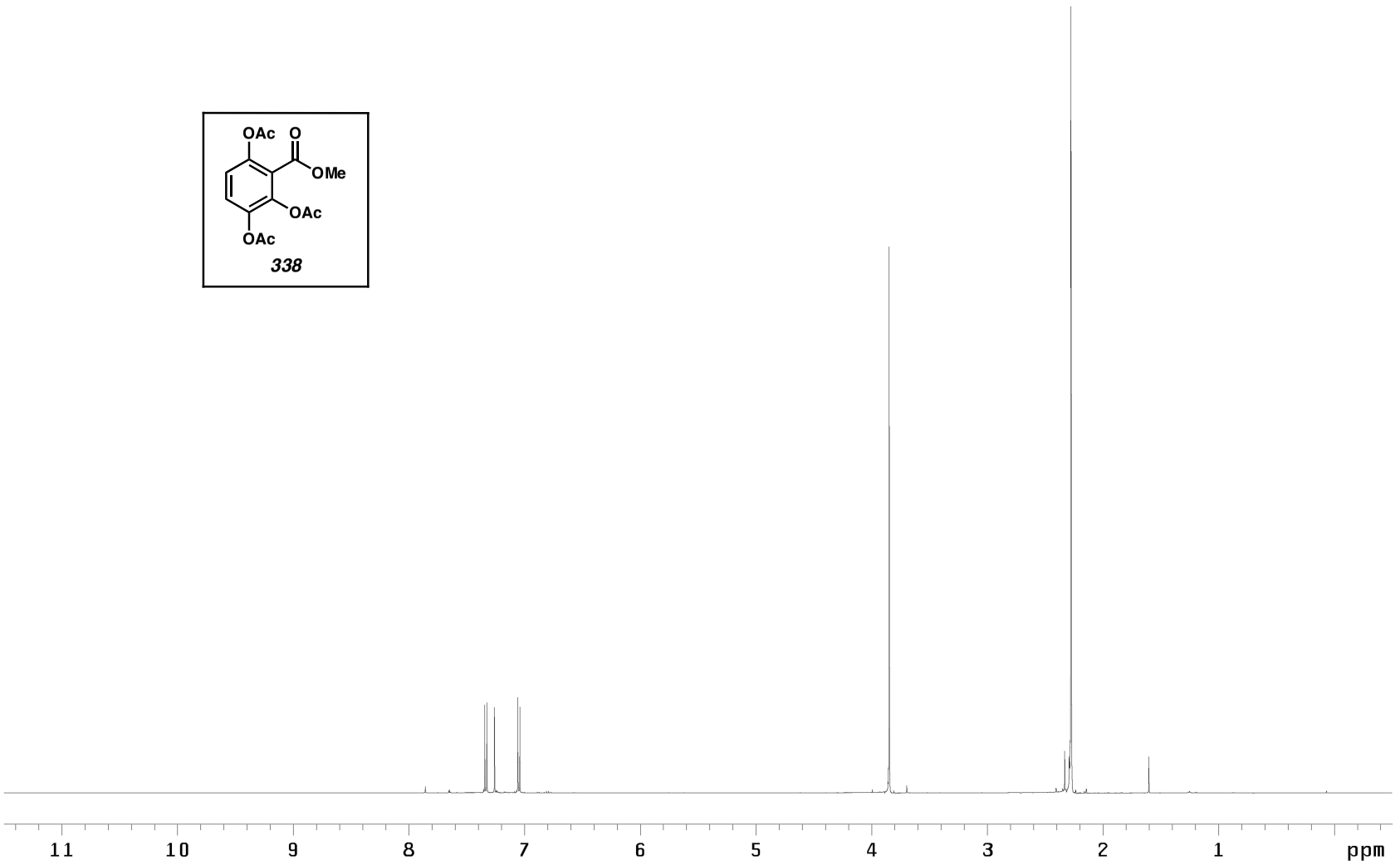


Figure A7.37 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **338**.

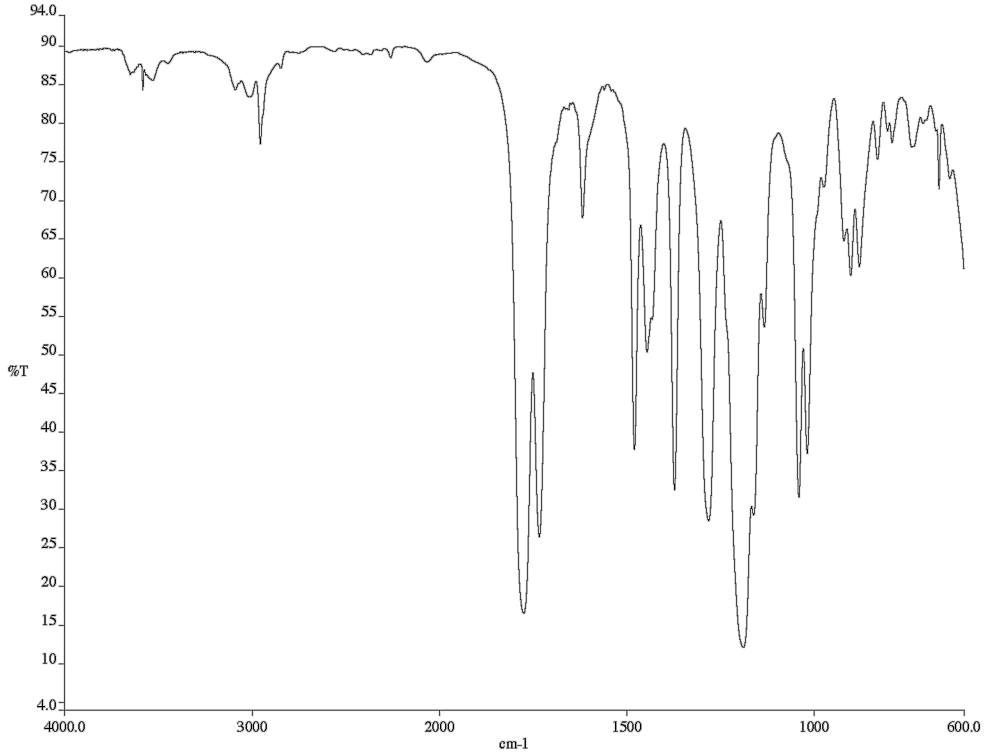


Figure A7.38 Infrared spectrum (NaCl/$CDCl_3$) of compound **338**.

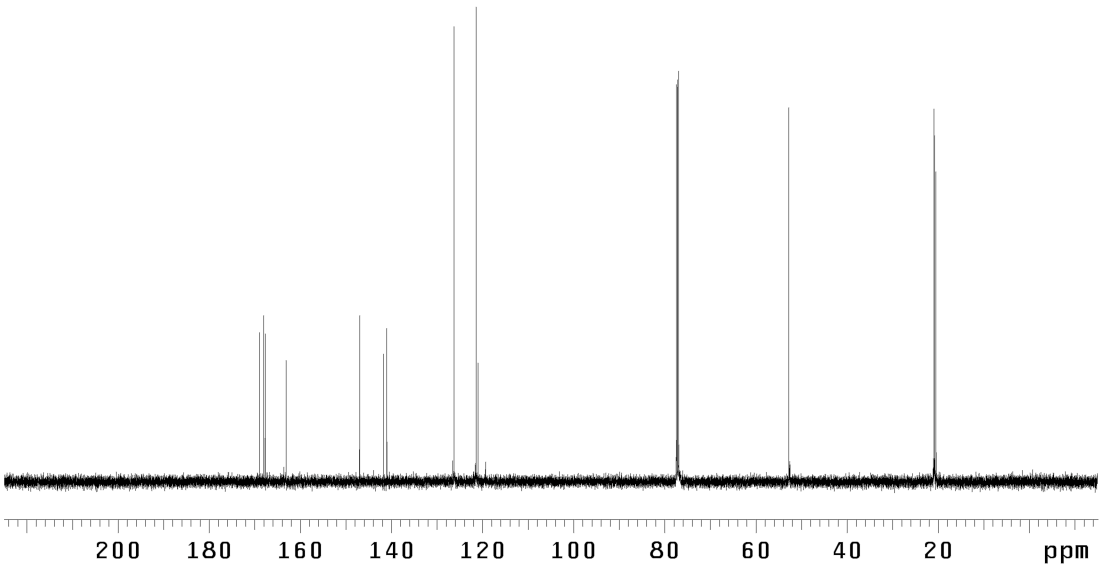


Figure A7.39 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **338**.

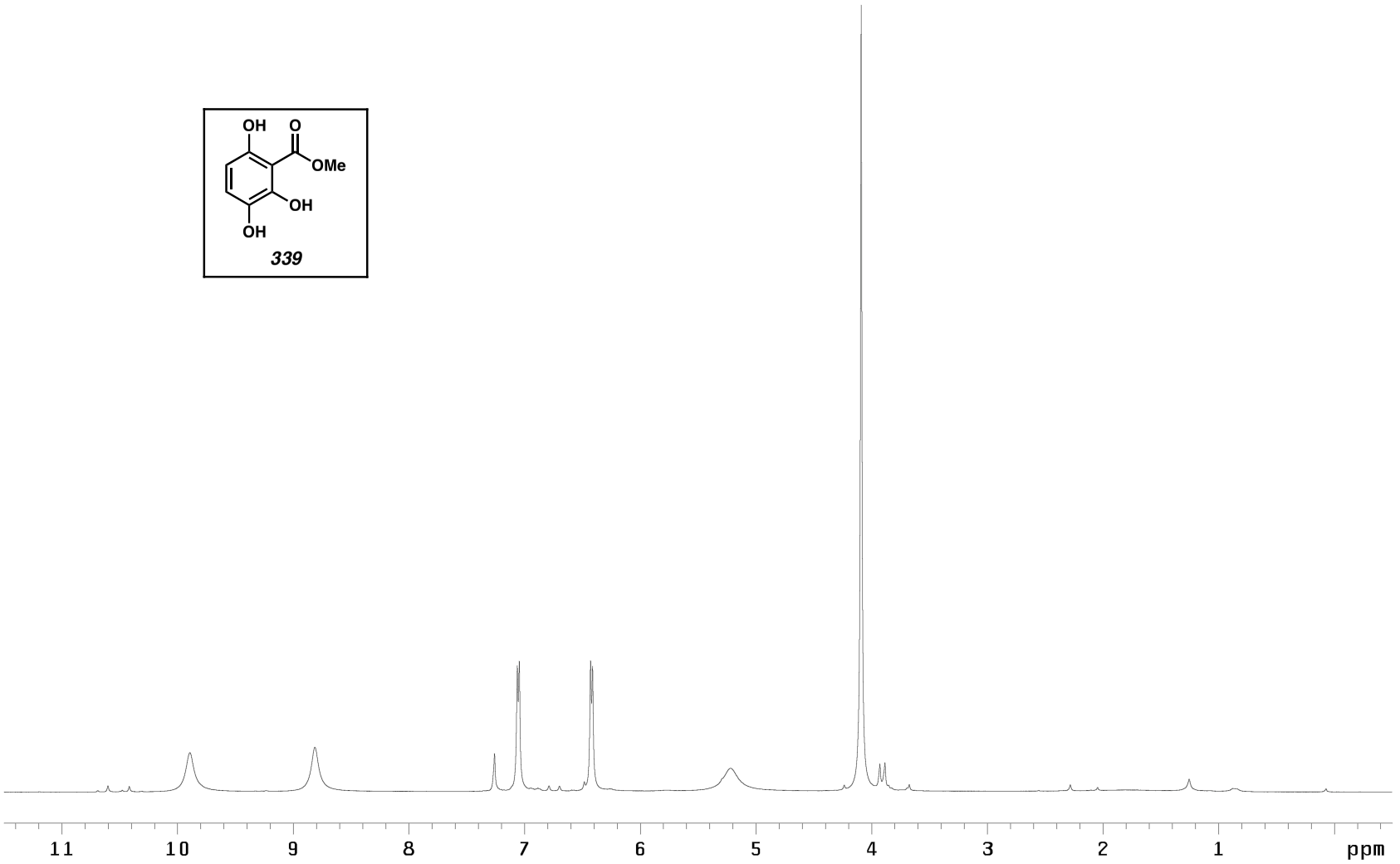


Figure A7.40 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **339**.

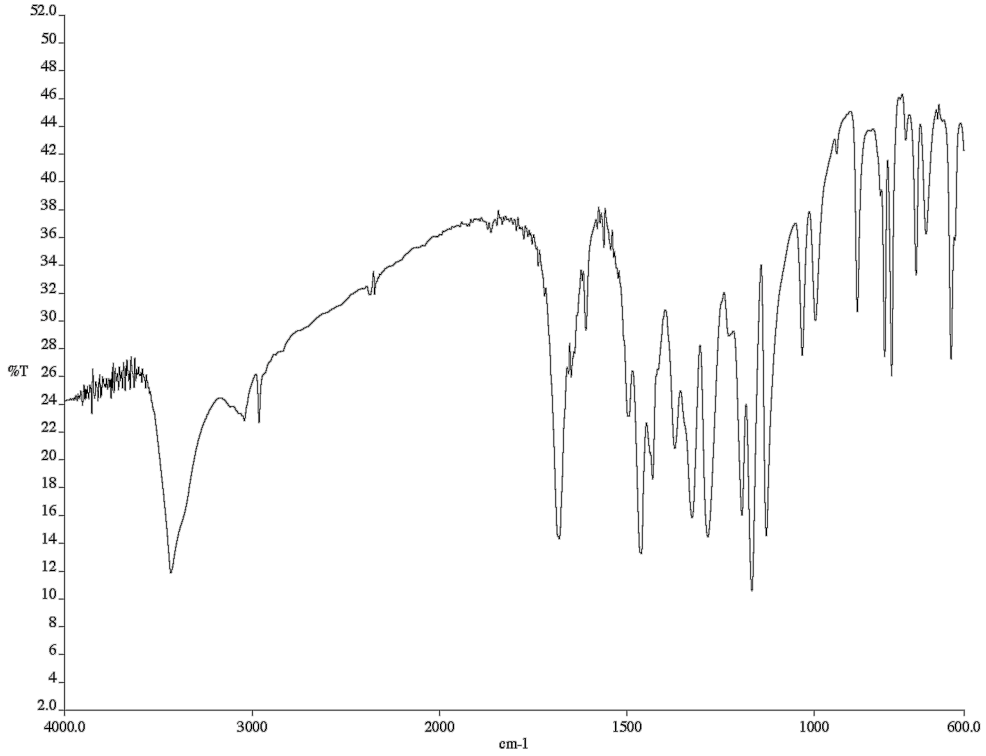


Figure A7.41 Infrared spectrum (KBr) of compound **339**.

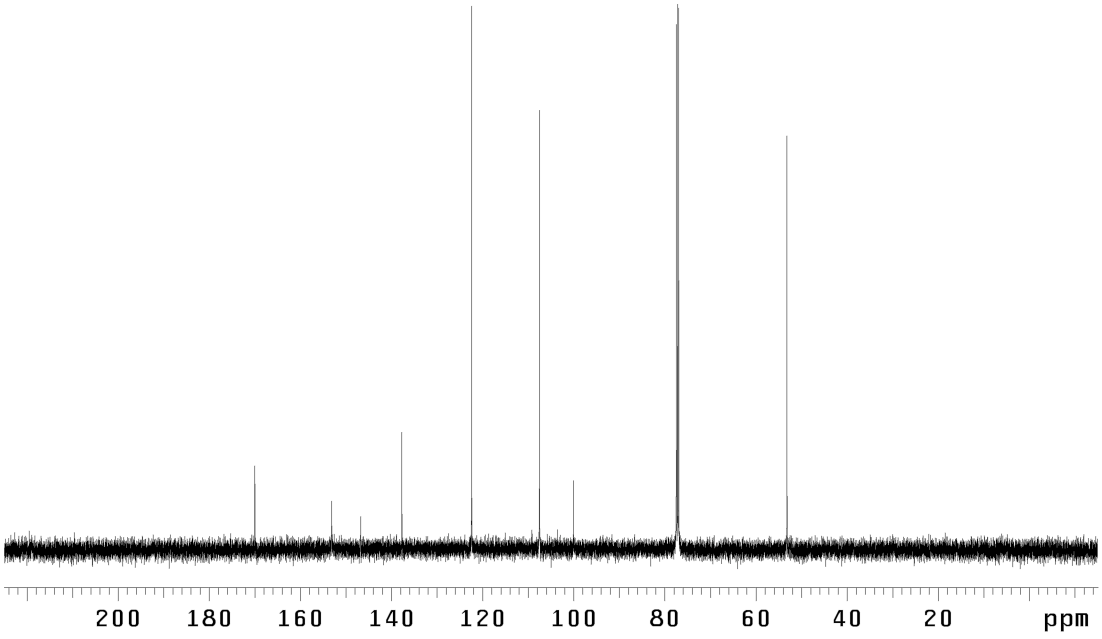


Figure A7.42 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **339**.

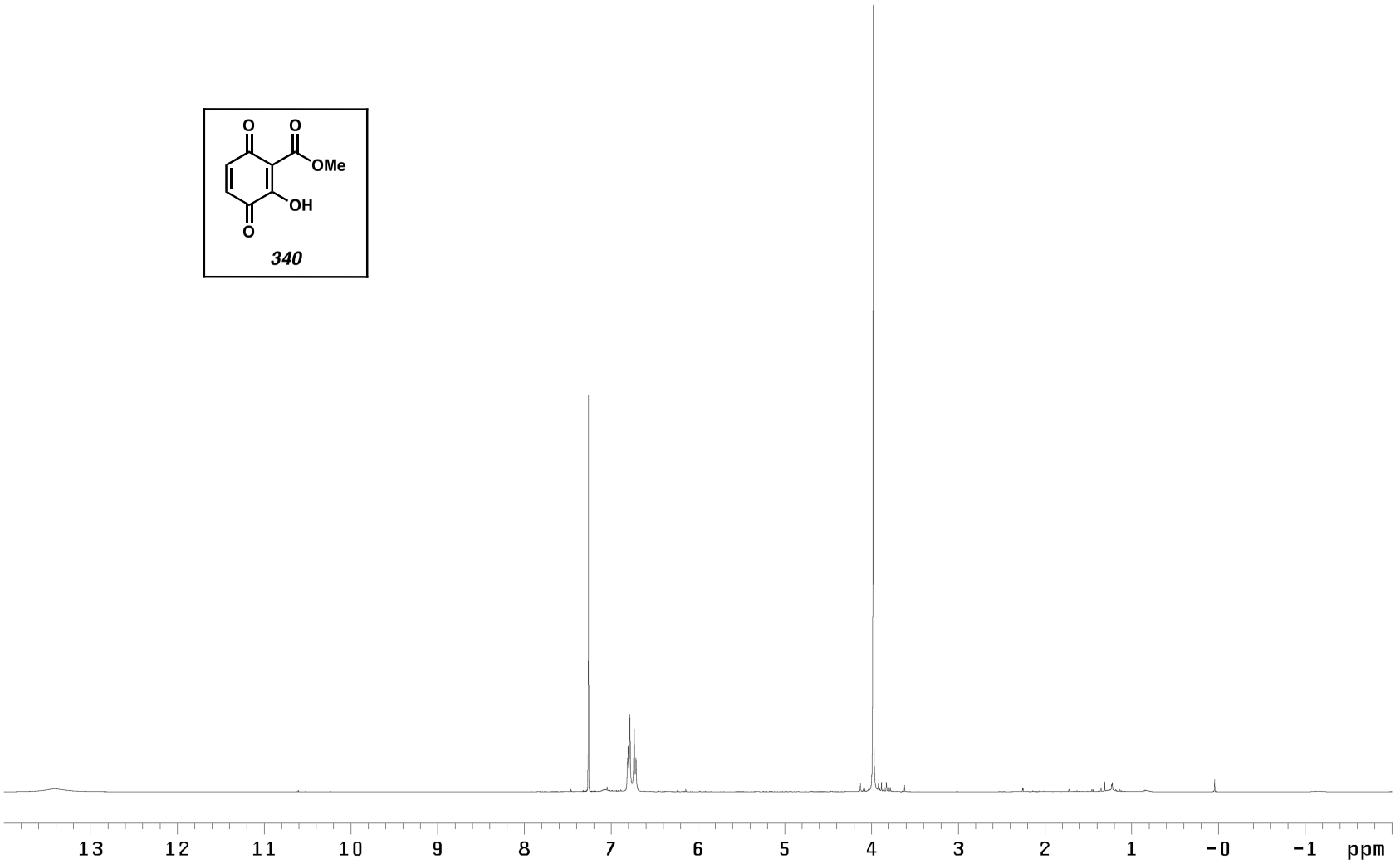


Figure A7.43 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **340**.

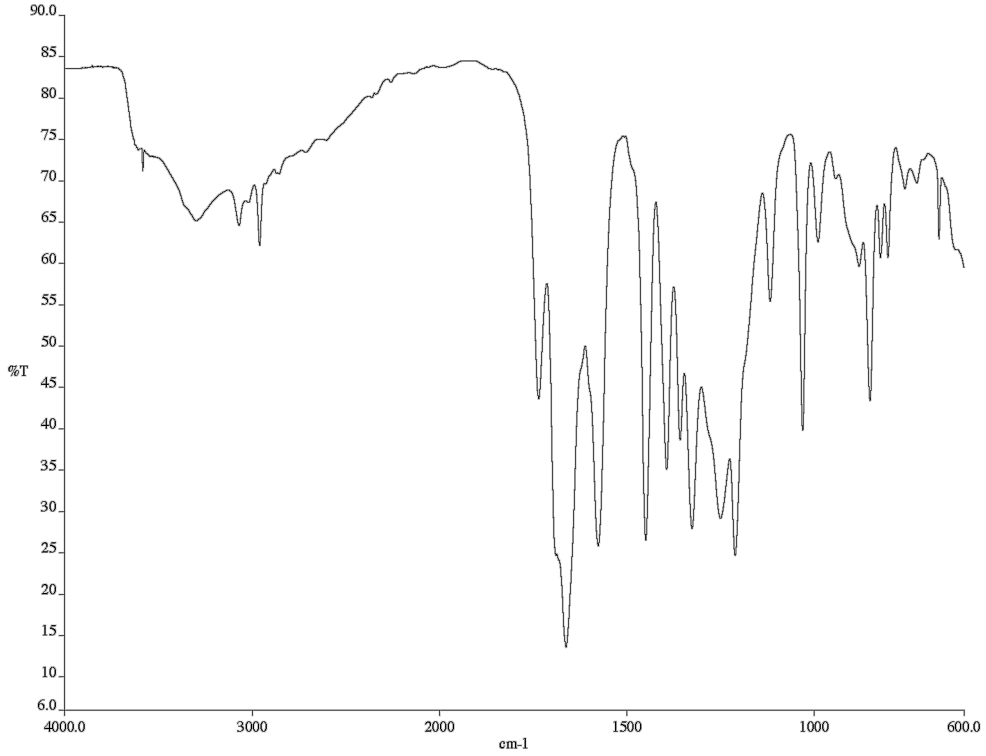


Figure A7.44 Infrared spectrum ($NaCl/CHCl_3/CDCl_3$) of compound **340**.

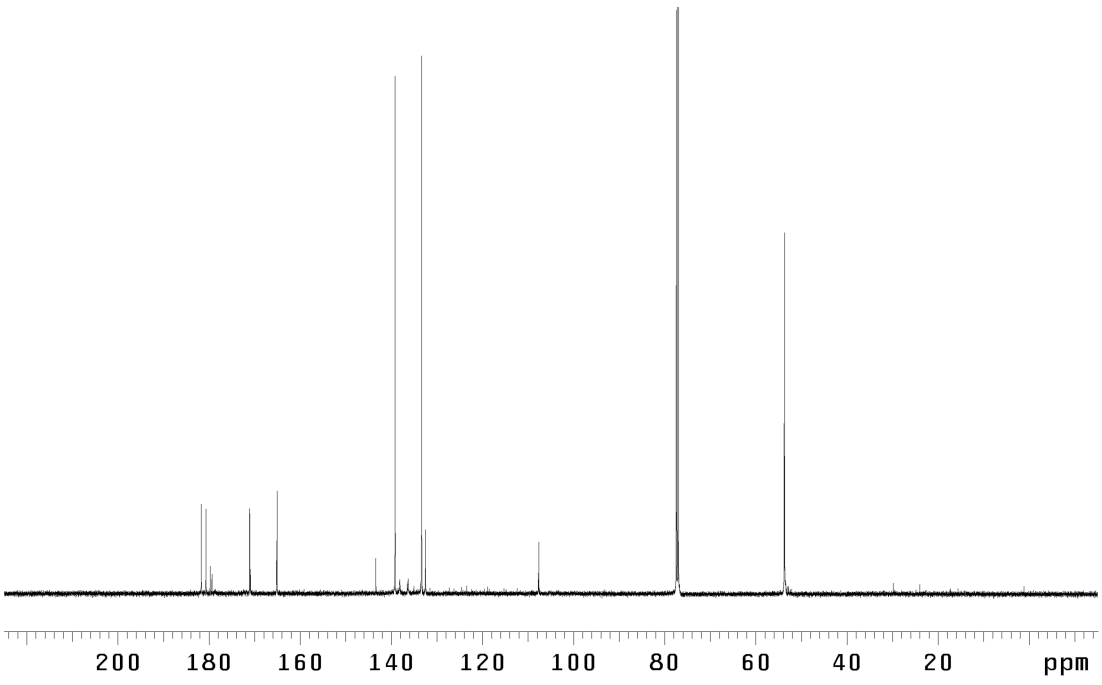


Figure A7.45 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **340**.

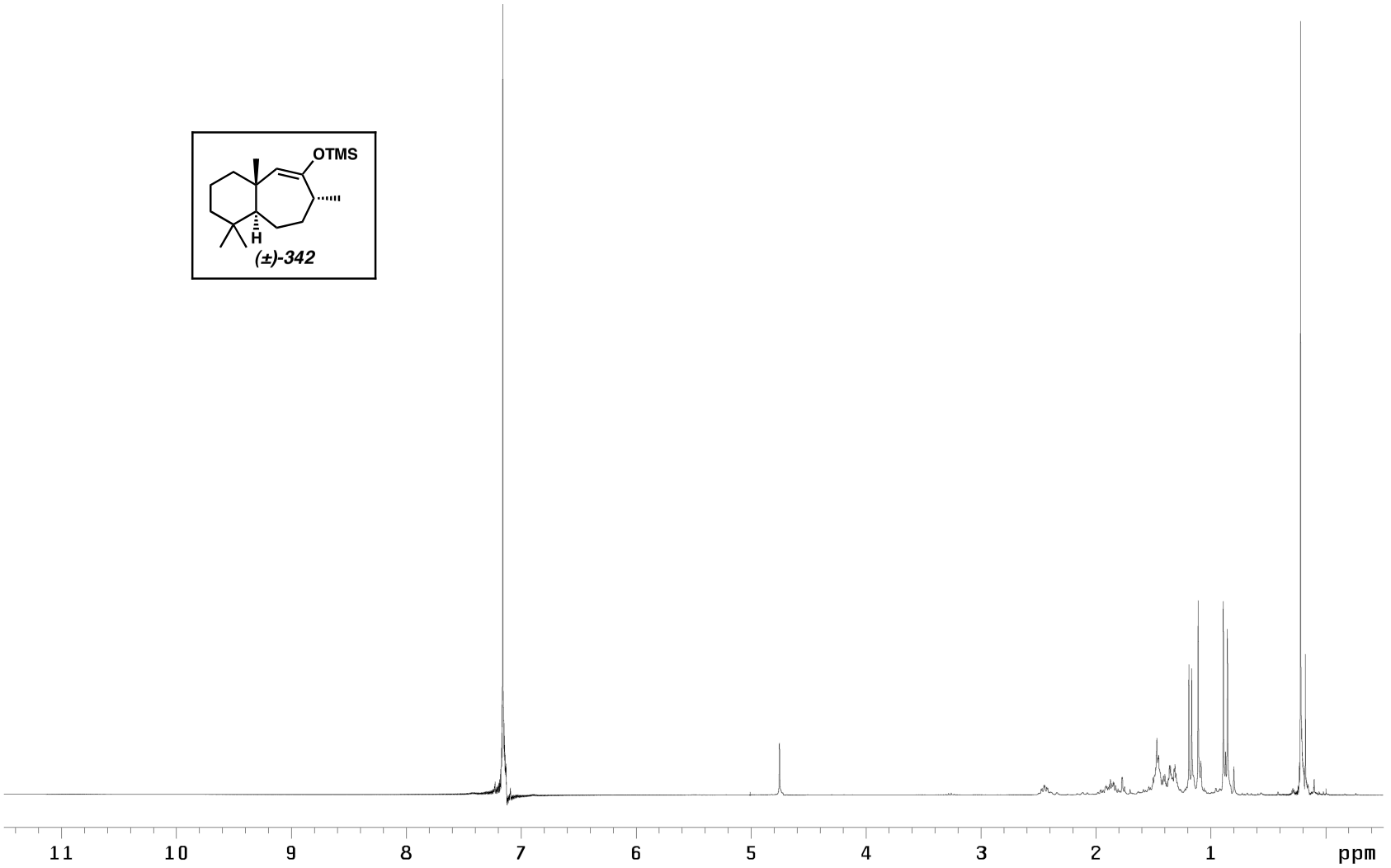


Figure A7.46 ^{1}H NMR (300 MHz, C_6D_6) of compound **342**.

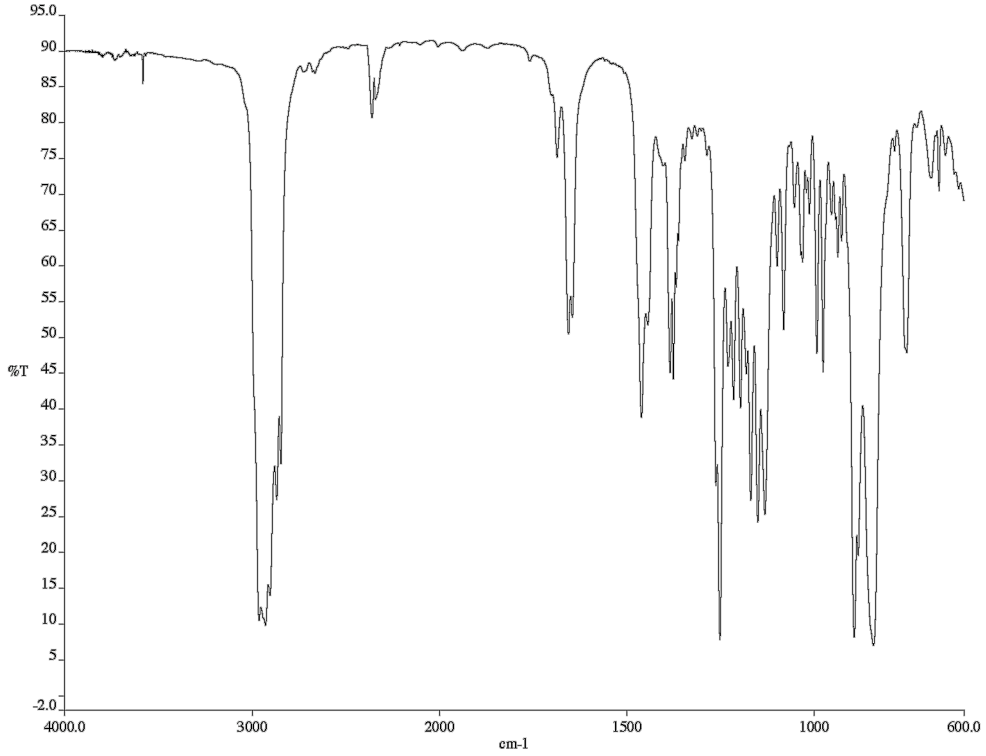


Figure A7.47 Infrared spectrum (NaCl/neat) of compound **342**.

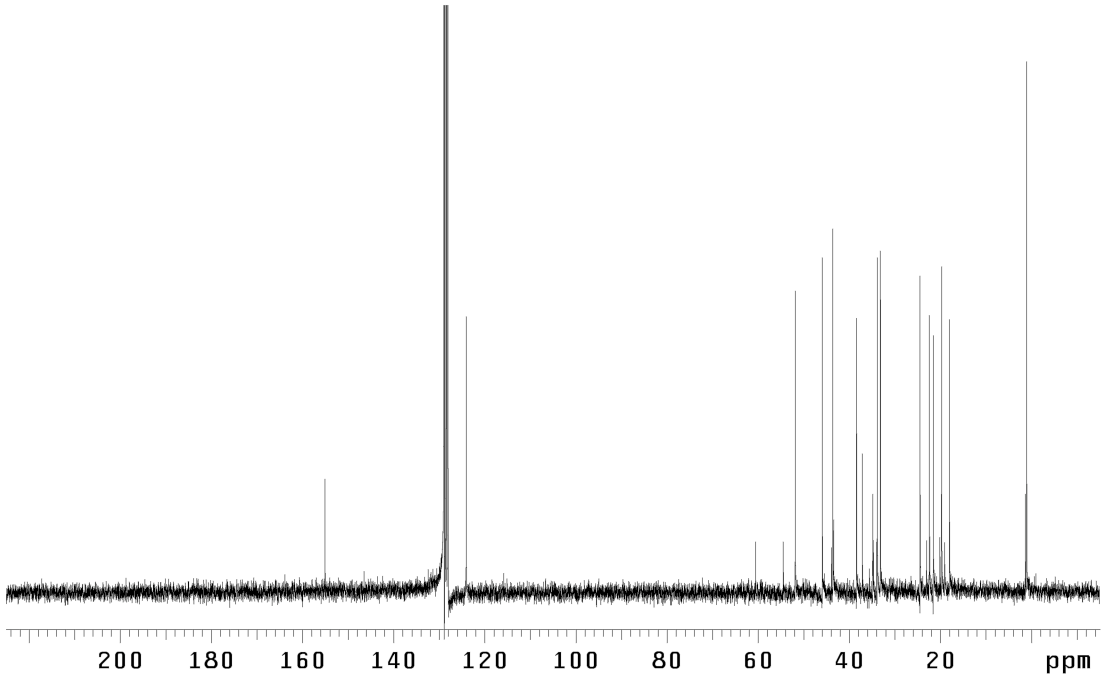


Figure A7.48 ^{13}C NMR (75 MHz, C_6D_6) of compound **342**.

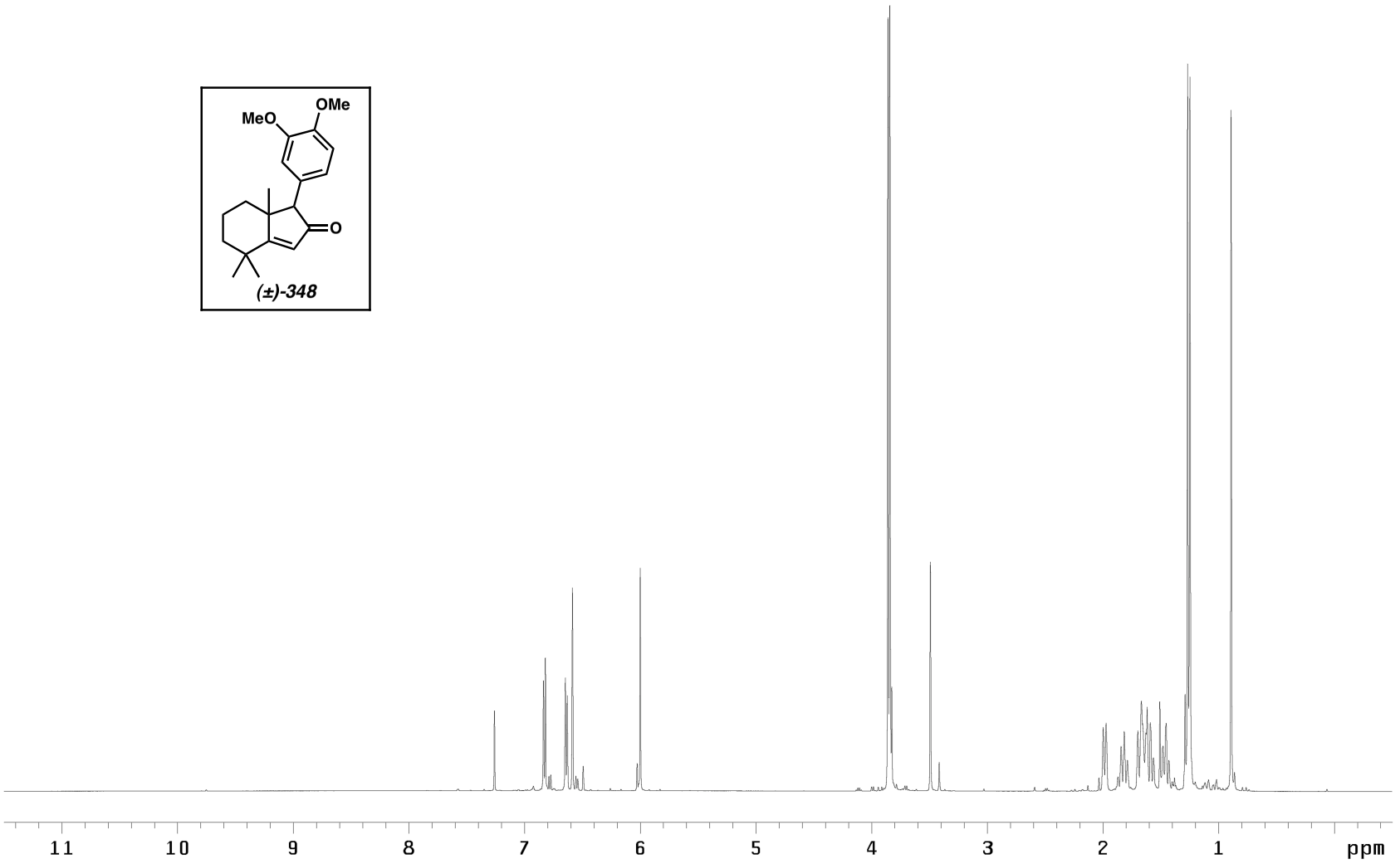


Figure A7.49 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **348**.

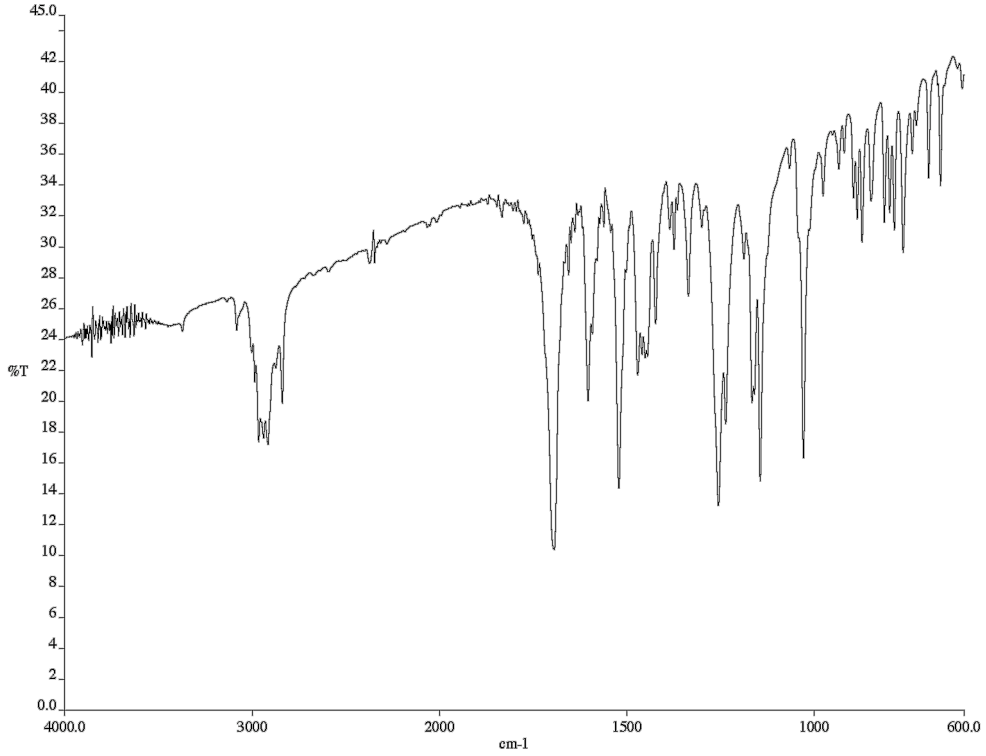


Figure A7.50 Infrared spectrum (KBr) of compound **348**.

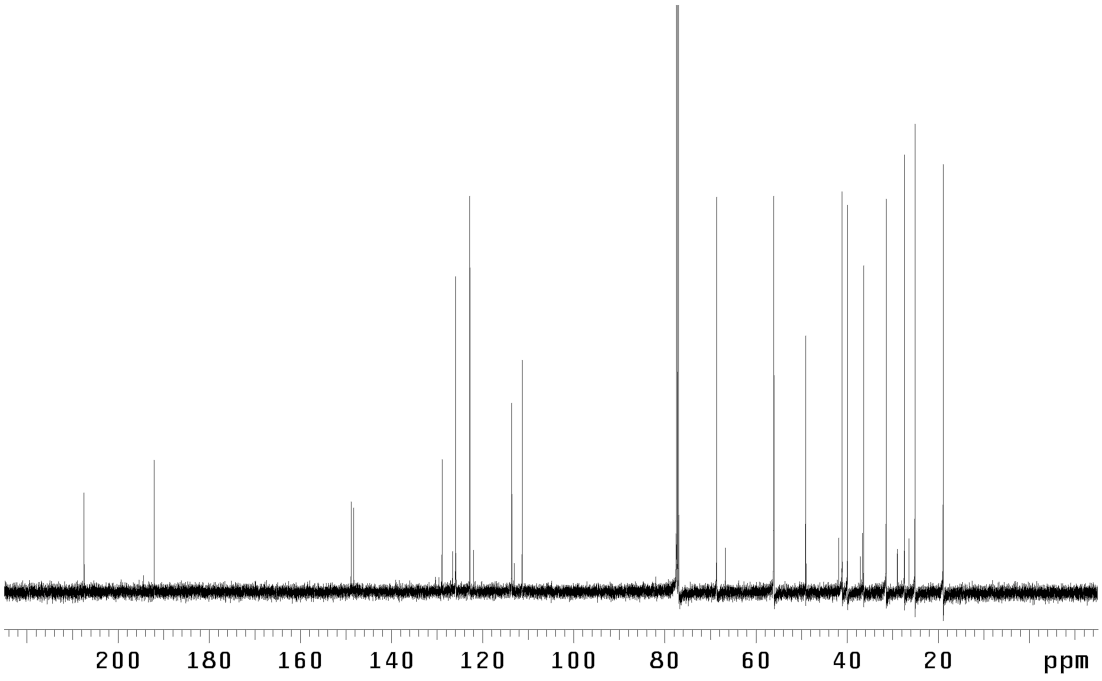


Figure A7.51 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **348**.

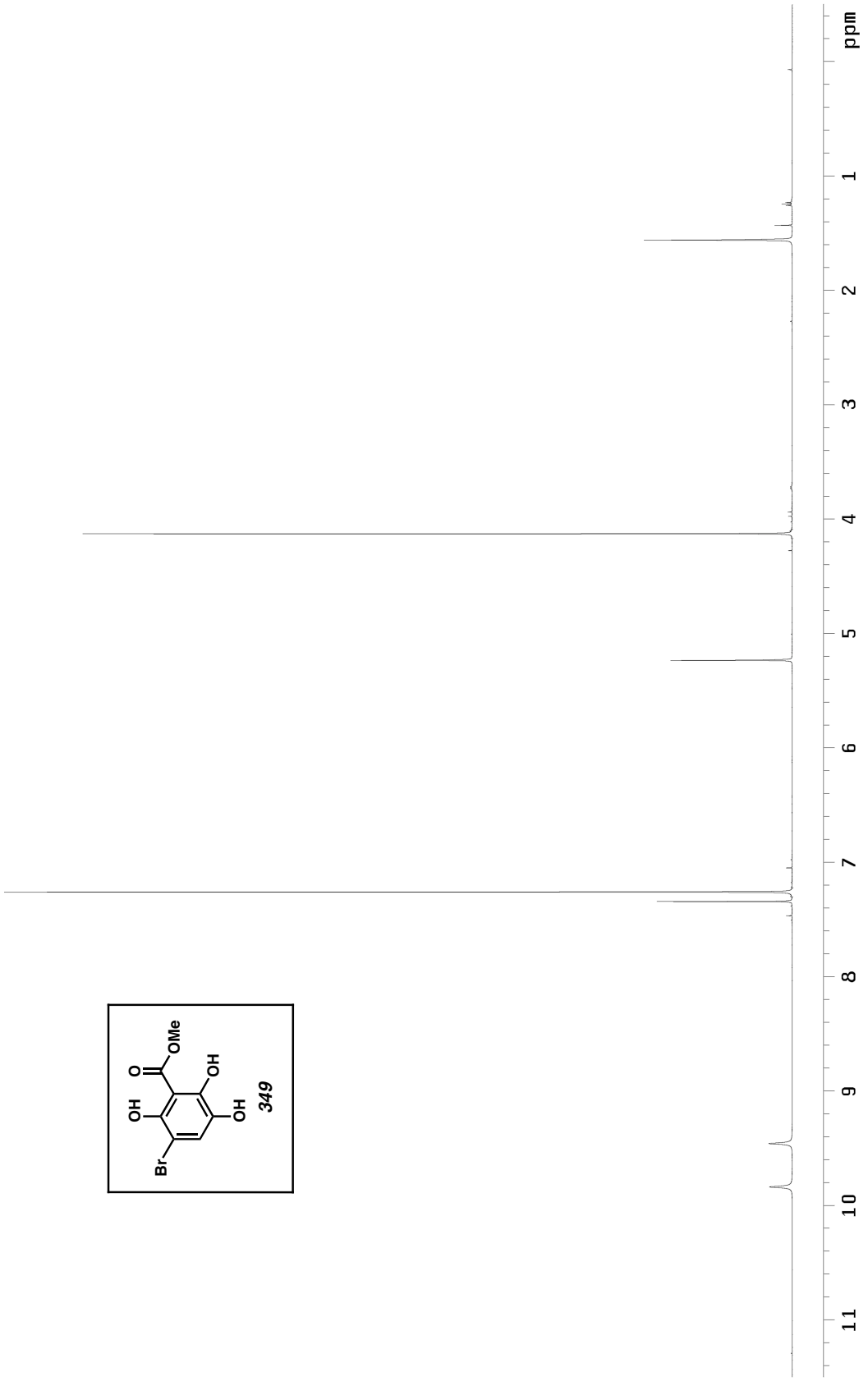


Figure A7.52 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **349**.

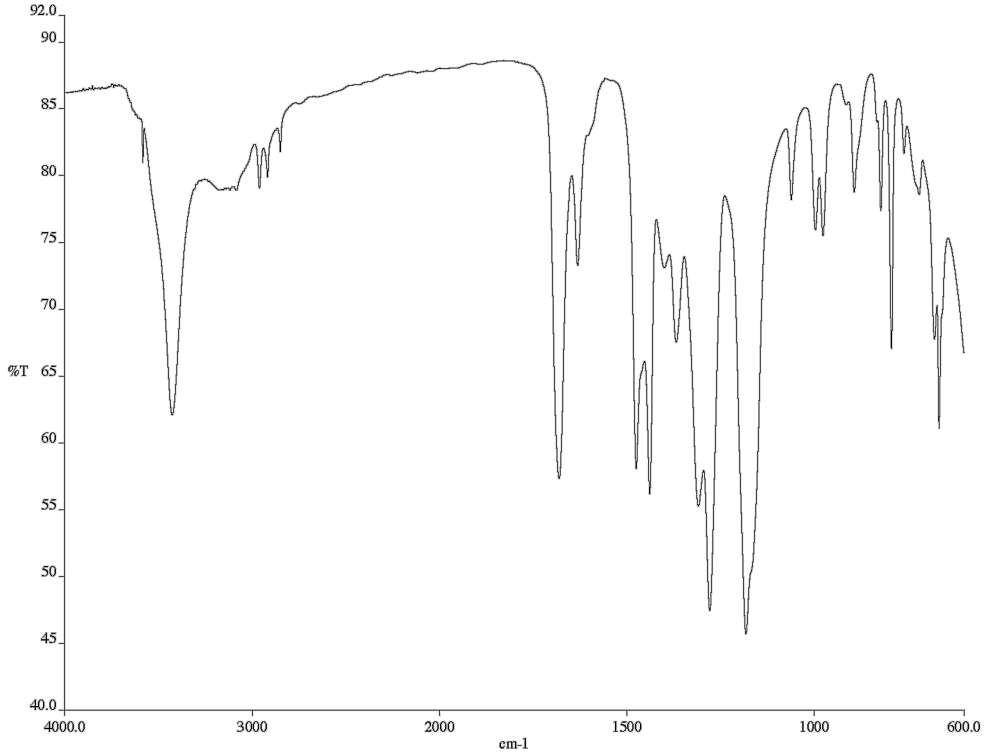


Figure A7.53 Infrared spectrum ($NaCl/CDCl_3$) of compound **349**.

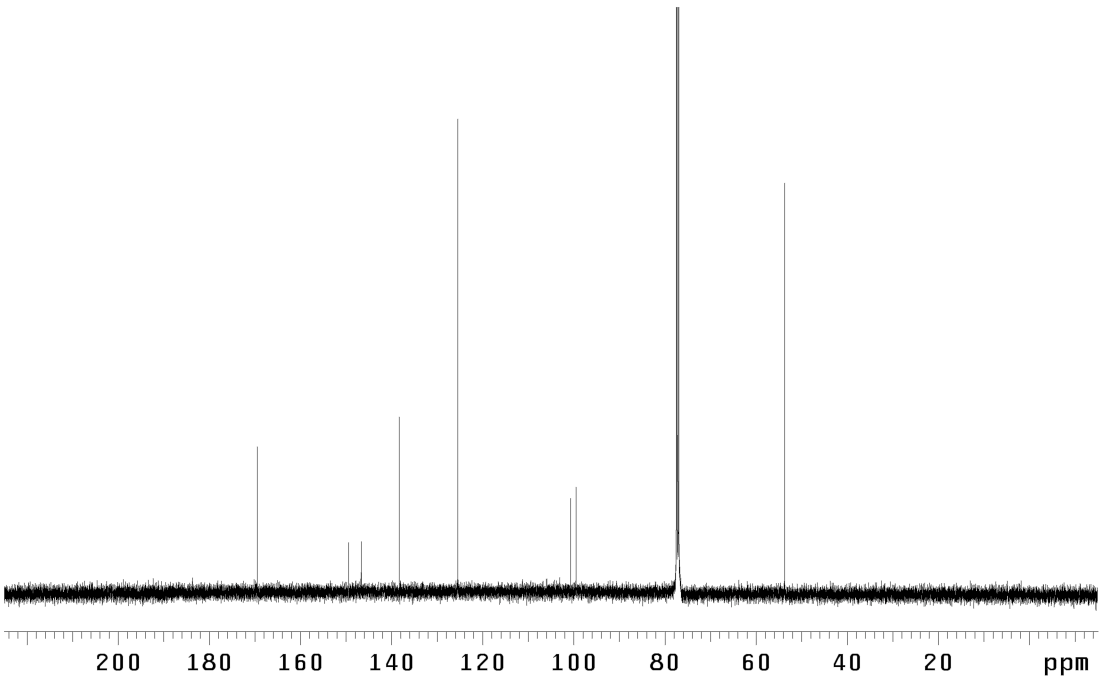


Figure A7.54 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **349**.

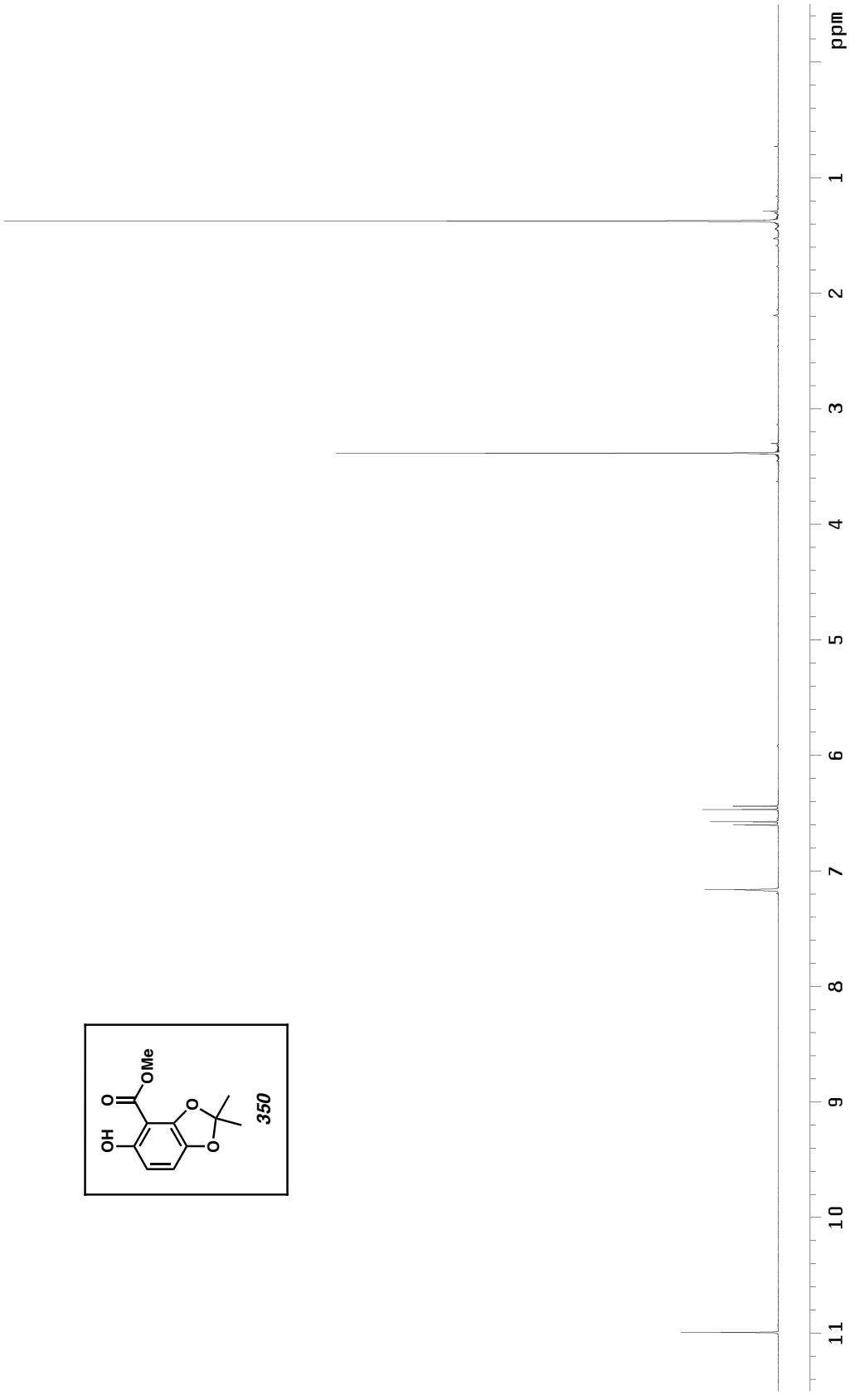


Figure A7.55 ^{1}H NMR (300 MHz, C_6D_6) of compound **350**.

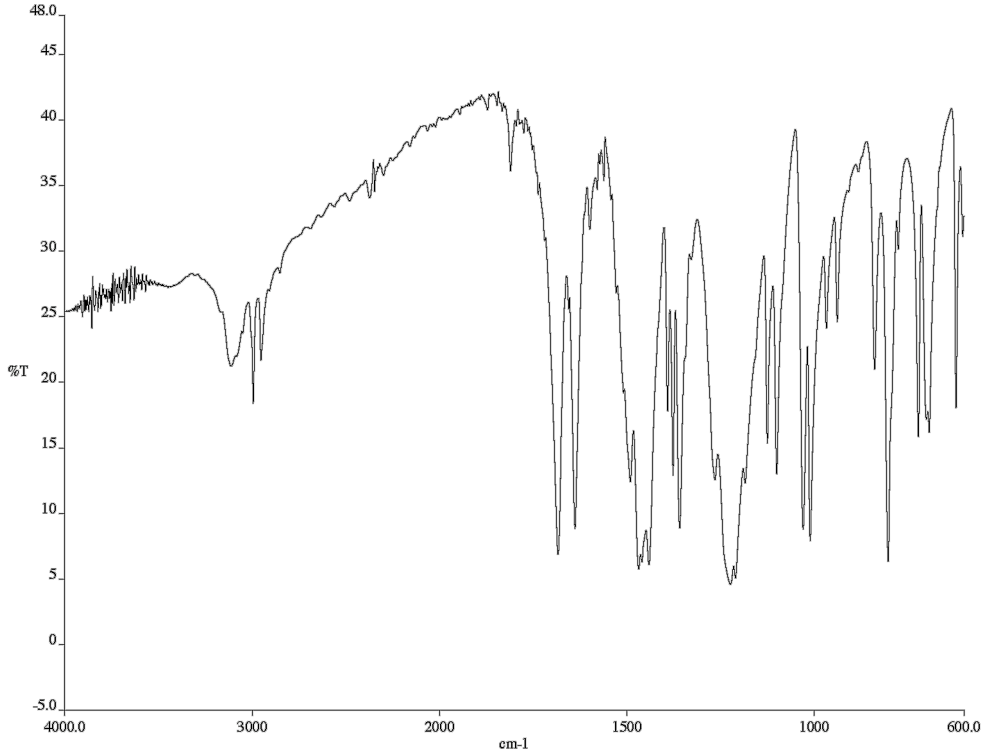


Figure A7.56 Infrared spectrum (KBr) of compound **350**.

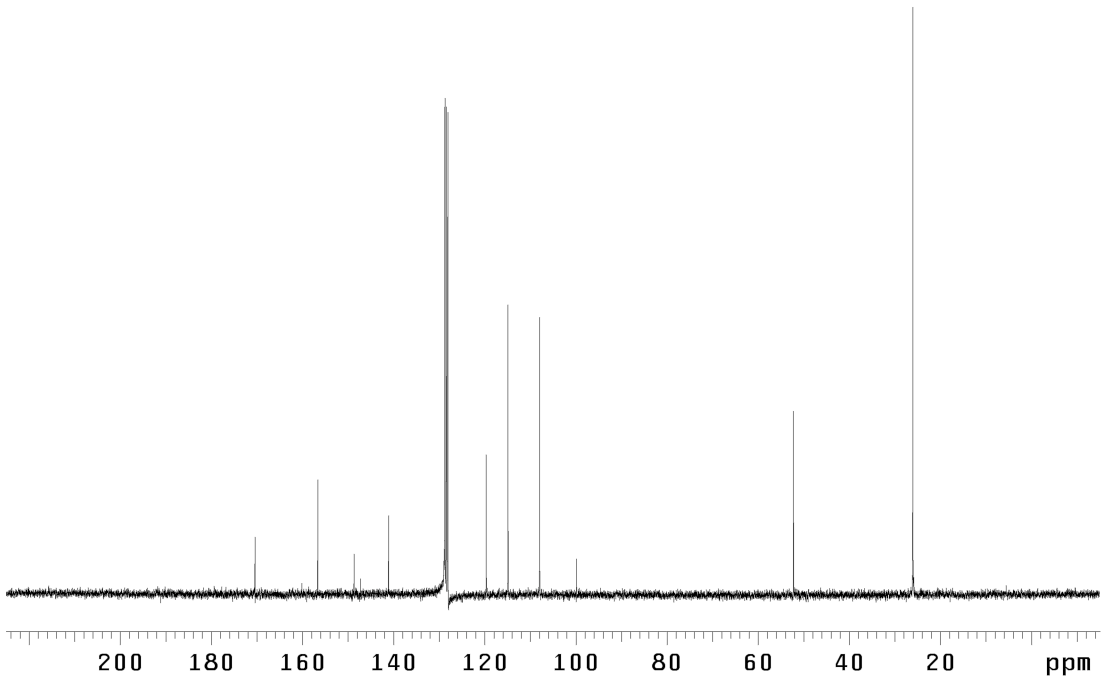


Figure A7.57 ^{13}C NMR (75 MHz, C_6D_6) of compound **350**.

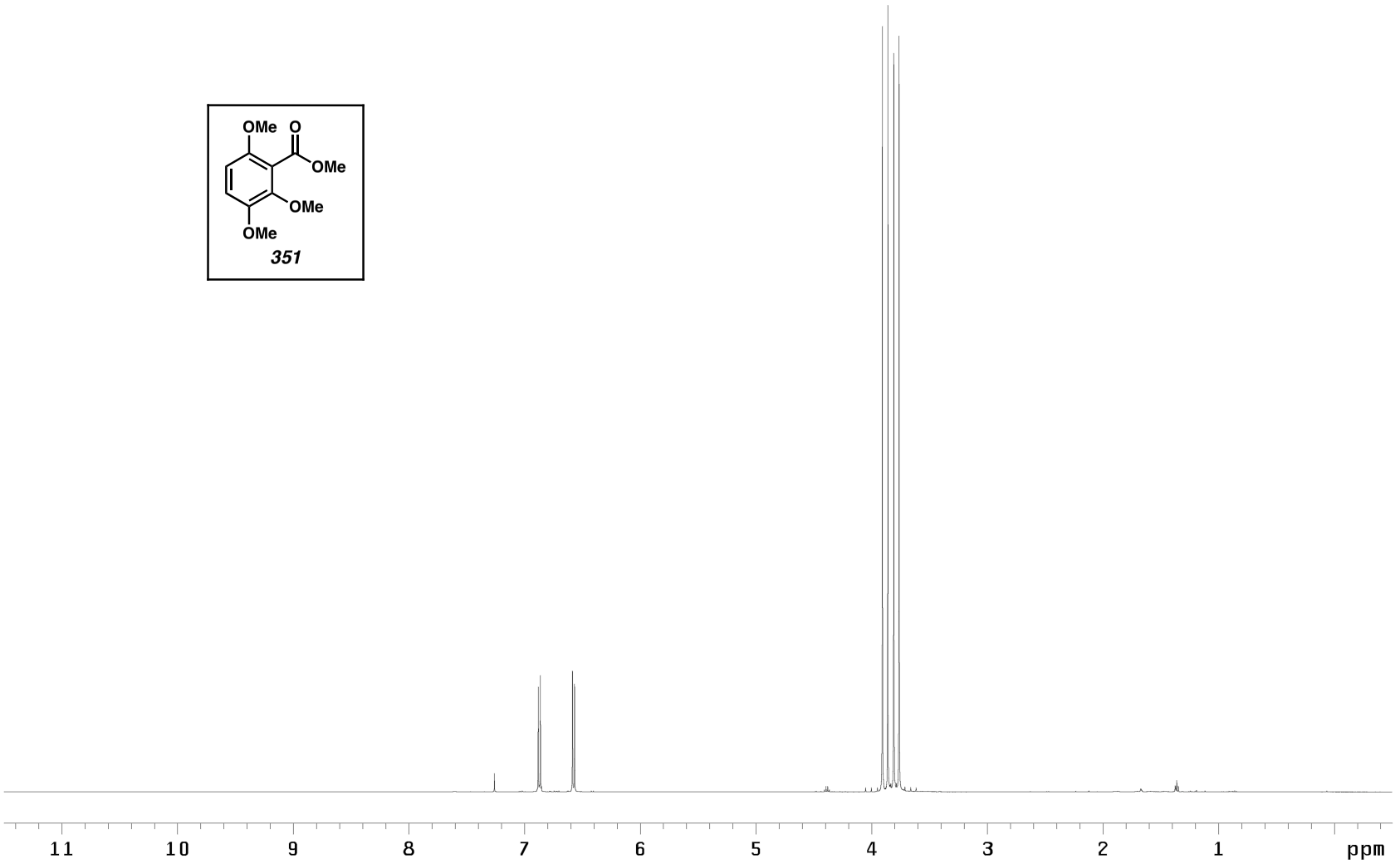


Figure A7.58 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **351**.

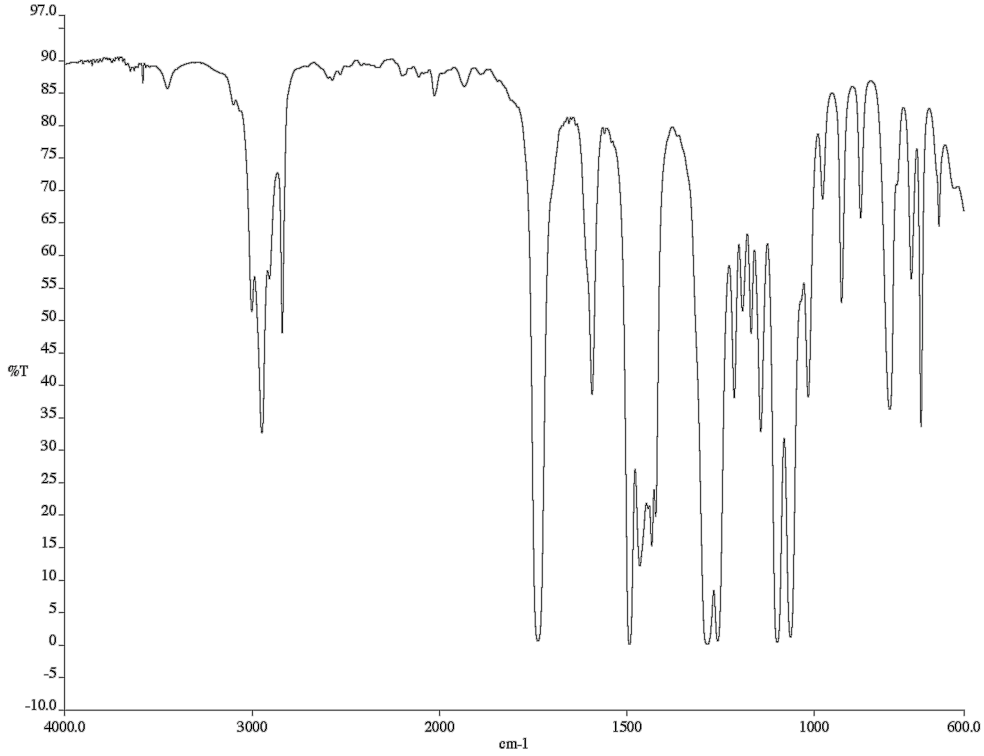


Figure A7.59 Infrared spectrum ($NaCl/CDCl_3$) of compound **351**.

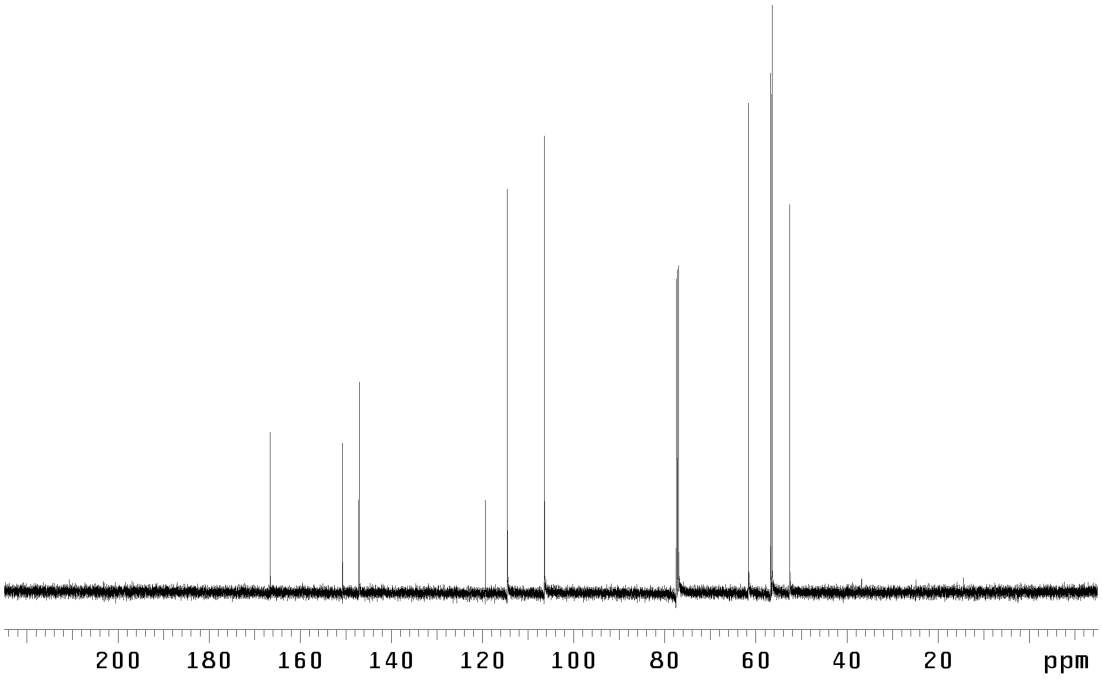


Figure A7.60 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **351**.

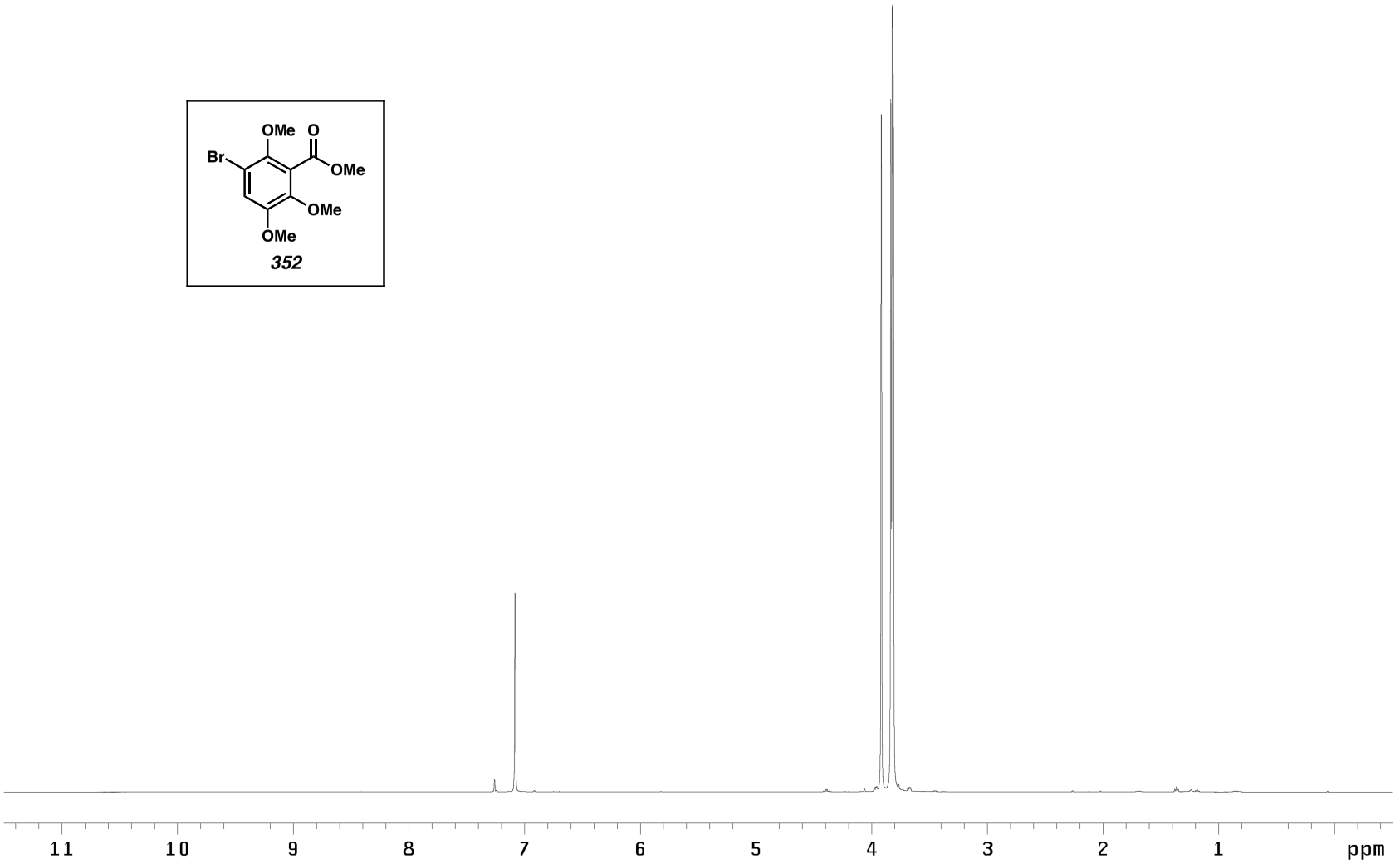


Figure A7.61 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **352**.

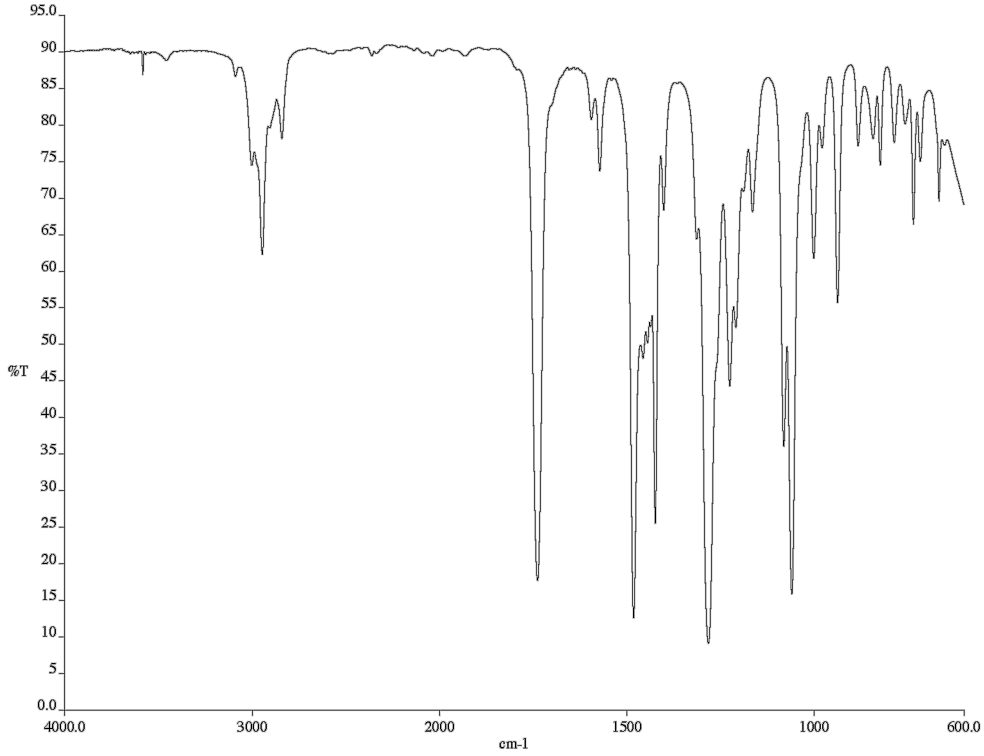


Figure A7.62 Infrared spectrum ($NaCl/CHCl_3$) of compound **352**.

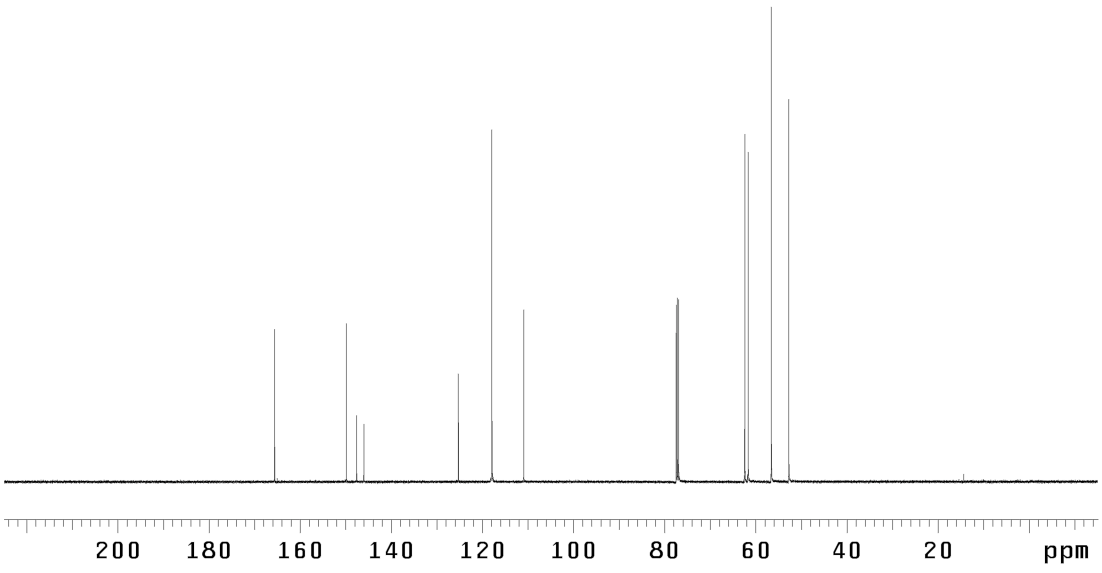


Figure A7.63 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **352**.

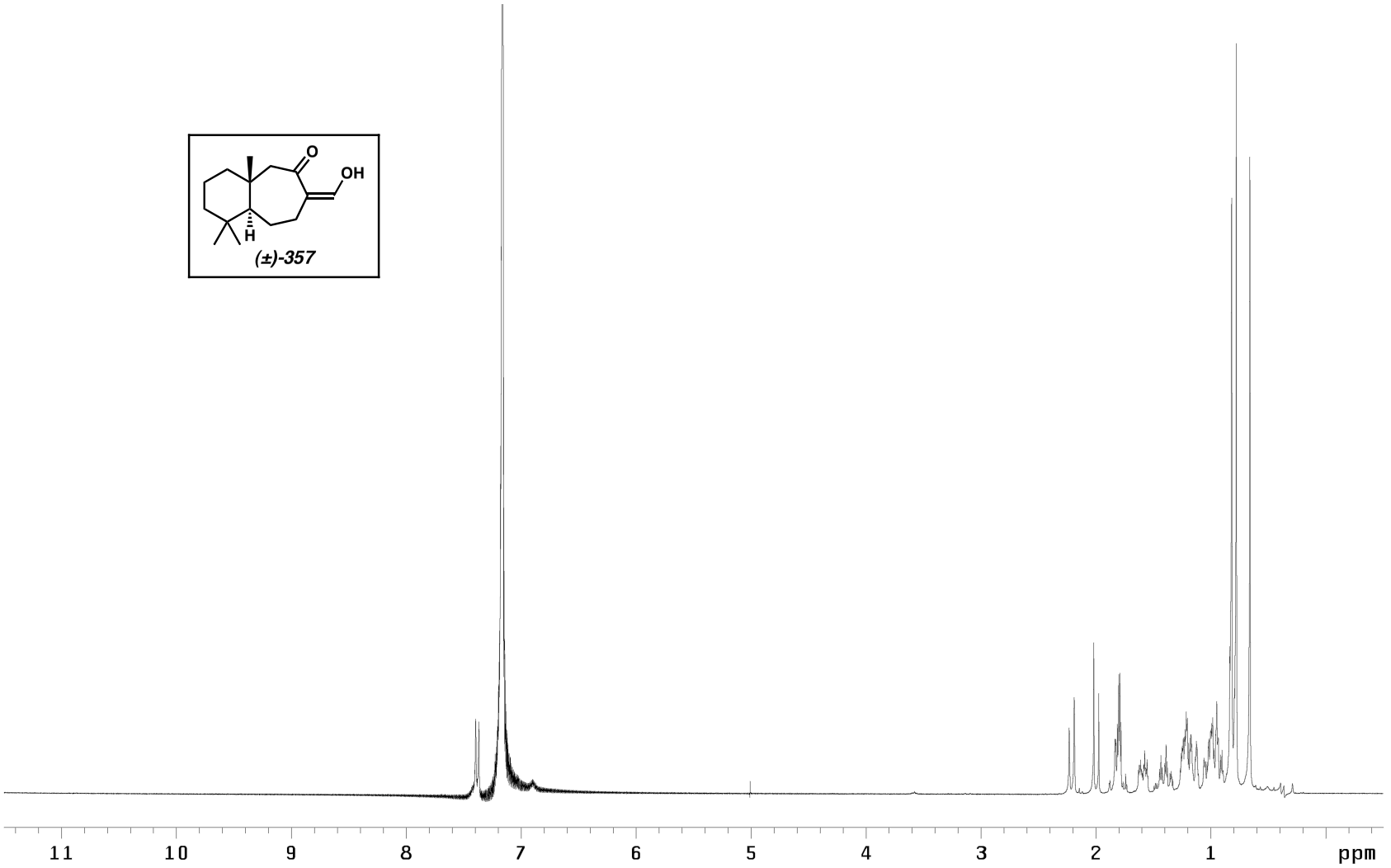


Figure A7.64 ^{1}H NMR (300 MHz, C_6D_6) of compound **357**.

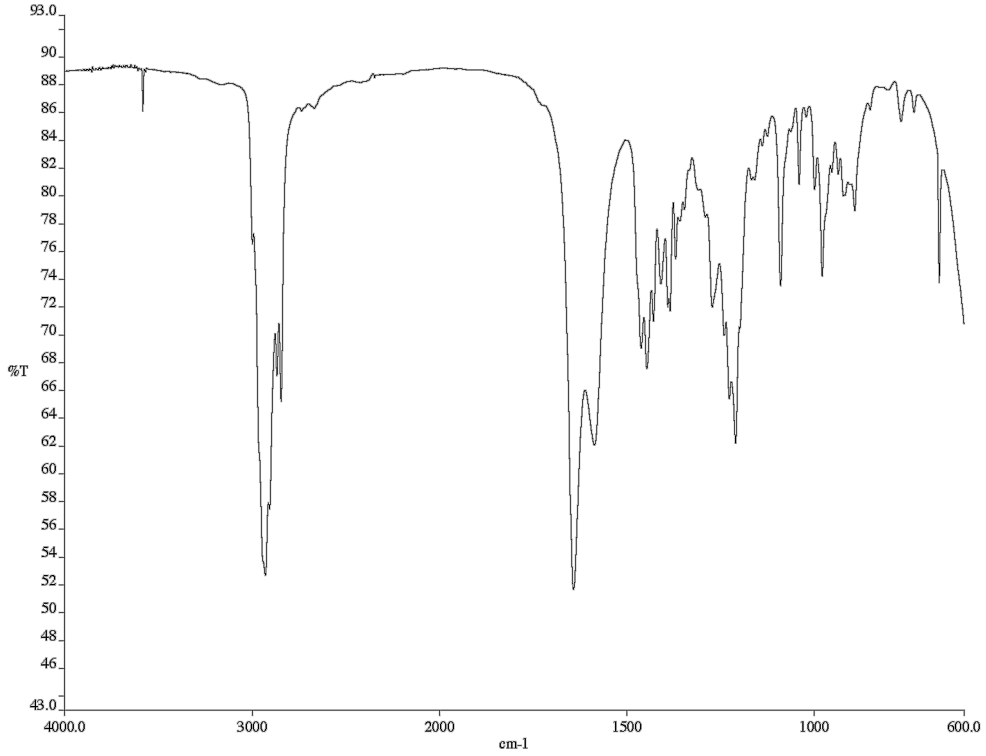


Figure A7.65 Infrared spectrum ($NaCl/CH_2Cl_2$) of compound **357**.

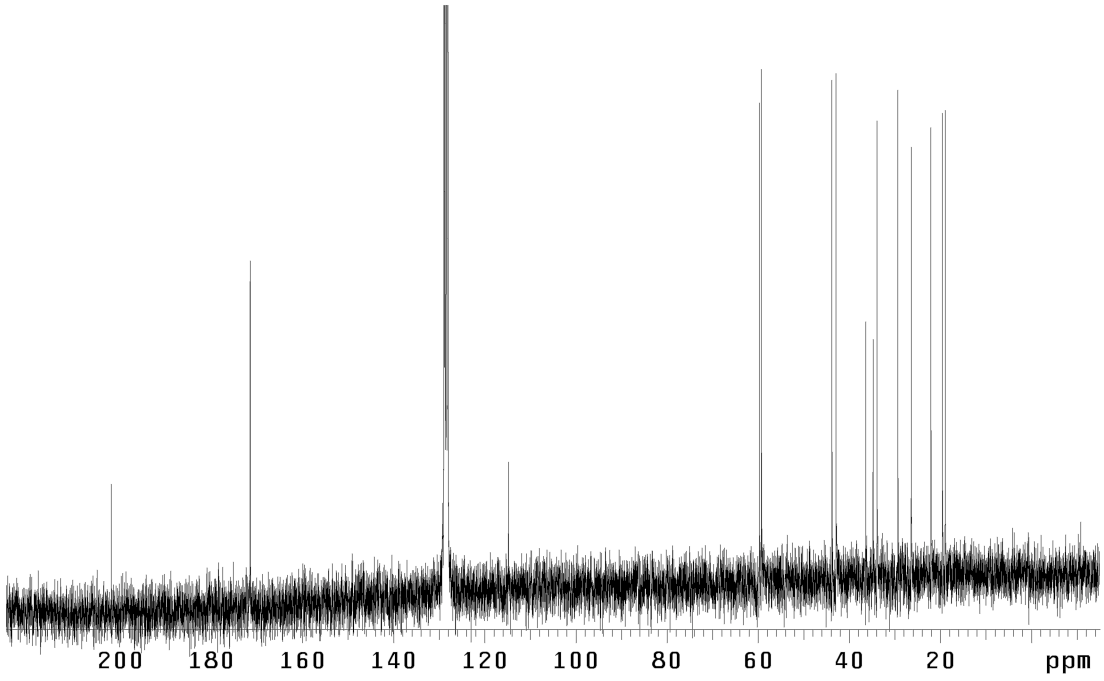


Figure A7.66 ^{13}C NMR (75 MHz, C_6D_6) of compound **357**.

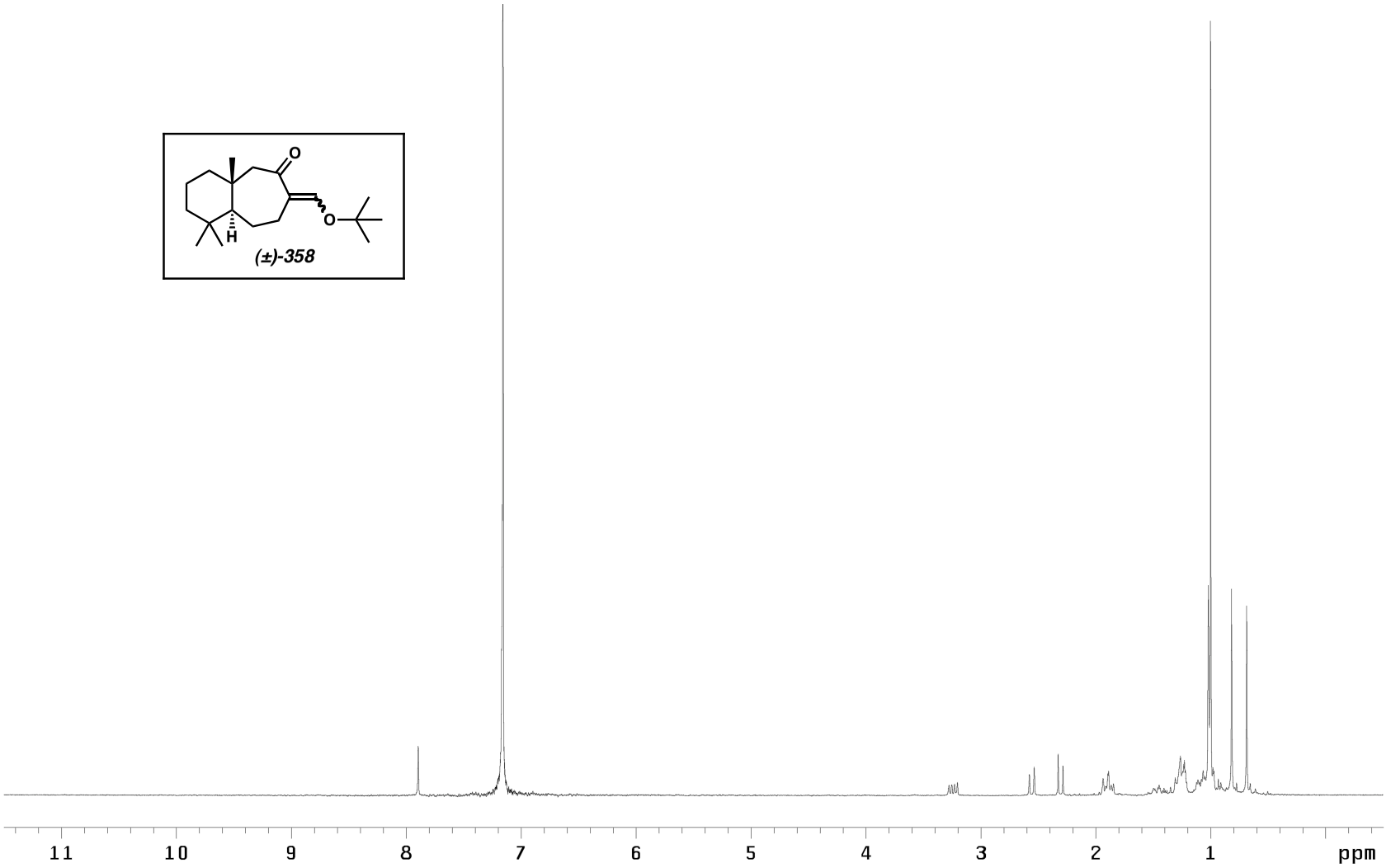


Figure A7.67 ^{1}H NMR (300 MHz, C_6D_6) of compound **358**.

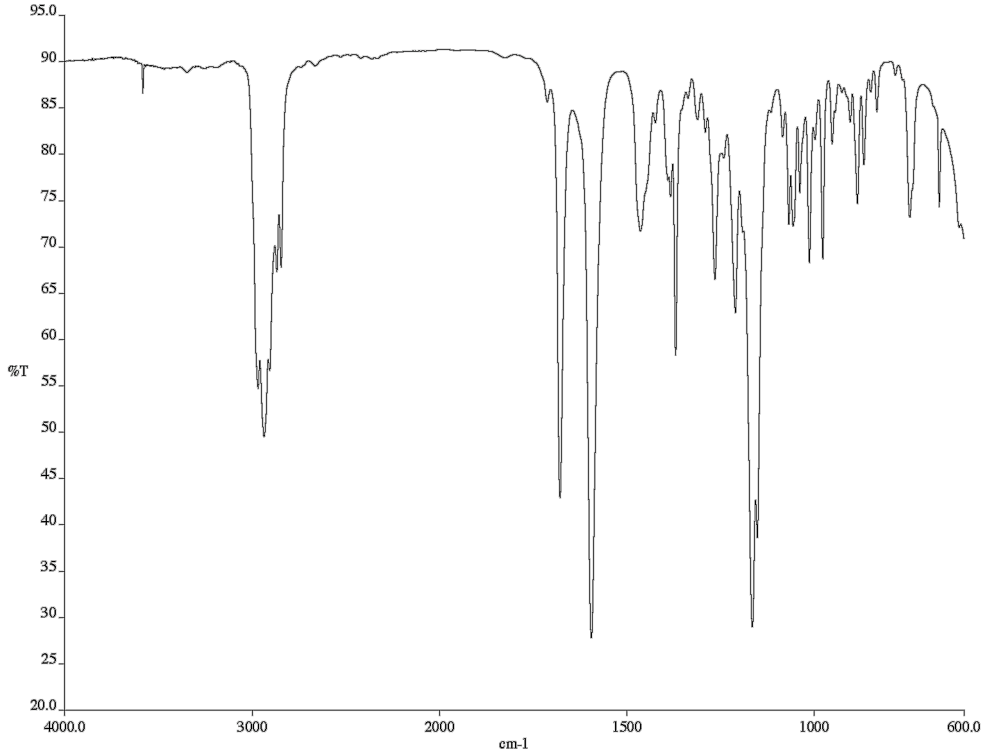


Figure A7.68 Infrared spectrum ($NaCl/CH_2Cl_2$) of compound **358**.

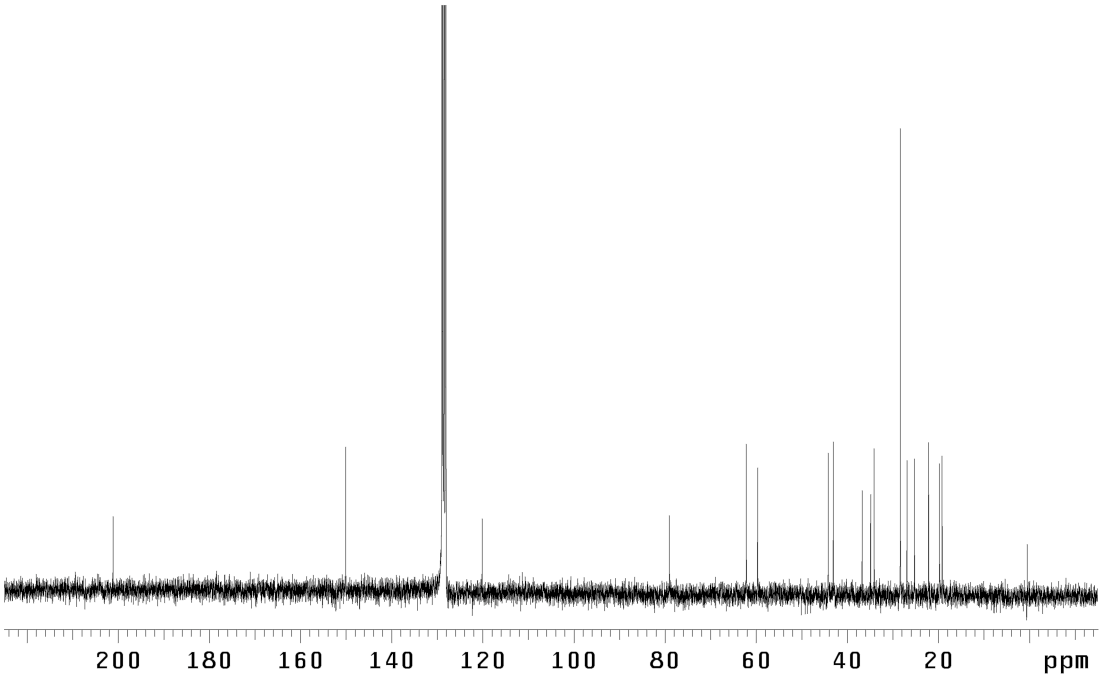


Figure A7.69 ^{13}C NMR (75 MHz, C_6D_6) of compound **358**.

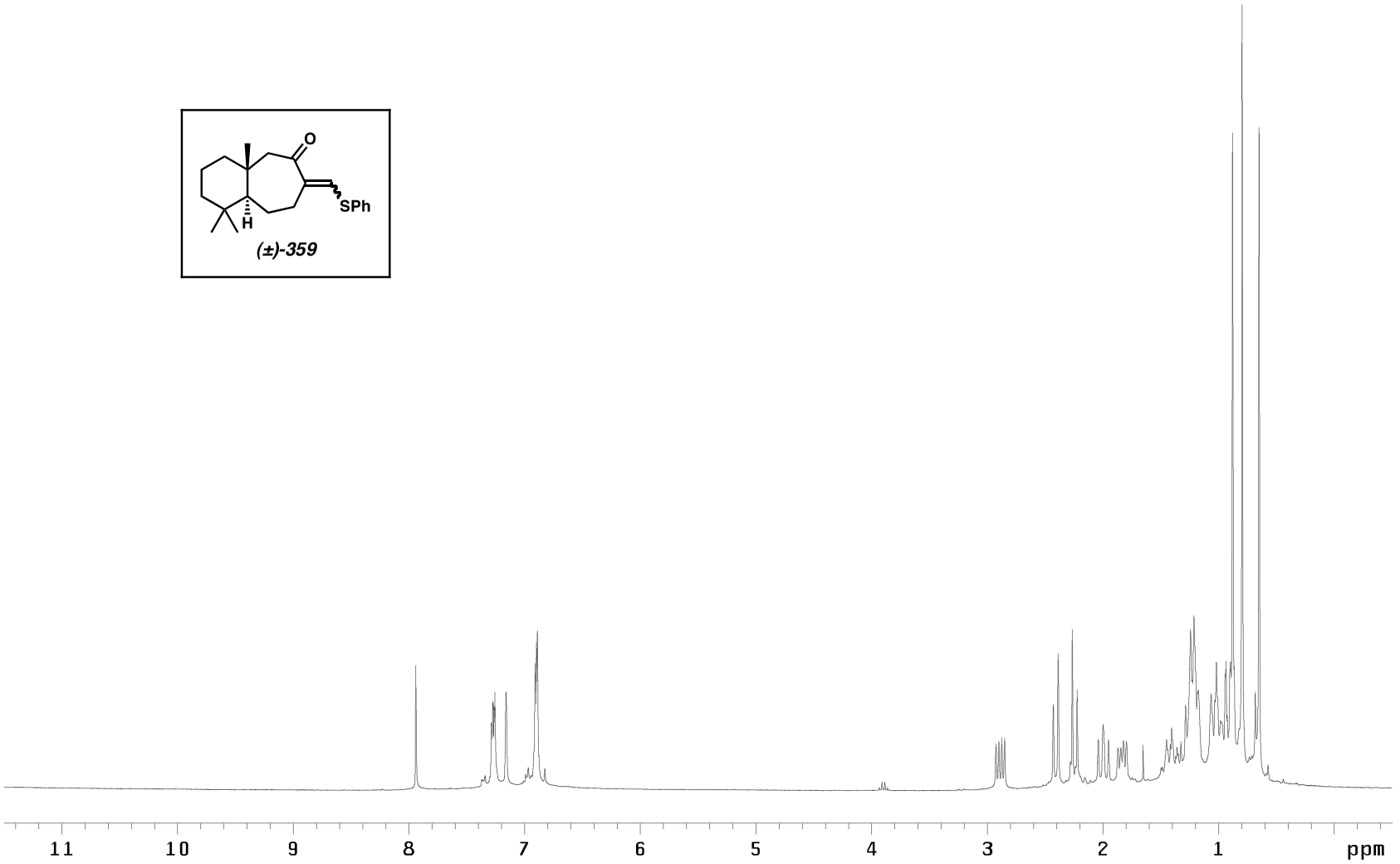


Figure A7.70 ^{1}H NMR (300 MHz, C_6D_6) of compound **359**.

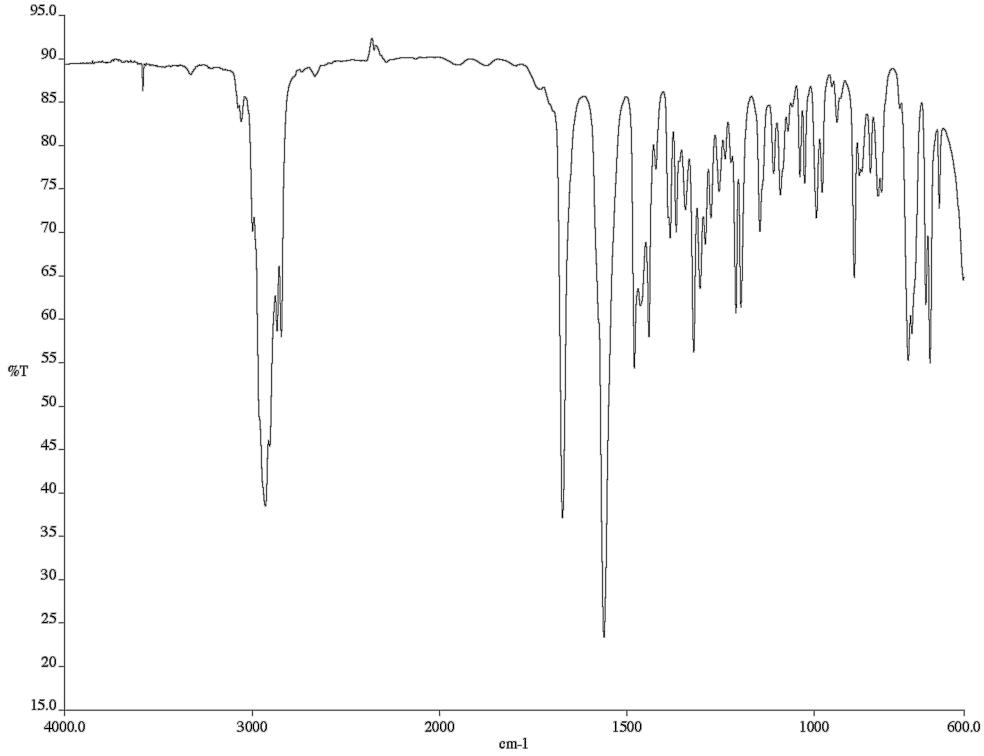


Figure A7.71 Infrared spectrum ($NaCl/CH_2Cl_2$) of compound **359**.

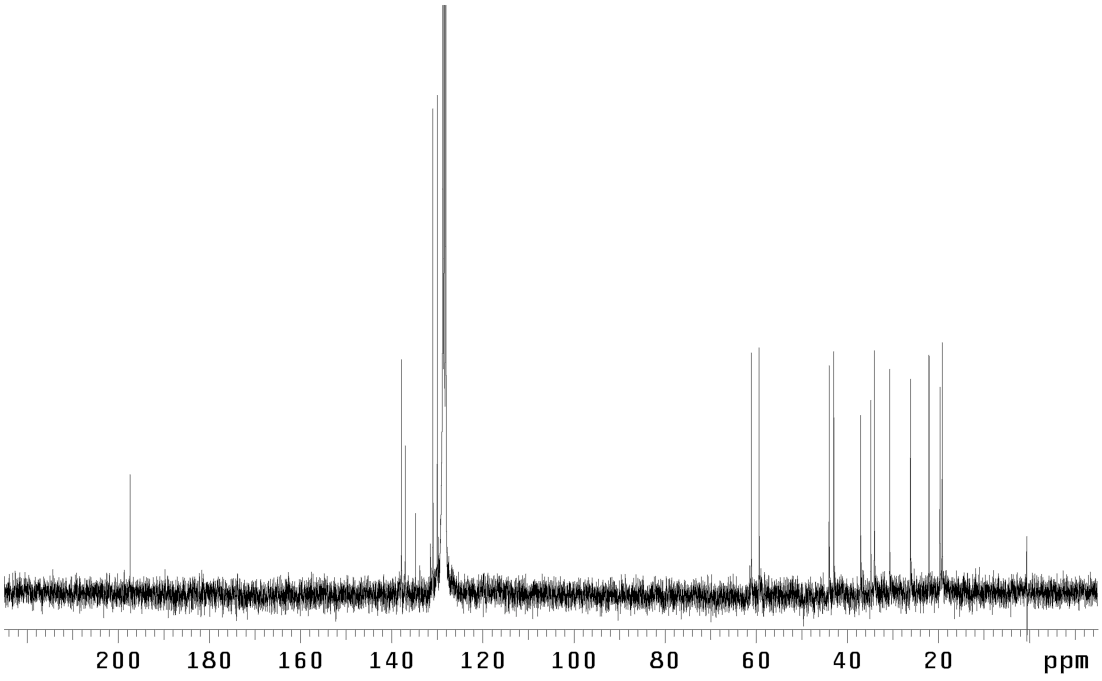


Figure A7.72 ^{13}C NMR (75 MHz, C_6D_6) of compound **359**.

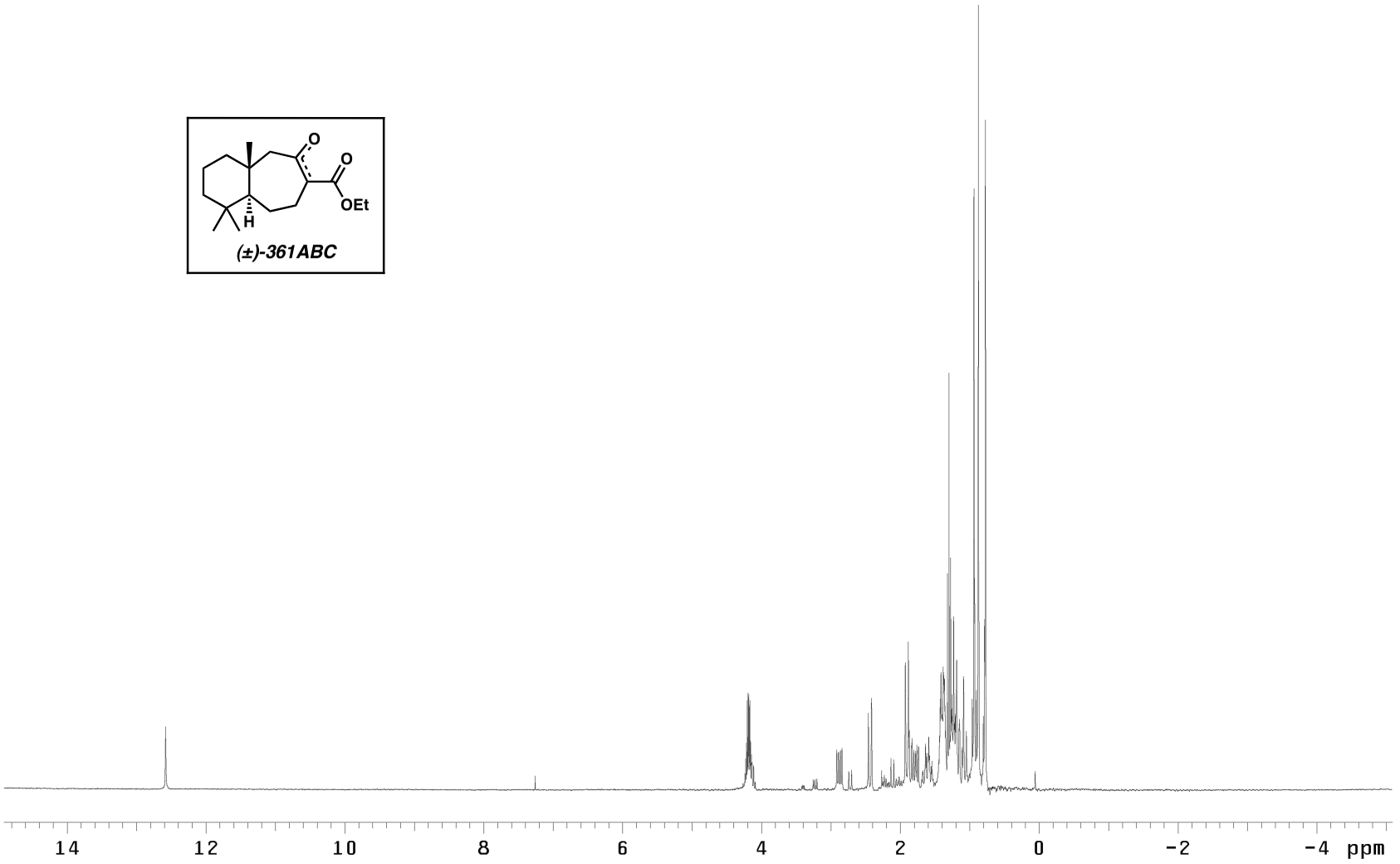


Figure A7.73 ^{1}H NMR (300 MHz, $CDCl_3$) of compounds **361A**, **361B**, and **361C**.

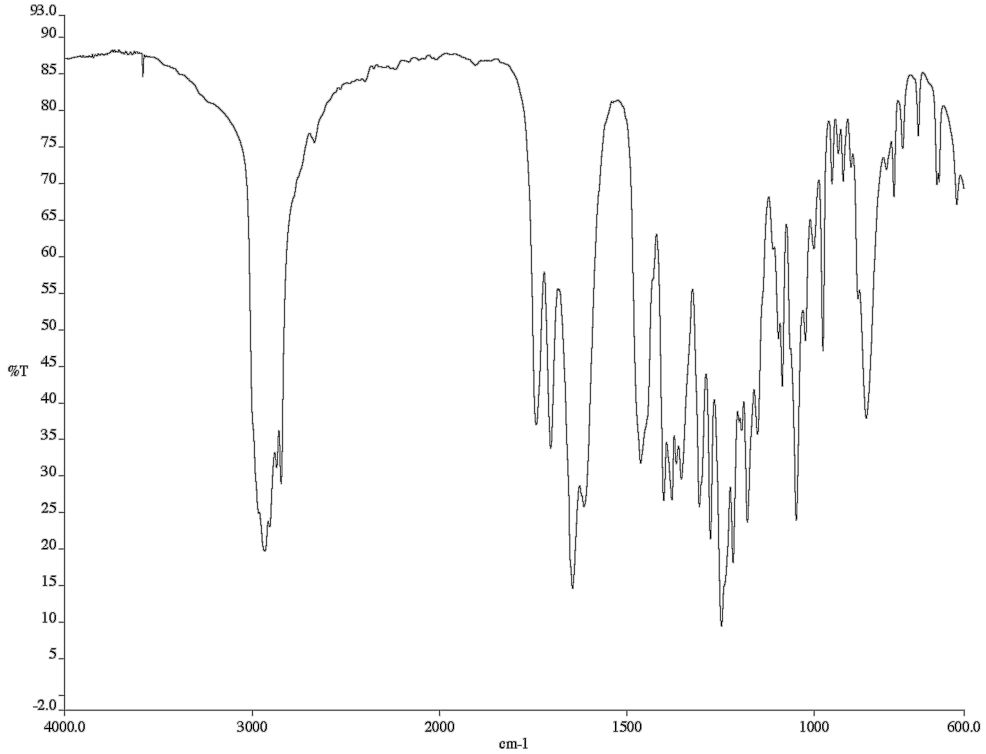


Figure A7.74 Infrared spectrum ($NaCl/CDCl_3$) of compounds **361A**, **361B**, and **361C**.

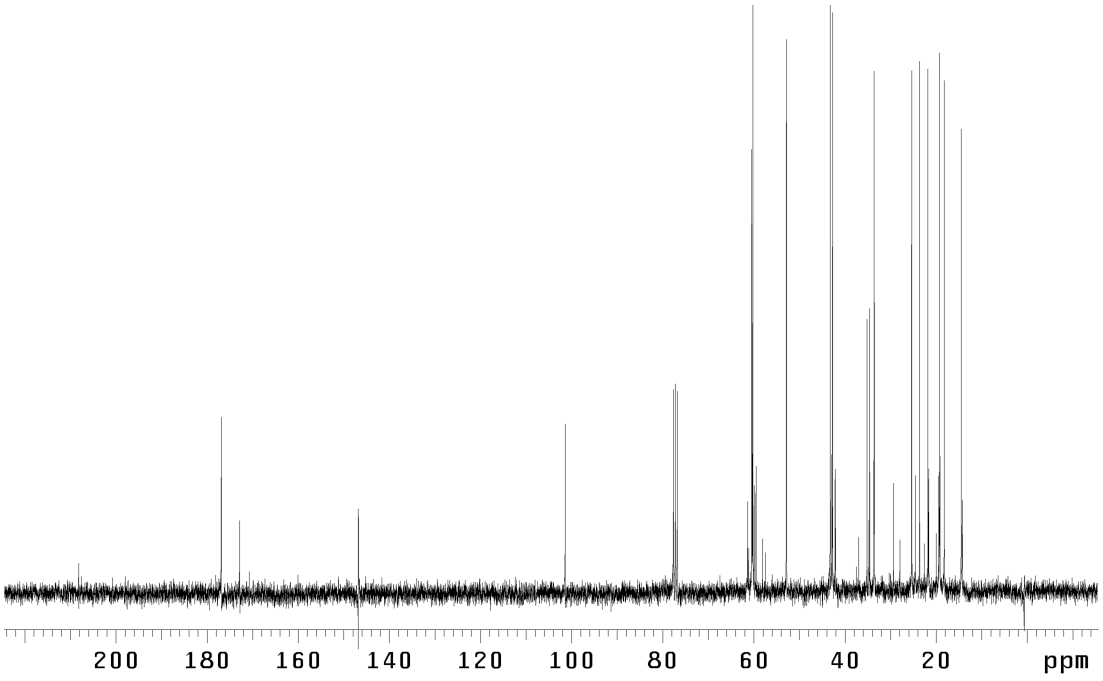


Figure A7.75 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **361A**, **361B**, and **361C**.

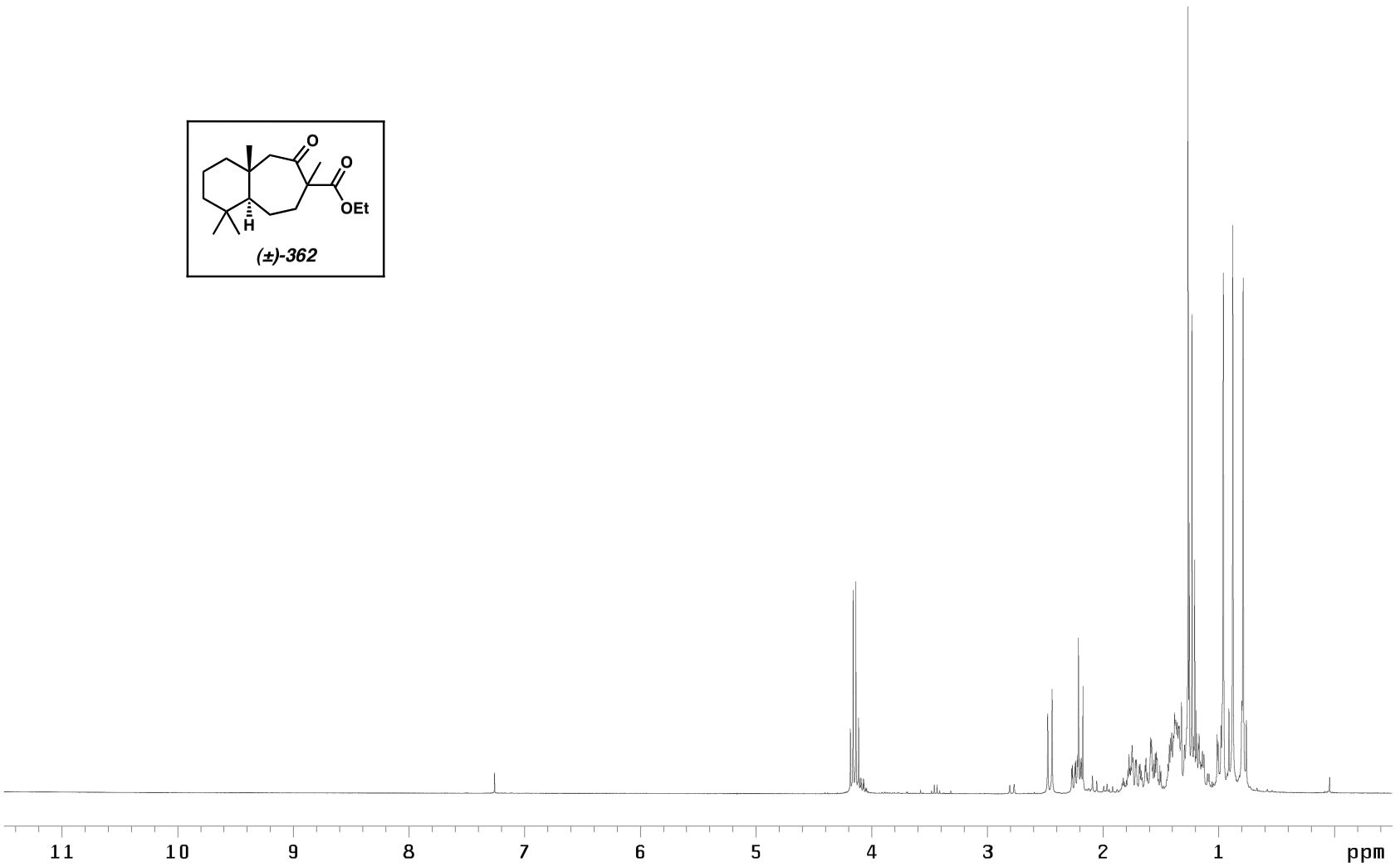


Figure A7.76 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **362**.

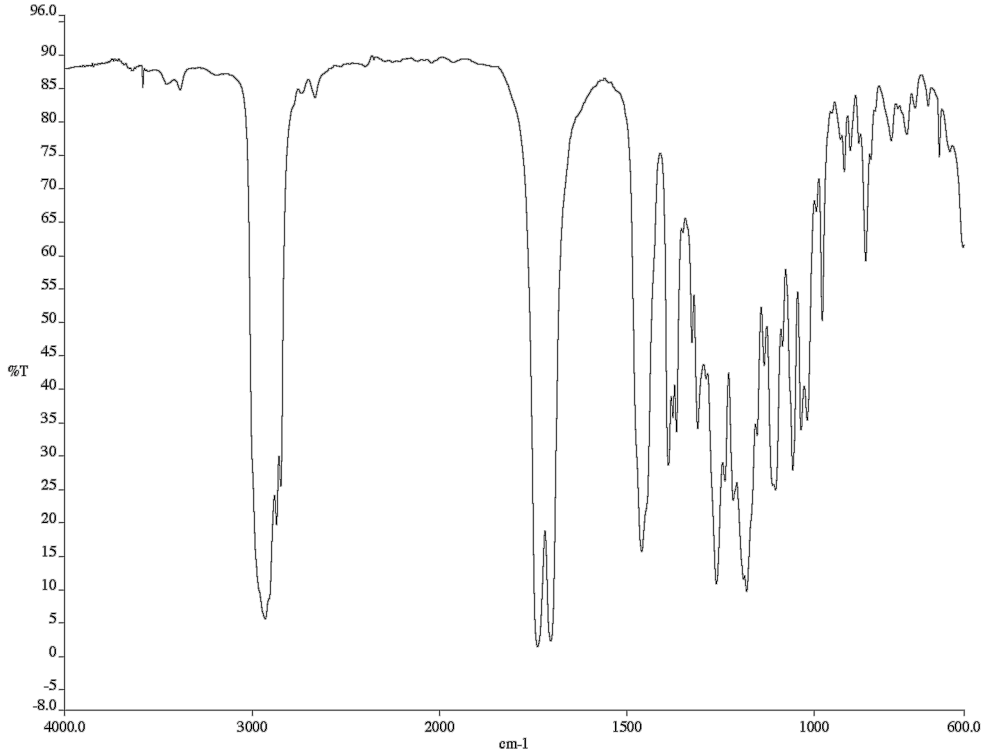


Figure A7.77 Infrared spectrum ($NaCl/CDCl_3$) of compound **362**.

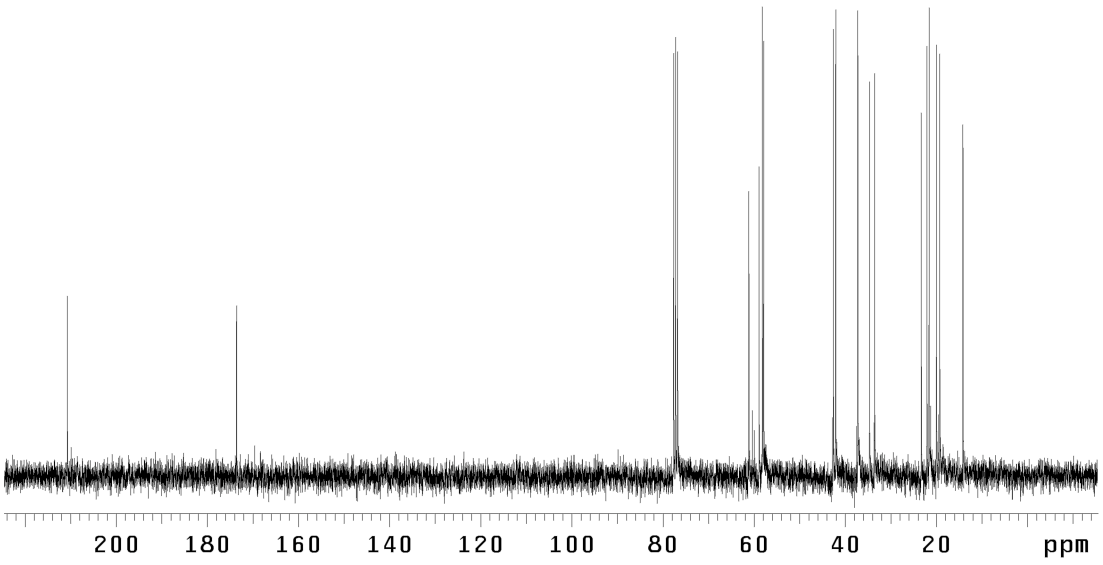


Figure A7.78 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **362**.

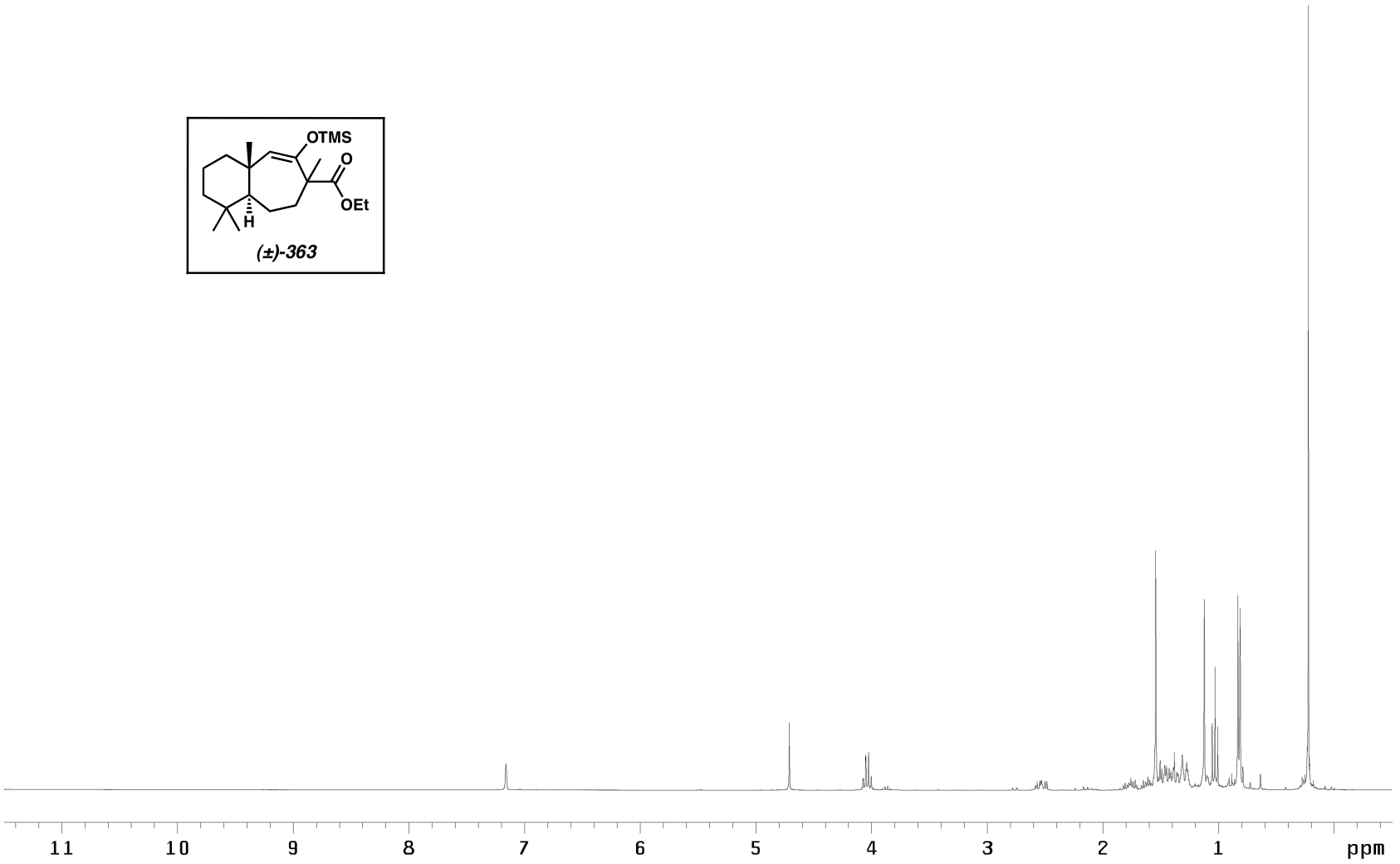


Figure A7.79 ^{1}H NMR (300 MHz, C_6D_6) of compound **363**.

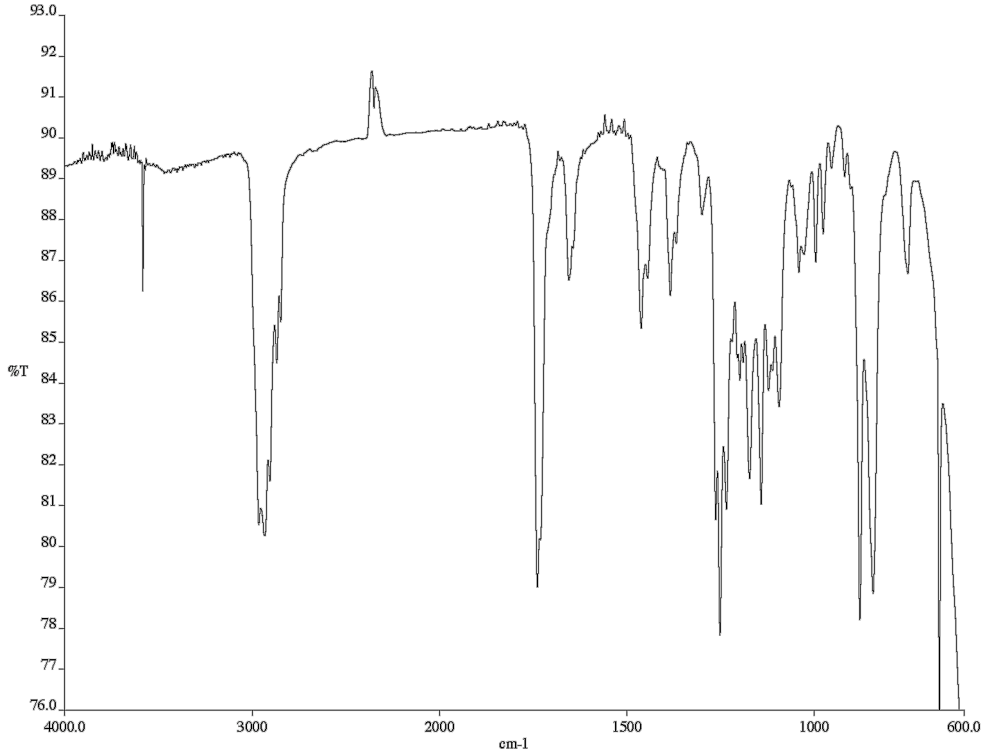


Figure A7.80 Infrared spectrum ($NaCl/CH_2Cl_2$) of compound **363**.

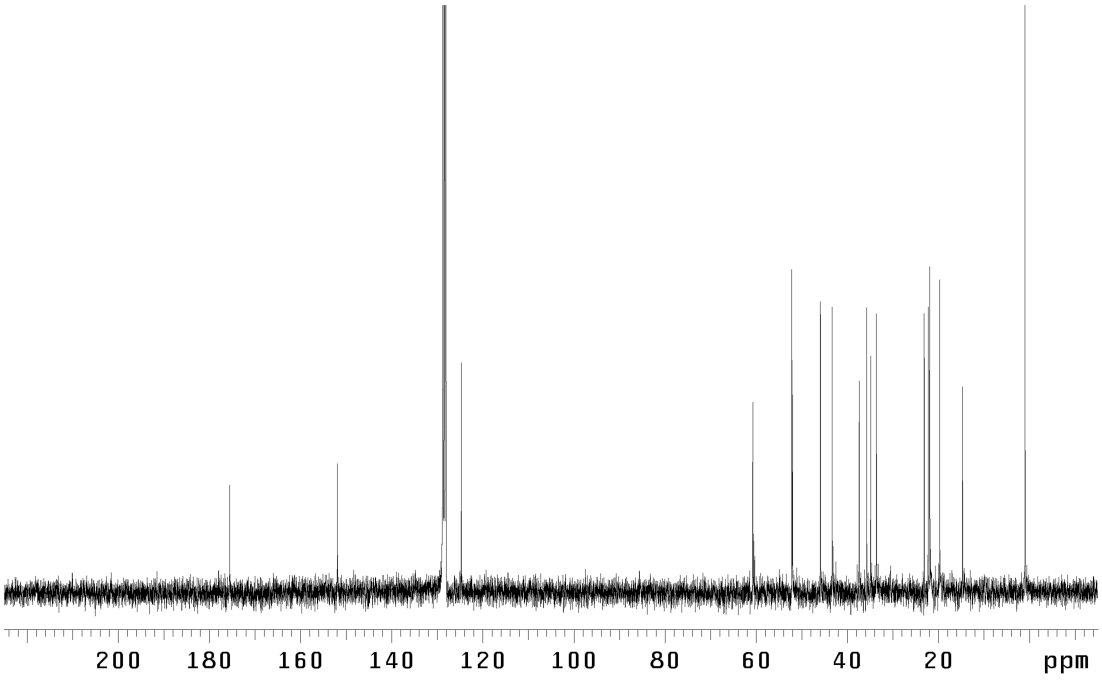


Figure A7.81 ^{13}C NMR (75 MHz, C_6D_6) of compound **363**.

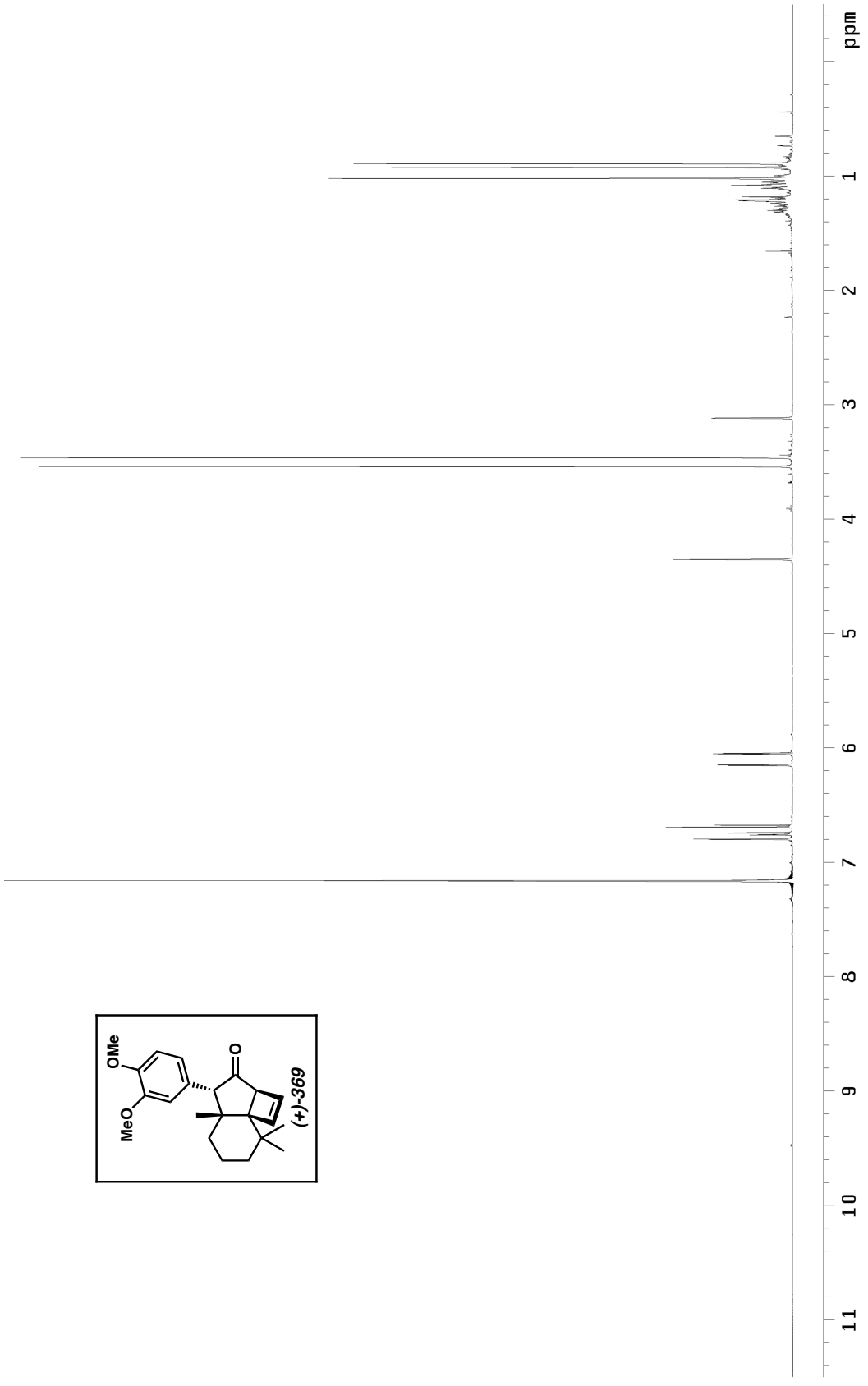


Figure A7.82 ^{1}H NMR (500 MHz, C_6D_6) of compound **369**.

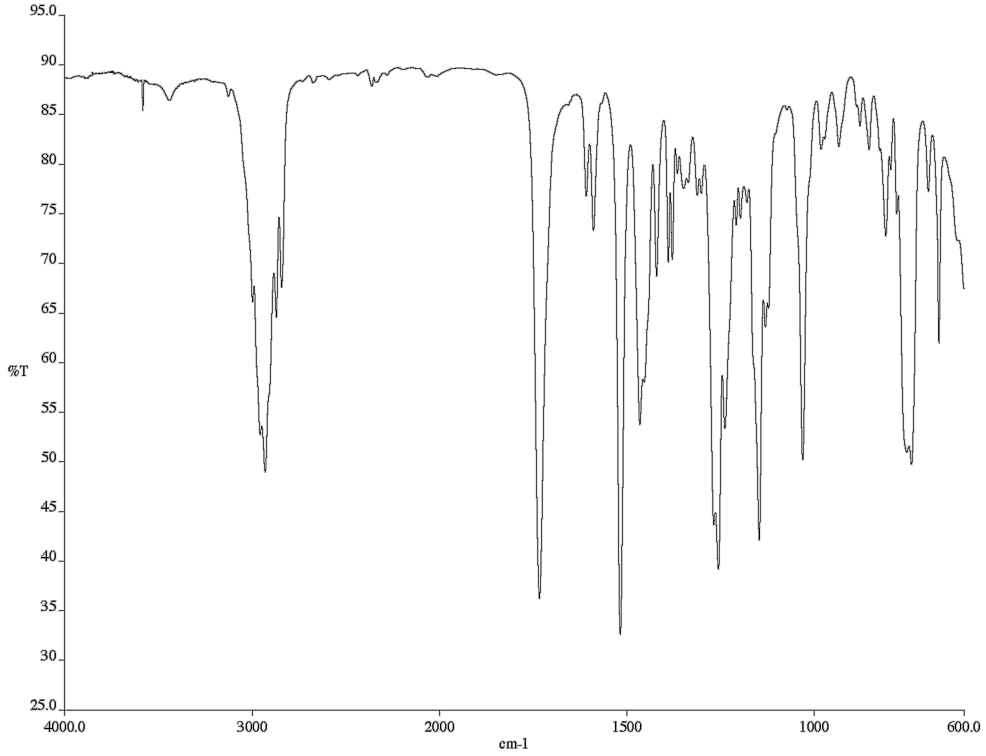


Figure A7.83 Infrared spectrum ($NaCl/CHCl_3$) of compound **369**.

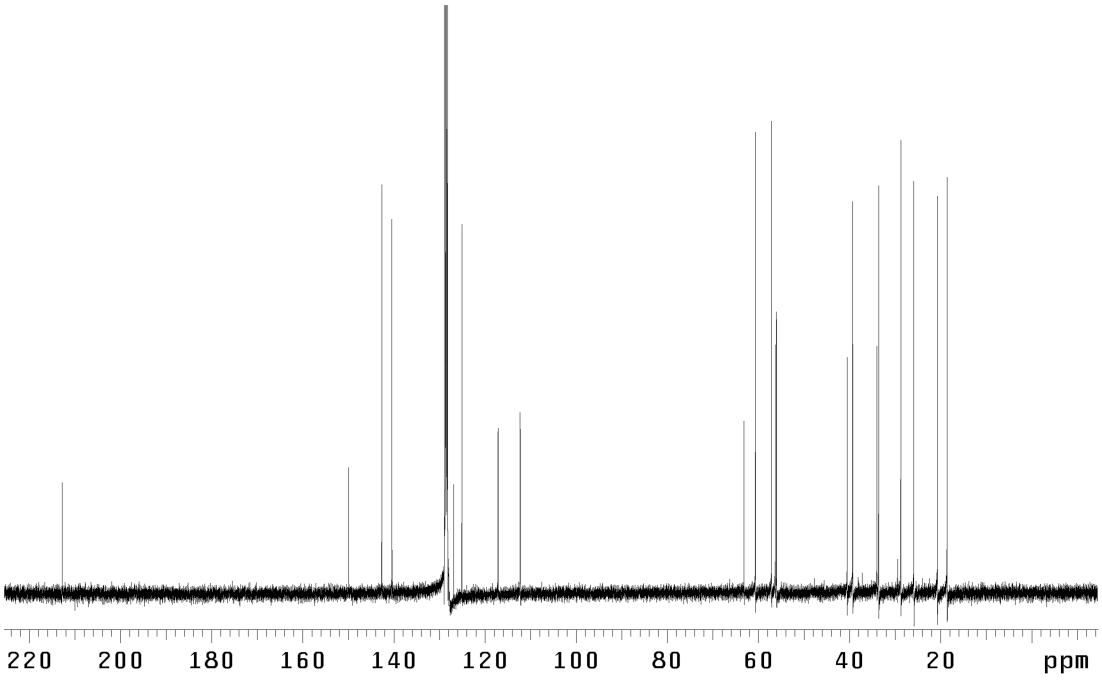


Figure A7.84 ^{13}C NMR (125 MHz, C_6D_6) of compound **369**.

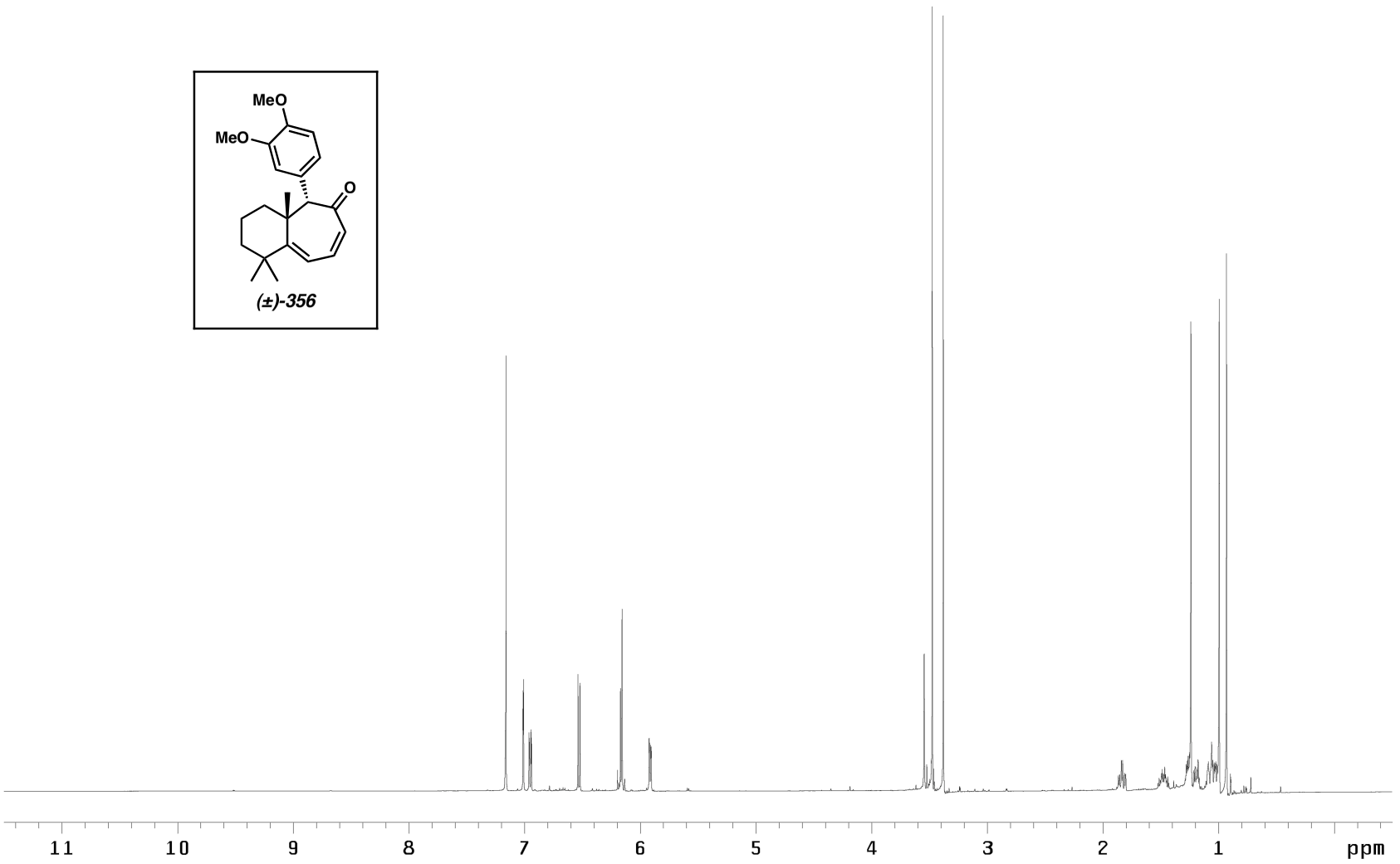


Figure A7.85 ^{1}H NMR (500 MHz, C_6D_6) of compound **356**.

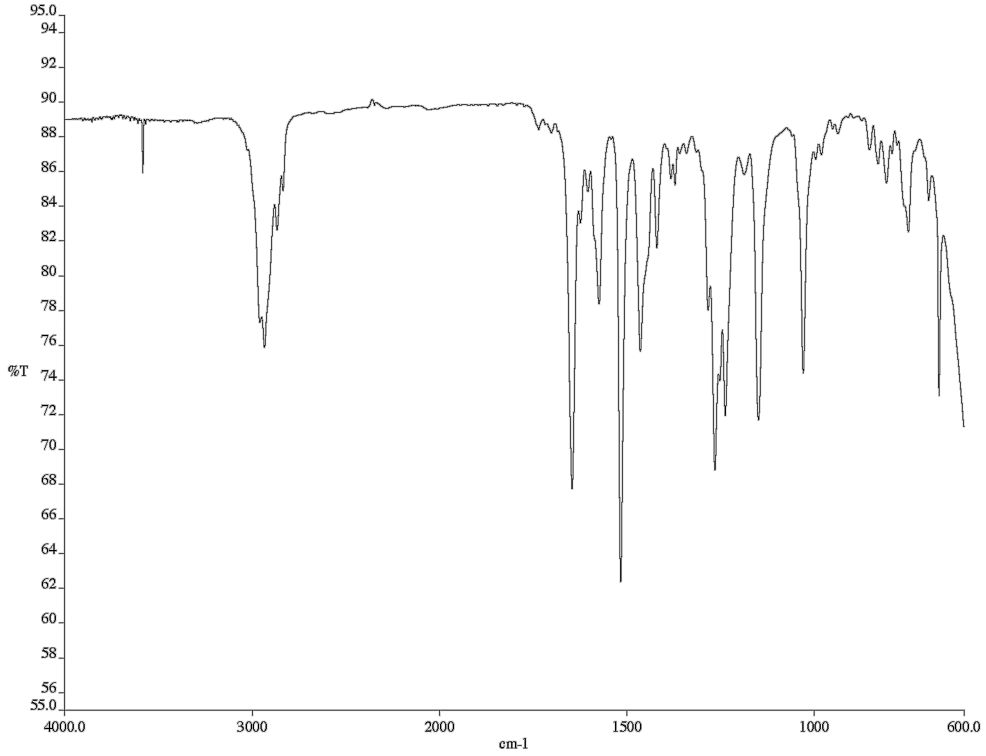


Figure A7.86 Infrared spectrum ($NaCl/CHCl_3$) of compound **356**.

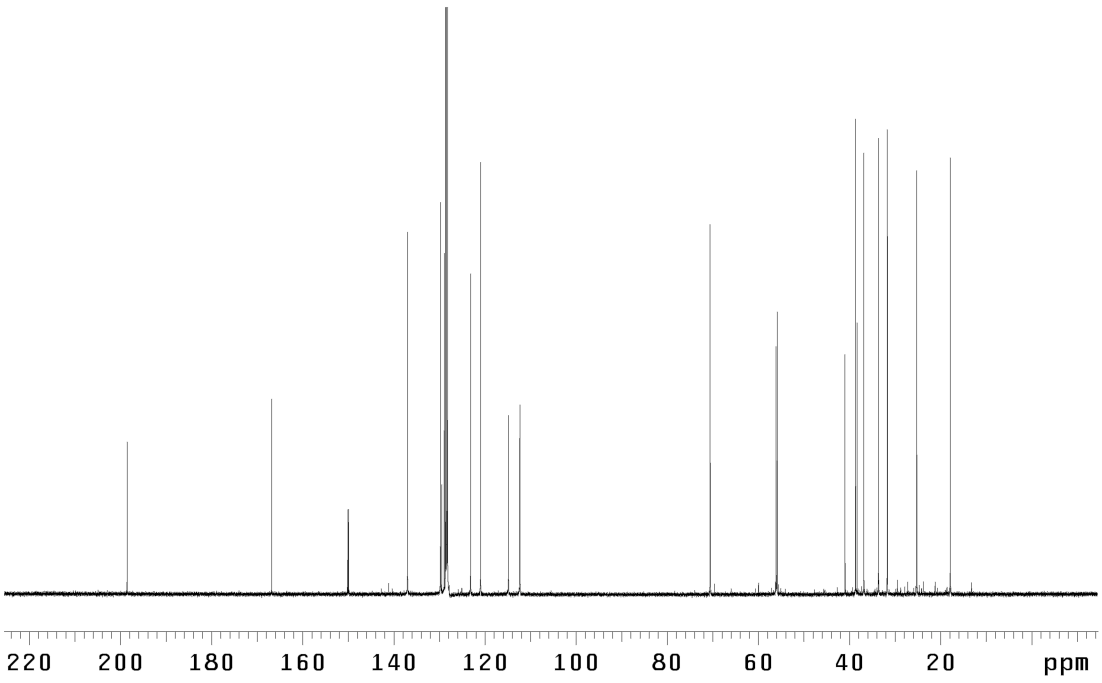


Figure A7.87 ^{13}C NMR (125 MHz, C_6D_6) of compound **356**.

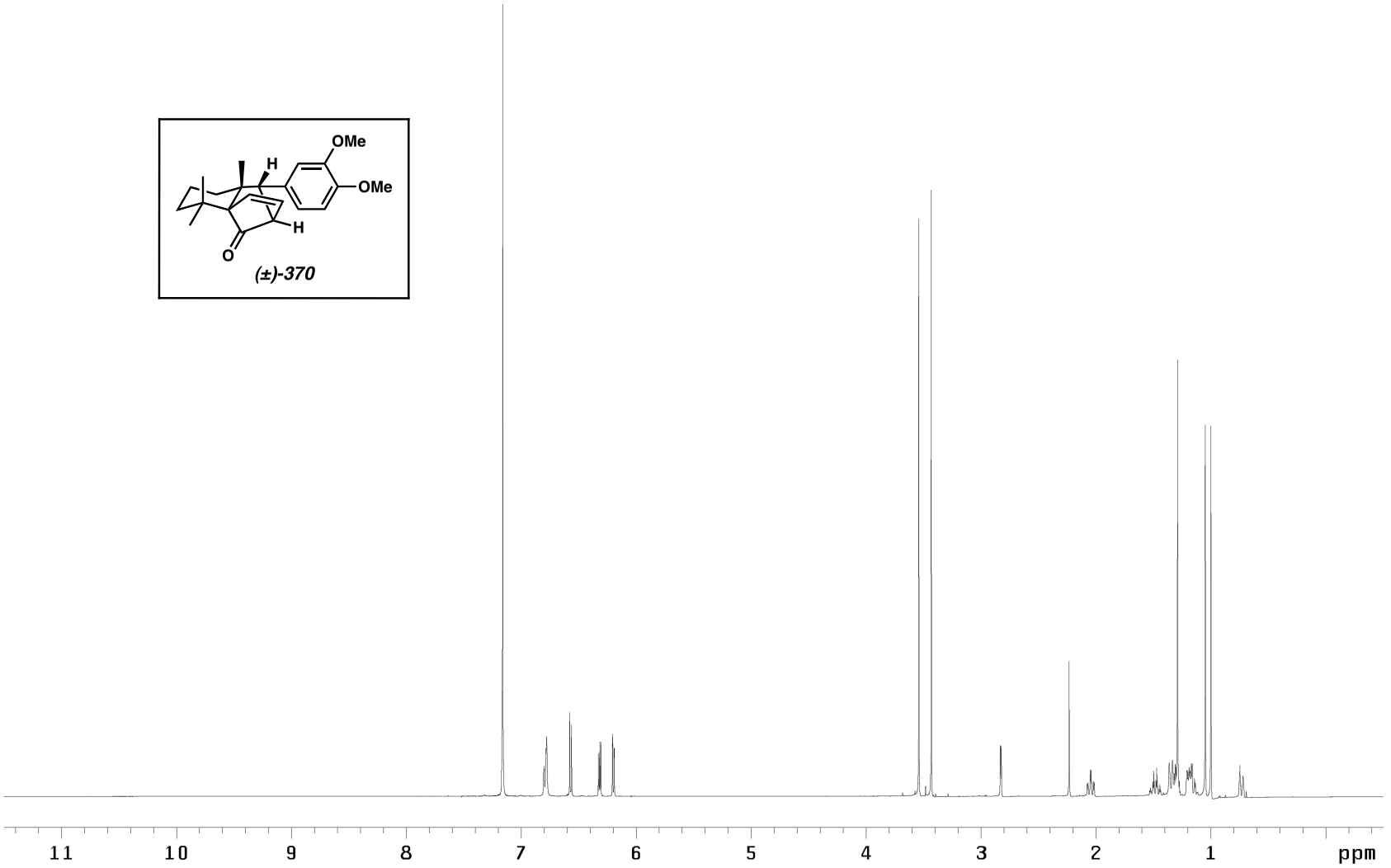


Figure A7.88 ^{1}H NMR (500 MHz, C_6D_6) of compound **370**.

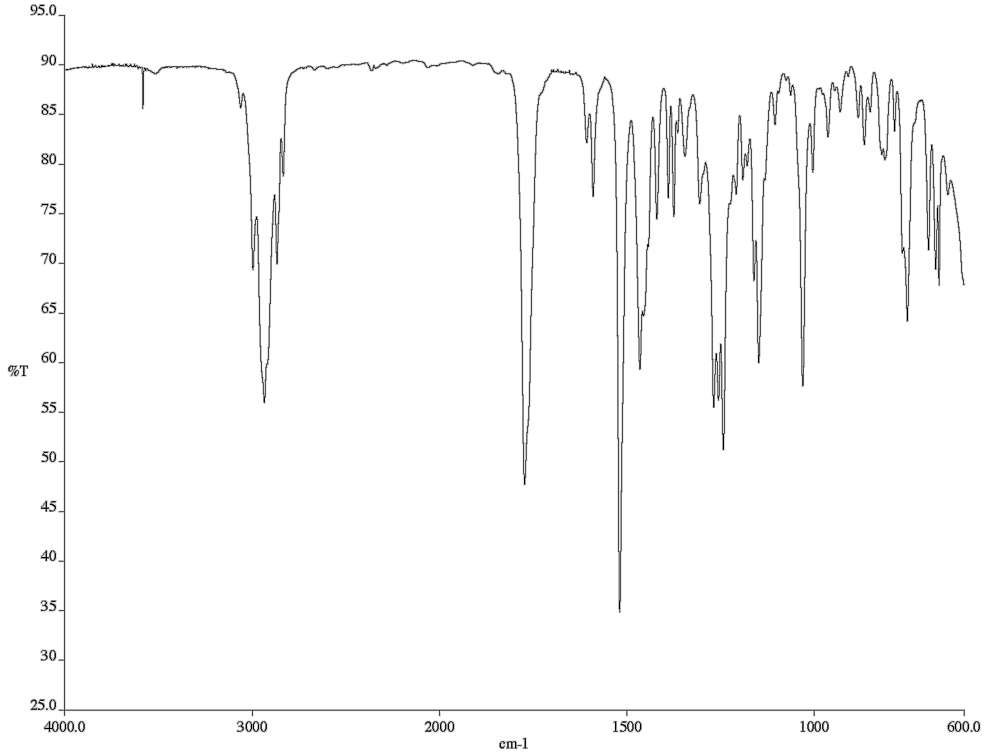


Figure A7.89 Infrared spectrum ($NaCl/CHCl_3$) of compound **370**.

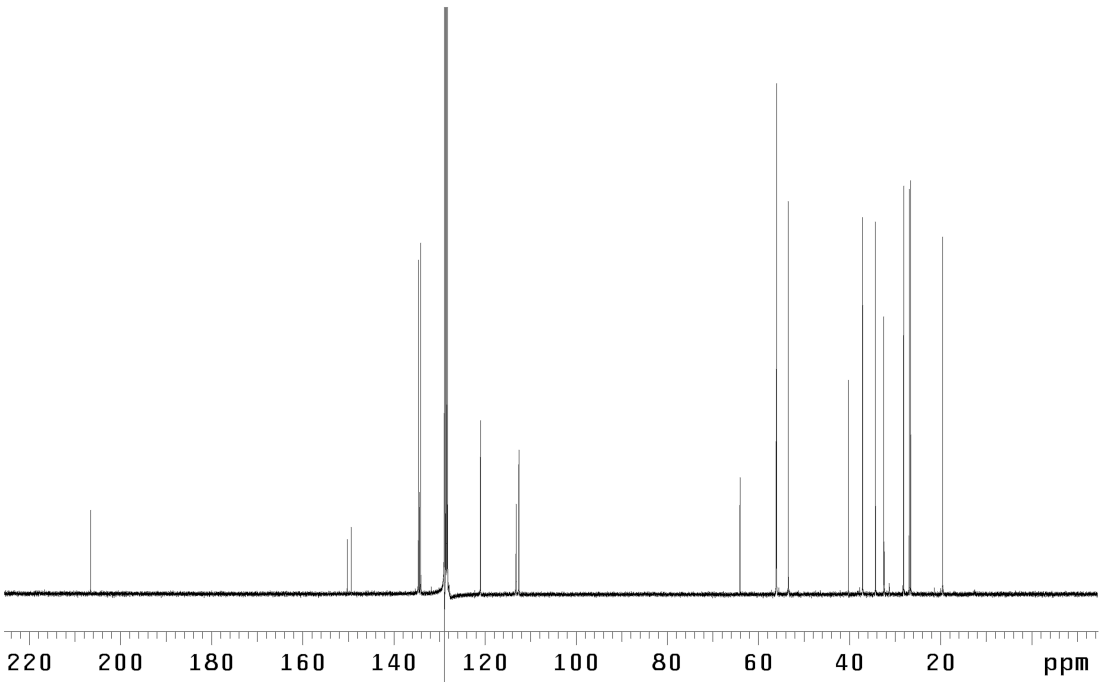


Figure A7.90 ^{13}C NMR (125 MHz, C_6D_6) of compound **370**.

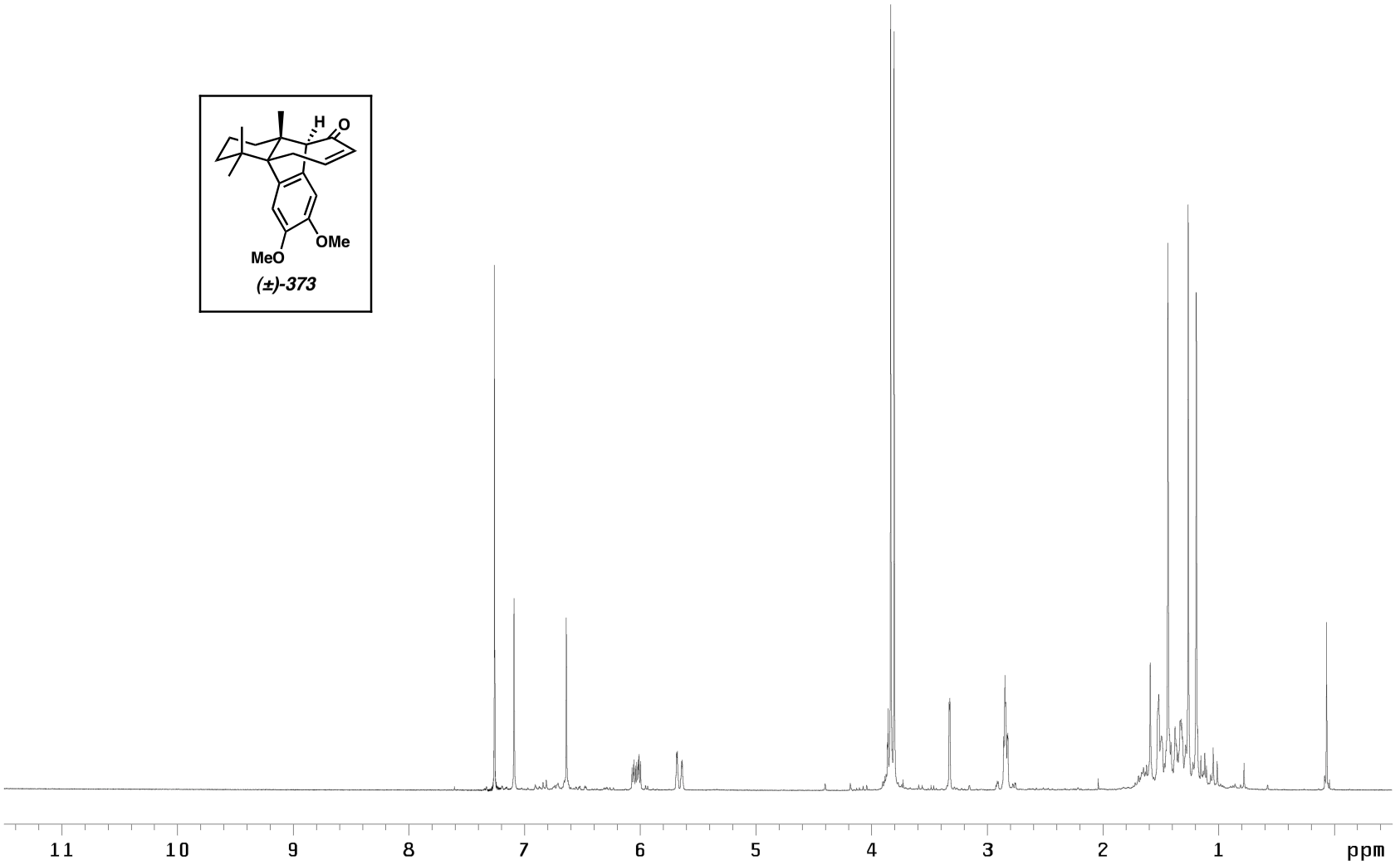


Figure A7.91 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **373**.

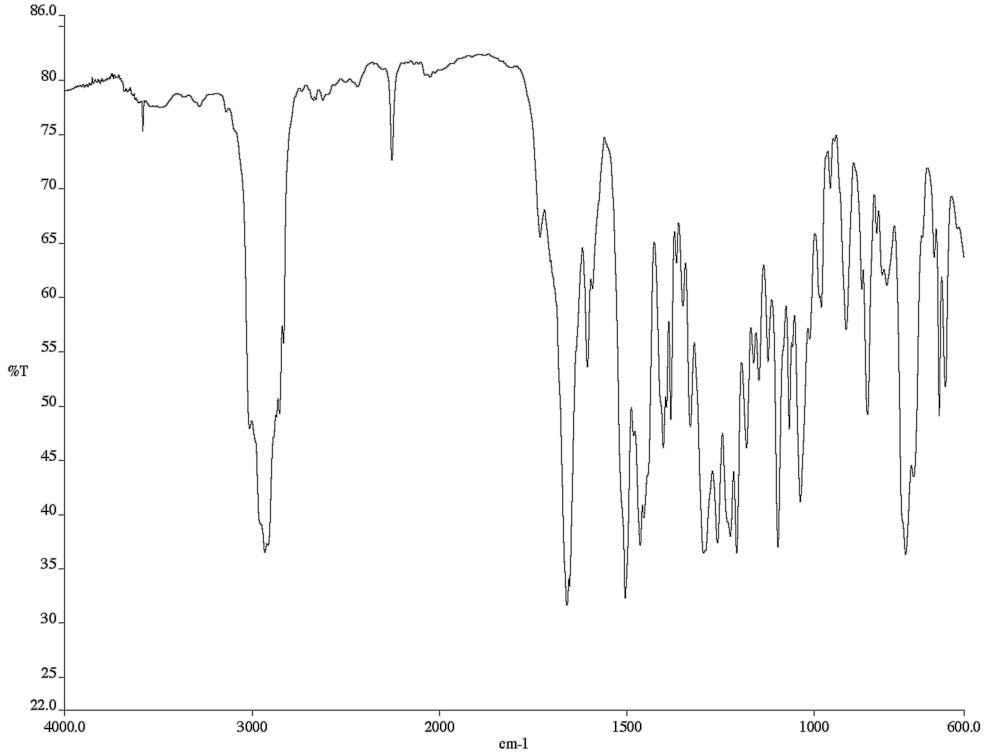


Figure A7.92 Infrared spectrum ($NaCl/CDCl_3$) of compound **373**.

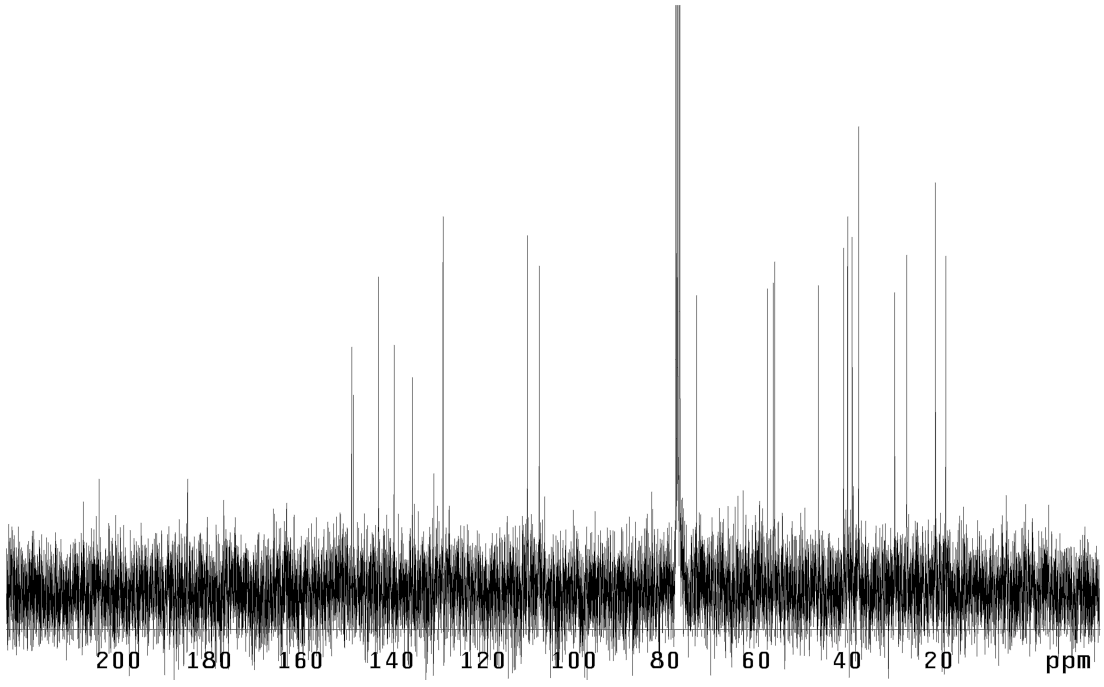


Figure A7.93 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **373**.

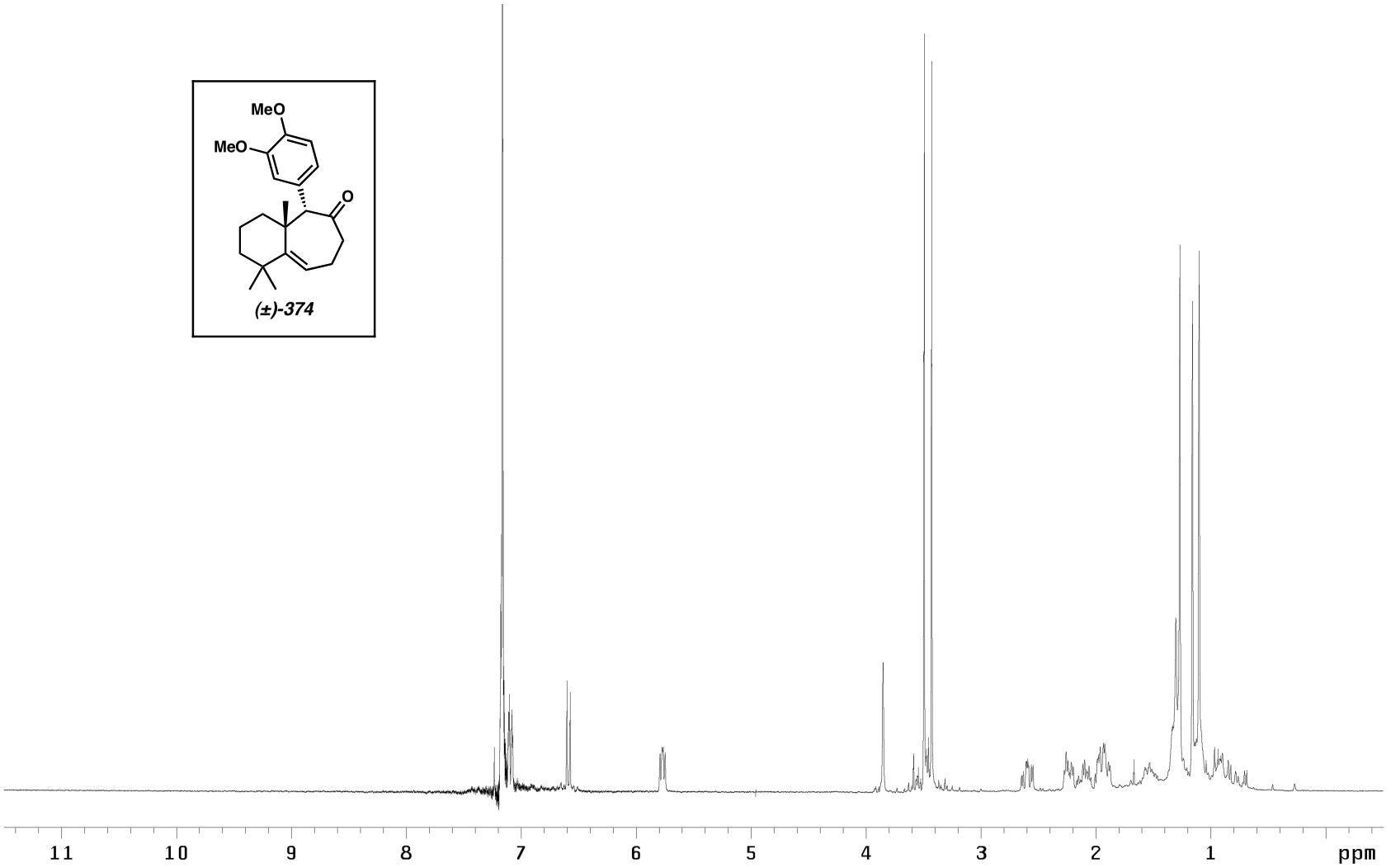


Figure A7.94 ^{1}H NMR (300 MHz, C_6D_6) of compound **374**.

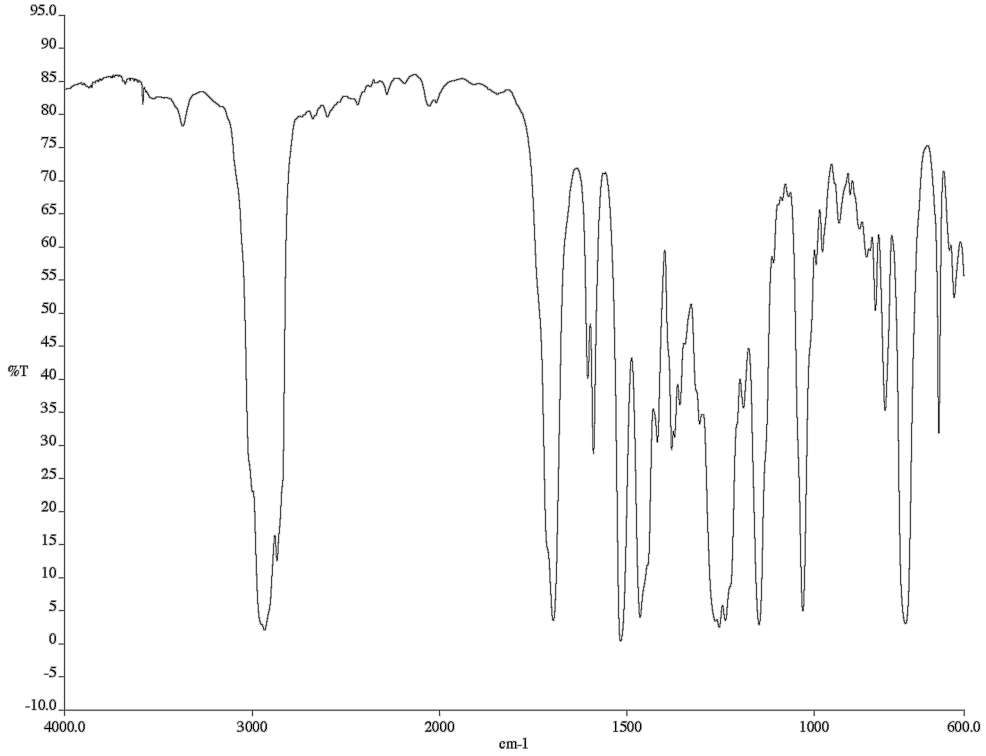


Figure A7.95 Infrared spectrum ($NaCl/CHCl_3$) of compound **374**.

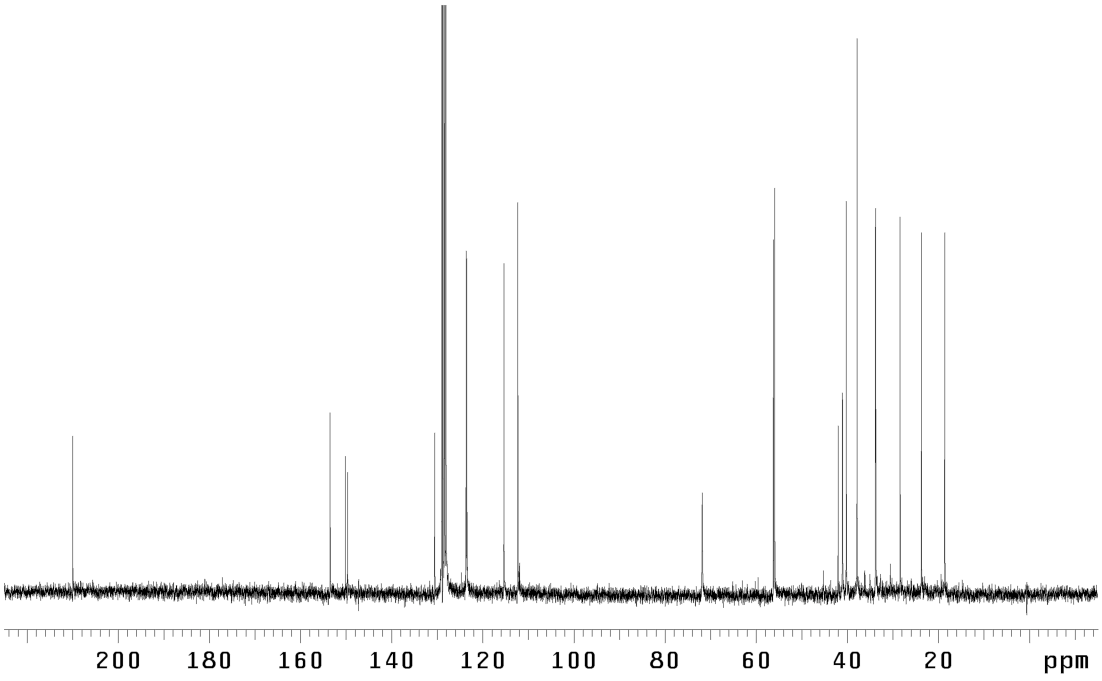


Figure A7.96 ^{13}C NMR (75 MHz, C_6D_6) of compound **374**.

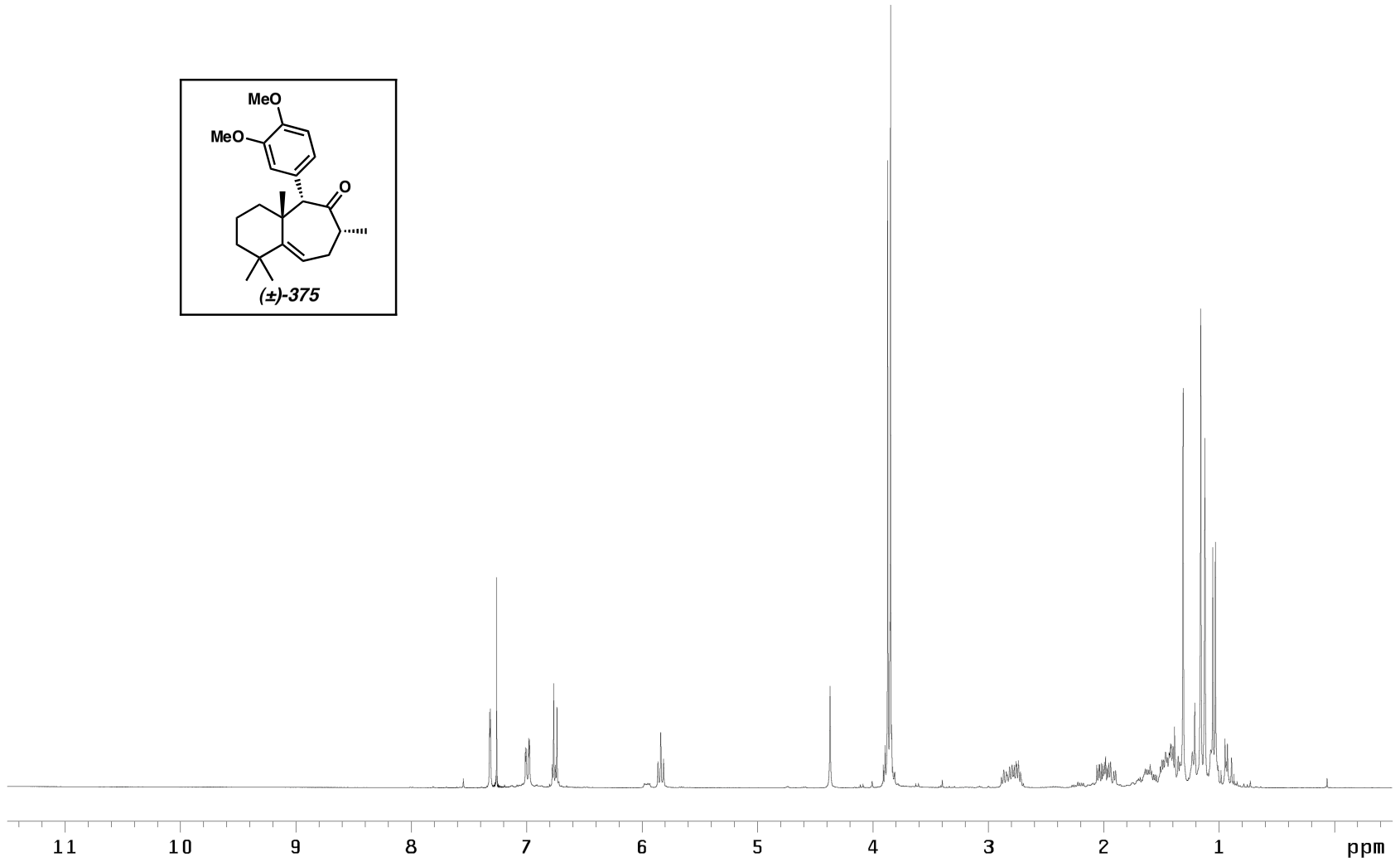


Figure A7.97 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **375**.

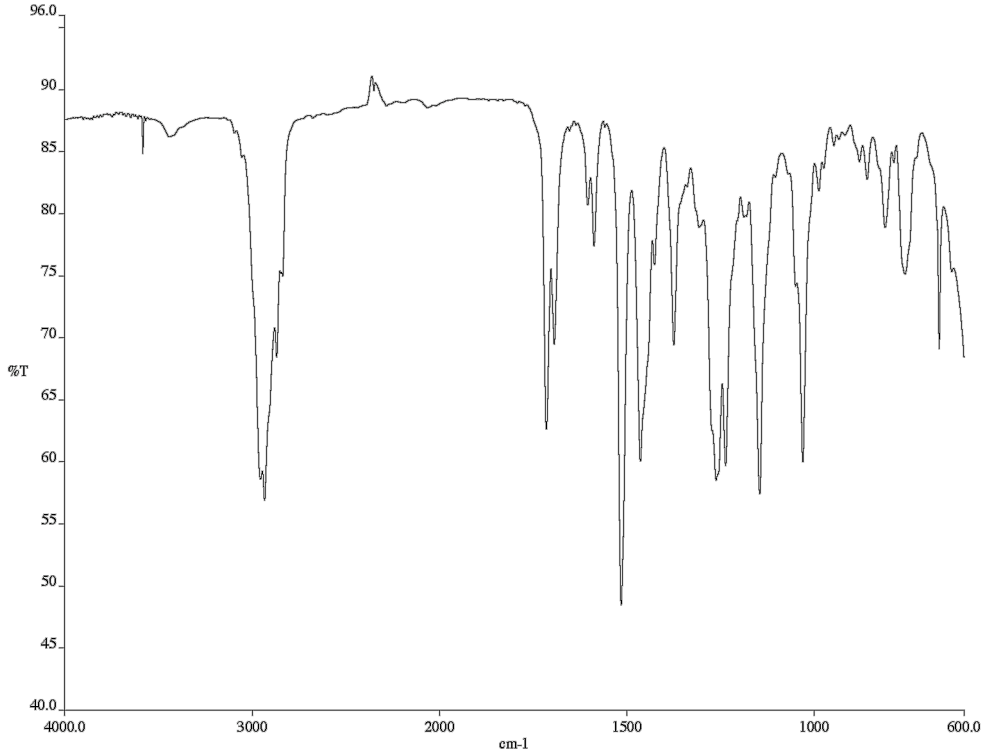


Figure A7.98 Infrared spectrum ($NaCl/CHCl_3$) of compound **375**.

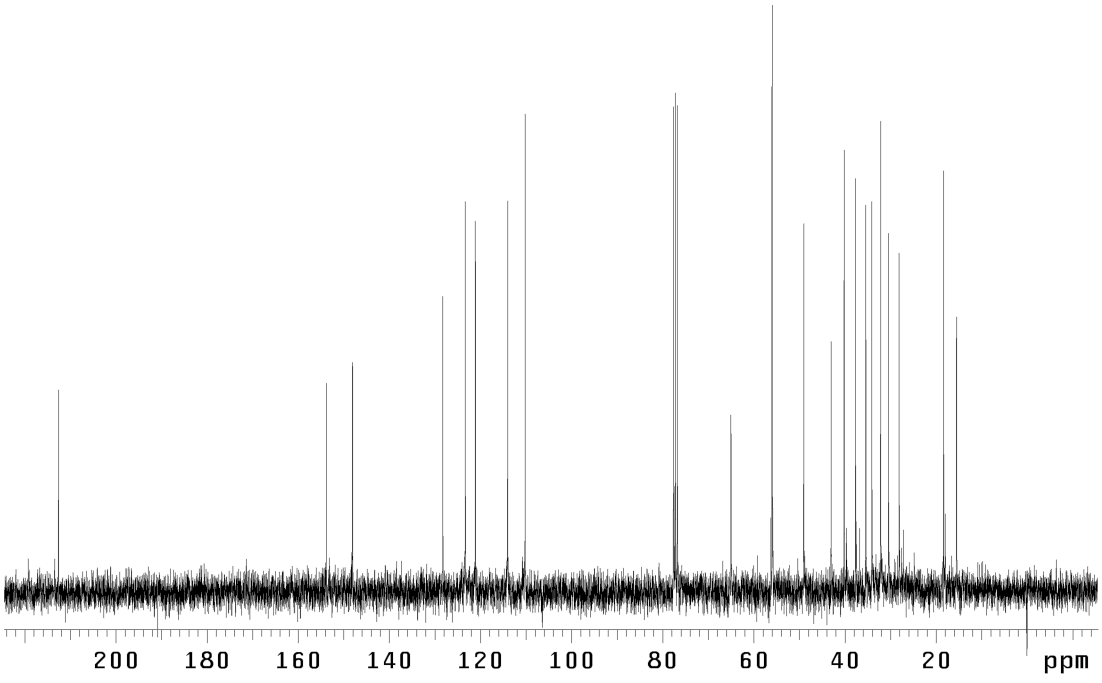


Figure A7.99 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **375**.

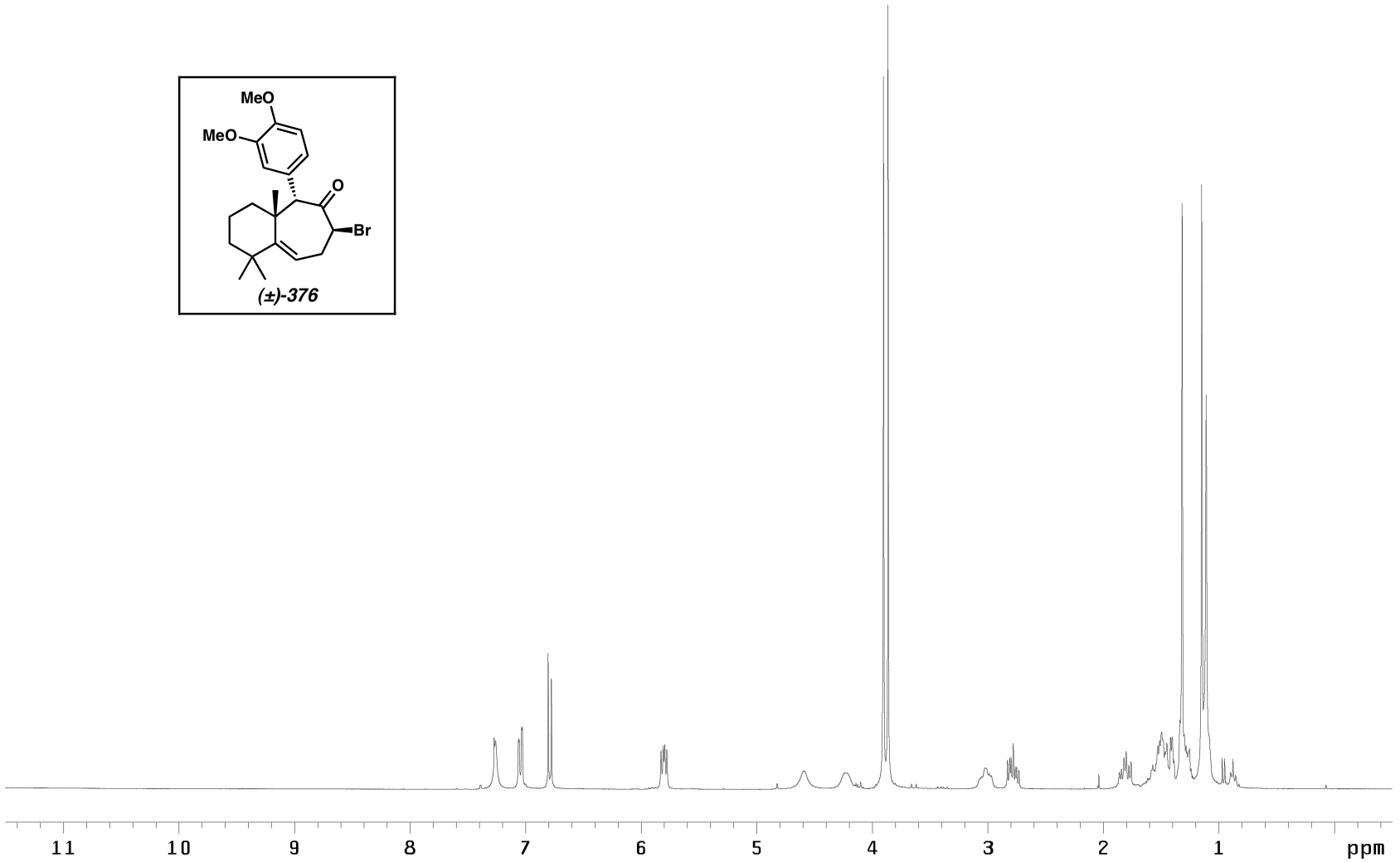


Figure A7.100 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **376**.

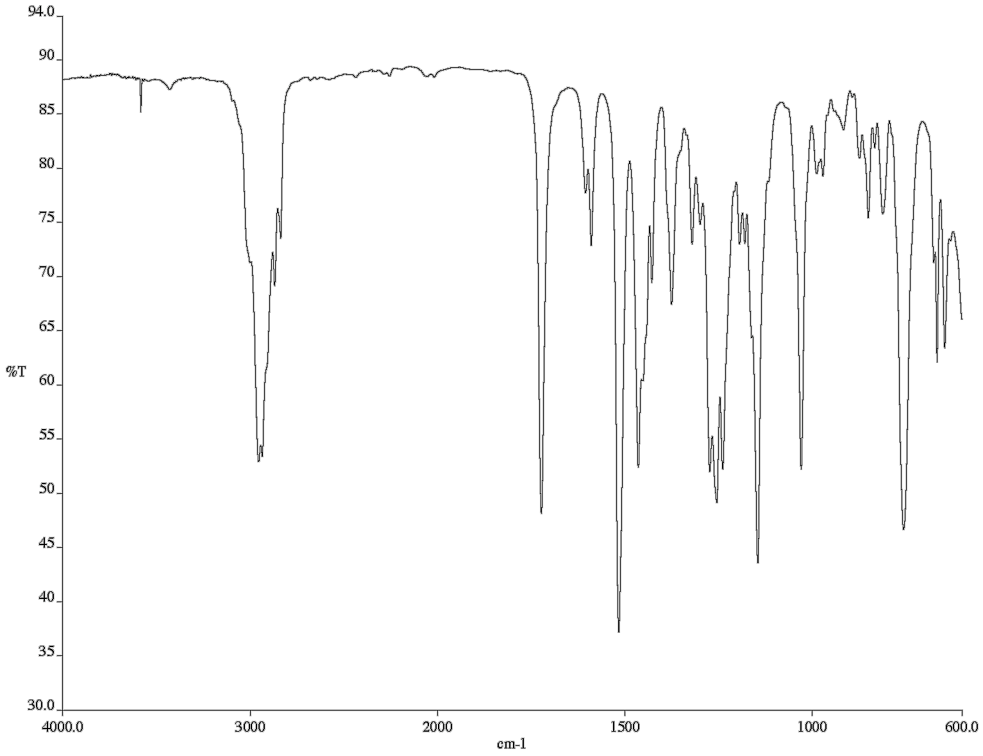


Figure A7.101 Infrared spectrum ($NaCl/CHCl_3$) of compound **376**.

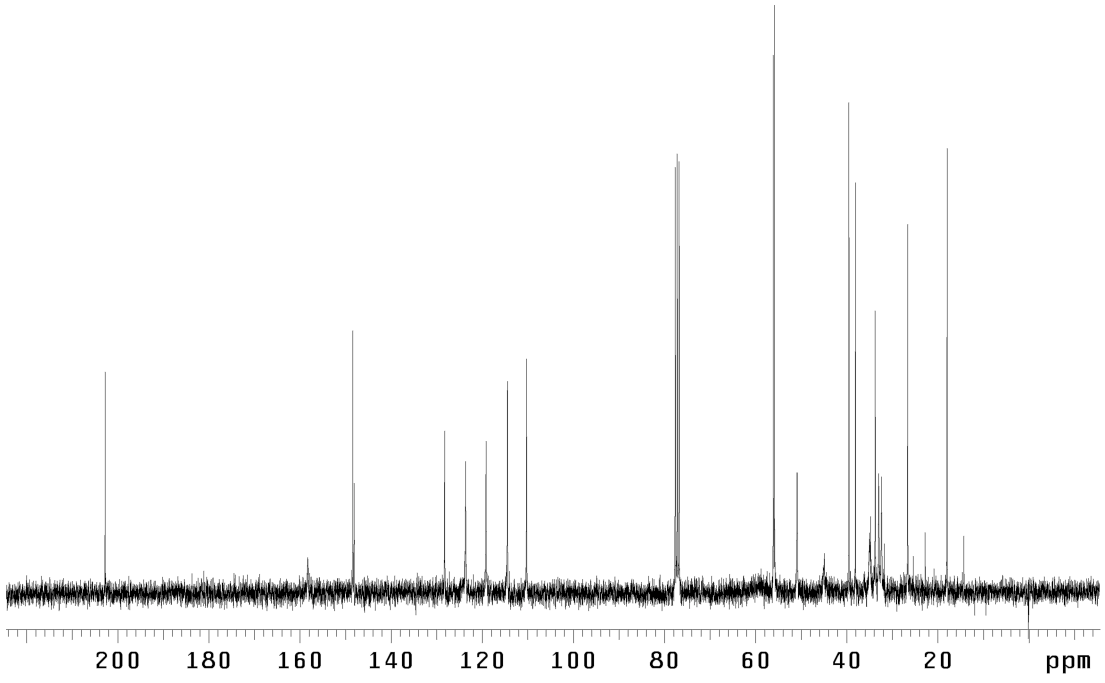


Figure A7.102 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **376**.

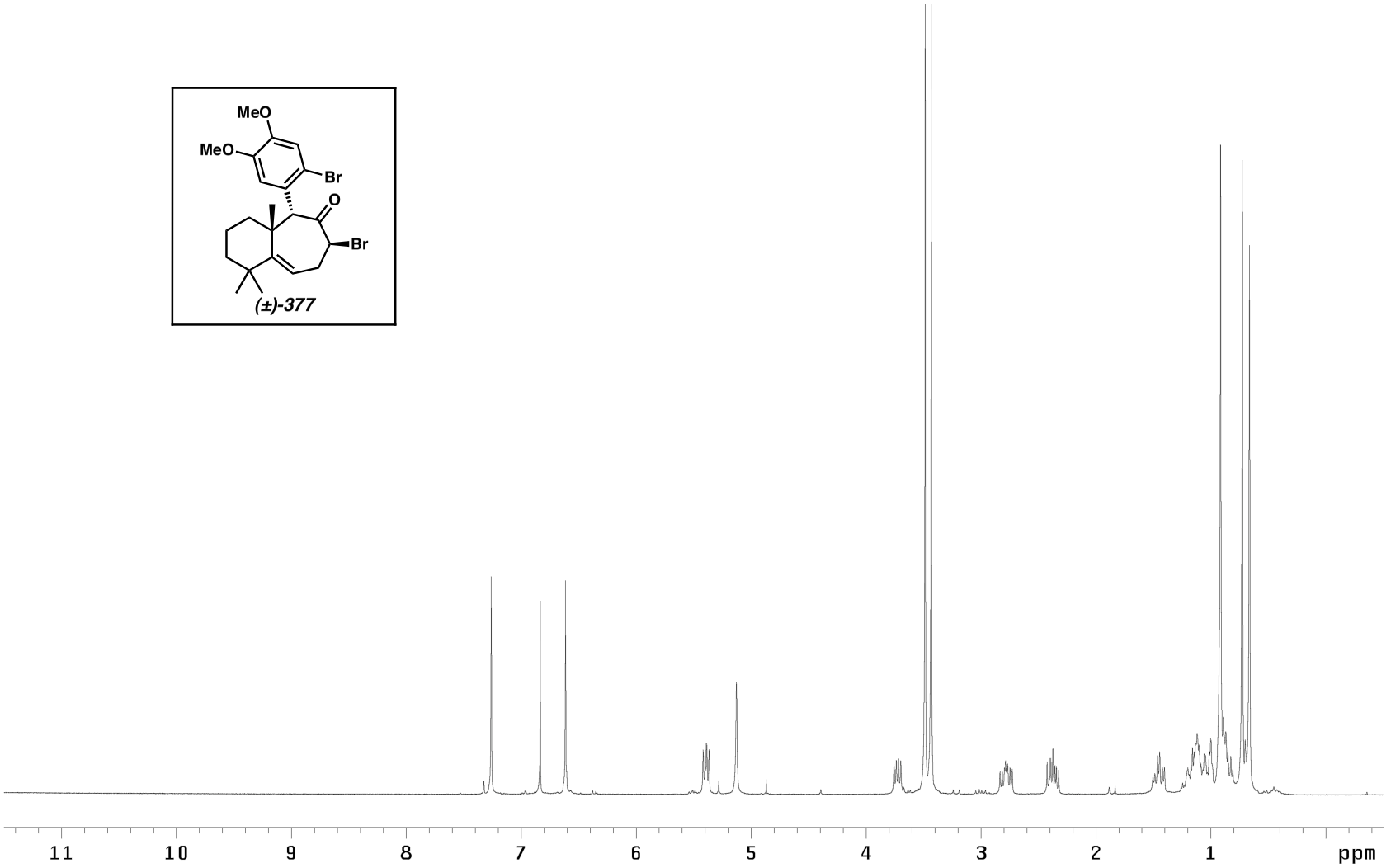


Figure A7.103 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **377**.

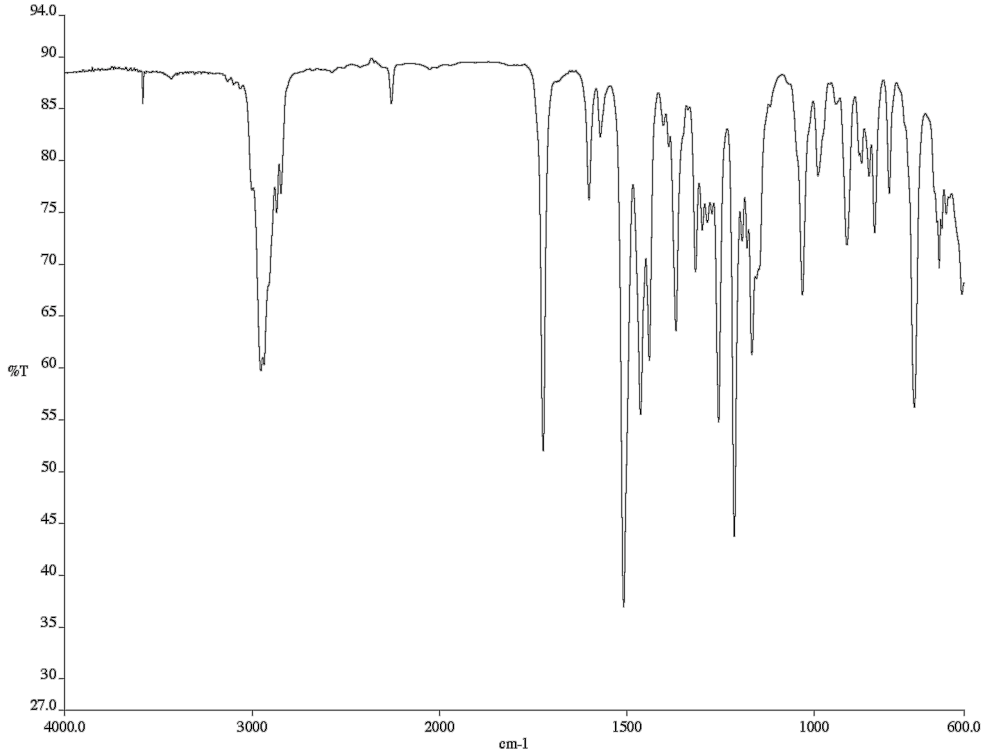


Figure A7.104 Infrared spectrum ($NaCl/CDCl_3$) of compound **377**.

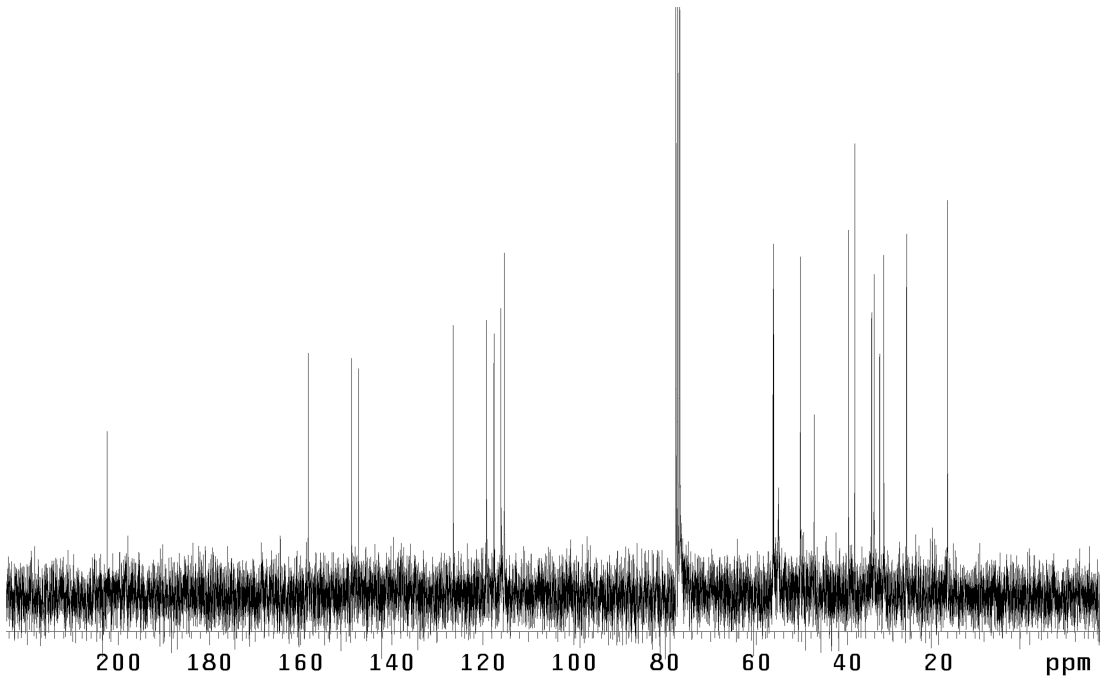


Figure A7.105 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **377**.

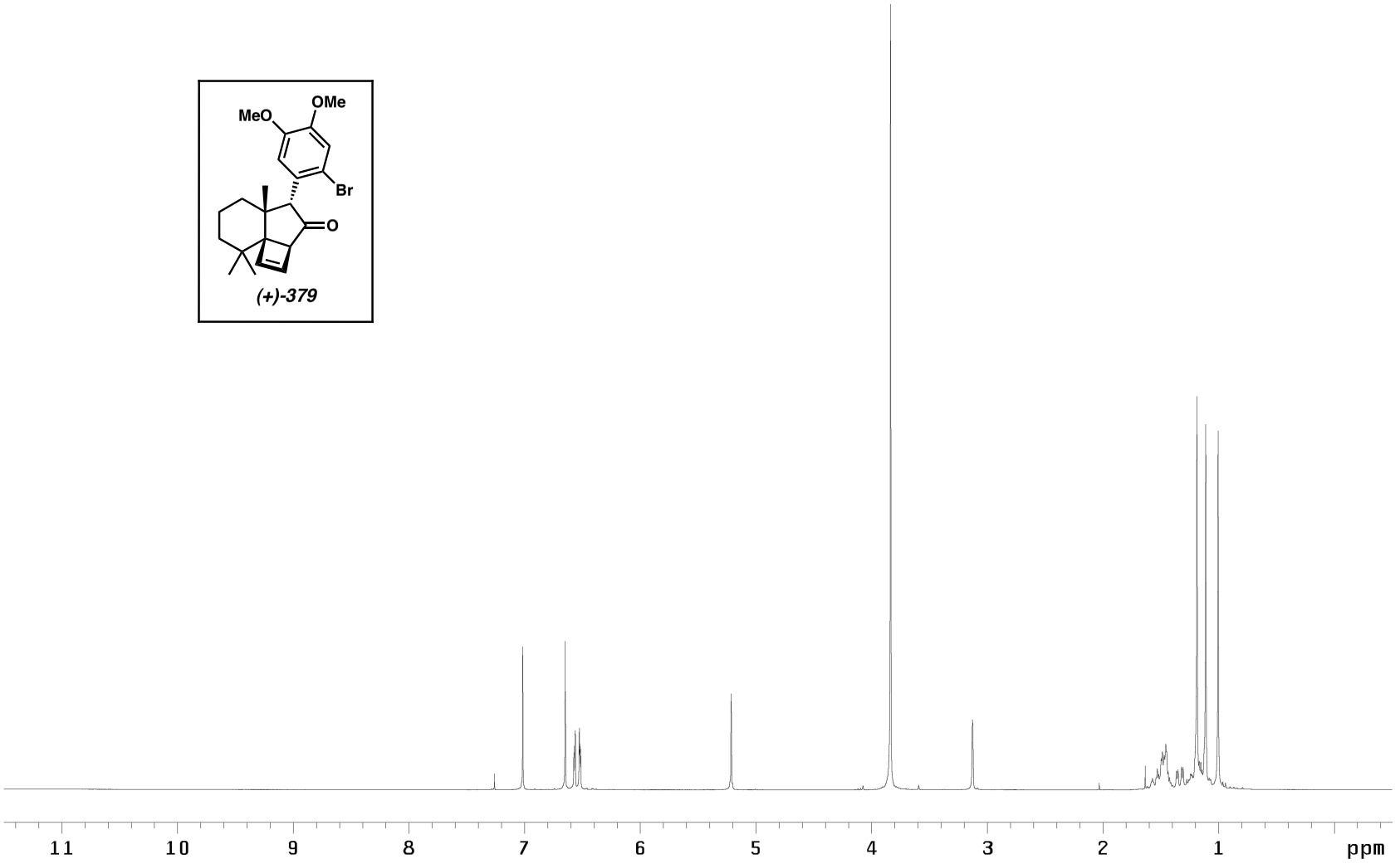


Figure A7.106 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **379**.

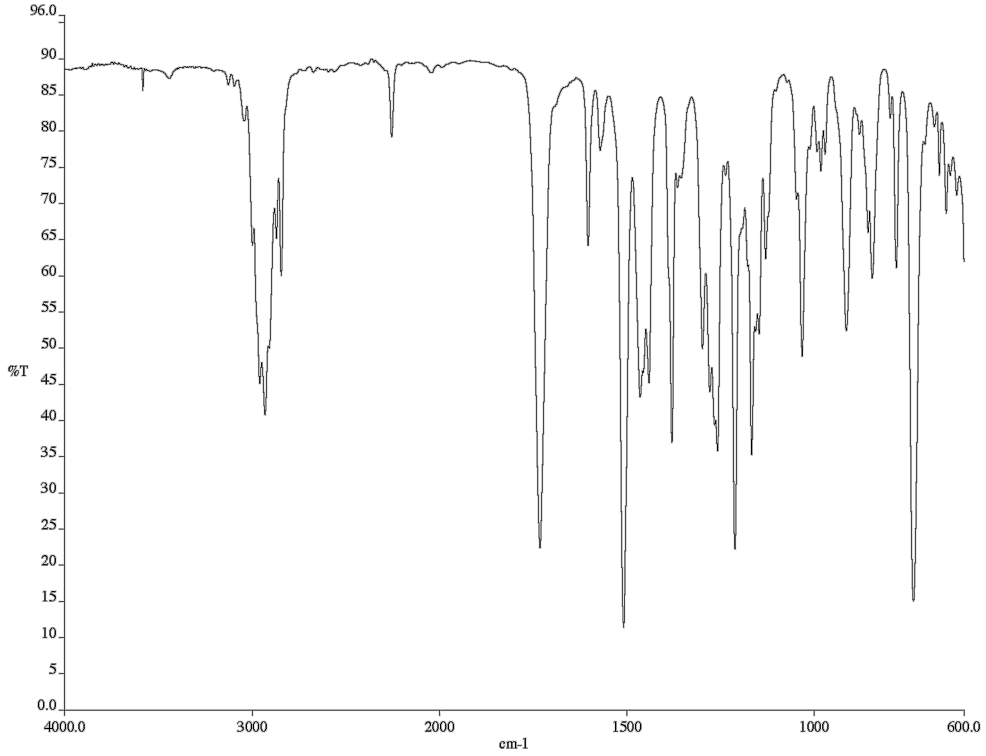


Figure A7.107 Infrared spectrum ($NaCl/CDCl_3$) of compound **379**.

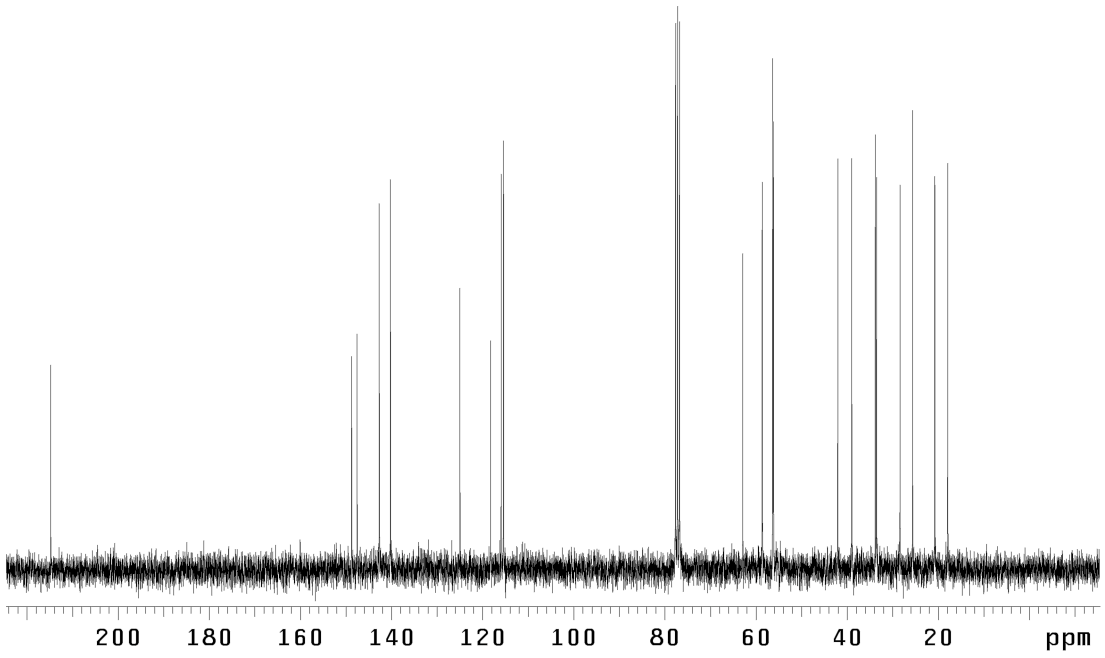


Figure A7.108 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **379**.

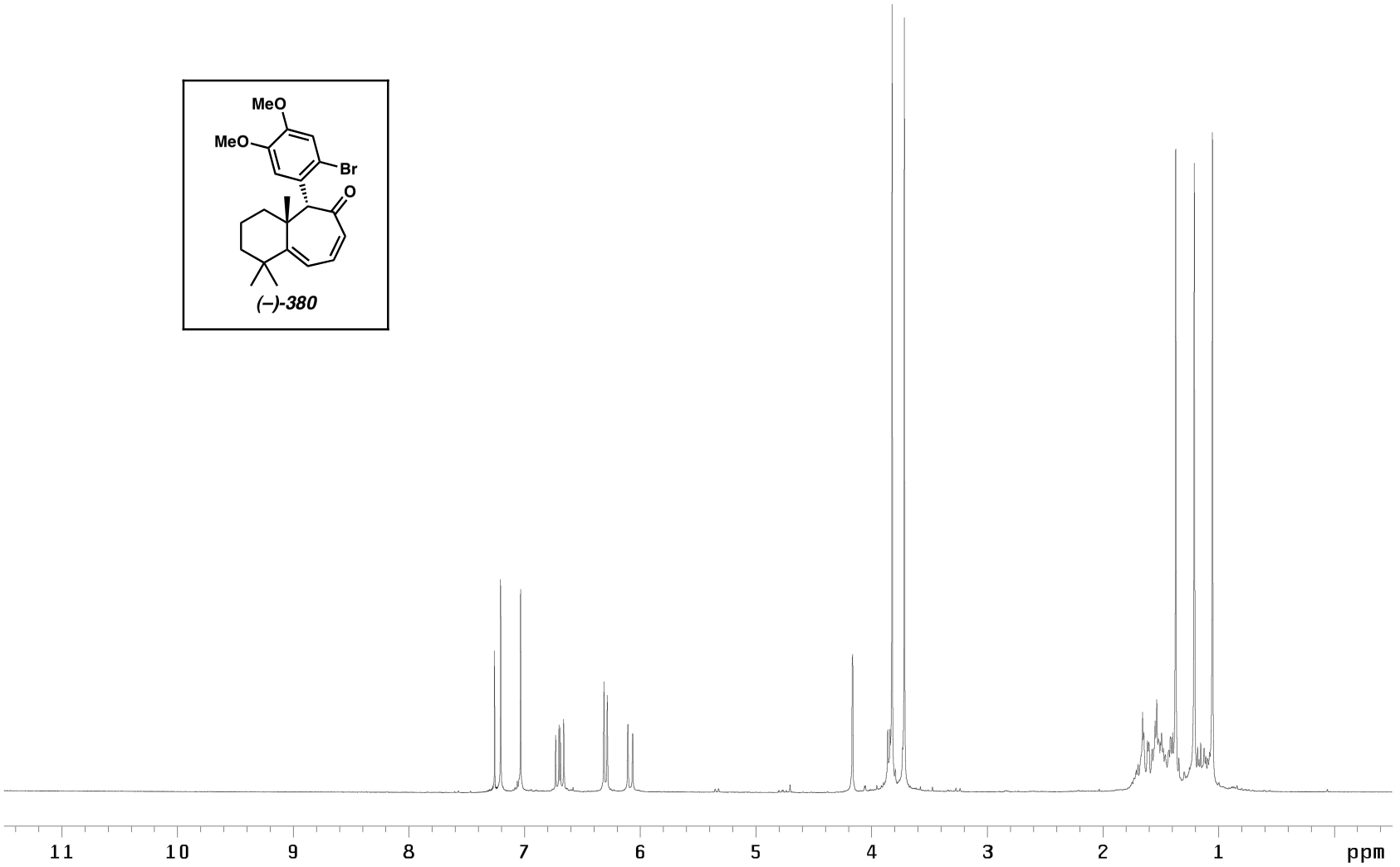


Figure A7.109 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **380**.

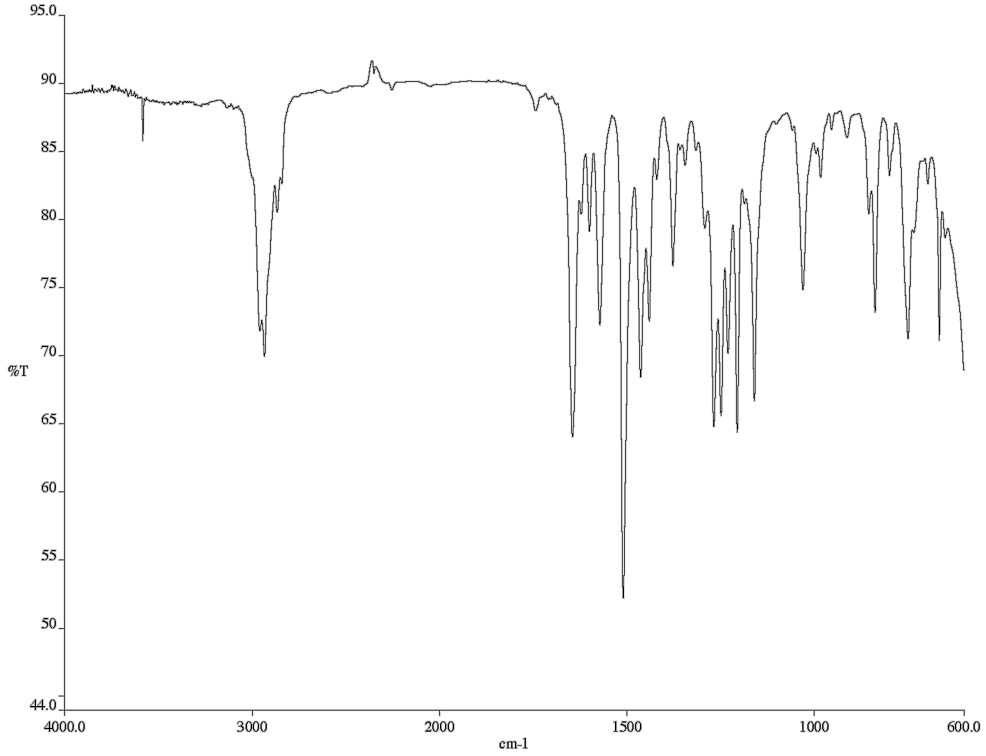


Figure A7.110 Infrared spectrum ($NaCl/CDCl_3$) of compound **380**.

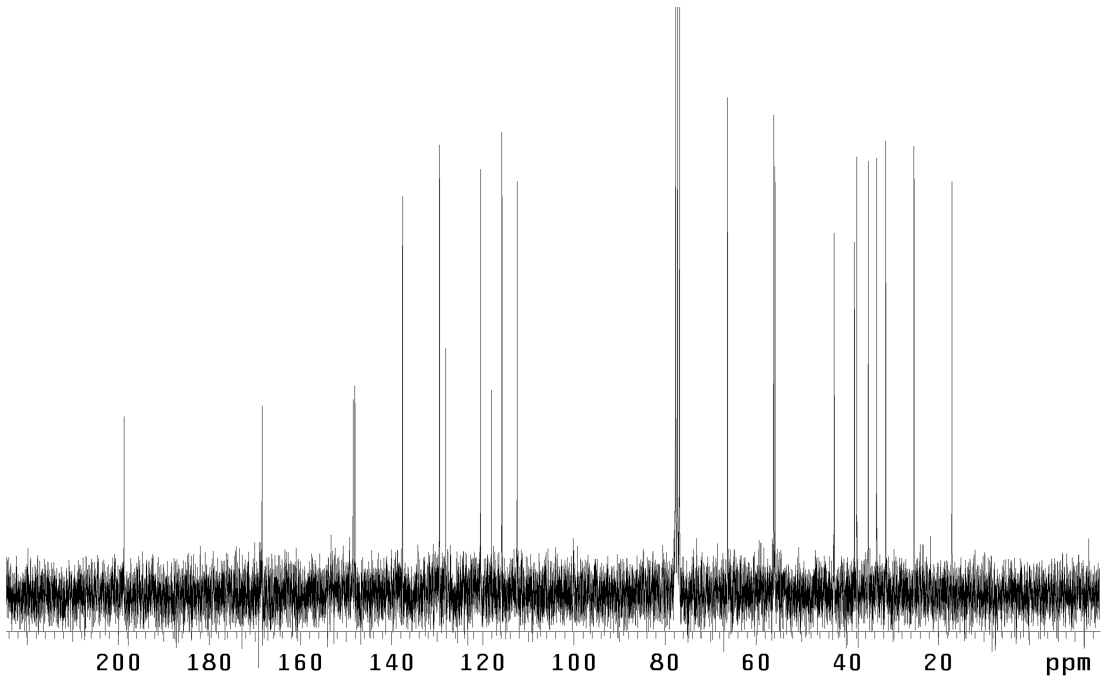


Figure A7.111 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **380**.

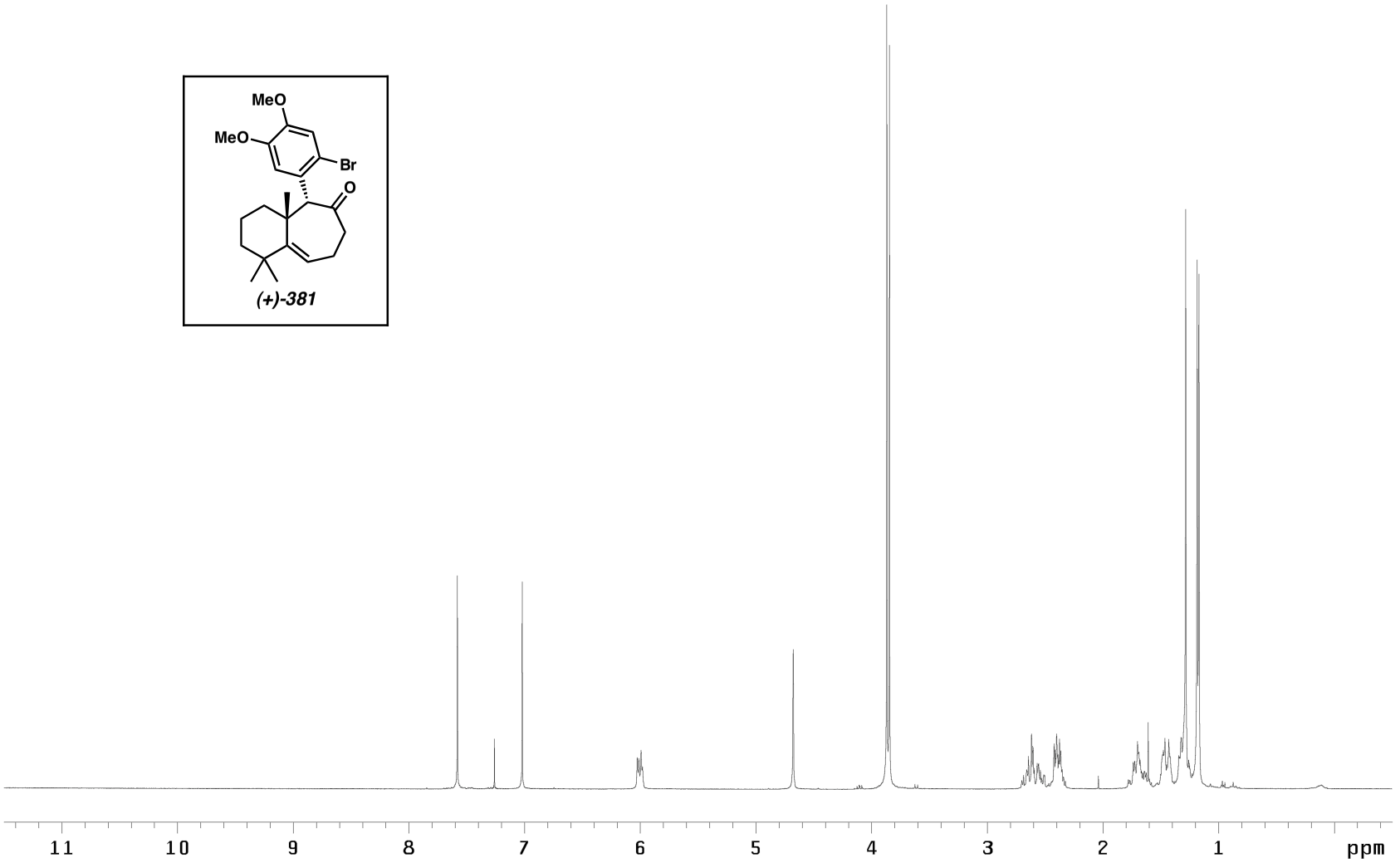


Figure A7.112 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **381**.

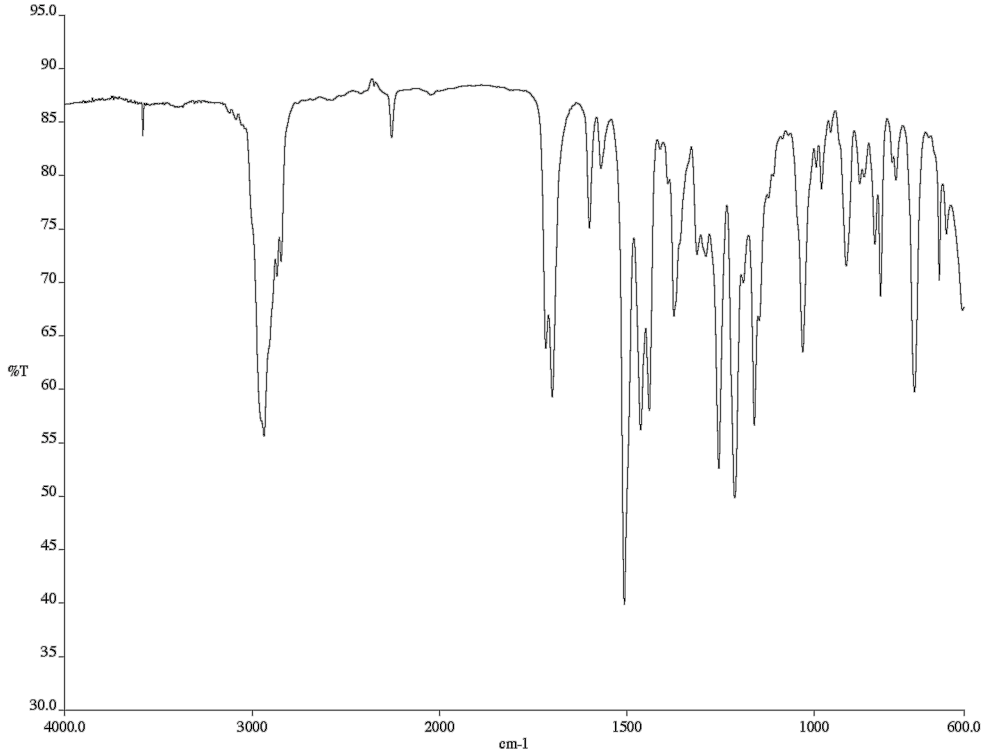


Figure A7.113 Infrared spectrum ($NaCl/CDCl_3$) of compound **381**.

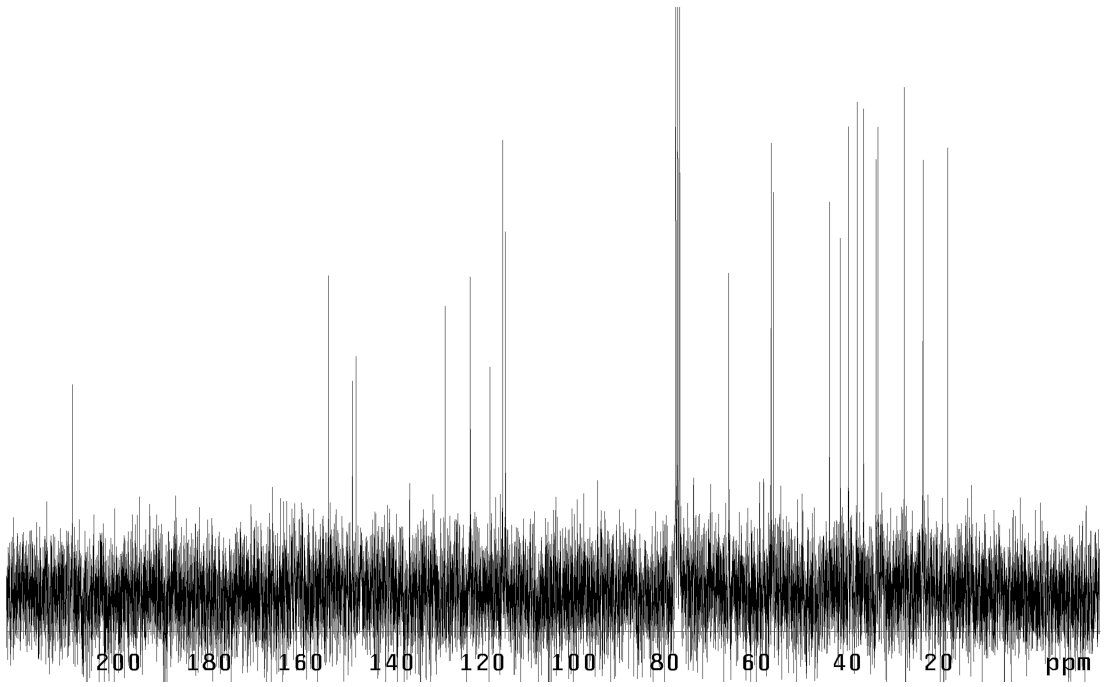


Figure A7.114 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **381**.

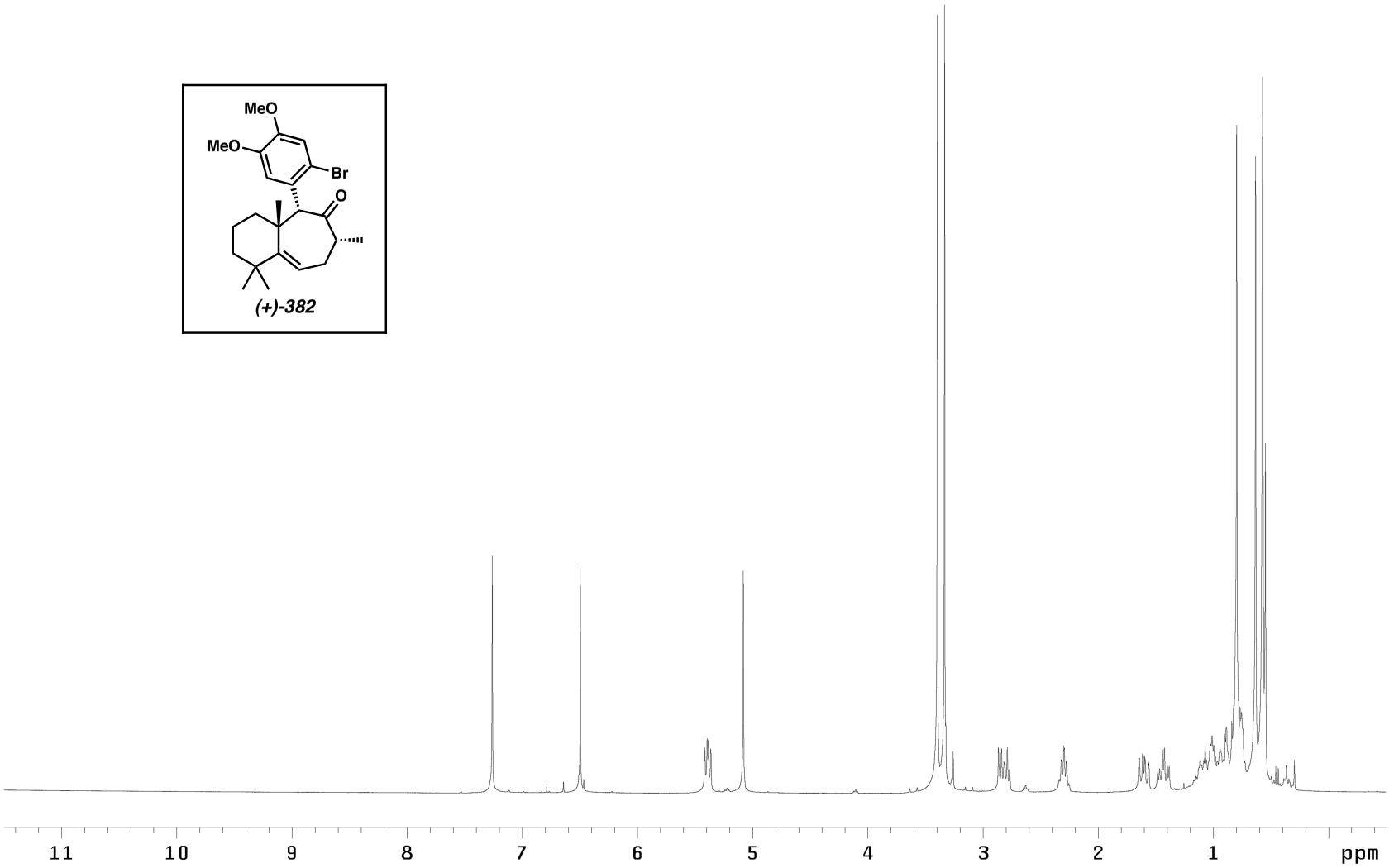


Figure A7.115 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **382**.

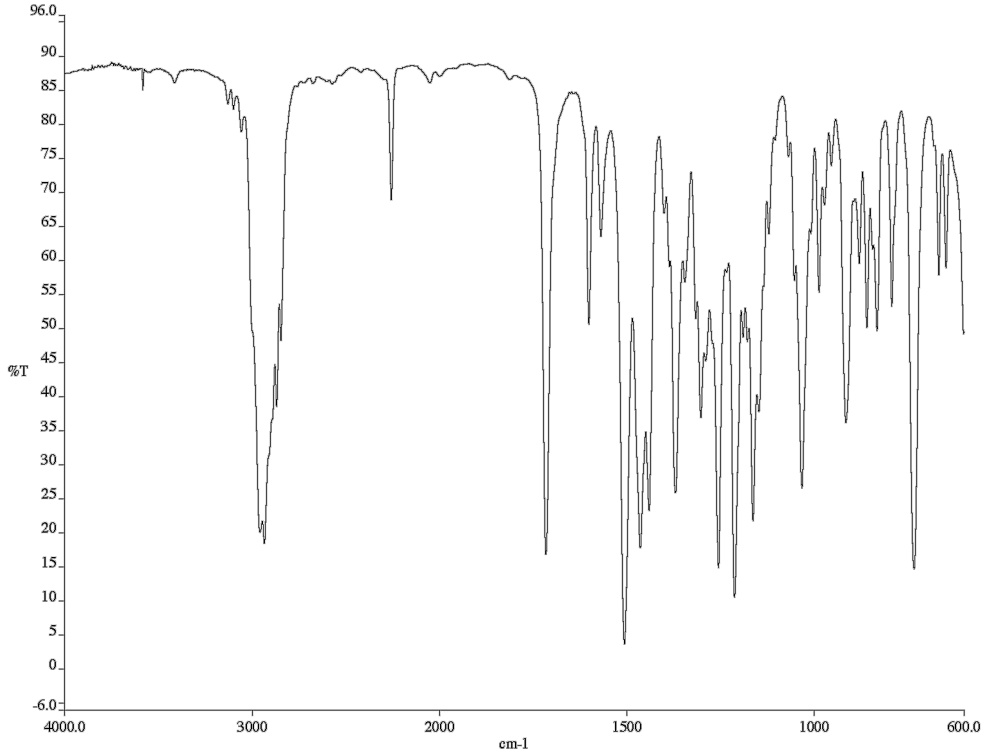


Figure A7.116 Infrared spectrum ($NaCl/CDCl_3$) of compound **382**.

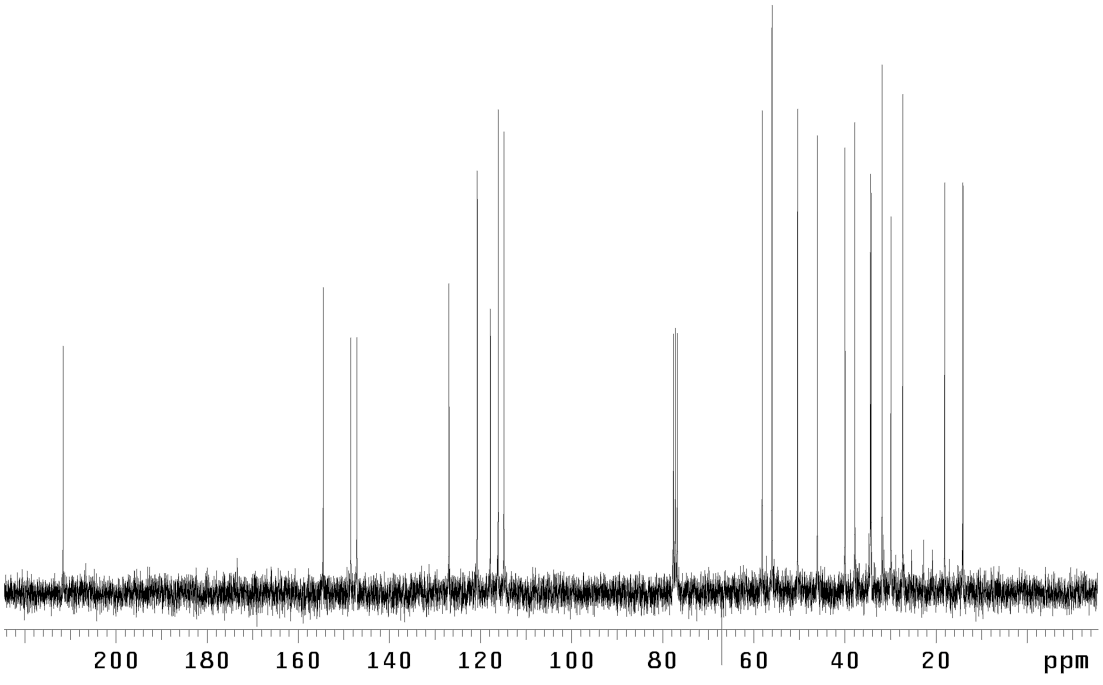


Figure A7.117 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **382**.

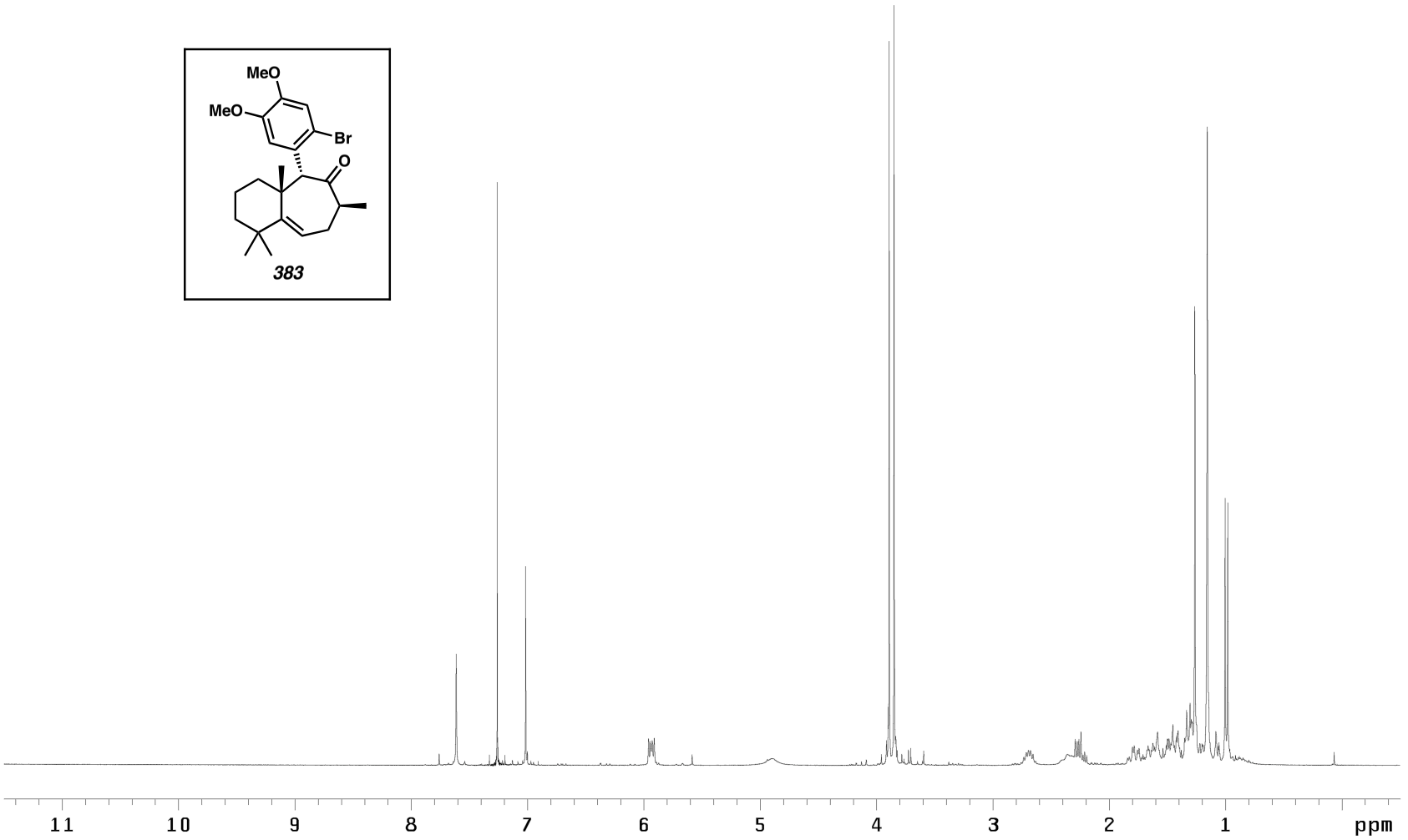


Figure A7.118 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **383**.

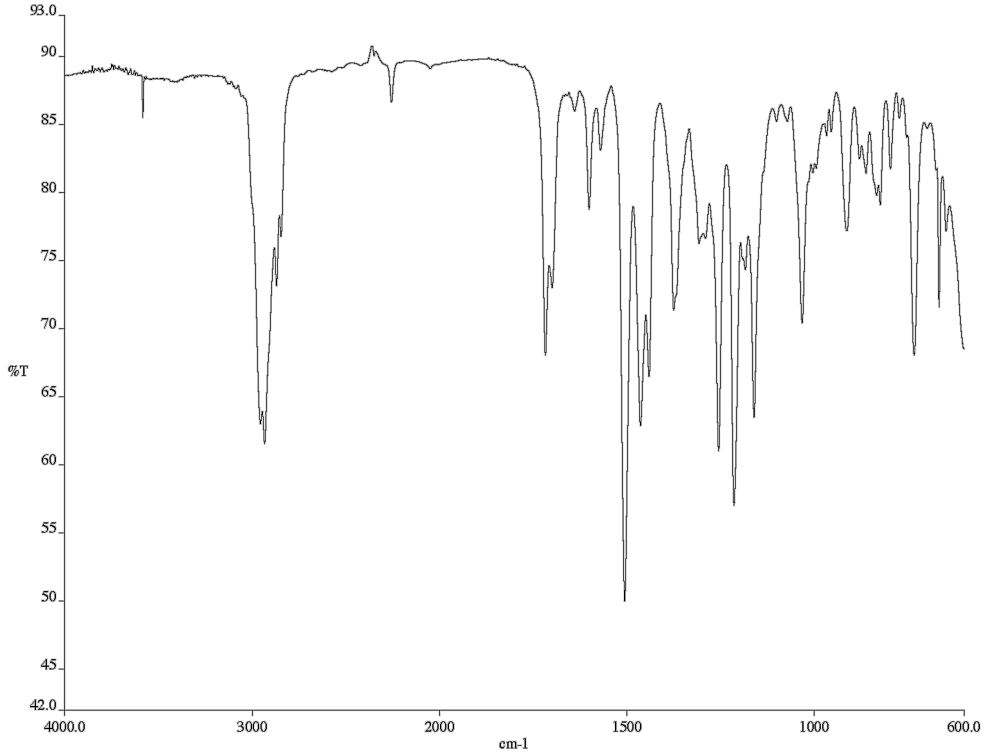


Figure A7.119 Infrared spectrum ($NaCl/CDCl_3$) of compound **383**.

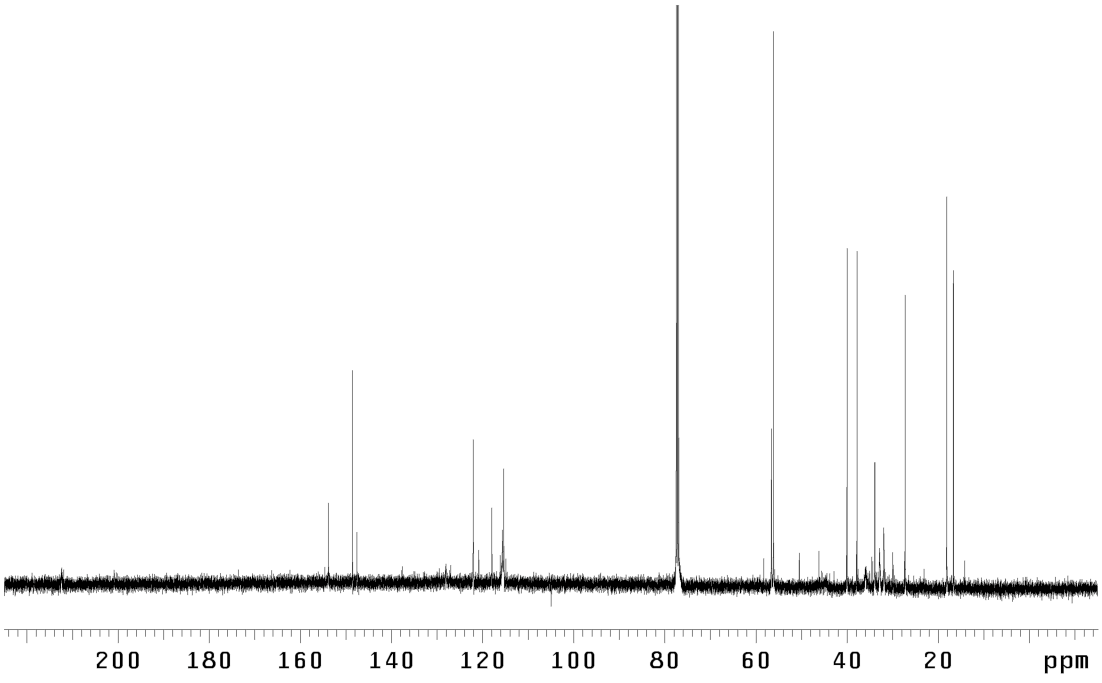


Figure A7.120 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **383**.

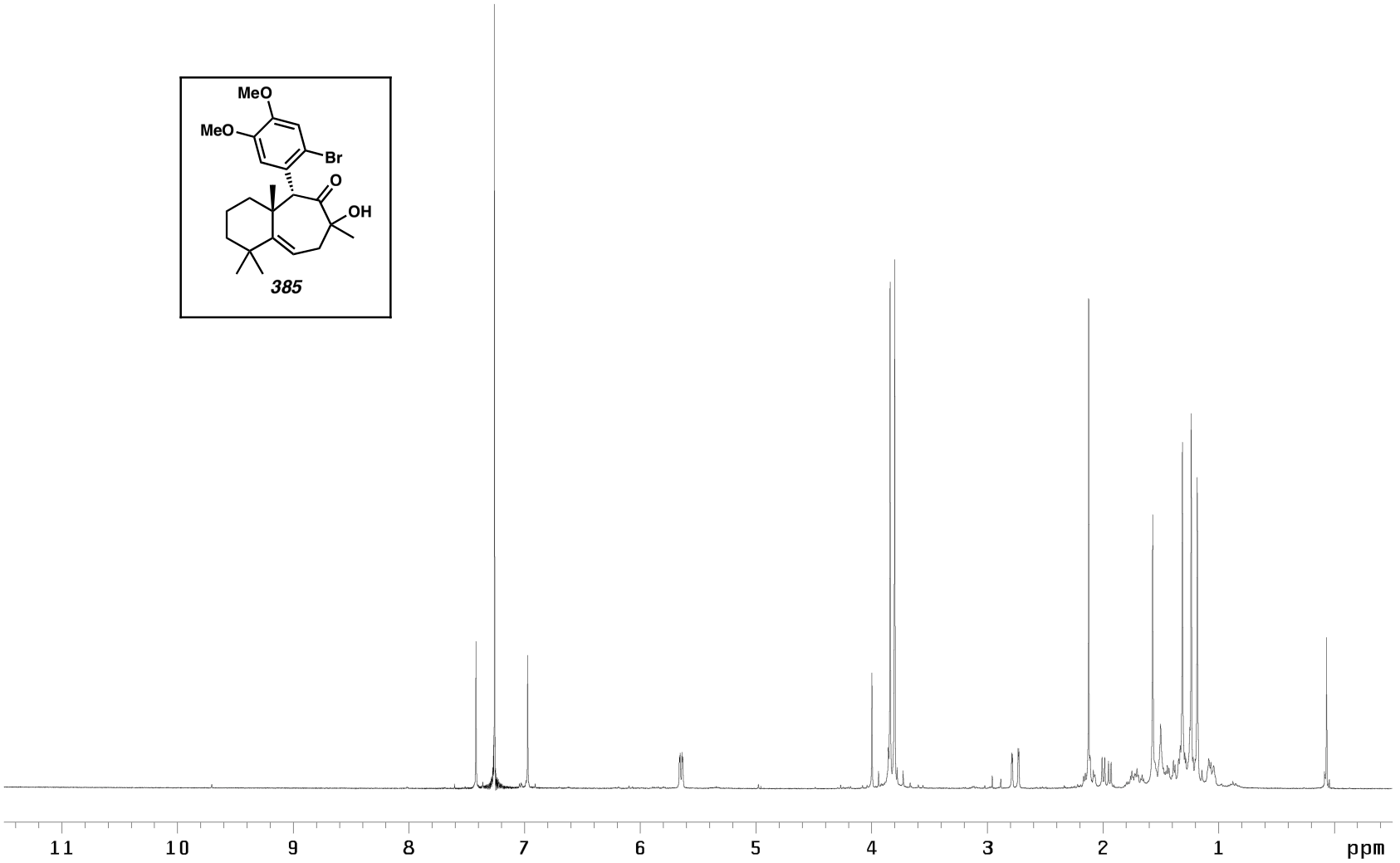


Figure A7.121 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **385**.

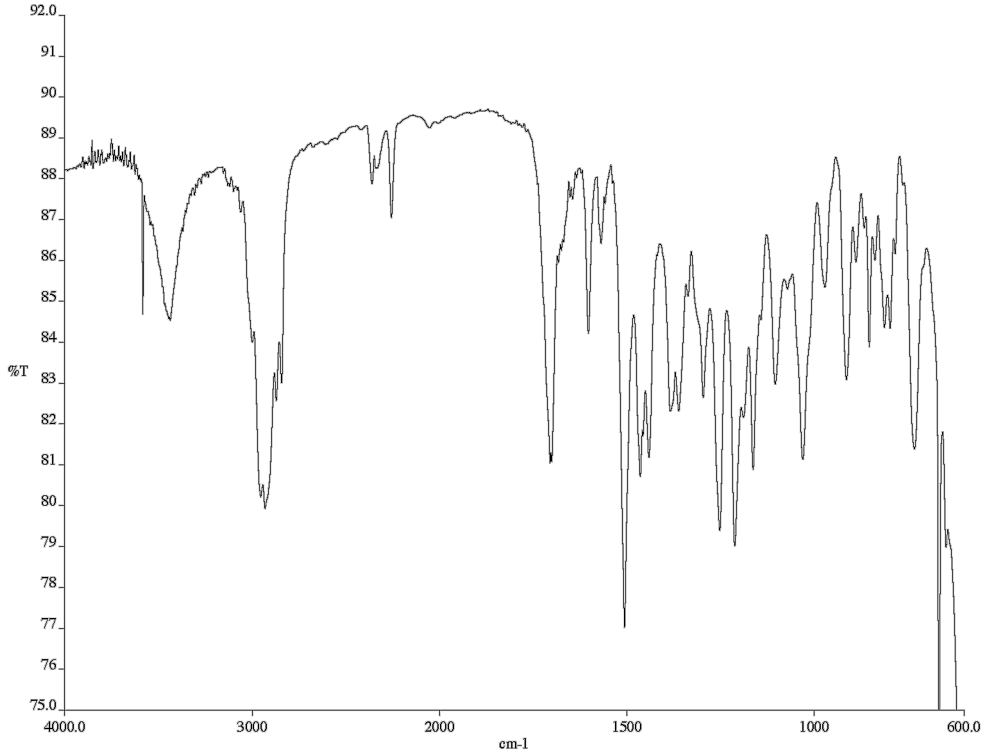


Figure A7.122 Infrared spectrum (NaCl/$CDCl_3$) of compound **385**.

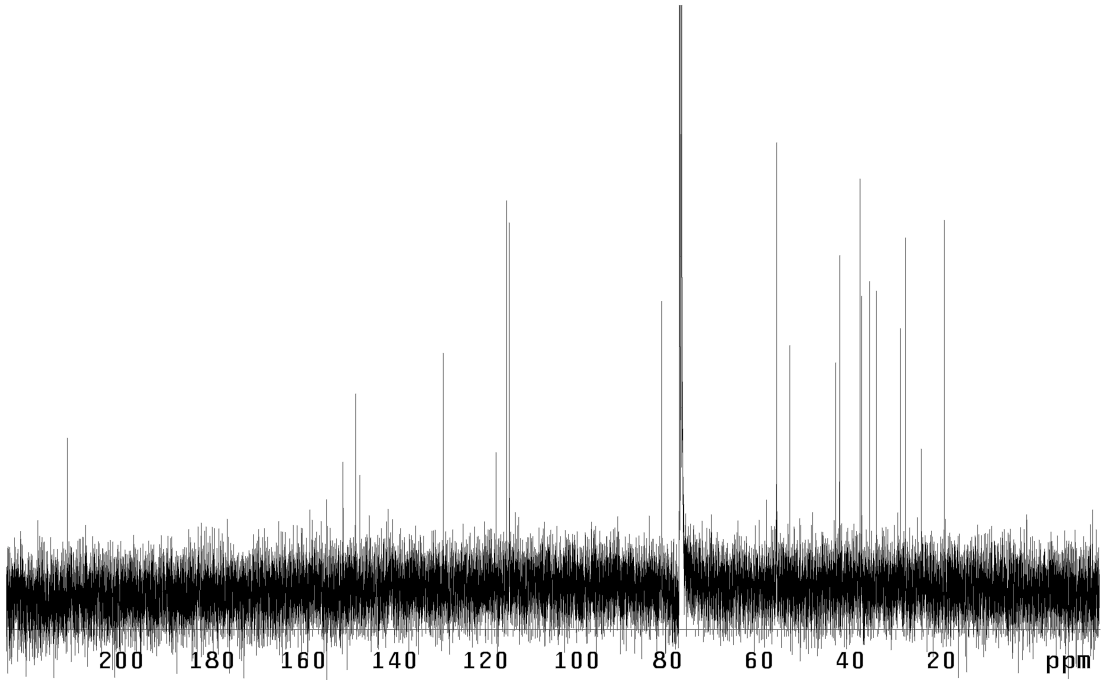


Figure A7.123 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **385**.

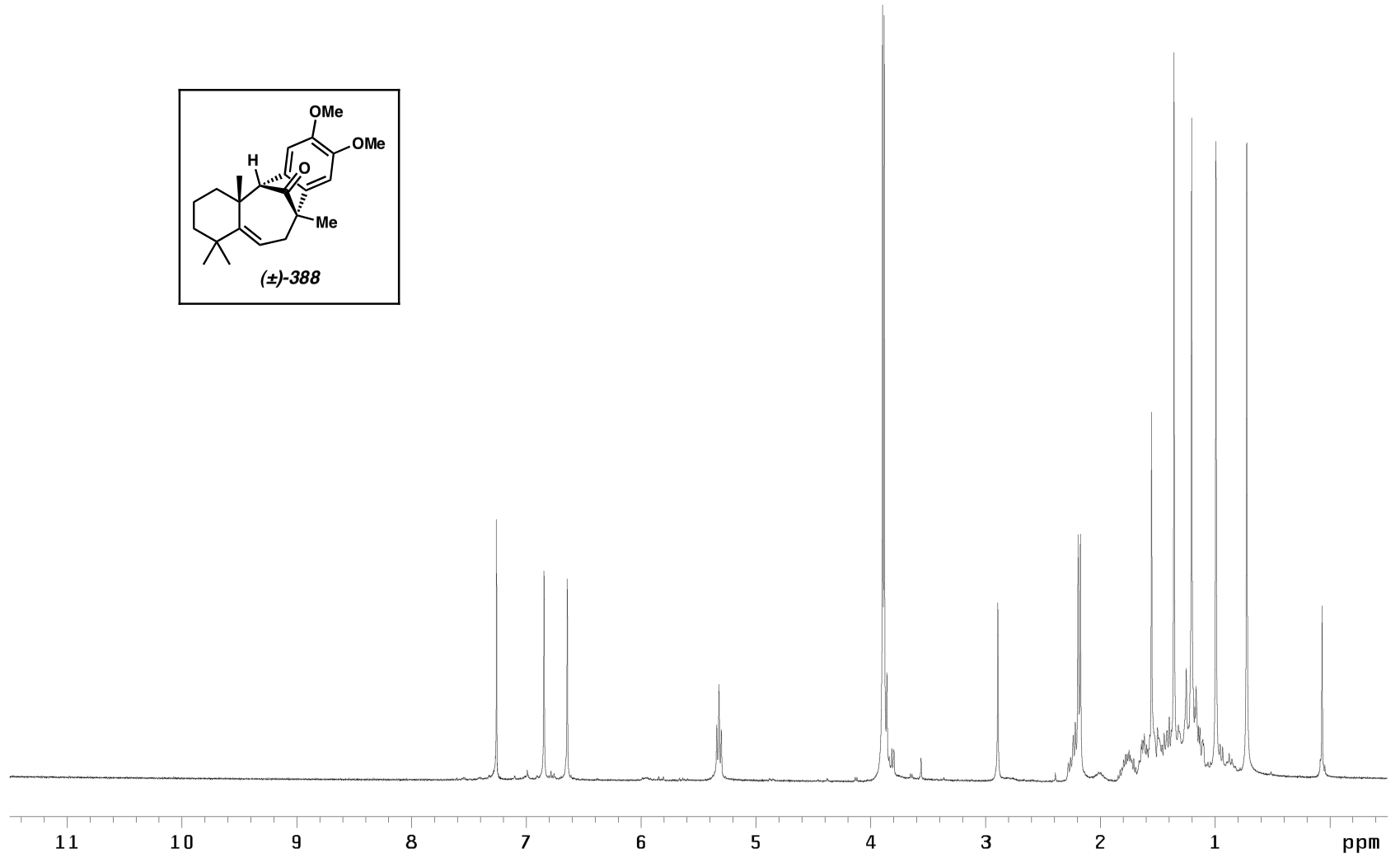


Figure A7.124 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **388**.

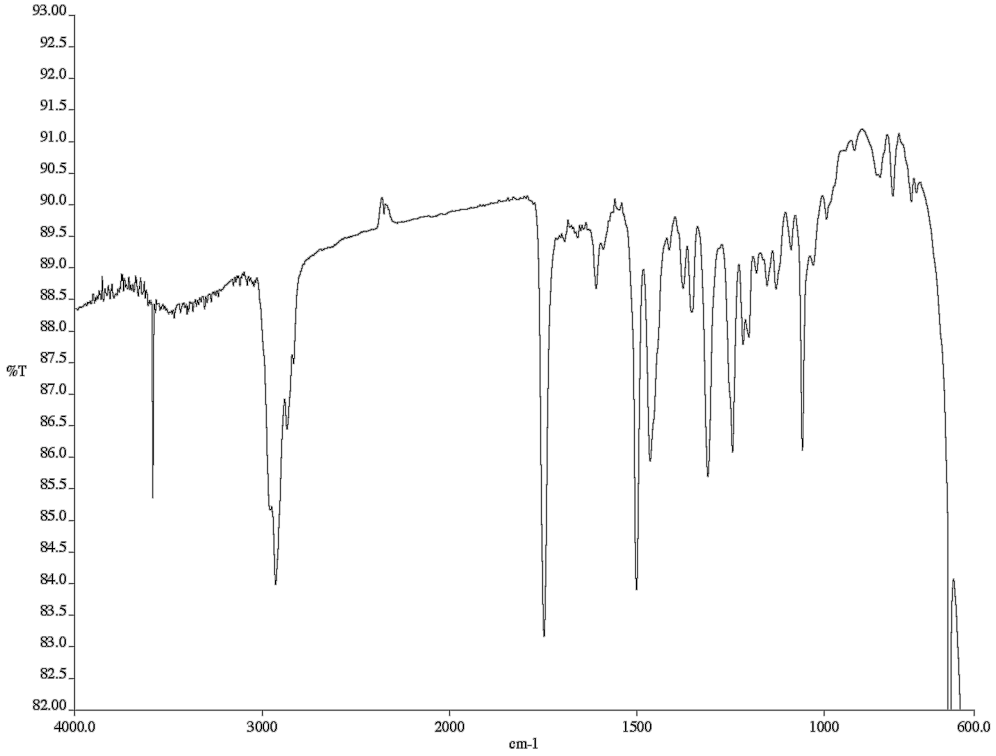


Figure A7.125 Infrared spectrum ($NaCl/CDCl_3$) of compound **388**.

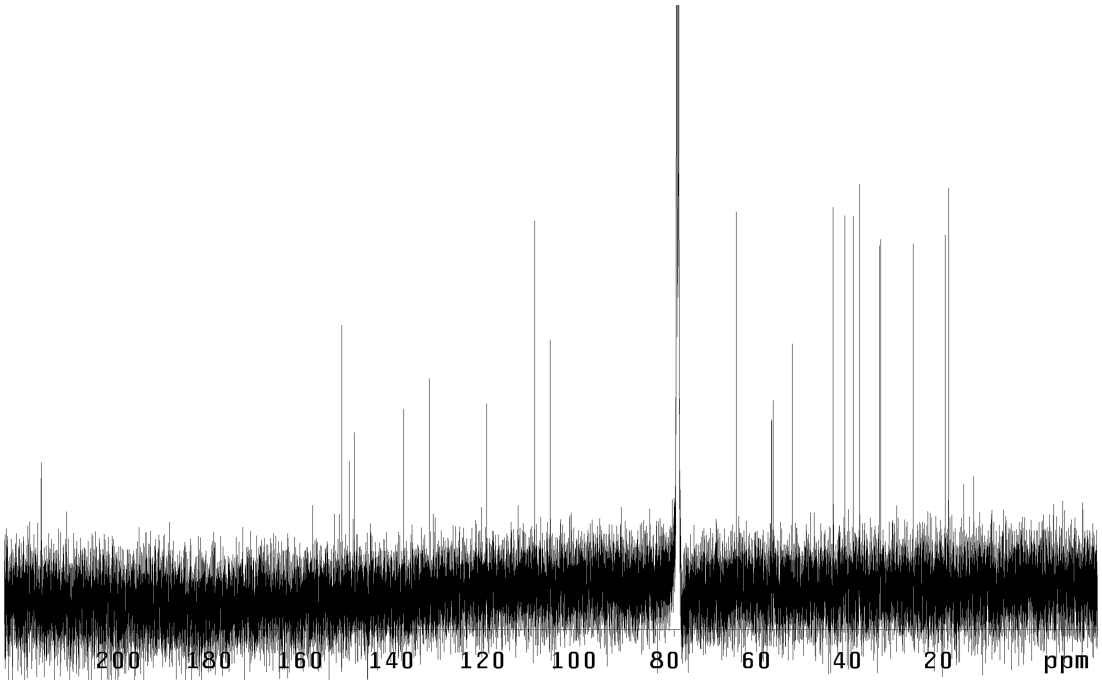


Figure A7.126 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **388**.

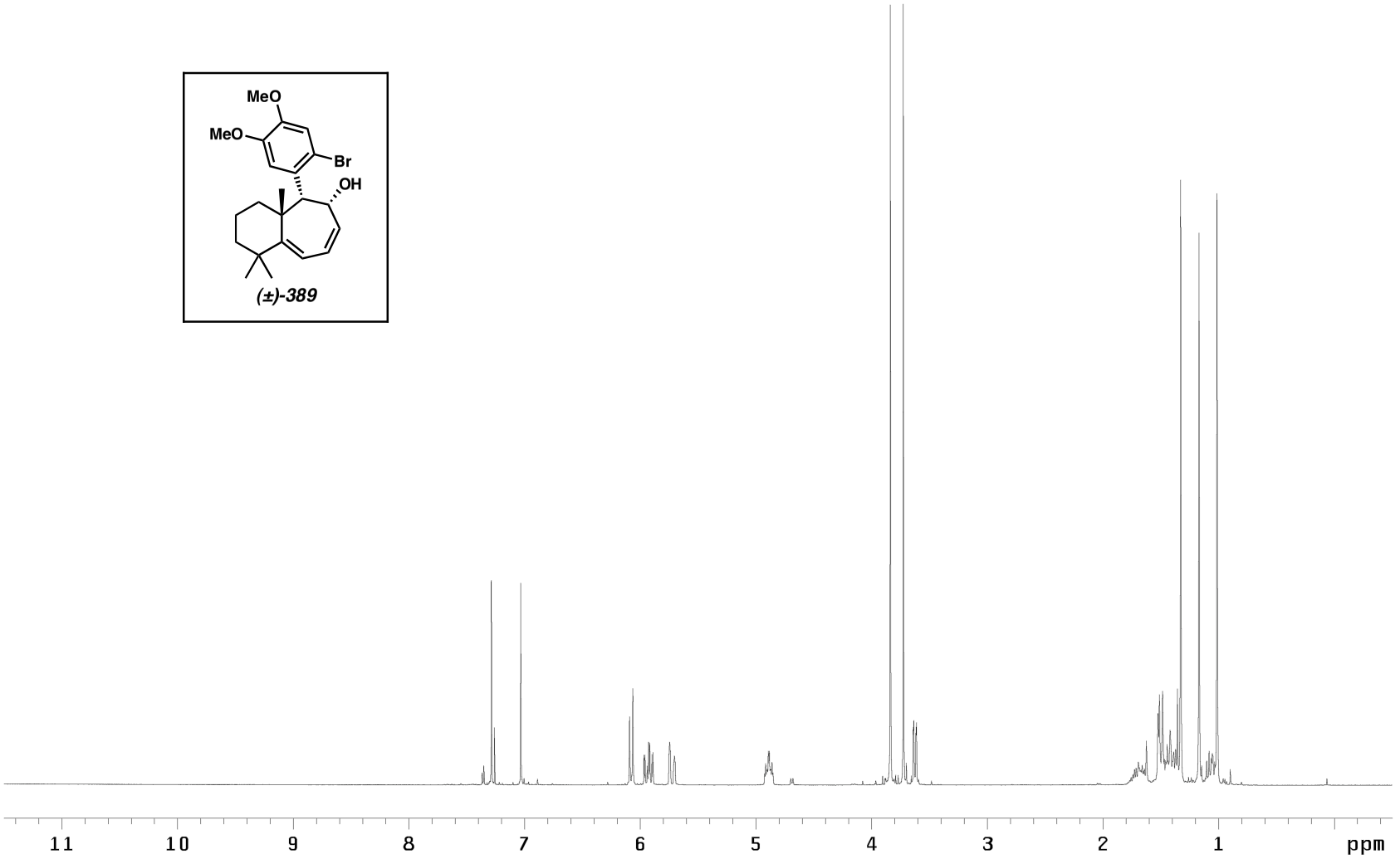


Figure A7.127 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **389**.

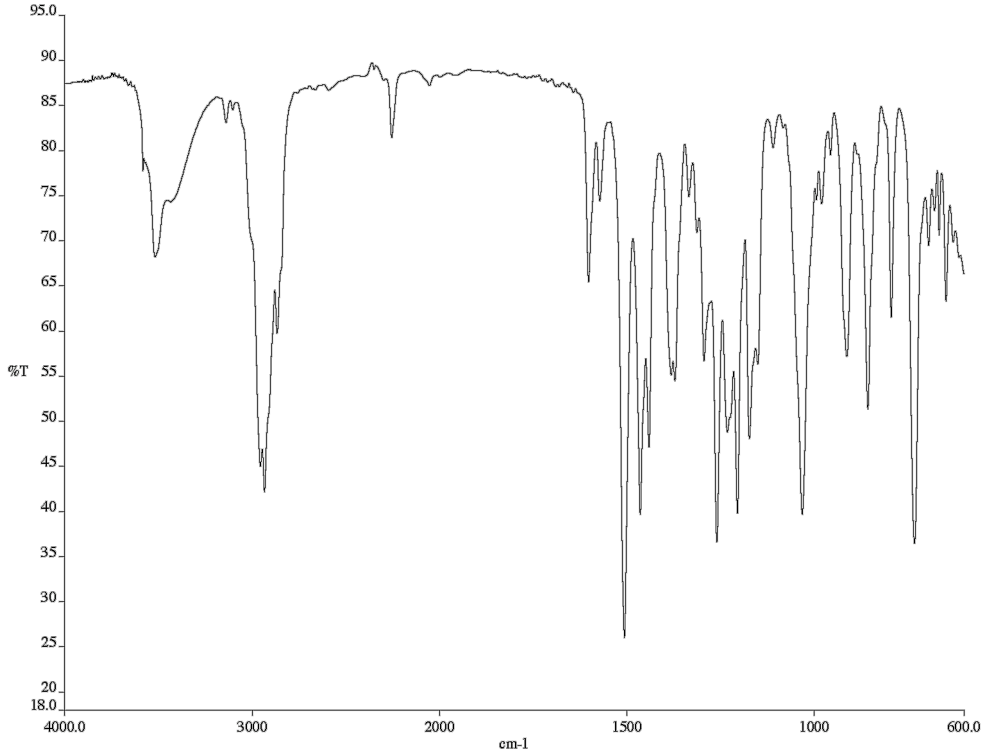


Figure A7.128 Infrared spectrum (NaCl/$CDCl_3$) of compound **389**.

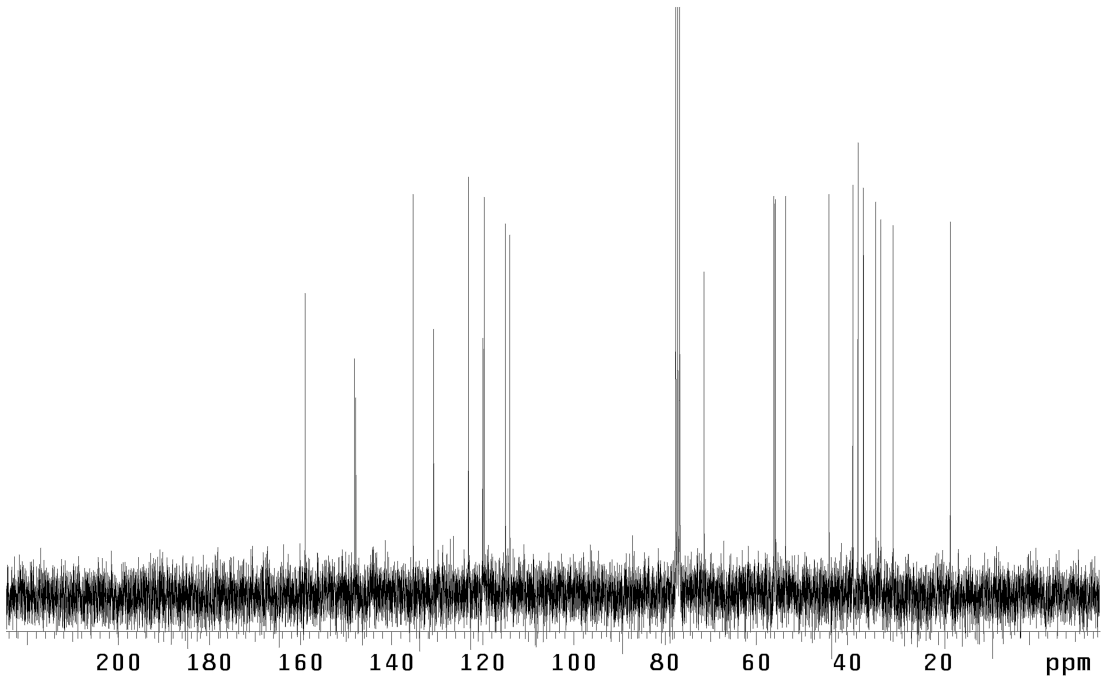


Figure A7.129 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **389**.

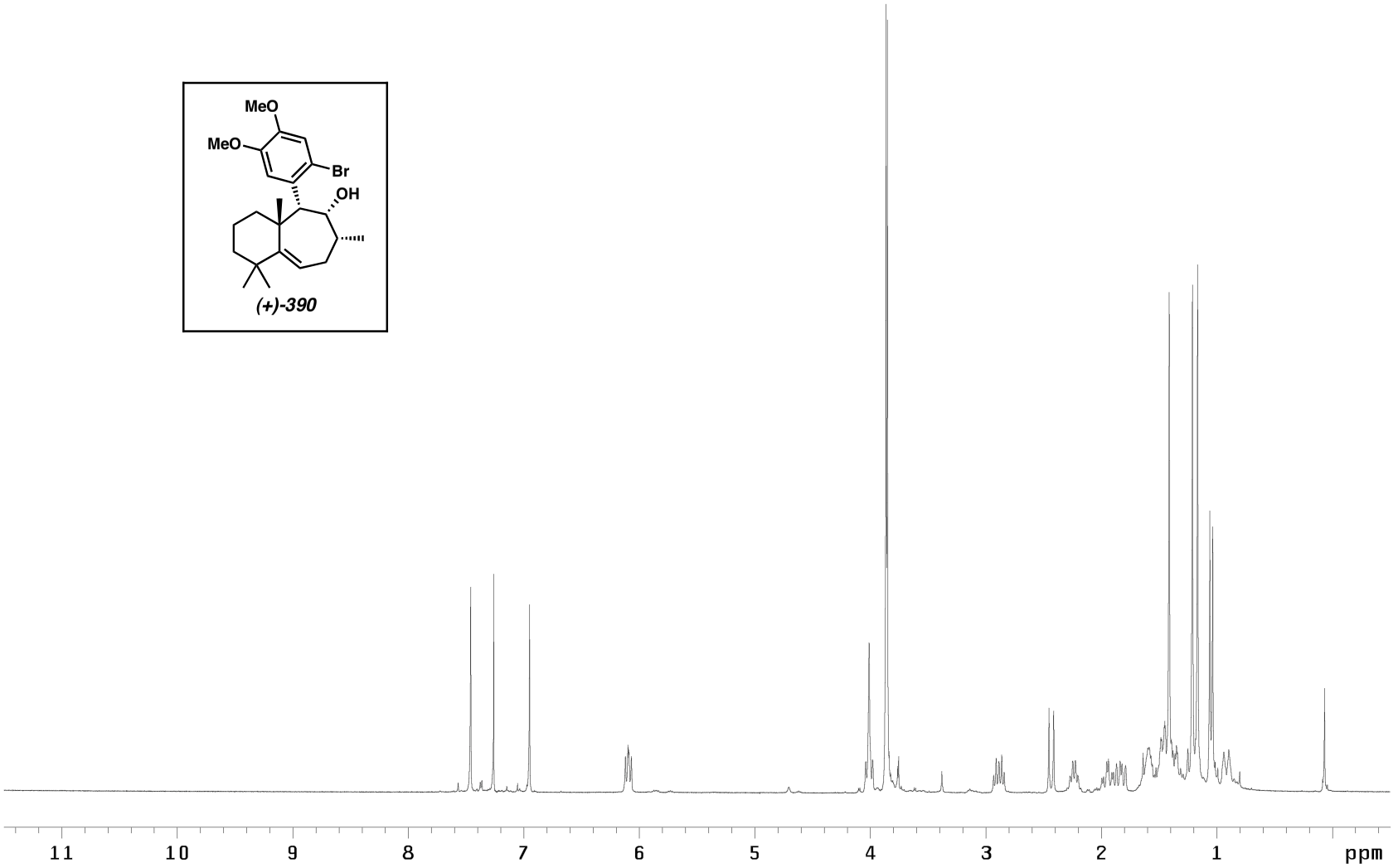


Figure A7.130 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **390**.

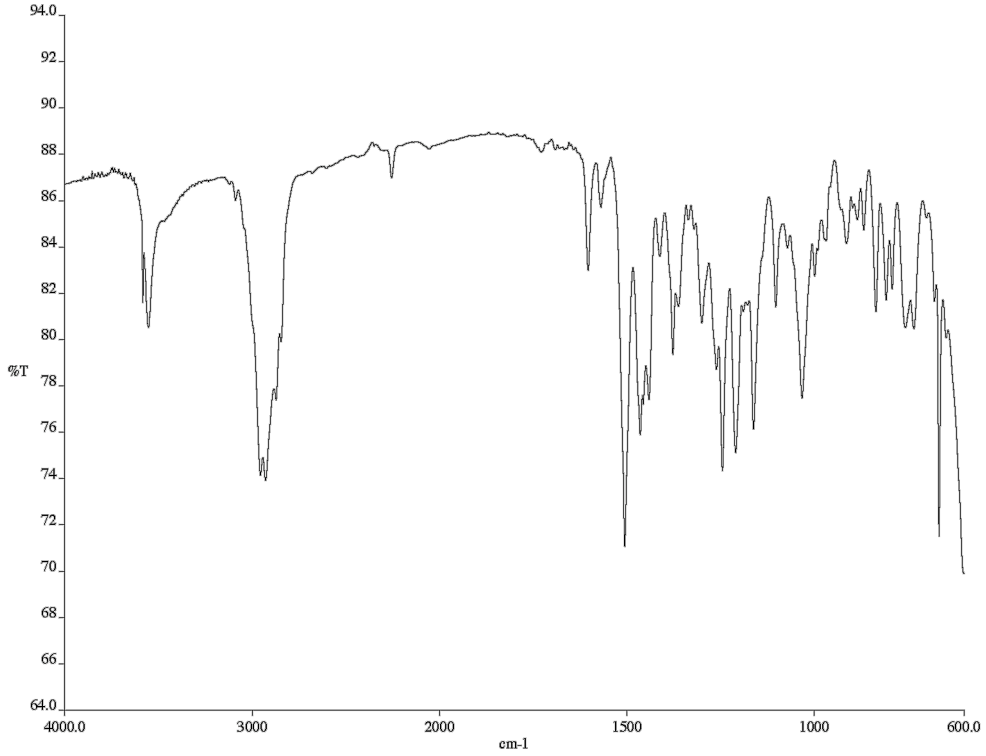


Figure A7.131 Infrared spectrum ($NaCl/CDCl_3$) of compound **390**.

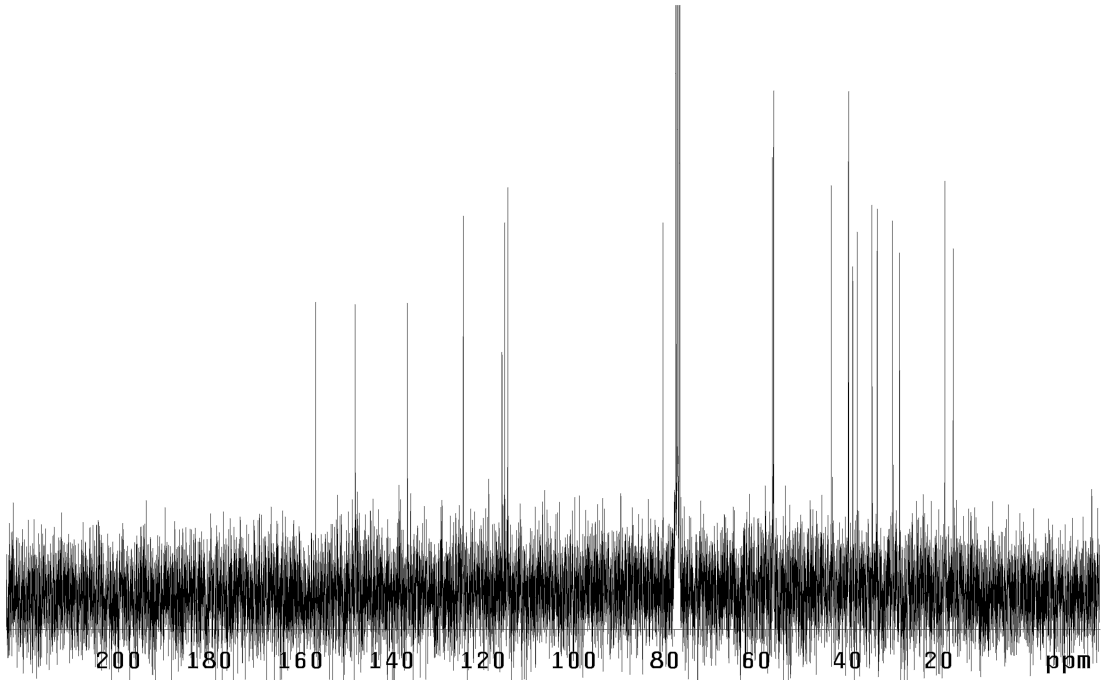


Figure A7.132 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **390**.

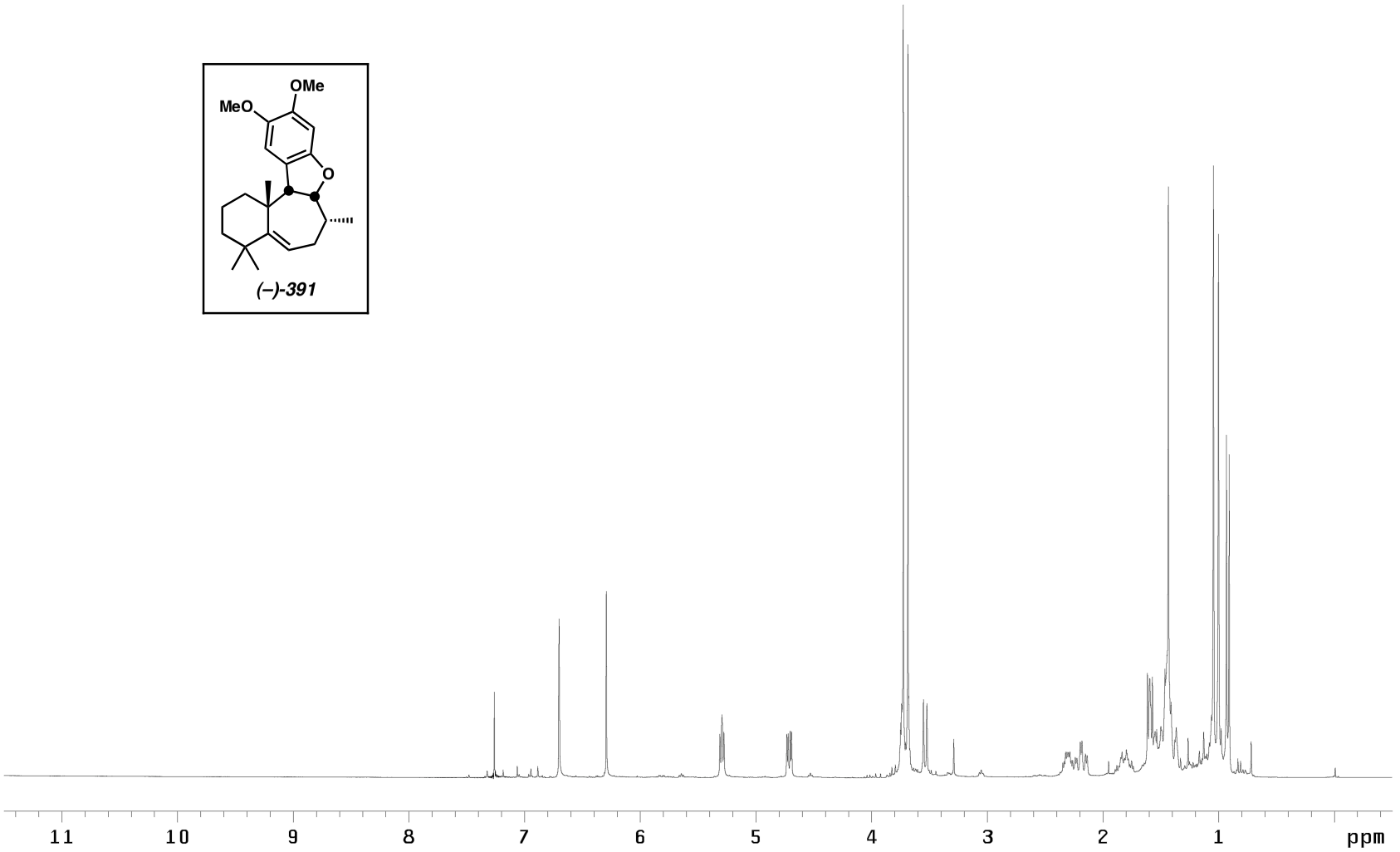


Figure A7.133 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **391**.

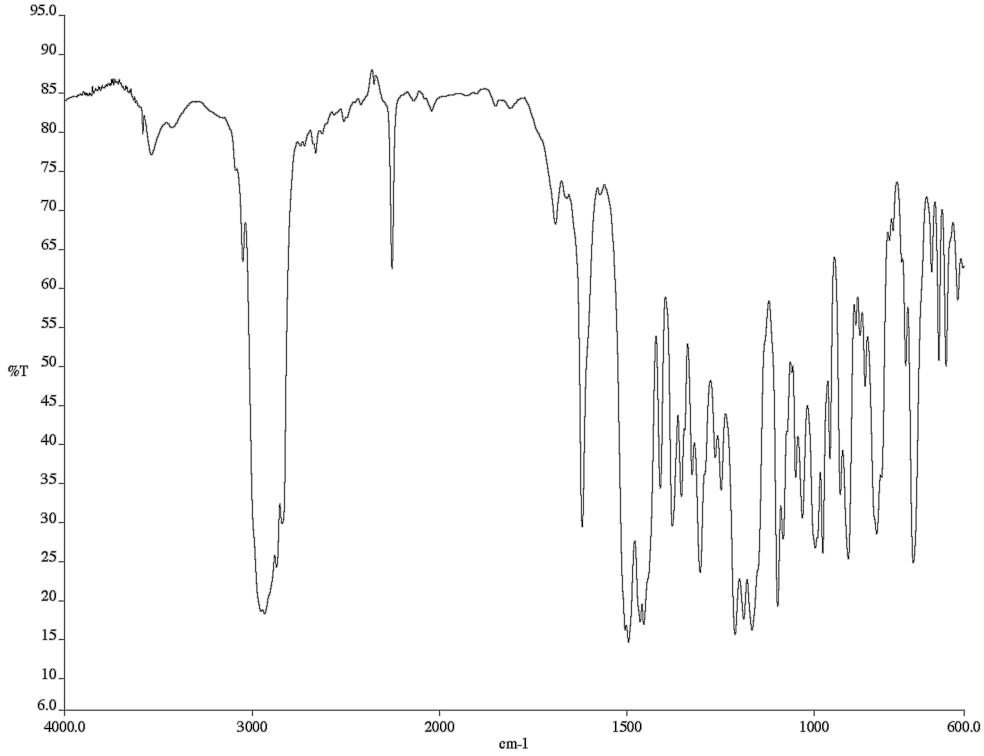


Figure A7.134 Infrared spectrum ($NaCl/CDCl_3$) of compound **391**.

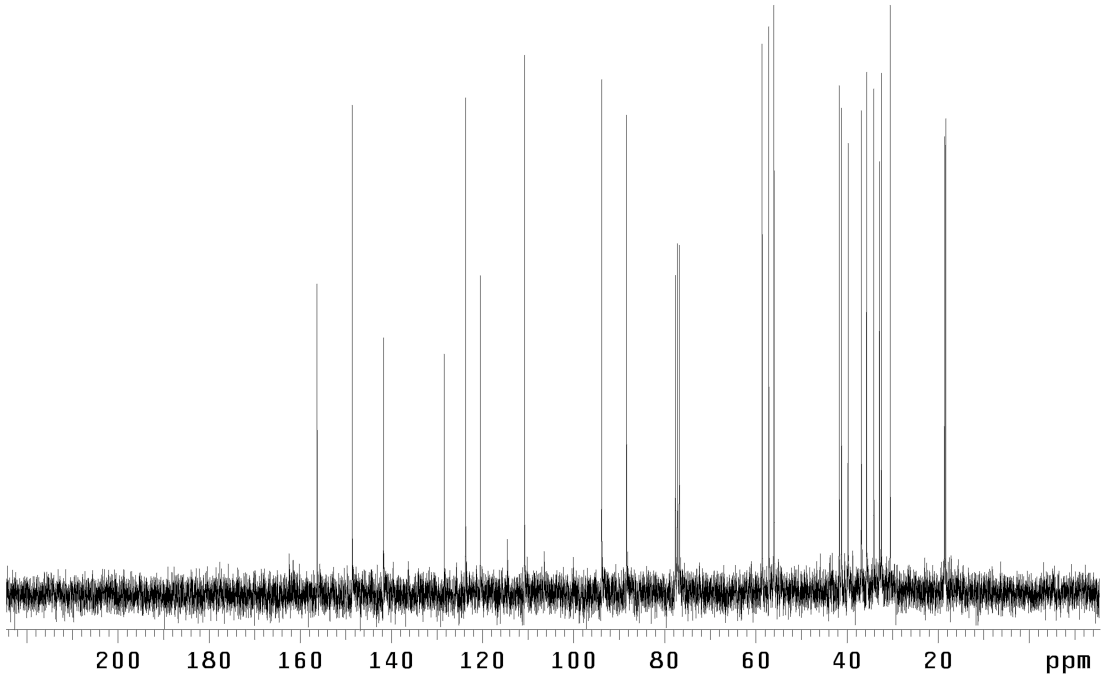


Figure A7.135 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **391**.

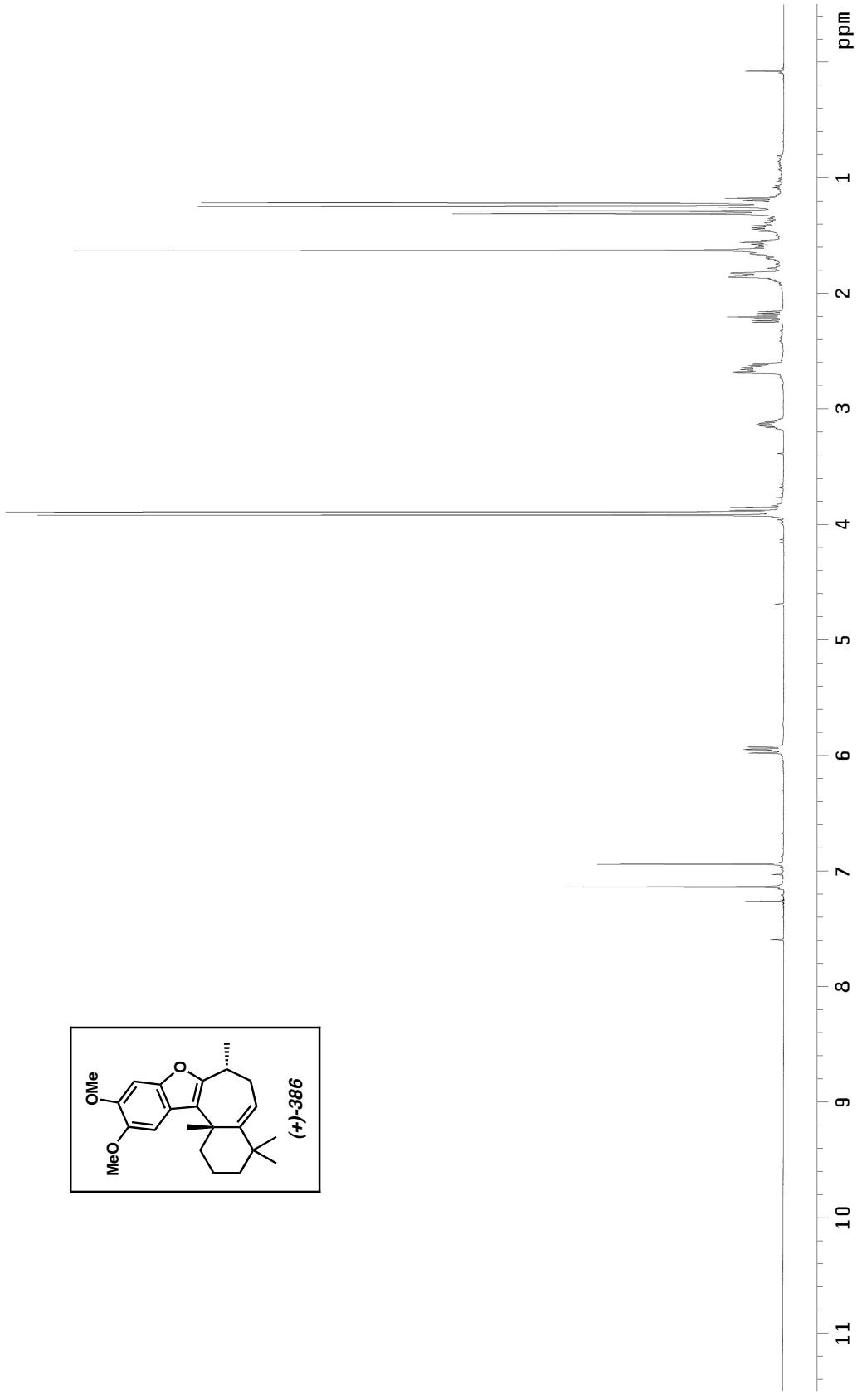


Figure A7.136 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **386**.

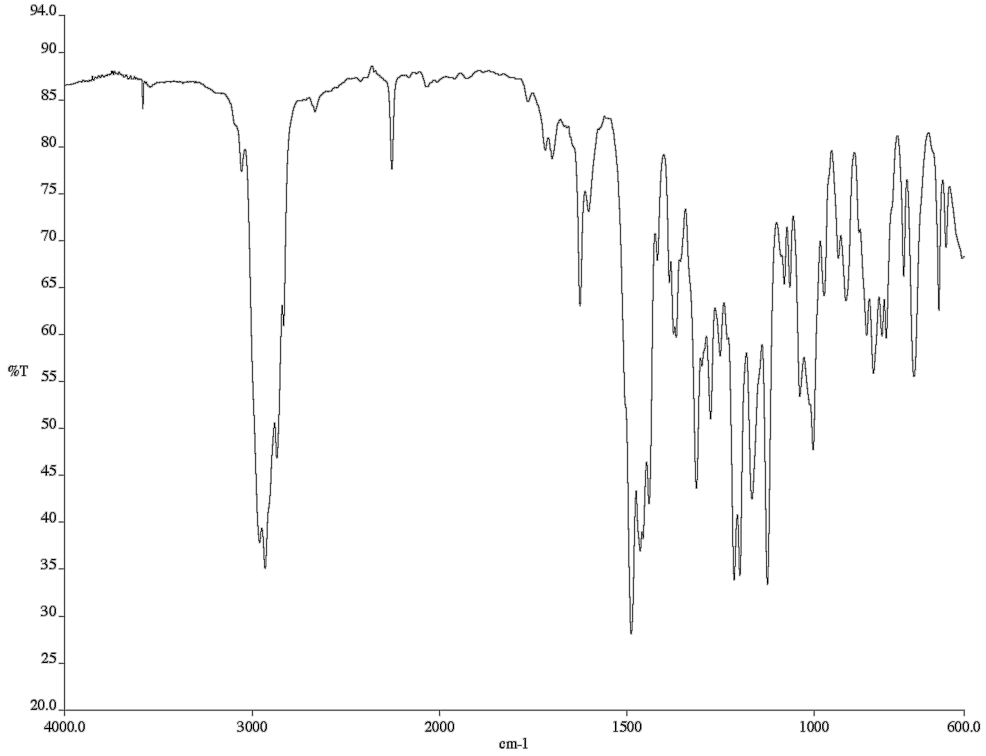


Figure A7.137 Infrared spectrum ($NaCl/CDCl_3$) of compound **386**.

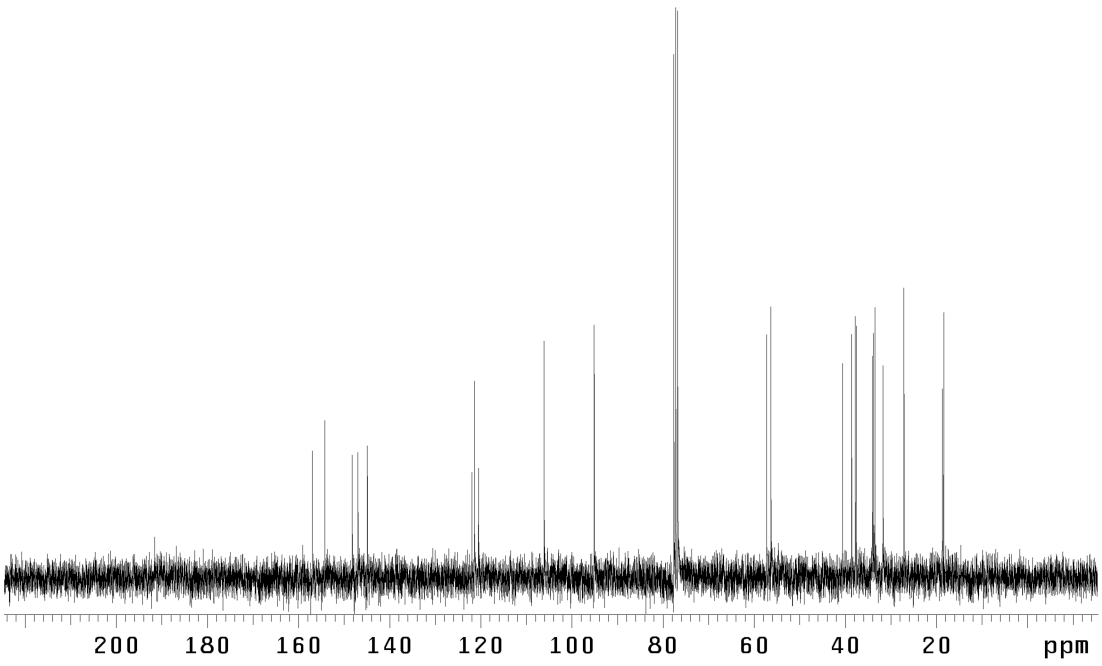


Figure A7.138 ^{13}C NMR (75 MHz, $CDCl_3$) of compound **386**.

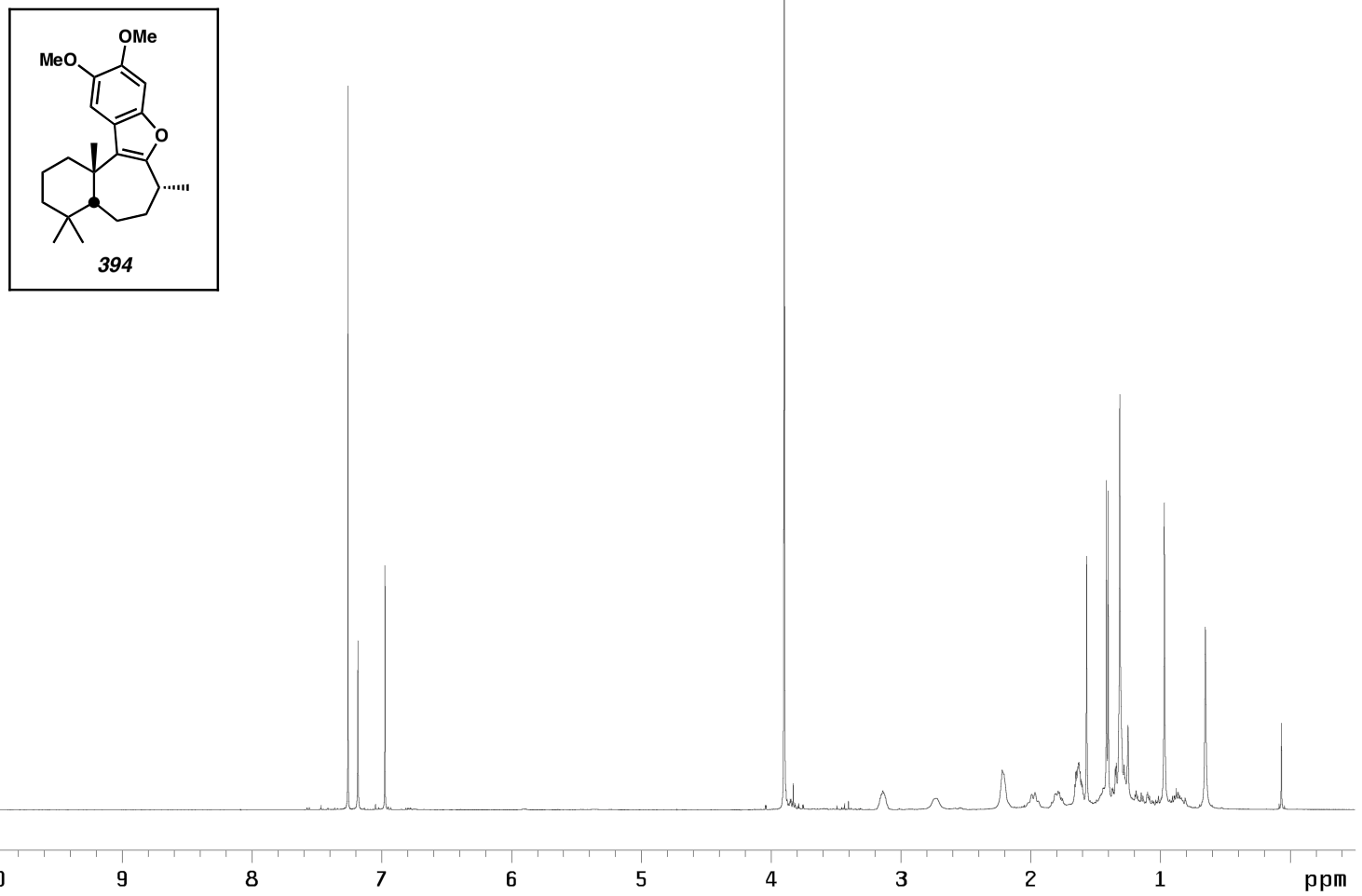


Figure A7.139 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **394**.

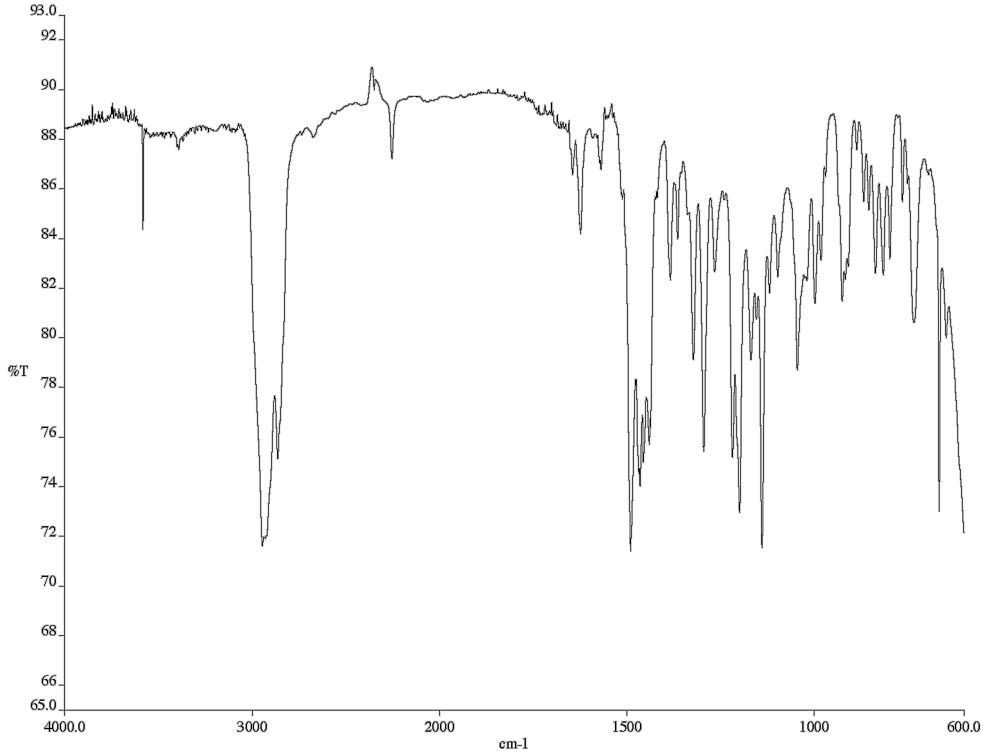


Figure A7.140 Infrared spectrum ($NaCl/CDCl_3$) of compound **394**.

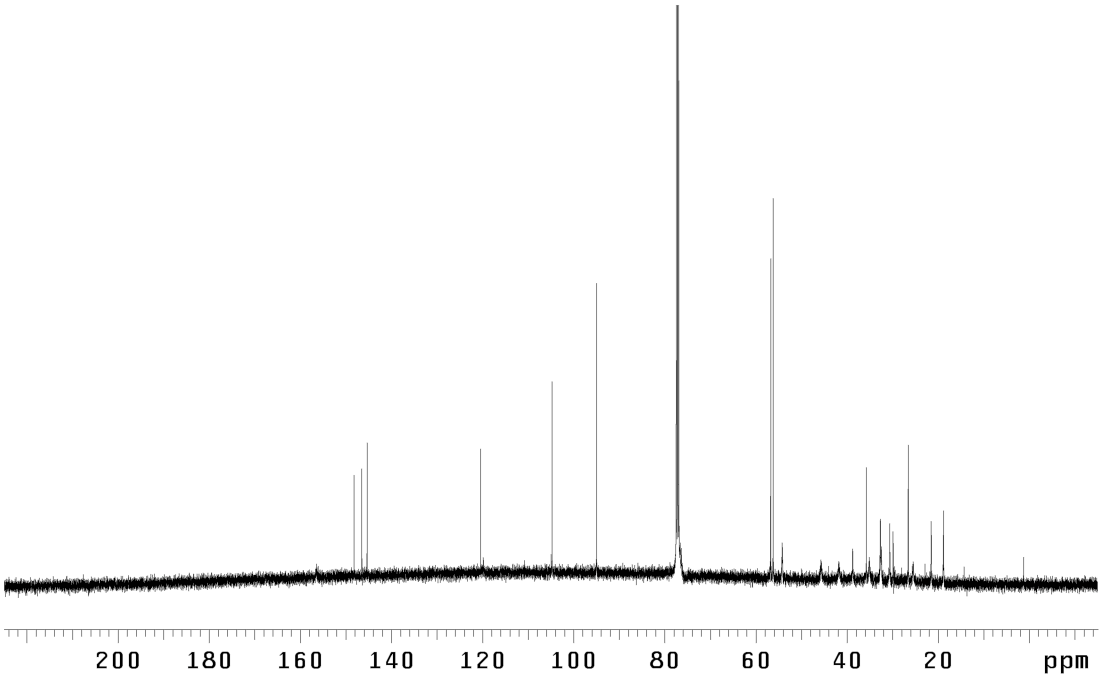


Figure A7.141 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **394**.

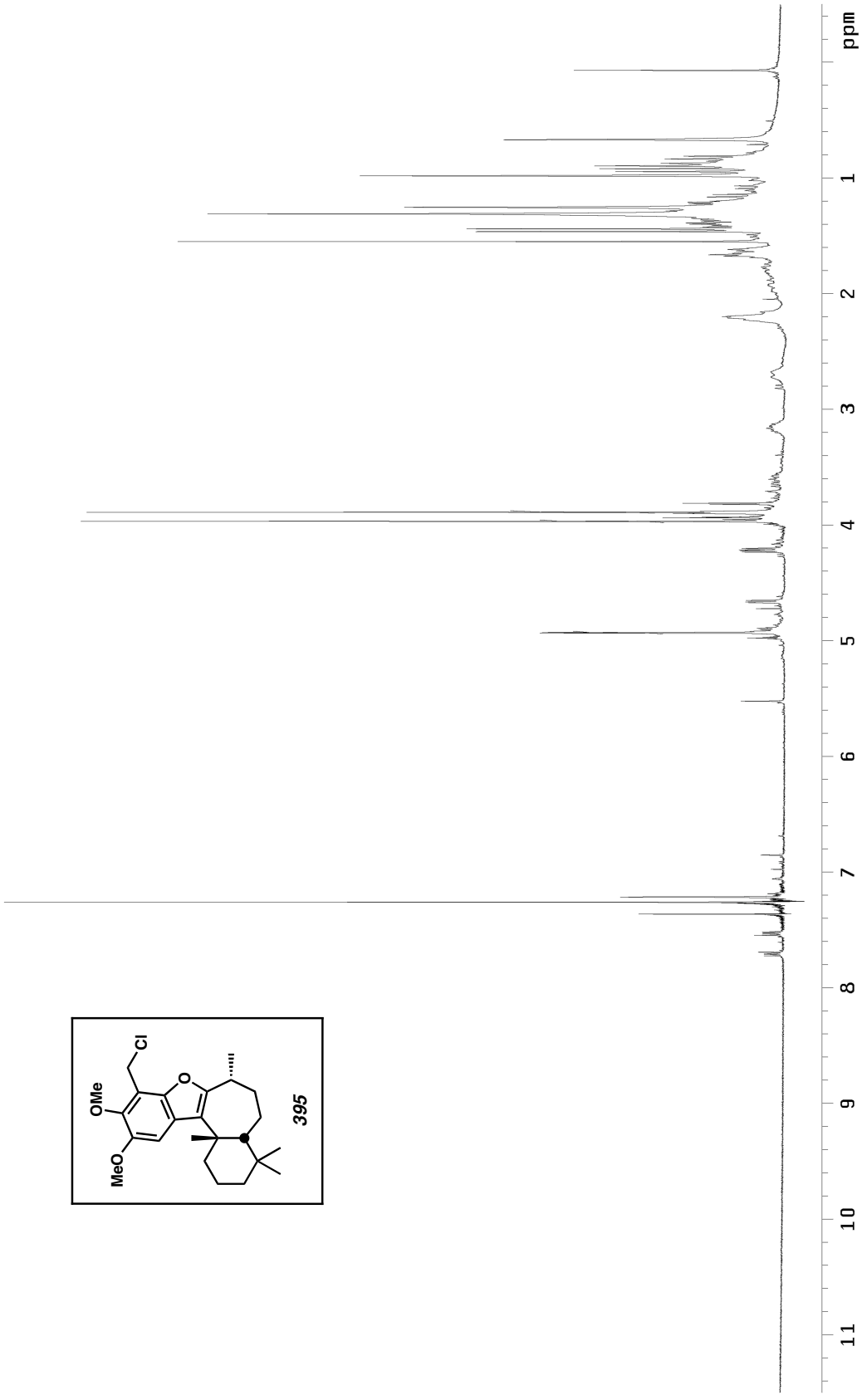


Figure A7.142 ^{1}H NMR (300 MHz, $CDCl_3$) of compound **395**.

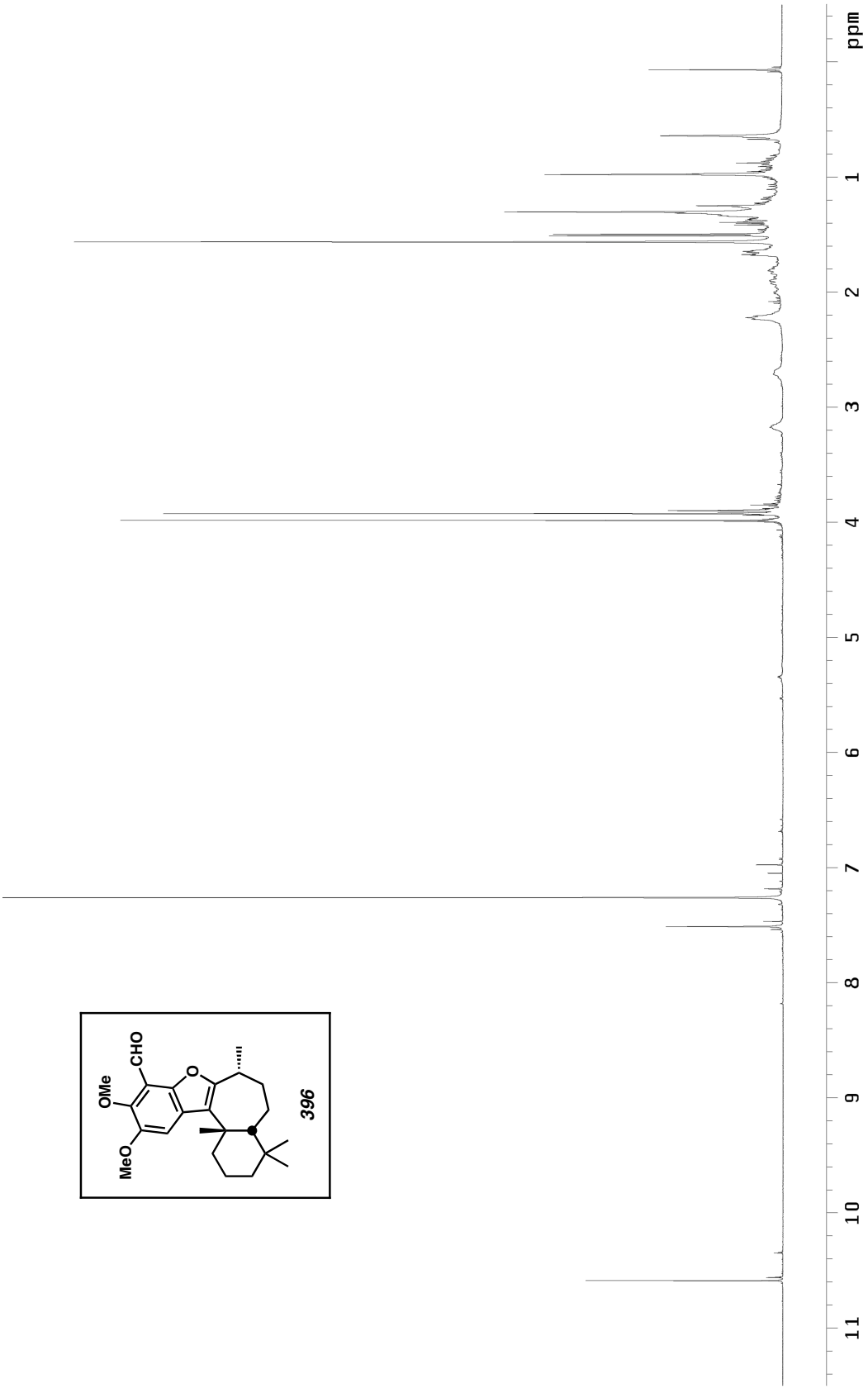


Figure A7.143 ^{1}H NMR (500 MHz, $CDCl_3$) of compound **396**.

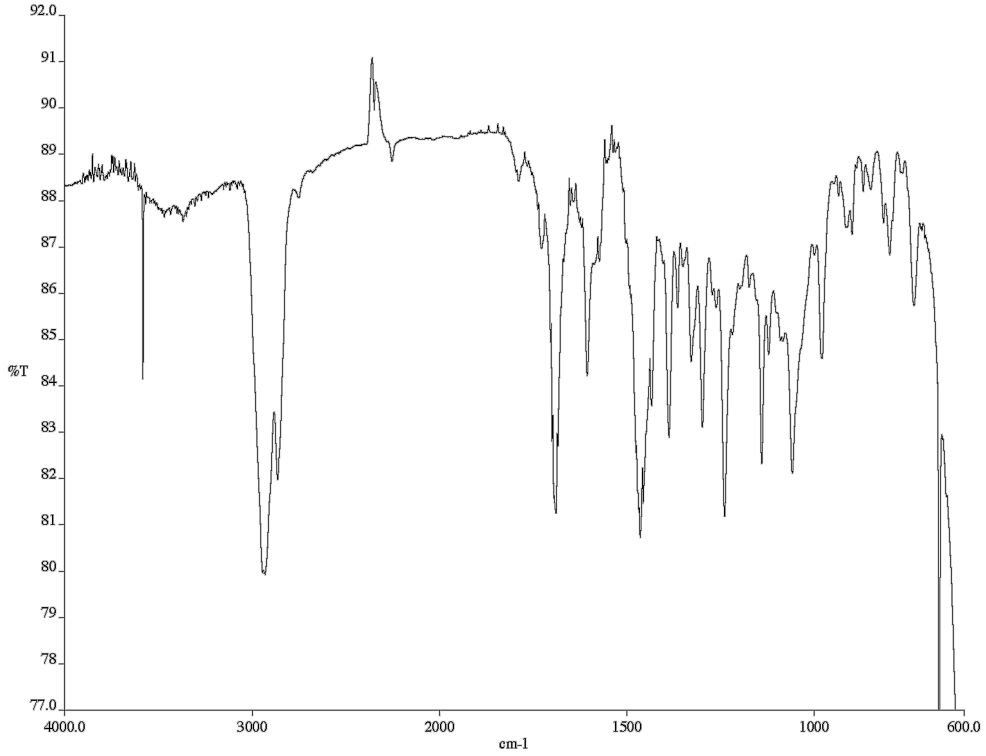


Figure A7.144 Infrared spectrum ($NaCl/CDCl_3$) of compound **396**.

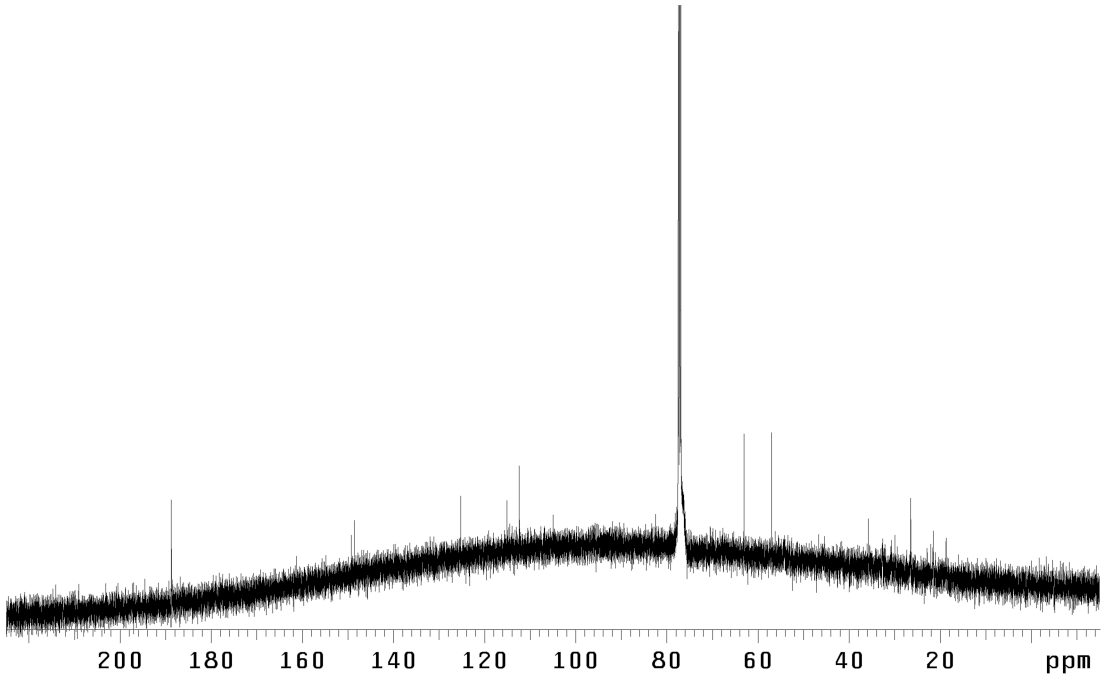


Figure A7.145 ^{13}C NMR (125 MHz, $CDCl_3$) of compound **396**.

Appendix EIGHT

X-Ray Crystallographic Data Relevant to Chapter 4

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 1 May 2006

Crystal Structure Analysis of:

319B

(shown below)

For Investigator: Ryan McFadden ext. 6131

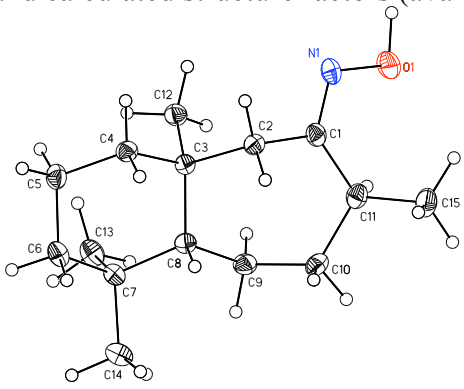
Advisor: B. M. Stoltz ext. 6064

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

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents



319B

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 606034. 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 606034."

Table 1. Crystal data and structure refinement for 319B (CCDC 606034).

Empirical formula	$C_{15}H_{27}NO$
Formula weight	237.38
Crystallization Solvent	Heptane
Crystal Habit	Column
Crystal size	0.41 x 0.15 x 0.13 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 6053 reflections used in lattice determination	2.39 to 30.07°	
Unit cell dimensions	a = 6.0159(7) Å b = 10.0422(12) Å c = 12.4023(14) Å	α= 74.349(2)° β= 81.140(2)° γ = 77.614(2)°
Volume	700.99(14) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.125 Mg/m^3	
F(000)	264	
Data collection program	Bruker SMART v5.630	
θ range for data collection	1.71 to 30.48°	
Completeness to θ = 30.48°	88.4 %	
Index ranges	$-8 \le h \le 8, -13 \le k \le 14, -17 \le l \le 17$	
Data collection scan type	ω scans at 7 ϕ settings	
Data reduction program	Bruker SAINT v6.45A	
Reflections collected	15201	
Independent reflections	3787 [R_{int}= 0.0535]	
Absorption coefficient	0.069 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.9911 and 0.9723	

Table 1 (cont.)

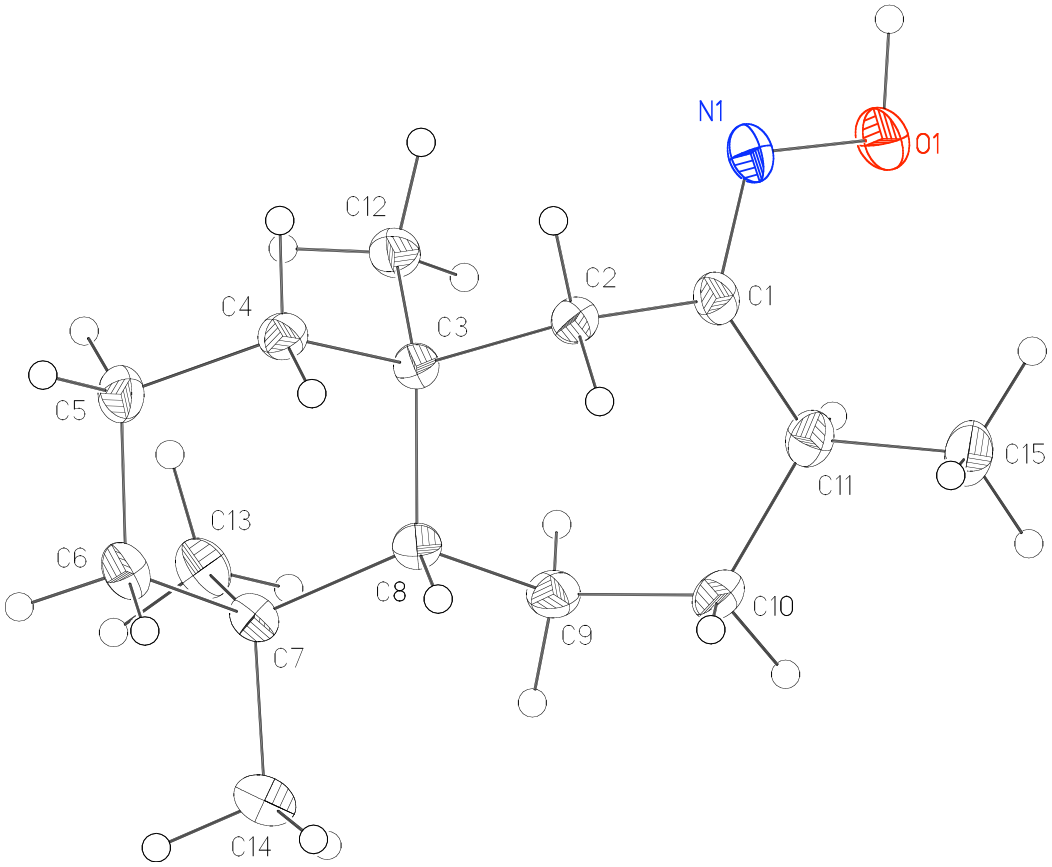
Structure solution and Refinement

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	3787 / 0 / 262
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.727
Final R indices [$I>2\sigma(I)$, 2680 reflections]	R1 = 0.0472, *w*R2 = 0.0748
R indices (all data)	R1 = 0.0689, *w*R2 = 0.0772
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.339 and -0.260 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.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C12
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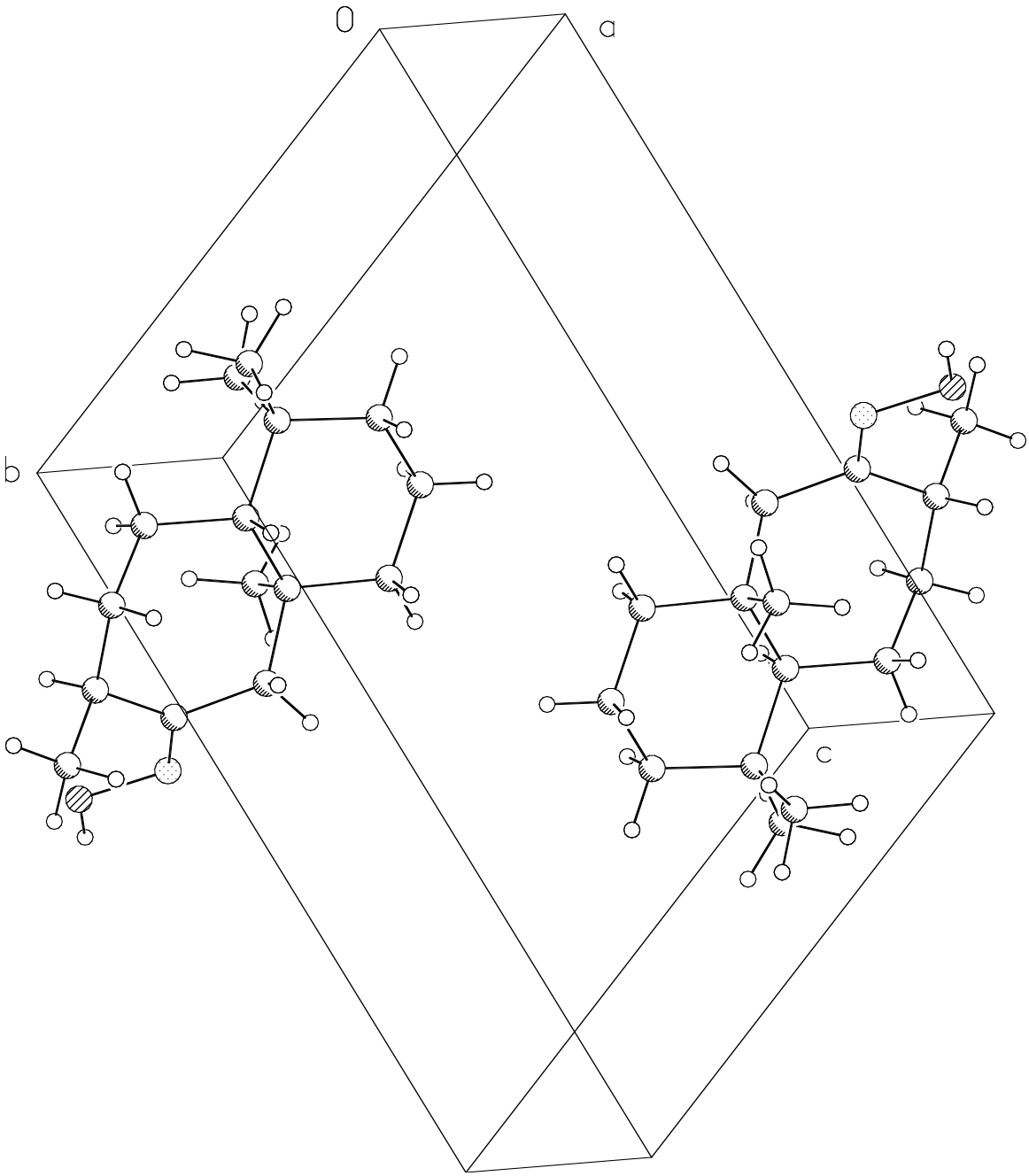
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a
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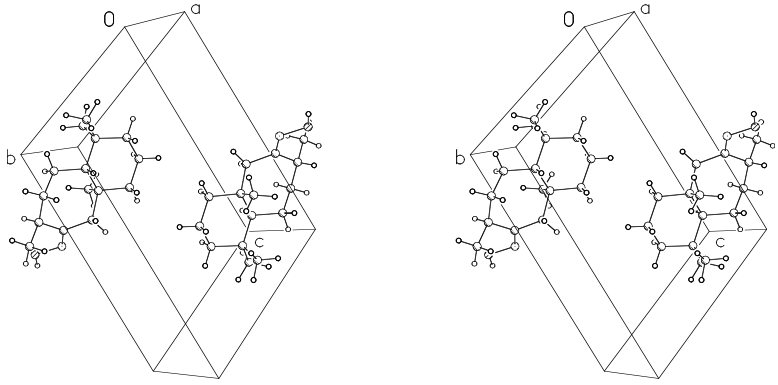

0
a
b
c
0
a
b
c

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 319B (CCDC 606034). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	-4505(1)	11144(1)	3840(1)	28(1)
N(1)	-2790(2)	9957(1)	4223(1)	21(1)
C(1)	-964(2)	9902(1)	3535(1)	18(1)
C(2)	877(2)	8645(1)	3887(1)	17(1)
C(3)	1046(2)	7415(1)	3314(1)	15(1)
C(4)	2524(2)	6123(1)	4021(1)	18(1)
C(5)	3103(2)	4868(1)	3493(1)	21(1)
C(6)	4334(2)	5257(1)	2315(1)	21(1)
C(7)	3040(2)	6534(1)	1514(1)	18(1)
C(8)	2286(2)	7777(1)	2102(1)	16(1)
C(9)	1074(2)	9121(1)	1332(1)	20(1)
C(10)	1234(2)	10493(1)	1604(1)	22(1)
C(11)	-655(2)	11007(1)	2448(1)	20(1)
C(12)	-1380(2)	7122(1)	3382(1)	19(1)
C(13)	1049(2)	6122(1)	1112(1)	24(1)
C(14)	4725(2)	6957(2)	471(1)	26(1)
C(15)	-230(3)	12347(1)	2687(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for 319B (CCDC 606034).

O(1)-N(1)	1.4241(11)	C(1)-C(2)-C(3)	115.86(9)
O(1)-H(1)	1.017(16)	C(1)-C(2)-H(2A)	109.5(6)
N(1)-C(1)	1.2844(14)	C(3)-C(2)-H(2A)	106.0(6)
C(1)-C(2)	1.5045(15)	C(1)-C(2)-H(2B)	109.3(6)
C(1)-C(11)	1.5119(15)	C(3)-C(2)-H(2B)	109.1(6)
C(2)-C(3)	1.5612(14)	H(2A)-C(2)-H(2B)	106.8(8)
C(2)-H(2A)	0.982(11)	C(12)-C(3)-C(4)	109.18(9)
C(2)-H(2B)	0.987(11)	C(12)-C(3)-C(8)	114.96(9)
C(3)-C(12)	1.5346(15)	C(4)-C(3)-C(8)	108.42(8)
C(3)-C(4)	1.5404(14)	C(12)-C(3)-C(2)	107.57(9)
C(3)-C(8)	1.5570(14)	C(4)-C(3)-C(2)	106.39(8)
C(4)-C(5)	1.5243(15)	C(8)-C(3)-C(2)	109.98(9)
C(4)-H(4A)	1.022(11)	C(5)-C(4)-C(3)	113.13(9)
C(4)-H(4B)	0.993(10)	C(5)-C(4)-H(4A)	109.2(6)
C(5)-C(6)	1.5226(16)	C(3)-C(4)-H(4A)	108.3(6)
C(5)-H(5A)	0.963(12)	C(5)-C(4)-H(4B)	110.5(6)
C(5)-H(5B)	1.017(11)	C(3)-C(4)-H(4B)	108.1(6)
C(6)-C(7)	1.5365(15)	H(4A)-C(4)-H(4B)	107.4(8)
C(6)-H(6A)	1.004(11)	C(6)-C(5)-C(4)	110.84(10)
C(6)-H(6B)	1.011(11)	C(6)-C(5)-H(5A)	109.6(7)
C(7)-C(13)	1.5369(15)	C(4)-C(5)-H(5A)	109.6(7)
C(7)-C(14)	1.5378(16)	C(6)-C(5)-H(5B)	110.0(6)
C(7)-C(8)	1.5626(15)	C(4)-C(5)-H(5B)	110.9(6)
C(8)-C(9)	1.5364(15)	H(5A)-C(5)-H(5B)	105.7(9)
C(8)-H(8)	0.985(10)	C(5)-C(6)-C(7)	114.42(10)
C(9)-C(10)	1.5297(16)	C(5)-C(6)-H(6A)	110.0(6)
C(9)-H(9A)	0.984(12)	C(7)-C(6)-H(6A)	109.6(6)
C(9)-H(9B)	1.021(10)	C(5)-C(6)-H(6B)	107.7(6)
C(10)-C(11)	1.5254(16)	C(7)-C(6)-H(6B)	109.0(6)
C(10)-H(10A)	0.980(11)	H(6A)-C(6)-H(6B)	105.8(8)
C(10)-H(10B)	0.985(11)	C(6)-C(7)-C(13)	110.26(10)
C(11)-C(15)	1.5327(16)	C(6)-C(7)-C(14)	106.92(9)
C(11)-H(11)	0.962(11)	C(13)-C(7)-C(14)	107.11(9)
C(12)-H(12A)	1.003(11)	C(6)-C(7)-C(8)	109.36(9)
C(12)-H(12B)	0.997(11)	C(13)-C(7)-C(8)	113.71(9)
C(12)-H(12C)	0.994(12)	C(14)-C(7)-C(8)	109.24(9)
C(13)-H(13A)	0.969(12)	C(9)-C(8)-C(3)	113.62(9)
C(13)-H(13B)	0.990(12)	C(9)-C(8)-C(7)	112.57(9)
C(13)-H(13C)	0.996(13)	C(3)-C(8)-C(7)	115.88(9)
C(14)-H(14A)	0.979(13)	C(9)-C(8)-H(8)	106.2(6)
C(14)-H(14B)	1.005(13)	C(3)-C(8)-H(8)	103.6(6)
C(14)-H(14C)	0.997(12)	C(7)-C(8)-H(8)	103.5(6)
C(15)-H(15A)	1.014(12)	C(10)-C(9)-C(8)	115.08(9)
C(15)-H(15B)	1.000(12)	C(10)-C(9)-H(9A)	107.3(6)
C(15)-H(15C)	0.989(13)	C(8)-C(9)-H(9A)	107.9(6)
		C(10)-C(9)-H(9B)	108.8(6)
N(1)-O(1)-H(1)	103.0(8)	C(8)-C(9)-H(9B)	111.7(6)
C(1)-N(1)-O(1)	112.92(9)	H(9A)-C(9)-H(9B)	105.6(9)
N(1)-C(1)-C(2)	114.97(10)	C(11)-C(10)-C(9)	115.95(10)
N(1)-C(1)-C(11)	123.26(10)	C(11)-C(10)-H(10A)	106.0(6)
C(2)-C(1)-C(11)	121.77(10)	C(9)-C(10)-H(10A)	109.8(6)

C(11)-C(10)-H(10B)	108.9(6)
C(9)-C(10)-H(10B)	110.2(6)
H(10A)-C(10)-H(10B)	105.5(9)
C(1)-C(11)-C(10)	113.20(9)
C(1)-C(11)-C(15)	110.49(9)
C(10)-C(11)-C(15)	110.64(10)
C(1)-C(11)-H(11)	106.7(7)
C(10)-C(11)-H(11)	107.9(7)
C(15)-C(11)-H(11)	107.6(7)
C(3)-C(12)-H(12A)	113.6(6)
C(3)-C(12)-H(12B)	114.1(7)
H(12A)-C(12)-H(12B)	106.8(9)
C(3)-C(12)-H(12C)	109.7(6)
H(12A)-C(12)-H(12C)	105.8(9)
H(12B)-C(12)-H(12C)	106.3(9)
C(7)-C(13)-H(13A)	109.4(7)
C(7)-C(13)-H(13B)	111.3(7)
H(13A)-C(13)-H(13B)	106.3(9)
C(7)-C(13)-H(13C)	112.7(7)
H(13A)-C(13)-H(13C)	107.4(9)
H(13B)-C(13)-H(13C)	109.5(9)
C(7)-C(14)-H(14A)	111.5(7)
C(7)-C(14)-H(14B)	113.5(7)
H(14A)-C(14)-H(14B)	107.7(10)
C(7)-C(14)-H(14C)	110.1(7)
H(14A)-C(14)-H(14C)	105.0(10)
H(14B)-C(14)-H(14C)	108.7(10)
C(11)-C(15)-H(15A)	111.2(7)
C(11)-C(15)-H(15B)	107.8(7)
H(15A)-C(15)-H(15B)	110.5(9)
C(11)-C(15)-H(15C)	110.3(7)
H(15A)-C(15)-H(15C)	107.5(10)
H(15B)-C(15)-H(15C)	109.6(10)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^4$) for 319B (CCDC 606034). 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)229(5)	225(5)	330(5)	-51(4)	-13(4)	65(4)
N(1)201(5)	170(5)	247(5)	-64(4)	-44(4)	23(4)
C(1)195(6)	172(6)	201(6)	-80(5)	-24(5)	-39(5)
C(2)175(6)	167(6)	161(6)	-36(5)	-17(5)	-42(5)
C(3)147(5)	158(6)	159(5)	-40(4)	-19(4)	-29(5)
C(4)185(6)	180(6)	162(6)	-23(5)	-13(5)	-25(5)
C(5)225(6)	159(6)	229(6)	-37(5)	-42(5)	2(5)
C(6)179(6)	205(6)	254(6)	-103(5)	-27(5)	4(5)
C(7)164(6)	193(6)	181(6)	-65(5)	-8(5)	-13(5)
C(8)147(6)	180(6)	165(6)	-40(5)	-21(5)	-36(5)
C(9)222(6)	212(6)	149(6)	-26(5)	-8(5)	-30(5)
C(10)250(7)	180(6)	195(6)	10(5)	-6(5)	-52(5)
C(11)205(6)	167(6)	227(6)	-22(5)	-51(5)	-17(5)
C(12)164(6)	202(7)	218(6)	-61(5)	-3(5)	-41(5)
C(13)228(7)	257(7)	247(7)	-112(6)	-42(6)	-10(6)
C(14)237(7)	306(8)	232(7)	-100(6)	35(5)	-33(6)
C(15)351(8)	171(7)	310(7)	-56(6)	-31(6)	-39(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 319B (CCDC 606034).

	x	y	z	U_{iso}
H(1)	-5840(30)	11001(16)	4446(13)	67(5)
H(2A)	611(17)	8240(11)	4700(9)	18(3)
H(2B)	2372(19)	8949(11)	3752(8)	18(3)
H(4A)	4005(19)	6406(11)	4113(9)	22(3)
H(4B)	1692(17)	5871(11)	4782(9)	14(3)
H(5A)	4060(20)	4102(13)	3959(10)	29(3)
H(5B)	1668(19)	4503(11)	3465(9)	24(3)
H(6A)	4678(17)	4427(12)	1973(9)	21(3)
H(6B)	5870(19)	5459(11)	2391(9)	21(3)
H(8)	3746(18)	7985(10)	2218(8)	12(3)
H(9A)	1780(19)	9161(11)	556(10)	23(3)
H(9B)	-608(19)	9093(11)	1319(9)	19(3)
H(10A)	1180(18)	11255(12)	916(10)	21(3)
H(10B)	2728(19)	10415(11)	1870(9)	18(3)
H(11)	-2074(19)	11239(11)	2116(9)	22(3)
H(12A)	-1412(17)	6178(12)	3264(9)	20(3)
H(12B)	-2364(19)	7833(12)	2839(10)	27(3)
H(12C)	-2179(19)	7128(11)	4145(10)	23(3)
H(13A)	1653(19)	5487(13)	629(10)	31(3)
H(13B)	110(20)	6953(13)	651(10)	29(3)
H(13C)	50(20)	5634(13)	1746(10)	35(4)
H(14A)	5910(20)	7379(12)	643(10)	31(3)
H(14B)	3970(20)	7639(13)	-182(11)	37(4)
H(14C)	5570(20)	6104(13)	222(10)	32(3)
H(15A)	-1510(20)	12715(12)	3225(10)	26(3)
H(15B)	-120(20)	13063(13)	1952(11)	31(3)
H(15C)	1210(20)	12151(13)	3037(10)	41(4)

Table 6. Hydrogen bonds for 319B (CCDC 606034) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(1)#1	1.017(16)	1.843(16)	2.7884(13)	153.2(12)
O(1)-H(1)...O(1)#1	1.017(16)	2.584(15)	3.2256(17)	120.8(10)

Symmetry transformations used to generate equivalent atoms:
#1 -x-1,-y+2,-z+1

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 23 January 2007

Crystal Structure Analysis of:

370

(shown below)

For Investigator: Ryan McFadden ext. 6131

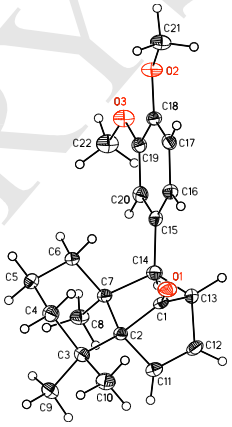
Advisor: B. M. Stoltz ext. 6064

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 has been placed on hold pending further instructions from me. The deposition number is 634511. 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 634511."

Table 1. Crystal data and structure refinement for 370 (CCDC 634511).

Empirical formula	$C_{22}H_{28}O_3$
Formula weight	340.44
Crystallization Solvent	Hexanes/ethylacetate
Crystal Habit	Fragment
Crystal size	0.26 x 0.22 x 0.17 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 8994 reflections used in lattice determination	2.29 to 34.45°
Unit cell dimensions	a = 23.2678(15) Å b = 13.8762(9) Å β= 108.548(2)° c = 11.8122(8) Å
Volume	3615.7(4) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	C2/c
Density (calculated)	1.251 Mg/m^3
F(000)	1472
Data collection program	Bruker SMART v5.630
θ range for data collection	1.73 to 34.57°
Completeness to θ = 34.57°	89.7 %
Index ranges	$-36 \le h \le 36$, $-21 \le k \le 21$, $-18 \le l \le 18$
Data collection scan type	ω scans at 5 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	37303
Independent reflections	37303 [R_{int}= 0.0000]
Absorption coefficient	0.081 mm^{-1}
Absorption correction	TWINABS
Max. and min. transmission	1.0000 and 0.7508

Table 1 (cont.)

Structure solution and Refinement

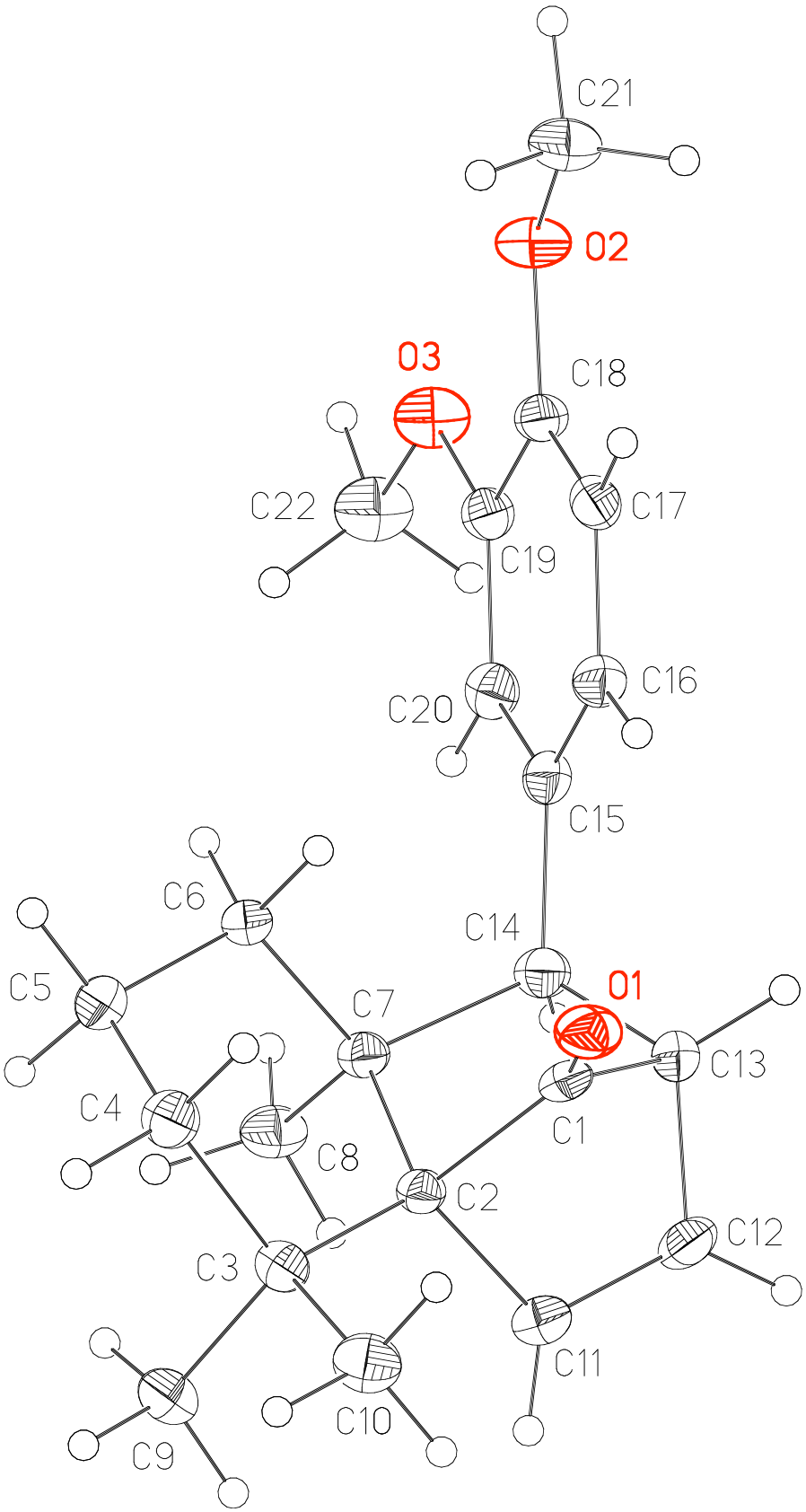
Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	37303 / 0 / 339
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.182
Final R indices [I>2σ(I), 21619 reflections]	R1 = 0.0601, *w*R2 = 0.1106
R indices (all data)	R1 = 0.1018, *w*R2 = 0.1173
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.570 and -0.427 e.Å^{-3}

Special Refinement Details

This crystal is a non-merohedral twin and data were integrated and the structure refined as such.. The twin law (179.8º rotation around the *c*-axis) was determined using CELL_NOW on a group of orientation reflections, 690/781 reflections were assigned to domain 1 and 452/781 were assigned to domain 2, 89 of which were exclusive to this domain.

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.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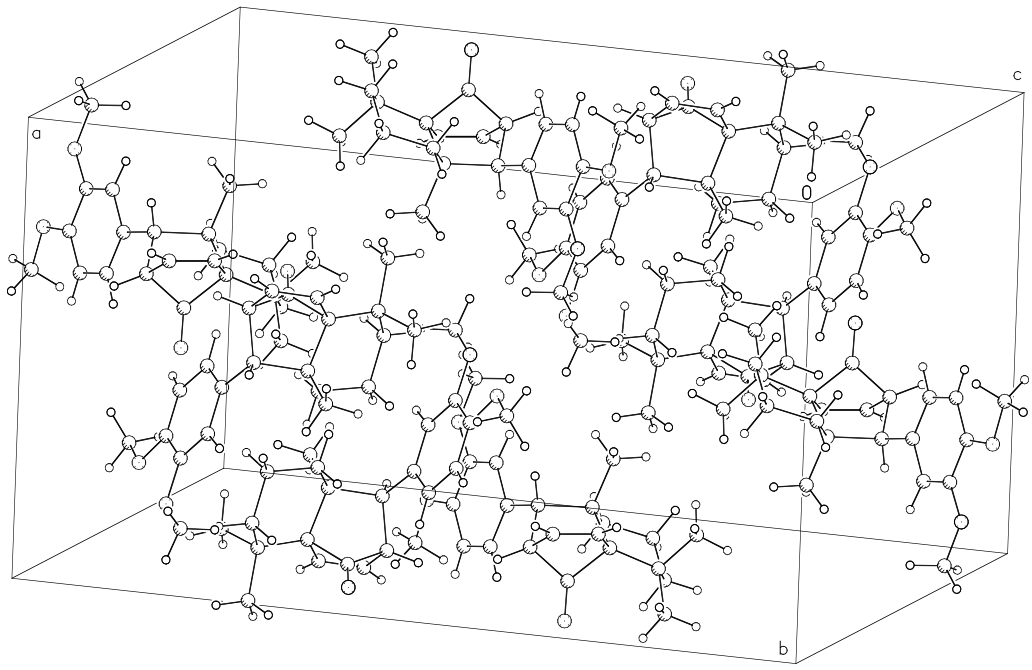
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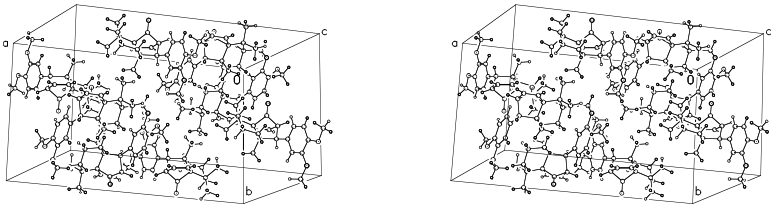
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a
c
b

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 370 (CCDC 634511). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	1481(1)	5234(1)	2876(1)	28(1)
O(2)	684(1)	1843(1)	6684(1)	28(1)
O(3)	623(1)	556(1)	5078(1)	28(1)
C(1)	1332(1)	4548(1)	2231(1)	21(1)
C(2)	1679(1)	3923(1)	1575(1)	16(1)
C(3)	2328(1)	4235(1)	1655(1)	20(1)
C(4)	2752(1)	4090(1)	2946(1)	24(1)
C(5)	2709(1)	3082(1)	3421(1)	25(1)
C(6)	2065(1)	2867(1)	3409(1)	20(1)
C(7)	1593(1)	2918(1)	2152(1)	19(1)
C(8)	1643(1)	2037(1)	1419(1)	25(1)
C(9)	2569(1)	3662(1)	794(1)	26(1)
C(10)	2332(1)	5298(1)	1303(1)	27(1)
C(11)	1203(1)	4003(1)	347(1)	21(1)
C(12)	657(1)	4078(1)	469(1)	25(1)
C(13)	721(1)	4029(1)	1779(1)	23(1)
C(14)	912(1)	2985(1)	2204(1)	21(1)
C(15)	836(1)	2720(1)	3400(1)	20(1)
C(16)	873(1)	3401(1)	4275(1)	22(1)
C(17)	826(1)	3130(1)	5385(1)	22(1)
C(18)	736(1)	2184(1)	5622(1)	20(1)
C(19)	699(1)	1478(1)	4742(1)	21(1)
C(20)	746(1)	1757(1)	3647(1)	21(1)
C(21)	803(1)	2524(1)	7636(1)	29(1)
C(22)	592(1)	-189(1)	4224(1)	33(1)

Table 3. Bond lengths [Å] and angles [°] for 370 (CCDC 634511).

O(1)-C(1)	1.1998(9)	C(21)-H(21B)	1.028(9)
O(2)-C(18)	1.3818(9)	C(21)-H(21C)	0.987(8)
O(2)-C(21)	1.4275(10)	C(22)-H(22A)	1.018(10)
O(3)-C(19)	1.3677(9)	C(22)-H(22B)	1.033(8)
O(3)-C(22)	1.4304(10)	C(22)-H(22C)	1.036(10)
C(1)-C(13)	1.5297(12)		
C(1)-C(2)	1.5508(11)	C(18)-O(2)-C(21)	115.88(7)
C(2)-C(11)	1.5236(10)	C(19)-O(3)-C(22)	116.95(7)
C(2)-C(3)	1.5449(11)	O(1)-C(1)-C(13)	130.05(8)
C(2)-C(7)	1.5923(11)	O(1)-C(1)-C(2)	132.08(8)
C(3)-C(9)	1.5311(12)	C(13)-C(1)-C(2)	97.86(7)
C(3)-C(10)	1.5324(12)	C(11)-C(2)-C(3)	115.97(7)
C(3)-C(4)	1.5432(11)	C(11)-C(2)-C(1)	95.61(6)
C(4)-C(5)	1.5230(12)	C(3)-C(2)-C(1)	117.85(6)
C(4)-H(4A)	0.992(8)	C(11)-C(2)-C(7)	108.61(6)
C(4)-H(4B)	0.996(8)	C(3)-C(2)-C(7)	118.24(6)
C(5)-C(6)	1.5221(12)	C(1)-C(2)-C(7)	96.91(6)
C(5)-H(5A)	1.030(8)	C(9)-C(3)-C(10)	106.53(7)
C(5)-H(5B)	0.966(8)	C(9)-C(3)-C(4)	109.50(7)
C(6)-C(7)	1.5426(10)	C(10)-C(3)-C(4)	109.68(7)
C(6)-H(6A)	0.988(8)	C(9)-C(3)-C(2)	111.79(7)
C(6)-H(6B)	0.996(7)	C(10)-C(3)-C(2)	110.12(7)
C(7)-C(8)	1.5238(11)	C(4)-C(3)-C(2)	109.18(7)
C(7)-C(14)	1.6080(11)	C(5)-C(4)-C(3)	112.82(7)
C(8)-H(8A)	0.980(8)	C(5)-C(4)-H(4A)	112.3(4)
C(8)-H(8B)	0.967(8)	C(3)-C(4)-H(4A)	107.6(5)
C(8)-H(8C)	0.992(9)	C(5)-C(4)-H(4B)	107.9(5)
C(9)-H(9A)	1.001(9)	C(3)-C(4)-H(4B)	108.1(4)
C(9)-H(9B)	0.993(9)	H(4A)-C(4)-H(4B)	108.0(6)
C(9)-H(9C)	0.981(9)	C(6)-C(5)-C(4)	110.87(7)
C(10)-H(10A)	0.988(9)	C(6)-C(5)-H(5A)	109.0(4)
C(10)-H(10B)	0.997(8)	C(4)-C(5)-H(5A)	110.2(4)
C(10)-H(10C)	0.982(9)	C(6)-C(5)-H(5B)	109.2(5)
C(11)-C(12)	1.3280(12)	C(4)-C(5)-H(5B)	109.6(5)
C(11)-H(11)	0.901(7)	H(5A)-C(5)-H(5B)	107.9(6)
C(12)-C(13)	1.5082(12)	C(5)-C(6)-C(7)	113.39(7)
C(12)-H(12)	0.951(8)	C(5)-C(6)-H(6A)	108.5(4)
C(13)-C(14)	1.5519(11)	C(7)-C(6)-H(6A)	109.1(4)
C(13)-H(13)	0.950(8)	C(5)-C(6)-H(6B)	111.6(4)
C(14)-C(15)	1.5240(11)	C(7)-C(6)-H(6B)	108.4(4)
C(14)-H(14)	0.968(7)	H(6A)-C(6)-H(6B)	105.5(6)
C(15)-C(16)	1.3829(11)	C(8)-C(7)-C(6)	110.53(7)
C(15)-C(20)	1.3977(11)	C(8)-C(7)-C(2)	114.65(7)
C(16)-C(17)	1.4002(12)	C(6)-C(7)-C(2)	107.68(6)
C(16)-H(16)	1.004(8)	C(8)-C(7)-C(14)	108.84(7)
C(17)-C(18)	1.3713(11)	C(6)-C(7)-C(14)	112.01(7)
C(17)-H(17)	0.939(8)	C(2)-C(7)-C(14)	102.98(6)
C(18)-C(19)	1.4120(11)	C(7)-C(8)-H(8A)	112.0(5)
C(19)-C(20)	1.3868(11)	C(7)-C(8)-H(8B)	111.8(5)
C(20)-H(20)	1.015(7)	H(8A)-C(8)-H(8B)	107.1(7)
C(21)-H(21A)	0.990(9)	C(7)-C(8)-H(8C)	109.6(5)

H(8A)-C(8)-H(8C)	109.5(7)	H(21A)-C(21)-H(21C)	108.8(7)
H(8B)-C(8)-H(8C)	106.7(7)	H(21B)-C(21)-H(21C)	110.8(7)
C(3)-C(9)-H(9A)	112.5(5)	O(3)-C(22)-H(22A)	109.2(5)
C(3)-C(9)-H(9B)	109.4(5)	O(3)-C(22)-H(22B)	106.3(5)
H(9A)-C(9)-H(9B)	110.4(7)	H(22A)-C(22)-H(22B)	109.3(7)
C(3)-C(9)-H(9C)	110.5(5)	O(3)-C(22)-H(22C)	109.9(5)
H(9A)-C(9)-H(9C)	106.6(7)	H(22A)-C(22)-H(22C)	110.2(7)
H(9B)-C(9)-H(9C)	107.2(7)	H(22B)-C(22)-H(22C)	111.8(7)
C(3)-C(10)-H(10A)	110.1(5)		
C(3)-C(10)-H(10B)	107.9(5)		
H(10A)-C(10)-H(10B)	108.8(7)		
C(3)-C(10)-H(10C)	113.3(5)		
H(10A)-C(10)-H(10C)	108.1(7)		
H(10B)-C(10)-H(10C)	108.5(7)		
C(12)-C(11)-C(2)	109.50(8)		
C(12)-C(11)-H(11)	123.9(4)		
C(2)-C(11)-H(11)	126.6(5)		
C(11)-C(12)-C(13)	108.78(8)		
C(11)-C(12)-H(12)	130.1(5)		
C(13)-C(12)-H(12)	121.1(5)		
C(12)-C(13)-C(1)	96.58(7)		
C(12)-C(13)-C(14)	107.33(7)		
C(1)-C(13)-C(14)	100.80(6)		
C(12)-C(13)-H(13)	116.9(5)		
C(1)-C(13)-H(13)	116.6(5)		
C(14)-C(13)-H(13)	115.8(5)		
C(15)-C(14)-C(13)	114.77(7)		
C(15)-C(14)-C(7)	115.31(6)		
C(13)-C(14)-C(7)	103.12(6)		
C(15)-C(14)-H(14)	108.7(4)		
C(13)-C(14)-H(14)	109.7(4)		
C(7)-C(14)-H(14)	104.6(5)		
C(16)-C(15)-C(20)	118.28(8)		
C(16)-C(15)-C(14)	122.09(7)		
C(20)-C(15)-C(14)	119.60(7)		
C(15)-C(16)-C(17)	120.80(8)		
C(15)-C(16)-H(16)	120.5(4)		
C(17)-C(16)-H(16)	118.7(4)		
C(18)-C(17)-C(16)	120.70(8)		
C(18)-C(17)-H(17)	120.1(5)		
C(16)-C(17)-H(17)	119.2(5)		
C(17)-C(18)-O(2)	125.25(7)		
C(17)-C(18)-C(19)	119.42(7)		
O(2)-C(18)-C(19)	115.32(7)		
O(3)-C(19)-C(20)	126.04(7)		
O(3)-C(19)-C(18)	114.77(7)		
C(20)-C(19)-C(18)	119.19(7)		
C(19)-C(20)-C(15)	121.61(8)		
C(19)-C(20)-H(20)	120.7(4)		
C(15)-C(20)-H(20)	117.6(4)		
O(2)-C(21)-H(21A)	109.7(5)		
O(2)-C(21)-H(21B)	103.5(4)		
H(21A)-C(21)-H(21B)	111.6(7)		
O(2)-C(21)-H(21C)	112.4(5)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 370 (CCDC 634511). 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)	395(4)	242(3)	222(3)	3(3)	138(3)	53(3)
O(2)	369(4)	292(3)	190(3)	-1(3)	115(3)	-64(3)
O(3)	365(4)	231(3)	251(3)	-21(3)	101(3)	-68(3)
C(1)	263(5)	231(5)	134(4)	83(4)	61(3)	32(4)
C(2)	179(4)	175(4)	143(4)	-1(3)	56(3)	3(3)
C(3)	204(4)	213(5)	192(4)	-6(3)	60(3)	-12(3)
C(4)	186(4)	314(5)	212(5)	-24(4)	56(4)	-23(4)
C(5)	197(5)	344(6)	191(4)	33(4)	47(4)	49(4)
C(6)	215(4)	237(5)	162(4)	19(4)	66(3)	43(4)
C(7)	190(4)	211(4)	154(4)	1(3)	54(3)	3(3)
C(8)	306(5)	232(5)	210(5)	-8(4)	94(4)	-18(4)
C(9)	260(5)	306(6)	255(5)	-1(4)	117(4)	3(4)
C(10)	265(5)	266(5)	290(5)	9(4)	98(4)	-44(4)
C(11)	259(5)	207(5)	166(4)	8(4)	55(4)	-14(4)
C(12)	222(5)	295(5)	197(4)	67(4)	10(4)	0(4)
C(13)	190(4)	293(5)	235(5)	58(4)	91(4)	56(4)
C(14)	212(4)	237(5)	177(4)	13(4)	50(3)	-12(4)
C(15)	140(4)	252(5)	207(4)	24(4)	39(3)	5(3)
C(16)	202(4)	227(5)	239(5)	35(4)	79(4)	9(4)
C(17)	192(4)	247(5)	207(4)	-27(4)	64(3)	16(4)
C(18)	170(4)	262(5)	183(4)	25(4)	57(3)	-14(4)
C(19)	152(4)	237(5)	222(4)	29(4)	38(3)	-25(4)
C(20)	171(4)	257(5)	202(4)	-18(4)	38(3)	-23(4)
C(21)	380(6)	307(6)	219(5)	-22(4)	128(4)	-24(5)
C(22)	453(7)	236(6)	314(6)	-27(4)	137(5)	-30(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 370 (CCDC 634511).

	x	y	z	U_{iso}
H(4A)	3170(4)	4250(5)	2959(7)	23(2)
H(4B)	2632(3)	4559(6)	3468(7)	23(2)
H(5A)	2835(3)	2575(6)	2907(7)	20(2)
H(5B)	2981(4)	3027(6)	4229(8)	32(2)
H(6A)	1955(3)	3335(5)	3935(6)	14(2)
H(6B)	2036(3)	2221(6)	3755(6)	14(2)
H(8A)	2064(4)	1905(5)	1462(7)	22(2)
H(8B)	1413(4)	2116(6)	584(8)	29(2)
H(8C)	1473(4)	1466(6)	1705(7)	28(2)
H(9A)	2575(4)	2951(6)	943(7)	30(2)
H(9B)	2982(4)	3894(6)	856(8)	35(3)
H(9C)	2312(4)	3763(6)	-34(8)	32(2)
H(10A)	2060(4)	5396(6)	478(8)	33(3)
H(10B)	2753(4)	5468(6)	1337(7)	26(2)
H(10C)	2205(4)	5737(6)	1830(7)	28(2)
H(11)	1272(3)	4011(5)	-362(6)	7(2)
H(12)	269(4)	4139(6)	-120(7)	26(2)
H(13)	399(4)	4292(5)	2014(7)	20(2)
H(14)	684(3)	2531(5)	1606(6)	15(2)
H(16)	941(3)	4098(6)	4131(6)	18(2)
H(17)	868(3)	3601(6)	5976(7)	20(2)
H(20)	739(3)	1260(5)	3013(7)	16(2)
H(21A)	1225(4)	2762(6)	7834(7)	31(2)
H(21B)	741(4)	2132(6)	8327(7)	31(2)
H(21C)	524(4)	3080(6)	7436(7)	30(2)
H(22A)	230(4)	-69(7)	3483(9)	51(3)
H(22B)	529(4)	-826(6)	4621(7)	29(2)
H(22C)	989(4)	-199(7)	4001(8)	47(3)

Appendix NINE

Compounds Submitted for PI3K Biological Screening

Table A9.1 Compounds Submitted for PI3K Biological Screening: Part 1

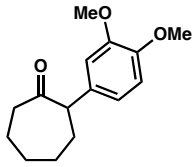
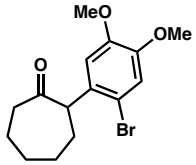
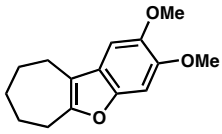
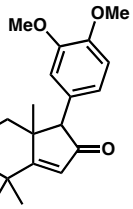
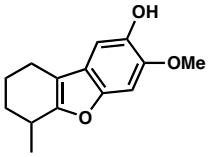
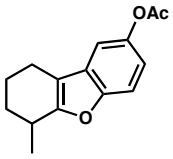
Compound Structure	Cantley#	Notebook#	%ee	Quantity (mg)	Storage Method
 ***(±)-398***	1	16RMM2-1129135	0	12	Solution in Benzene
 ***(±)-399***	2	16RMM1-1212203	0	6.8	Solution in Benzene
 ***(±)-400***	3	16RMM1-1213207	NA	4.3	Solution in Benzene
 (7.5 to 1.0 dr) ***(±)-348***	4	16RMM1-1107101	0	6.1	Solid
 ***(±)-334***	5	15RMM1-0917163	0	4.0	Solution in Benzene
 ***(±)-401***	6	14RMM1-0809259	0	1.5	Solution in Benzene

Table A9.2 Compounds Submitted for PI3K Biological Screening: Part 2

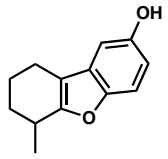
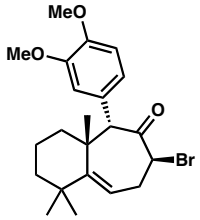
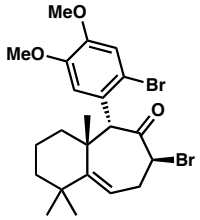
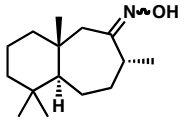
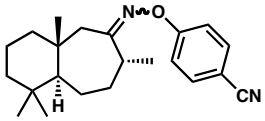
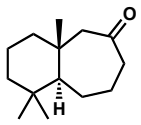
Compound Structure	Cantley#	Notebook#	%ee	Quantity (mg)	Storage Method
 *(±)-331*	7	14RMM1-0706161	0	5	Solution in Benzene
 *(±)-376*	8	16RMM2-0121289	0	30±5	Solution in Benzene
 *(±)-377*	9	16RMM1-0119289	0	2.0	Solid
 *(±)-319A and (±)-319B*	10	17RMM1-0227145	0	9.7	Solid
 *(±)-323A and (±)-323B*	11	14RMM1-0619109	0	3.0	Solution in Benzene
 *(±)-305*	12	16RMM2-0118287	0	3.1	Solution in Benzene

Table A9.3 Compounds Submitted for PI3K Biological Screening: Part 3

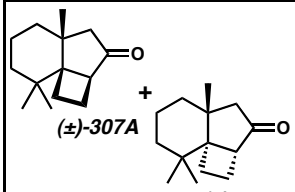
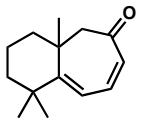
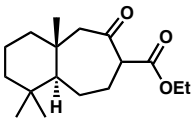
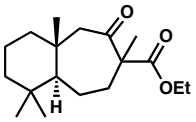
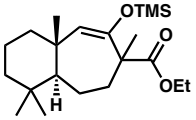
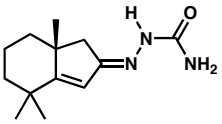
Compound Structure	Cantley#	Notebook#	%ee	Quantity (mg)	Storage Method
 ***(±)-307A*** + ***(±)-307B*** (2 : 1 mixture; major diastereomer unassigned)	13	13RMM1-0324231	0	8.7	Solid
 ***(±)-318***	14	13RMM2-0907277	0	2.2	Solid
 ***(±)-361ABC*** (tautomeric mixture)	15	17RMM1-012437	0	2.1	Solid
 ***(±)-362***	16	17RMMc-0209103	0	6.0	Solution in Benzene
 ***(±)-363***	17	17RMMc-0211107	0	8.6	Solution in Benzene
 ***(+)-246***	18	15RMM1-0906111	95	16	Solid

Table A9.4 Compounds Submitted for PI3K Biological Screening: Part 4

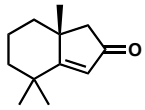
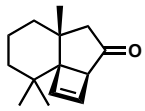
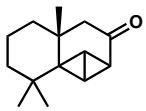
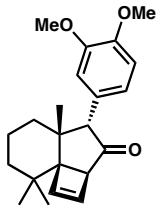
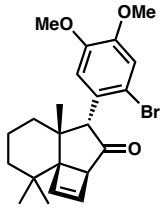
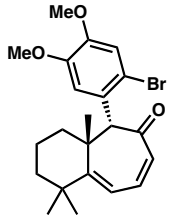
Compound Structure	Cantley#	Notebook#	%ee	Quantity (mg)	Storage Method
 *(+)-143*	19	19RMM6-090937	95	10	Neat Oil
 *(+)-312*	20	19RMM1-091151	95	8±3 Compound is Volatile!	Solution in Benzene
 *(–)-313*	21	19RMM4-090937	95	2.6±0.6	Solution in Benzene
 *(±)-369*	22	17RMM2-0211113	0	7.3	Solid
 *(+)-379*	23	19RMM1-091471	95	2.1	Solid
 *(–)-380*	24	19RMM1-091675	95	6.0	Solid

Table A9.5 Compounds Submitted for PI3K Biological Screening: Part 5

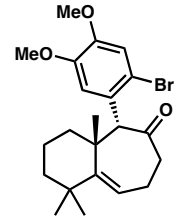
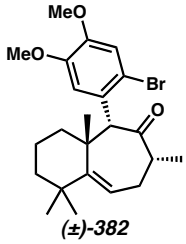
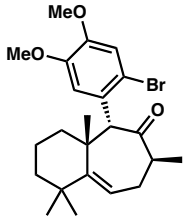
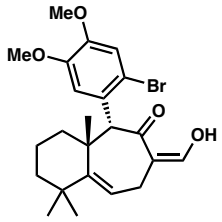
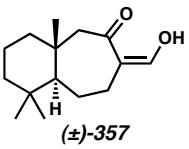
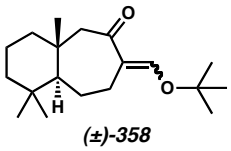
Compound Structure	Cantley#	Notebook#	%ee	Quantity (mg)	Storage Method
 *(+)-381*	25	19RMM1-091889	95	1.6	Solid
 *(±)-382*	26	17RMM1-0425227	0	3.3	Solution in Benzene
 *(8R,10S,11R)-383*	27	19RMMmethylepi	95	3.8	Solution in Benzene
 *(±)-402*	28	19RMM1-091155	0	3.2	Solution in Benzene
 *(±)-357*	29	16RMM1-0103235	0	3.3	Solution in Benzene
 *(±)-358*	30	16RMM2-0103235	0	3.5	Solution in Benzene

Table A9.6 Compounds Submitted for PI3K Biological Screening: Part 6

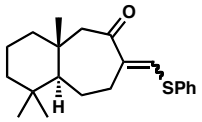
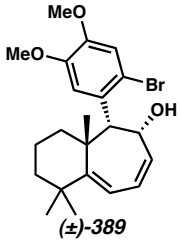
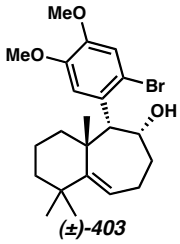
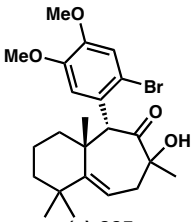
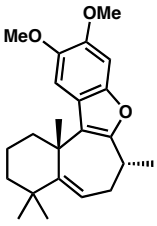
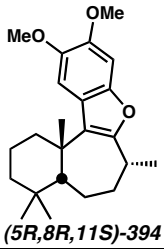
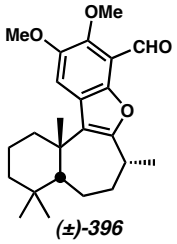
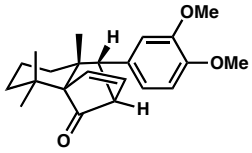
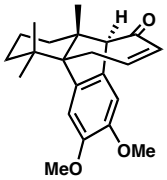
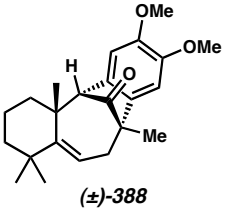
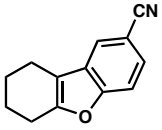
Compound Structure	Cantley#	Notebook#	%ee	Quantity (mg)	Storage Method
 *(±)-359*	31	16RMM3-0114261	0	6.8	Solution in Benzene
 *(±)-389*	32	18RMM2-071897	0	1.8	Solution in Benzene
 *(±)-403*	33	18RMMx-0718101	0	8±2	Solution in Benzene
 *(±)-385*	34	18RMM5-070851	0	4.2	Solution in Benzene
 *(±)-386*	35	18RMMc-0722119	0	1.5	Solution in Benzene

Table A9.7 Compounds Submitted for PI3K Biological Screening: Part 7

Compound Structure	Cantley#	Notebook#	%ee	Quantity (mg)	Storage Method
 *(5R,8R,11S)-394*	36	19RMM1-1026197	95	2.5	Solution in Benzene
 *(±)-396*	37	19RMM1-1024191	0	1.0	Solution in Benzene
 *(±)-370*	38	16RMM5-1130137	0	4.0	Solution in Benzene
 *(±)-373*	39	17RMM2-0318197	0	2.0±0.5	Solution in Benzene
 *(±)-388*	40	17RMM1-0504233	0	1.4	Solution in Benzene
 *322*	41	17RMM1-0312171	NA	1.0	Solid

Appendix Ten

Cross References to Characterization Binders and Notebooks

Table A10.1 Cross References for Compounds from Chapter 2: Thujopsene

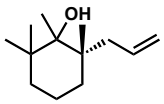
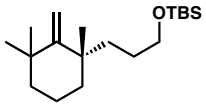
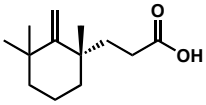
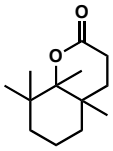
Characterization Binder #	Structure (Thesis #)	Spectral Data
TH01	 *99A and 99B*	^{1}H NMR: 1-jm-062007-112H ^{13}C NMR : 1-jm-062007-112C13C IR: jm-1-061907-111NaCD
TH02	 *(–)-104*	^{1}H NMR: 18RMM1-0820221H ^{13}C NMR : 18RMM1-0820221C13C IR: 18RMM1-0820221NaCD
TH03	 *(–)-94*	^{1}H NMR: 18RMM1-0822229H ^{13}C NMR : 18RMM1-822229C13C IR: 1jm-072707157NaCD
TH04	 *103A and 103B*	^{1}H NMR: 19RMMx-lactoneH ^{13}C NMR : 19RMMx-lactoneC IR: 19RMMx-lactoneNaCD

Table A10.2 Cross References for Compounds from Chapter 2: Dysidiolide

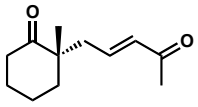
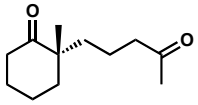
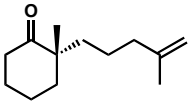
Characterization Binder #	Structure (Thesis #)	Spectral Data
DY01	 *(–)-113*	^{1}H NMR: 7RMM1-0211109H ^{13}C NMR : 17RMM1-0211109C13C IR: 17RMM1-0211109NaCD
DY02	 *(–)-112*	^{1}H NMR: 17RMMc-0212115H ^{13}C NMR : 17RMMc-0212115C13C IR: 17RMMc-0212115NaCD
DY03	 *(–)-109*	^{1}H NMR: 17RMM1-0219139H ^{13}C NMR : 17RMM1-0219137C13C IR: 17RMM1-0218137NaCD

Table A10.3 Cross References for Compounds from Chapter 2: Aspidospermine

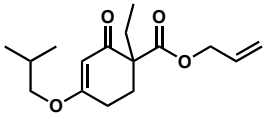
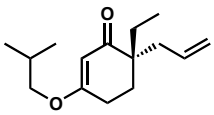
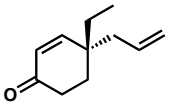
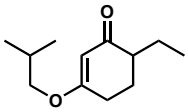
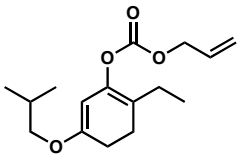
Characterization Binder #	Structure (Thesis #)	Spectral Data
AS01	 ***121***	^{1}H NMR: 17RMM2-0228151H ^{13}C NMR : 17RMM2-0228151C13C IR: 17RMM2-0228151NaCD
AS02	 ***(+)-79***	^{1}H NMR: 18RMM1-0726157H ^{13}C NMR : 17RMM1-0312169C13C IR: 17RMM1-0312169NaCD
AS03	 ***(+)-120***	^{1}H NMR: 18RMM1-0729161H ^{13}C NMR : 18RMM1-0729161C13C IR: 18RMM1-0729161NaCD
AS04	 ***125***	^{1}H NMR: 17RMM2-0401201H ^{13}C NMR : 17RMM2-0401201C13C IR: 17RMM2-0401201NaCD
AS05	 ***124***	^{1}H NMR: 17RMM1-0402209H ^{13}C NMR : 17RMM1-0402209C13C IR: 17RMM2-0402209NaCD

Table A10.4 Cross References for Compounds from Chapter 3: Dichroanone: Part 1

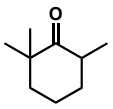
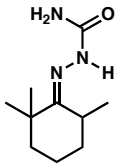
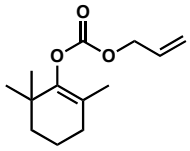
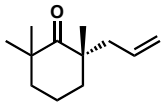
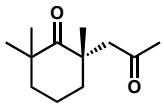
Characterization Binder #	Structure (Thesis #)	Spectral Data
DM01	 ***101***	^{1}H NMR: 11RMM1-0916107CH1H ^{13}C NMR : 11RMM1-0916107CC13C IR: 11RMM1-0916107ClRNaCD
DM02	 ***222***	^{1}H NMR: 11RMMC-918111CH1H ^{13}C NMR : 11RMMC-0918111CC13C IR: 11RMMC-0918111ClRKBr
DM03	 ***100***	^{1}H NMR: 13RMM3-0321215H ^{13}C NMR : 11RMM1-1003179CC13C IR: 11RMM1-1003179ClRNaCD
DM04	 ***(–)-75***	^{1}H NMR: 17RMM1-0617255CH1H ^{13}C NMR : 17RMM1-0617255C13C IR: 11RMM1-1006193ClRNaCD
DM05	 ***(+)-219***	^{1}H NMR: 11RMM1-1013203CH1H ^{13}C NMR : 11RMM1-1013203CC13C IR: 11RMM1-1013203ClRNaCD

Table A10.5 Cross References for Compounds from Chapter 3: Dichroanone: Part 2

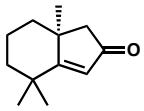
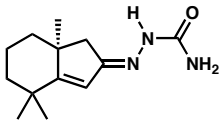
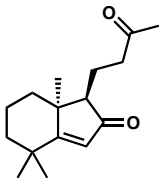
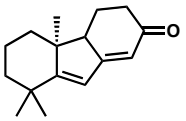
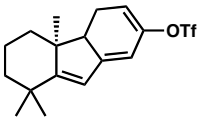
Characterization Binder #	Structure (Thesis #)	Spectral Data
DM06	 *(–)-143*	^{1}H NMR: 12RMM3-0110665CH1H ^{13}C NMR : 11RMM1-1016215CC13C IR: 11RMM1-1016215ClRNaCD
DM07	 *(–)-246*	^{1}H NMR: 12RMM2-110665CH1H ^{13}C NMR : 12RMM2-110665CC13C IR: 12RMM2-110665KBr
DM08	 *(–)-233*	^{1}H NMR: 11RMM2-1018221CH1H ^{13}C NMR : 1RMM2-1018221CC13C IR: 11RMM2-1018221ClRKBr
DM09	 *(–)-234*	^{1}H NMR: 12RMM2-111679CH1H ^{13}C NMR : 12RMM2-111679CC13C IR: 12RMM2-111679ClRNaCD
DM10	 *(–)-250*	^{1}H NMR: 12RMM1-112189CH1H ^{13}C NMR : 12RMM1-112189CC13C ^{19}F NMR: 12RMM1-112189CF19F IR: 12RMM1-112189ClRNaHex

Table A10.6 Cross References for Compounds from Chapter 3: Dichroanone: Part 3

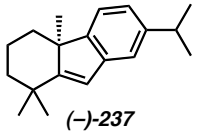
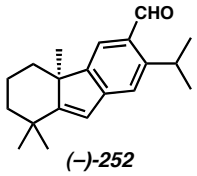
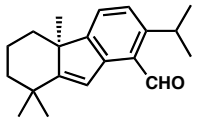
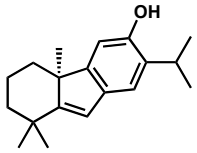
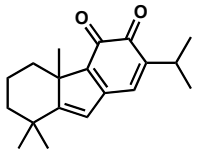
Characterization Binder #	Structure (Thesis #)	Spectral Data
DM11	 *(–)-237*	^{1}H NMR: 12RMM1-112087CH1H ^{13}C NMR : 12RMM1-112087CC13C IR: 12RMM1-112087ClRNaCD
DM12	 *(–)-252*	^{1}H NMR: 12RMM2-112293CH1H ^{13}C NMR : 12RMM2-112293CC13C IR: 12RMM2-112293ClRNaCD
DM13	 *(+)-253*	^{1}H NMR: 12RMM1-112293CH1H ^{13}C NMR :12RMM1-112293CC13C IR: 12RMM1-112293ClRNaCD
DM14	 *(–)-242*	^{1}H NMR: 12RMM1-1204105CC13C ^{13}C NMR : 12RMM1-112599CH1H IR: 12RMM1-112599ClRKBr
DM15	 *(±)-260*	^{1}H NMR: 11RMM1-0920123-100H ^{13}C NMR : IR: RacoQuinoneNaNeat

Table A10.7 Cross References for Compounds from Chapter 3: Dichroanone: Part 4

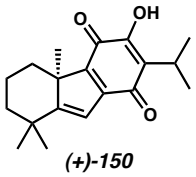
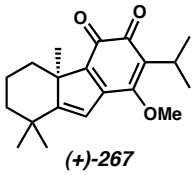
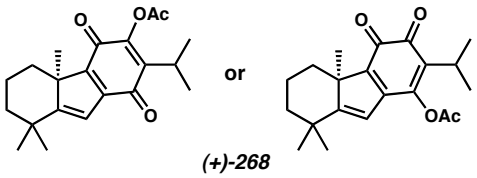
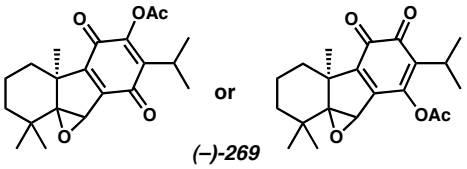
Characterization Binder #	Structure (Thesis #)	Spectral Data
DM16	 *(+)-150*	^{1}H NMR: 12RMM1-1128101CH1H ^{13}C NMR : 12RMM1-1128101C13C IR: 12RMM1-1128101KBr DichroanoneNaCl
DM17	 *(+)-267*	^{1}H NMR: 12RMM1-1213109CH1H ^{13}C NMR : 12RMM1-1213109CC13C IR: 12RMM1-1213109ClRNaCD
DM18	 *(+)-268*	^{1}H NMR: 13RMM1-0209121CH1H ^{13}C NMR : 13RMM1-0209121CC13C IR: 13RMM1-0209121ClRNaCH
DM19	 *(–)-269*	^{1}H NMR: 13RMM4-0212123CH1H ^{13}C NMR : 13RMM4-0212123CC13xC IR: 13RMM4-0212123ClRNaCH

Table A10.8 Cross References for Compounds from Chapter 3: Dichroanone: Part 5

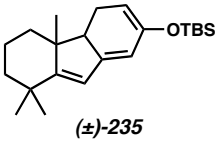
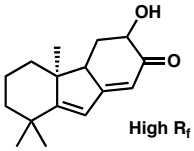
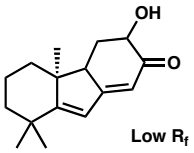
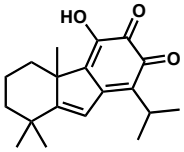
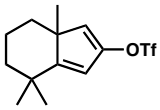
Characterization Binder #	Structure (Thesis #)	Spectral Data
DX01	 *(±)-235*	^{1}H NMR: 8RMM1-020739CH1H ^{13}C NMR : 8RMM1-020739CC13C IR: 8RMM1-020739CIRNeat
DX02	 *(±)-236A*	^{1}H NMR: 8RMM1-020947CH1H ^{13}C NMR : 8RMM1-020947CC13C IR: 8RMM1-020947CIRNaCD
DX03	 *(±)-236B*	^{1}H NMR: 8RMM2-020947CH1H ^{13}C NMR : 8RMM2-020947CC13C IR: 8RMM2-020947CIRNaCD
DX04	 *(±)-240*	^{1}H NMR: 7RMMx-0116235CH1H ^{13}C NMR : 7RMM1-0116235CC13-500C IR: 7RMMx-0116235CIR2NaCD
DX05	 *(±)-229*	^{1}H NMR: 8RMM1-0327143CH1H ^{13}C NMR : 8RMM1-0327143CC13C ^{19}F NMR: 8RMM1-0327143CF19F

Table A10.9 Cross References for Compounds from Chapter 3: Dichroanone: Part 6

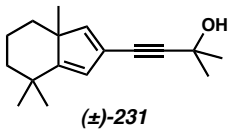
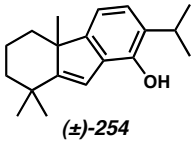
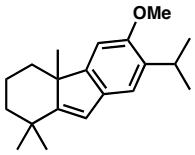
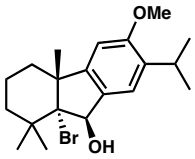
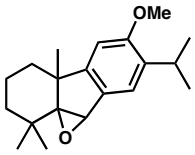
Characterization Binder #	Structure (Thesis #)	Spectral Data
DX06	 ***(±)-231***	^{1}H NMR: 8RMM1-0324141CH1H ^{13}C NMR : 8RMM1-0324141CC13C IR: 8RMM1-0324141NaCD
DX07	 ***(±)-254***	^{1}H NMR: 8RMM1-0408181CH1H ^{13}C NMR : 8RMM1-0408181CC13C IR: 8RMM1-0408181ClRNaCD
DX08	 ***(±)-257***	^{1}H NMR: 8RMM1-0408185CH1H ^{13}C NMR : 8RMM1-0408185CC13C IR: 8RMM1-0408185ClRNaCD
DX09	 ***(±)-258***	^{1}H NMR: 8RMM2-0410187H ^{13}C NMR : 8RMM2-0414187C13C IR: 8RMM2-0410187IRNaCD
DX10	 ***(±)-259***	^{1}H NMR: 8RMM1-0414205H ^{13}C NMR : 8RMM1-0414205C13C IR: 8RMM1-0414205NaCDD2O

Table A10.10 Cross References for Compounds from Chapter 3: Dichroanone: Part 7

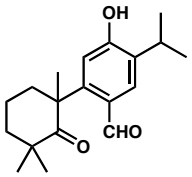
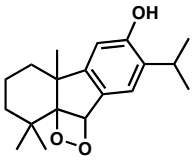
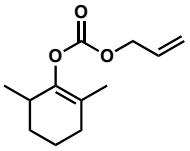
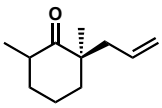
Characterization Binder #	Structure (Thesis #)	Spectral Data
DX11	 *245A and 245B*	^{1}H NMR: 10RMMx-0901249H ^{13}C NMR : 10RMMx-0901249C13C IR: 11RMM4-1005191NaCD
DX12	 *244*	^{1}H NMR: 11RMM3-1005191H ^{13}C NMR : None IR: None
LI32	 *(±)-255*	^{1}H NMR: 17RMM1-012961H ^{13}C NMR : 17RMM1-012961C13C IR: 17RMM1-012961NaCD
LI33	 *(±)-256*	^{1}H NMR: 17RMM1-013163H ^{13}C NMR : 17RMM1-013163C13C IR: 17RMM1-013163NaCD

Table A10.11 Cross References for Compounds from Chapter 4: Liphagal: Part 1

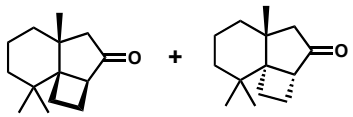
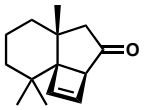
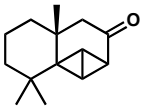
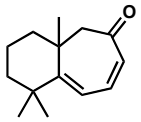
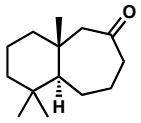
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI01	 *(±)-307A* *(±)-307B*	^{1}H NMR: 13RMM1-0324231CH1H ^{13}C NMR : 13RMM1-0324231C13C IR: 13RMM1-0324231CIRKBr
LI02	 *(+)-312*	^{1}H NMR: 15RMM1-cyclobuteneH ^{13}C NMR : 15RMM1-cyclobuteneCC13C IR: 15RMM1-cyclobuteneCIRNaCH
LI03	 *(–)-313*	^{1}H NMR: 14RMM3-0814271CH1H ^{13}C NMR : 14RMM3-0814271CC13C IR: 14RMM3-0814271CIRNaNeat
LI04	 *(±)-318*	^{1}H NMR: 13RMM2-0407275CH1H. ^{13}C NMR : 13RMM2-0407275CC13C IR: 13RMM2-0407275CIRNaCD
LI05	 *(±)-305*	^{1}H NMR: 14RMM1-061599CH1H. ^{13}C NMR : 14RMM1-061599CC13C IR: 14RMM1-061599CIRNaCD

Table A10.12 Cross References for Compounds from Chapter 4: Liphagal: Part 2

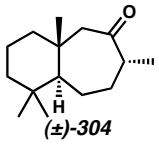
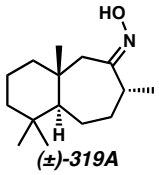
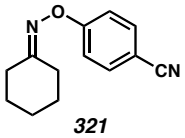
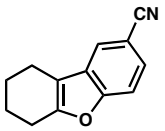
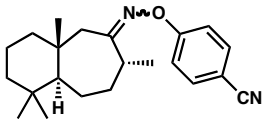
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI06	 *(±)-304*	^{1}H NMR: 13RMM1-0411287CH1H ^{13}C NMR : 13RMM1-0411287CC13C IR: 13RMM1-0411287ClRNaCD
LI07	 *(±)-319A*	^{1}H NMR: 14RMM1-0618107CH1H ^{13}C NMR : 14RMM1-0618107CC13C IR: 14RMM1-0618107ClRNaNaCD
LI08	 *321*	^{1}H NMR: 14RMM1-061397CH1H ^{13}C NMR : 14RMM1-061397CC13C IR: 14RMM1-061397ClRNaCD
LI09	 *322*	^{1}H NMR: 17RMM1-0312171H ^{13}C NMR : 17RMM1-0312171C13C IR: 17RMM1-0312171NaCD
LI10	 *(±)-323A and (±)-323B*	^{1}H NMR: 14RMM1-0619109CH1H ^{13}C NMR : 14RMM1-0619109CC13C IR: 14RMM1-0619109ClRNaCD

Table A10.13 Cross References for Compounds from Chapter 4: Liphagal: Part 3

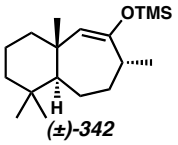
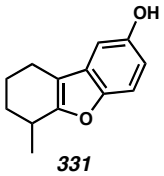
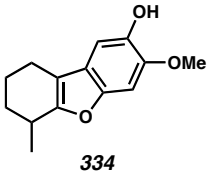
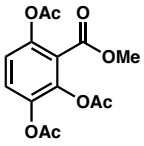
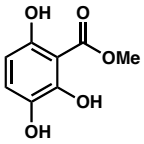
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI11	 *(±)-342*	^{1}H NMR: 14RMMc-0625125H ^{13}C NMR : 14RMMc-0625125C13C IR: 14RMM1-0625125NaNeat
LI12	 *331*	^{1}H NMR: 14RMM1-0703151CH1H ^{13}C NMR : 14RMM1-0703151CC13C IR: 14RMM1-0703151ClRNaCD
LI13	 *334*	^{1}H NMR: 15RMM1-0917163H ^{13}C NMR : 15RMM1-0917163CC13C IR: 15RMM1-0917163KBr
LI14	 *338*	^{1}H NMR: 15RMM1-0921189CH1H ^{13}C NMR : 15RMM1-0921189CC13C IR: 15RMM1-0921189ClRNaCD
LI15	 *339*	^{1}H NMR: 15RMM1-1001207CH1H ^{13}C NMR : 15RMM1-1001207CC13C IR: 15RMM1-1001207ClRxKBr

Table A10.14 Cross References for Compounds from Chapter 4: Liphagal: Part 4

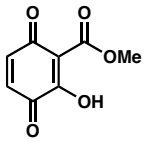
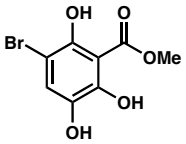
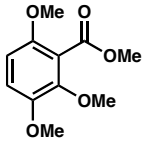
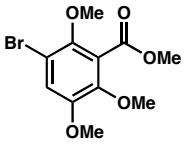
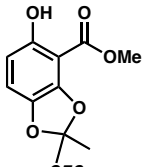
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI16	 *340*	^{1}H NMR: 15RMMc-1002215H ^{13}C NMR : 15RMMc-1002215C13C. IR: 15RMMc-1002215NaCDCH
LI17	 *349*	^{1}H NMR: 15RMM1-1008263H ^{13}C NMR : 15RMM1-1008263C13C IR: 15RMM1-1008263NaCD
LI18	 *351*	^{1}H NMR: 16RMM1-102651CH1H. ^{13}C NMR : 16RMM1-102651CC13C IR: 16RMM1-102651ClRNaCD
LI19	 *352*	^{1}H NMR: 16RMM2-110389CH1H ^{13}C NMR : 16RMM2-110389CC13C IR: 16RMM2-110389ClRNaCH
LI20	 *350*	^{1}H NMR: 16RMM1-102445CH1H ^{13}C NMR : 16RMM1-102445CC13C IR: 16RMM1-102445ClRKBr

Table A10.15 Cross References for Compounds from Chapter 4: Liphagal: Part 5

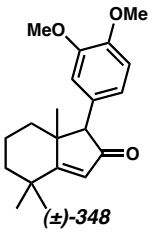
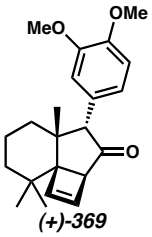
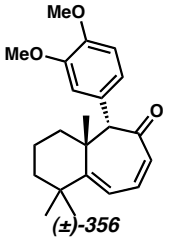
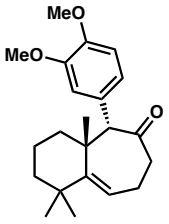
Characterization Binder #	Structure (Thesis #)	Spectral Data
Li21	 (±)-348	^{1}H NMR: 16RMM1-1107101H ^{13}C NMR : 16RMM1-1107101C13C IR: 16RMM1-1107101KBr
LI22	 (+)-369	^{1}H NMR: 16RMM1-1126123H ^{13}C NMR : 16RMM1-1126123C13C IR: 16RMM1-1126123NaCH
LI23	 (±)-356	^{1}H NMR: 16RMM2-1130137H ^{13}C NMR : 16RMM2-1130137C13C IR: 16RMM2-1130137NaCH
LI24	 (±)-374	^{1}H NMR: 16RMMc-1201145H ^{13}C NMR : 16RMMc-1201145C13C IR: 16RMMc-1201145NaCH

Table A10.16 Cross References for Compounds from Chapter 4: Liphagal: Part 6

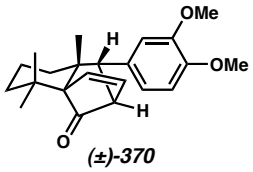
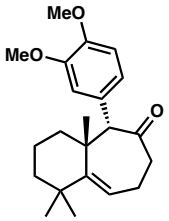
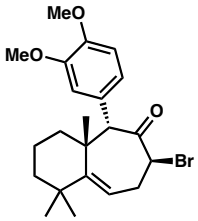
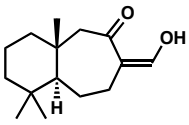
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI25	 *(±)-370*	^{1}H NMR: 16RMM4-1130137H ^{13}C NMR : 16RMM4-1130137C13C IR: 16RMM4-1130137NaCH
LI26	 *(±)-374*	^{1}H NMR: 16RMMc-1201145H ^{13}C NMR : 16RMMc-1201145C13C IR: 16RMMc-1201145NaCH
LI27	 *(±)-376*	^{1}H NMR: 16RMM1-0103237H ^{13}C NMR : 16RMM1-0103237C13C IR: 16RMM1-0103237NaCH
LI28	 *(±)-357*	^{1}H NMR: 16RMM1-0103235H ^{13}C NMR : 16RMM1-0103235C13C IR: 16RMM1-0103235

Table A10.17 Cross References for Compounds from Chapter 4: Liphagal: Part 7

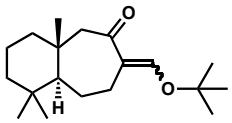
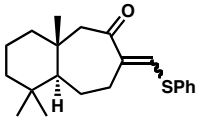
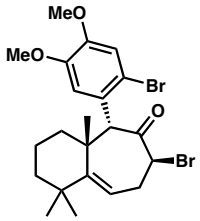
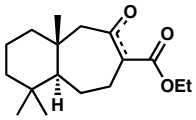
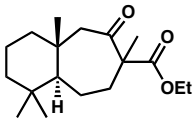
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI29	 *(±)-358*	^{1}H NMR: 16RMM2-0103235H ^{13}C NMR : 16RMM2-0103235C13C IR: 16RMM2-0103235NaDCM
LI30	 *(±)-359*	^{1}H NMR: 16RMM3-0114261CH1H ^{13}C NMR : 16RMM3-0114261CC13C IR: 16RMM3-0114261NaDCM
LI31	 *(±)-377*	^{1}H NMR: 16RMM1-0119289H ^{13}C NMR : 16RMM1-0119289C13xC IR: 16RMM1-0119289NaCD
LI34	 *(±)-361ABC*	^{1}H NMR: 17RMM1-013169C ^{13}C NMR : 17RMM1-013169C13C IR: 17RMM1-013169NaCD
LI35	 *(±)-362*	^{1}H NMR: 17RMM1-020175H ^{13}C NMR : 17RMM1-020175C13C IR: 17RMM1-020175

Table A10.18 Cross References for Compounds from Chapter 4: Liphagal: Part 8

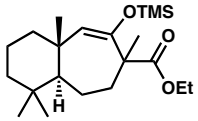
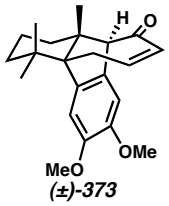
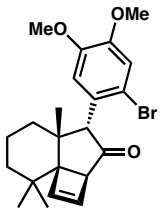
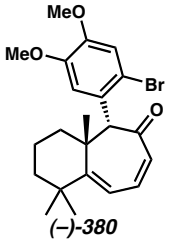
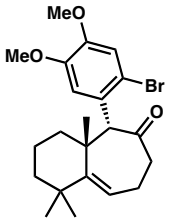
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI36	 *(±)-363*	^{1}H NMR: 17RMMc-0211107H ^{13}C NMR : 17RMMc-0211107C13C IR: 17RMMc-0211107NaDCM
LI37	 *(±)-373*	^{1}H NMR: 17RMM2-0318197H ^{13}C NMR : 17RMM2-0318197C13C IR: 17RMM2-0318197NaCD
LI38	 *(+)-379*	^{1}H NMR: 17RMM1-0406219H ^{13}C NMR : 17RMM1-0406219C13C IR: 17RMM1-0406219NaCD
LI39	 *(–)-380*	^{1}H NMR: 17RMM2-0401205H ^{13}C NMR : 17RMM2-0401205C13C IR: 17RMM2-0401205NaCD
LI40	 *(+)-381*	^{1}H NMR: 17RMMx-0422223H ^{13}C NMR : 17RMMx-0422223C13C IR: 17RMMx-0422223NaCD

Table A10.19 Cross References for Compounds from Chapter 4: Liphagal: Part 9

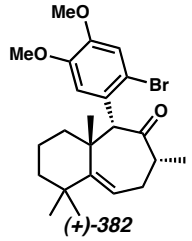
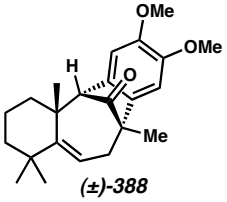
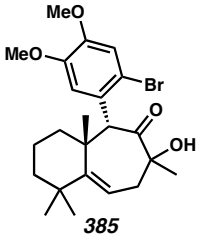
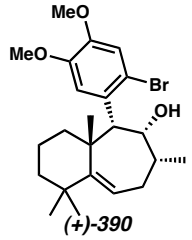
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI41	 *(+)-382*	^{1}H NMR: 17RMM1-0425227H ^{13}C NMR : 17RMM1-0425227C13C IR: 17RMM1-0425227NaCD
LI42	 *(±)-388*	^{1}H NMR: 17RMM3-0503231H ^{13}C NMR : 17RMM1-0504233C IR: 17RMM1-0504233NaCD
LI43	 *385*	^{1}H NMR: 18RMM5-070851H ^{13}C NMR : 18RMM5-070851C13C IR: 18RMM5-070851NaCD
LI44	 *(+)-390*	^{1}H NMR: 18RMMc-071065H ^{13}C NMR : 18RMMc-071065C13C IR: 18RMMc-071065NaCD

Table A10.20 Cross References for Compounds from Chapter 4: Liphagal: Part 10

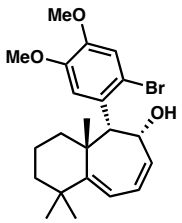
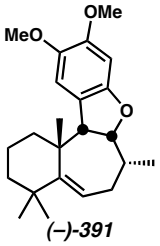
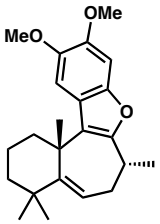
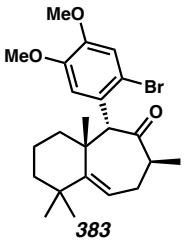
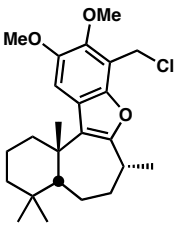
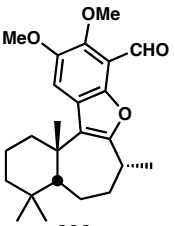
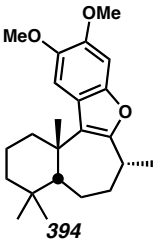
Characterization Binder #	Structure (Thesis #)	Spectral Data
LI45	 *(±)-389*	^{1}H NMR: 18RMM2-071897H ^{13}C NMR : 18RMM2-071897C13C IR: 18RMM2-071897NaCD
LI46	 *(–)-391*	^{1}H NMR: 18RMM1-0828251H ^{13}C NMR : 18RMM1-0828251C13C IR: 18RMM1-0828251
LI47	 *(+)-386*	^{1}H NMR: 19RMM1-0926127H ^{13}C NMR : 19RMM1-0926127C13C IR: 19RMM1-0926127NaCD
LI48	 *383*	^{1}H NMR: 19RMMx-MethylEpiH ^{13}C NMR : 19RMMx-MethylEpiC13C IR: 19RMMx-MethylEpiNaCD

Table A10.21 Cross References for Compounds from Chapter 4: Liphagal: Part 11

Characterization Binder #	Structure (Thesis #)	Spectral Data
LI49	 ***395***	^{1}H NMR: 19RMM1-0924121H ^{13}C NMR : None IR: None
LI50	 ***396***	^{1}H NMR: 19RMM1-1024191H ^{13}C NMR : 19RMM1-1024191C13C IR: 19RMM1-1024191NaCD
LI51	 ***394***	^{1}H NMR: 19RMM1-1026197H ^{13}C NMR : 19RMM1-1026197C13C IR: 19RMM1-1026197NaCD