

APPENDIX C

Spectra and X-Ray Crystallographic Data:
Radical Cyclization Approaches Toward
the Tricyclic Core of Zoanthenol

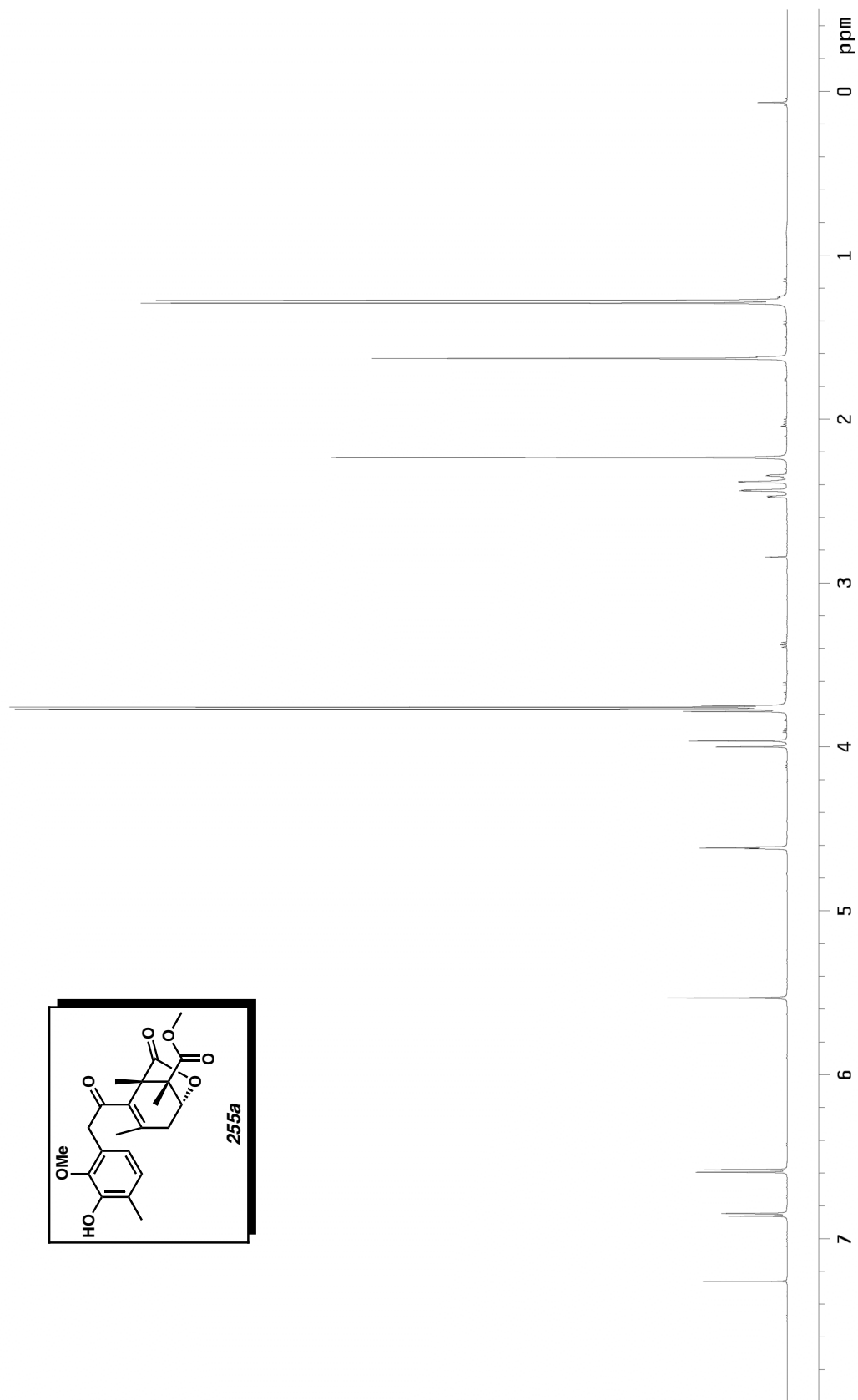


Figure C.1 ¹H NMR (500 MHz, CDCl₃) of compound **255a**.

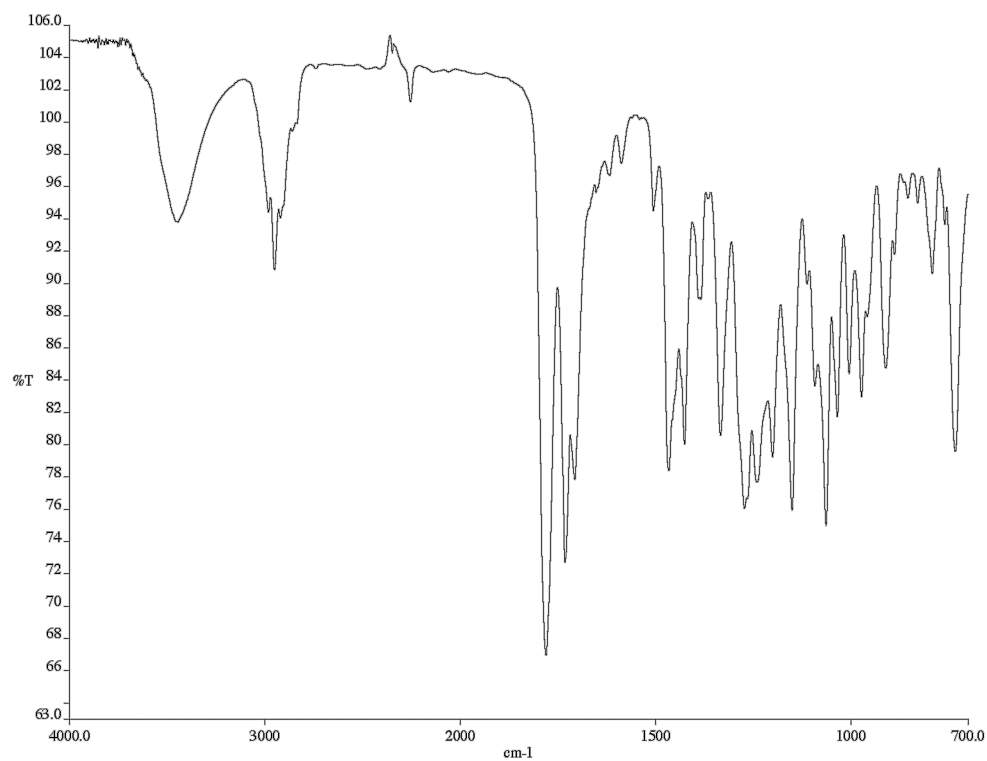


Figure C.2 Infrared spectrum (thin film/NaCl) of compound **255a**.

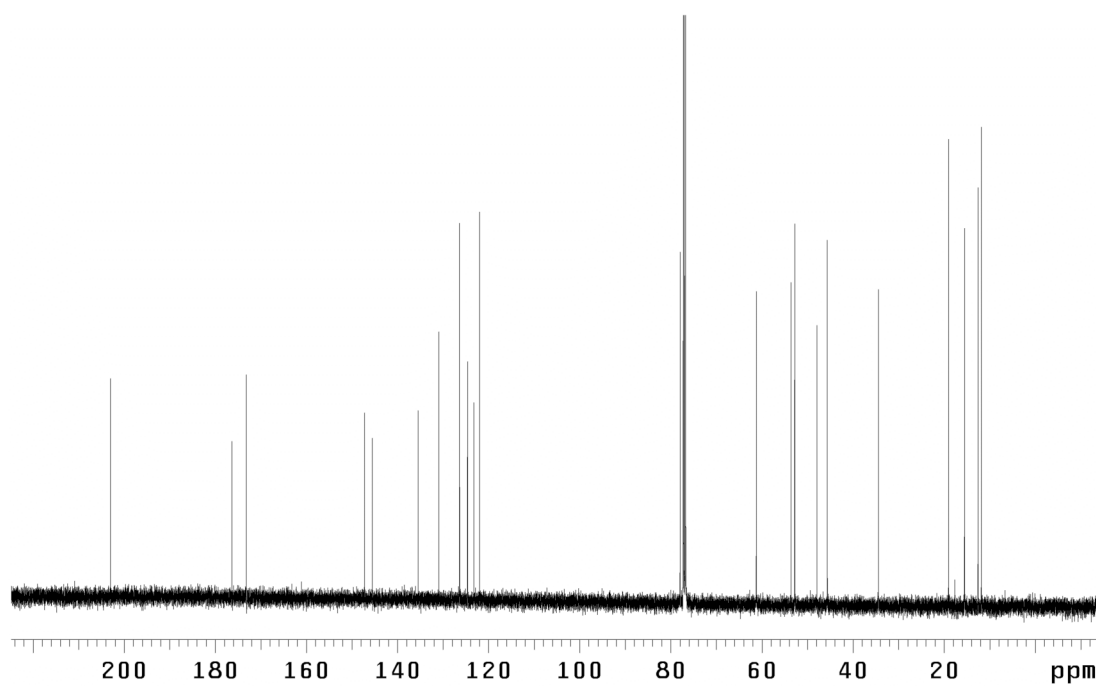


Figure C.3 ¹³C NMR (125 MHz, CDCl₃) of compound **255a**.

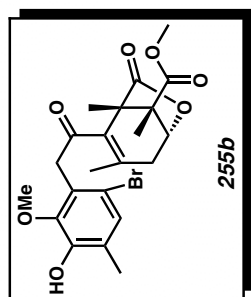
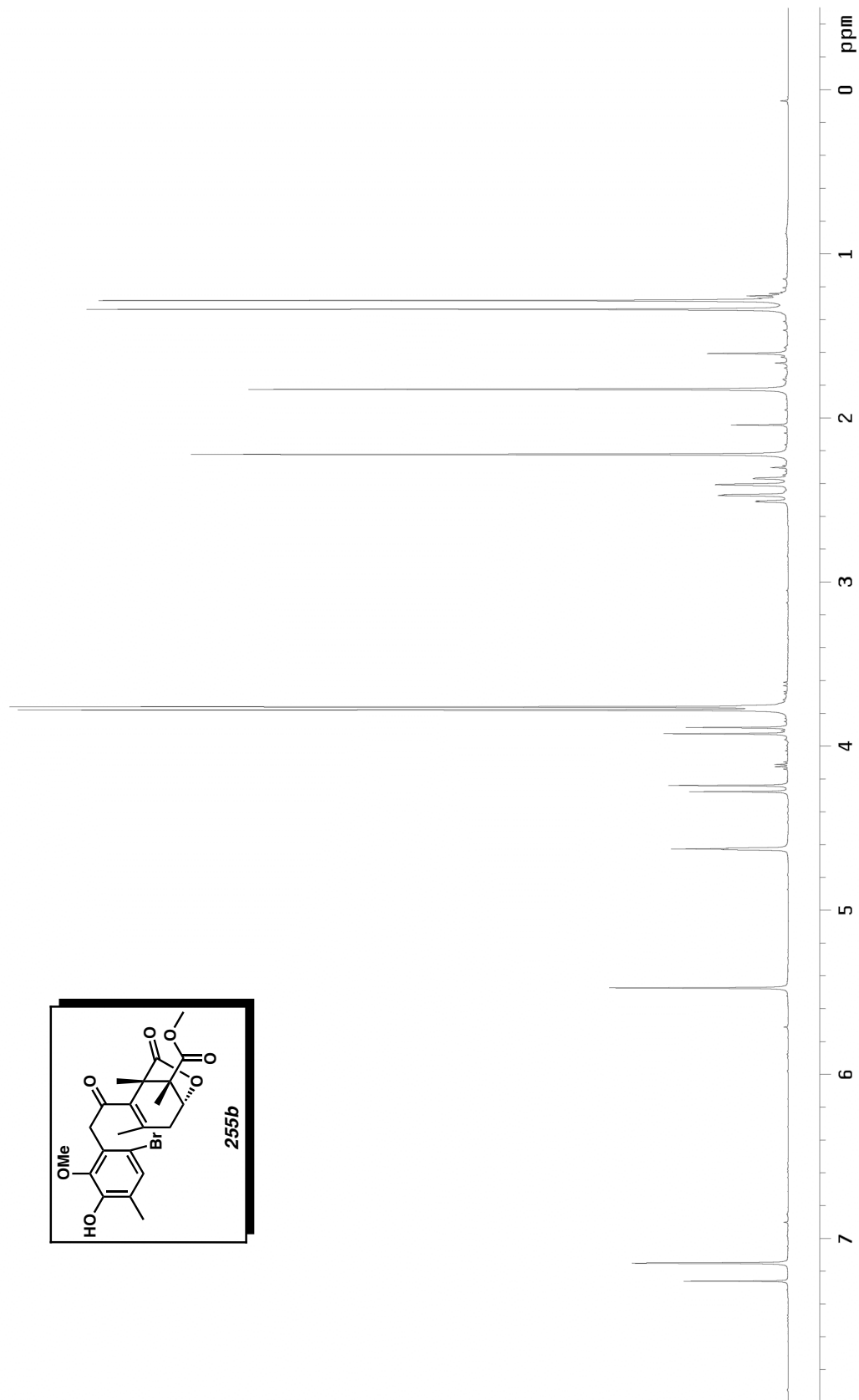


Figure C.4 ^1H NMR (500 MHz, CDCl_3) of compound **255b**.

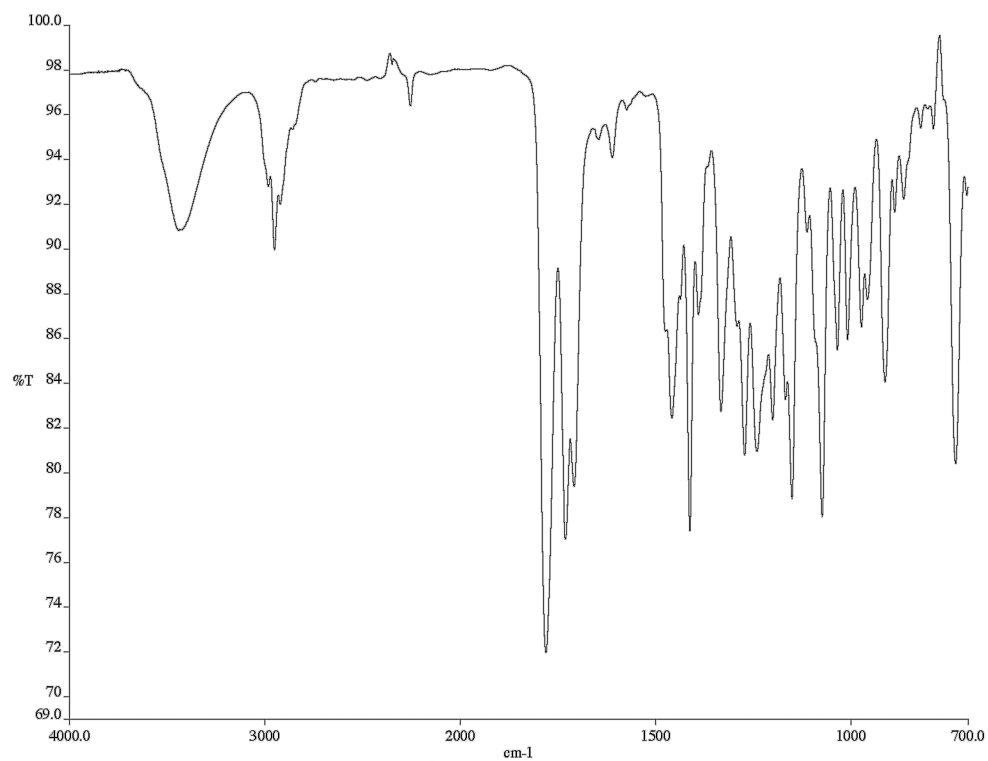


Figure C.5 Infrared spectrum (thin film/NaCl) of compound **255b**.

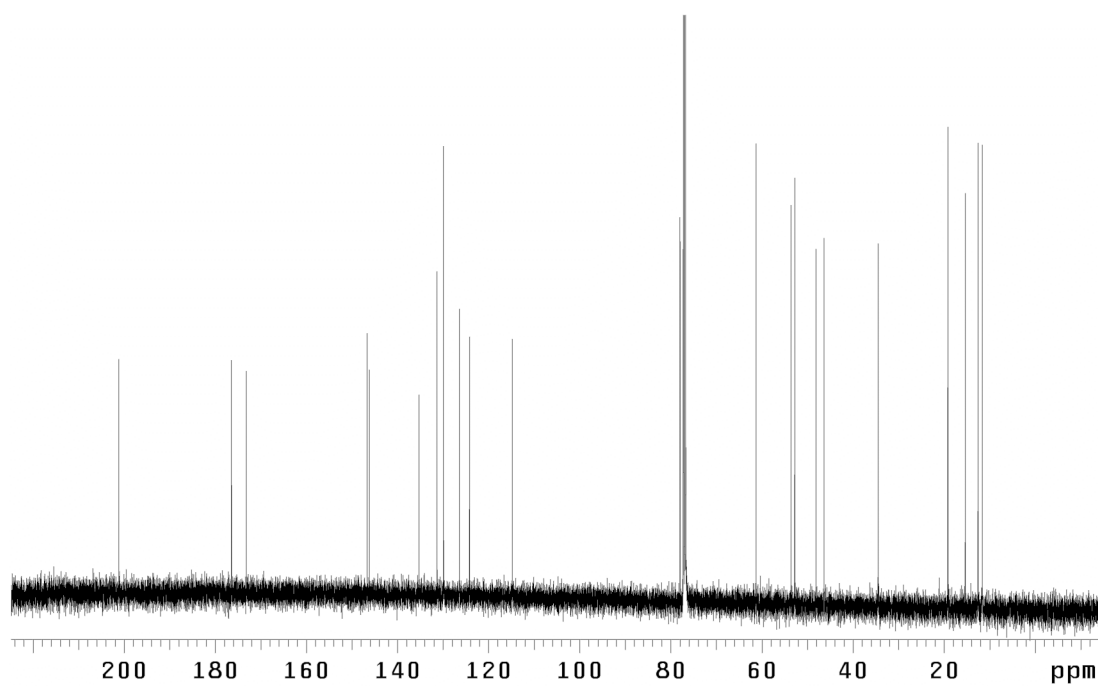


Figure C.6 ¹³C NMR (125 MHz, CDCl₃) of compound **255b**.

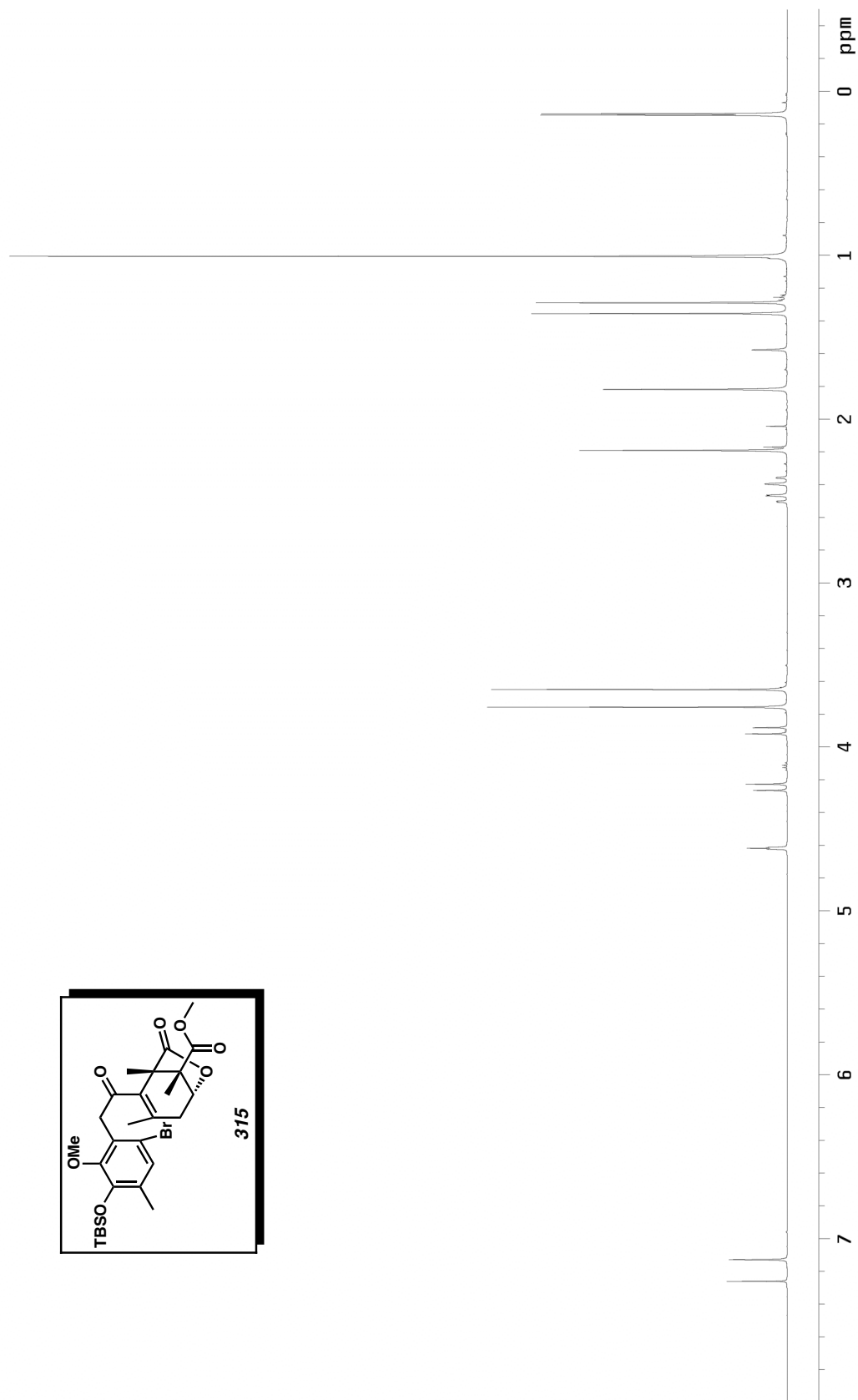
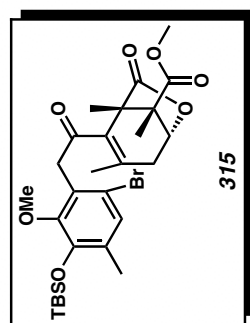


Figure C.7 ¹H NMR (500 MHz, CDCl₃) of compound **315**.



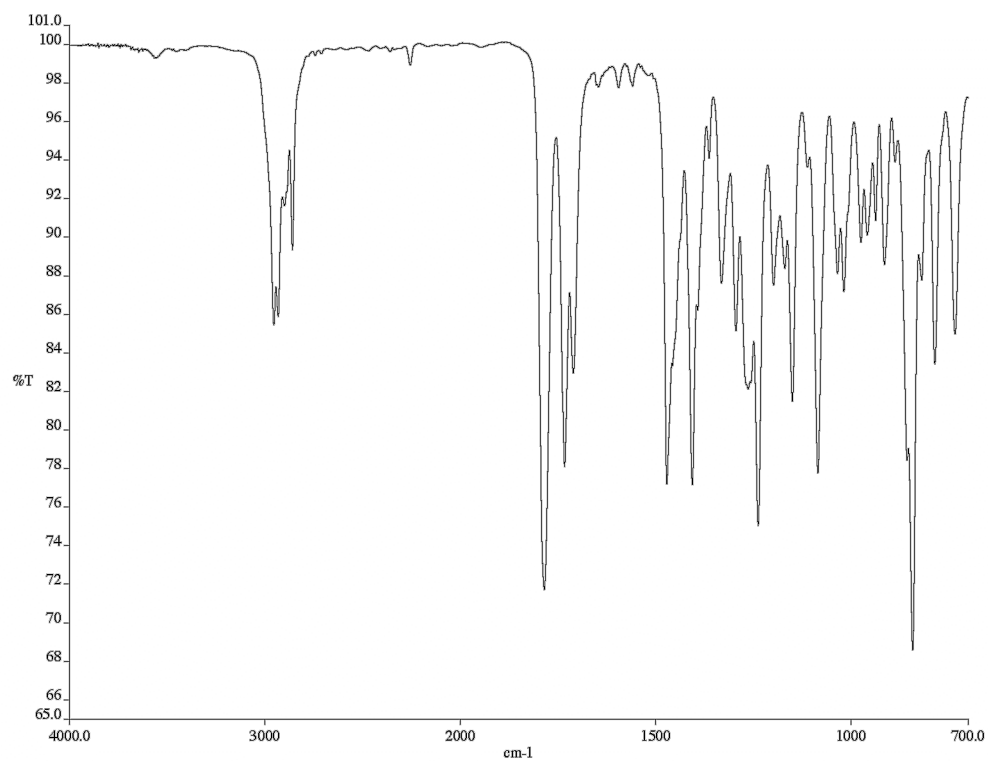


Figure C.8 Infrared spectrum (thin film/NaCl) of compound **315**.

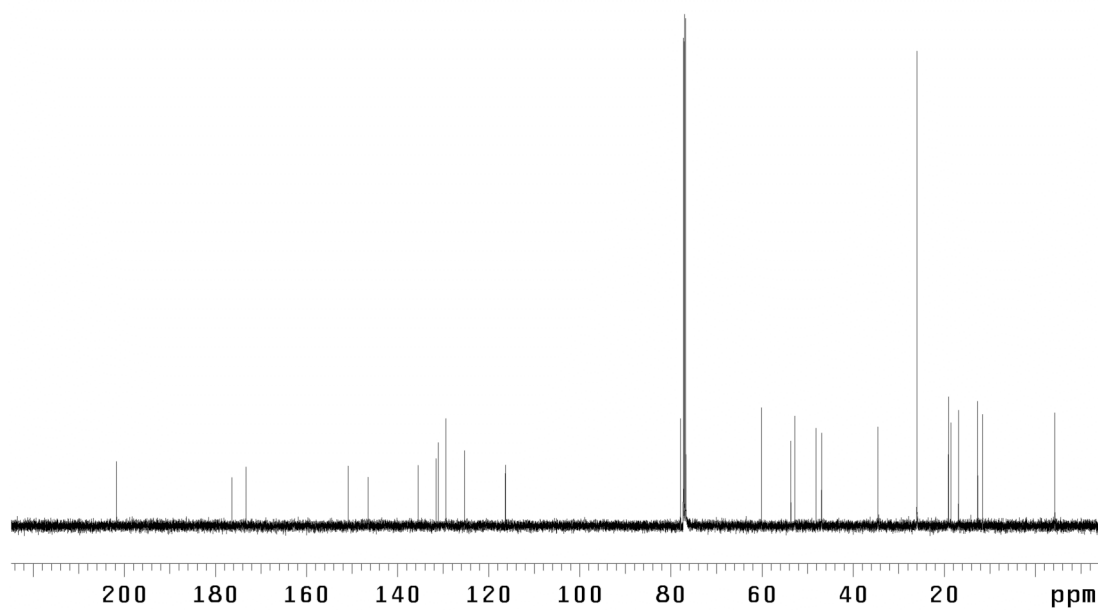


Figure C.9 ¹³C NMR (125 MHz, CDCl₃) of compound **315**.

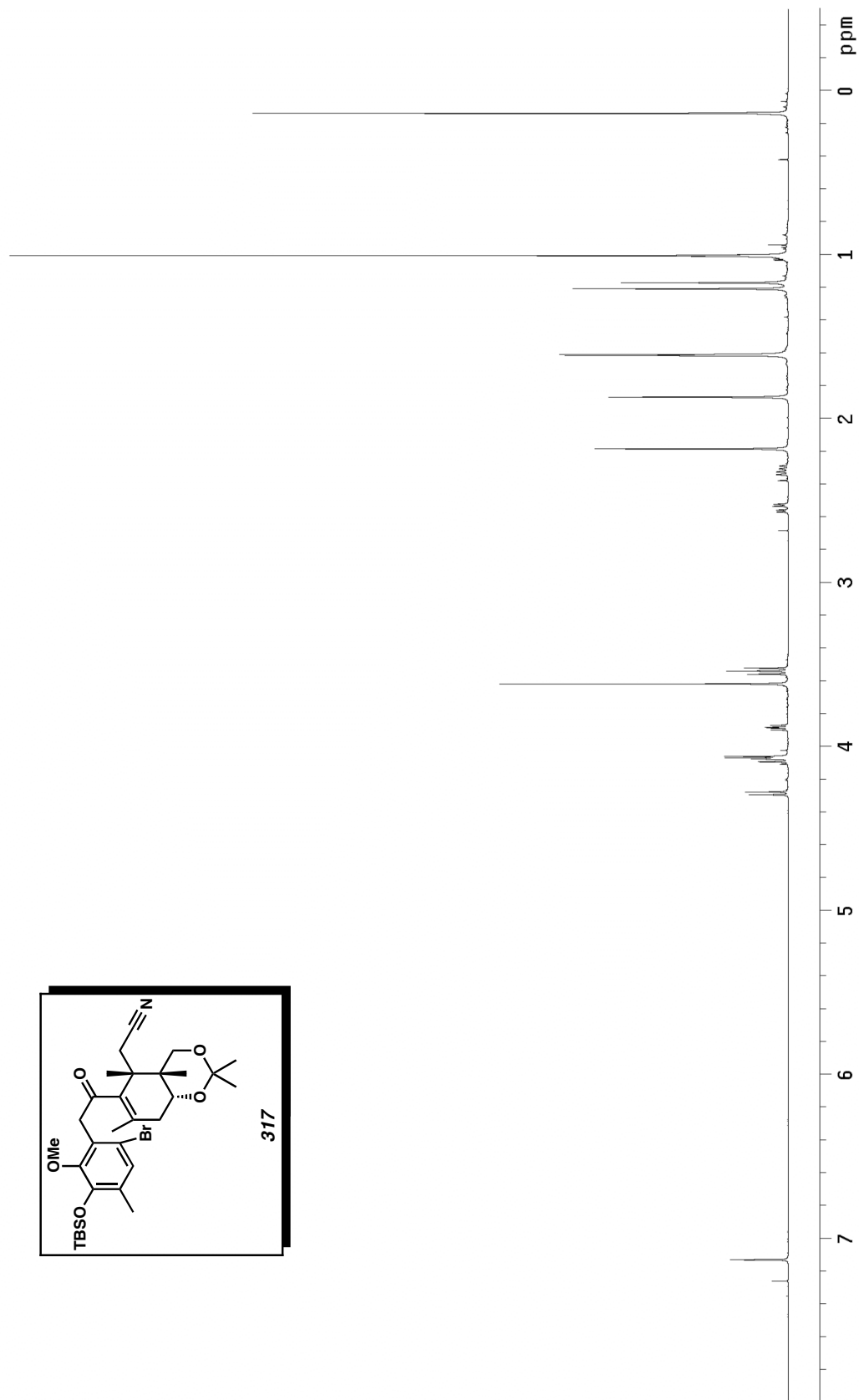


Figure C.10 ^1H NMR (500 MHz, CDCl_3) of compound **317**.

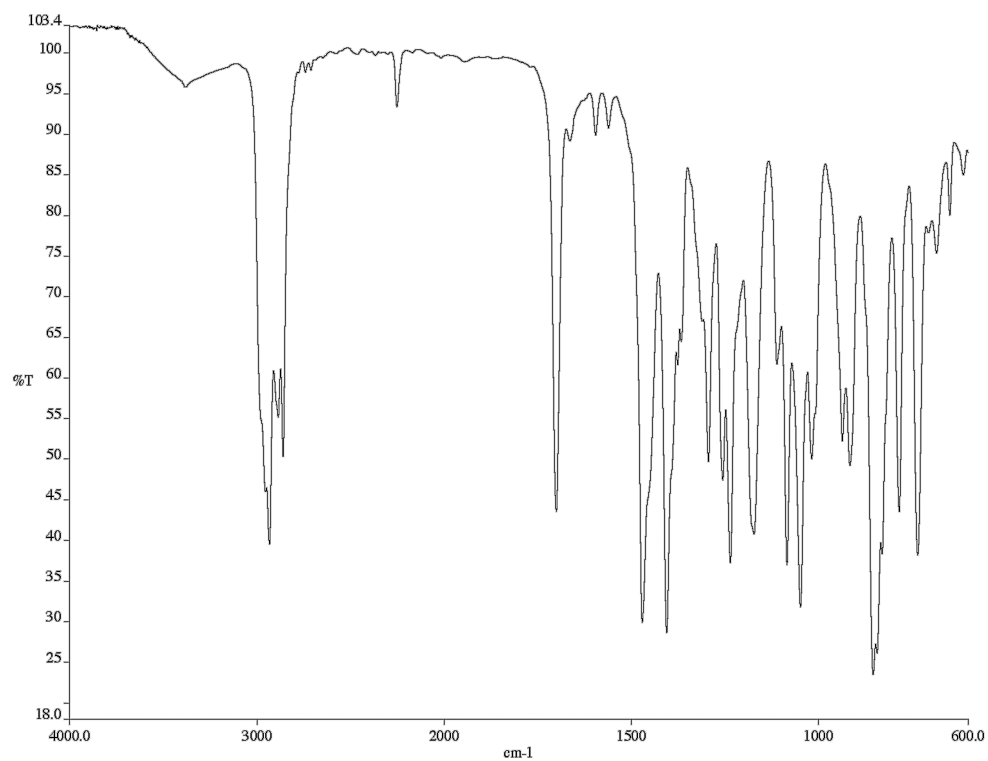


Figure C.11 Infrared spectrum (thin film/NaCl) of compound **317**.

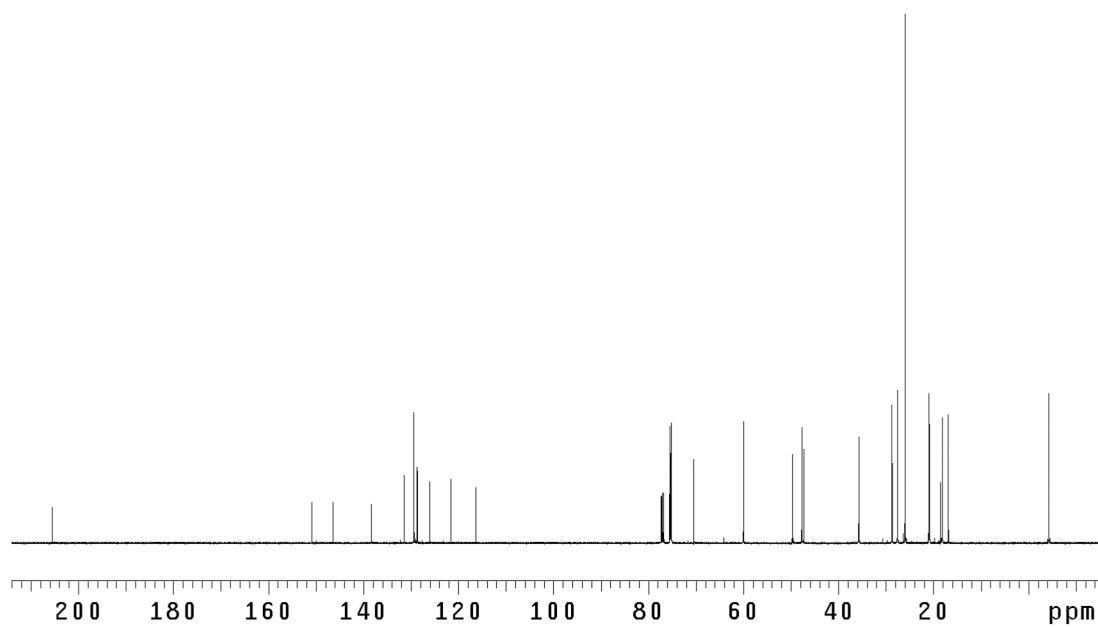


Figure C.12 ¹³C NMR (125 MHz, CDCl₃) of compound **317**.

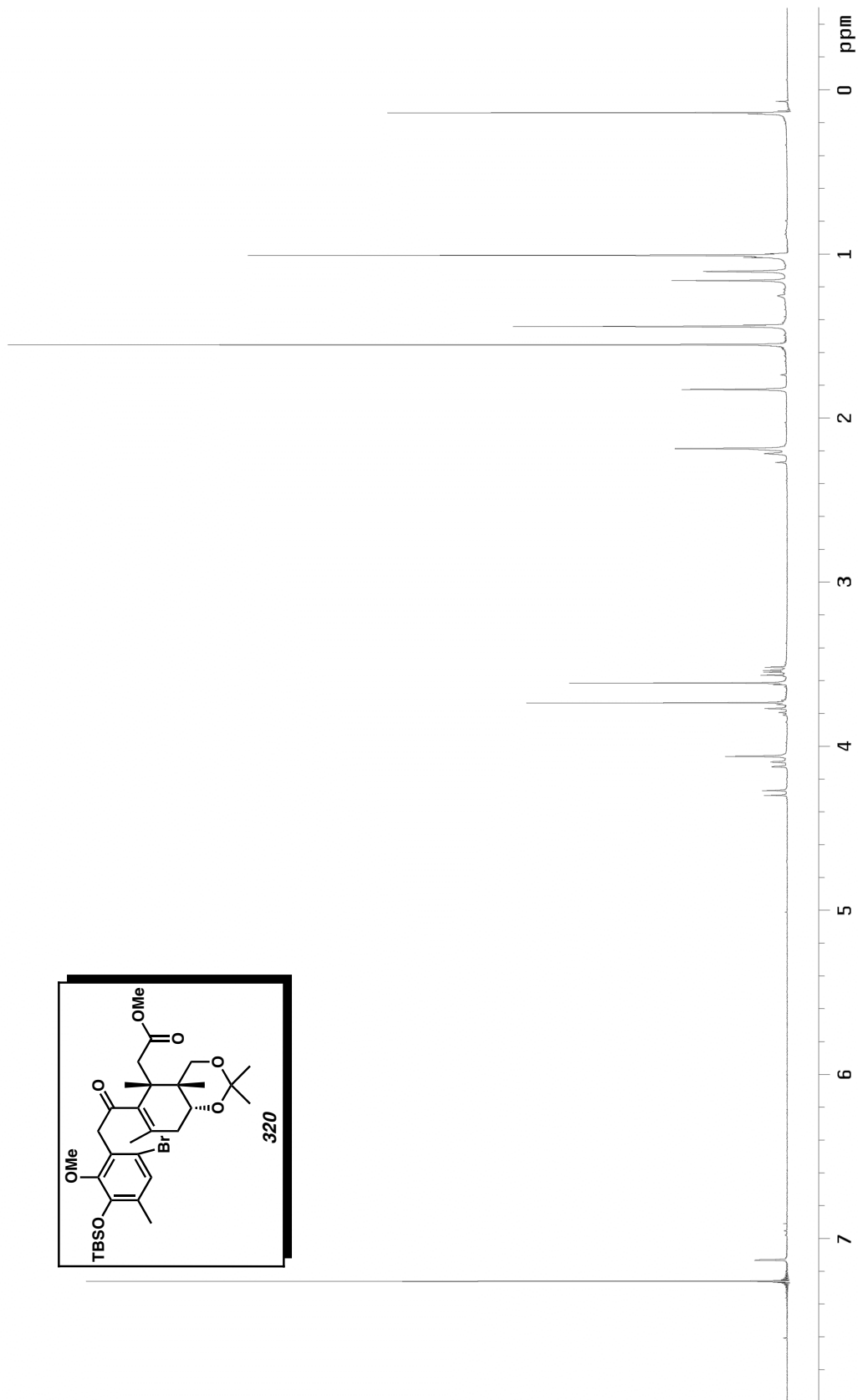


Figure C.13 ^1H NMR (300 MHz, CDCl_3) of compound **320**.

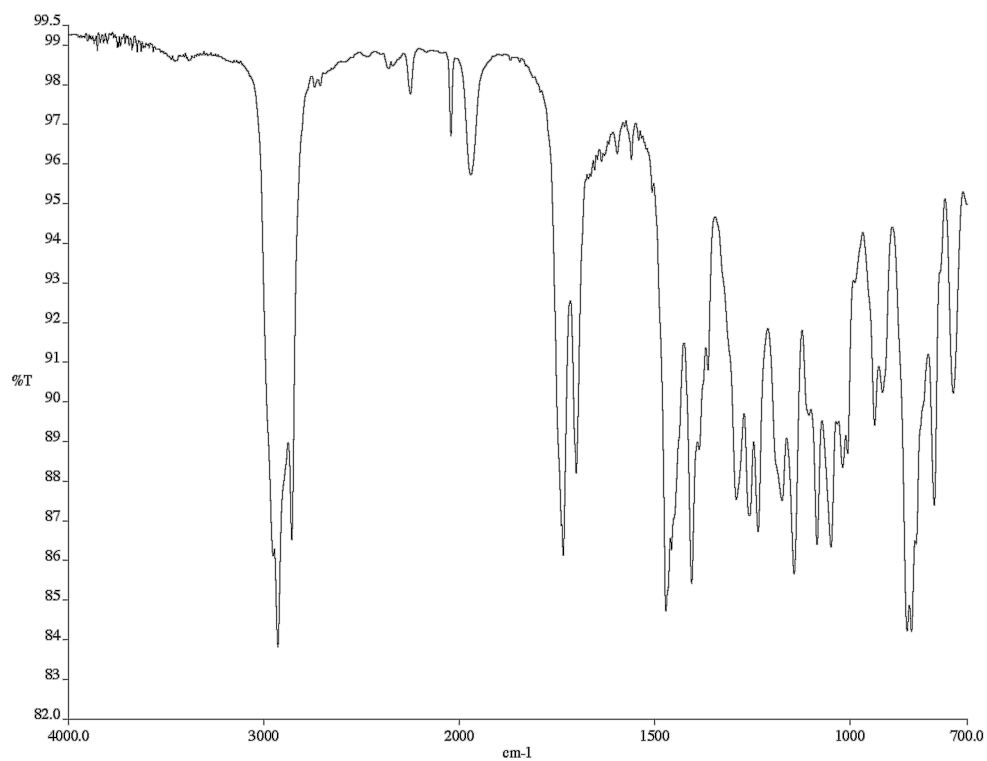


Figure C.14 Infrared spectrum (thin film/NaCl) of compound **320**.

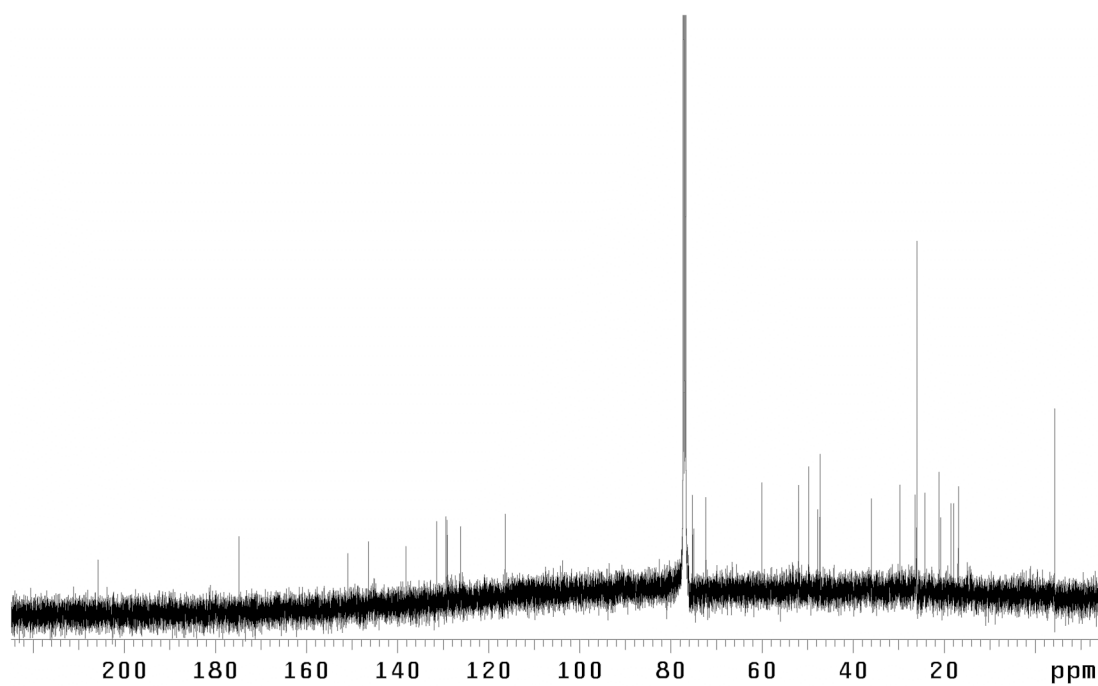


Figure C.15 ¹³C NMR (75 MHz, CDCl₃) of compound **320**.

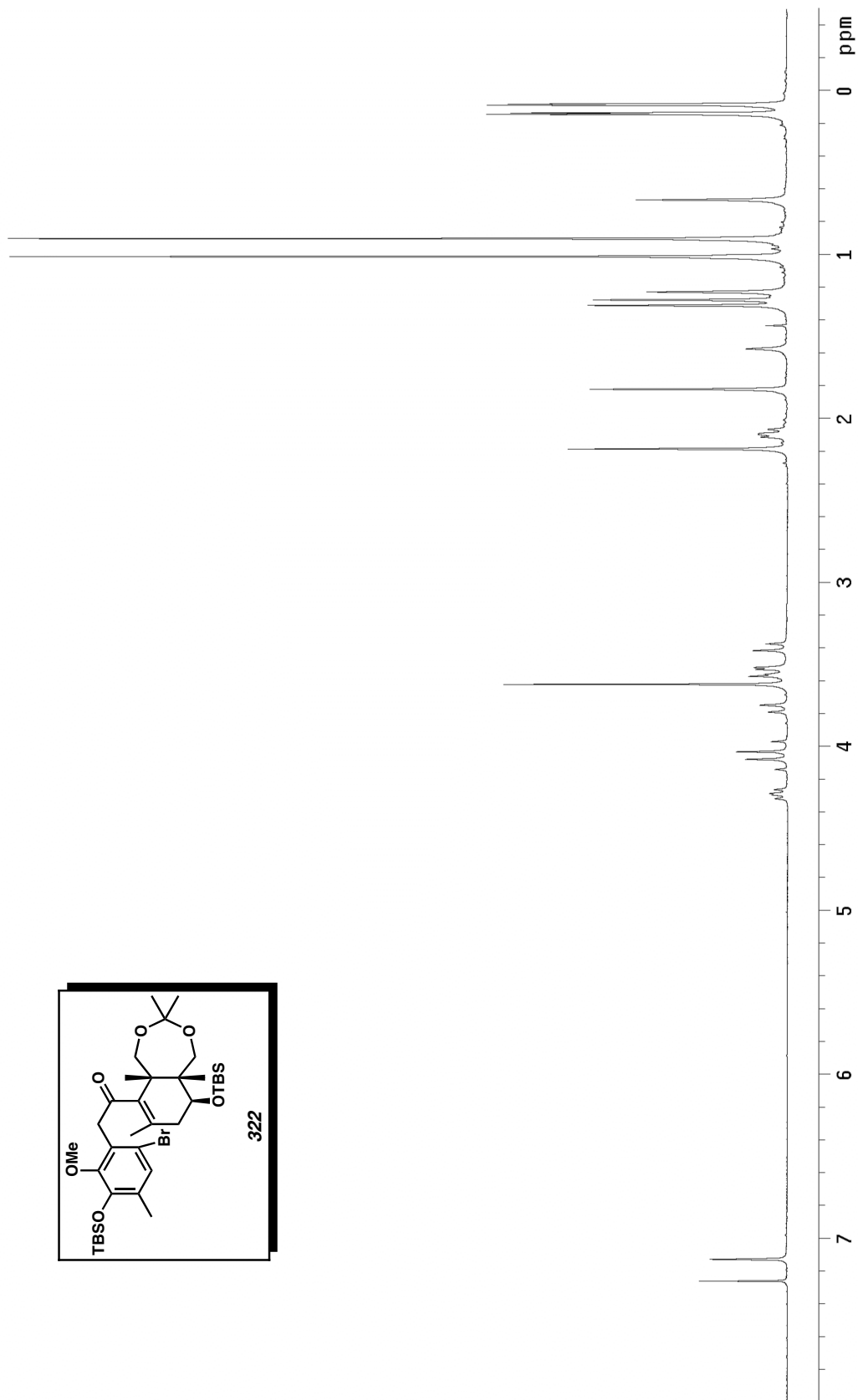
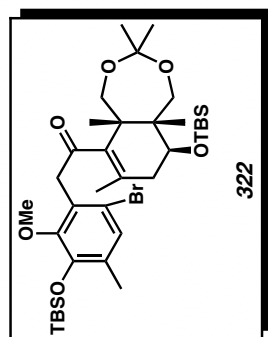


Figure C.16 ^1H NMR (300 MHz, CDCl_3) of compound **322**.

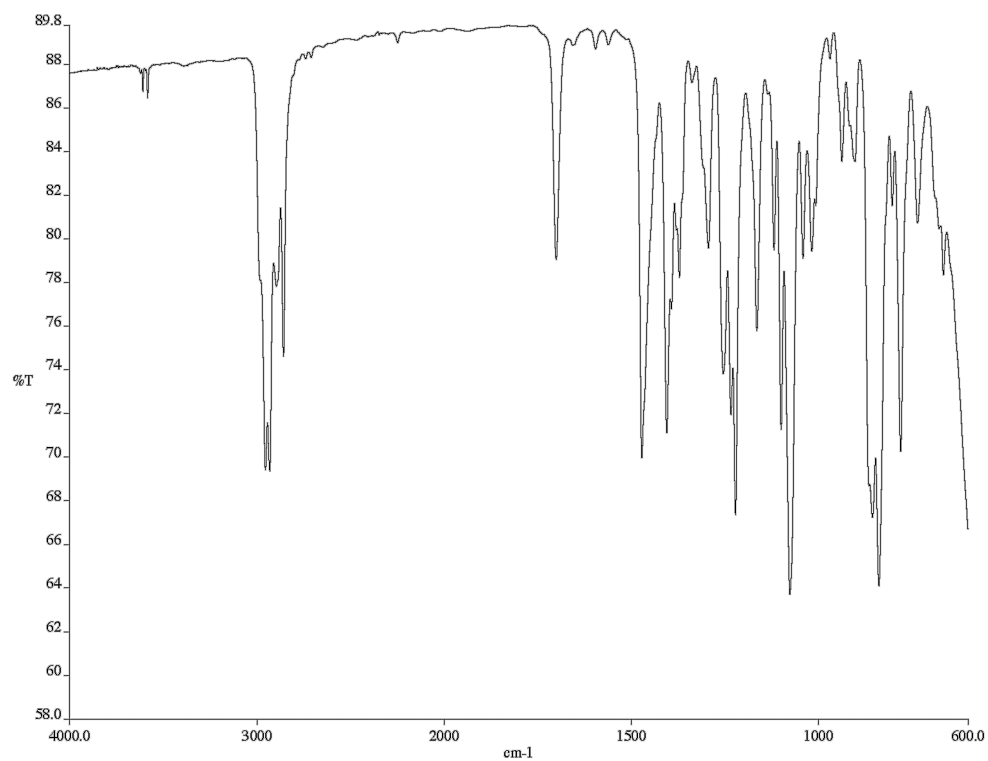


Figure C.17 Infrared spectrum (thin film/NaCl) of compound **322**.

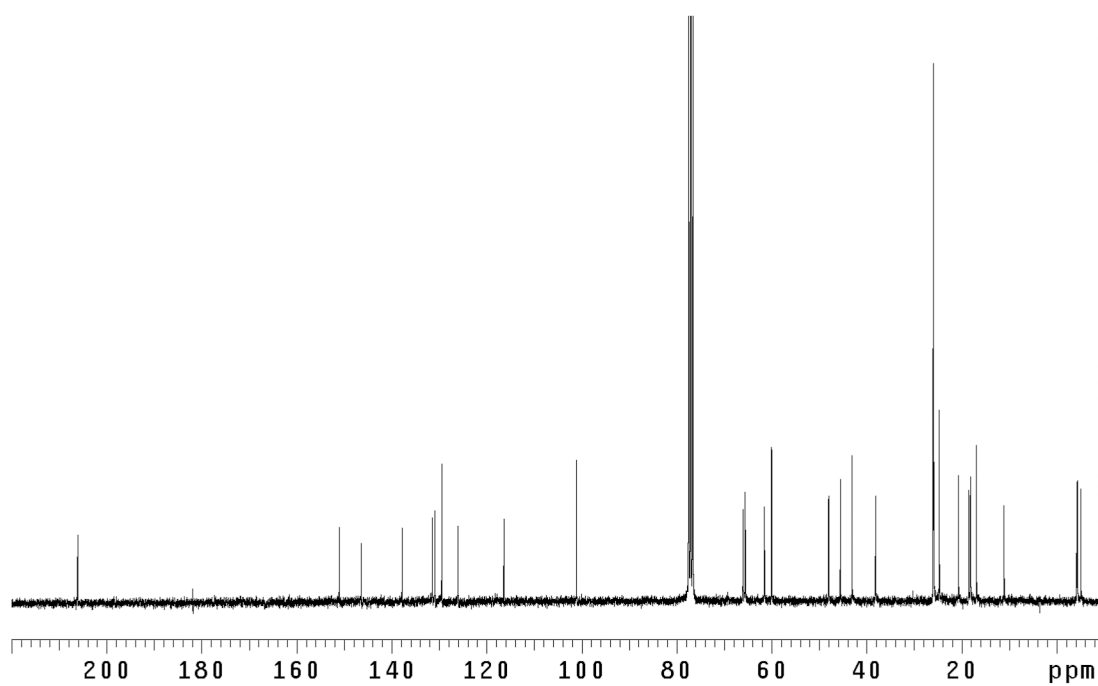


Figure C.18 ¹³C NMR (75 MHz, CDCl₃) of compound **322**.

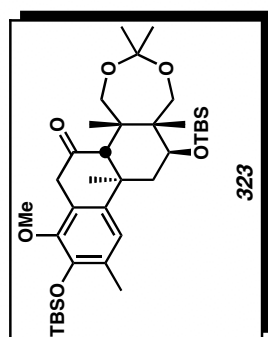
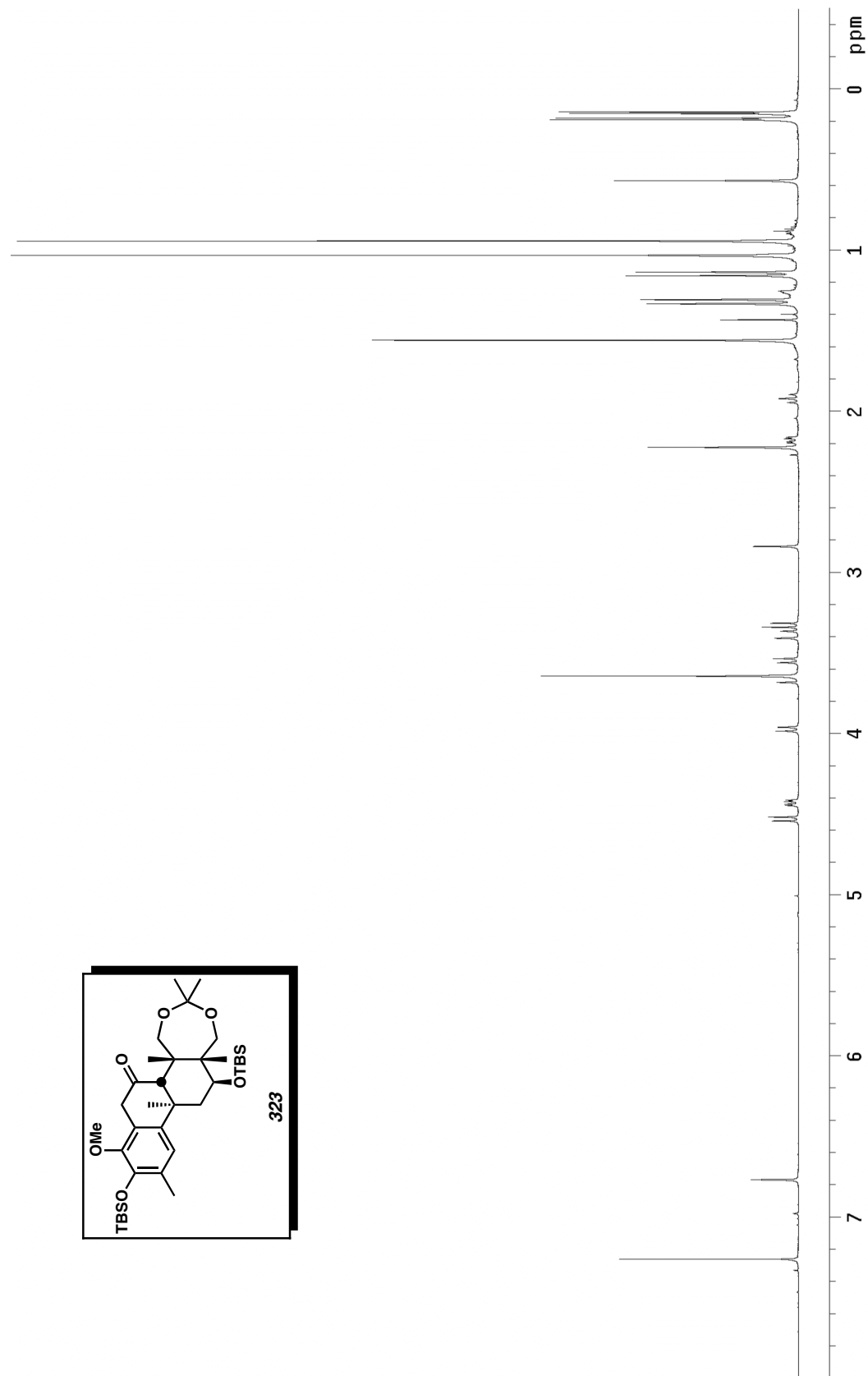


Figure C.19 ¹H NMR (500 MHz, CDCl₃) of compound **323**.

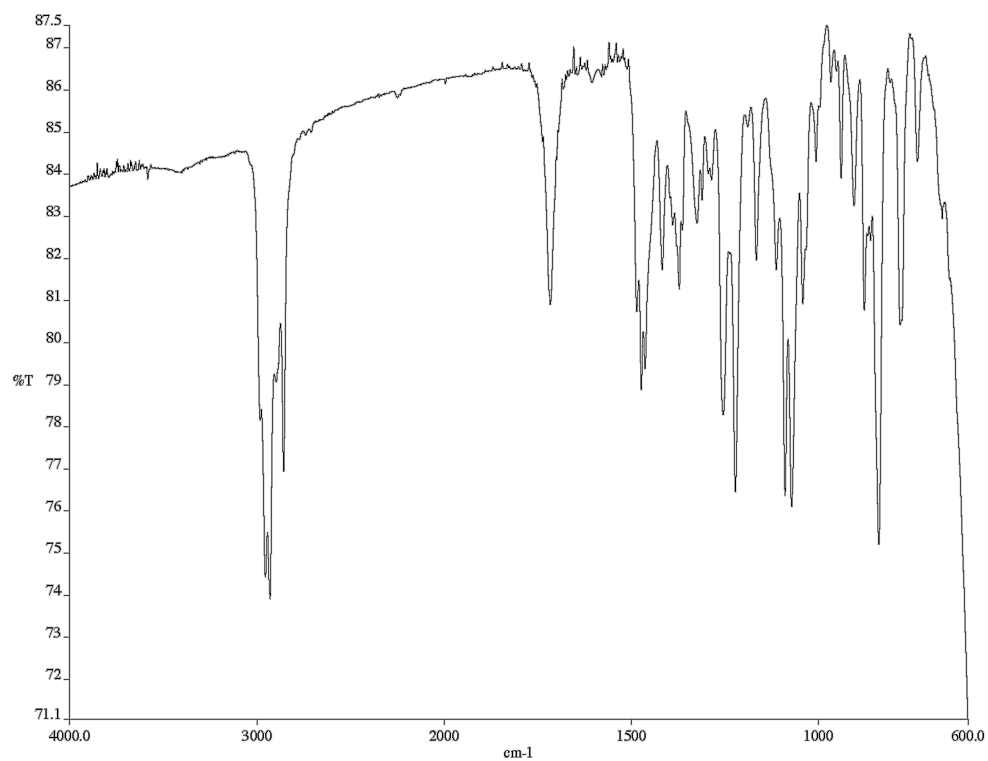


Figure C.20 Infrared spectrum (thin film/NaCl) of compound **323**.

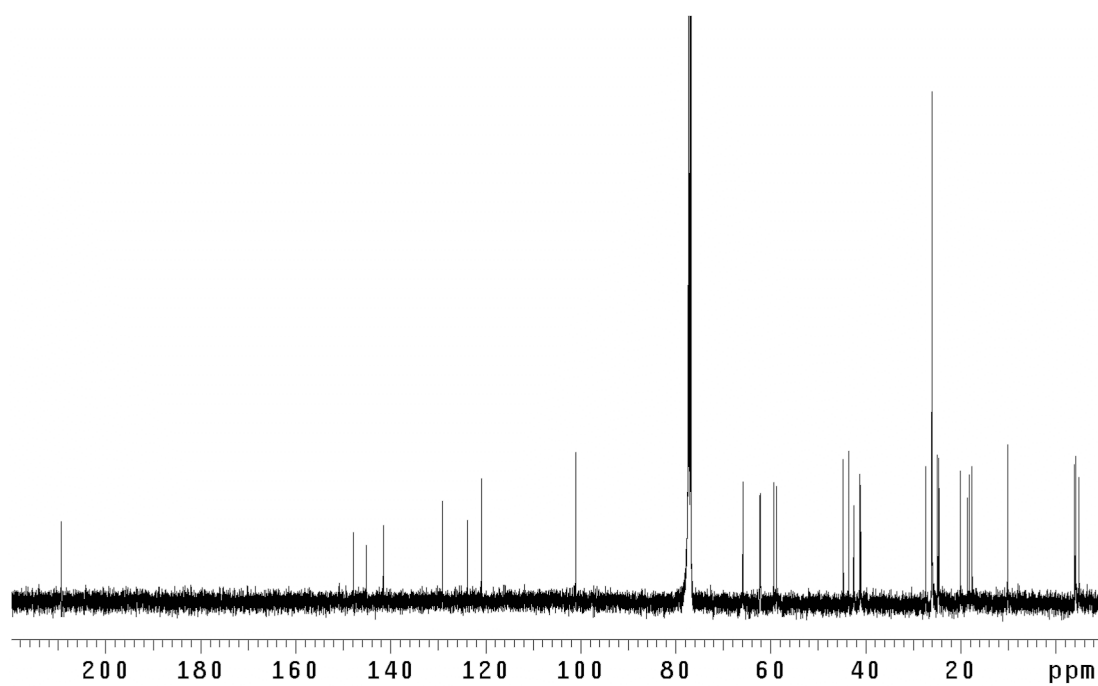


Figure C.21 ¹³C NMR (125 MHz, CDCl₃) of compound **323**.

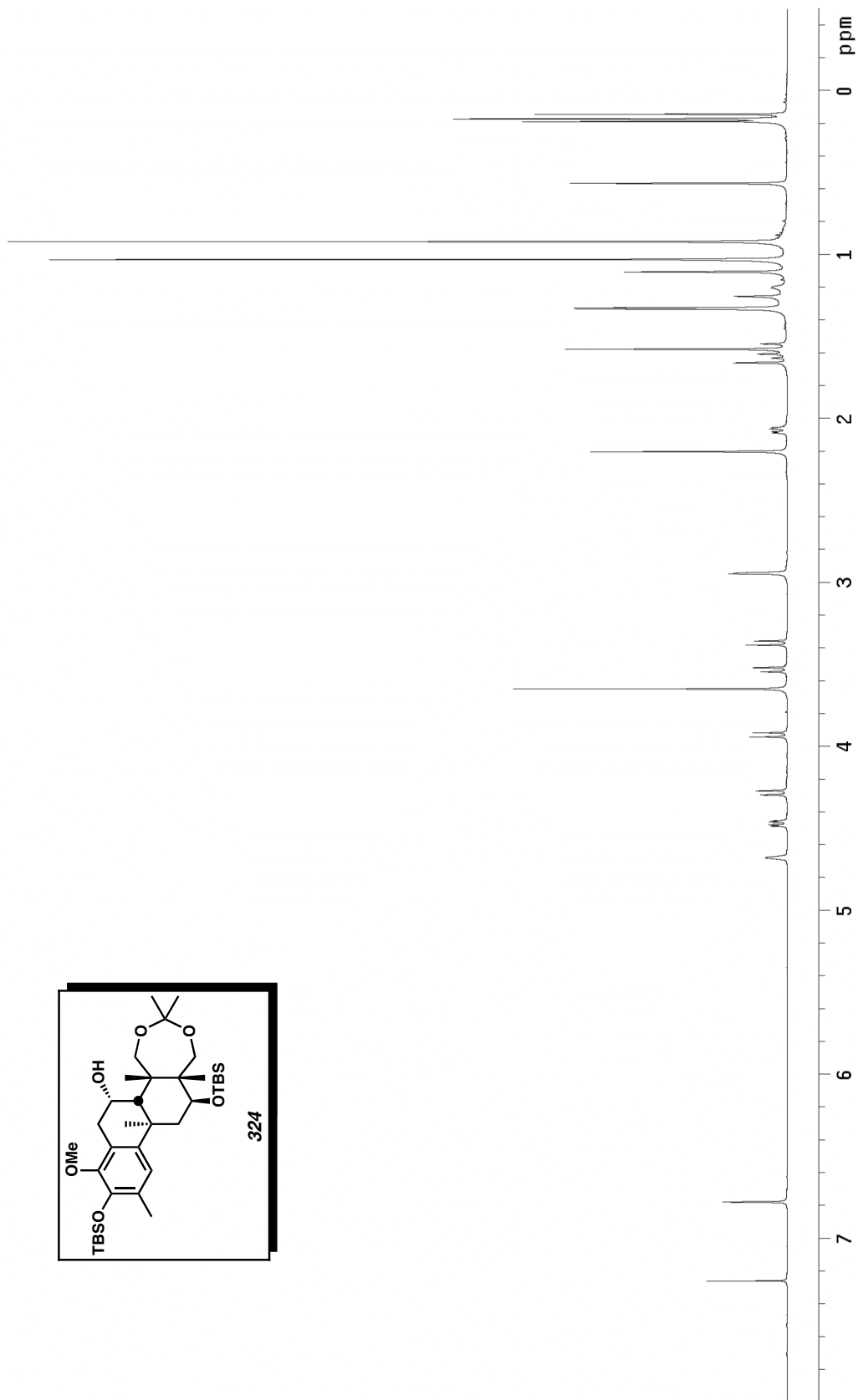
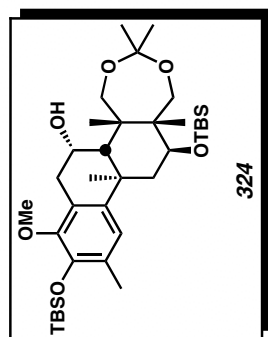


Figure C.22 ^1H NMR (500 MHz, CDCl_3) of compound **324**.

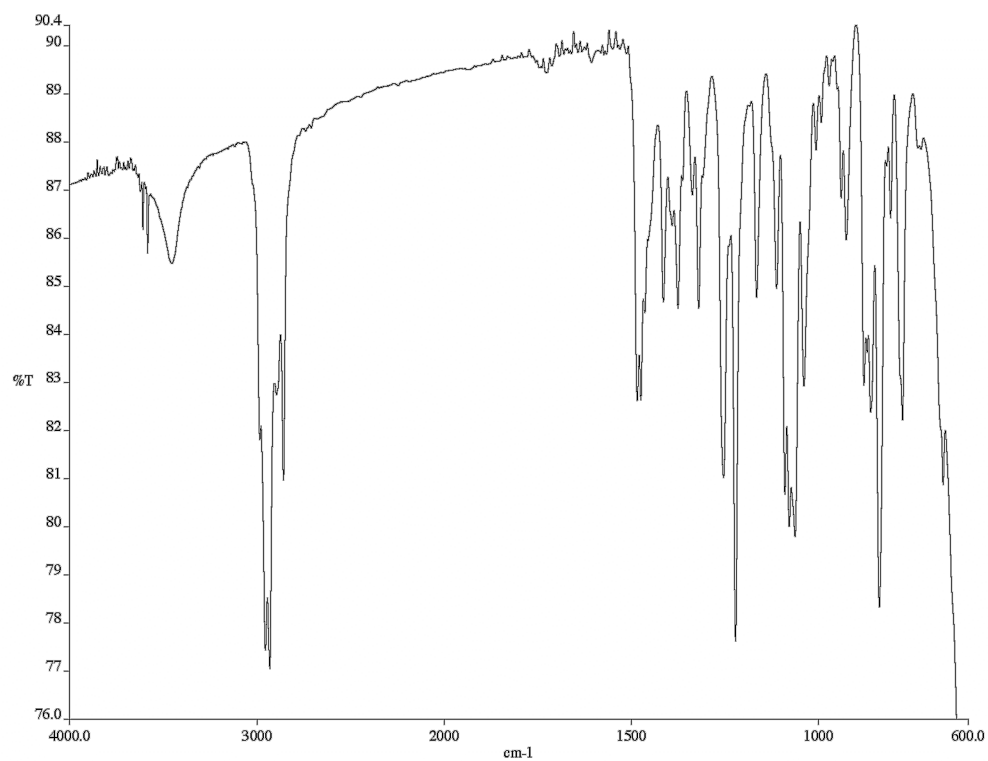


Figure C.23 Infrared spectrum (thin film/NaCl) of compound **324**.

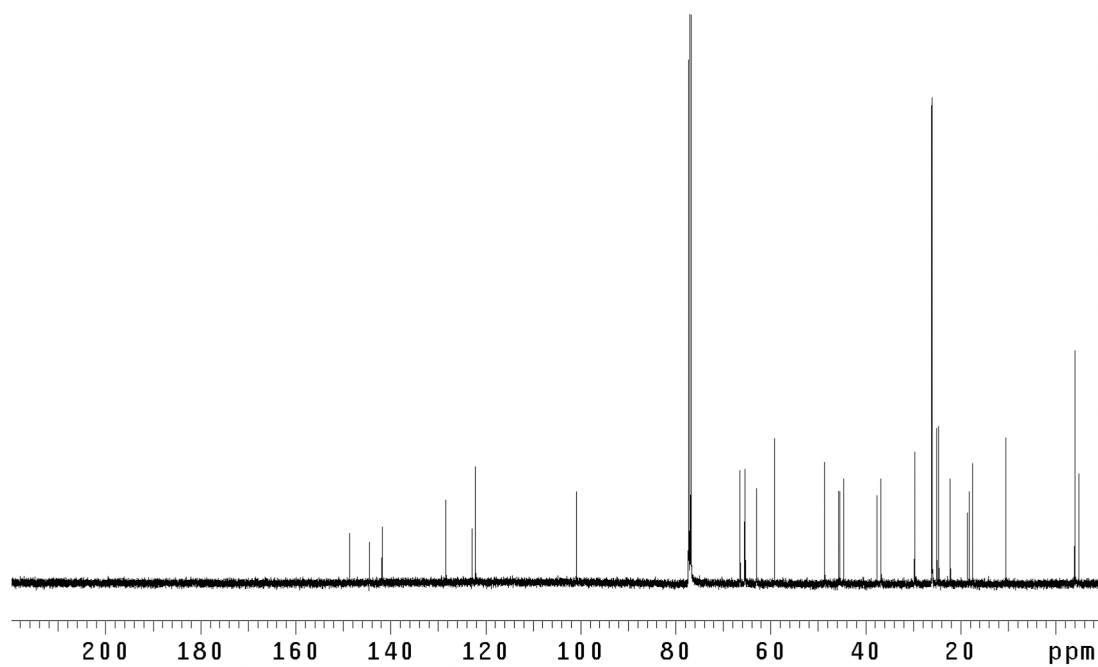


Figure C.24 ¹³C NMR (125 MHz, CDCl₃) of compound **324**.

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Crystal Structure Analysis of:

Alcohol **324** (DCB34)Contents:

Table C.1	Crystal data.
Table C.2	Atomic coordinates.
Table C.3	Full bond distances and angles.

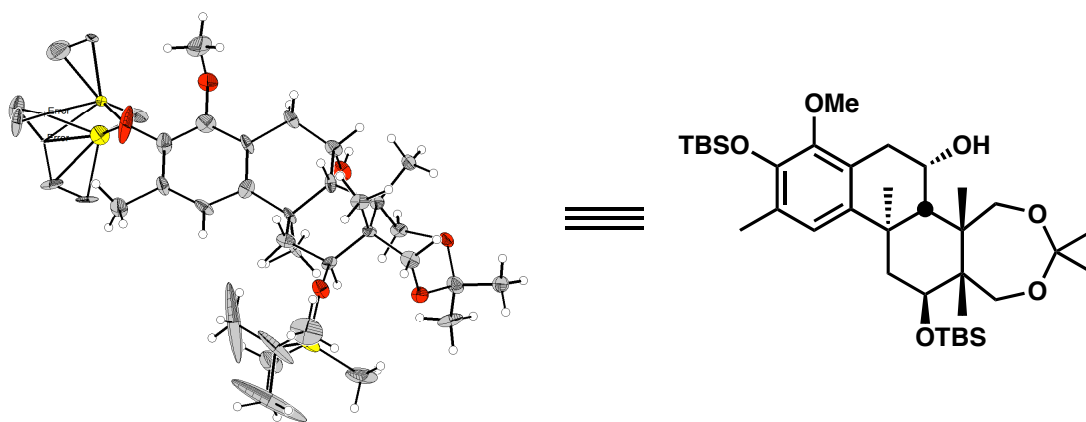
Figure C.25 Representation of Alcohol **324**.

Table C.1 Crystal data and structure refinement for dcb34.

Empirical formula	C ₃₆ H ₄₉ O ₆ Si ₂
Formula weight	633.93
Crystallization Solvent	Methylene Chloride
Crystal Habit	Fragment
Crystal size	0.45 x 0.20 x 0.19 mm ³
Crystal color	Colorless

Data Collection

Preliminary Photos		
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoK α	
Data Collection Temperature	100(2) K	
θ range for 2391 reflections used in lattice determination	2.25 to 25.75°	
Unit cell dimensions	a = 8.012(3) Å b = 12.103(5) Å c = 21.064(8) Å	α = 104.652(5)° β = 92.405(7)° γ = 98.610(6)°
Volume	1947.0(12) Å ³	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.081 Mg/m ³	
F(000)	682	
θ range for data collection	1.76 to 27.12°	
Completeness to θ = 27.12°	78.9 %	
Index ranges	-10 ≤ h ≤ 8, -15 ≤ k ≤ 15, -26 ≤ l ≤ 12	
Data collection scan type	scans at 3 settings	
Reflections collected	8155	
Independent reflections	6807 [R _{int} = 0.0961; GOF _{merge} =]	
Absorption coefficient	0.129 mm ⁻¹	
Absorption correction	None	

Table C.1 (cont.)**Structure Solution and Refinement**

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	direct
Secondary solution method	difmap
Hydrogen placement	geom
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6807 / 0 / 456
Treatment of hydrogen atoms	mixed
Goodness-of-fit on F^2	2.722
Final R indices [$I > 2\sigma(I)$, 4077 reflections]	$R_1 = 0.1484$, $wR_2 = 0.1836$
R indices (all data)	$R_1 = 0.2120$, $wR_2 = 0.1890$
Type of weighting scheme used	calc
Weighting scheme used	calc
$w = 1 / [\sigma^2(F_o^2) + (0.0000P)^2 + 0.0000P]$ where $P = (F_o^2 + 2F_c^2) / 3$	
Max shift/error	1.254
Average shift/error	0.004
Largest diff. peak and hole	0.655 and -0.594 e.Å ⁻³

Table C.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for dcb34. $U(\text{eq})$ is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Si(2A)	11898(6)	1267(5)	4132(2)	15(2)	0.480(9)
Si(2B)	12395(6)	2036(5)	4004(2)	32(2)	0.520(9)
O(6)	2561(6)	4434(4)	2066(2)	26(1)	1
O(4)	3040(6)	1577(4)	-102(2)	21(1)	1
O(3)	7053(6)	620(4)	947(2)	27(1)	1
O(5)	2281(6)	3355(4)	432(2)	24(1)	1
O(1A)	10070(40)	1775(16)	4115(16)	23(7)	0.480(9)
C(1)	2380(8)	2466(5)	1362(3)	16(2)	1
O(2)	8803(7)	-67(4)	2989(3)	41(2)	1
C(2)	4738(9)	3387(6)	2278(3)	23(2)	1
C(3)	4299(8)	1754(6)	459(3)	21(2)	1
C(4)	4798(8)	1409(6)	1584(3)	20(2)	1
C(5)	5795(9)	384(6)	1376(3)	23(2)	1
C(6)	5952(8)	2528(5)	1996(3)	19(2)	1
C(7)	7591(9)	3162(6)	3129(4)	25(2)	1
C(8)	7268(8)	3098(6)	1588(3)	21(2)	1
C(9)	3425(8)	1492(6)	1051(3)	16(2)	1
C(10)	3552(8)	3555(5)	1752(3)	19(2)	1
C(11)	8602(9)	3023(6)	3647(3)	24(2)	1
C(12)	6986(9)	2280(7)	2562(3)	24(2)	1
C(13)	7315(8)	1161(6)	2542(3)	22(2)	1
C(14)	1097(8)	2053(6)	1829(3)	20(2)	1
C(15)	1296(8)	2793(6)	853(3)	22(2)	1
C(16)	8395(9)	1028(6)	3049(4)	30(2)	1
C(17)	9097(10)	1930(7)	3580(4)	30(2)	1
C(18)	976(8)	2272(6)	-653(3)	25(2)	1
C(19)	2236(8)	320(5)	817(3)	23(2)	1
C(20)	6564(9)	111(6)	1978(3)	24(2)	1
C(21)	9165(10)	4017(6)	4246(3)	38(2)	1
C(22)	2536(10)	2627(6)	-208(4)	28(2)	1
C(23)	5312(9)	6404(7)	2242(4)	45(2)	1
C(24)	3956(9)	3325(6)	-466(4)	34(2)	1
C(25)	2088(11)	6074(7)	1347(5)	71(3)	1
C(26)	26(11)	6041(8)	2774(4)	64(3)	1
C(27)	2062(17)	7851(9)	2892(9)	241(12)	1
C(28)	1911(11)	6533(7)	2886(6)	80(4)	1
C(29)	2709(15)	6347(16)	3472(5)	225(13)	1
C(30)	7871(15)	-666(8)	3383(5)	95(5)	1
C(34)	15112(10)	2027(7)	4889(4)	39(2)	1
C(33)	12570(10)	2764(7)	5392(3)	43(2)	1
C(32)	13620(60)	2710(70)	4690(20)	330(60)	0.480(9)
O(1B)	10270(40)	1780(20)	4019(18)	67(10)	0.520(9)
C(37)	13940(30)	3570(18)	4427(13)	49(8)	0.480(9)
C(38)	12530(30)	502(17)	4794(9)	62(7)	0.520(9)
C(39)	13340(30)	2090(30)	4776(15)	42(7)	0.520(9)
C(42)	12884(10)	1006(6)	3290(3)	33(2)	1
C(40)	11720(20)	-94(12)	4414(8)	21(4)	0.480(9)

C(41)	13220(20)	3598(12)	3960(8)	30(4)	0.520(9)
Si(1)	2960(3)	5826(2)	2116(1)	36(1)	1

Table C.3 Bond lengths [Å] and angles [°] for dcb34.

Si(2A)-O(1A)	1.68(3)	C(14)-H(14A)	0.9800
Si(2A)-C(40)	1.876(15)	C(14)-H(14B)	0.9800
Si(2A)-C(42)	1.943(8)	C(14)-H(14C)	0.9800
Si(2A)-C(32)	2.11(7)	C(15)-H(15A)	0.9900
Si(2B)-O(1B)	1.69(3)	C(15)-H(15B)	0.9900
Si(2B)-C(39)	1.75(3)	C(16)-C(17)	1.381(10)
Si(2B)-C(42)	1.793(8)	C(17)-O(1B)	1.35(3)
Si(2B)-C(41)	1.934(15)	C(18)-C(22)	1.470(9)
O(6)-C(10)	1.464(7)	C(18)-H(18A)	0.9800
O(6)-Si(1)	1.643(5)	C(18)-H(18B)	0.9800
O(4)-C(22)	1.456(8)	C(18)-H(18C)	0.9800
O(4)-C(3)	1.471(7)	C(19)-H(19A)	0.9800
O(3)-C(5)	1.426(8)	C(19)-H(19B)	0.9800
O(3)-H(3)	0.8400	C(19)-H(19C)	0.9800
O(5)-C(15)	1.441(7)	C(20)-H(20A)	0.9900
O(5)-C(22)	1.454(8)	C(20)-H(20B)	0.9900
O(1A)-C(17)	1.41(3)	C(21)-H(21A)	0.9800
C(1)-C(15)	1.516(9)	C(21)-H(21B)	0.9800
C(1)-C(10)	1.520(9)	C(21)-H(21C)	0.9800
C(1)-C(14)	1.567(9)	C(22)-C(24)	1.516(9)
C(1)-C(9)	1.572(8)	C(23)-Si(1)	1.892(8)
O(2)-C(16)	1.388(8)	C(23)-H(23A)	0.9800
O(2)-C(30)	1.403(11)	C(23)-H(23B)	0.9800
C(2)-C(10)	1.502(8)	C(23)-H(23C)	0.9800
C(2)-C(6)	1.554(8)	C(24)-H(24A)	0.9800
C(2)-H(2A)	0.9900	C(24)-H(24B)	0.9800
C(2)-H(2B)	0.9900	C(24)-H(24C)	0.9800
C(3)-C(9)	1.535(9)	C(25)-Si(1)	1.847(8)
C(3)-H(3A)	0.9900	C(25)-H(25A)	0.9800
C(3)-H(3B)	0.9900	C(25)-H(25B)	0.9800
C(4)-C(6)	1.551(9)	C(25)-H(25C)	0.9800
C(4)-C(5)	1.556(8)	C(26)-C(28)	1.523(11)
C(4)-C(9)	1.570(9)	C(26)-H(26A)	0.9800
C(4)-H(4)	1.0000	C(26)-H(26B)	0.9800
C(5)-C(20)	1.519(9)	C(26)-H(26C)	0.9800
C(5)-H(5)	1.0000	C(27)-C(28)	1.578(15)
C(6)-C(12)	1.540(9)	C(27)-H(27A)	0.9800
C(6)-C(8)	1.576(9)	C(27)-H(27B)	0.9800
C(7)-C(11)	1.391(9)	C(27)-H(27C)	0.9800
C(7)-C(12)	1.397(9)	C(28)-C(29)	1.449(17)
C(7)-H(7)	0.9500	C(28)-Si(1)	1.923(9)
C(8)-H(8A)	0.9800	C(29)-H(29A)	0.9800
C(8)-H(8B)	0.9800	C(29)-H(29B)	0.9800
C(8)-H(8C)	0.9800	C(29)-H(29C)	0.9800
C(9)-C(19)	1.537(9)	C(30)-H(30A)	0.9800
C(10)-H(10)	1.0000	C(30)-H(30B)	0.9800
C(11)-C(17)	1.412(10)	C(30)-H(30C)	0.9800
C(11)-C(21)	1.505(9)	C(34)-C(39)	1.45(3)
C(12)-C(13)	1.410(9)	C(34)-C(32)	1.65(5)
C(13)-C(16)	1.402(9)	C(33)-C(39)	1.55(3)
C(13)-C(20)	1.528(8)	C(33)-C(32)	1.73(5)

C(32)-C(37)	1.29(9)	C(4)-C(6)-C(8)	113.9(5)
C(38)-C(39)	1.94(4)	C(2)-C(6)-C(8)	109.6(5)
O(1A)-Si(2A)-C(40)	113.4(11)	C(11)-C(7)-C(12)	124.2(7)
O(1A)-Si(2A)-C(42)	112.9(13)	C(11)-C(7)-H(7)	117.9
C(40)-Si(2A)-C(42)	108.8(5)	C(12)-C(7)-H(7)	117.9
O(1A)-Si(2A)-C(32)	103.6(15)	C(6)-C(8)-H(8A)	109.5
C(40)-Si(2A)-C(32)	117(2)	C(6)-C(8)-H(8B)	109.5
C(42)-Si(2A)-C(32)	100.4(15)	H(8A)-C(8)-H(8B)	109.5
O(1B)-Si(2B)-C(39)	109.1(16)	C(6)-C(8)-H(8C)	109.5
O(1B)-Si(2B)-C(42)	106.2(11)	H(8A)-C(8)-H(8C)	109.5
C(39)-Si(2B)-C(42)	119.3(11)	H(8B)-C(8)-H(8C)	109.5
O(1B)-Si(2B)-C(41)	112.0(12)	C(3)-C(9)-C(19)	108.6(5)
C(39)-Si(2B)-C(41)	99.8(12)	C(3)-C(9)-C(4)	109.4(5)
C(42)-Si(2B)-C(41)	110.5(6)	C(19)-C(9)-C(4)	108.9(5)
C(10)-O(6)-Si(1)	126.8(4)	C(3)-C(9)-C(1)	110.8(5)
C(22)-O(4)-C(3)	115.3(5)	C(19)-C(9)-C(1)	109.7(5)
C(5)-O(3)-H(3)	109.5	C(4)-C(9)-C(1)	109.4(5)
C(15)-O(5)-C(22)	116.3(5)	O(6)-C(10)-C(2)	107.6(5)
C(17)-O(1A)-Si(2A)	130(2)	O(6)-C(10)-C(1)	110.2(5)
C(15)-C(1)-C(10)	107.9(5)	C(2)-C(10)-C(1)	115.2(6)
C(15)-C(1)-C(14)	104.9(5)	O(6)-C(10)-H(10)	107.9
C(10)-C(1)-C(14)	108.9(5)	C(2)-C(10)-H(10)	107.9
C(15)-C(1)-C(9)	113.1(6)	C(1)-C(10)-H(10)	107.9
C(10)-C(1)-C(9)	110.7(5)	C(7)-C(11)-C(17)	117.5(7)
C(14)-C(1)-C(9)	111.1(5)	C(7)-C(11)-C(21)	120.5(6)
C(16)-O(2)-C(30)	112.3(6)	C(17)-C(11)-C(21)	122.0(7)
C(10)-C(2)-C(6)	112.6(5)	C(7)-C(12)-C(13)	117.3(6)
C(10)-C(2)-H(2A)	109.1	C(7)-C(12)-C(6)	120.7(6)
C(6)-C(2)-H(2A)	109.1	C(13)-C(12)-C(6)	121.9(6)
C(10)-C(2)-H(2B)	109.1	C(16)-C(13)-C(12)	118.3(6)
C(6)-C(2)-H(2B)	109.1	C(16)-C(13)-C(20)	120.0(6)
H(2A)-C(2)-H(2B)	107.8	C(12)-C(13)-C(20)	121.7(6)
O(4)-C(3)-C(9)	110.2(5)	C(1)-C(14)-H(14A)	109.5
O(4)-C(3)-H(3A)	109.6	C(1)-C(14)-H(14B)	109.5
C(9)-C(3)-H(3A)	109.6	H(14A)-C(14)-H(14B)	109.5
O(4)-C(3)-H(3B)	109.6	C(1)-C(14)-H(14C)	109.5
C(9)-C(3)-H(3B)	109.6	H(14A)-C(14)-H(14C)	109.5
H(3A)-C(3)-H(3B)	108.1	H(14B)-C(14)-H(14C)	109.5
C(6)-C(4)-C(5)	112.0(5)	O(5)-C(15)-C(1)	113.0(6)
C(6)-C(4)-C(9)	119.5(6)	O(5)-C(15)-H(15A)	109.0
C(5)-C(4)-C(9)	115.5(5)	C(1)-C(15)-H(15A)	109.0
C(6)-C(4)-H(4)	102.2	O(5)-C(15)-H(15B)	109.0
C(5)-C(4)-H(4)	102.2	C(1)-C(15)-H(15B)	109.0
C(9)-C(4)-H(4)	102.2	H(15A)-C(15)-H(15B)	107.8
O(3)-C(5)-C(20)	111.5(6)	C(17)-C(16)-O(2)	119.7(7)
O(3)-C(5)-C(4)	111.1(6)	C(17)-C(16)-C(13)	123.3(7)
C(20)-C(5)-C(4)	110.5(6)	O(2)-C(16)-C(13)	117.0(7)
O(3)-C(5)-H(5)	107.9	O(1B)-C(17)-C(16)	120.7(14)
C(20)-C(5)-H(5)	107.9	O(1B)-C(17)-O(1A)	11(3)
C(4)-C(5)-H(5)	107.9	C(16)-C(17)-O(1A)	123.0(10)
C(12)-C(6)-C(4)	110.9(6)	O(1B)-C(17)-C(11)	120.6(14)
C(12)-C(6)-C(2)	110.1(5)	C(16)-C(17)-C(11)	118.6(7)
C(4)-C(6)-C(2)	105.8(5)	O(1A)-C(17)-C(11)	117.5(11)
C(12)-C(6)-C(8)	106.6(6)	C(22)-C(18)-H(18A)	109.5

C(22)-C(18)-H(18B)	109.5	C(28)-C(27)-H(27B)	109.5
H(18A)-C(18)-H(18B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(22)-C(18)-H(18C)	109.5	C(28)-C(27)-H(27C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(18B)-C(18)-H(18C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(9)-C(19)-H(19A)	109.5	C(29)-C(28)-C(26)	112.9(11)
C(9)-C(19)-H(19B)	109.5	C(29)-C(28)-C(27)	113.7(11)
H(19A)-C(19)-H(19B)	109.5	C(26)-C(28)-C(27)	106.1(9)
C(9)-C(19)-H(19C)	109.5	C(29)-C(28)-Si(1)	110.7(7)
H(19A)-C(19)-H(19C)	109.5	C(26)-C(28)-Si(1)	107.6(6)
H(19B)-C(19)-H(19C)	109.5	C(27)-C(28)-Si(1)	105.4(8)
C(5)-C(20)-C(13)	115.6(6)	C(28)-C(29)-H(29A)	109.5
C(5)-C(20)-H(20A)	108.4	C(28)-C(29)-H(29B)	109.5
C(13)-C(20)-H(20A)	108.4	H(29A)-C(29)-H(29B)	109.5
C(5)-C(20)-H(20B)	108.4	C(28)-C(29)-H(29C)	109.5
C(13)-C(20)-H(20B)	108.4	H(29A)-C(29)-H(29C)	109.5
H(20A)-C(20)-H(20B)	107.5	H(29B)-C(29)-H(29C)	109.5
C(11)-C(21)-H(21A)	109.5	O(2)-C(30)-H(30A)	109.5
C(11)-C(21)-H(21B)	109.5	O(2)-C(30)-H(30B)	109.5
H(21A)-C(21)-H(21B)	109.5	H(30A)-C(30)-H(30B)	109.5
C(11)-C(21)-H(21C)	109.5	O(2)-C(30)-H(30C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(21B)-C(21)-H(21C)	109.5	H(30B)-C(30)-H(30C)	109.5
O(5)-C(22)-O(4)	107.4(5)	C(39)-C(34)-C(32)	30(4)
O(5)-C(22)-C(18)	112.5(6)	C(39)-C(33)-C(32)	28(3)
O(4)-C(22)-C(18)	107.1(6)	C(37)-C(32)-C(34)	123(4)
O(5)-C(22)-C(24)	105.3(6)	C(37)-C(32)-C(33)	124(4)
O(4)-C(22)-C(24)	111.1(6)	C(34)-C(32)-C(33)	96(4)
C(18)-C(22)-C(24)	113.4(7)	C(37)-C(32)-Si(2A)	116(3)
Si(1)-C(23)-H(23A)	109.5	C(34)-C(32)-Si(2A)	99(4)
Si(1)-C(23)-H(23B)	109.5	C(33)-C(32)-Si(2A)	93(3)
H(23A)-C(23)-H(23B)	109.5	C(17)-O(1B)-Si(2B)	127(3)
Si(1)-C(23)-H(23C)	109.5	C(34)-C(39)-C(33)	113.8(18)
H(23A)-C(23)-H(23C)	109.5	C(34)-C(39)-Si(2B)	123(2)
H(23B)-C(23)-H(23C)	109.5	C(33)-C(39)-Si(2B)	117(2)
C(22)-C(24)-H(24A)	109.5	C(34)-C(39)-C(38)	95.0(19)
C(22)-C(24)-H(24B)	109.5	C(33)-C(39)-C(38)	100.8(16)
H(24A)-C(24)-H(24B)	109.5	Si(2B)-C(39)-C(38)	98.6(14)
C(22)-C(24)-H(24C)	109.5	Si(2B)-C(42)-Si(2A)	32.6(2)
H(24A)-C(24)-H(24C)	109.5	O(6)-Si(1)-C(25)	108.9(3)
H(24B)-C(24)-H(24C)	109.5	O(6)-Si(1)-C(23)	111.8(3)
Si(1)-C(25)-H(25A)	109.5	C(25)-Si(1)-C(23)	109.2(4)
Si(1)-C(25)-H(25B)	109.5	O(6)-Si(1)-C(28)	104.3(4)
H(25A)-C(25)-H(25B)	109.5	C(25)-Si(1)-C(28)	113.9(5)
Si(1)-C(25)-H(25C)	109.5	C(23)-Si(1)-C(28)	108.8(4)
H(25A)-C(25)-H(25C)	109.5		
H(25B)-C(25)-H(25C)	109.5		
C(28)-C(26)-H(26A)	109.5		
C(28)-C(26)-H(26B)	109.5		
H(26A)-C(26)-H(26B)	109.5		
C(28)-C(26)-H(26C)	109.5		
H(26A)-C(26)-H(26C)	109.5		
H(26B)-C(26)-H(26C)	109.5		
C(28)-C(27)-H(27A)	109.5		