Supporting Information

Conception and Evolution of Stereocontrolled Strategies toward Functionalized 8-Aryloctanoic Acids Related to the Total Synthesis of Aliskiren

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X-Ray

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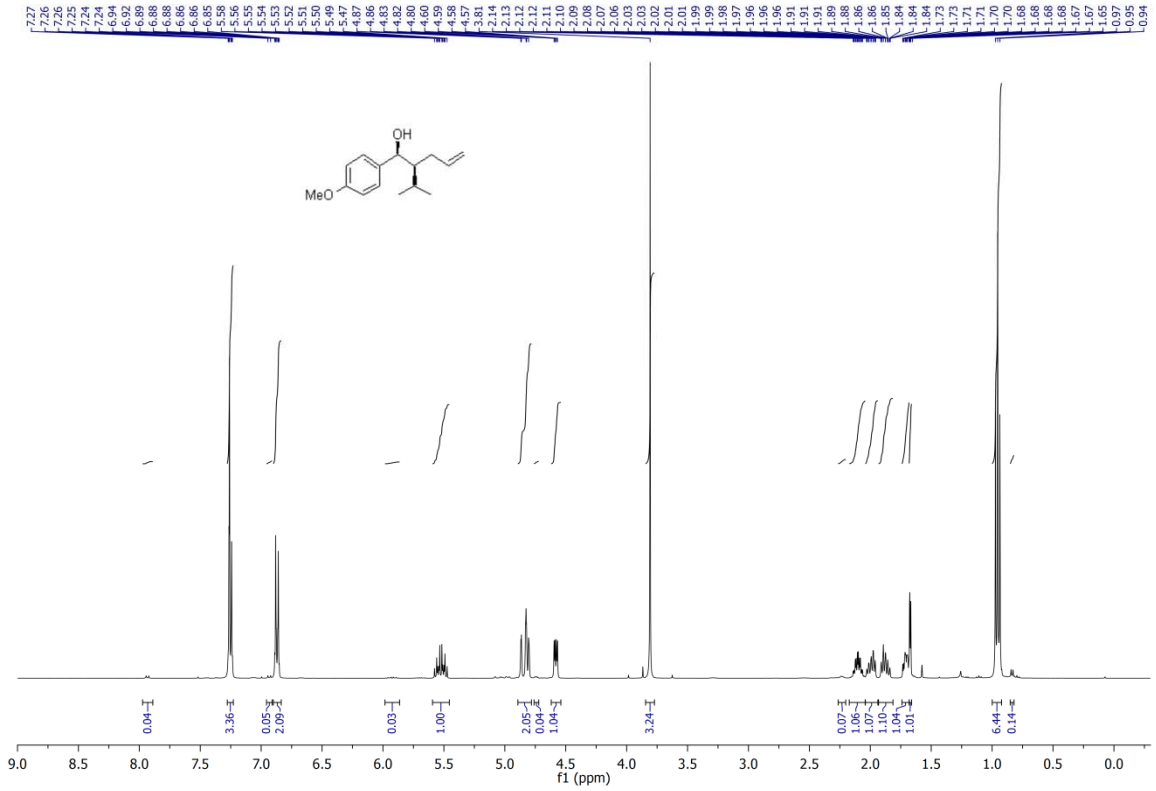
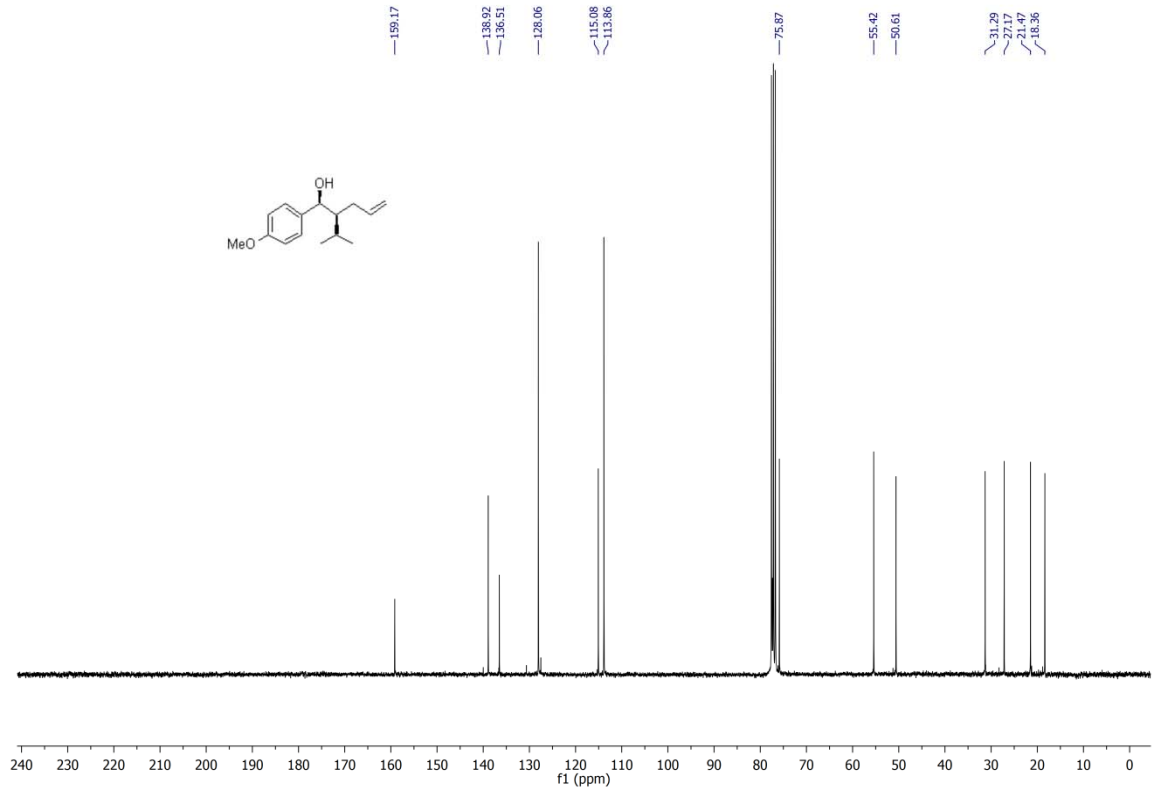
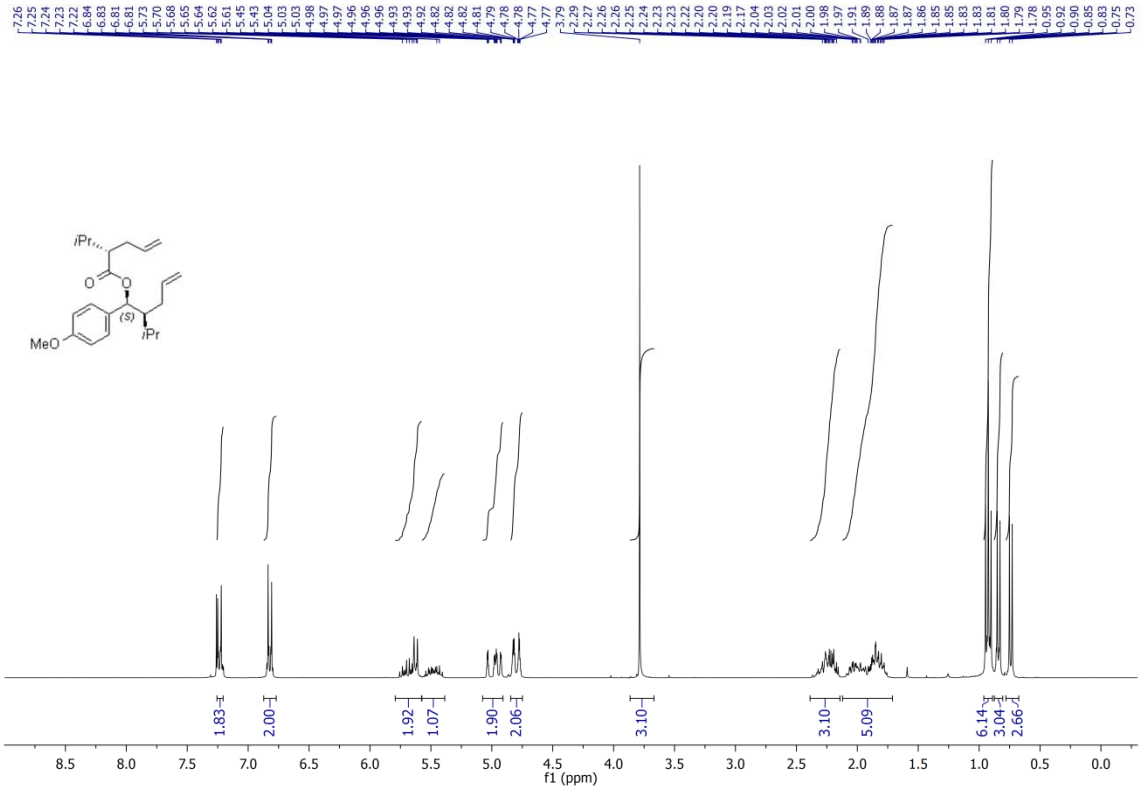


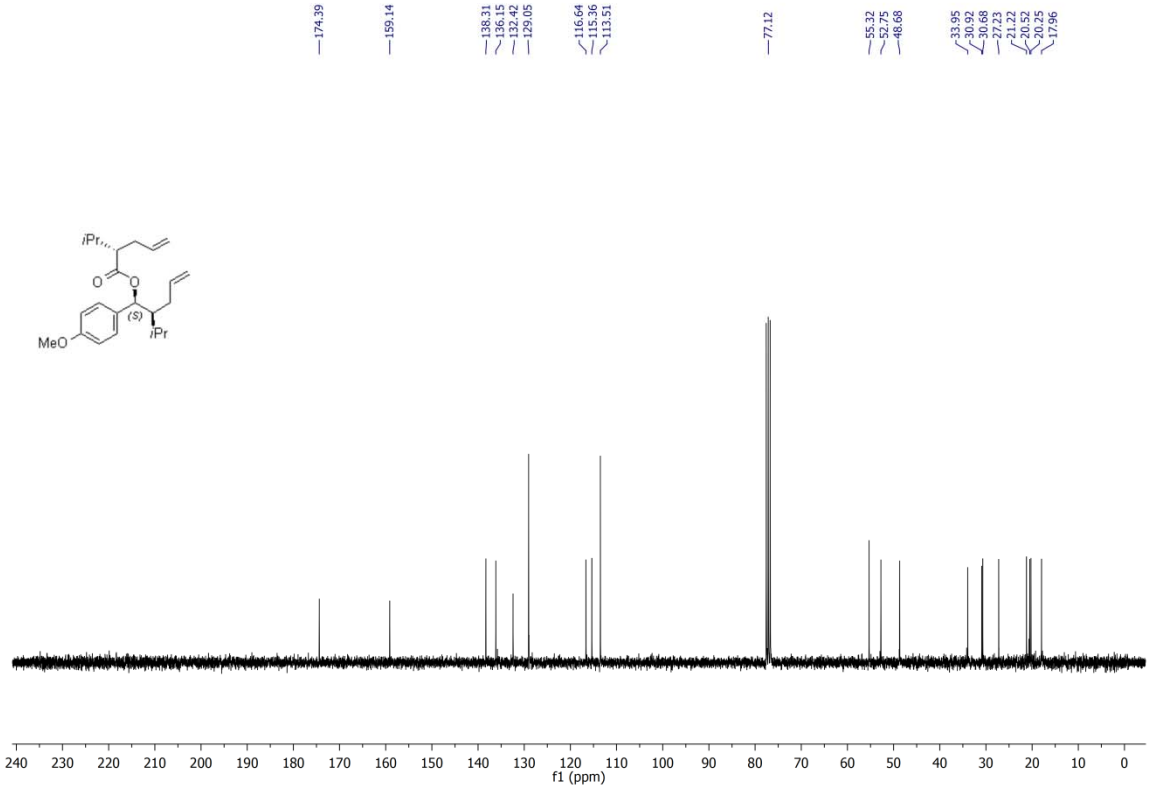
75 MHz, $CDCl_3$



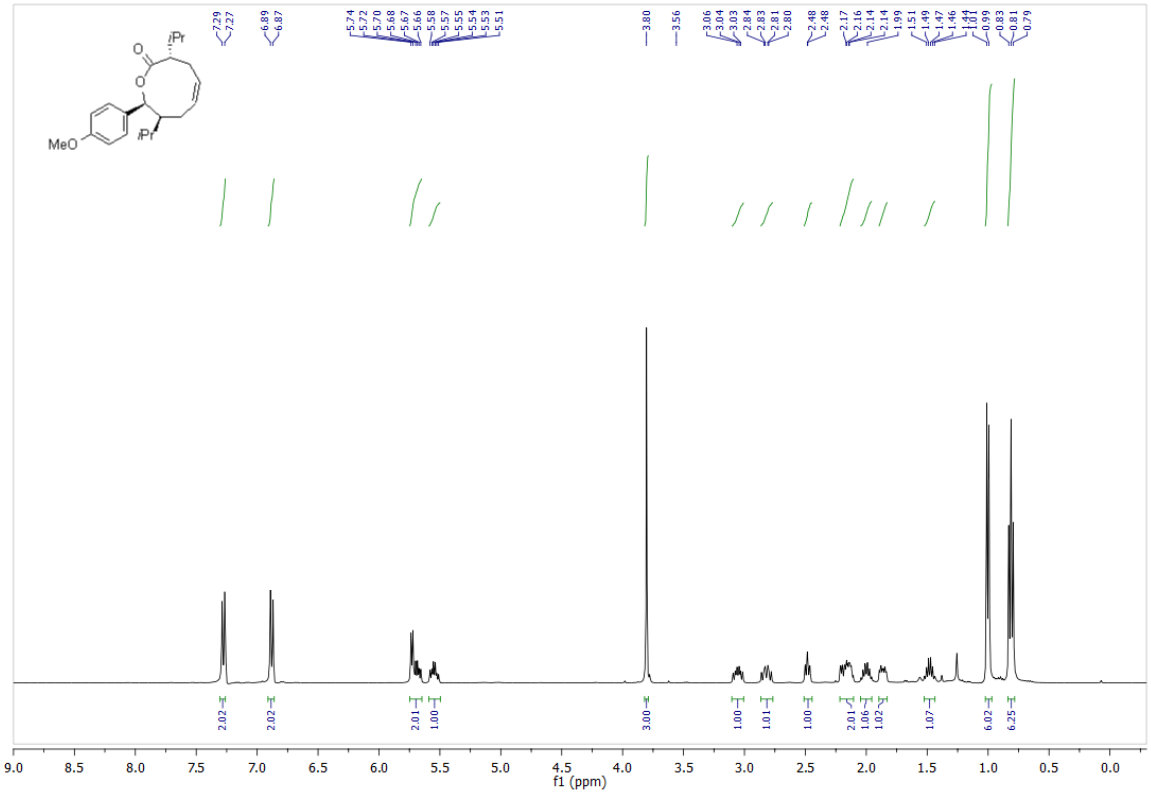
Ester **16**, 300 MHz, $CDCl_3$



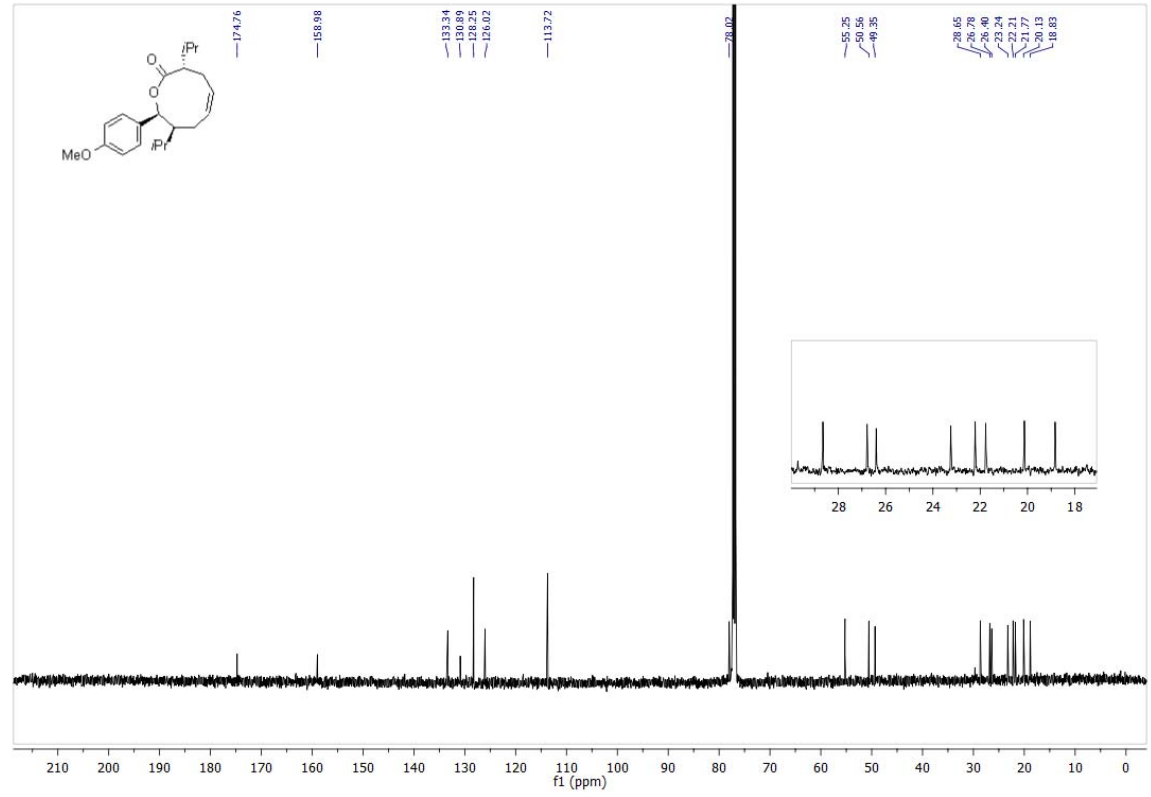
75 MHz, $CDCl_3$



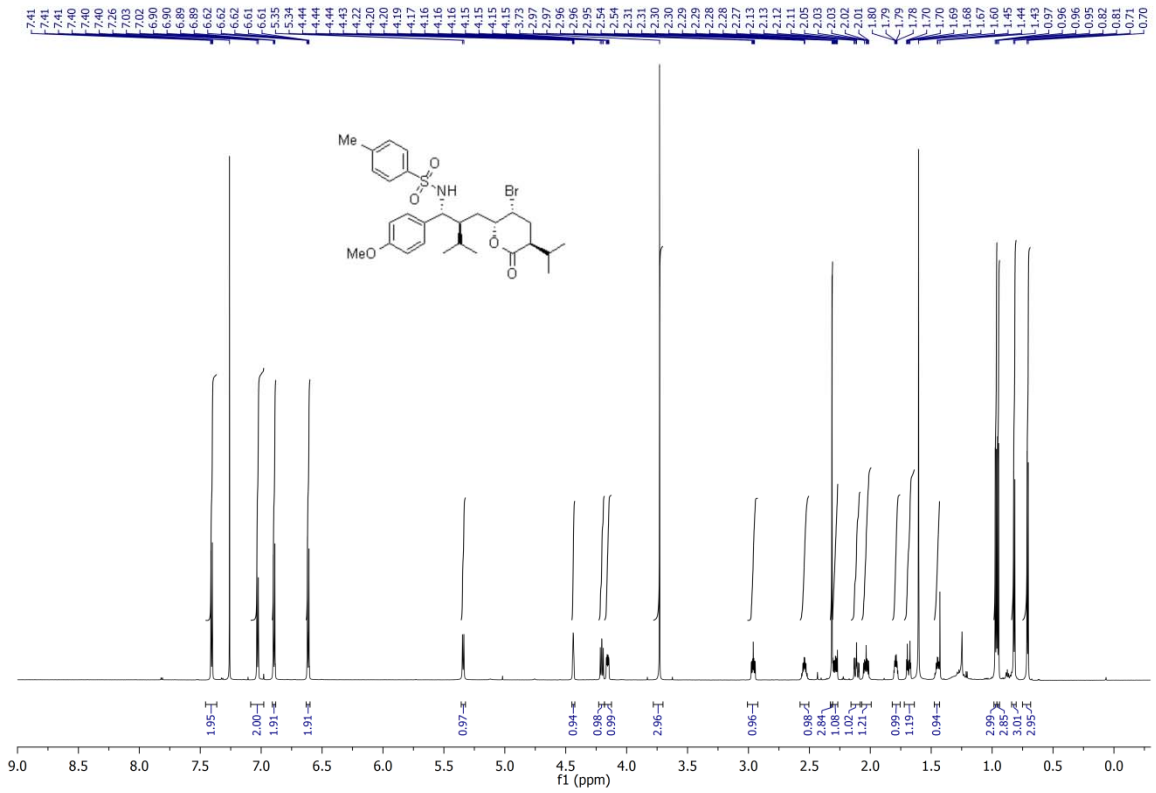
Lactone **20**, 400 MHz, CDCl3



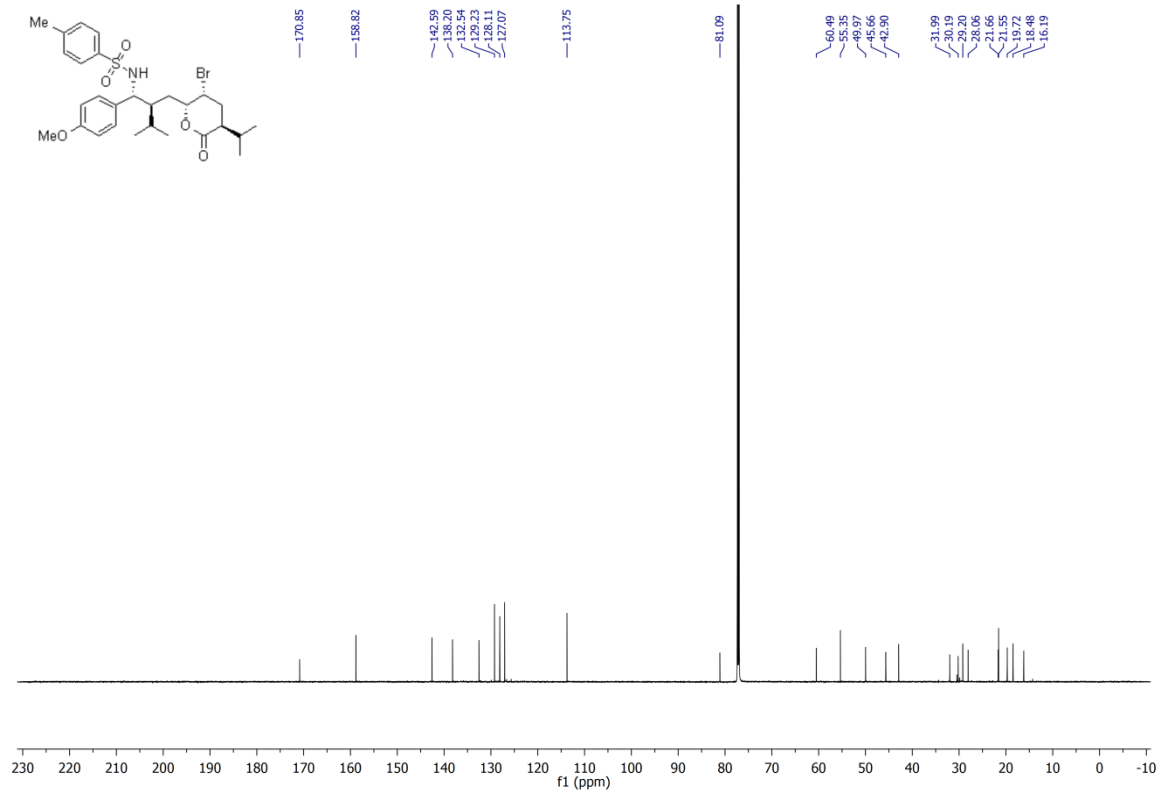
126 MHz, $CDCl_3$



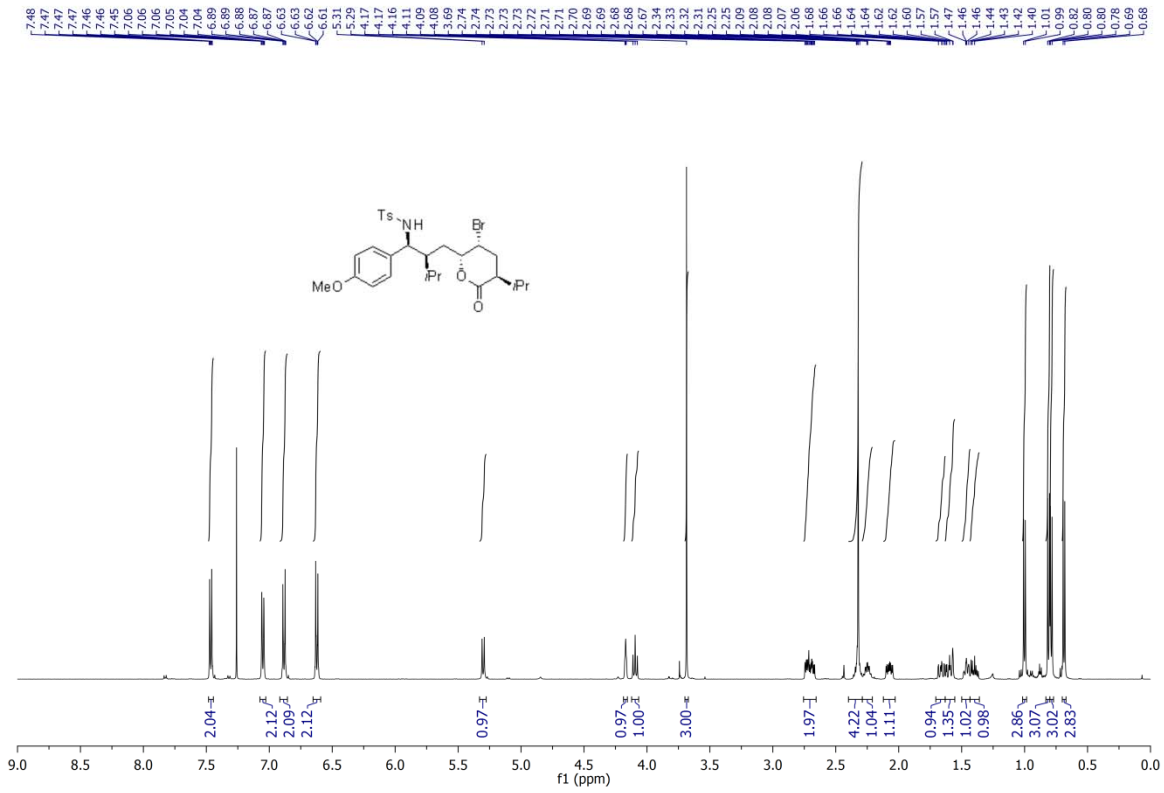
Bromolactone **24**, 700 MHz, $CDCl_3$



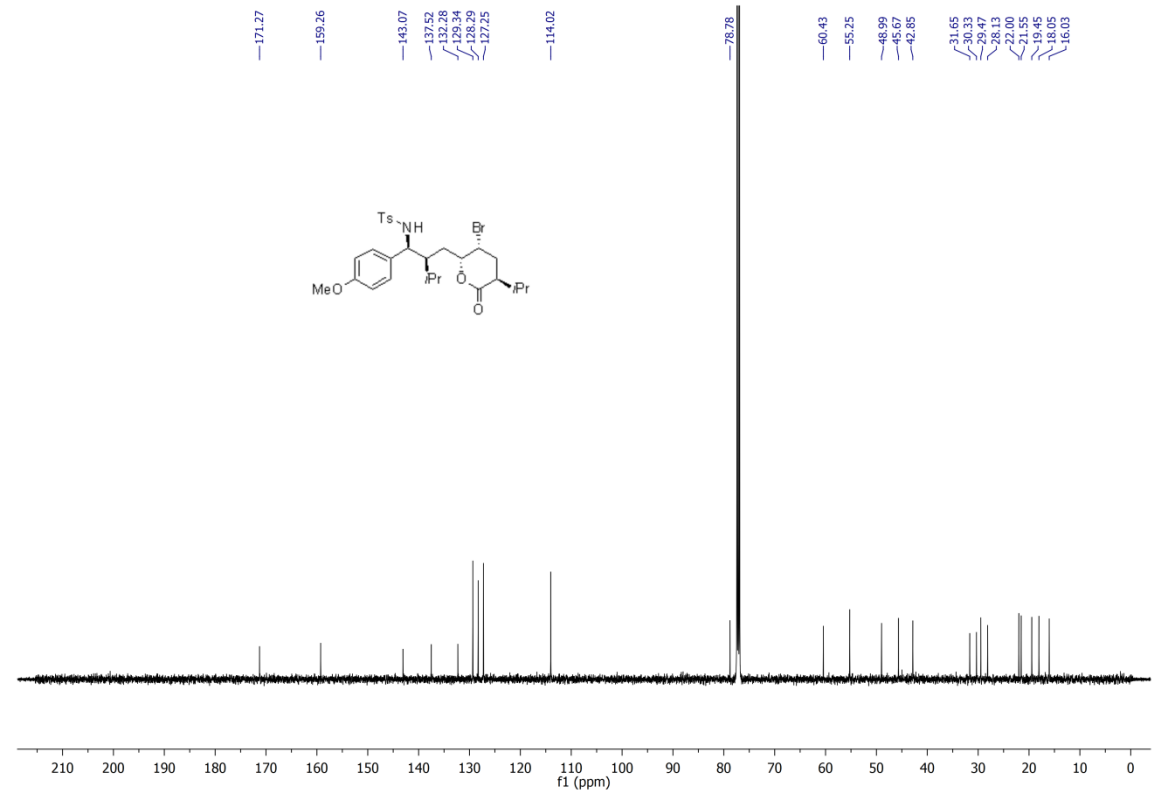
176 MHz, $CDCl_3$



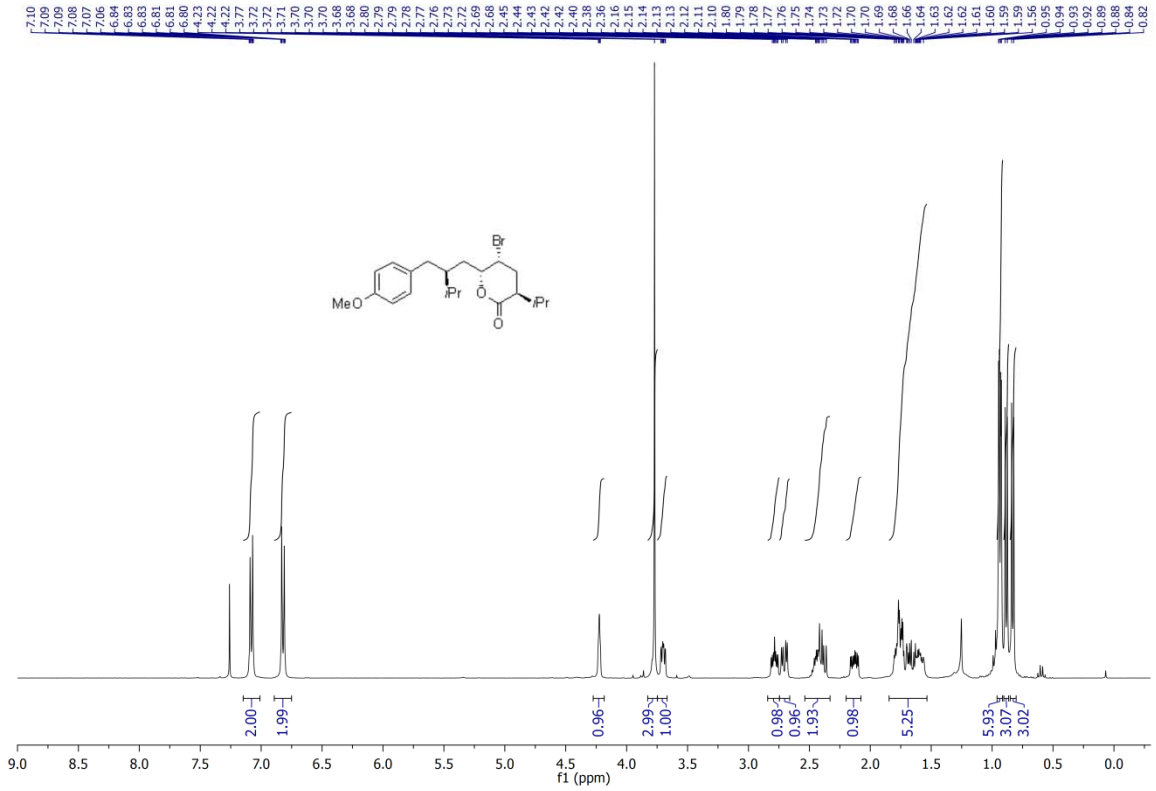
Bromolactone **25**, 500 MHz, $CDCl_3$



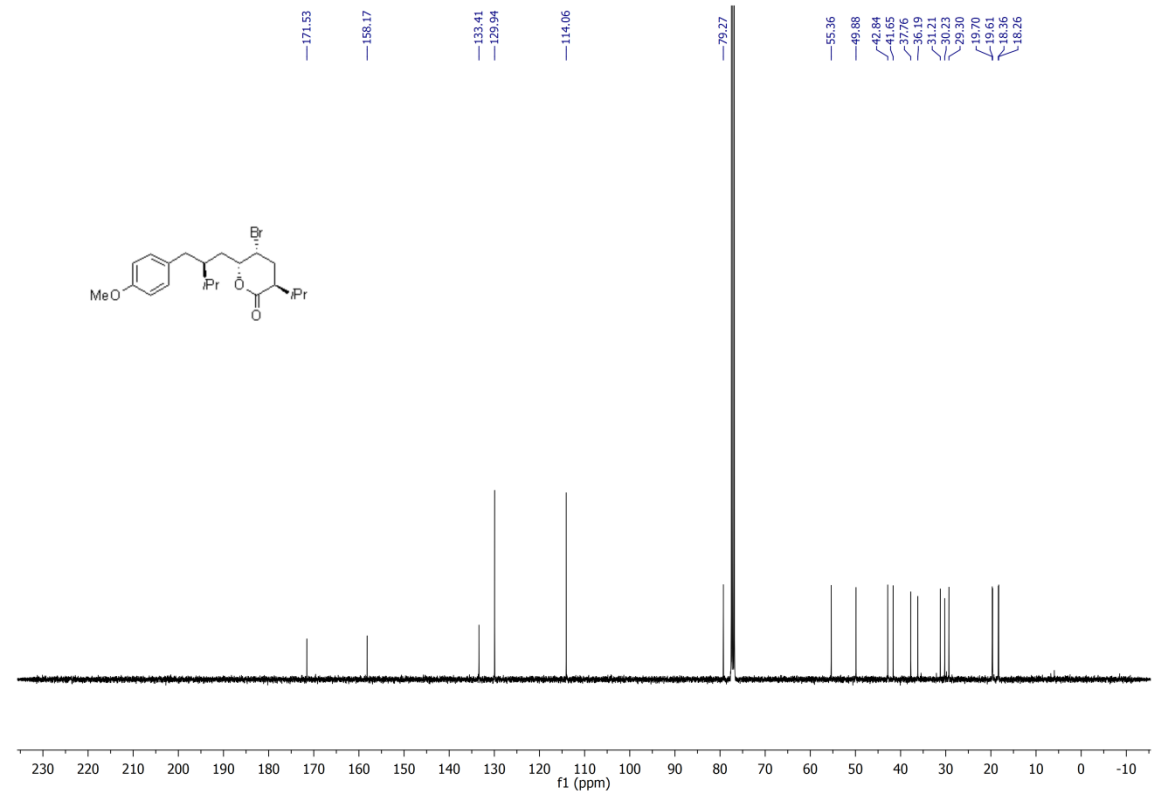
176 MHz, $CDCl_3$



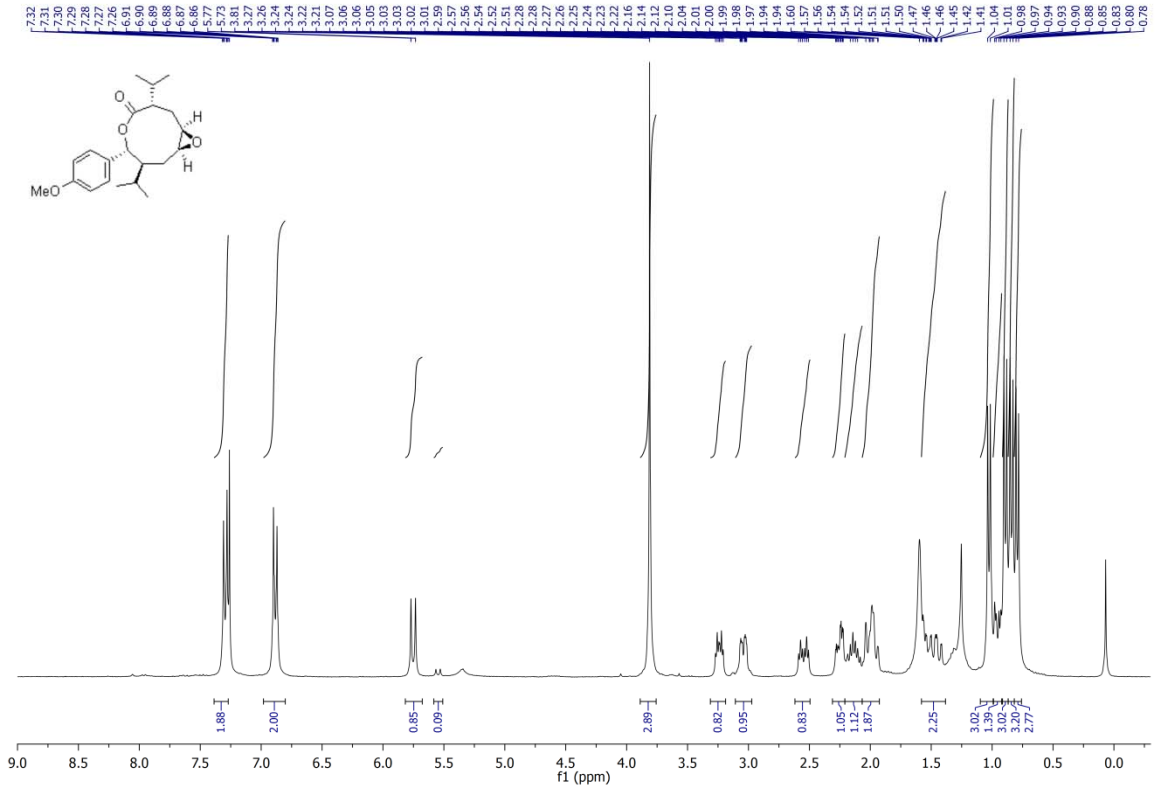
Bromolactone **26**, 400 MHz, $CDCl_3$



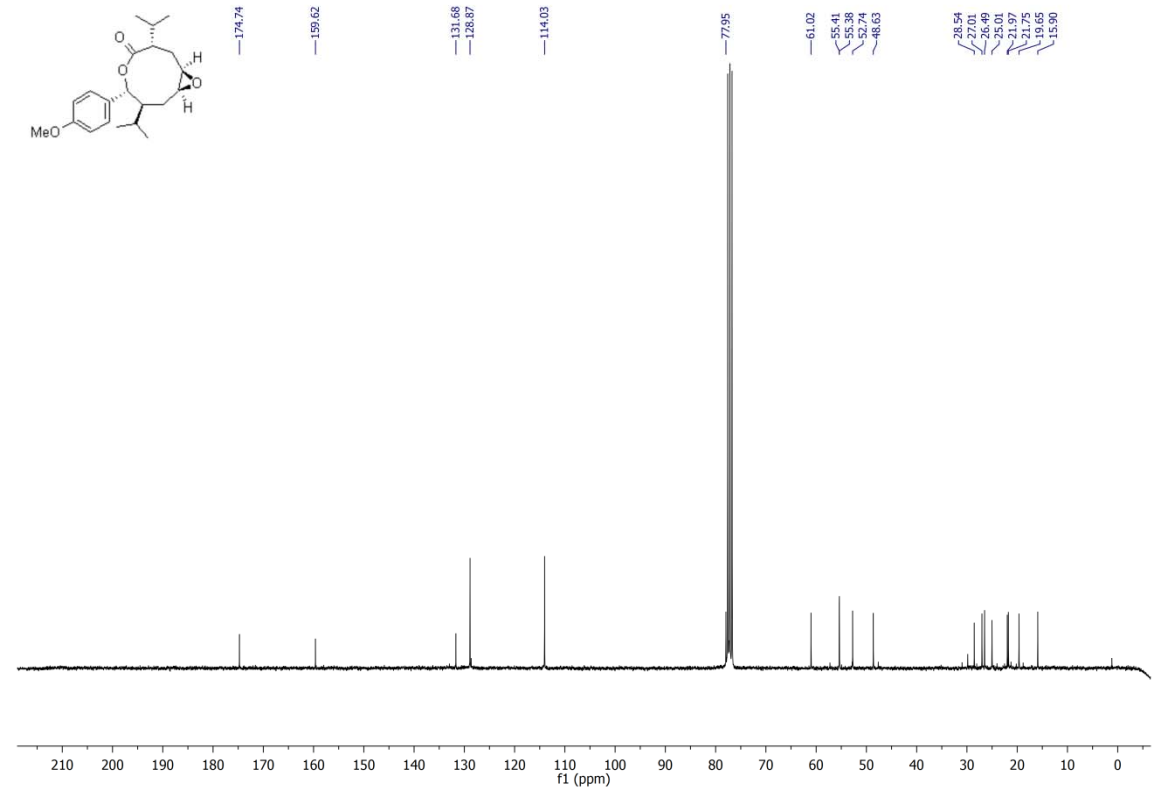
101 MHz, $CDCl_3$



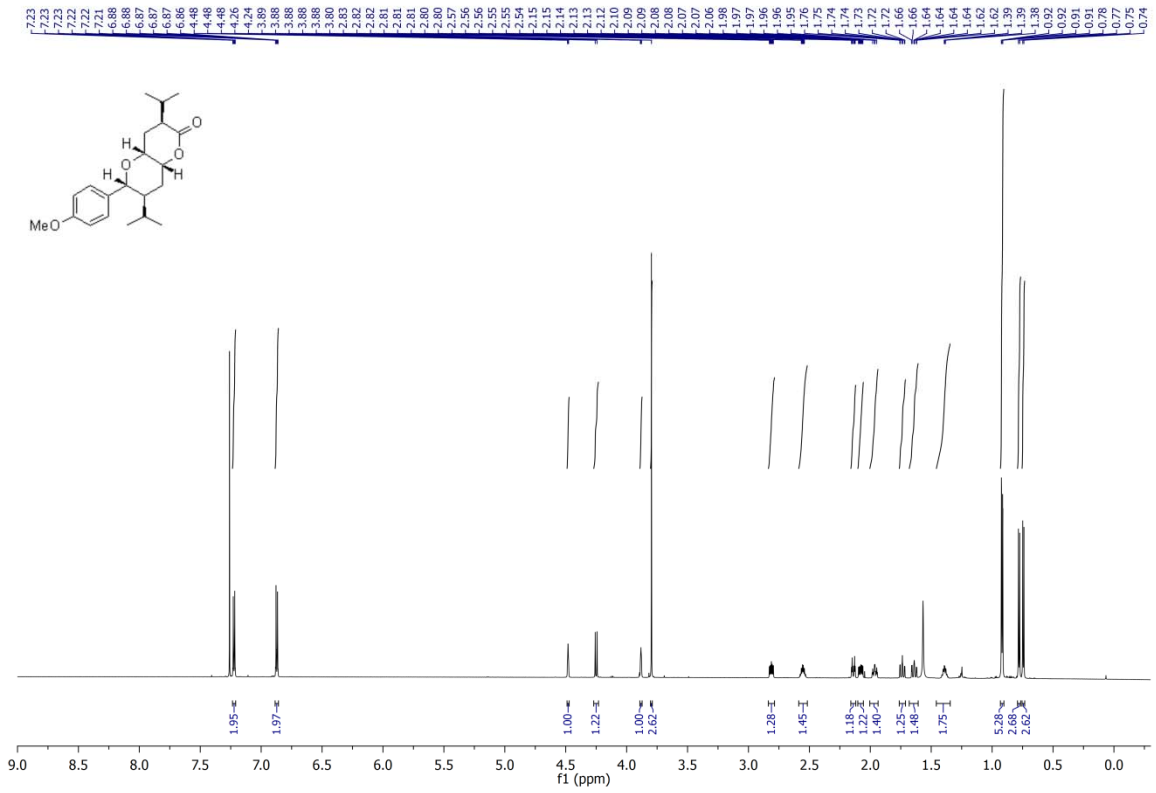
Epoxide **28**, 300 MHz, $CDCl_3$



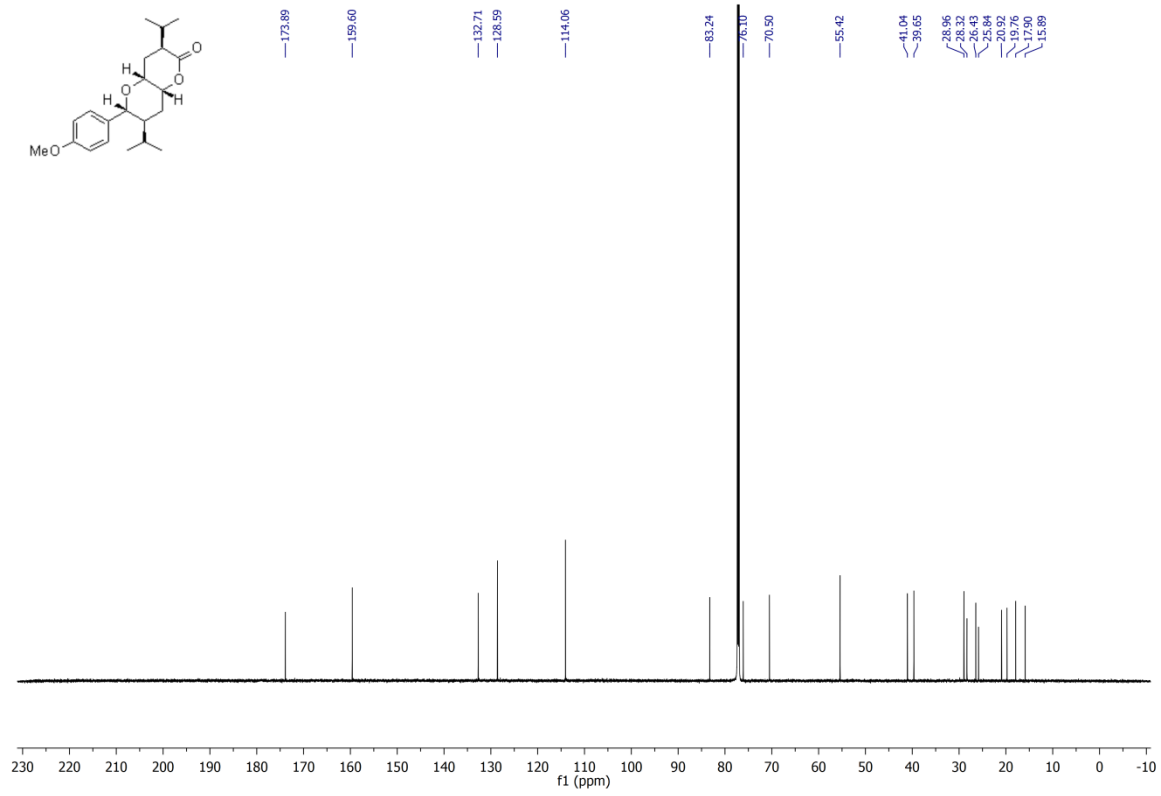
75 MHz, $CDCl_3$



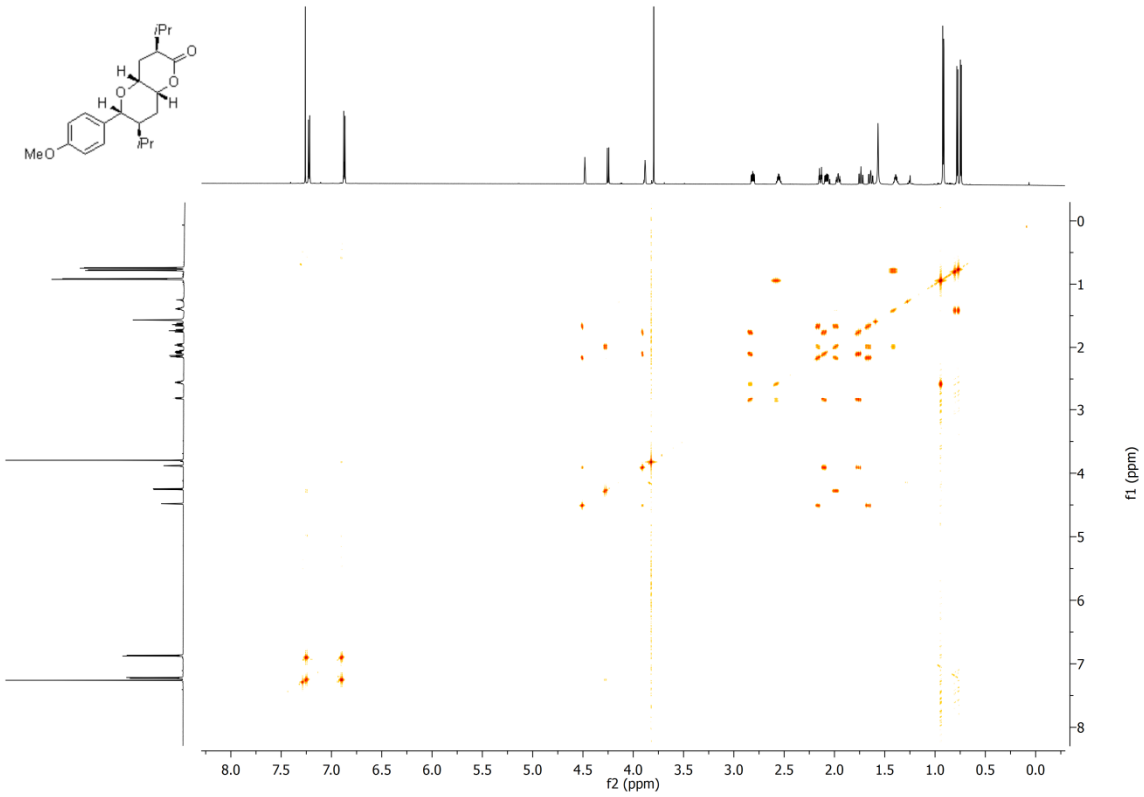
Lactone **29**, 700 MHz, $CDCl_3$



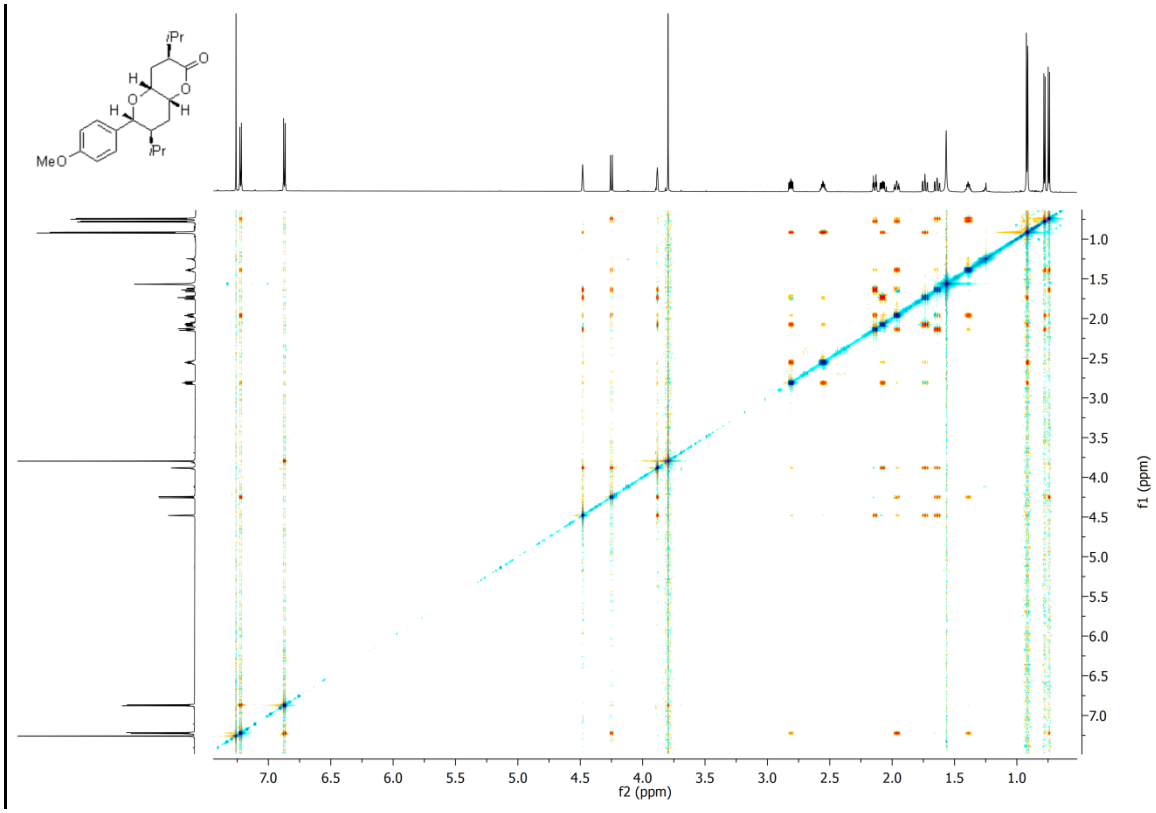
176 MHz, $CDCl_3$



Lactone **29**, COSY, 700 MHz, $CDCl_3$



NOESY, 700 MHz, $CDCl_3$



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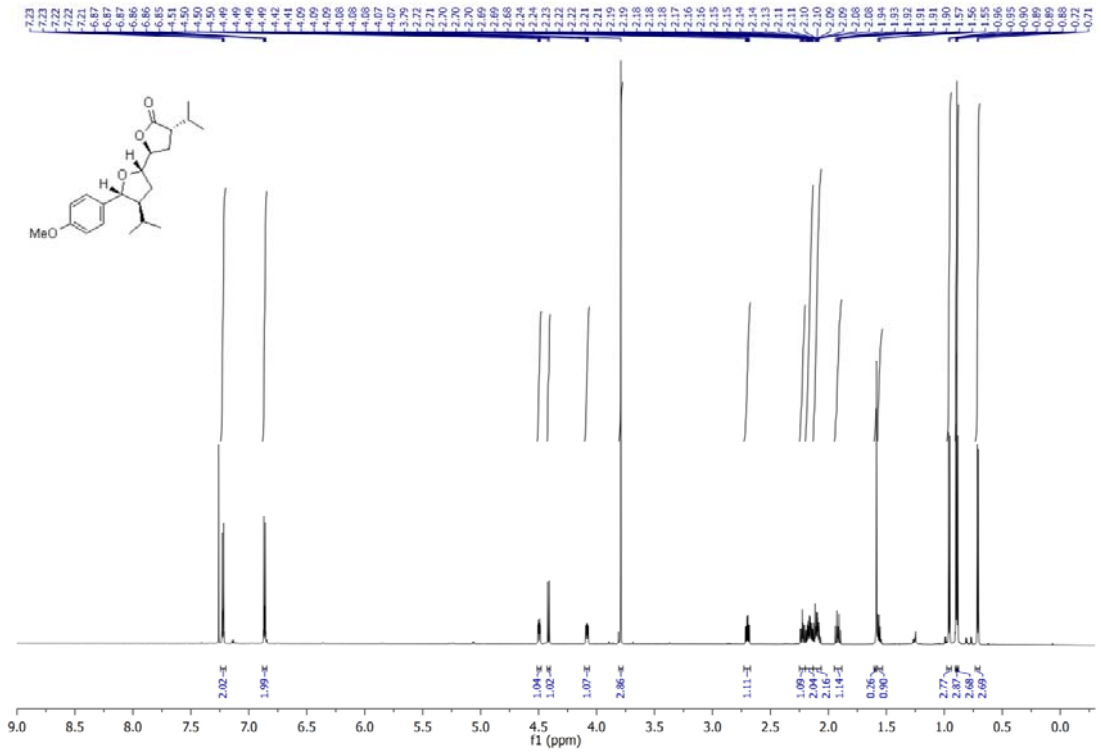
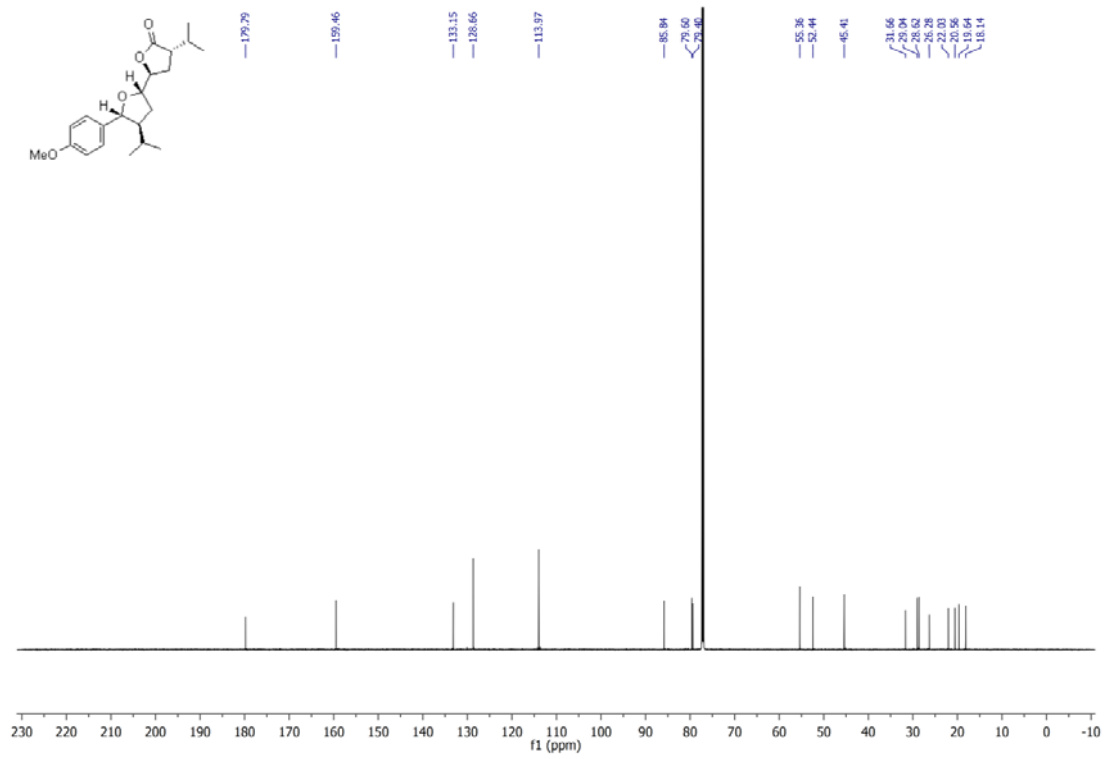
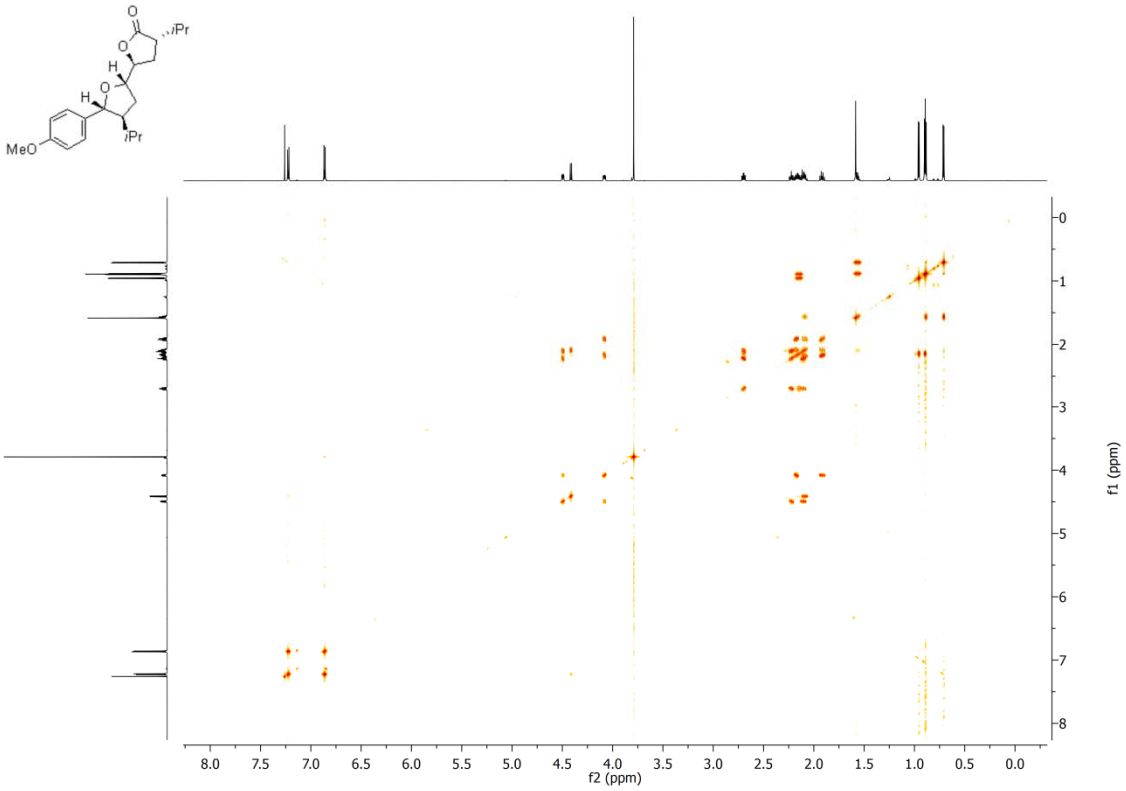


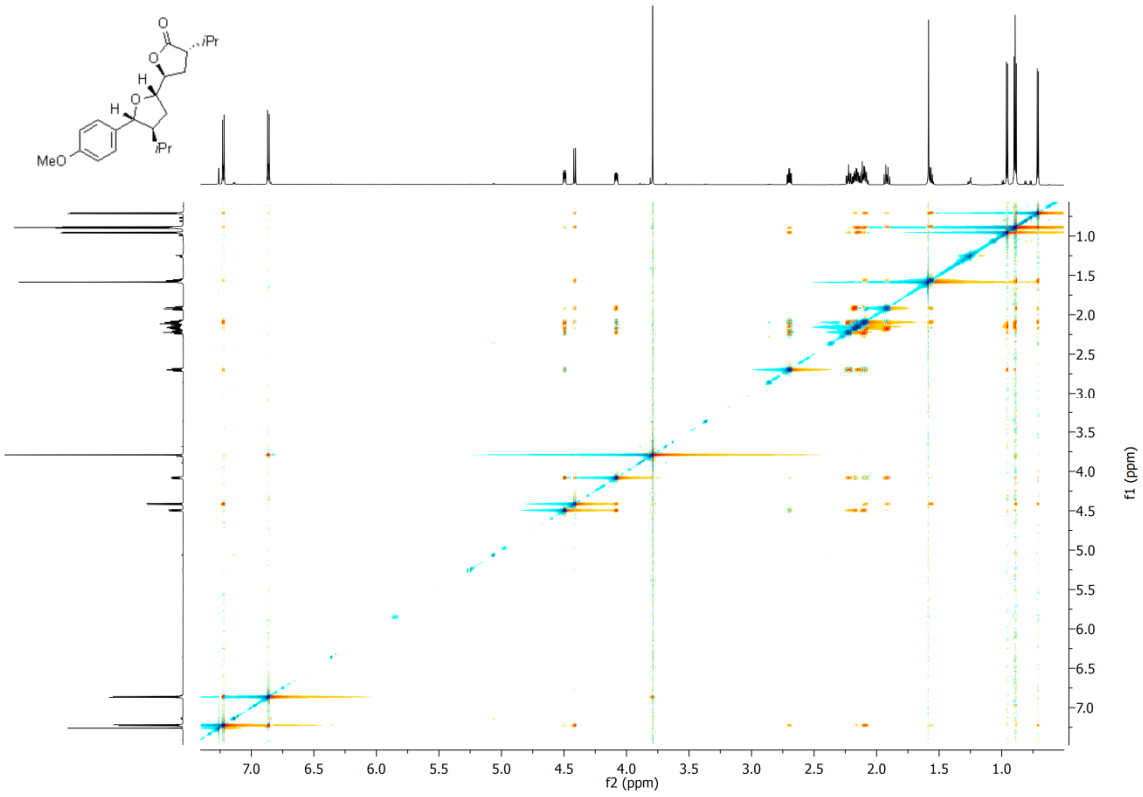
176 MHz, $CDCl_3$



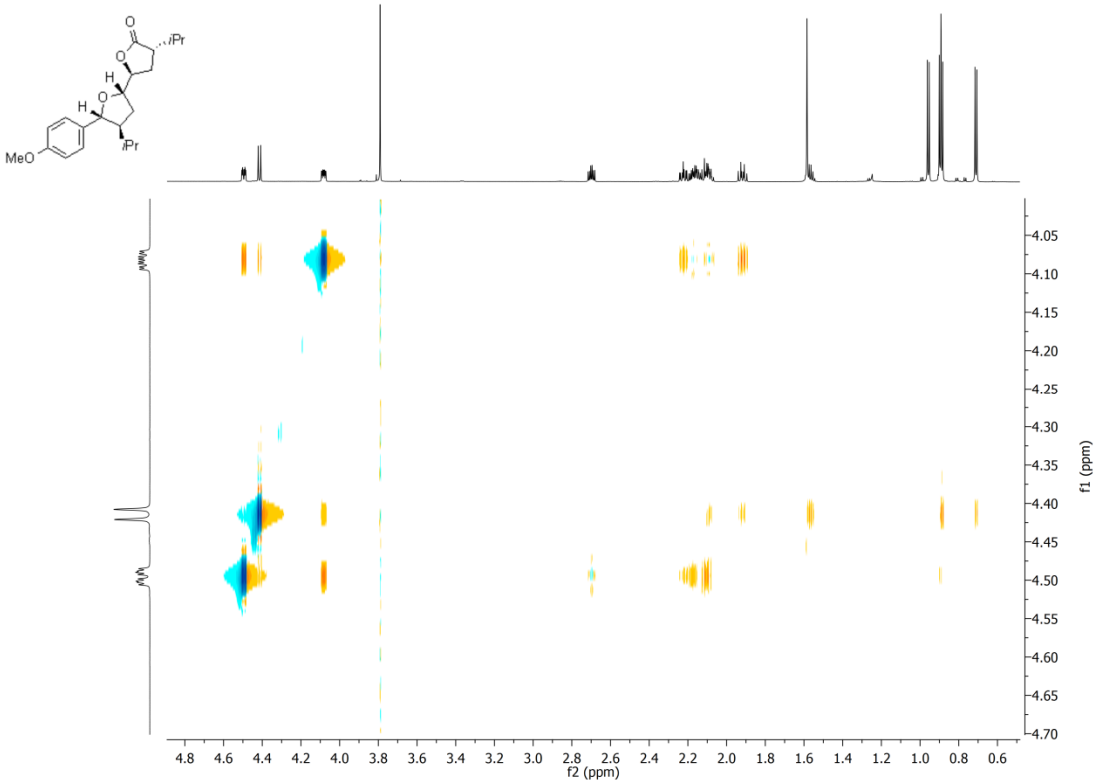
Lactone **30**, 700 MHz, $CDCl_3$, COSY



NOESY, 700 MHz, $CDCl_3$



Lactone **30**, NOESY ZOOM, 700 MHz, $CDCl_3$



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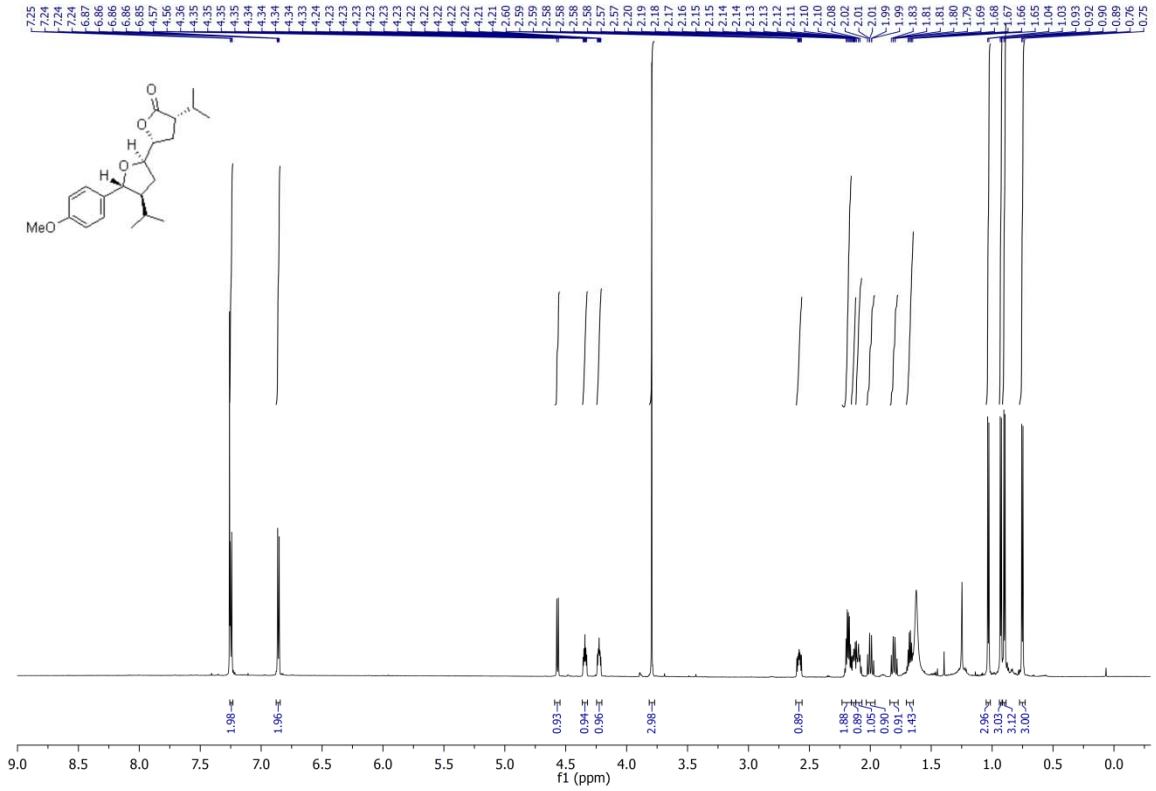
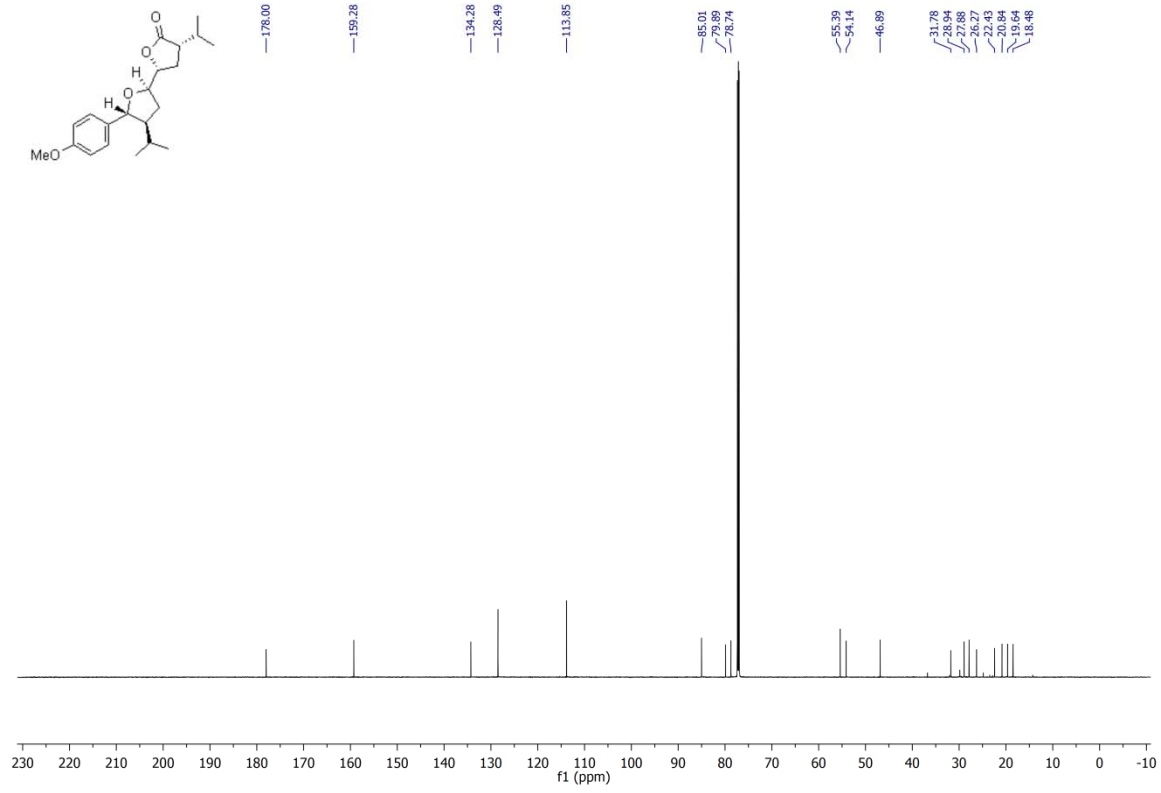
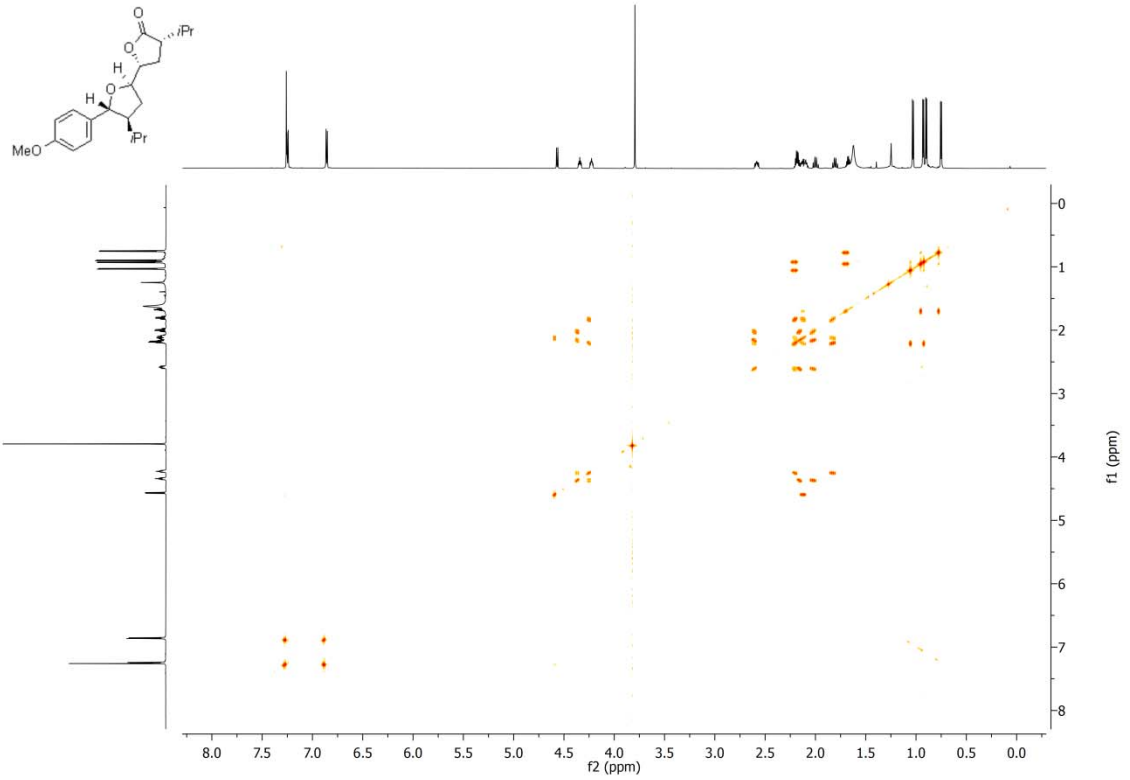


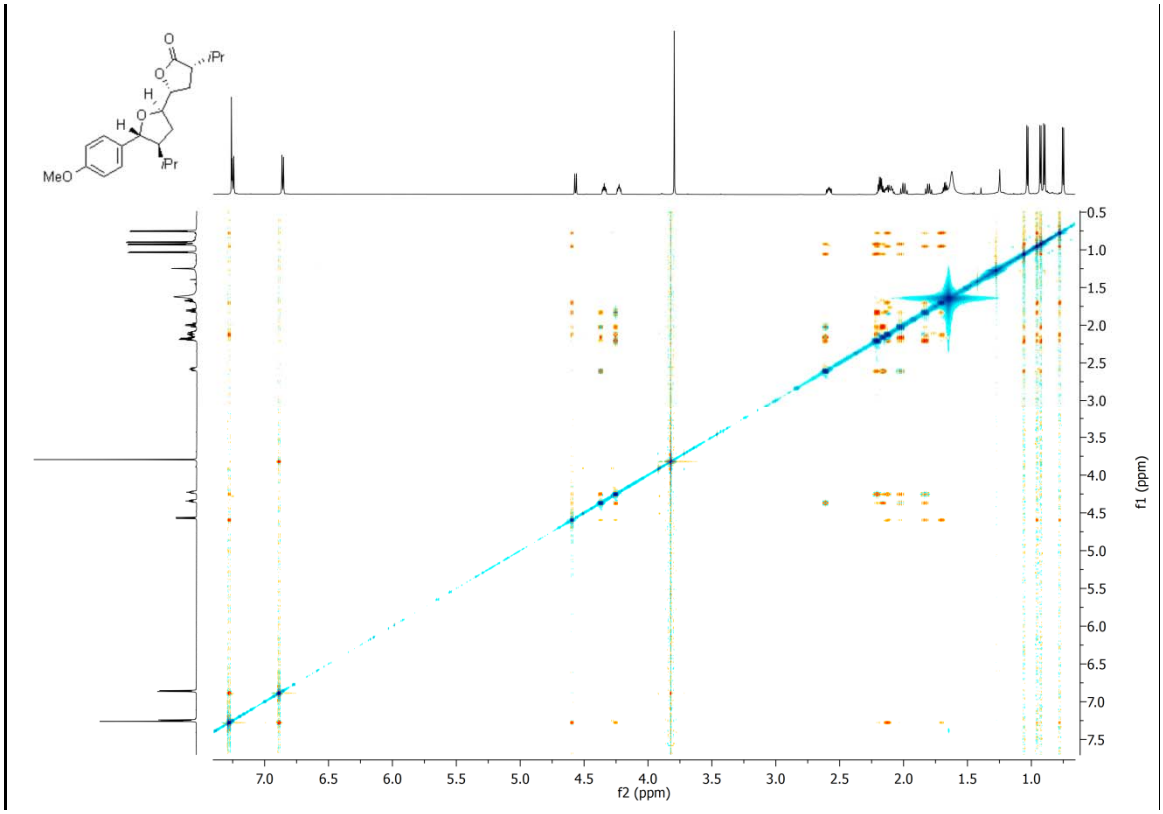
176 MHz, $CDCl_3$



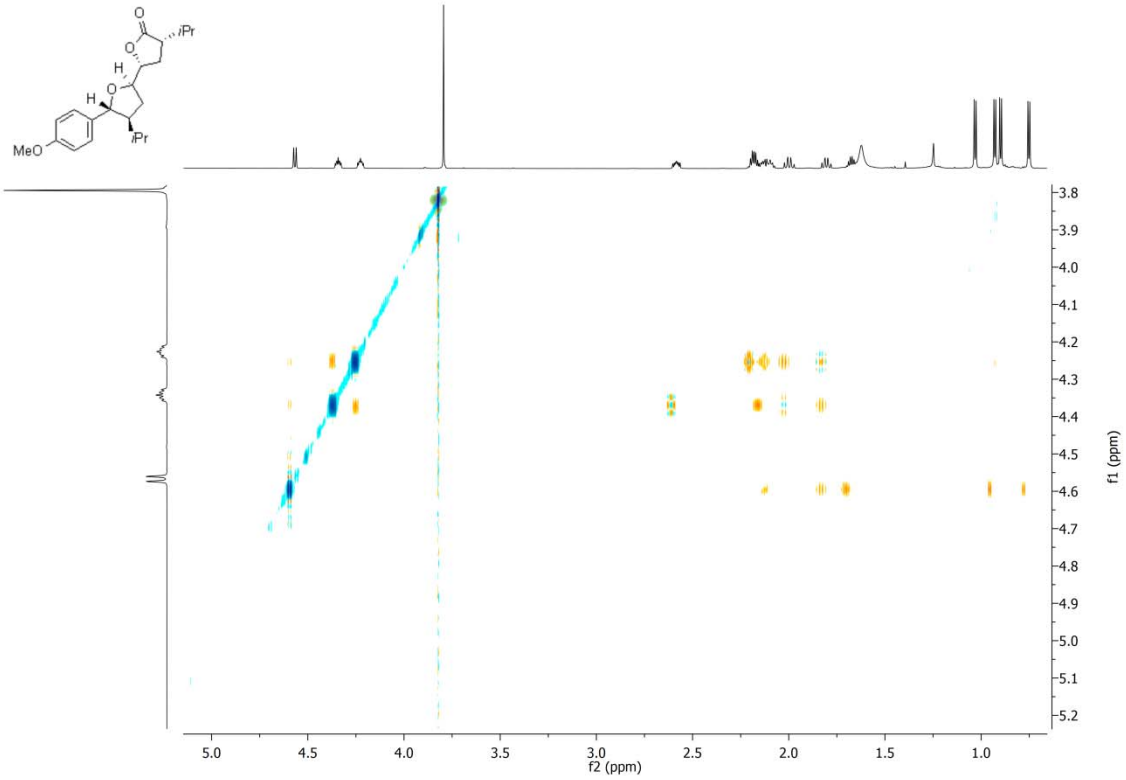
Lactone **31**, COSY, 700 MHz, $CDCl_3$



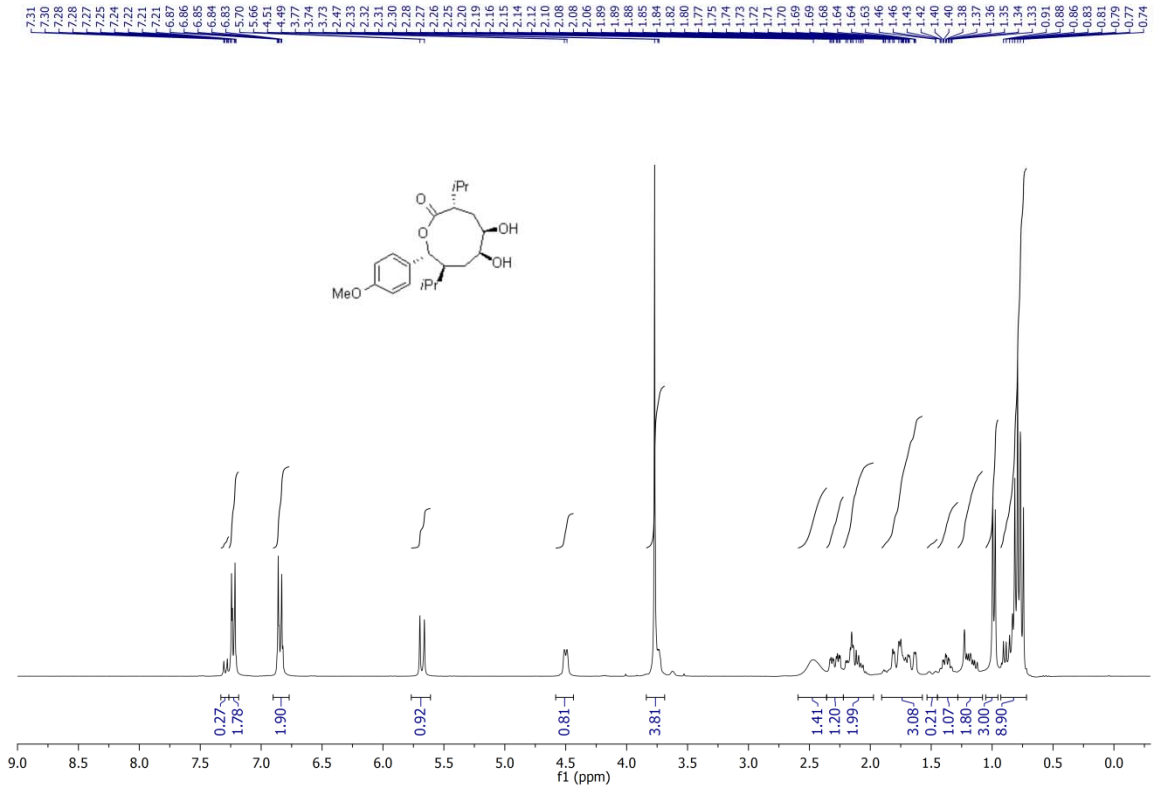
NOESY, 700 MHz, $CDCl_3$



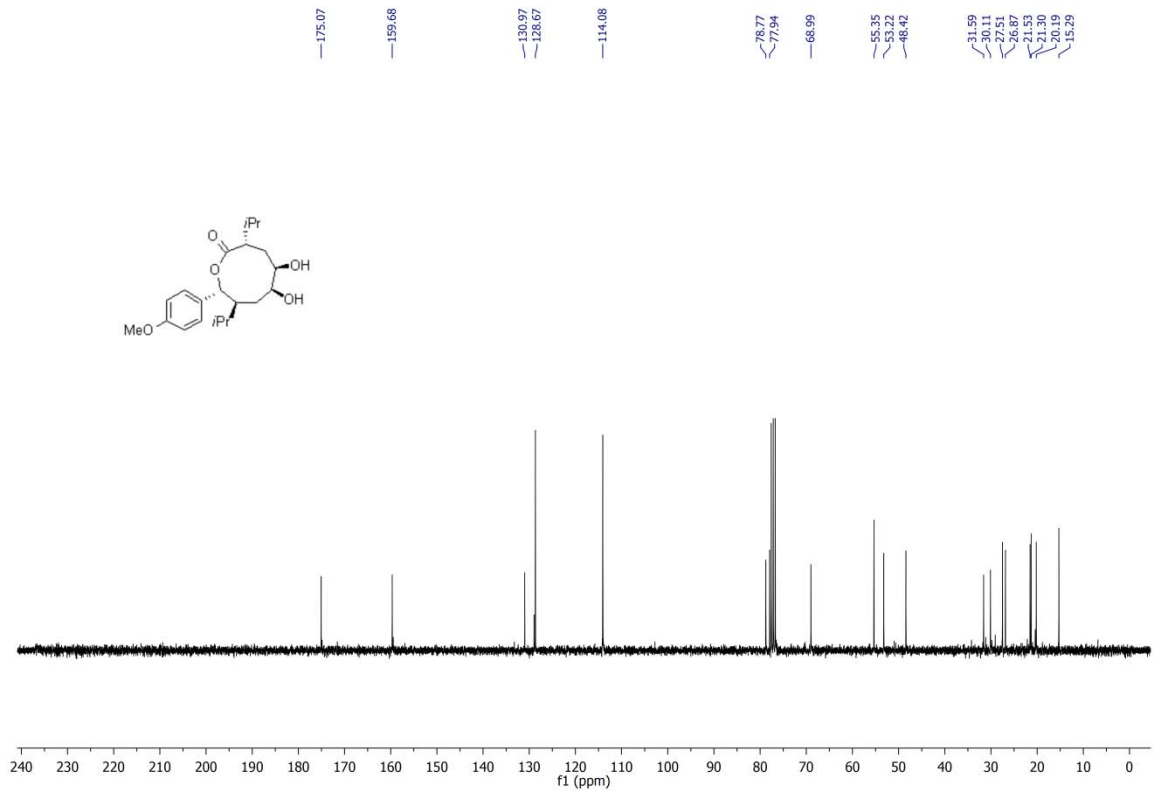
Lactone **31**, 700 MHz, $CDCl_3$, NOESY (ZOOM)



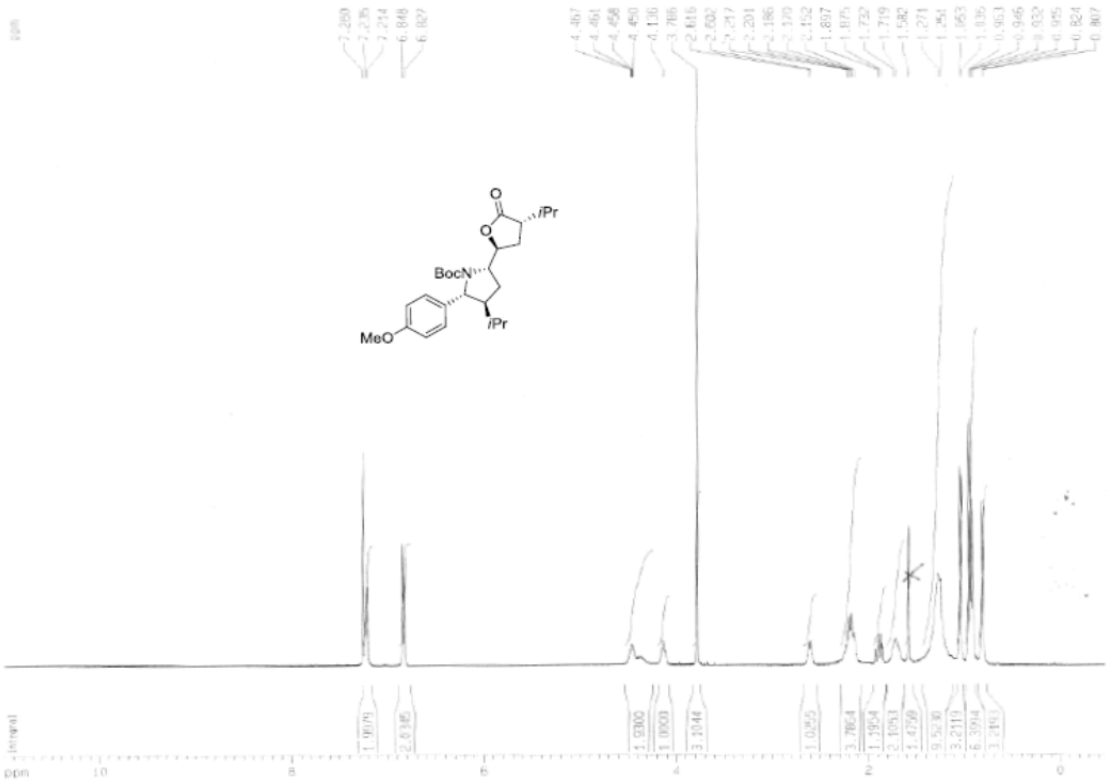
Diol **32**, 300 MHz, $CDCl_3$



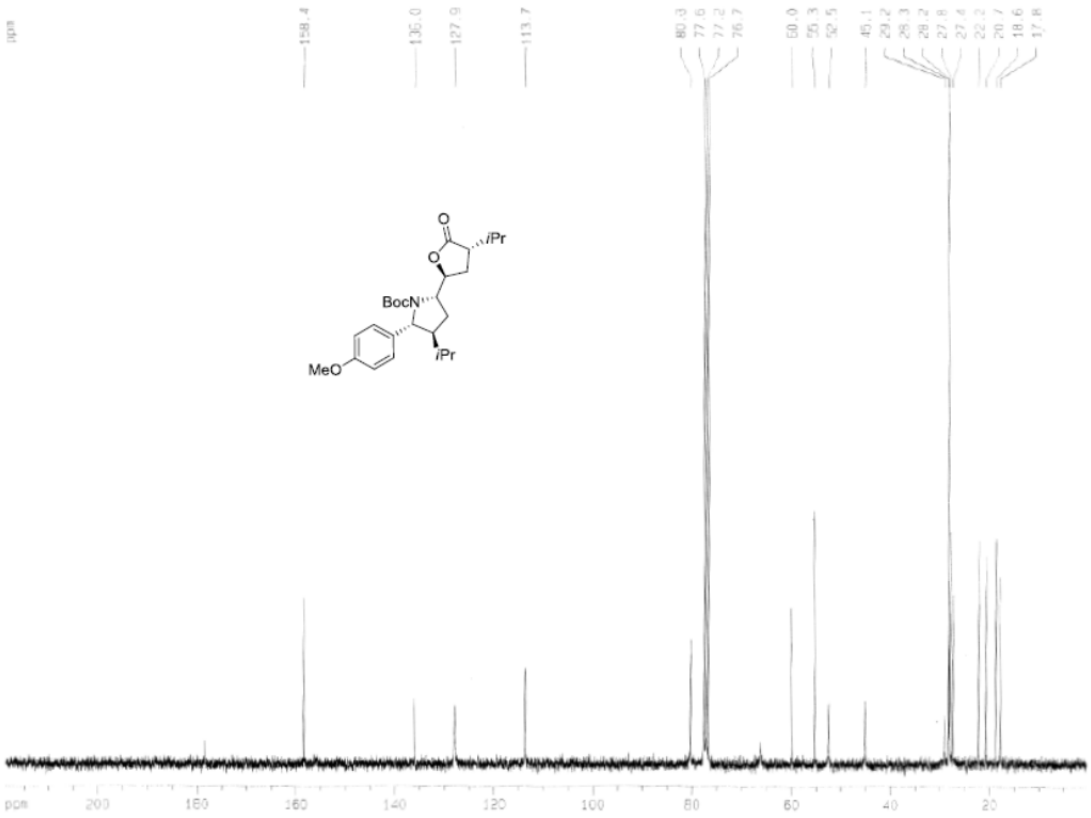
75 MHz, $CDCl_3$



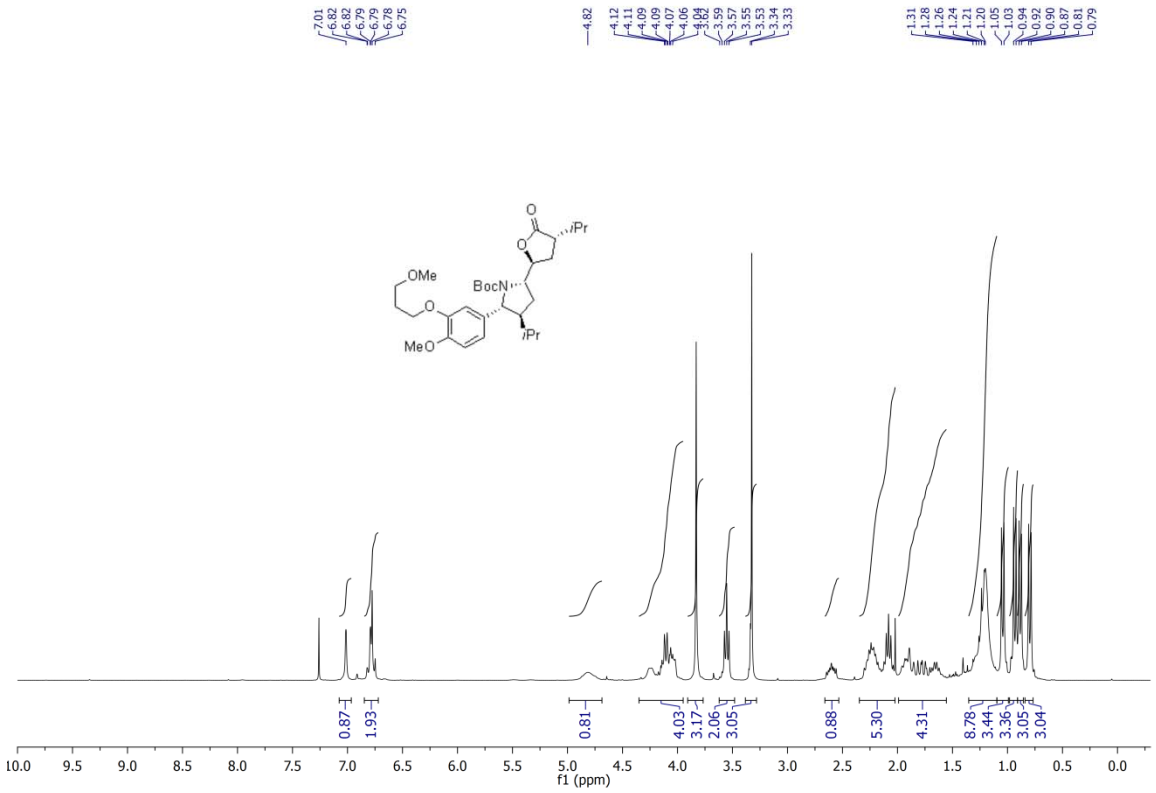
Lactone **39**, 400 MHz, $CDCl_3$



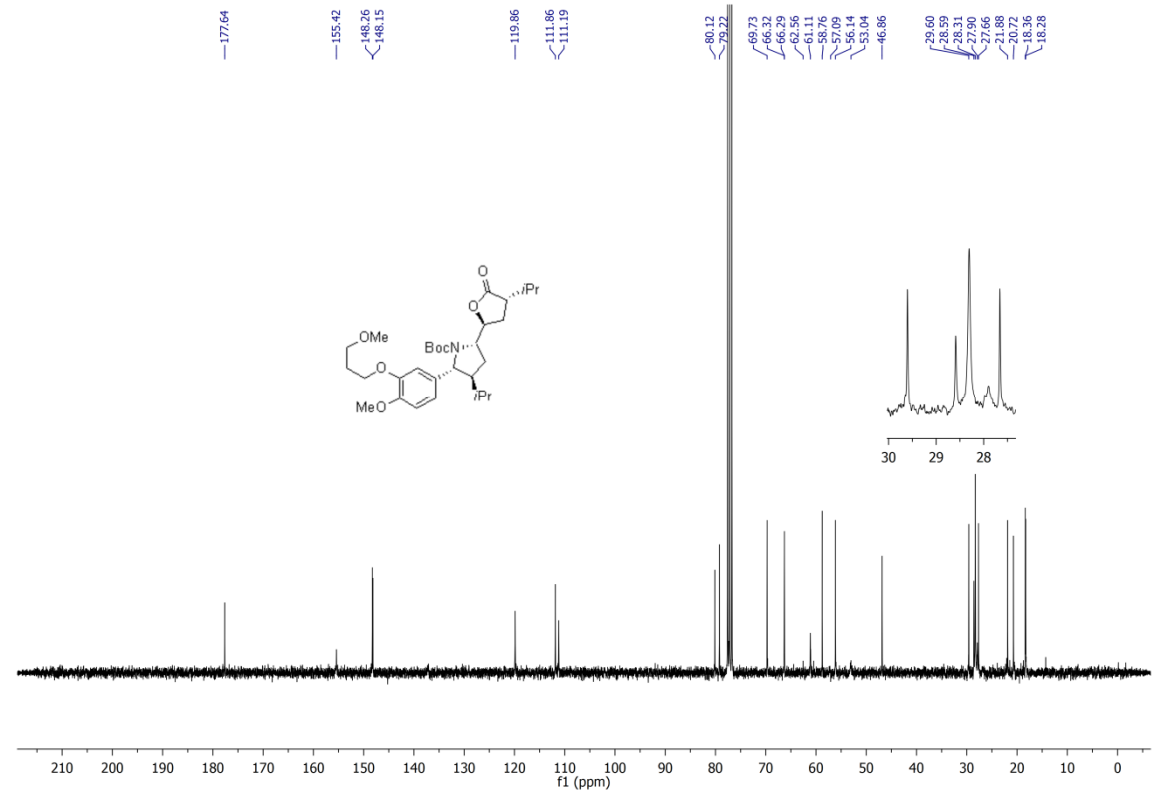
126 MHz, $CDCl_3$



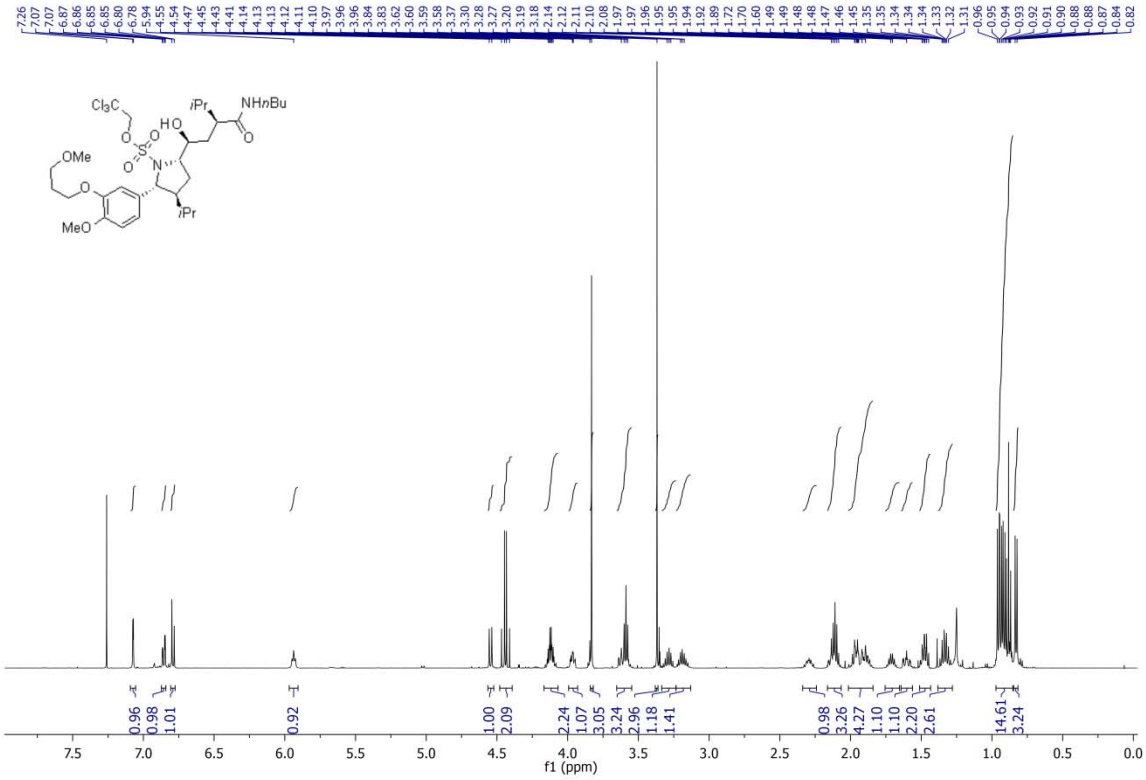
Lactone **41**, 300 MHz, $CDCl_3$



75 MHz, $CDCl_3$



Amide **42**, 500 MHz, $CDCl_3$



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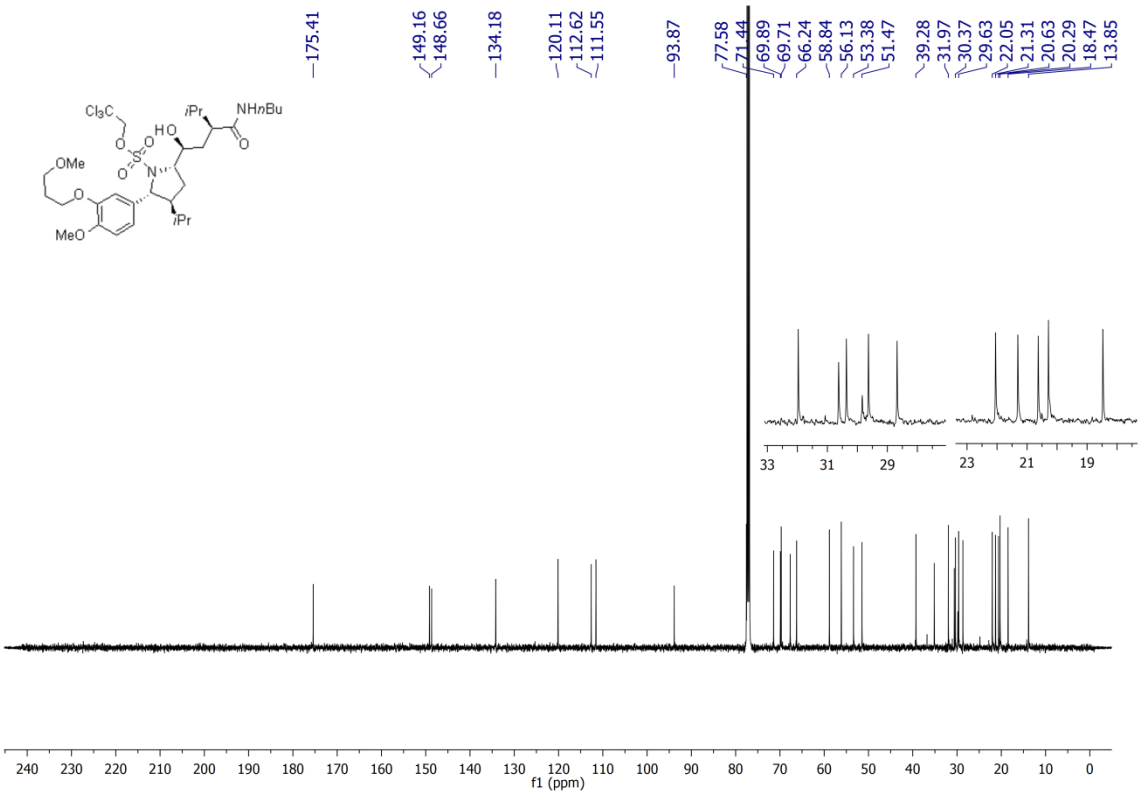
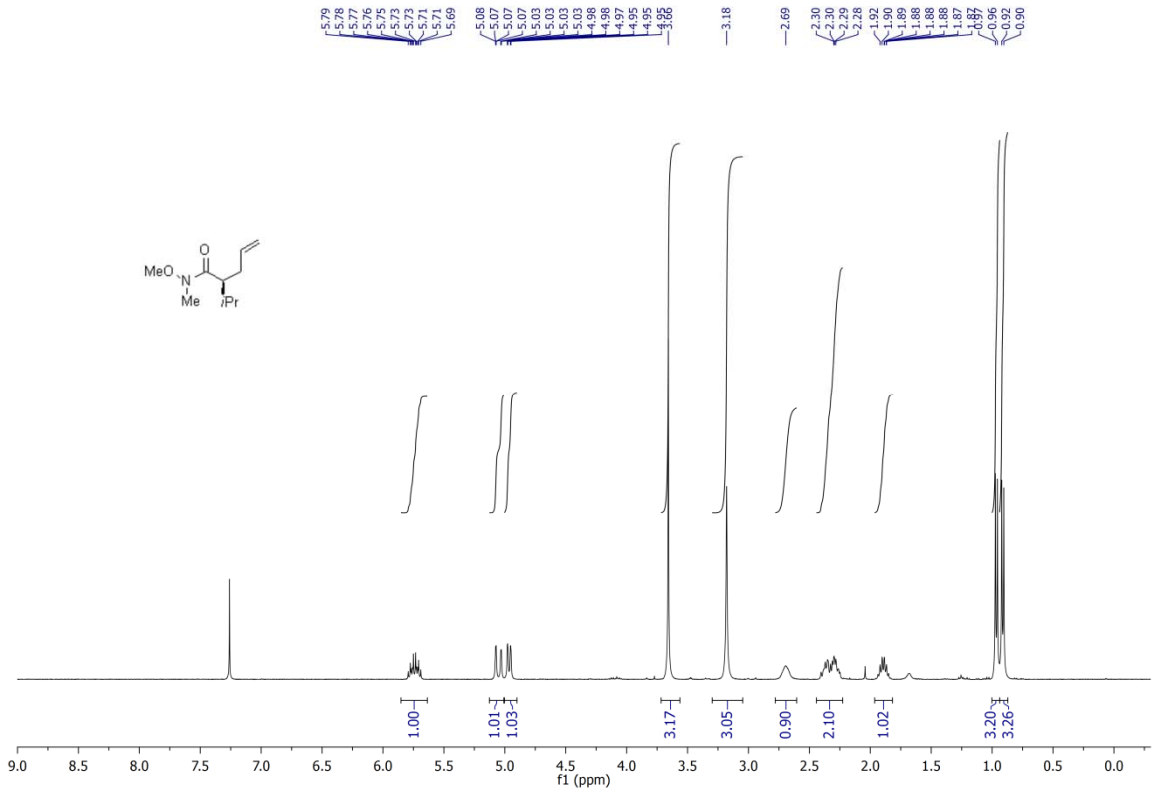
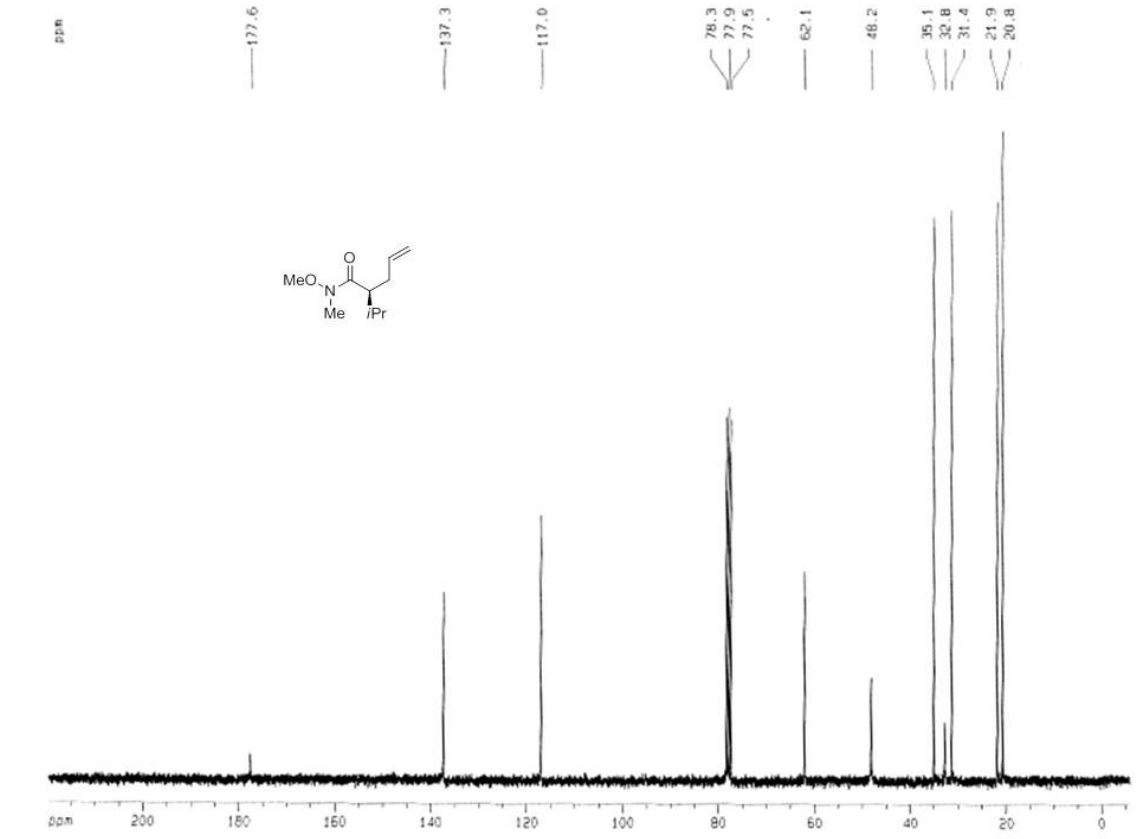


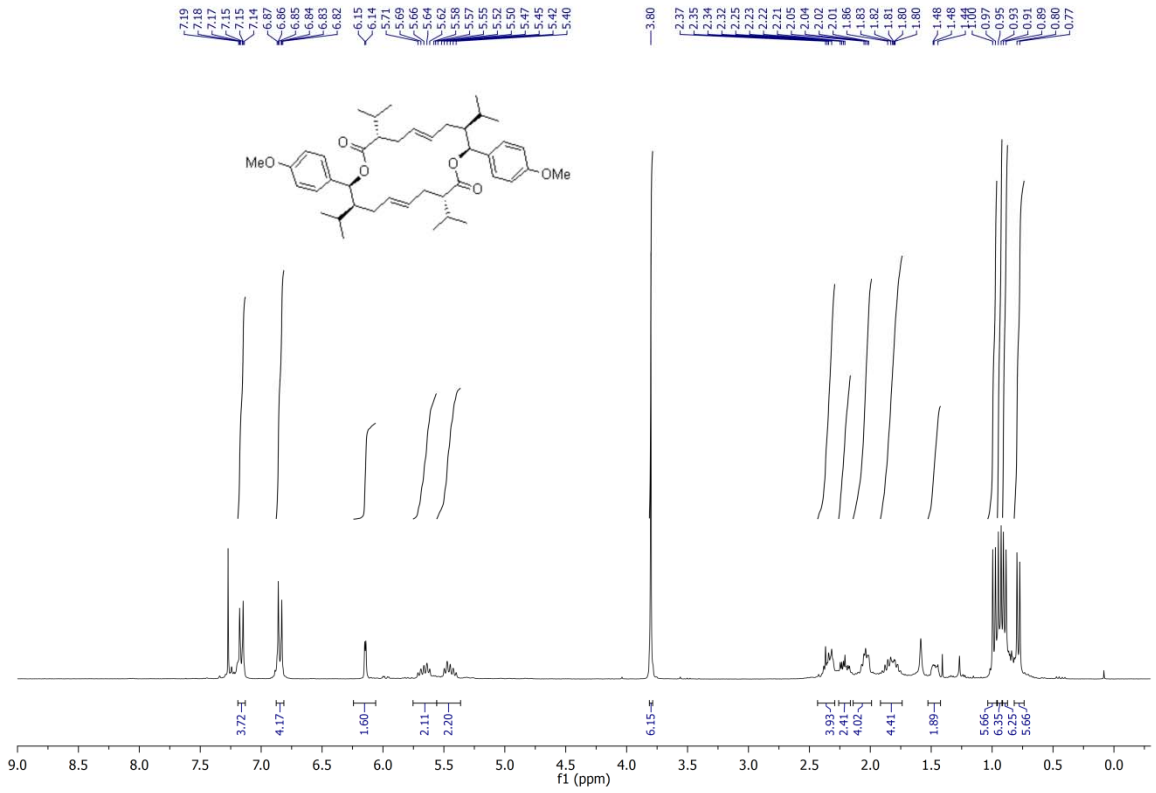
Weinreb amide **47**, 400 MHz, $CDCl_3$



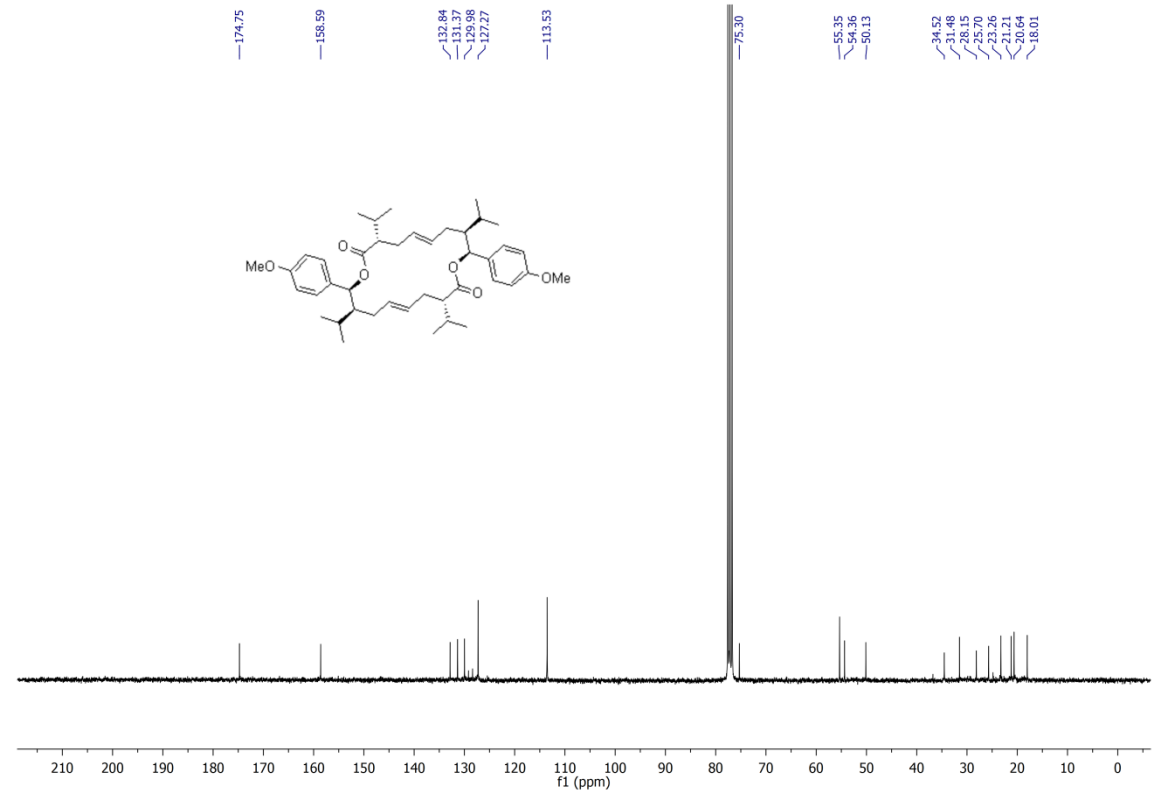
75 MHz, $CDCl_3$



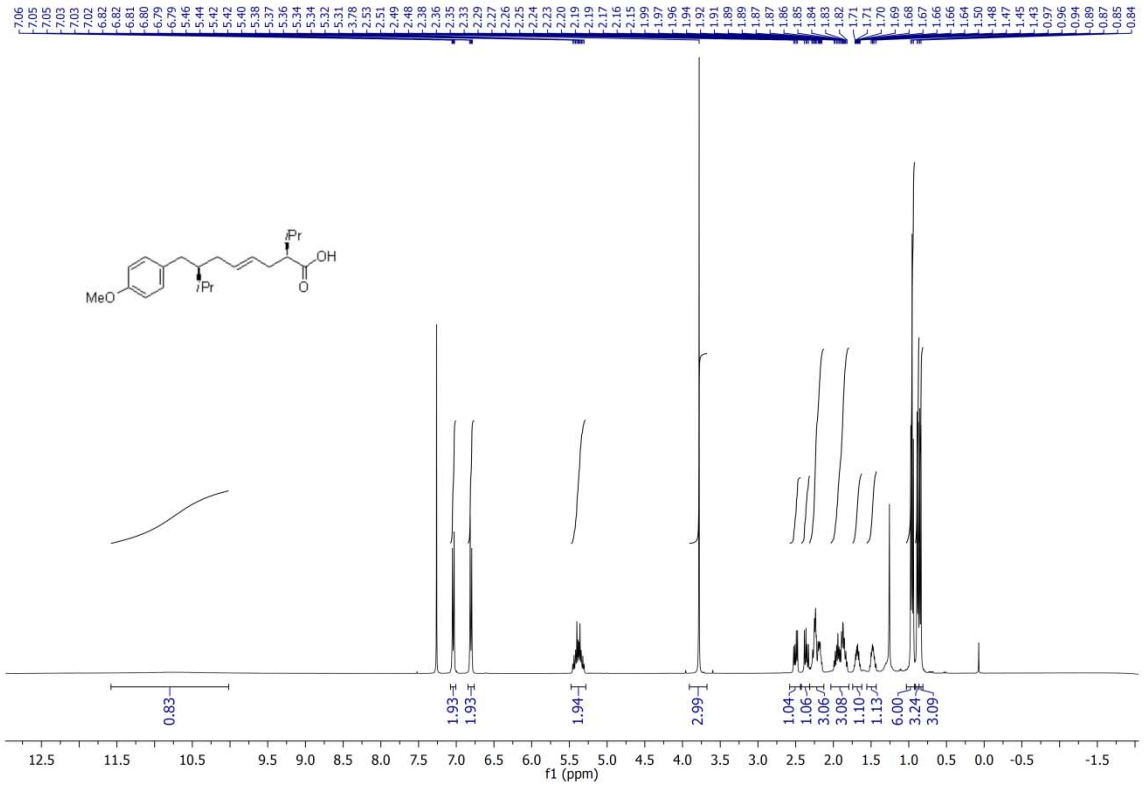
Dilactone **49**, 300 MHz, $CDCl_3$



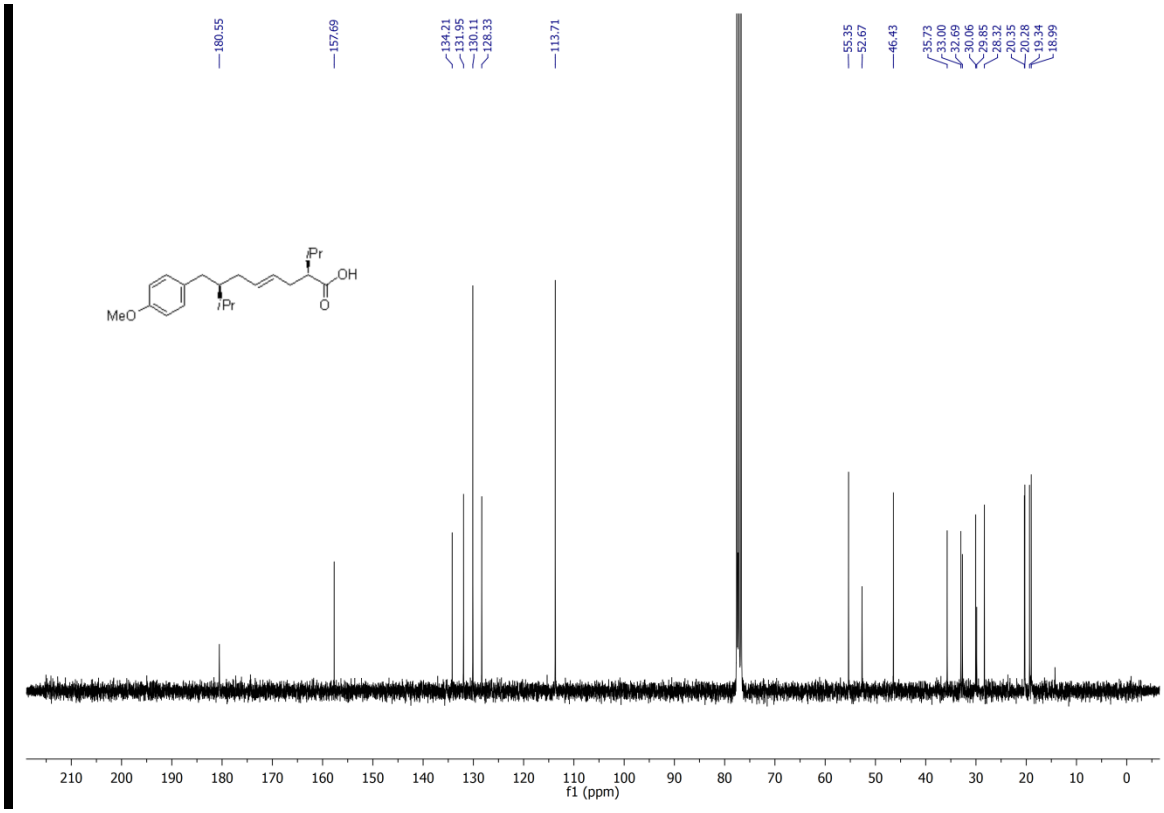
75 MHz, $CDCl_3$



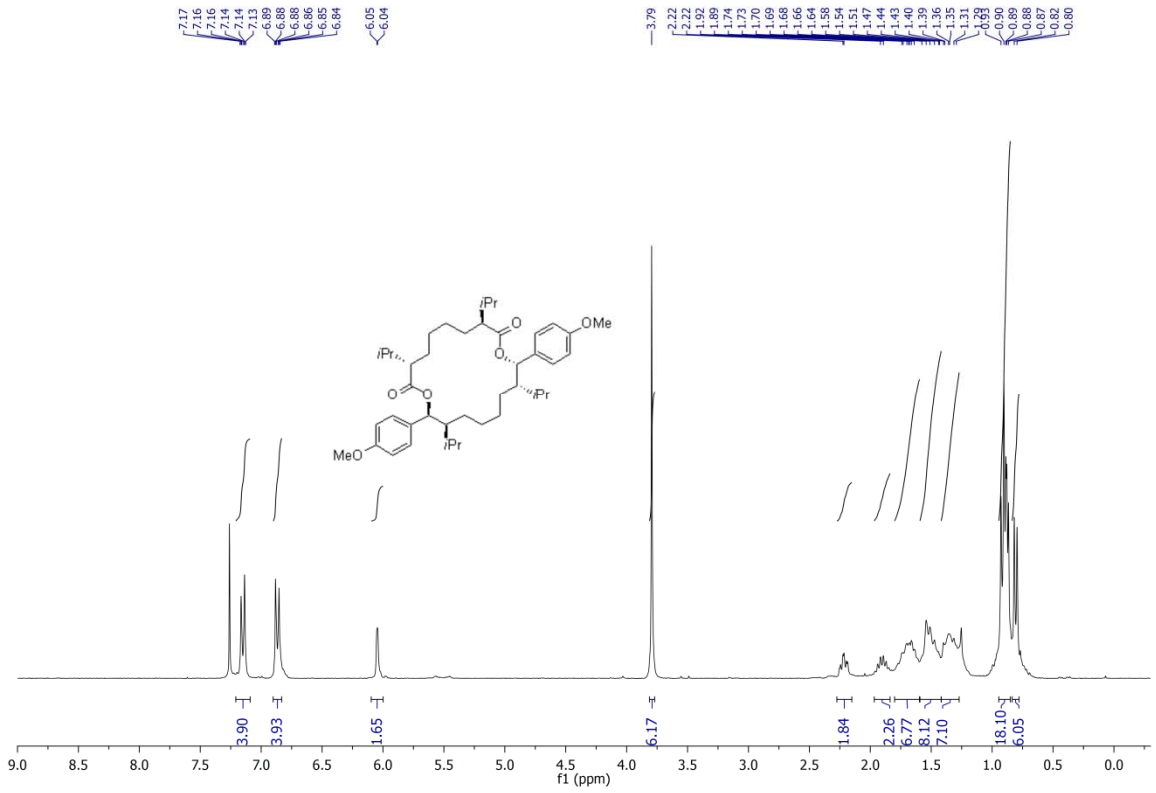
Acid **51**, 400 MHz, $CDCl_3$



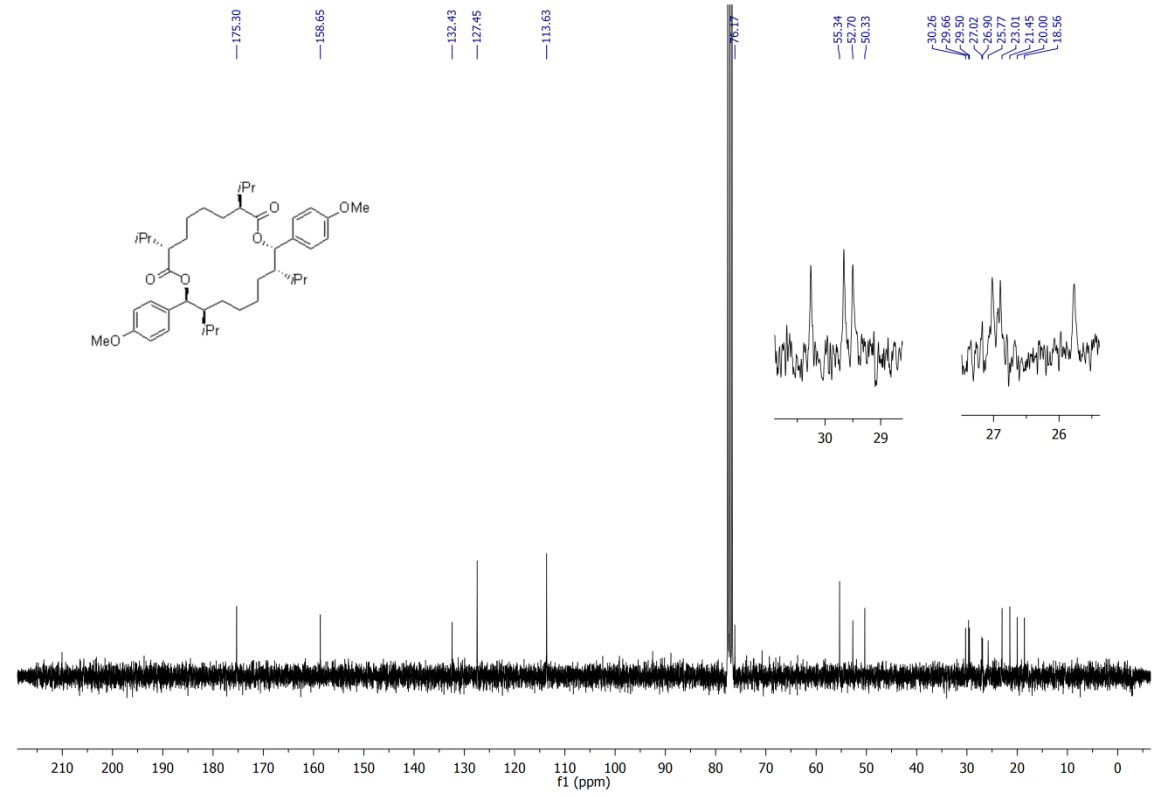
101 MHz, $CDCl_3$



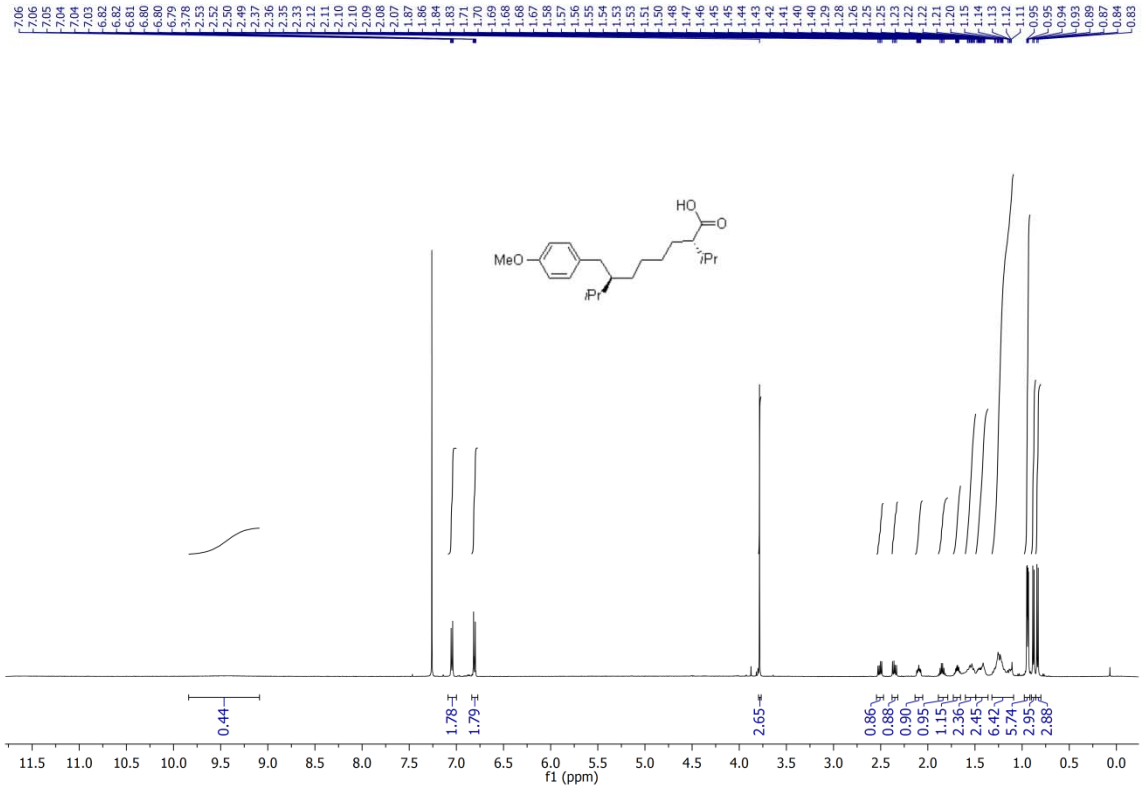
dilactone **52**, 300 MHz, $CDCl_3$



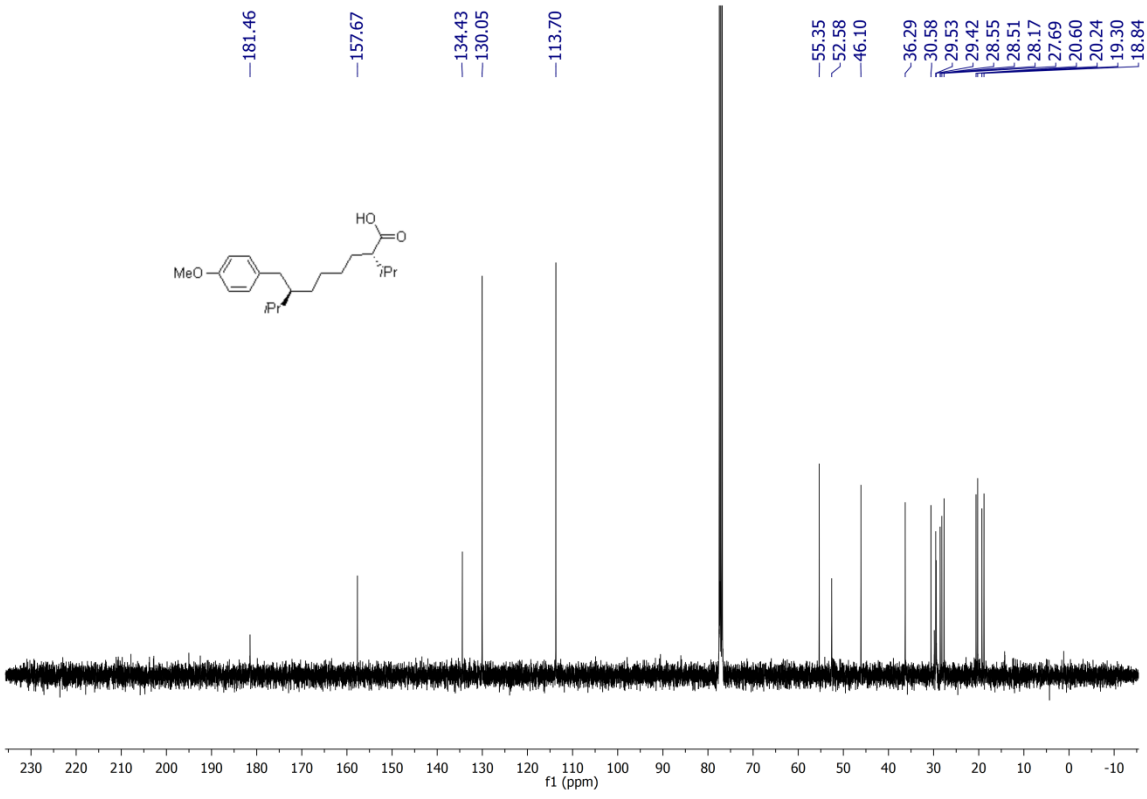
75 MHz, $CDCl_3$



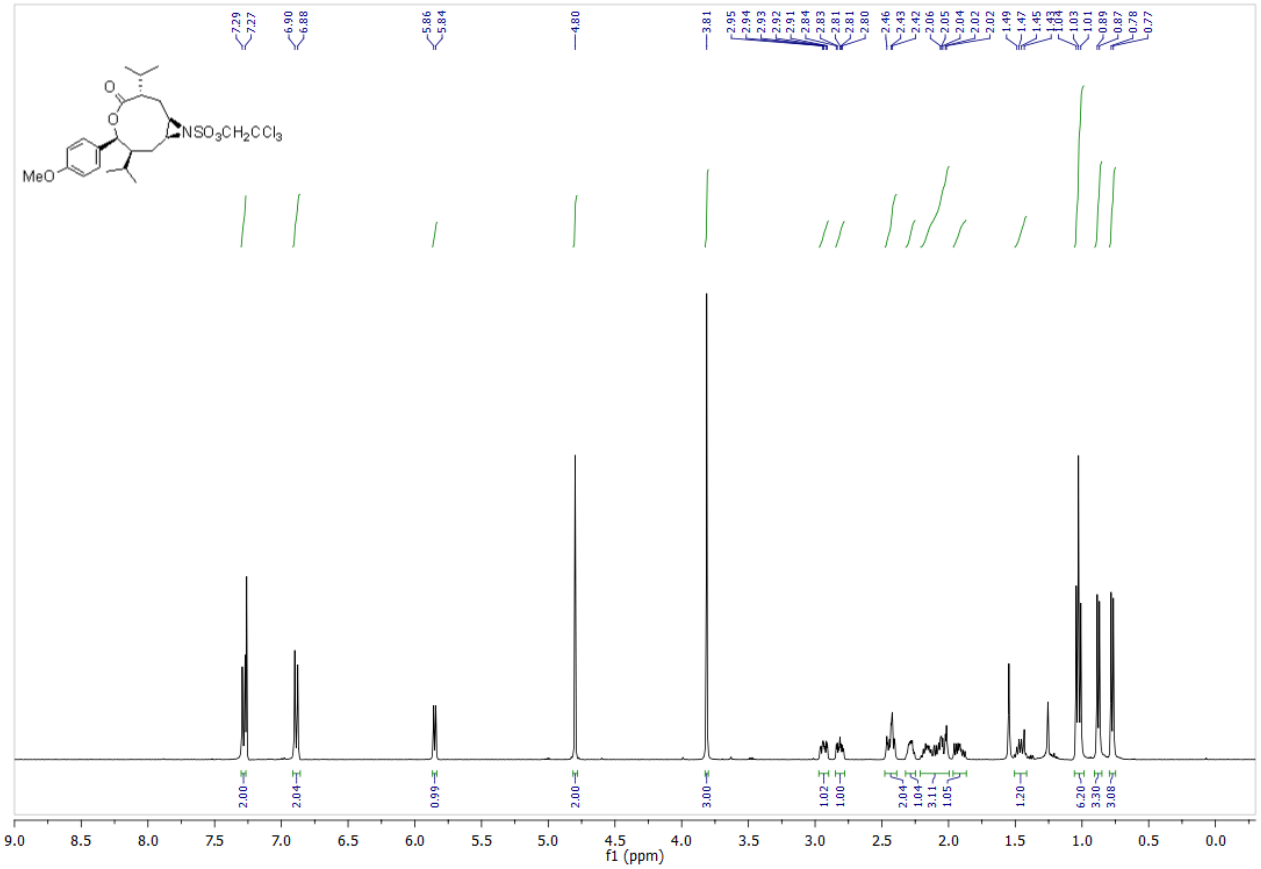
acid **54**, 500 MHz, $CDCl_3$



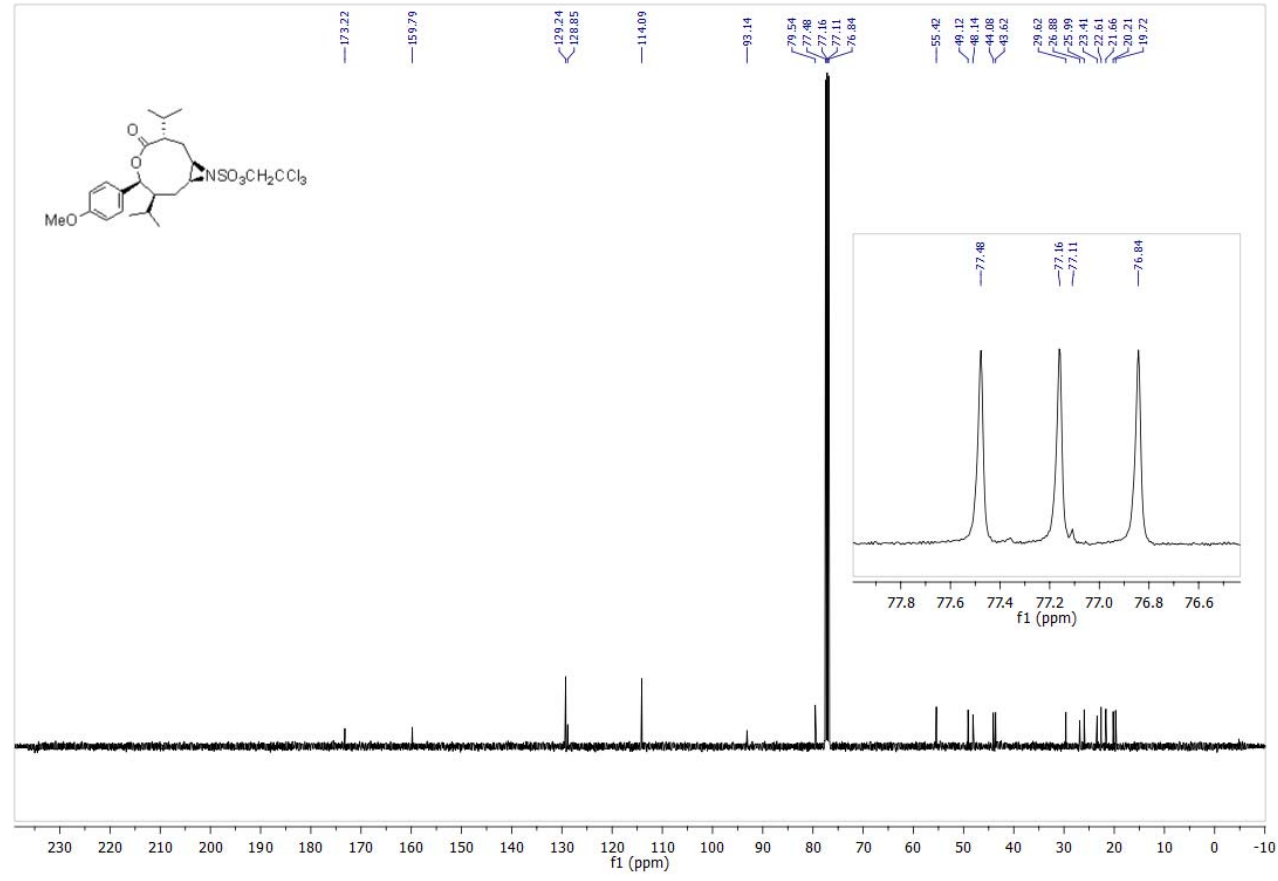
175 MHz, $CDCl_3$



Lactone **55**, 400 MHz, $CDCl_3$



101 MHz, $CDCl_3$



Lactone **20**

Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C21 H30 O3 COMPOUND (ROBE48)

Equipe Hanessian

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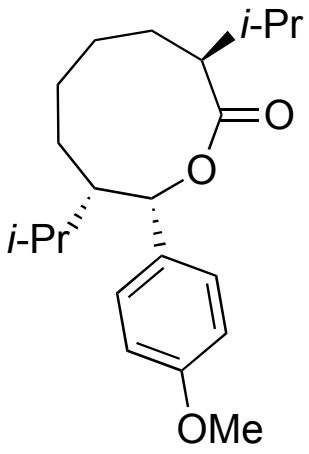


Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Robert D. Giacometti.

Table 1. Crystal data and structure refinement for C21 H30 O3.

Identification code	ROBE48
Empirical formula	$C_{21}H_{30}O_3$
Formula weight	330.45
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1$
a/Å	9.63600(9)
b/Å	9.33460(9)
c/Å	10.49330(10)
α/°	90
β/°	100.0230(3)
γ/°	90
Volume/Å^3	929.448(15)
Z	2
ρ_{calc}g/cm^3	1.181
μ/mm^{-1}	0.607
F(000)	360.0
Crystal size/mm^3	0.16 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.556 to 143.38
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -12 ≤ l ≤ 12
Reflections collected	19284
Independent reflections	3466 [R_{int} = 0.0177, R_{sigma} = 0.0130]
Data/restraints/parameters	3466/1/222

Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0276, wR_2 = 0.0729
Final R indexes [all data]	R_1 = 0.0278, wR_2 = 0.0731
Largest diff. peak/hole / e $Å^{-3}$	0.19/-0.15
Flack parameter	0.06(3)

Table 2. Fractional atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for C21 H30 O3.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	9570.4(15)	3317.6(17)	928.7(14)	15.3(3)
C2	9651.1(16)	2748.3(17)	-415.7(14)	17.8(3)
C3	8102.9(17)	2605(2)	-1141.8(15)	23.1(3)
C4	7316.3(17)	4001(2)	-1201.8(15)	25.4(4)
C5	6498.0(17)	4443(2)	-380.0(16)	25.0(4)
C6	6170.4(16)	3626(2)	772.2(15)	22.6(3)
C7	7083.3(15)	4149.7(17)	2075.2(15)	18.1(3)
C8	8216.7(15)	3033.9(16)	2631.7(14)	15.7(3)
C9	7751.5(15)	1787.9(17)	3371.0(14)	16.2(3)
C10	8570.3(16)	1388.7(17)	4541.8(15)	17.6(3)
C11	8189.4(16)	269.0(18)	5291.2(14)	18.2(3)
C12	6952.9(15)	-487.1(18)	4848.3(14)	17.1(3)
C13	6117.1(16)	-109.6(18)	3672.7(15)	18.8(3)
C14	6508.7(16)	1012.4(18)	2953.5(14)	18.2(3)
C15	10604.2(16)	3683.1(17)	-1115.7(14)	18.7(3)
C16	10484.3(18)	3246(2)	-2536.3(15)	24.5(4)
C17	12141.9(17)	3566(2)	-448.8(15)	25.1(4)
C18	6199.6(17)	4647.5(19)	3089.0(17)	22.8(3)
C19	7122.4(19)	5074(2)	4371.3(17)	27.9(4)
C20	5272(2)	5922(2)	2571(2)	33.2(4)
C21	7274.0(18)	-2023.6(19)	6685.1(16)	25.2(4)
O1	8804.6(11)	2421.6(12)	1546.7(10)	16.3(2)
O2	10060.0(11)	4429.2(12)	1390.2(10)	18.3(2)
O3	6460.2(11)	-1608.7(13)	5477(1)	20.6(2)

Table 3. Hydrogen atom coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for C21 H30 O3.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	*x*	*y*	*z*	U(eq)
H2	10069	1766	-315	21
H3A	8108	2260	-2033	28
H3B	7606	1883	-696	28
H4	7413	4629	-1894	30
H5	6080	5363	-534	30
H6A	6347	2593	656	27
H6B	5160	3744	820	27
H7	7608	5014	1854	22
H8	8991	3546	3214	19
H10	9419	1896	4842	21
H11	8765	26	6092	22
H13	5276	-626	3366	23
H14	5924	1264	2160	22
H15	10300	4704	-1080	22
H16A	10636	2211	-2591	37
H16B	11197	3757	-2923	37
H16C	9543	3489	-3005	37
H17A	12228	3878	453	38
H17B	12730	4176	-898	38
H17C	12454	2568	-474	38
H18	5574	3840	3257	27
H19A	7640	4233	4760	42
H19B	6525	5446	4962	42
H19C	7792	5815	4213	42

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for C21 H30 O3.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	13.1(6)	15.3(7)	17.0(7)	1.7(6)	0.7(5)	1.7(5)
C2	22.3(7)	15.5(8)	15.7(7)	-0.6(6)	3.8(6)	-1.6(6)
C3	25.6(8)	27.5(9)	15.5(7)	-1.5(7)	1.5(6)	-8.3(7)
C4	22.3(8)	32.7(10)	18.1(7)	7.1(7)	-5.4(6)	-4.9(7)
C5	19.7(7)	27.3(9)	24.3(8)	7.1(7)	-6.6(6)	1.0(7)
C6	15.4(7)	27.7(9)	22.9(7)	3.4(7)	-1.1(5)	0.8(6)
C7	15.2(7)	17.9(8)	21.2(7)	1.2(6)	3.1(6)	0.2(6)
C8	14.8(6)	17.6(8)	14.9(6)	-2.8(6)	2.9(5)	-0.3(5)
C9	15.4(7)	18.5(8)	15.2(7)	-2.2(6)	4.1(6)	1.1(6)
C10	15.3(7)	20.1(8)	17.1(7)	-3.9(6)	2.1(5)	-0.7(6)
C11	17.8(7)	22.0(8)	14.3(7)	-0.5(6)	1.4(5)	1.9(6)
C12	18.5(7)	17.6(7)	16.6(7)	-1.5(6)	7.0(5)	0.3(6)
C13	14.9(7)	21.5(8)	19.6(7)	-1.3(6)	2.3(6)	-1.5(6)
C14	17.1(7)	21.0(8)	15.8(7)	-0.6(6)	0.6(5)	0.1(6)
C15	23.1(8)	16.4(8)	17.0(7)	0.6(6)	4.7(5)	-1.2(6)
C16	30.6(8)	26.8(9)	17.0(7)	-0.2(6)	6.6(6)	-5.6(7)
C17	22.3(8)	33.9(10)	19.9(7)	1.9(7)	6.1(6)	-1.2(7)
C18	19.9(7)	20.3(8)	29.9(8)	0.5(7)	9.2(6)	1.8(6)
C19	31.5(9)	25.9(9)	28.6(9)	-4.9(7)	11.8(7)	4.1(7)
C20	27.2(9)	28.7(10)	45.5(11)	2.0(9)	11.5(8)	9.2(8)
C21	26.7(8)	28.2(9)	20.4(8)	6.9(7)	3.3(6)	-1.3(7)
O1	17.9(5)	16.8(6)	14.6(5)	-1.2(4)	4.3(4)	-0.4(4)
O2	19.1(5)	17.5(6)	18.0(5)	-1.8(4)	2.8(4)	-2.4(4)
O3	21.5(5)	22.2(6)	18.3(5)	2.8(5)	3.8(4)	-3.1(5)

Table 5. Bond lengths [Å] for C21 H30 O3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.522(2)	C9	C10	1.390(2)
C1	O1	1.3531(18)	C9	C14	1.403(2)
C1	O2	1.2060(19)	C10	C11	1.395(2)
C2	C3	1.558(2)	C11	C12	1.393(2)
C2	C15	1.543(2)	C12	C13	1.396(2)
C3	C4	1.503(3)	C12	O3	1.3659(19)
C4	C5	1.331(3)	C13	C14	1.381(2)
C5	C6	1.509(2)	C15	C16	1.530(2)
C6	C7	1.570(2)	C15	C17	1.528(2)
C7	C8	1.548(2)	C18	C19	1.531(2)
C7	C18	1.545(2)	C18	C20	1.530(2)
C8	C9	1.509(2)	C21	O3	1.4234(19)
C8	O1	1.4725(17)			

Table 6. Bond angles [Å] for C21 H30 O3.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	C1	C2	110.39(13)	C10	C9	C14	117.39(14)
O2	C1	C2	126.37(14)	C14	C9	C8	123.44(14)
O2	C1	O1	123.18(13)	C9	C10	C11	122.30(15)
C1	C2	C3	106.51(12)	C12	C11	C10	119.03(14)
C1	C2	C15	112.00(13)	C11	C12	C13	119.68(14)
C15	C2	C3	114.48(12)	O3	C12	C11	125.18(13)
C4	C3	C2	112.27(14)	O3	C12	C13	115.13(13)
C5	C4	C3	126.35(16)	C14	C13	C12	120.25(14)
C4	C5	C6	126.33(17)	C13	C14	C9	121.35(14)
C5	C6	C7	112.14(14)	C16	C15	C2	111.26(13)
C8	C7	C6	111.75(12)	C17	C15	C2	110.58(13)
C18	C7	C6	113.63(12)	C17	C15	C16	109.25(13)

C18	C7	C8	112.31(13)	C19	C18	C7	112.21(13)
C9	C8	C7	117.34(12)	C20	C18	C7	110.32(14)
O1	C8	C7	108.10(12)	C20	C18	C19	108.90(15)
O1	C8	C9	106.68(12)	C1	O1	C8	116.48(12)
C10	C9	C8	119.16(13)	C12	O3	C21	117.05(12)

Table 7. Torsion angles [°] for C21 H30 O3.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	57.39(16)	C9	C8	O1	C1	-165.59(12)
C1	C2	C15	C16	-170.69(13)	C9	C10	C11	C12	0.6(2)
C1	C2	C15	C17	67.72(17)	C10	C9	C14	C13	-0.4(2)
C2	C1	O1	C8	-159.39(11)	C10	C11	C12	C13	-0.3(2)
C2	C3	C4	C5	-94.36(19)	C10	C11	C12	O3	179.56(14)
C3	C2	C15	C16	-49.31(18)	C11	C12	C13	C14	-0.3(2)
C3	C2	C15	C17	-170.90(14)	C11	C12	O3	C21	0.6(2)
C3	C4	C5	C6	-1.0(3)	C12	C13	C14	C9	0.7(2)
C4	C5	C6	C7	100.2(2)	C13	C12	O3	C21	-179.54(13)
C5	C6	C7	C8	-108.33(16)	C14	C9	C10	C11	-0.3(2)
C5	C6	C7	C18	123.29(15)	C15	C2	C3	C4	-66.96(17)
C6	C7	C8	C9	-80.64(16)	C18	C7	C8	C9	48.43(18)
C6	C7	C8	O1	39.95(16)	C18	C7	C8	O1	169.02(12)
C6	C7	C18	C19	176.91(14)	O1	C1	C2	C3	58.23(16)
C6	C7	C18	C20	-61.47(19)	O1	C1	C2	C15	-175.91(12)
C7	C8	C9	C10	-134.57(15)	O1	C8	C9	C10	104.10(14)
C7	C8	C9	C14	44.2(2)	O1	C8	C9	C14	-77.17(17)
C7	C8	O1	C1	67.37(15)	O2	C1	C2	C3	-119.15(16)
C8	C7	C18	C19	48.82(19)	O2	C1	C2	C15	6.7(2)
C8	C7	C18	C20	170.44(14)	O2	C1	O1	C8	18.1(2)
C8	C9	C10	C11	178.54(14)	O3	C12	C13	C14	179.79(13)
C8	C9	C14	C13	-179.14(14)					

Experimental

Single crystals of $C_{21}H_{30}O_3$ [ROBE481] were obtained by slow recrystallized from diethyl ether. A suitable crystal was selected and mounted on a loop fiber on a Bruker APEX-II CCD diffractometer. The crystal was kept at 100 K during data collection. Using Olex2 [1], the structure was solved with the XT [2] structure solution program using Direct Methods and refined with the ShelXL [2] refinement package using Least Squares minimization.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. APEX2 (2008), Bruker AXS Inc., Madison, WI 53719-1173.
4. SAINT (2013) V8.34A, Bruker AXS Inc., Madison, WI 53719-1173.
5. XPREP (2013); X-ray data Preparation and Reciprocal space Exploration Program. Bruker AXS Inc., Madison, WI 53719-1173.

Crystal structure determination of ROBE481:

Crystal Data for $C_{21}H_{30}O_3$ (M =330.45 g/mol): monoclinic, space group $P2_1$ (no. 4), a = 9.63600(9) Å, b = 9.33460(9) Å, c = 10.49330(10) Å, β = 100.0230(3)°, V = 929.448(15) Å^3, Z = 2, T = 100 K, μ(CuKα) = 0.607 mm^{-1}, $Dcalc$ = 1.181 g/cm^3, 19284 reflections measured (8.556° ≤ 2Θ ≤ 143.38°), 3466 unique (R_{int} = 0.0177, R_{sigma} = 0.0130) which were used in all calculations. The final R_1 was 0.0276 (I > 2σ(I)) and wR_2 was 0.0731 (all data).

Refinement model description

Number of restraints - 1, number of constraints - unknown.

Details:

1. Fixed Uiso

At 1.2 times of:

All C(H) groups, All C(H,H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

C2(H2), C7(H7), C8(H8), C15(H15), C18(H18)

2.b Secondary CH2 refined with riding coordinates:

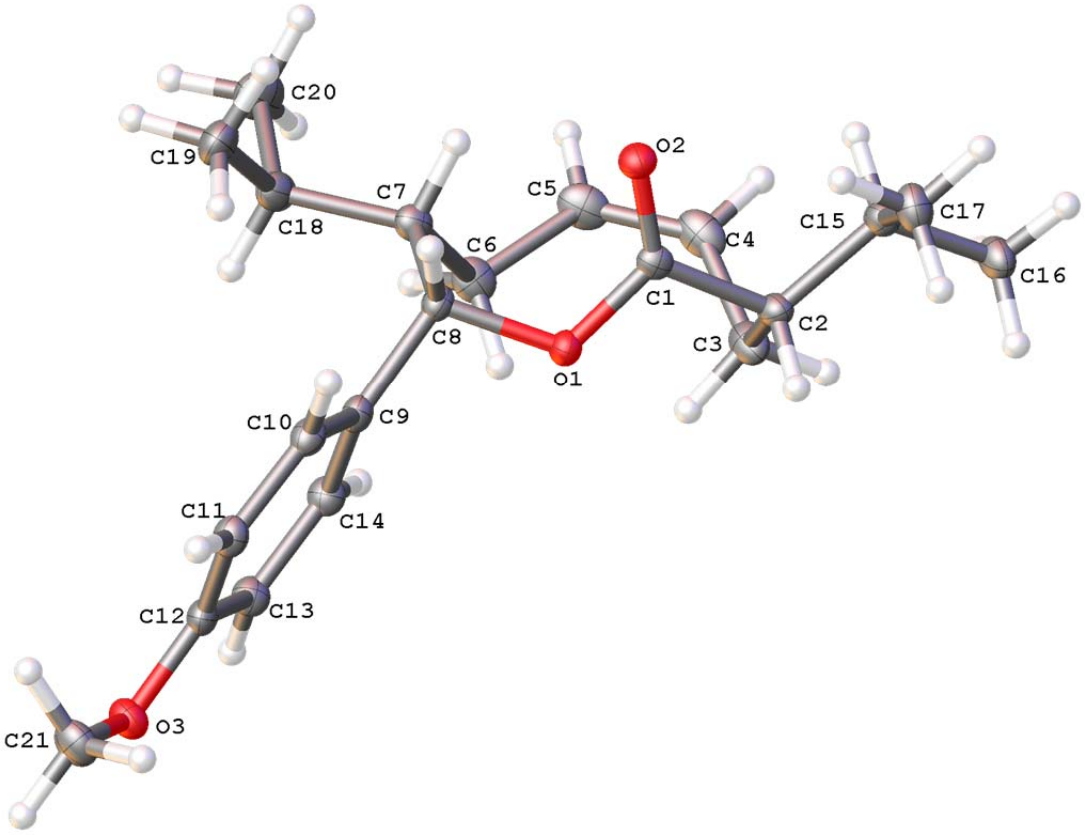
C3(H3A,H3B), C6(H6A,H6B)

2.c Aromatic/amide H refined with riding coordinates:

C4(H4), C5(H5), C10(H10), C11(H11), C13(H13), C14(H14)

2.d Idealized Me refined as rotating group:

C16(H16A,H16B,H16C), C17(H17A,H17B,H17C), C19(H19A,H19B,H19C), C20(H20A,H20B,
H20C), C21(H21A,H21B,H21C)



ORTEP view of the C21 H30 O3 compound with the numbering scheme adopted. Ellipsoids are drawn at the 50% probability level. Hydrogen atoms are represented by spheres of arbitrary size.

Bromolactone **25**

Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C28 H38 Br N O5 S COMPOUND (rober7)

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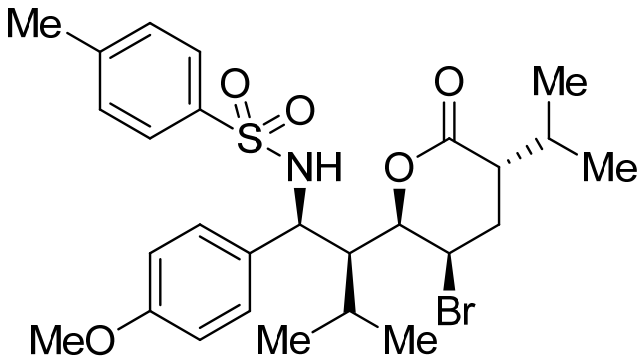


Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Robert D. Giacometti.

Table 1. Crystal data and structure refinement for C28 H38 Br N O5 S.

Identification code	rober7
Empirical formula	C28 H38 Br N O5 S
Formula weight	580.56
Temperature	150K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P212121
Unit cell dimensions	a = 8.2272(4) Å α = 90° b = 18.3055(8) Å β = 90° c = 18.5334(9) Å γ = 90°
Volume	2791.2(2)Å^3
Z	4
Density (calculated)	1.382 g/cm^3
Absorption coefficient	3.010 mm^{-1}
F(000)	1216
Crystal size	0.20 x 0.05 x 0.05 mm
Theta range for data collection	3.39 to 69.75°
Index ranges	$-9 \le h \le 9$, $-22 \le k \le 20$, $-22 \le l \le 22$
Reflections collected	56291
Independent reflections	5227 [R_{int} = 0.049]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8603 and 0.6653
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5227 / 0 / 332
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R_1 = 0.0276, wR_2 = 0.0743
R indices (all data)	R_1 = 0.0281, wR_2 = 0.0747

Absolute structure parameter	-0.023(12)
Extinction coefficient	0.00119(11)
Largest diff. peak and hole	0.386 and -0.317 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for C28 H38 Br N O5 S.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U_{eq}
Br(1)	3977(1)	2598(1)	9671(1)	49(1)
S(1)	10004(1)	5154(1)	7447(1)	29(1)
O(1)	2396(2)	4064(1)	9050(1)	29(1)
O(2)	-53(2)	4069(1)	9483(1)	34(1)
O(3)	9317(2)	5001(1)	6754(1)	37(1)
O(4)	11707(2)	5032(1)	7571(1)	37(1)
O(5)	4739(2)	6831(1)	10008(1)	41(1)
N(1)	9057(2)	4677(1)	8042(1)	28(1)
C(1)	1396(2)	4049(1)	9617(1)	27(1)
C(2)	2017(2)	3998(1)	10381(1)	31(1)
C(3)	3880(3)	3945(1)	10447(1)	38(1)
C(4)	4651(3)	3625(1)	9779(1)	35(1)
C(5)	4157(2)	4078(1)	9134(1)	26(1)
C(6)	4832(2)	3866(1)	8403(1)	26(1)
C(7)	6703(2)	3903(1)	8336(1)	24(1)
C(8)	7270(2)	4675(1)	8097(1)	25(1)
C(9)	6637(2)	5281(1)	8586(1)	26(1)
C(10)	5435(3)	5750(1)	8351(1)	31(1)
C(11)	4765(3)	6281(1)	8807(1)	35(1)
C(12)	5316(3)	6334(1)	9510(1)	31(1)
C(13)	6530(3)	5867(1)	9757(1)	32(1)
C(14)	7184(3)	5348(1)	9297(1)	29(1)
C(15)	3356(4)	7247(2)	9813(2)	63(1)
C(16)	1345(3)	4621(2)	10858(1)	46(1)
C(17)	1525(4)	5366(2)	10496(2)	67(1)
C(18)	-400(3)	4485(2)	11102(2)	59(1)
C(19)	7375(3)	3303(1)	7828(1)	29(1)
C(20)	7135(3)	2537(1)	8137(1)	41(1)
C(21)	6704(3)	3346(1)	7064(1)	42(1)
C(22)	9577(2)	6081(1)	7631(1)	29(1)
C(23)	8698(3)	6493(1)	7146(1)	33(1)
C(24)	8354(3)	7223(1)	7306(1)	35(1)
C(25)	8873(3)	7531(1)	7950(1)	33(1)
C(26)	9768(3)	7102(1)	8428(1)	34(1)
C(27)	10126(3)	6381(1)	8274(1)	34(1)
C(28)	8465(3)	8309(1)	8139(2)	45(1)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for C28 H38 Br N O5 S.

	x	y	z	U_{eq}
H(1)	9624	4408	8344	34
H(2)	1572	3533	10584	37
H(3A)	4331	4439	10532	46
H(3B)	4157	3637	10868	46
H(4)	5860	3645	9831	42
H(5)	4485	4595	9231	32
H(6A)	4351	4192	8033	31
H(6B)	4478	3362	8292	31
H(7)	7164	3811	8827	29
H(8)	6826	4765	7603	30
H(10)	5053	5711	7869	37
H(11)	3942	6601	8635	42
H(13)	6910	5905	10239	38
H(14)	8017	5033	9467	35
H(15A)	2484	6918	9657	94
H(15B)	3638	7578	9417	94
H(15C)	2988	7532	10229	94
H(16)	2029	4634	11304	55
H(17A)	835	5385	10065	100
H(17B)	2662	5441	10356	100
H(17C)	1194	5751	10833	100
H(18A)	-460	4017	11357	89
H(18B)	-1117	4472	10680	89
H(18C)	-744	4879	11427	89
H(19)	8575	3384	7792	35
H(20A)	7690	2181	7829	61
H(20B)	5972	2424	8155	61
H(20C)	7590	2516	8625	61
H(21A)	5517	3301	7078	63
H(21B)	7159	2948	6774	63
H(21C)	7002	3816	6848	63
H(23)	8328	6283	6708	40
H(24)	7761	7511	6970	42
H(26)	10139	7309	8869	41
H(27)	10739	6095	8603	40
H(28A)	7504	8318	8452	67
H(28B)	8238	8584	7697	67
H(28C)	9385	8532	8392	67

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C28 H38 Br N O5 S.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Br(1)	56(1)	36(1)	56(1)	15(1)	21(1)	14(1)
S(1)	31(1)	25(1)	32(1)	1(1)	5(1)	-1(1)
O(1)	23(1)	37(1)	27(1)	5(1)	0(1)	3(1)
O(2)	24(1)	42(1)	35(1)	0(1)	0(1)	5(1)
O(3)	48(1)	34(1)	31(1)	0(1)	4(1)	-4(1)
O(4)	29(1)	32(1)	49(1)	3(1)	8(1)	1(1)
O(5)	48(1)	38(1)	38(1)	-11(1)	-4(1)	17(1)
N(1)	27(1)	26(1)	33(1)	5(1)	3(1)	0(1)
C(1)	28(1)	23(1)	30(1)	0(1)	2(1)	1(1)
C(2)	28(1)	37(1)	27(1)	0(1)	1(1)	-3(1)
C(3)	29(1)	59(1)	27(1)	-2(1)	-1(1)	-5(1)
C(4)	26(1)	50(1)	30(1)	6(1)	-1(1)	3(1)
C(5)	20(1)	32(1)	27(1)	0(1)	0(1)	-1(1)
C(6)	23(1)	27(1)	27(1)	-2(1)	1(1)	-3(1)
C(7)	25(1)	22(1)	26(1)	1(1)	2(1)	-4(1)
C(8)	26(1)	23(1)	28(1)	1(1)	1(1)	-1(1)
C(9)	28(1)	21(1)	29(1)	1(1)	1(1)	-3(1)
C(10)	35(1)	29(1)	29(1)	0(1)	-1(1)	3(1)
C(11)	39(1)	31(1)	35(1)	0(1)	-3(1)	11(1)
C(12)	35(1)	25(1)	34(1)	-4(1)	1(1)	4(1)
C(13)	33(1)	30(1)	33(1)	-5(1)	-6(1)	1(1)
C(14)	28(1)	27(1)	33(1)	-2(1)	-3(1)	2(1)
C(15)	75(2)	65(2)	48(2)	-18(1)	-14(1)	46(2)
C(16)	40(1)	59(2)	37(1)	-18(1)	5(1)	-1(1)
C(17)	74(2)	40(1)	86(2)	-28(2)	6(2)	-6(1)
C(18)	45(2)	90(2)	44(1)	-14(2)	10(1)	9(1)
C(19)	30(1)	23(1)	35(1)	-2(1)	6(1)	0(1)
C(20)	46(1)	24(1)	52(1)	1(1)	12(1)	0(1)
C(21)	52(1)	41(1)	34(1)	-9(1)	2(1)	5(1)
C(22)	28(1)	22(1)	36(1)	2(1)	5(1)	-3(1)
C(23)	31(1)	34(1)	34(1)	-2(1)	0(1)	-2(1)
C(24)	33(1)	29(1)	44(1)	4(1)	-1(1)	5(1)
C(25)	31(1)	26(1)	44(1)	0(1)	5(1)	0(1)
C(26)	37(1)	30(1)	37(1)	-2(1)	2(1)	-4(1)
C(27)	39(1)	28(1)	34(1)	4(1)	0(1)	1(1)
C(28)	45(1)	29(1)	60(2)	-5(1)	4(1)	4(1)

Table 5. Bond lengths [Å] and angles [°] for C28 H38 Br N O5 S

Br(1)-C(4)	1.969(2)	O(2)-C(1)-O(1)	116.23(18)
S(1)-O(3)	1.4306(16)	O(2)-C(1)-C(2)	121.66(18)
S(1)-O(4)	1.4370(16)	O(1)-C(1)-C(2)	122.11(17)
S(1)-N(1)	1.6080(16)	C(1)-C(2)-C(3)	114.58(18)
S(1)-C(22)	1.766(2)	C(1)-C(2)-C(16)	111.78(19)
O(1)-C(1)	1.336(2)	C(3)-C(2)-C(16)	110.91(19)
O(1)-C(5)	1.457(2)	C(4)-C(3)-C(2)	112.18(18)
O(2)-C(1)	1.218(3)	C(3)-C(4)-C(5)	108.78(18)
O(5)-C(12)	1.380(3)	C(3)-C(4)-BR1	109.61(16)
O(5)-C(15)	1.416(3)	C(5)-C(4)-BR1	111.60(15)
N(1)-C(8)	1.473(3)	O(1)-C(5)-C(4)	110.02(16)
		O(1)-C(5)-C(6)	105.34(15)
C(1)-C(2)	1.508(3)	C(4)-C(5)-C(6)	117.88(17)
C(2)-C(3)	1.540(3)	C(5)-C(6)-C(7)	115.22(16)
C(2)-C(16)	1.546(3)	C(6)-C(7)-C(19)	111.98(16)
C(3)-C(4)	1.510(3)	C(6)-C(7)-C(8)	111.22(16)
C(4)-C(5)	1.512(3)	C(19)-C(7)-C(8)	111.42(16)
C(5)-C(6)	1.515(3)	N(1)-C(8)-C(9)	112.41(16)
C(6)-C(7)	1.545(3)	N(1)-C(8)-C(7)	108.77(15)
C(7)-C(19)	1.547(3)	C(9)-C(8)-C(7)	112.98(16)
C(7)-C(8)	1.553(3)	C(10)-C(9)-C(14)	118.24(19)
C(8)-C(9)	1.523(3)	C(10)-C(9)-C(8)	120.68(19)
C(9)-C(10)	1.380(3)	C(14)-C(9)-C(8)	120.96(18)
C(9)-C(14)	1.398(3)	C(9)-C(10)-C(11)	121.6(2)
C(10)-C(11)	1.402(3)	C(12)-C(11)-C(10)	119.1(2)
C(11)-C(12)	1.383(3)	O(5)-C(12)-C(11)	124.26(19)
C(12)-C(13)	1.391(3)	O(5)-C(12)-C(13)	115.59(18)
C(13)-C(14)	1.386(3)	C(11)-C(12)-C(13)	120.16(19)
C(16)-C(18)	1.526(4)	C(14)-C(13)-C(12)	119.8(2)
C(16)-C(17)	1.527(4)	C(13)-C(14)-C(9)	121.02(19)
C(19)-C(21)	1.523(3)	C(18)-C(16)-C(17)	111.6(3)
C(19)-C(20)	1.527(3)	C(18)-C(16)-C(2)	112.7(2)
C(22)-C(23)	1.378(3)	C(17)-C(16)-C(2)	111.8(2)
C(22)-C(27)	1.388(3)	C(21)-C(19)-C(20)	110.41(19)
C(23)-C(24)	1.397(3)	C(21)-C(19)-C(7)	113.52(18)
C(24)-C(25)	1.387(3)	C(20)-C(19)-C(7)	112.17(17)
C(25)-C(26)	1.395(3)		
C(25)-C(28)	1.505(3)	C(23)-C(22)-C(27)	120.91(19)
C(26)-C(27)	1.381(3)	C(23)-C(22)-S(1)	120.32(17)
		C(27)-C(22)-S(1)	118.77(16)
O(3)-S(1)-O(4)	119.86(10)	C(22)-C(23)-C(24)	119.5(2)
O(3)-S(1)-N(1)	108.50(9)	C(25)-C(24)-C(23)	120.5(2)
O(4)-S(1)-N(1)	106.20(10)	C(24)-C(25)-C(26)	118.72(19)
O(3)-S(1)-C(22)	106.39(10)	C(24)-C(25)-C(28)	121.1(2)
O(4)-S(1)-C(22)	108.24(10)	C(26)-C(25)-C(28)	120.2(2)
N(1)-S(1)-C(22)	107.06(9)	C(27)-C(26)-C(25)	121.2(2)
C(1)-O(1)-C(5)	121.92(16)	C(26)-C(27)-C(22)	119.1(2)
C(12)-O(5)-C(15)	117.40(18)		
C(8)-N(1)-S(1)	122.19(14)		

Table 6. Torsion angles [°] for C28 H38 Br N O5 S.

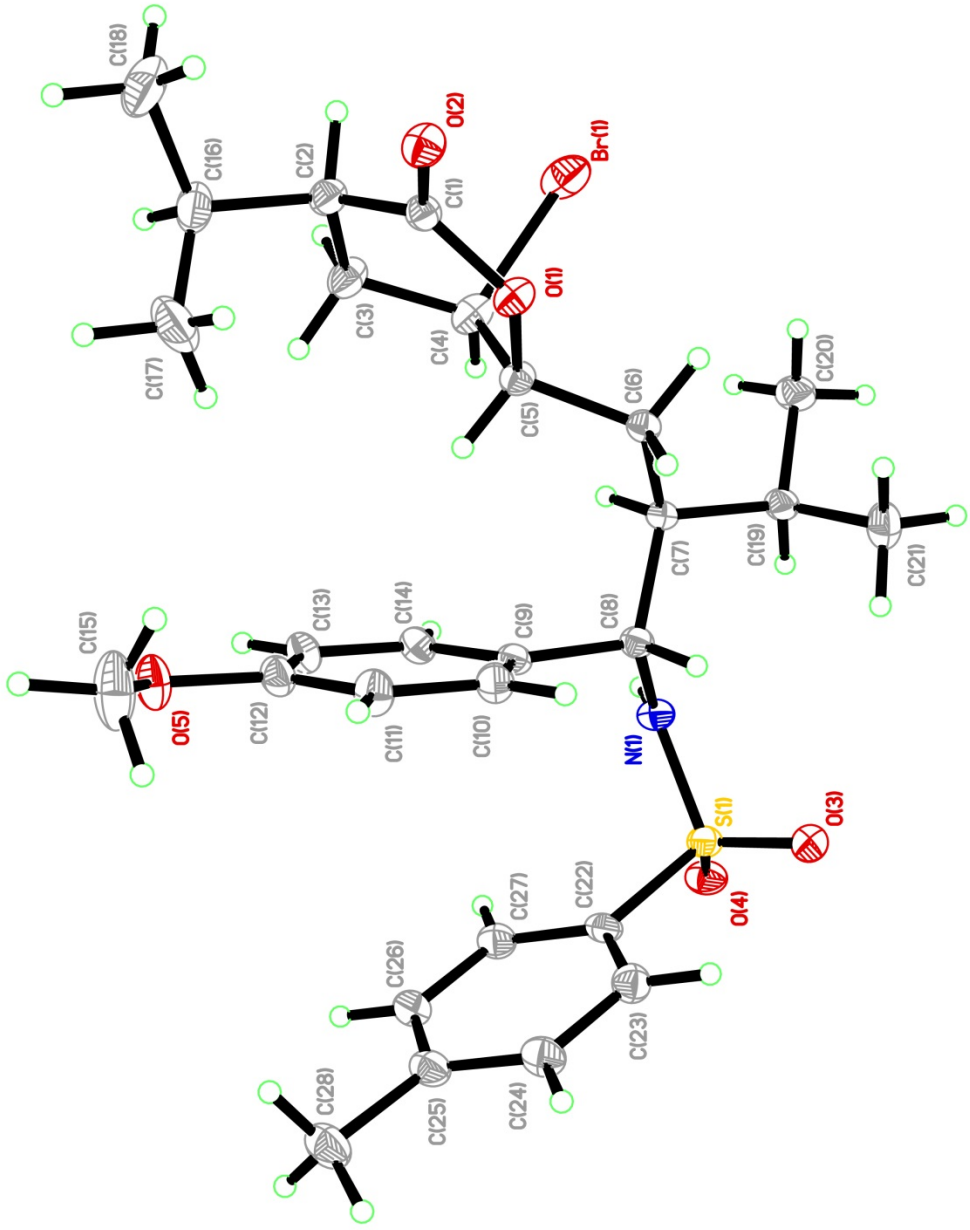
O(3)-S(1)-N(1)-C(8)	-51.38(18)
O(4)-S(1)-N(1)-C(8)	178.54(15)
C(22)-S(1)-N(1)-C(8)	63.06(18)
C(5)-O(1)-C(1)-O(2)	176.98(18)
C(5)-O(1)-C(1)-C(2)	-3.8(3)
O(2)-C(1)-C(2)-C(3)	177.5(2)
O(1)-C(1)-C(2)-C(3)	-1.6(3)
O(2)-C(1)-C(2)-C(16)	-55.2(3)
O(1)-C(1)-C(2)-C(16)	125.6(2)
C(1)-C(2)-C(3)-C(4)	-25.4(3)
C(16)-C(2)-C(3)-C(4)	-153.1(2)
C(2)-C(3)-C(4)-C(5)	56.3(3)
C(2)-C(3)-C(4)-BR1	-66.0(2)
C(1)-O(1)-C(5)-C(4)	35.5(2)
C(1)-O(1)-C(5)-C(6)	163.49(17)
C(3)-C(4)-C(5)-O(1)	-60.8(2)
BR1-C(4)-C(5)-O(1)	60.22(19)
C(3)-C(4)-C(5)-C(6)	178.42(18)
BR1-C(4)-C(5)-C(6)	-60.5(2)
O(1)-C(5)-C(6)-C(7)	175.22(16)
C(4)-C(5)-C(6)-C(7)	-61.6(2)
C(5)-C(6)-C(7)-C(19)	146.17(17)
C(5)-C(6)-C(7)-C(8)	-88.4(2)
S(1)-N(1)-C(8)-C(9)	-88.15(19)
S(1)-N(1)-C(8)-C(7)	145.97(14)
C(6)-C(7)-C(8)-N(1)	-179.92(16)
C(19)-C(7)-C(8)-N(1)	-54.2(2)
C(6)-C(7)-C(8)-C(9)	54.5(2)
C(19)-C(7)-C(8)-C(9)	-179.78(17)
N(1)-C(8)-C(9)-C(10)	128.7(2)
C(7)-C(8)-C(9)-C(10)	-107.7(2)
N(1)-C(8)-C(9)-C(14)	-55.3(2)
C(7)-C(8)-C(9)-C(14)	68.3(2)
C(14)-C(9)-C(10)-C(11)	-0.2(3)
C(8)-C(9)-C(10)-C(11)	176.0(2)
C(9)-C(10)-C(11)-C(12)	-0.4(3)
C(15)-O(5)-C(12)-C(11)	8.6(4)
C(15)-O(5)-C(12)-C(13)	-171.5(2)
C(10)-C(11)-C(12)-O(5)	-179.6(2)
C(10)-C(11)-C(12)-C(13)	0.6(3)
O(5)-C(12)-C(13)-C(14)	179.9(2)
C(11)-C(12)-C(13)-C(14)	-0.2(3)
C(12)-C(13)-C(14)-C(9)	-0.4(3)
C(10)-C(9)-C(14)-C(13)	0.5(3)
C(8)-C(9)-C(14)-C(13)	-175.61(19)
C(1)-C(2)-C(16)-C(18)	78.3(3)
C(3)-C(2)-C(16)-C(18)	-152.5(2)
C(1)-C(2)-C(16)-C(17)	-48.4(3)
C(3)-C(2)-C(16)-C(17)	80.8(3)
C(6)-C(7)-C(19)-C(21)	59.3(2)
C(8)-C(7)-C(19)-C(21)	-65.9(2)
C(6)-C(7)-C(19)-C(20)	-66.7(2)
C(8)-C(7)-C(19)-C(20)	168.05(18)
O(3)-S(1)-C(22)-C(23)	1.4(2)
O(4)-S(1)-C(22)-C(23)	131.46(17)
N(1)-S(1)-C(22)-C(23)	-114.44(18)
O(3)-S(1)-C(22)-C(27)	-179.33(17)
O(4)-S(1)-C(22)-C(27)	-49.3(2)
N(1)-S(1)-C(22)-C(27)	64.81(19)
C(27)-C(22)-C(23)-C(24)	0.0(3)
S(1)-C(22)-C(23)-C(24)	179.19(16)
C(22)-C(23)-C(24)-C(25)	-0.8(3)
C(23)-C(24)-C(25)-C(26)	1.2(3)
C(23)-C(24)-C(25)-C(28)	-178.0(2)
C(24)-C(25)-C(26)-C(27)	-0.7(3)
C(28)-C(25)-C(26)-C(27)	178.5(2)
C(25)-C(26)-C(27)-C(22)	-0.2(3)
C(23)-C(22)-C(27)-C(26)	0.6(3)
S(1)-C(22)-C(27)-C(26)	-178.70(17)

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C28 H38 Br N O5 S.

D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
N(1)-H(1)	O(2)#1	0.88	2.22	2.985(2)	145.8

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z



ORTEP view of the C28 H38 Br N O5 S compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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Lactone diol **32**

Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C21 H32 O5 COMPOUND (robe17)

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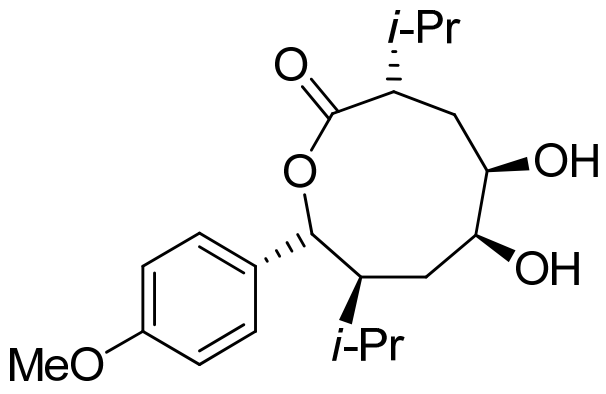


As Ether or Hexane Solvate (Solvent Squeezed Out)

Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Robert D. Giacometti.

Table 1. Crystal data and structure refinement for C21 H32 O5.

Identification code	robe17
Empirical formula	C21 H32 O5 (after squeeze)
Formula weight	364.47 (after squeeze)
Temperature	150K
Wavelength	1.54178 Å
Crystal system	Trigonal
Space group	P32
Unit cell dimensions	a = 25.5016(5) Å α = 90° b = 25.5016(5) Å β = 90° c = 5.8826(1) Å γ = 120°
Volume	3313.10(11)Å^3
Z	6
Density (calculated)	1.096 g/cm^3 (after squeeze)
Absorption coefficient	0.621 mm^{-1} (after squeeze)
F(000)	1188 (after squeeze)
Crystal size	0.21 x 0.06 x 0.02 mm
Theta range for data collection	2.00 to 71.18°
Index ranges	$-31 \leq h \leq 31$, $-30 \leq k \leq 29$, $-7 \leq l \leq 7$
Reflections collected	44115
Independent reflections	8463 [R_{int} = 0.059]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9877 and 0.8428
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8463 / 583 / 782
Goodness-of-fit on F^2	1.075
Final R indices [I>2sigma(I)]	R_1 = 0.0477, wR_2 = 0.1379
R indices (all data)	R_1 = 0.0512, wR_2 = 0.1421
Absolute structure parameter	0.09(17)

Largest diff. peak and hole	0.241 and -0.151 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for C21 H32 O5.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ.	x	y	z	U_{eq}
C(12)	1	8035(1)	7995(1)	2709(4)	51(1)
C(17)	1	9700(1)	7982(1)	2264(4)	43(1)
C(18)	1	9111(1)	7440(1)	3189(4)	44(1)
C(22)	1	3372(1)	4703(1)	6038(4)	51(1)
C(27)	1	5051(1)	6368(1)	5599(4)	44(1)
C(28)	1	5004(1)	5777(1)	6521(4)	43(1)
C(115)	1	7609(1)	7600(1)	811(4)	52(1)
C(116)	1	7117(1)	7005(1)	1790(6)	72(1)
C(117)	1	7335(2)	7924(2)	-491(6)	76(1)
C(118)	1	10259(1)	7955(1)	3137(4)	48(1)
C(119)	1	10833(1)	8404(1)	1870(5)	61(1)
C(120)	1	10352(1)	8064(2)	5688(5)	62(1)
C(215)	1	3342(1)	4275(1)	4142(4)	51(1)
C(216)	1	3440(2)	3783(1)	5121(6)	72(1)
C(217)	1	2743(2)	4003(2)	2853(6)	77(1)
C(218)	1	5636(1)	6927(1)	6469(4)	48(1)
C(219)	1	5764(1)	7499(1)	5196(5)	62(1)
C(220)	1	5623(1)	7020(1)	9022(5)	63(1)
O(11)	0.740(6)	8642(2)	7554(2)	2360(6)	33(1)
O(12)	0.740(6)	8297(2)	7535(2)	5914(5)	67(1)
O(13)	0.740(6)	8947(2)	8958(2)	-1975(7)	70(1)
O(14)	0.740(6)	9839(2)	9535(1)	1340(10)	65(1)
O(15)	0.740(6)	8786(2)	5214(2)	-11(8)	74(1)
O(21)	0.740(6)	4420(1)	5309(3)	5692(6)	34(1)
O(22)	0.740(6)	4096(2)	4961(2)	9247(5)	67(1)
O(23)	0.740(6)	3319(2)	5615(1)	1364(7)	69(1)
O(24)	0.740(6)	3638(2)	6507(2)	4696(9)	65(1)
O(25)	0.740(6)	6856(2)	5386(3)	3122(11)	89(2)
C(11)	0.740(6)	8333(2)	7678(2)	3926(6)	51(1)
C(13)	0.740(6)	8543(2)	8610(2)	1843(9)	57(1)
C(14)	0.740(6)	8968(2)	8627(2)	-22(8)	49(1)
C(15)	0.740(6)	9634(2)	8916(2)	711(8)	50(1)
C(16)	0.740(6)	9767(2)	8615(2)	2725(7)	45(1)
C(19)	0.740(6)	8998(1)	6846(2)	2366(7)	45(1)
C(110)	0.740(6)	8757(2)	6611(2)	243(9)	51(1)
C(111)	0.740(6)	8690(2)	6064(2)	-452(9)	55(1)
C(112)	0.740(6)	8861(2)	5740(2)	921(9)	55(1)
C(113)	0.740(6)	9087(3)	5955(2)	3022(9)	57(1)
C(114)	0.740(6)	9156(3)	6508(2)	3754(8)	54(1)
C(121)	0.740(6)	8986(3)	4877(2)	1256(12)	86(1)
C(21)	0.740(6)	3989(2)	5001(2)	7260(6)	52(1)
C(23)	0.740(6)	3263(2)	5207(2)	5177(9)	58(1)
C(24)	0.740(6)	3677(2)	5636(2)	3313(8)	49(1)

C(25)	0.740(6) 4049(2)	6298(2)	4065(9)	48(1)
C(26)	0.740(6) 4487(2)	6430(2)	6046(7)	46(1)
C(29)	0.740(6) 5482(1)	5642(1)	5643(8)	43(1)
C(210)	0.740(6) 5451(2)	5395(2)	3519(8)	45(1)
C(211)	0.740(6) 5915(2)	5310(3)	2762(9)	54(1)
C(212)	0.740(6) 6416(2)	5470(3)	4073(10)	61(1)
C(213)	0.740(6) 6452(2)	5705(3)	6203(10)	63(1)
C(214)	0.740(6) 5985(2)	5786(3)	6959(9)	55(1)
C(221)	0.740(6) 7404(3)	5585(4)	4351(14)	96(2)
O(31)	0.260(6) 8562(7)	7447(7)	2493(18)	58(5)
O(32)	0.260(6) 8470(5)	7857(5)	5785(13)	59(2)
O(33)	0.260(6) 9056(6)	9177(7)	-1320(20)	93(4)
O(34)	0.260(6) 9896(6)	9548(4)	2090(30)	71(4)
O(35)	0.260(6) 8583(6)	5147(4)	-570(20)	92(3)
O(41)	0.260(6) 4448(3)	5222(9)	5828(18)	54(6)
O(42)	0.260(6) 3945(4)	5133(5)	9116(13)	57(2)
O(43)	0.260(6) 3208(5)	5734(5)	2035(19)	91(4)
O(44)	0.260(6) 3682(6)	6573(6)	5450(30)	86(5)
O(45)	0.260(6) 6966(4)	5523(7)	3570(20)	69(2)
C(31)	0.260(6) 8338(5)	7722(5)	3810(13)	51(1)
C(33)	0.260(6) 8546(5)	8705(5)	2230(20)	54(2)
C(34)	0.260(6) 8989(4)	8745(4)	400(19)	63(4)
C(35)	0.260(6) 9628(4)	8935(4)	1279(18)	51(3)
C(36)	0.260(6) 9671(6)	8549(6)	3200(20)	48(2)
C(39)	0.260(6) 8978(3)	6794(3)	2320(17)	43(3)
C(310)	0.260(6) 8722(5)	6613(4)	177(18)	44(3)
C(311)	0.260(6) 8598(6)	6061(4)	-698(18)	55(4)
C(312)	0.260(6) 8726(5)	5678(4)	511(19)	63(4)
C(313)	0.260(6) 8972(7)	5843(5)	2620(20)	73(5)
C(314)	0.260(6) 9100(7)	6402(5)	3532(18)	50(3)
C(321)	0.260(6) 8722(9)	4739(6)	520(30)	92(4)
C(41)	0.260(6) 3950(3)	5005(5)	7135(13)	52(1)
C(43)	0.260(6) 3174(5)	5216(5)	5560(20)	54(2)
C(44)	0.260(6) 3582(4)	5667(4)	3739(19)	68(4)
C(45)	0.260(6) 4024(4)	6300(4)	4643(19)	67(5)
C(46)	0.260(6) 4455(5)	6344(7)	6530(20)	45(2)
C(49)	0.260(6) 5529(3)	5709(3)	5807(17)	41(3)
C(410)	0.260(6) 5530(4)	5475(6)	3686(19)	49(3)
C(411)	0.260(6) 6017(4)	5418(7)	3008(19)	56(4)
C(412)	0.260(6) 6504(4)	5589(6)	4407(19)	50(3)
C(413)	0.260(6) 6512(5)	5820(8)	6520(20)	54(3)
C(414)	0.260(6) 6024(5)	5876(7)	7194(18)	44(2)
C(421)	0.260(6) 7500(5)	5753(8)	4920(30)	76(3)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for C21 H32 O5.

	Occ.	x	y	z	U_{eq}
H(12)	1	7791	8072	3850	62
H(17)	1	9692	7933	576	52
H(18)	1	9116	7446	4889	53
H(22)	1	3051	4458	7180	61
H(27)	1	5092	6359	3911	53
H(28)	1	5006	5781	8221	52
H(115)	1	7851	7507	-286	62
H(11A)	1	7303	6813	2661	108
H(11B)	1	6875	6737	550	108
H(11C)	1	6856	7082	2792	108
H(11D)	1	7118	8045	570	113
H(11E)	1	7052	7651	-1640	113
H(11F)	1	7659	8285	-1238	113
H(118)	1	10188	7539	2826	58
H(11G)	1	10923	8818	2190	92
H(11H)	1	10772	8327	232	92
H(11I)	1	11172	8354	2373	92
H(12A)	1	10722	8067	6147	93
H(12B)	1	10005	7741	6498	93
H(12C)	1	10387	8455	6061	93
H(215)	1	3676	4515	3041	61
H(21A)	1	3106	3530	6151	108
H(21B)	1	3823	3968	5963	108
H(21C)	1	3455	3533	3885	108
H(21D)	1	2407	3787	3920	115
H(21E)	1	2731	3719	1701	115
H(21F)	1	2706	4327	2111	115
H(218)	1	5980	6854	6157	58
H(21G)	1	5439	7589	5500	92
H(21H)	1	5784	7439	3560	92
H(21I)	1	6151	7839	5709	92
H(22A)	1	5999	7383	9484	94
H(22B)	1	5585	6667	9830	94
H(22C)	1	5277	7072	9394	94
H(13)	0.740(6)	9263	9300	-2017	106
H(14)	0.740(6)	10127	9768	490	98
H(23)	0.740(6)	3326	5946	1244	103
H(24)	0.740(6)	3680	6781	3798	97
H(13A)	0.740(6)	8351	8840	1287	69
H(13B)	0.740(6)	8796	8833	3167	69
H(14A)	0.740(6)	8827	8201	-507	59
H(15)	0.740(6)	9877	8916	-625	60
H(16A)	0.740(6)	9492	8572	3988	54
H(16B)	0.740(6)	10186	8891	3247	54
H(110)	0.740(6)	8638	6828	-739	61

H(111)	0.740(6) 8523	5908	-1907	66
H(113)	0.740(6) 9198	5729	3997	68
H(114)	0.740(6) 9315	6655	5226	64
H(12D)	0.740(6) 9416	5135	1626	129
H(12E)	0.740(6) 8931	4530	357	129
H(12F)	0.740(6) 8751	4734	2664	129
H(23A)	0.740(6) 3288	5458	6501	69
H(23B)	0.740(6) 2842	5013	4606	69
H(24A)	0.740(6) 3963	5496	2823	58
H(25)	0.740(6) 4290	6541	2728	58
H(26A)	0.740(6) 4256	6156	7313	55
H(26B)	0.740(6) 4628	6849	6570	55
H(210)	0.740(6) 5108	5283	2579	55
H(211)	0.740(6) 5886	5138	1304	65
H(213)	0.740(6) 6794	5810	7144	76
H(214)	0.740(6) 6010	5946	8439	66
H(22D)	0.740(6) 7585	6018	4694	144
H(22E)	0.740(6) 7686	5519	3433	144
H(22F)	0.740(6) 7317	5356	5773	144
H(33)	0.260(6) 9190	9520	-725	140
H(34)	0.260(6) 9739	9552	3342	107
H(43)	0.260(6) 3117	5991	2477	136
H(44)	0.260(6) 3335	6300	5846	129
H(33A)	0.260(6) 8343	8930	1726	65
H(33B)	0.260(6) 8769	8893	3650	65
H(34A)	0.260(6) 8820	8338	-334	75
H(35)	0.260(6) 9875	8929	-33	61
H(36A)	0.260(6) 9315	8407	4208	57
H(36B)	0.260(6) 10038	8804	4116	57
H(310)	0.260(6) 8631	6871	-694	53
H(311)	0.260(6) 8422	5943	-2165	66
H(313)	0.260(6) 9057	5579	3478	87
H(314)	0.260(6) 9273	6514	5006	60
H(12G)	0.260(6) 8382	4463	1484	138
H(12H)	0.260(6) 9086	4965	1453	138
H(12I)	0.260(6) 8796	4505	-631	138
H(43A)	0.260(6) 2747	5015	5054	65
H(43B)	0.260(6) 3208	5436	6991	65
H(44A)	0.260(6) 3820	5501	2988	81
H(45)	0.260(6) 4276	6548	3334	80
H(46A)	0.260(6) 4241	5990	7550	54
H(46B)	0.260(6) 4571	6712	7442	54
H(410)	0.260(6) 5194	5353	2695	59
H(411)	0.260(6) 6013	5257	1548	67
H(413)	0.260(6) 6848	5939	7507	64
H(414)	0.260(6) 6029	6036	8659	53
H(42D)	0.260(6) 7396	5561	6418	113
H(42E)	0.260(6) 7680	6192	5086	113
H(42F)	0.260(6) 7790	5664	4173	113

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C21 H32 O5.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(12)	41(1)	55(1)	63(1)	-11(1)	4(1)	28(1)
C(17)	39(1)	49(1)	42(1)	-4(1)	-5(1)	22(1)
C(18)	44(1)	57(1)	36(1)	0(1)	-1(1)	29(1)
C(22)	40(1)	42(1)	61(1)	2(1)	14(1)	13(1)
C(27)	45(1)	40(1)	42(1)	-5(1)	-1(1)	17(1)
C(28)	43(1)	41(1)	36(1)	-1(1)	-1(1)	13(1)
C(115)	46(1)	53(1)	59(1)	-3(1)	-2(1)	27(1)
C(116)	54(1)	60(2)	88(2)	3(1)	-9(1)	17(1)
C(117)	64(2)	75(2)	91(2)	7(2)	-8(1)	38(1)
C(118)	42(1)	58(1)	48(1)	-9(1)	-7(1)	27(1)
C(119)	40(1)	78(2)	62(1)	-7(1)	-4(1)	26(1)
C(120)	55(1)	82(2)	50(1)	-9(1)	-12(1)	35(1)
C(215)	46(1)	45(1)	57(1)	-1(1)	2(1)	19(1)
C(216)	75(2)	53(1)	89(2)	-8(1)	-10(1)	33(1)
C(217)	63(2)	62(2)	92(2)	-6(1)	-15(2)	22(1)
C(218)	44(1)	43(1)	47(1)	-7(1)	4(1)	14(1)
C(219)	64(2)	41(1)	63(1)	-4(1)	4(1)	14(1)
C(220)	66(2)	57(1)	51(1)	-13(1)	-3(1)	21(1)
O(11)	29(1)	37(1)	35(2)	-4(1)	0(1)	17(1)
O(12)	78(2)	96(3)	44(1)	12(2)	17(1)	57(2)
O(13)	55(2)	58(2)	97(2)	30(2)	6(1)	27(1)
O(14)	63(2)	42(1)	85(4)	-1(1)	25(2)	21(1)
O(15)	83(3)	57(2)	99(2)	-5(1)	6(2)	47(2)
O(21)	32(2)	30(1)	36(2)	2(1)	4(1)	13(1)
O(22)	58(2)	80(2)	44(1)	18(1)	6(1)	21(2)
O(23)	58(2)	55(1)	95(2)	5(1)	-25(1)	29(1)
O(24)	61(2)	60(2)	87(3)	26(2)	27(2)	41(2)
O(25)	59(2)	100(4)	108(3)	12(2)	14(2)	40(2)
C(11)	45(1)	67(2)	44(1)	-9(1)	3(1)	30(1)
C(13)	46(1)	41(2)	93(3)	-14(2)	4(2)	28(1)
C(14)	47(2)	37(2)	66(2)	3(2)	10(1)	22(1)
C(15)	49(2)	45(2)	55(2)	3(1)	16(1)	23(1)
C(16)	32(2)	48(2)	48(2)	-2(1)	11(1)	14(1)
C(19)	38(2)	50(2)	46(2)	9(2)	4(2)	23(2)
C(110)	53(2)	51(2)	49(2)	3(2)	2(2)	27(2)
C(111)	59(2)	54(2)	56(2)	-3(2)	8(2)	30(2)
C(112)	48(2)	44(2)	78(3)	9(2)	13(2)	26(2)
C(113)	53(2)	53(2)	74(2)	16(2)	6(2)	34(2)
C(114)	56(2)	53(2)	54(2)	8(1)	1(2)	28(2)
C(121)	101(3)	71(2)	112(3)	1(2)	4(2)	62(2)
C(21)	52(1)	45(1)	45(1)	3(1)	13(1)	14(1)
C(23)	32(2)	45(1)	95(3)	4(2)	20(2)	19(1)

C(24)	37(2)	48(2)	66(2)	9(1)	5(2)	25(1)
C(25)	44(2)	48(2)	57(2)	14(1)	11(1)	27(2)
C(26)	50(1)	33(2)	48(2)	12(1)	14(1)	16(1)
C(29)	38(2)	35(2)	46(2)	5(1)	-4(1)	10(1)
C(210)	40(2)	48(2)	44(2)	0(1)	-1(1)	18(2)
C(211)	51(2)	52(2)	57(2)	8(2)	9(2)	24(2)
C(212)	39(2)	55(3)	84(3)	19(2)	14(2)	21(2)
C(213)	41(2)	54(3)	81(3)	7(2)	-14(2)	13(2)
C(214)	52(2)	47(2)	57(2)	-2(2)	-8(2)	17(2)
C(221)	68(2)	114(3)	113(3)	6(2)	3(2)	51(2)
O(31)	55(8)	66(9)	48(6)	15(5)	8(4)	27(6)
O(32)	66(5)	76(6)	38(4)	6(4)	9(3)	39(5)
O(33)	87(6)	85(6)	111(6)	1(4)	-7(4)	47(4)
O(34)	65(5)	63(5)	80(9)	1(4)	12(5)	28(4)
O(35)	92(6)	79(4)	107(5)	-4(4)	-1(5)	45(4)
O(41)	61(7)	51(8)	45(5)	5(4)	-5(4)	23(5)
O(42)	59(5)	70(5)	38(4)	9(3)	5(3)	28(4)
O(43)	82(5)	84(5)	108(6)	-11(4)	-4(4)	42(4)
O(44)	75(6)	74(6)	98(10)	10(5)	10(6)	31(5)
O(45)	38(3)	82(5)	101(5)	6(4)	8(3)	41(4)
C(31)	45(1)	67(2)	44(1)	-9(1)	3(1)	30(1)
C(33)	46(3)	35(3)	91(4)	-20(3)	6(3)	27(2)
C(34)	66(6)	30(5)	98(8)	-7(5)	-5(6)	28(4)
C(35)	42(3)	51(4)	65(5)	-2(4)	14(3)	28(3)
C(36)	31(3)	51(2)	50(3)	-3(2)	9(2)	12(2)
C(39)	37(4)	48(4)	49(4)	5(4)	15(4)	26(3)
C(310)	50(4)	49(4)	44(4)	-3(4)	8(4)	32(3)
C(311)	47(5)	62(6)	61(6)	7(5)	2(4)	30(4)
C(312)	46(6)	65(7)	75(7)	-8(5)	13(5)	27(5)
C(313)	55(7)	65(7)	96(9)	11(6)	7(6)	29(5)
C(314)	45(4)	59(5)	57(4)	11(4)	4(3)	35(4)
C(321)	94(5)	88(5)	99(5)	-2(3)	-1(3)	50(3)
C(41)	52(1)	45(1)	45(1)	3(1)	13(1)	14(1)
C(43)	30(2)	44(2)	94(3)	2(2)	23(2)	23(2)
C(44)	44(5)	66(6)	106(9)	-1(6)	12(5)	37(4)
C(45)	56(6)	46(6)	82(8)	10(5)	24(5)	13(5)
C(46)	52(2)	30(2)	50(3)	9(2)	14(2)	18(2)
C(49)	40(4)	35(4)	41(4)	-1(3)	1(4)	13(3)
C(410)	47(4)	46(4)	53(4)	1(4)	-5(4)	20(4)
C(411)	49(6)	53(6)	60(6)	2(5)	6(5)	22(5)
C(412)	35(5)	42(5)	68(6)	3(4)	-14(4)	16(4)
C(413)	37(4)	50(5)	70(4)	-5(4)	-15(3)	18(4)
C(414)	38(3)	48(4)	49(4)	-7(3)	-14(3)	23(3)
C(421)	67(4)	82(4)	84(4)	-3(3)	-2(3)	41(3)

Table 5. Bond lengths [Å] and angles [°] for C21 H32 O5

C(12)-C(31)	1.429(7)
C(12)-C(115)	1.532(3)
C(12)-C(11)	1.535(4)
C(12)-C(13)	1.538(5)
C(12)-C(33)	1.642(10)
C(17)-C(18)	1.546(3)
C(17)-C(118)	1.549(3)
C(17)-C(16)	1.557(5)
C(17)-C(36)	1.583(13)
C(18)-O(11)	1.448(3)
C(18)-O(31)	1.468(11)
C(18)-C(19)	1.476(4)
C(18)-C(39)	1.591(7)
C(22)-C(41)	1.430(7)
C(22)-C(23)	1.531(5)
C(22)-C(215)	1.536(3)
C(22)-C(21)	1.540(4)
C(22)-C(43)	1.644(10)
C(27)-C(218)	1.547(3)
C(27)-C(28)	1.547(3)
C(27)-C(26)	1.548(5)
C(27)-C(46)	1.588(12)
C(28)-O(21)	1.450(4)
C(28)-O(41)	1.475(13)
C(28)-C(49)	1.494(7)
C(28)-C(29)	1.515(4)
C(115)-C(116)	1.517(4)
C(115)-C(117)	1.529(4)
C(118)-C(120)	1.523(3)
C(118)-C(119)	1.527(4)
C(215)-C(216)	1.509(4)
C(215)-C(217)	1.526(4)
C(218)-C(220)	1.524(3)
C(218)-C(219)	1.525(4)
O(11)-C(11)	1.349(3)
O(12)-C(11)	1.214(4)
O(13)-C(14)	1.443(4)
O(14)-C(15)	1.441(4)
O(15)-C(112)	1.370(4)
O(15)-C(121)	1.412(6)
O(21)-C(21)	1.347(3)
O(22)-C(21)	1.216(4)
O(23)-C(24)	1.451(4)
O(24)-C(25)	1.442(4)
O(25)-C(212)	1.361(4)
O(25)-C(221)	1.422(7)
C(13)-C(14)	1.527(5)
C(14)-C(15)	1.538(4)
C(15)-C(16)	1.539(5)
C(19)-C(114)	1.385(4)
C(19)-C(110)	1.388(4)
C(110)-C(111)	1.380(4)
C(111)-C(112)	1.372(6)
C(112)-C(113)	1.358(7)
C(113)-C(114)	1.400(6)
C(23)-C(24)	1.536(5)
C(24)-C(25)	1.531(5)
C(25)-C(26)	1.529(5)
C(29)-C(214)	1.381(4)
C(29)-C(210)	1.383(4)
C(210)-C(211)	1.380(4)
C(211)-C(212)	1.369(6)
C(212)-C(213)	1.372(7)
C(213)-C(214)	1.381(5)
O(31)-C(31)	1.346(3)
O(32)-C(31)	1.211(4)
O(33)-C(34)	1.444(4)
O(34)-C(35)	1.441(5)
O(35)-C(312)	1.369(5)
O(35)-C(321)	1.411(6)
O(41)-C(41)	1.344(3)
O(42)-C(41)	1.213(4)
O(43)-C(44)	1.452(4)
O(44)-C(45)	1.441(5)
O(45)-C(412)	1.362(5)
O(45)-C(421)	1.425(7)
C(33)-C(34)	1.527(6)
C(34)-C(35)	1.537(5)
C(35)-C(36)	1.538(5)
C(39)-C(314)	1.384(4)
C(39)-C(310)	1.389(4)
C(310)-C(311)	1.380(4)
C(311)-C(312)	1.372(6)
C(312)-C(313)	1.358(7)
C(313)-C(314)	1.400(6)
C(43)-C(44)	1.536(5)
C(44)-C(45)	1.530(5)
C(45)-C(46)	1.528(5)
C(49)-C(414)	1.380(4)
C(49)-C(410)	1.383(4)
C(410)-C(411)	1.380(4)
C(411)-C(412)	1.368(6)
C(412)-C(413)	1.372(7)
C(413)-C(414)	1.381(5)
C(31)-C(12)-C(115)	112.9(4)
C(31)-C(12)-C(11)	2.6(6)
C(115)-C(12)-C(11)	111.6(2)
C(31)-C(12)-C(13)	105.2(6)
C(115)-C(12)-C(13)	112.8(3)

C(11)-C(12)-C(13) 107.8(3)
C(31)-C(12)-C(33) 107.0(5)
C(115)-C(12)-C(33) 120.7(6)
C(11)-C(12)-C(33) 109.5(5)
C(13)-C(12)-C(33) 11.3(5)
C(18)-C(17)-C(118) 110.42(18)
C(18)-C(17)-C(16) 114.8(2)
C(118)-C(17)-C(16) 111.2(2)
C(18)-C(17)-C(36) 103.1(6)
C(118)-C(17)-C(36) 113.0(5)
C(16)-C(17)-C(36) 12.9(5)
O(11)-C(18)-O(31) 10.1(8)
O(11)-C(18)-C(19) 109.8(2)
O(31)-C(18)-C(19) 102.9(6)
O(11)-C(18)-C(17) 103.5(3)

O(31)-C(18)-C(17) 113.5(7)
C(19)-C(18)-C(17) 113.95(18)
O(11)-C(18)-C(39) 109.2(4)
O(31)-C(18)-C(39) 102.3(5)
C(19)-C(18)-C(39) 1.0(3)
C(17)-C(18)-C(39) 114.9(2)
C(41)-C(22)-C(23) 105.6(6)
C(41)-C(22)-C(215) 112.5(4)
C(23)-C(22)-C(215) 113.0(3)
C(41)-C(22)-C(21) 2.5(6)
C(23)-C(22)-C(21) 108.1(3)
C(215)-C(22)-C(21) 111.5(2)
C(41)-C(22)-C(43) 107.0(5)
C(23)-C(22)-C(43) 11.2(5)
C(215)-C(22)-C(43) 121.1(6)
C(21)-C(22)-C(43) 109.3(5)
C(218)-C(27)-C(28) 110.49(18)
C(218)-C(27)-C(26) 111.5(2)
C(28)-C(27)-C(26) 114.7(2)
C(218)-C(27)-C(46) 112.7(5)
C(28)-C(27)-C(46) 103.6(6)
C(26)-C(27)-C(46) 12.5(6)
O(21)-C(28)-O(41) 10.8(10)
O(21)-C(28)-C(49) 114.8(5)
O(41)-C(28)-C(49) 107.3(7)
O(21)-C(28)-C(29) 108.0(3)
O(41)-C(28)-C(29) 100.6(7)
C(49)-C(28)-C(29) 6.8(5)
O(21)-C(28)-C(27) 103.4(3)
O(41)-C(28)-C(27) 114.0(8)
C(49)-C(28)-C(27) 112.2(3)
C(29)-C(28)-C(27) 115.00(18)
C(116)-C(115)-C(117) 111.0(2)
C(116)-C(115)-C(12) 109.9(2)
C(117)-C(115)-C(12) 112.1(2)
C(120)-C(118)-C(119) 110.0(2)
C(120)-C(118)-C(17) 112.34(18)
C(119)-C(118)-C(17) 111.3(2)
C(216)-C(215)-C(217) 110.8(2)
C(216)-C(215)-C(22) 110.0(2)
C(217)-C(215)-C(22) 111.6(2)
C(220)-C(218)-C(219) 110.1(2)
C(220)-C(218)-C(27) 112.56(19)
C(219)-C(218)-C(27) 111.5(2)
C(11)-O(11)-C(18) 117.1(2)
C(112)-O(15)-C(121) 117.9(4)
C(21)-O(21)-C(28) 116.9(2)
C(212)-O(25)-C(221) 118.3(5)
O(12)-C(11)-O(11) 123.6(3)
O(12)-C(11)-C(12) 128.6(3)
O(11)-C(11)-C(12) 107.8(3)
C(14)-C(13)-C(12) 119.4(4)
O(13)-C(14)-C(13) 110.8(3)
O(13)-C(14)-C(15) 107.3(3)
C(13)-C(14)-C(15) 114.2(4)
O(14)-C(15)-C(14) 107.8(3)
O(14)-C(15)-C(16) 107.4(3)
C(14)-C(15)-C(16) 116.3(3)
C(15)-C(16)-C(17) 116.4(3)
C(114)-C(19)-C(110) 117.7(3)
C(114)-C(19)-C(18) 118.5(3)
C(110)-C(19)-C(18) 123.8(3)
C(111)-C(110)-C(19) 120.5(3)
C(112)-C(111)-C(110) 121.2(4)
C(113)-C(112)-O(15) 125.6(4)
C(113)-C(112)-C(111) 119.4(3)
O(15)-C(112)-C(111) 115.0(4)
C(112)-C(113)-C(114) 120.1(3)
C(19)-C(114)-C(113) 121.1(3)
O(22)-C(21)-O(21) 123.7(3)
O(22)-C(21)-C(22) 128.6(3)
O(21)-C(21)-C(22) 107.6(3)
C(22)-C(23)-C(24) 119.0(4)
O(23)-C(24)-C(25) 107.5(3)
O(23)-C(24)-C(23) 109.9(3)
C(25)-C(24)-C(23) 113.9(4)
O(24)-C(25)-C(26) 107.8(4)
O(24)-C(25)-C(24) 108.5(3)
C(26)-C(25)-C(24) 116.4(3)
C(25)-C(26)-C(27) 117.4(3)
C(214)-C(29)-C(210) 117.6(3)
C(214)-C(29)-C(28) 119.7(3)
C(210)-C(29)-C(28) 122.8(3)
C(211)-C(210)-C(29) 120.2(3)
C(212)-C(211)-C(210) 121.3(4)
O(25)-C(212)-C(211) 116.2(5)
O(25)-C(212)-C(213) 124.3(4)
C(211)-C(212)-C(213) 119.5(3)
C(212)-C(213)-C(214) 119.0(3)
C(29)-C(214)-C(213) 122.4(4)
C(31)-O(31)-C(18) 120.0(7)
C(312)-O(35)-C(321) 118.5(6)
C(41)-O(41)-C(28) 119.6(8)
C(412)-O(45)-C(421) 116.9(6)

O(32)-C(31)-O(31)	124.9(5)	O(42)-C(41)-C(22)	115.5(6)
O(32)-C(31)-C(12)	115.8(6)	O(41)-C(41)-C(22)	118.1(5)
O(31)-C(31)-C(12)	117.7(6)	C(44)-C(43)-C(22)	110.6(8)
C(34)-C(33)-C(12)	110.3(8)	O(43)-C(44)-C(45)	107.2(4)
O(33)-C(34)-C(33)	110.2(4)	O(43)-C(44)-C(43)	109.3(4)
O(33)-C(34)-C(35)	107.1(4)	C(45)-C(44)-C(43)	114.4(5)
C(33)-C(34)-C(35)	114.7(5)	O(44)-C(45)-C(46)	108.2(5)
O(34)-C(35)-C(34)	107.9(4)	O(44)-C(45)-C(44)	108.7(4)
O(34)-C(35)-C(36)	107.6(4)	C(46)-C(45)-C(44)	116.9(4)
C(34)-C(35)-C(36)	116.7(4)	C(45)-C(46)-C(27)	113.1(8)
C(35)-C(36)-C(17)	112.3(8)	C(414)-C(49)-C(410)	118.0(3)
C(314)-C(39)-C(310)	117.7(4)	C(414)-C(49)-C(28)	122.1(6)
C(314)-C(39)-C(18)	125.1(6)	C(410)-C(49)-C(28)	119.9(6)
C(310)-C(39)-C(18)	117.2(6)	C(411)-C(410)-C(49)	120.1(4)
C(311)-C(310)-C(39)	120.5(4)	C(412)-C(411)-C(410)	121.0(4)
C(312)-C(311)-C(310)	121.3(4)	O(45)-C(412)-C(411)	116.4(5)
C(313)-C(312)-O(35)	125.8(5)	O(45)-C(412)-C(413)	123.7(5)
C(313)-C(312)-C(311)	119.3(4)	C(411)-C(412)-C(413)	119.9(4)
O(35)-C(312)-C(311)	114.9(5)	C(412)-C(413)-C(414)	119.0(4)
C(312)-C(313)-C(314)	120.1(4)	C(49)-C(414)-C(413)	122.1(4)
C(39)-C(314)-C(313)	121.1(4)		
O(42)-C(41)-O(41)	125.1(5)		

Table 6. Torsion angles [°] for C21 H32 O5.

C(118)-C(17)-C(18)-O(11) 176.24(18)
C(16)-C(17)-C(18)-O(11) 49.6(3)
C(36)-C(17)-C(18)-O(11) 55.3(4)
C(118)-C(17)-C(18)-O(31) 178.0(4)
C(16)-C(17)-C(18)-O(31) 51.4(5)
C(36)-C(17)-C(18)-O(31) 57.1(6)
C(118)-C(17)-C(18)-C(19) -64.6(3)
C(16)-C(17)-C(18)-C(19) 168.8(3)
C(36)-C(17)-C(18)-C(19) 174.5(4)
C(118)-C(17)-C(18)-C(39) -64.7(5)
C(16)-C(17)-C(18)-C(39) 168.6(5)
C(36)-C(17)-C(18)-C(39) 174.3(6)
C(218)-C(27)-C(28)-O(21) 176.18(19)
C(26)-C(27)-C(28)-O(21) 49.1(3)
C(46)-C(27)-C(28)-O(21) 55.3(4)
C(218)-C(27)-C(28)-O(41) 178.2(4)
C(26)-C(27)-C(28)-O(41) 51.1(5)
C(46)-C(27)-C(28)-O(41) 57.4(6)
C(218)-C(27)-C(28)-C(49) -59.6(5)
C(26)-C(27)-C(28)-C(49) 173.3(5)
C(46)-C(27)-C(28)-C(49) 179.5(6)
C(218)-C(27)-C(28)-C(29) -66.3(3)
C(26)-C(27)-C(28)-C(29) 166.6(3)
C(46)-C(27)-C(28)-C(29) 172.8(4)
C(31)-C(12)-C(115)-C(116) 61.5(5)
C(11)-C(12)-C(115)-C(116) 59.0(3)
C(13)-C(12)-C(115)-C(116) -179.4(3)
C(33)-C(12)-C(115)-C(116) -170.3(5)
C(31)-C(12)-C(115)-C(117) -174.6(5)
C(11)-C(12)-C(115)-C(117) -177.1(3)
C(13)-C(12)-C(115)-C(117) -55.6(3)
C(33)-C(12)-C(115)-C(117) -46.4(5)
C(18)-C(17)-C(118)-C(120) -68.1(3)
C(16)-C(17)-C(118)-C(120) 60.5(3)
C(36)-C(17)-C(118)-C(120) 46.7(6)
C(18)-C(17)-C(118)-C(119) 168.06(19)
C(16)-C(17)-C(118)-C(119) -63.3(3)
C(36)-C(17)-C(118)-C(119) -77.1(6)
C(41)-C(22)-C(215)-C(216) 61.8(5)
C(23)-C(22)-C(215)-C(216) -178.8(2)
C(21)-C(22)-C(215)-C(216) 59.3(3)
C(43)-C(22)-C(215)-C(216) -170.0(5)
C(41)-C(22)-C(215)-C(217) -174.8(5)
C(23)-C(22)-C(215)-C(217) -55.3(3)
C(21)-C(22)-C(215)-C(217) -177.2(3)
C(43)-C(22)-C(215)-C(217) -46.6(5)
C(28)-C(27)-C(218)-C(220) -68.0(3)
C(26)-C(27)-C(218)-C(220) 60.8(3)
C(46)-C(27)-C(218)-C(220) 47.3(6)
C(28)-C(27)-C(218)-C(219) 167.66(19)
C(26)-C(27)-C(218)-C(219) -63.5(3)
C(46)-C(27)-C(218)-C(219) -77.0(6)
O(31)-C(18)-O(11)-C(11) 76(2)
C(19)-C(18)-O(11)-C(11) 124.4(4)
C(17)-C(18)-O(11)-C(11) -113.6(4)
C(39)-C(18)-O(11)-C(11) 123.6(5)
O(41)-C(28)-O(21)-C(21) 77(2)

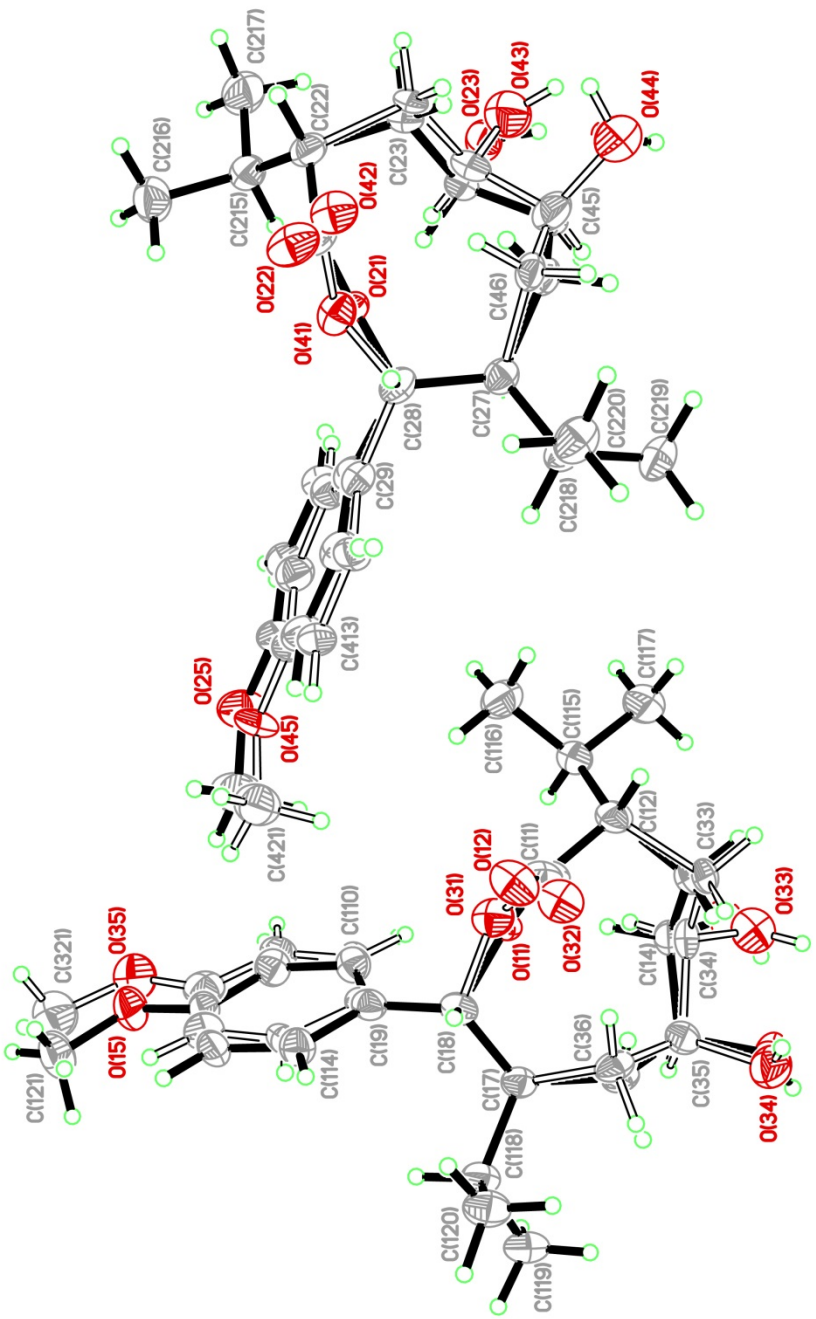
C(49)-C(28)-O(21)-C(21) 124.0(6)
C(29)-C(28)-O(21)-C(21) 124.2(5)
C(27)-C(28)-O(21)-C(21) -113.5(5)
C(18)-O(11)-C(11)-O(12) -21.7(7)
C(18)-O(11)-C(11)-C(12) 160.3(4)
C(31)-C(12)-C(11)-O(12) 122(10)
C(115)-C(12)-C(11)-O(12)-119.1(5)
C(13)-C(12)-C(11)-O(12) 116.5(6)
C(33)-C(12)-C(11)-O(12) 104.7(8)
C(31)-C(12)-C(11)-O(11) -60(9)
C(115)-C(12)-C(11)-O(11) 58.8(4)
C(13)-C(12)-C(11)-O(11) -65.6(5)
C(33)-C(12)-C(11)-O(11) -77.4(6)
C(31)-C(12)-C(13)-C(14) 66.3(5)
C(115)-C(12)-C(13)-C(14) -57.2(4)
C(11)-C(12)-C(13)-C(14) 66.5(4)
C(33)-C(12)-C(13)-C(14) 167(3)
C(12)-C(13)-C(14)-O(13) 121.7(4)
C(12)-C(13)-C(14)-C(15) -116.9(4)
O(13)-C(14)-C(15)-O(14) 61.9(5)
C(13)-C(14)-C(15)-O(14) -61.4(4)
O(13)-C(14)-C(15)-C(16) -177.5(4)
C(13)-C(14)-C(15)-C(16) 59.2(5)
O(14)-C(15)-C(16)-C(17) -168.5(3)
C(14)-C(15)-C(16)-C(17) 70.7(4)
C(18)-C(17)-C(16)-C(15) -102.2(3)
C(118)-C(17)-C(16)-C(15) 131.5(2)
C(36)-C(17)-C(16)-C(15) -128(2)
O(11)-C(18)-C(19)-C(114) -146.3(4)
O(31)-C(18)-C(19)-C(114) -138.6(6)
C(17)-C(18)-C(19)-C(114) 98.2(3)
C(39)-C(18)-C(19)-C(114) -90(32)
O(11)-C(18)-C(19)-C(110) 35.7(4)
O(31)-C(18)-C(19)-C(110) 43.4(7)
C(17)-C(18)-C(19)-C(110) -79.9(3)
C(39)-C(18)-C(19)-C(110) 91(32)
C(114)-C(19)-C(110)-C(111) -1.0(2)
C(18)-C(19)-C(110)-C(111) 177.0(2)
C(19)-C(110)-C(111)-C(112) -0.3(2)
C(121)-O(15)-C(112)-C(113) -3.3(6)
C(121)-O(15)-C(112)-C(111) 176.3(4)

C(110)-C(111)-C(112)-C(113) 1.5(5)
C(110)-C(111)-C(112)-O(15) -178.1(2)
O(15)-C(112)-C(113)-C(114) 178.2(4)
C(111)-C(112)-C(113)-C(114) -1.4(6)
C(110)-C(19)-C(114)-C(113) 1.2(4)
C(18)-C(19)-C(114)-C(113) -177.0(3)
C(112)-C(113)-C(114)-C(19) 0.0(6)
C(28)-O(21)-C(21)-O(22) -22.3(8)
C(28)-O(21)-C(21)-C(22) 160.4(5)
C(41)-C(22)-C(21)-O(22) 128(11)
C(23)-C(22)-C(21)-O(22) 117.1(6)
C(215)-C(22)-C(21)-O(22) -118.2(5)
C(43)-C(22)-C(21)-O(22) 105.3(8)
C(41)-C(22)-C(21)-O(21) -55(10)
C(23)-C(22)-C(21)-O(21) -65.8(5)
C(215)-C(22)-C(21)-O(21) 58.9(4)
C(43)-C(22)-C(21)-O(21) -77.5(7)
C(41)-C(22)-C(23)-C(24) 65.5(5)
C(215)-C(22)-C(23)-C(24) -57.8(4)
C(21)-C(22)-C(23)-C(24) 66.0(4)
C(43)-C(22)-C(23)-C(24) 164(3)
C(22)-C(23)-C(24)-O(23) 122.5(4)
C(22)-C(23)-C(24)-C(25) -116.8(4)
O(23)-C(24)-C(25)-O(24) 60.9(5)
C(23)-C(24)-C(25)-O(24) -61.1(5)
O(23)-C(24)-C(25)-C(26) -177.3(4)
C(23)-C(24)-C(25)-C(26) 60.7(5)
O(24)-C(25)-C(26)-C(27) -167.9(3)
C(24)-C(25)-C(26)-C(27) 69.9(5)
C(218)-C(27)-C(26)-C(25) 131.5(3)
C(28)-C(27)-C(26)-C(25) -101.9(3)
C(46)-C(27)-C(26)-C(25) -131(3)
O(21)-C(28)-C(29)-C(214)-146.4(4)
O(41)-C(28)-C(29)-C(214)-138.3(7)
C(49)-C(28)-C(29)-C(214) 32(3)
C(27)-C(28)-C(29)-C(214) 98.7(3)
O(21)-C(28)-C(29)-C(210) 35.7(4)
O(41)-C(28)-C(29)-C(210) 43.8(7)
C(49)-C(28)-C(29)-C(210)-146(4)
C(27)-C(28)-C(29)-C(210) -79.2(3)
C(214)-C(29)-C(210)-C(211) -1.3(2)
C(28)-C(29)-C(210)-C(211) 176.7(2)
C(29)-C(210)-C(211)-C(212) -0.3(2)
C(221)-O(25)-C(212)-C(211) 175.6(6)
C(221)-O(25)-C(212)-C(213) -3.7(8)
C(210)-C(211)-C(212)-O(25) -177.7(3)
C(210)-C(211)-C(212)-C(213) 1.6(5)
O(25)-C(212)-C(213)-C(214) 178.0(4)
C(211)-C(212)-C(213)-C(214) -1.2(6)
C(210)-C(29)-C(214)-C(213) 1.7(4)
C(28)-C(29)-C(214)-C(213) -176.3(3)
C(212)-C(213)-C(214)-C(29) -0.4(6)
O(11)-C(18)-O(31)-C(31) -81(3)
C(19)-C(18)-O(31)-C(31) 145.4(11)
C(17)-C(18)-O(31)-C(31) -91.0(11)
C(39)-C(18)-O(31)-C(31) 144.6(10)
O(21)-C(28)-O(41)-C(41) -79(3)
C(49)-C(28)-O(41)-C(41) 145.3(12)
C(29)-C(28)-O(41)-C(41) 146.5(13)
C(27)-C(28)-O(41)-C(41) -89.9(13)
C(18)-O(31)-C(31)-O(32) -16.8(17)
C(18)-O(31)-C(31)-C(12) 148.3(11)
C(115)-C(12)-C(31)-O(32) -150.5(8)
C(11)-C(12)-C(31)-O(32) -88(10)
C(13)-C(12)-C(31)-O(32) 86.1(9)
C(33)-C(12)-C(31)-O(32) 74.5(10)
C(115)-C(12)-C(31)-O(31) 43.0(10)
C(11)-C(12)-C(31)-O(31) 105(10)
C(13)-C(12)-C(31)-O(31) -80.4(10)
C(33)-C(12)-C(31)-O(31) -92.0(11)
C(31)-C(12)-C(33)-C(34) 69.5(8)
C(115)-C(12)-C(33)-C(34) -61.2(7)
C(11)-C(12)-C(33)-C(34) 70.3(7)
C(13)-C(12)-C(33)-C(34) -13(2)
C(12)-C(33)-C(34)-O(33) 130.3(9)
C(12)-C(33)-C(34)-C(35) -108.9(8)
O(33)-C(34)-C(35)-O(34) 56.9(9)
C(33)-C(34)-C(35)-O(34) -65.7(9)
O(33)-C(34)-C(35)-C(36) 178.1(9)
C(33)-C(34)-C(35)-C(36) 55.6(9)
O(34)-C(35)-C(36)-C(17) -152.0(9)
C(34)-C(35)-C(36)-C(17) 86.6(10)
C(18)-C(17)-C(36)-C(35) -116.0(6)
C(118)-C(17)-C(36)-C(35) 124.8(5)
C(16)-C(17)-C(36)-C(35) 40(2)
O(11)-C(18)-C(39)-C(314) -145.3(7)
O(31)-C(18)-C(39)-C(314) -137.6(9)
C(19)-C(18)-C(39)-C(314) 90(32)
C(17)-C(18)-C(39)-C(314) 99.0(7)
O(11)-C(18)-C(39)-C(310) 35.0(7)
O(31)-C(18)-C(39)-C(310) 42.6(8)
C(19)-C(18)-C(39)-C(310) -89(32)
C(17)-C(18)-C(39)-C(310) -80.8(7)
C(314)-C(39)-C(310)-C(311) -0.3(3)
C(18)-C(39)-C(310)-C(311) 179.4(3)
C(39)-C(310)-C(311)-C(312) -0.3(3)
C(321)-O(35)-C(312)-C(313) -3.1(16)
C(321)-O(35)-C(312)-C(311) 177.5(13)
C(310)-C(311)-C(312)-C(313) 0.8(7)
C(310)-C(311)-C(312)-O(35) -179.7(4)
O(35)-C(312)-C(313)-C(314) 179.7(6)
C(311)-C(312)-C(313)-C(314) -0.8(9)
C(310)-C(39)-C(314)-C(313) 0.3(7)
C(18)-C(39)-C(314)-C(313) -179.4(5)
C(312)-C(313)-C(314)-C(39) 0.3(9)
C(28)-O(41)-C(41)-O(42) -18.8(19)
C(28)-O(41)-C(41)-C(22) 147.4(13)
C(23)-C(22)-C(41)-O(42) 86.3(10)
C(215)-C(22)-C(41)-O(42) -150.0(8)
C(21)-C(22)-C(41)-O(42) -83(10)

C(43)-C(22)-C(41)-O(42) 74.8(11)
C(23)-C(22)-C(41)-O(41) -81.1(11)
C(215)-C(22)-C(41)-O(41) 42.6(11)
C(21)-C(22)-C(41)-O(41) 109(11)
C(43)-C(22)-C(41)-O(41) -92.7(12)
C(41)-C(22)-C(43)-C(44) 69.0(7)
C(23)-C(22)-C(43)-C(44) -16(2)
C(215)-C(22)-C(43)-C(44) -61.5(7)
C(21)-C(22)-C(43)-C(44) 70.0(7)
C(22)-C(43)-C(44)-O(43) 130.6(9)
C(22)-C(43)-C(44)-C(45) -109.1(8)
O(43)-C(44)-C(45)-O(44) 55.2(9)
C(43)-C(44)-C(45)-O(44) -66.2(9)
O(43)-C(44)-C(45)-C(46) 178.0(9)
C(43)-C(44)-C(45)-C(46) 56.6(9)
O(44)-C(45)-C(46)-C(27) -152.0(9)
C(44)-C(45)-C(46)-C(27) 84.9(10)
C(218)-C(27)-C(46)-C(45) 124.8(5)
C(28)-C(27)-C(46)-C(45) -115.8(6)
C(26)-C(27)-C(46)-C(45) 37(2)
O(21)-C(28)-C(49)-C(414) -145.6(8)
O(41)-C(28)-C(49)-C(414) -137.3(10)
C(29)-C(28)-C(49)-C(414) -147(4)
C(27)-C(28)-C(49)-C(414) 96.7(8)
O(21)-C(28)-C(49)-C(410) 34.8(8)
O(41)-C(28)-C(49)-C(410) 43.1(10)
C(29)-C(28)-C(49)-C(410) 33(3)
C(27)-C(28)-C(49)-C(410) -82.8(7)
C(414)-C(49)-C(410)-C(411) -0.4(3)
C(28)-C(49)-C(410)-C(411) 179.2(3)
C(49)-C(410)-C(411)-C(412) 0.1(3)
C(421)-O(45)-C(412)-C(411) 174.2(14)
C(421)-O(45)-C(412)-C(413) -5.1(16)
C(410)-C(411)-C(412)-O(45) -179.1(4)
C(410)-C(411)-C(412)-C(413) 0.2(7)
O(45)-C(412)-C(413)-C(414) 179.0(6)
C(411)-C(412)-C(413)-C(414) -0.2(9)
C(410)-C(49)-C(414)-C(413) 0.4(7)
C(28)-C(49)-C(414)-C(413) -179.2(5)
C(412)-C(413)-C(414)-C(49) -0.1(10)

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C21 H32 O5.

D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(13)-H(13)	O(14)	0.84	2.35	2.792(6)	113.1
O(23)-H(23)	O(24)	0.84	2.38	2.797(6)	111.4
O(33)-H(33)	O(34)	0.84	2.42	2.739(12)	103.1
O(43)-H(43)	O(44)	0.84	2.28	2.738(12)	114.5



ORTEP view of the C21 H32 O5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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Lactone dibenzoate **33**

Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C35 H40 O7 COMPOUND (12)

Friday, October 23, 2009

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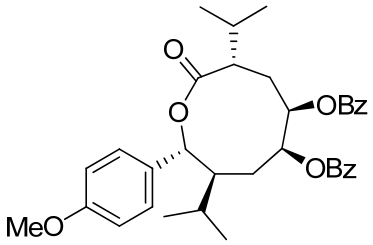


12
$C_{35}H_{40}O_7$
MW 572.69

Structure solved and refined in the laboratory of X-ray diffraction
Université de Montréal by Michel Simard.

Table 1. Crystal data and structure refinement for C35 H40 O7.

Identification code	12
Empirical formula	C35 H40 O7
Formula weight	572.67
Temperature	100(2)K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2R_1$
Unit cell dimensions	a = 12.6491(2) Å α = 90° b = 7.4042(1) Å β = 101.056(1)° c = 16.8171(3) Å γ = 90°
Volume	1545.80(4)ÅP^{3P}
Z	2
Density (calculated)	1.230 g/cm^3
Absorption coefficient	0.686 mmP^{-1P}
F(000)	612
Crystal size	0.28 x 0.20 x 0.04 mm
Theta range for data collection	2.68 to 67.77°
Index ranges	$-15 \leq h \leq 15$, $-7 \leq k \leq 8$, $-20 \leq l \leq 20$
Reflections collected	24377
Independent reflections	5122 [R_{int} = 0.031]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9800 and 0.6400
Refinement method	Full-matrix least-squares on FP^{2P}
Data / restraints / parameters	5122 / 1 / 385
Goodness-of-fit on FP^{2P}	1.069
Final R indices [I>2sigma(I)]	RR_{1R} = 0.0263, wRR_{2R} = 0.0665
R indices (all data)	RR_{1R} = 0.0271, wRR_{2R} = 0.0673
Absolute structure parameter	0.06(10)

Extinction coefficient	0.0026(2)
Largest diff. peak and hole	0.150 and -0.133 e/ÅP^{3P}

Table 2. Atomic coordinates (x $10P^{4P}$) and equivalent isotropic displacement parameters (ÅP^{2P} x $10P^{3P}$) for C35 H40 O7.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U_{eq}
O(1)	5833(1)	6624(1)	7372(1)	25(1)
O(2)	6113(1)	5077(2)	6272(1)	35(1)
O(3)	2547(1)	8121(1)	7060(1)	27(1)
O(4)	3129(1)	9397(2)	8280(1)	43(1)
O(5)	2515(1)	4416(1)	7018(1)	27(1)
O(6)	1344(1)	5232(2)	7817(1)	31(1)
O(7)	10007(1)	8167(1)	9873(1)	30(1)
C(1)	5696(1)	6303(2)	6570(1)	25(1)
C(2)	4869(1)	7603(2)	6118(1)	26(1)
C(3)	3760(1)	6944(2)	6258(1)	27(1)
C(4)	3558(1)	7123(2)	7128(1)	25(1)
C(5)	3398(1)	5340(2)	7546(1)	25(1)
C(6)	4342(1)	4027(2)	7692(1)	26(1)
C(7)	5314(1)	4659(2)	8344(1)	25(1)
C(8)	6258(1)	5171(2)	7940(1)	24(1)
C(9)	5123(1)	9592(2)	6324(1)	29(1)
C(10)	6214(1)	10098(2)	6124(1)	40(1)
C(11)	4237(1)	10827(2)	5873(1)	34(1)
C(12)	5648(1)	3281(2)	9034(1)	28(1)
C(13)	4735(1)	2936(2)	9494(1)	34(1)
C(14)	6056(1)	1499(2)	8751(1)	38(1)
C(15)	2409(1)	9101(2)	7712(1)	28(1)
C(16)	1278(1)	9707(2)	7648(1)	29(1)
C(17)	461(1)	9130(2)	7022(1)	32(1)
C(18)	-597(1)	9605(2)	7026(1)	37(1)
C(19)	-841(1)	10651(2)	7650(1)	41(1)
C(20)	-30(1)	11256(2)	8263(1)	41(1)
C(21)	1030(1)	10793(2)	8263(1)	34(1)
C(22)	1518(1)	4600(2)	7193(1)	26(1)
C(23)	669(1)	3944(2)	6516(1)	27(1)
C(24)	908(1)	2940(2)	5875(1)	31(1)
C(25)	85(1)	2344(2)	5268(1)	39(1)
C(26)	-973(1)	2754(3)	5297(1)	43(1)
C(27)	-1221(1)	3771(3)	5925(1)	41(1)
C(28)	-396(1)	4367(2)	6538(1)	33(1)
C(29)	7260(1)	5891(2)	8482(1)	24(1)
C(30)	7216(1)	7019(2)	9134(1)	27(1)
C(31)	8149(1)	7724(2)	9593(1)	28(1)
C(32)	9147(1)	7337(2)	9397(1)	26(1)
C(33)	9208(1)	6196(2)	8755(1)	27(1)
C(34)	8262(1)	5479(2)	8309(1)	27(1)
C(35)	11059(1)	7624(2)	9782(1)	33(1)

Table 3. Hydrogen coordinates (x $10P^{4P}$) and isotropic displacement parameters ($ÅP^{2P}$ x $10P^{3P}$) for C35 H40 O7.

	x	y	z	U_{eq}
H(2)	4872	7450	5527	31
H(3A)	3193	7630	5893	33
H(3B)	3677	5657	6098	33
H(4)	4158	7822	7465	30
H(5)	3180	5605	8074	30
H(6A)	4592	3838	7175	31
H(6B)	4087	2849	7860	31
H(7)	5085	5783	8594	29
H(8)	6454	4112	7629	29
H(9)	5163	9760	6919	35
H(10A)	6774	9321	6431	60
H(10B)	6376	11363	6271	60
H(10C)	6191	9935	5543	60
H(11A)	4474	12088	5939	52
H(11B)	3580	10669	6094	52
H(11C)	4089	10516	5296	52
H(12)	6257	3830	9427	34
H(13A)	4165	2236	9152	51
H(13B)	4441	4093	9634	51
H(13C)	5014	2259	9991	51
H(14A)	6302	717	9220	57
H(14B)	6657	1736	8474	57
H(14C)	5472	900	8376	57
H(17)	628	8414	6594	38
H(18)	-1156	9212	6601	45
H(19)	-1569	10955	7655	49
H(20)	-201	11991	8684	49
H(21)	1587	11215	8683	41
H(24)	1635	2663	5853	37
H(25)	246	1652	4831	47
H(26)	-1535	2333	4880	52
H(27)	-1949	4059	5938	49
H(28)	-560	5065	6973	40
H(30)	6539	7309	9266	32
H(31)	8109	8477	10043	34
H(33)	9885	5909	8621	33
H(34)	8303	4683	7873	32
H(35A)	11169	6349	9932	50
H(35B)	11598	8362	10135	50
H(35C)	11133	7789	9217	50

Table 4. Anisotropic parameters (ÅP^{2P} x 10P^{3P}) for C35 H40 O7.

The anisotropic displacement factor exponent takes the form:

$$-2\,\pi^{2P}\,[\,h^{2P}\,a^{*2P}\,U_{11R} + \ldots + 2\,h\,k\,a^{*}\,b^{*}\,U_{12R}\,]$$

	U11	U22	U33	U23	U13	U12
O(1)	26(1)	26(1)	22(1)	1(1)	1(1)	2(1)
O(2)	40(1)	36(1)	29(1)	0(1)	9(1)	10(1)
O(3)	24(1)	29(1)	26(1)	-3(1)	3(1)	3(1)
O(4)	35(1)	50(1)	41(1)	-18(1)	-3(1)	5(1)
O(5)	21(1)	30(1)	30(1)	-6(1)	3(1)	-4(1)
O(6)	29(1)	35(1)	31(1)	-4(1)	8(1)	-2(1)
O(7)	25(1)	31(1)	33(1)	-5(1)	0(1)	-3(1)
C(1)	25(1)	28(1)	24(1)	1(1)	5(1)	-3(1)
C(2)	27(1)	30(1)	21(1)	0(1)	3(1)	2(1)
C(3)	26(1)	30(1)	25(1)	-2(1)	2(1)	1(1)
C(4)	21(1)	27(1)	27(1)	-3(1)	2(1)	0(1)
C(5)	21(1)	27(1)	26(1)	-3(1)	1(1)	-3(1)
C(6)	26(1)	24(1)	28(1)	-2(1)	3(1)	-2(1)
C(7)	24(1)	24(1)	25(1)	0(1)	3(1)	0(1)
C(8)	24(1)	22(1)	24(1)	1(1)	2(1)	2(1)
C(9)	33(1)	31(1)	22(1)	1(1)	2(1)	-1(1)
C(10)	36(1)	36(1)	47(1)	6(1)	5(1)	-5(1)
C(11)	39(1)	33(1)	30(1)	2(1)	6(1)	5(1)
C(12)	29(1)	28(1)	28(1)	2(1)	4(1)	-1(1)
C(13)	40(1)	30(1)	34(1)	3(1)	11(1)	-1(1)
C(14)	43(1)	33(1)	41(1)	8(1)	13(1)	9(1)
C(15)	31(1)	24(1)	29(1)	-3(1)	4(1)	0(1)
C(16)	32(1)	24(1)	31(1)	2(1)	7(1)	4(1)
C(17)	31(1)	28(1)	35(1)	-1(1)	5(1)	3(1)
C(18)	30(1)	34(1)	47(1)	2(1)	5(1)	3(1)
C(19)	35(1)	39(1)	52(1)	8(1)	15(1)	12(1)
C(20)	51(1)	37(1)	39(1)	4(1)	19(1)	17(1)
C(21)	42(1)	29(1)	30(1)	0(1)	7(1)	7(1)
C(22)	23(1)	23(1)	31(1)	3(1)	5(1)	0(1)
C(23)	24(1)	26(1)	30(1)	3(1)	2(1)	-3(1)
C(24)	29(1)	27(1)	35(1)	0(1)	1(1)	1(1)
C(25)	41(1)	35(1)	37(1)	-3(1)	-5(1)	0(1)
C(26)	34(1)	46(1)	43(1)	1(1)	-10(1)	-8(1)
C(27)	24(1)	49(1)	47(1)	10(1)	-1(1)	-3(1)
C(28)	28(1)	36(1)	36(1)	5(1)	7(1)	0(1)
C(29)	24(1)	23(1)	24(1)	2(1)	1(1)	1(1)
C(30)	24(1)	26(1)	31(1)	-2(1)	6(1)	1(1)
C(31)	30(1)	25(1)	29(1)	-3(1)	5(1)	0(1)
C(32)	26(1)	23(1)	26(1)	3(1)	0(1)	-2(1)
C(33)	23(1)	30(1)	29(1)	1(1)	5(1)	1(1)
C(34)	28(1)	28(1)	23(1)	-1(1)	5(1)	2(1)
C(35)	24(1)	33(1)	40(1)	1(1)	0(1)	-1(1)

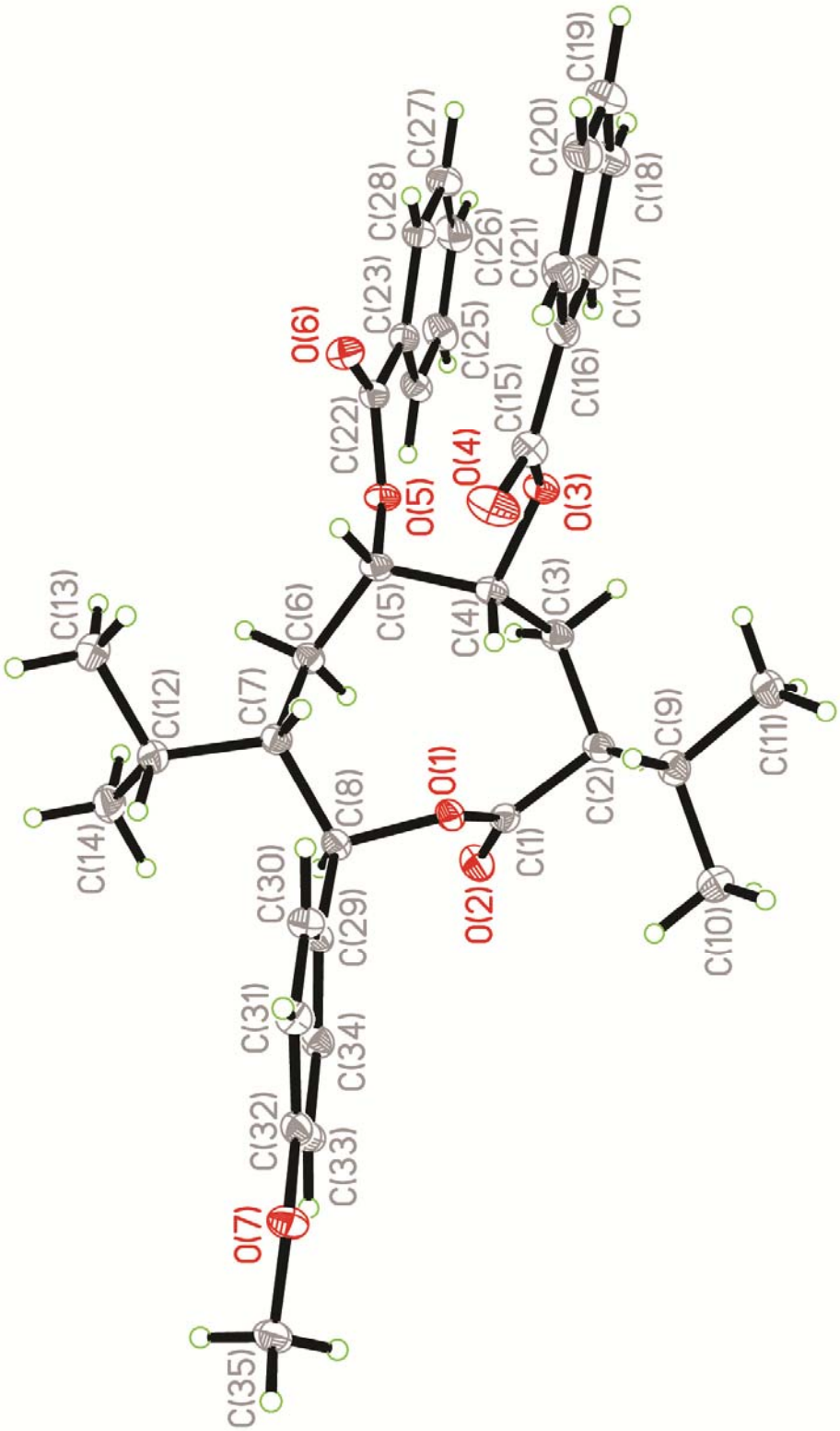
Table 5. Bond lengths [Å] and angles [°] for C35 H40 O7

		O(1)-C(1)-C(2)	109.55(11)
O(1)-C(1)	1.3472(14)	C(1)-C(2)-C(9)	113.73(10)
O(1)-C(8)	1.4707(16)	C(1)-C(2)-C(3)	106.39(11)
O(2)-C(1)	1.2063(17)		
O(3)-C(15)	1.3529(16)		
O(3)-C(4)	1.4627(15)	C(9)-C(2)-C(3)	115.19(11)
O(4)-C(15)	1.2069(16)	C(4)-C(3)-C(2)	116.04(10)
O(5)-C(22)	1.3562(14)	O(3)-C(4)-C(5)	106.33(9)
O(5)-C(5)	1.4570(14)	O(3)-C(4)-C(3)	105.79(9)
O(6)-C(22)	1.2070(16)	C(5)-C(4)-C(3)	115.06(12)
O(7)-C(32)	1.3656(15)	O(5)-C(5)-C(6)	106.55(11)
O(7)-C(35)	1.4261(16)	O(5)-C(5)-C(4)	106.23(9)
C(1)-C(2)	1.5146(18)	C(6)-C(5)-C(4)	117.21(10)
C(2)-C(9)	1.533(2)	C(5)-C(6)-C(7)	114.31(11)
C(2)-C(3)	1.5460(17)	C(8)-C(7)-C(12)	111.92(10)
C(3)-C(4)	1.5375(16)	C(8)-C(7)-C(6)	109.86(9)
C(4)-C(5)	1.527(2)	C(12)-C(7)-C(6)	113.43(11)
C(5)-C(6)	1.5229(18)	O(1)-C(8)-C(29)	107.12(11)
C(6)-C(7)	1.5540(16)	O(1)-C(8)-C(7)	104.48(9)
C(7)-C(8)	1.5315(16)	C(29)-C(8)-C(7)	117.09(10)
C(7)-C(12)	1.5418(18)	C(10)-C(9)-C(11)	110.54(12)
C(8)-C(29)	1.5090(16)	C(10)-C(9)-C(2)	110.16(12)
C(9)-C(10)	1.5281(19)	C(11)-C(9)-C(2)	111.13(11)
C(9)-C(11)	1.5301(19)	C(14)-C(12)-C(13)	110.30(13)
C(12)-C(14)	1.526(2)	C(14)-C(12)-C(7)	113.42(11)
C(12)-C(13)	1.5300(18)	C(13)-C(12)-C(7)	111.49(11)
C(15)-C(16)	1.4831(18)	O(4)-C(15)-O(3)	122.95(12)
C(16)-C(21)	1.3929(19)	O(4)-C(15)-C(16)	124.97(12)
C(16)-C(17)	1.3941(19)	O(3)-C(15)-C(16)	112.06(10)
C(17)-C(18)	1.3847(19)	C(21)-C(16)-C(17)	119.83(12)
C(18)-C(19)	1.385(2)	C(21)-C(16)-C(15)	118.21(12)
C(19)-C(20)	1.382(2)	C(17)-C(16)-C(15)	121.84(12)
C(20)-C(21)	1.384(2)	C(18)-C(17)-C(16)	119.69(13)
C(22)-C(23)	1.4881(17)	C(17)-C(18)-C(19)	120.16(14)
C(23)-C(24)	1.390(2)	C(20)-C(19)-C(18)	120.30(13)
C(23)-C(28)	1.3907(17)	C(19)-C(20)-C(21)	119.99(14)
C(24)-C(25)	1.3826(19)	C(20)-C(21)-C(16)	119.99(14)
C(25)-C(26)	1.381(2)	O(6)-C(22)-O(5)	124.00(11)
C(26)-C(27)	1.382(2)	O(6)-C(22)-C(23)	124.53(11)
C(27)-C(28)	1.3910(19)	O(5)-C(22)-C(23)	111.46(10)
C(29)-C(34)	1.3875(17)	C(24)-C(23)-C(28)	119.81(12)
C(29)-C(30)	1.3881(18)	C(24)-C(23)-C(22)	122.41(11)
C(30)-C(31)	1.3822(18)	C(28)-C(23)-C(22)	117.78(12)
C(31)-C(32)	1.3944(18)	C(25)-C(24)-C(23)	119.89(12)
C(32)-C(33)	1.3853(19)	C(26)-C(25)-C(24)	120.08(14)
C(33)-C(34)	1.3902(18)	C(25)-C(26)-C(27)	120.67(13)
		C(26)-C(27)-C(28)	119.44(13)
C(1)-O(1)-C(8)	118.80(11)	C(23)-C(28)-C(27)	120.10(14)
C(15)-O(3)-C(4)	117.05(9)	C(34)-C(29)-C(30)	118.32(11)
C(22)-O(5)-C(5)	117.23(9)	C(34)-C(29)-C(8)	119.39(11)
C(32)-O(7)-C(35)	117.73(10)	C(30)-C(29)-C(8)	122.24(11)
O(2)-C(1)-O(1)	124.50(12)	C(31)-C(30)-C(29)	120.59(11)
O(2)-C(1)-C(2)	125.74(11)	C(30)-C(31)-C(32)	120.39(12)

O(7)-C(32)-C(33)	125.01(11)	C(29)-C(34)-C(33)	121.98(12)
O(7)-C(32)-C(31)	115.17(11)		
C(33)-C(32)-C(31)	119.82(11)		
C(32)-C(33)-C(34)	118.87(11)		

Table 6. Torsion angles [°] for C35 H40 O7.

C(8)-O(1)-C(1)-O(2)	-17.70(18)
C(8)-O(1)-C(1)-C(2)	157.25(10)
O(2)-C(1)-C(2)-C(9)	-131.52(14)
O(1)-C(1)-C(2)-C(9)	53.61(13)
O(2)-C(1)-C(2)-C(3)	100.61(15)
O(1)-C(1)-C(2)-C(3)	-74.26(13)
C(1)-C(2)-C(3)-C(4)	68.04(15)
C(9)-C(2)-C(3)-C(4)	-58.96(15)
C(15)-O(3)-C(4)-C(5)	84.22(13)
C(15)-O(3)-C(4)-C(3)	-152.99(11)
C(2)-C(3)-C(4)-O(3)	126.57(12)
C(2)-C(3)-C(4)-C(5)	-116.37(13)
C(22)-O(5)-C(5)-C(6)	137.84(11)
C(22)-O(5)-C(5)-C(4)	-96.47(12)
O(3)-C(4)-C(5)-O(5)	61.08(11)
C(3)-C(4)-C(5)-O(5)	-55.67(12)
O(3)-C(4)-C(5)-C(6)	179.98(10)
C(3)-C(4)-C(5)-C(6)	63.23(14)
O(5)-C(5)-C(6)-C(7)	-171.5(1)
C(4)-C(5)-C(6)-C(7)	69.77(14)
C(5)-C(6)-C(7)-C(8)	-109.40(13)
C(5)-C(6)-C(7)-C(12)	124.52(12)
C(1)-O(1)-C(8)-C(29)	123.07(11)
C(1)-O(1)-C(8)-C(7)	-112.06(11)
C(12)-C(7)-C(8)-O(1)	-173.74(10)
C(6)-C(7)-C(8)-O(1)	59.32(13)
C(12)-C(7)-C(8)-C(29)	-55.48(16)
C(6)-C(7)-C(8)-C(29)	177.58(12)
C(1)-C(2)-C(9)-C(10)	59.33(13)
C(3)-C(2)-C(9)-C(10)	-177.49(11)
C(1)-C(2)-C(9)-C(11)	-177.81(10)
C(3)-C(2)-C(9)-C(11)	-54.62(13)
C(8)-C(7)-C(12)-C(14)	-61.03(15)
C(6)-C(7)-C(12)-C(14)	63.95(14)
C(8)-C(7)-C(12)-C(13)	173.74(11)
C(6)-C(7)-C(12)-C(13)	-61.27(15)
C(4)-O(3)-C(15)-O(4)	11.4(2)
C(4)-O(3)-C(15)-C(16)	-167.08(11)
O(4)-C(15)-C(16)-C(21)	4.1(2)
O(3)-C(15)-C(16)-C(21)	-177.43(13)
O(4)-C(15)-C(16)-C(17)	-171.90(15)
O(3)-C(15)-C(16)-C(17)	6.6(2)
C(21)-C(16)-C(17)-C(18)	-1.6(2)
C(15)-C(16)-C(17)-C(18)	174.38(14)
C(16)-C(17)-C(18)-C(19)	0.1(2)
C(17)-C(18)-C(19)-C(20)	1.2(3)
C(18)-C(19)-C(20)-C(21)	-1.1(3)
C(19)-C(20)-C(21)-C(16)	-0.4(2)
C(17)-C(16)-C(21)-C(20)	1.7(2)
C(15)-C(16)-C(21)-C(20)	-174.37(14)
C(5)-O(5)-C(22)-O(6)	-11.88(19)
C(5)-O(5)-C(22)-C(23)	167.45(11)
O(6)-C(22)-C(23)-C(24)	-168.30(14)
O(5)-C(22)-C(23)-C(24)	12.37(19)
O(6)-C(22)-C(23)-C(28)	11.7(2)
O(5)-C(22)-C(23)-C(28)	-167.61(12)
C(28)-C(23)-C(24)-C(25)	-0.9(2)
C(22)-C(23)-C(24)-C(25)	179.08(14)
C(23)-C(24)-C(25)-C(26)	0.3(2)
C(24)-C(25)-C(26)-C(27)	0.5(3)
C(25)-C(26)-C(27)-C(28)	-0.7(3)
C(24)-C(23)-C(28)-C(27)	0.7(2)
C(22)-C(23)-C(28)-C(27)	-179.30(13)
C(26)-C(27)-C(28)-C(23)	0.1(2)
O(1)-C(8)-C(29)-C(34)	-97.97(14)
C(7)-C(8)-C(29)-C(34)	145.19(13)
O(1)-C(8)-C(29)-C(30)	79.38(14)
C(7)-C(8)-C(29)-C(30)	-37.46(19)
C(34)-C(29)-C(30)-C(31)	0.6(2)
C(8)-C(29)-C(30)-C(31)	-176.74(13)
C(29)-C(30)-C(31)-C(32)	1.1(2)
C(35)-O(7)-C(32)-C(33)	-9.68(19)
C(35)-O(7)-C(32)-C(31)	170.99(12)
C(30)-C(31)-C(32)-O(7)	177.46(13)
C(30)-C(31)-C(32)-C(33)	-1.9(2)
O(7)-C(32)-C(33)-C(34)	-178.38(13)
C(31)-C(32)-C(33)-C(34)	0.9(2)
C(30)-C(29)-C(34)-C(33)	-1.6(2)
C(8)-C(29)-C(34)-C(33)	175.81(13)
C(32)-C(33)-C(34)-C(29)	0.9(2)



ORTEP view of the C35 H40 O7 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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Lactone **39**

Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C26 H39 N O5 COMPOUND (bent38)

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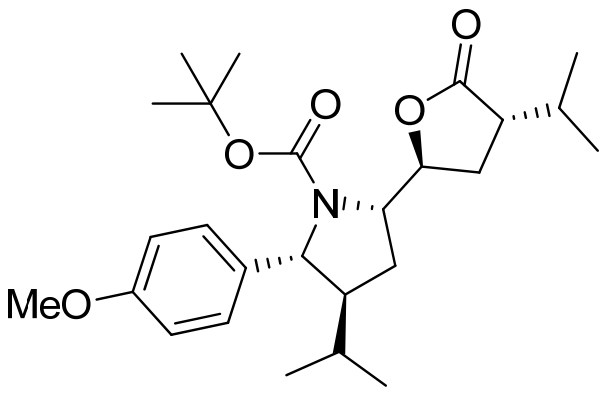


Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Benoît Deschênes Simard.

Table 1. Crystal data and structure refinement for C26 H39 N O5.

Identification code	bent38
Empirical formula	C26 H39 N O5
Formula weight	445.58
Temperature	175K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P212121
Unit cell dimensions	a = 10.2176(1) Å α = 90° b = 10.2887(1) Å β = 90° c = 24.2502(3) Å γ = 90°
Volume	2549.32(5)Å^3
Z	4
Density (calculated)	1.161 g/cm^3
Absorption coefficient	0.636 mm^{-1}
F(000)	968
Crystal size	0.22 x 0.20 x 0.18 mm
Theta range for data collection	3.65 to 72.43°
Index ranges	$-12 \leq h \leq 12$, $-12 \leq k \leq 12$, $-29 \leq l \leq 28$
Reflections collected	33232
Independent reflections	4996 [R_{int} = 0.035]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8918 and 0.8079
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4996 / 54 / 349
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R_1 = 0.0376, wR_2 = 0.0945

R indices (all data)	$R_1 = 0.0381$, $wR_2 = 0.0953$
Absolute structure parameter	0.02(15)
Extinction coefficient	0.0220(6)
Largest diff. peak and hole	0.182 and -0.221 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for C26 H39 N O5.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ.	x	y	z	U_{eq}
O(4)	1	7813(1)	4192(1)	7683(1)	39(1)
O(5)	1	7281(1)	4370(1)	6772(1)	36(1)
N(1)	1	9056(1)	5364(1)	7086(1)	33(1)
C(1)	1	9373(1)	5782(1)	6517(1)	32(1)
C(2)	1	10731(1)	6419(1)	6595(1)	33(1)
C(3)	1	11321(1)	5652(1)	7080(1)	36(1)
C(4)	1	10153(1)	5490(1)	7469(1)	34(1)
C(5)	1	10032(1)	6655(1)	7864(1)	38(1)
C(15)	1	11561(1)	6518(1)	6068(1)	40(1)
C(16)	1	11870(2)	5208(2)	5805(1)	57(1)
C(17)	1	12809(2)	7278(2)	6175(1)	52(1)
C(21)	1	8014(1)	4609(1)	7220(1)	32(1)
C(22)	1	5931(1)	3882(1)	6820(1)	37(1)
C(23)	1	5477(2)	3900(2)	6226(1)	51(1)
C(24)	1	5915(1)	2517(2)	7050(1)	52(1)
C(25)	1	5142(2)	4815(2)	7170(1)	60(1)
O(1A)	0.75	7189(2)	6731(3)	8635(1)	60(1)
O(2A)	0.75	8690(2)	7015(3)	7983(1)	39(1)
O(3A)	0.75	5542(2)	8966(2)	5488(1)	49(1)
C(6A)	0.75	10580(2)	6283(2)	8449(1)	38(1)
C(7A)	0.75	9368(2)	5728(2)	8732(1)	40(1)
C(8A)	0.75	8274(2)	6512(4)	8467(1)	43(1)
C(9A)	0.75	8349(1)	6650(2)	6260(1)	32(1)
C(10A)	0.75	7997(2)	6485(2)	5708(1)	36(1)
C(11A)	0.75	7063(2)	7275(2)	5464(1)	39(1)
C(12A)	0.75	6453(2)	8243(2)	5768(1)	38(1)
C(13A)	0.75	6785(2)	8416(3)	6320(1)	40(1)
C(14A)	0.75	7732(2)	7618(2)	6558(1)	37(1)
C(18A)	0.75	9330(2)	5700(2)	9368(1)	50(1)
C(19A)	0.75	9336(4)	7038(3)	9620(1)	86(1)
C(20A)	0.75	10418(2)	4853(3)	9594(1)	60(1)
C(26A)	0.75	4955(3)	10020(2)	5770(2)	59(1)
O(1B)	0.25	7204(6)	6498(13)	8603(4)	60(1)
O(2B)	0.25	8633(6)	6912(9)	7937(3)	39(1)
O(3B)	0.25	5740(6)	9173(6)	5491(3)	49(1)
C(6B)	0.25	10647(5)	6594(9)	8389(3)	38(1)
C(7B)	0.25	9550(5)	6008(8)	8739(2)	40(1)
C(8B)	0.25	8322(5)	6483(12)	8448(3)	43(1)
C(9B)	0.25	8387(3)	6721(4)	6280(2)	32(1)
C(10B)	0.25	8179(5)	6679(5)	5711(2)	36(1)
C(11B)	0.25	7289(6)	7509(6)	5461(2)	39(1)
C(12B)	0.25	6596(5)	8396(6)	5776(2)	38(1)
C(13B)	0.25	6787(7)	8449(7)	6345(2)	40(1)
C(14B)	0.25	7686(7)	7608(7)	6589(3)	37(1)

C(18B)	0.25	9609(5)	6362(7)	9358(2)	50(1)
C(19B)	0.25	8487(7)	5755(8)	9672(3)	86(1)
C(20B)	0.25	10944(6)	6000(8)	9581(2)	60(1)
C(26B)	0.25	5208(11)	10248(9)	5780(6)	59(1)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for C26 H39 N O5.

	Occ.	x	y	z	U_{eq}
H(1)	1	9478	4991	6282	38
H(2)	1	10577	7326	6729	39
H(3A)	1	11660	4799	6957	43
H(3B)	1	12037	6145	7259	43
H(4)	1	10252	4670	7687	40
H(5)	1	10520	7418	7713	45
H(15)	1	11038	7025	5794	48
H(16A)	1	12352	4667	6068	85
H(16B)	1	12404	5343	5474	85
H(16C)	1	11052	4773	5703	85
H(17A)	1	13271	7419	5826	78
H(17B)	1	13372	6786	6427	78
H(17C)	1	12591	8119	6341	78
H(23A)	1	5511	4792	6085	76
H(23B)	1	4576	3576	6205	76
H(23C)	1	6050	3344	6004	76
H(24A)	1	6173	2536	7439	78
H(24B)	1	6530	1974	6842	78
H(24C)	1	5031	2156	7017	78
H(25A)	1	5211	5693	7016	91
H(25B)	1	5481	4812	7548	91
H(25C)	1	4222	4544	7172	91
H(6A)	0.75	11285	5626	8422	45
H(6B)	0.75	10916	7057	8647	45
H(7A)	0.75	9269	4810	8603	48
H(10A)	0.75	8405	5821	5496	43
H(11A)	0.75	6840	7153	5087	47
H(13A)	0.75	6369	9072	6533	48
H(14A)	0.75	7959	7743	6934	44
H(18A)	0.75	8485	5281	9475	60
H(19A)	0.75	8638	7563	9454	129
H(19B)	0.75	10183	7453	9552	129
H(19C)	0.75	9188	6969	10018	129
H(20A)	0.75	10295	4735	9991	89
H(20B)	0.75	11264	5273	9526	89
H(20C)	0.75	10399	4005	9410	89
H(26A)	0.75	4455	9692	6085	88
H(26B)	0.75	4366	10484	5519	88
H(26C)	0.75	5637	10615	5901	88
H(6C)	0.25	10899	7469	8522	45
H(6D)	0.25	11429	6026	8382	45
H(7B)	0.25	9591	5040	8704	48
H(10B)	0.25	8654	6074	5492	43
H(11B)	0.25	7155	7469	5074	47
H(13B)	0.25	6310	9052	6563	48
H(14B)	0.25	7820	7646	6976	44

H(18B)	0.25	9518	7327	9389	60
H(19D)	0.25	8626	4815	9701	129
H(19E)	0.25	7665	5923	9477	129
H(19F)	0.25	8443	6133	10043	129
H(20D)	0.25	11605	6584	9425	89
H(20E)	0.25	11149	5102	9478	89
H(20F)	0.25	10942	6080	9983	89
H(26D)	0.25	4754	9938	6111	88
H(26E)	0.25	4588	10709	5542	88
H(26F)	0.25	5915	10839	5888	88

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C26 H39 N O5.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(4)	41(1)	42(1)	35(1)	8(1)	-4(1)	-7(1)
O(5)	34(1)	41(1)	35(1)	1(1)	-5(1)	-7(1)
N(1)	33(1)	36(1)	29(1)	4(1)	-5(1)	-4(1)
C(1)	34(1)	33(1)	29(1)	1(1)	-1(1)	1(1)
C(2)	30(1)	36(1)	33(1)	1(1)	-1(1)	0(1)
C(3)	32(1)	42(1)	35(1)	1(1)	-4(1)	0(1)
C(4)	33(1)	36(1)	32(1)	3(1)	-5(1)	-3(1)
C(5)	37(1)	40(1)	36(1)	0(1)	-1(1)	-8(1)
C(15)	34(1)	52(1)	33(1)	3(1)	3(1)	4(1)
C(16)	52(1)	69(1)	51(1)	-14(1)	10(1)	8(1)
C(17)	38(1)	69(1)	48(1)	2(1)	11(1)	-6(1)
C(21)	33(1)	30(1)	33(1)	1(1)	-4(1)	0(1)
C(22)	28(1)	39(1)	42(1)	4(1)	-6(1)	-1(1)
C(23)	43(1)	62(1)	47(1)	5(1)	-15(1)	-12(1)
C(24)	43(1)	45(1)	68(1)	13(1)	-16(1)	-13(1)
C(25)	45(1)	76(1)	61(1)	-5(1)	-1(1)	17(1)
O(1A)	42(1)	77(2)	63(1)	2(1)	7(1)	16(1)
O(2A)	42(1)	39(1)	37(1)	-1(1)	-5(1)	5(1)
O(3A)	41(1)	53(1)	54(1)	10(1)	-10(1)	7(1)
C(6A)	36(1)	43(1)	34(1)	-2(1)	-6(1)	-4(1)
C(7A)	38(1)	50(1)	33(1)	2(1)	0(1)	5(1)
C(8A)	40(1)	49(1)	40(1)	1(1)	1(1)	6(1)
C(9A)	30(1)	36(1)	30(1)	3(1)	-2(1)	-3(1)
C(10A)	37(1)	39(1)	32(1)	-1(1)	-3(1)	-2(1)
C(11A)	39(1)	47(1)	33(1)	4(1)	-8(1)	-5(1)
C(12A)	31(1)	40(1)	43(1)	9(1)	-5(1)	-3(1)
C(13A)	38(1)	41(1)	41(1)	2(1)	2(1)	4(1)
C(14A)	39(1)	41(1)	30(1)	2(1)	-1(1)	1(1)
C(18A)	59(1)	58(1)	33(1)	8(1)	6(1)	13(1)
C(19A)	146(3)	72(2)	41(1)	-2(1)	8(2)	28(2)
C(20A)	64(1)	79(1)	37(1)	9(1)	-5(1)	16(1)
C(26A)	49(2)	46(1)	80(1)	7(1)	-16(1)	10(1)
O(1B)	42(1)	77(2)	63(1)	2(1)	7(1)	16(1)
O(2B)	42(1)	39(1)	37(1)	-1(1)	-5(1)	5(1)
O(3B)	41(1)	53(1)	54(1)	10(1)	-10(1)	7(1)
C(6B)	36(1)	43(1)	34(1)	-2(1)	-6(1)	-4(1)
C(7B)	38(1)	50(1)	33(1)	2(1)	0(1)	5(1)
C(8B)	40(1)	49(1)	40(1)	1(1)	1(1)	6(1)
C(9B)	30(1)	36(1)	30(1)	3(1)	-2(1)	-3(1)
C(10B)	37(1)	39(1)	32(1)	-1(1)	-3(1)	-2(1)
C(11B)	39(1)	47(1)	33(1)	4(1)	-8(1)	-5(1)
C(12B)	31(1)	40(1)	43(1)	9(1)	-5(1)	-3(1)
C(13B)	38(1)	41(1)	41(1)	2(1)	2(1)	4(1)
C(14B)	39(1)	41(1)	30(1)	2(1)	-1(1)	1(1)

C(18B)	59(1)	58(1)	33(1)	8(1)	6(1)	13(1)
C(19B)	146(3)	72(2)	41(1)	-2(1)	8(2)	28(2)
C(20B)	64(1)	79(1)	37(1)	9(1)	-5(1)	16(1)
C(26B)	49(2)	46(1)	80(1)	7(1)	-16(1)	10(1)

Table 5. Bond lengths [Å] and angles [°] for C26 H39 N O5

O(4)-C(21)	1.2191(15)
O(5)-C(21)	1.3420(14)
O(5)-C(22)	1.4726(15)
N(1)-C(21)	1.3576(16)
N(1)-C(4)	1.4628(15)
N(1)-C(1)	1.4794(14)
C(1)-C(9a)	1.511(2)
C(1)-C(9b)	1.511(4)
C(1)-C(2)	1.5457(16)
C(2)-C(15)	1.5376(17)
C(2)-C(3)	1.5378(17)
C(3)-C(4)	1.5314(17)
C(4)-C(5)	1.5384(18)
C(5)-C(6b)	1.421(7)
C(5)-O(2a)	1.449(3)
C(5)-O(2b)	1.465(7)
C(5)-C(6a)	1.573(2)
C(15)-C(17)	1.519(2)
C(15)-C(16)	1.524(2)
C(22)-C(24)	1.5106(19)
C(22)-C(25)	1.514(2)
C(22)-C(23)	1.5146(19)
O(1a)-C(8a)	1.203(2)
O(2a)-C(8a)	1.352(2)
O(3a)-C(12a)	1.3712(19)
O(3a)-C(26a)	1.416(2)
C(6a)-C(7a)	1.527(2)
C(7a)-C(8a)	1.521(2)
C(7a)-C(18a)	1.542(2)
C(9a)-C(14a)	1.382(2)
C(9a)-C(10a)	1.398(2)
C(10a)-C(11a)	1.386(2)
C(11a)-C(12a)	1.386(2)
C(12a)-C(13a)	1.393(2)
C(13a)-C(14a)	1.394(2)
C(18a)-C(19a)	1.507(3)
C(18a)-C(20a)	1.515(3)
O(1b)-C(8b)	1.202(4)
O(2b)-C(8b)	1.353(4)
O(3b)-C(12b)	1.372(4)
O(3b)-C(26b)	1.418(5)
C(6b)-C(7b)	1.529(5)
C(7b)-C(8b)	1.520(4)
C(7b)-C(18b)	1.547(4)
C(9b)-C(14b)	1.381(4)
C(9b)-C(10b)	1.396(4)
C(10b)-C(11b)	1.387(4)
C(11b)-C(12b)	1.385(4)
C(12b)-C(13b)	1.393(4)
C(13b)-C(14b)	1.394(4)
C(18b)-C(19b)	1.512(5)
C(18b)-C(20b)	1.513(5)
C(21)-O(5)-C(22)	121.40(10)
C(21)-N(1)-C(4)	119.91(10)
C(21)-N(1)-C(1)	124.19(9)
C(4)-N(1)-C(1)	113.52(9)
N(1)-C(1)-C(9A)	113.83(10)
N(1)-C(1)-C(9B)	113.3(2)
C(9A)-C(1)-C(9B)	3.6(2)
N(1)-C(1)-C(2)	101.88(9)
C(9A)-C(1)-C(2)	114.95(8)
C(9B)-C(1)-C(2)	111.99(10)
C(15)-C(2)-C(3)	116.95(10)
C(15)-C(2)-C(1)	114.90(10)
C(3)-C(2)-C(1)	103.19(9)
C(4)-C(3)-C(2)	102.80(9)
N(1)-C(4)-C(3)	102.37(9)
N(1)-C(4)-C(5)	113.81(10)
C(3)-C(4)-C(5)	111.19(10)
C(6B)-C(5)-O(2A)	104.6(3)
C(6B)-C(5)-O(2B)	109.3(4)
O(2A)-C(5)-O(2B)	6.4(5)
C(6B)-C(5)-C(4)	119.2(4)
O(2A)-C(5)-C(4)	113.48(14)
O(2B)-C(5)-C(4)	107.1(4)
C(6B)-C(5)-C(6A)	12.5(4)
O(2A)-C(5)-C(6A)	102.72(13)
O(2B)-C(5)-C(6A)	106.4(2)
C(4)-C(5)-C(6A)	110.10(13)
C(17)-C(15)-C(16)	110.65(12)
C(17)-C(15)-C(2)	110.84(11)
C(16)-C(15)-C(2)	113.82(12)
O(4)-C(21)-O(5)	125.91(11)
O(4)-C(21)-N(1)	123.69(11)
O(5)-C(21)-N(1)	110.37(10)
O(5)-C(22)-C(24)	110.88(10)
O(5)-C(22)-C(25)	109.11(11)
C(24)-C(22)-C(25)	112.18(13)
O(5)-C(22)-C(23)	101.96(10)
C(24)-C(22)-C(23)	111.02(12)
C(25)-C(22)-C(23)	111.22(12)
C(8A)-O(2A)-C(5)	111.84(16)
C(12A)-O(3A)-C(26A)	117.7(2)
C(7A)-C(6A)-C(5)	101.95(14)
C(8A)-C(7A)-C(6A)	101.99(15)
C(8A)-C(7A)-C(18A)	114.48(17)
C(6A)-C(7A)-C(18A)	118.45(17)
O(1A)-C(8A)-O(2A)	120.8(2)
O(1A)-C(8A)-C(7A)	129.3(2)

O(2A)-C(8A)-C(7A)	109.85(16)
C(14A)-C(9A)-C(10A)	118.11(16)
C(14A)-C(9A)-C(1)	121.79(17)
C(10A)-C(9A)-C(1)	120.09(16)
C(11A)-C(10A)-C(9A)	120.91(17)
C(12A)-C(11A)-C(10A)	120.34(17)
O(3A)-C(12A)-C(11A)	115.62(17)
O(3A)-C(12A)-C(13A)	124.84(18)
C(11A)-C(12A)-C(13A)	119.54(16)
C(12A)-C(13A)-C(14A)	119.41(18)
C(9A)-C(14A)-C(13A)	121.68(18)
C(19A)-C(18A)-C(20A)	112.0(2)
C(19A)-C(18A)-C(7A)	112.85(18)
C(20A)-C(18A)-C(7A)	110.75(16)
C(8B)-O(2B)-C(5)	106.3(4)
C(12B)-O(3B)-C(26B)	116.6(6)
C(5)-C(6B)-C(7B)	101.0(4)
C(8B)-C(7B)-C(6B)	102.7(4)
C(8B)-C(7B)-C(18B)	114.0(5)
C(6B)-C(7B)-C(18B)	114.7(5)
O(1B)-C(8B)-O(2B)	120.3(5)
O(1B)-C(8B)-C(7B)	130.1(5)
O(2B)-C(8B)-C(7B)	109.6(4)
C(14B)-C(9B)-C(10B)	118.6(4)
C(14B)-C(9B)-C(1)	124.1(4)
C(10B)-C(9B)-C(1)	117.3(4)
C(11B)-C(10B)-C(9B)	120.8(4)
C(12B)-C(11B)-C(10B)	120.1(4)
O(3B)-C(12B)-C(11B)	115.6(4)
O(3B)-C(12B)-C(13B)	124.4(4)
C(11B)-C(12B)-C(13B)	120.0(4)
C(12B)-C(13B)-C(14B)	119.2(4)
C(9B)-C(14B)-C(13B)	121.4(4)
C(19B)-C(18B)-C(20B)	113.7(5)
C(19B)-C(18B)-C(7B)	111.3(4)
C(20B)-C(18B)-C(7B)	108.9(4)

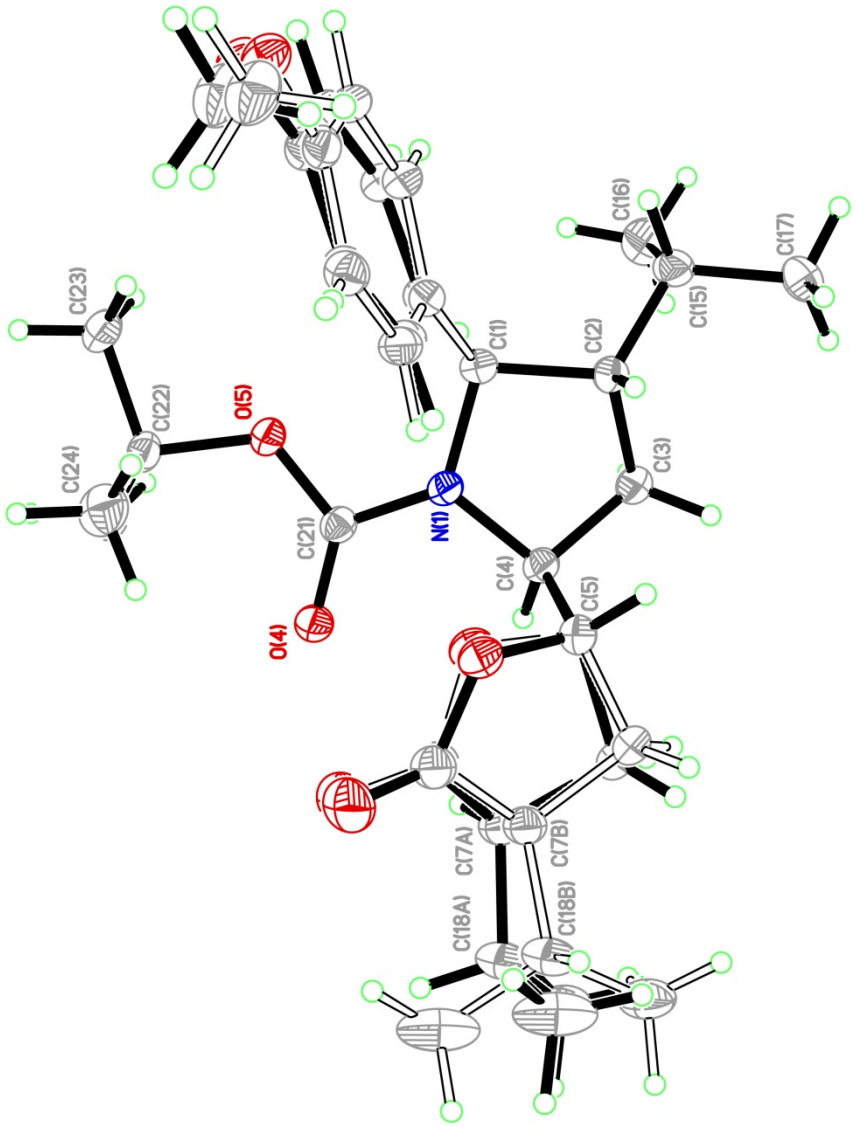
Table 6. Torsion angles [°] for C26 H39 N O5.

C(21)-N(1)-C(1)-C(9A) 63.88(15)
C(4)-N(1)-C(1)-C(9A) -133.73(11)
C(21)-N(1)-C(1)-C(9B) 67.78(19)
C(4)-N(1)-C(1)-C(9B) -129.84(17)
C(21)-N(1)-C(1)-C(2) -171.77(11)
C(4)-N(1)-C(1)-C(2) -9.38(12)
N(1)-C(1)-C(2)-C(15) 158.90(10)
C(9A)-C(1)-C(2)-C(15) -77.50(15)
C(9B)-C(1)-C(2)-C(15) -79.8(3)
N(1)-C(1)-C(2)-C(3) 30.44(11)
C(9A)-C(1)-C(2)-C(3) 154.03(12)
C(9B)-C(1)-C(2)-C(3) 151.8(3)
C(15)-C(2)-C(3)-C(4) -167.80(11)
C(1)-C(2)-C(3)-C(4) -40.62(11)
C(21)-N(1)-C(4)-C(3) 147.61(11)
C(1)-N(1)-C(4)-C(3) -15.61(13)
C(21)-N(1)-C(4)-C(5) -92.31(13)
C(1)-N(1)-C(4)-C(5) 104.48(12)
C(2)-C(3)-C(4)-N(1) 34.12(12)
C(2)-C(3)-C(4)-C(5) -87.77(11)
N(1)-C(4)-C(5)-C(6B) 152.5(3)
C(3)-C(4)-C(5)-C(6B) -92.6(3)
N(1)-C(4)-C(5)-O(2A) 28.60(16)
C(3)-C(4)-C(5)-O(2A) 143.57(13)
N(1)-C(4)-C(5)-O(2B) 27.8(3)
C(3)-C(4)-C(5)-O(2B) 142.7(3)
N(1)-C(4)-C(5)-C(6A) 143.09(12)
C(3)-C(4)-C(5)-C(6A) -101.94(13)
C(3)-C(2)-C(15)-C(17) -64.63(16)
C(1)-C(2)-C(15)-C(17) 174.15(11)
C(3)-C(2)-C(15)-C(16) 60.85(16)
C(1)-C(2)-C(15)-C(16) -60.36(15)
C(22)-O(5)-C(21)-O(4) 18.28(18)
C(22)-O(5)-C(21)-N(1) -163.50(10)
C(4)-N(1)-C(21)-O(4) 13.15(18)
C(1)-N(1)-C(21)-O(4) 174.48(11)
C(4)-N(1)-C(21)-O(5) -165.11(10)
C(1)-N(1)-C(21)-O(5) -3.78(16)
C(21)-O(5)-C(22)-C(24) -67.36(15)
C(21)-O(5)-C(22)-C(25) 56.69(15)
C(21)-O(5)-C(22)-C(23) 174.39(11)
C(6B)-C(5)-O(2A)-C(8A) -33.5(5)
O(2B)-C(5)-O(2A)-C(8A) 105(3)
C(4)-C(5)-O(2A)-C(8A) 98.1(3)
C(6A)-C(5)-O(2A)-C(8A) -20.8(3)
C(6B)-C(5)-C(6A)-C(7A) 132.3(16)
O(2A)-C(5)-C(6A)-C(7A) 32.3(2)
O(2B)-C(5)-C(6A)-C(7A) 26.9(4)
C(4)-C(5)-C(6A)-C(7A) -88.89(16)
C(5)-C(6A)-C(7A)-C(8A) -31.6(2)

C(5)-C(6A)-C(7A)-C(18A) -158.23(17)
C(5)-O(2A)-C(8A)-O(1A) 178.7(3)
C(5)-O(2A)-C(8A)-C(7A) 0.2(4)
C(6A)-C(7A)-C(8A)-O(1A) -157.3(4)
C(18A)-C(7A)-C(8A)-O(1A) -28.1(5)
C(6A)-C(7A)-C(8A)-O(2A) 21.0(3)

C(18A)-C(7A)-C(8A)-O(2A) 150.2(3)
N(1)-C(1)-C(9A)-C(14A) 40.68(15)
C(9B)-C(1)-C(9A)-C(14A) -41(3)
C(2)-C(1)-C(9A)-C(14A) -76.30(16)
N(1)-C(1)-C(9A)-C(10A) -139.15(13)
C(9B)-C(1)-C(9A)-C(10A) 139(3)
C(2)-C(1)-C(9A)-C(10A) 103.86(14)
C(14A)-C(9A)-C(10A)-C(11A) 0.42(19)
C(1)-C(9A)-C(10A)-C(11A) -179.74(12)
C(9A)-C(10A)-C(11A)-C(12A) -0.4(2)
C(26A)-O(3A)-C(12A)-C(11A) -175.9(2)
C(26A)-O(3A)-C(12A)-C(13A) 4.3(3)
C(10A)-C(11A)-C(12A)-O(3A) -179.80(16)
C(10A)-C(11A)-C(12A)-C(13A) 0.0(3)
O(3A)-C(12A)-C(13A)-C(14A) -179.83(19)
C(11A)-C(12A)-C(13A)-C(14A) 0.4(3)
C(10A)-C(9A)-C(14A)-C(13A) 0.0(2)
C(1)-C(9A)-C(14A)-C(13A) -179.86(15)
C(12A)-C(13A)-C(14A)-C(9A) -0.4(3)
C(8A)-C(7A)-C(18A)-C(19A) -55.8(3)
C(6A)-C(7A)-C(18A)-C(19A) 64.6(3)
C(8A)-C(7A)-C(18A)-C(20A) 177.6(2)
C(6A)-C(7A)-C(18A)-C(20A) -62.0(3)
C(6B)-C(5)-O(2B)-C(8B) -24.5(9)
O(2A)-C(5)-O(2B)-C(8B) -67(3)
C(4)-C(5)-O(2B)-C(8B) 105.9(7)
C(6A)-C(5)-O(2B)-C(8B) -11.8(8)
O(2A)-C(5)-C(6B)-C(7B) 37.8(6)
O(2B)-C(5)-C(6B)-C(7B) 33.4(7)
C(4)-C(5)-C(6B)-C(7B) -90.3(5)
C(6A)-C(5)-C(6B)-C(7B) -45.1(12)
C(5)-C(6B)-C(7B)-C(8B) -29.1(7)
C(5)-C(6B)-C(7B)-C(18B) -153.4(5)
C(5)-O(2B)-C(8B)-O(1B) -175.1(11)
C(5)-O(2B)-C(8B)-C(7B) 3.7(10)
C(6B)-C(7B)-C(8B)-O(1B) -165.3(13)
C(18B)-C(7B)-C(8B)-O(1B) -40.6(15)
C(6B)-C(7B)-C(8B)-O(2B) 16.1(10)
C(18B)-C(7B)-C(8B)-O(2B) 140.8(8)
N(1)-C(1)-C(9B)-C(14B) 31.4(3)
C(9A)-C(1)-C(9B)-C(14B) 131(3)

C(2)-C(1)-C(9B)-C(14B) -83.1(4)
N(1)-C(1)-C(9B)-C(10B) -148.6(3)
C(9A)-C(1)-C(9B)-C(10B) -49(3)
C(2)-C(1)-C(9B)-C(10B) 96.9(3)
C(14B)-C(9B)-C(10B)-C(11B) 0.0(4)
C(1)-C(9B)-C(10B)-C(11B) 180.0(2)
C(9B)-C(10B)-C(11B)-C(12B) 0.2(5)
C(26B)-O(3B)-C(12B)-C(11B) -168.2(8)
C(26B)-O(3B)-C(12B)-C(13B) 12.1(10)
C(10B)-C(11B)-C(12B)-O(3B) 180.0(4)
C(10B)-C(11B)-C(12B)-C(13B) -0.3(7)
O(3B)-C(12B)-C(13B)-C(14B) -180.0(5)
C(11B)-C(12B)-C(13B)-C(14B) 0.4(7)
C(10B)-C(9B)-C(14B)-C(13B) 0.0(5)
C(1)-C(9B)-C(14B)-C(13B) -179.9(3)
C(12B)-C(13B)-C(14B)-C(9B) -0.2(7)
C(8B)-C(7B)-C(18B)-C(19B) 61.5(8)
C(6B)-C(7B)-C(18B)-C(19B) 179.5(6)
C(8B)-C(7B)-C(18B)-C(20B) -172.5(6)
C(6B)-C(7B)-C(18B)-C(20B) -54.4(8)



ORTEP view of the C26 H39 N O5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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Dilactone **49**

Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C42 H60 O6 COMPOUND (bent69)

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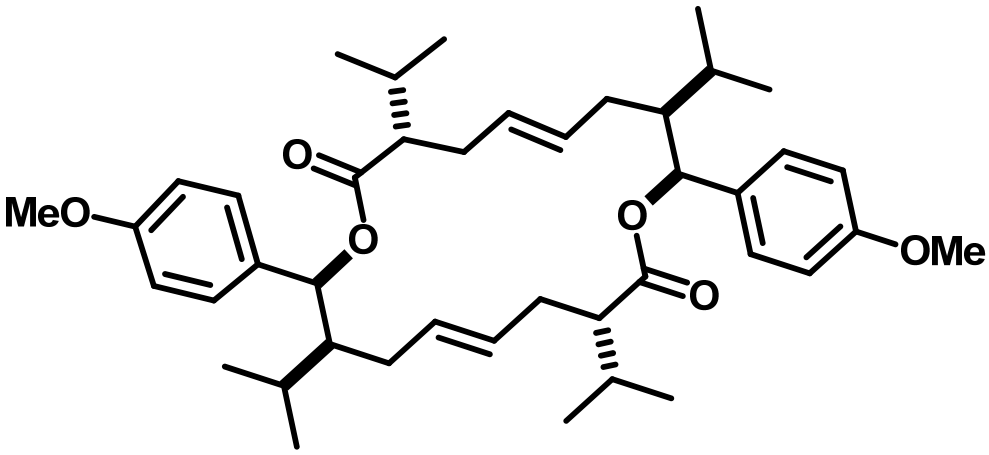


Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Benoît Deschênes Simard.

Table 1. Crystal data and structure refinement for C42 H60 O6.

Identification code	bent69
Empirical formula	C42 H60 O6
Formula weight	660.90
Temperature	200K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P212121
Unit cell dimensions	a = 8.2377(2) Å α = 90° b = 12.7351(4) Å β = 90° c = 38.5075(10) Å γ = 90°
Volume	4039.74(19)Å^3
Z	4
Density (calculated)	1.087 g/cm^3
Absorption coefficient	0.558 mm^{-1}
F(000)	1440
Crystal size	0.18 x 0.16 x 0.07 mm
Theta range for data collection	2.29 to 56.09°
Index ranges	$-8 \leq h \leq 8$, $-13 \leq k \leq 13$, $-40 \leq l \leq 41$
Reflections collected	53912
Independent reflections	5254 [R_{int} = 0.056]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9617 and 0.7039
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5254 / 126 / 531
Goodness-of-fit on F^2	0.913
Final R indices [I>2sigma(I)]	R_1 = 0.0455, wR_2 = 0.1130
R indices (all data)	R_1 = 0.0849, wR_2 = 0.1238
Absolute structure parameter	0.0(3)

Largest diff. peak and hole	0.170 and -0.158 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for C42 H60 O6.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ.	x	y	z	U_{eq}
O(12)	1	7863(3)	1278(2)	8220(1)	79(1)
O(13)	1	8990(4)	7183(2)	10672(1)	111(1)
O(11)	0.683(4)	6127(8)	2294(5)	8521(2)	108(2)
C(11)	0.683(4)	6908(10)	1503(6)	8495(2)	87(2)
C(12)	0.683(4)	6871(11)	624(6)	8757(2)	85(1)
C(13)	0.683(4)	7183(8)	1064(4)	9126(2)	89(2)
C(14)	0.683(4)	8838(8)	1518(4)	9168(1)	88(2)
C(15)	0.683(4)	9153(9)	2542(4)	9167(2)	78(2)
C(16)	0.683(4)	10858(9)	2960(8)	9202(4)	84(1)
C(17)	0.683(4)	11073(10)	3702(5)	9514(3)	77(1)
C(115)	0.683(4)	5285(15)	-18(9)	8741(2)	94(2)
C(116)	0.683(4)	5110(20)	-543(14)	8393(3)	116(4)
C(117)	0.683(4)	3765(16)	595(19)	8830(5)	115(5)
C(118)	0.683(4)	12873(10)	3930(9)	9587(3)	82(2)
C(119)	0.683(4)	13641(18)	3037(13)	9783(3)	105(4)
C(120)	0.683(4)	13851(15)	4172(17)	9264(4)	103(4)
C(22)	0.683(4)	10046(11)	6345(5)	8687(2)	76(1)
C(23)	0.683(4)	9560(20)	5831(7)	8345(2)	96(2)
C(24)	0.683(4)	10398(7)	4815(5)	8289(2)	89(2)
C(25)	0.683(4)	9625(7)	3899(5)	8285(2)	92(2)
C(26)	0.683(4)	10450(11)	2838(5)	8205(3)	93(2)
C(27)	0.683(4)	9743(5)	2339(6)	7872(2)	86(1)
C(215)	0.683(4)	9391(18)	7477(5)	8710(3)	97(2)
C(216)	0.683(4)	9910(30)	8011(10)	9046(3)	125(5)
C(217)	0.683(4)	9889(13)	8127(9)	8400(4)	131(5)
C(218)	0.683(4)	10831(8)	1517(5)	7705(3)	83(2)
C(219)	0.683(4)	12365(10)	1983(6)	7554(3)	117(3)
C(220)	0.683(4)	11245(19)	596(10)	7930(4)	113(3)
O(31)	0.317(4)	5659(18)	2106(12)	8379(4)	108(2)
C(31)	0.317(4)	6648(19)	1448(12)	8451(3)	87(2)
C(32)	0.317(4)	6770(20)	794(11)	8778(3)	85(1)
C(33)	0.317(4)	7009(17)	1575(11)	9082(3)	89(2)
C(34)	0.317(4)	8436(13)	2281(10)	9032(3)	88(2)
C(35)	0.317(4)	9704(19)	2257(11)	9245(5)	78(2)
C(36)	0.317(4)	11123(19)	3002(17)	9227(8)	84(1)
C(37)	0.317(4)	11155(19)	3764(10)	9537(5)	77(1)
C(315)	0.317(4)	5280(40)	80(20)	8826(5)	94(2)
C(316)	0.317(4)	5010(50)	-580(30)	8510(9)	116(4)
C(317)	0.317(4)	3740(30)	640(40)	8935(15)	115(5)
C(318)	0.317(4)	12880(20)	4041(19)	9654(8)	82(2)
C(319)	0.317(4)	13590(40)	3200(30)	9880(10)	105(4)
C(320)	0.317(4)	14030(30)	4290(40)	9359(11)	103(4)
C(42)	0.317(4)	10060(20)	6250(11)	8668(4)	76(1)

C(43)	0.317(4)	9470(50)	5682(14)	8343(4)	96(2)
C(44)	0.317(4)	9660(20)	4518(12)	8365(4)	89(2)
C(45)	0.317(4)	10483(15)	3987(10)	8125(4)	92(2)
C(46)	0.317(4)	10660(20)	2782(11)	8146(7)	93(2)
C(47)	0.317(4)	9783(7)	2177(11)	7857(4)	86(1)
C(415)	0.317(4)	9510(40)	7408(10)	8689(6)	97(2)
C(416)	0.317(4)	9610(90)	7790(20)	9066(7)	125(5)
C(417)	0.317(4)	10520(40)	8110(20)	8460(10)	131(5)
C(418)	0.317(4)	10691(19)	1182(13)	7743(6)	83(2)
C(419)	0.317(4)	12280(20)	1444(14)	7566(7)	117(3)
C(420)	0.317(4)	10950(50)	390(20)	8025(11)	113(3)
C(18)	1	9950(5)	4654(3)	9477(1)	77(1)
C(19)	1	9754(5)	5371(3)	9786(1)	72(1)
C(110)	1	8500(5)	5175(3)	10015(1)	83(1)
C(111)	1	8287(5)	5802(3)	10308(1)	94(1)
C(112)	1	9314(6)	6620(3)	10372(1)	87(1)
C(113)	1	10569(5)	6842(3)	10146(1)	91(1)
C(114)	1	10766(5)	6211(3)	9855(1)	89(1)
C(121)	1	10122(6)	7986(3)	10766(1)	122(2)
O(21)	1	7932(4)	5565(2)	9024(1)	94(1)
O(22)	1	10521(3)	5271(2)	9179(1)	72(1)
O(23)	1	5111(3)	629(2)	6677(1)	105(1)
C(21)	1	9390(6)	5682(3)	8973(1)	74(1)
C(28)	1	7975(4)	2017(3)	7931(1)	77(1)
C(29)	1	7134(4)	1586(3)	7618(1)	68(1)
C(210)	1	6725(5)	2285(3)	7353(1)	87(1)
C(211)	1	6067(5)	1952(4)	7053(1)	96(1)
C(212)	1	5787(4)	902(4)	7000(1)	80(1)
C(213)	1	6111(4)	164(3)	7255(1)	81(1)
C(214)	1	6811(4)	539(3)	7565(1)	80(1)
C(221)	1	4821(5)	-452(3)	6621(1)	118(2)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for C42 H60 O6.

	Occ.	x	y	z	U_{eq}
H(12D)	0.683(4)	7785	136	8701	102
H(13A)	0.683(4)	6368	1614	9177	106
H(13B)	0.683(4)	7037	493	9298	106
H(14A)	0.683(4)	9723	1048	9196	106
H(15A)	0.683(4)	8279	3025	9145	93
H(16A)	0.683(4)	11149	3340	8986	101
H(16B)	0.683(4)	11616	2361	9226	101
H(17A)	0.683(4)	10667	3305	9720	92
H(11A)	0.683(4)	5384	-590	8918	112
H(11B)	0.683(4)	6090	-952	8343	174
H(11C)	0.683(4)	4959	-8	8213	174
H(11D)	0.683(4)	4166	-1011	8397	174
H(11E)	0.683(4)	2831	118	8834	172
H(11F)	0.683(4)	3589	1141	8655	172
H(11G)	0.683(4)	3892	921	9059	172
H(11H)	0.683(4)	12921	4564	9740	98
H(11I)	0.683(4)	13074	2937	10004	157
H(11J)	0.683(4)	14785	3199	9828	157
H(11K)	0.683(4)	13565	2393	9645	157
H(12E)	0.683(4)	14940	4406	9331	155
H(12F)	0.683(4)	13310	4729	9132	155
H(12G)	0.683(4)	13934	3539	9121	155
H(22D)	0.683(4)	11257	6361	8704	91
H(23A)	0.683(4)	8368	5713	8344	115
H(23B)	0.683(4)	9818	6312	8151	115
H(24A)	0.683(4)	11539	4819	8254	107
H(25A)	0.683(4)	8496	3897	8335	110
H(26A)	0.683(4)	11631	2948	8175	112
H(26B)	0.683(4)	10289	2353	8403	112
H(27A)	0.683(4)	9692	2926	7700	103
H(21A)	0.683(4)	8179	7437	8711	117
H(21B)	0.683(4)	9510	8735	9049	188
H(21C)	0.683(4)	11100	8014	9062	188
H(21D)	0.683(4)	9462	7627	9245	188
H(21E)	0.683(4)	9413	8830	8419	197
H(21F)	0.683(4)	9503	7789	8187	197
H(21G)	0.683(4)	11075	8184	8393	197
H(21H)	0.683(4)	10206	1228	7504	99
H(21I)	0.683(4)	12833	1492	7385	175
H(21J)	0.683(4)	13148	2111	7741	175
H(21K)	0.683(4)	12108	2647	7438	175
H(22E)	0.683(4)	12035	149	7810	170
H(22F)	0.683(4)	10259	191	7978	170
H(22G)	0.683(4)	11712	846	8149	170
H(32A)	0.317(4)	7760	341	8761	102
H(33A)	0.317(4)	6018	2008	9106	106

H(33B)	0.317(4) 7153	1174	9300	106
H(34A)	0.317(4) 8438	2760	8842	106
H(35A)	0.317(4) 9717	1734	9421	93
H(36A)	0.317(4)11058	3411	9008	101
H(36B)	0.317(4)12145	2593	9222	101
H(37A)	0.317(4)10689	3352	9735	92
H(31A)	0.317(4) 5554	-415	9019	112
H(31B)	0.317(4) 5973	-1021	8469	174
H(31C)	0.317(4) 4828	-129	8309	174
H(31D)	0.317(4) 4064	-1034	8546	174
H(31E)	0.317(4) 3903	966	9163	172
H(31F)	0.317(4) 2844	139	8947	172
H(31G)	0.317(4) 3481	1189	8764	172
H(31H)	0.317(4)12800	4690	9800	98
H(31I)	0.317(4)14245	3518	10064	157
H(31J)	0.317(4)14281	2736	9739	157
H(31K)	0.317(4)12714	2783	9985	157
H(32B)	0.317(4)15013	4620	9451	155
H(32C)	0.317(4)13501	4761	9194	155
H(32D)	0.317(4)14329	3633	9240	155
H(42A)	0.317(4)11270	6220	8676	91
H(43A)	0.317(4) 8309	5849	8305	115
H(43B)	0.317(4)10084	5945	8140	115
H(44A)	0.317(4) 9194	4150	8554	107
H(45A)	0.317(4)10965	4355	7936	110
H(46A)	0.317(4)11833	2604	8138	112
H(46B)	0.317(4)10240	2543	8374	112
H(47A)	0.317(4) 9820	2653	7650	103
H(41A)	0.317(4) 8355	7453	8611	117
H(41B)	0.317(4) 9038	8465	9087	188
H(41C)	0.317(4)10752	7889	9131	188
H(41D)	0.317(4) 9109	7275	9220	188
H(41E)	0.317(4)10506	7839	8222	197
H(41F)	0.317(4)11641	8121	8546	197
H(41G)	0.317(4)10074	8821	8464	197
H(41H)	0.317(4) 9995	835	7564	99
H(41I)	0.317(4)12792	796	7482	175
H(41J)	0.317(4)13011	1789	7732	175
H(41K)	0.317(4)12081	1915	7369	175
H(42B)	0.317(4) 9894	174	8120	170
H(42C)	0.317(4)11605	702	8211	170
H(42D)	0.317(4)11511	-224	7930	170
H(18)	1	8847	4381	9417	92
H(110)	1	7778	4608	9973	100
H(111)	1	7421	5659	10463	112
H(113)	1	11281	7415	10188	109
H(114)	1	11626	6361	9699	107
H(12A)	1	10061	8561	10598	184
H(12B)	1	11223	7694	10767	184
H(12C)	1	9857	8252	10998	184
H(28)	1	7372	2664	8001	92
H(210)	1	6918	3014	7385	105
H(211)	1	5795	2445	6878	115
H(213)	1	5874	-559	7222	97
H(214)	1	7068	52	7744	95

H(22A)	1	4300	-754	6827	177
H(22B)	1	5854	-812	6578	177
H(22C)	1	4108	-541	6420	177

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C42 H60 O6.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(12)	84(2)	70(2)	82(2)	-9(2)	9(2)	6(1)
O(13)	111(2)	107(2)	114(2)	-38(2)	-3(2)	6(2)
O(11)	137(4)	64(3)	124(6)	-7(3)	49(4)	10(3)
C(11)	95(4)	52(3)	114(4)	-17(3)	18(3)	-6(3)
C(12)	93(3)	71(3)	90(3)	-8(3)	9(2)	-4(3)
C(13)	136(4)	48(5)	82(4)	1(4)	9(3)	-20(4)
C(14)	113(5)	78(3)	74(4)	3(3)	-15(3)	-20(4)
C(15)	82(6)	85(4)	67(5)	-11(3)	-18(4)	-2(4)
C(16)	99(4)	73(2)	80(3)	-14(2)	0(4)	-18(3)
C(17)	104(4)	57(2)	69(3)	0(2)	0(2)	-8(2)
C(115)	108(3)	75(4)	98(5)	-8(4)	18(4)	-12(3)
C(116)	117(4)	97(3)	134(10)	-33(7)	29(7)	-33(3)
C(117)	122(4)	123(4)	99(14)	-10(8)	25(5)	-10(4)
C(118)	95(3)	67(3)	84(5)	-10(3)	-17(3)	6(3)
C(119)	136(4)	101(6)	77(9)	-1(6)	-20(5)	28(4)
C(120)	85(4)	97(6)	129(11)	19(8)	-21(5)	-6(4)
C(22)	70(2)	67(3)	90(3)	2(2)	2(2)	-6(2)
C(23)	112(4)	82(4)	94(3)	13(3)	4(3)	15(4)
C(24)	77(6)	94(5)	95(5)	-4(4)	3(4)	1(4)
C(25)	58(5)	92(4)	126(6)	4(4)	-16(4)	-7(4)
C(26)	90(4)	84(3)	106(5)	-17(3)	-13(4)	-4(3)
C(27)	79(3)	78(3)	102(3)	-5(3)	-7(2)	-11(2)
C(215)	107(4)	57(2)	127(4)	13(3)	2(3)	7(2)
C(216)	135(12)	69(6)	173(5)	-31(4)	-42(5)	-2(8)
C(217)	102(12)	107(4)	185(8)	37(4)	28(8)	8(5)
C(218)	58(3)	83(5)	108(4)	-1(4)	10(3)	-18(3)
C(219)	76(4)	119(8)	155(5)	14(8)	19(3)	-22(6)
C(220)	117(7)	94(6)	129(11)	26(5)	47(5)	35(6)
O(31)	137(4)	64(3)	124(6)	-7(3)	49(4)	10(3)
C(31)	95(4)	52(3)	114(4)	-17(3)	18(3)	-6(3)
C(32)	93(3)	71(3)	90(3)	-8(3)	9(2)	-4(3)
C(33)	136(4)	48(5)	82(4)	1(4)	9(3)	-20(4)
C(34)	113(5)	78(3)	74(4)	3(3)	-15(3)	-20(4)
C(35)	82(6)	85(4)	67(5)	-11(3)	-18(4)	-2(4)
C(36)	99(4)	73(2)	80(3)	-14(2)	0(4)	-18(3)
C(37)	104(4)	57(2)	69(3)	0(2)	0(2)	-8(2)
C(315)	108(3)	75(4)	98(5)	-8(4)	18(4)	-12(3)
C(316)	117(4)	97(3)	134(10)	-33(7)	29(7)	-33(3)
C(317)	122(4)	123(4)	99(14)	-10(8)	25(5)	-10(4)
C(318)	95(3)	67(3)	84(5)	-10(3)	-17(3)	6(3)
C(319)	136(4)	101(6)	77(9)	-1(6)	-20(5)	28(4)
C(320)	85(4)	97(6)	129(11)	19(8)	-21(5)	-6(4)
C(42)	70(2)	67(3)	90(3)	2(2)	2(2)	-6(2)

C(43)	112(4)	82(4)	94(3)	13(3)	4(3)	15(4)
C(44)	77(6)	94(5)	95(5)	-4(4)	3(4)	1(4)
C(45)	58(5)	92(4)	126(6)	4(4)	-16(4)	-7(4)
C(46)	90(4)	84(3)	106(5)	-17(3)	-13(4)	-4(3)
C(47)	79(3)	78(3)	102(3)	-5(3)	-7(2)	-11(2)
C(415)	107(4)	57(2)	127(4)	13(3)	2(3)	7(2)
C(416)	135(12)	69(6)	173(5)	-31(4)	-42(5)	-2(8)
C(417)	102(12)	107(4)	185(8)	37(4)	28(8)	8(5)
C(418)	58(3)	83(5)	108(4)	-1(4)	10(3)	-18(3)
C(419)	76(4)	119(8)	155(5)	14(8)	19(3)	-22(6)
C(420)	117(7)	94(6)	129(11)	26(5)	47(5)	35(6)
C(18)	85(3)	68(2)	78(3)	-4(2)	-7(2)	-5(2)
C(19)	73(3)	64(2)	79(3)	0(2)	-4(2)	-2(2)
C(110)	91(3)	75(2)	83(3)	-6(2)	1(3)	-11(2)
C(111)	94(3)	94(3)	93(3)	-10(3)	11(2)	-5(3)
C(112)	96(4)	77(3)	86(3)	-13(3)	-6(3)	4(3)
C(113)	87(3)	75(3)	111(3)	-10(3)	-2(3)	-11(2)
C(114)	88(3)	87(3)	91(3)	-20(2)	5(2)	-16(3)
C(121)	129(4)	95(3)	143(4)	-44(3)	-27(3)	0(3)
O(21)	72(2)	101(2)	108(2)	10(2)	-5(2)	-1(2)
O(22)	68(2)	73(2)	76(2)	8(1)	-7(1)	-4(1)
O(23)	102(2)	101(2)	113(2)	9(2)	-10(2)	-7(2)
C(21)	65(3)	70(2)	89(3)	-12(2)	-1(3)	1(2)
C(28)	69(3)	65(2)	95(3)	-6(2)	15(2)	-3(2)
C(29)	57(2)	64(3)	85(3)	-1(2)	5(2)	6(2)
C(210)	76(3)	82(3)	105(3)	1(3)	-5(2)	-11(2)
C(211)	78(3)	93(3)	116(4)	16(3)	-7(3)	-8(3)
C(212)	60(2)	87(3)	93(3)	-1(3)	7(2)	-1(2)
C(213)	70(2)	64(2)	107(3)	-12(3)	16(2)	1(2)
C(214)	72(3)	73(3)	94(3)	-15(2)	6(2)	16(2)
C(221)	84(3)	96(2)	175(4)	-34(3)	-6(3)	1(2)

Table 5. Bond lengths [Å] and angles [°] for C42 H60 O6

O(12)-C(11)	1.349(6)	C(44)-C(45)	1.3294(8)
O(12)-C(31)	1.357(11)	C(45)-C(46)	1.544(9)
O(12)-C(28)	1.461(4)	C(46)-C(47)	1.538(8)
O(13)-C(112)	1.385(4)	C(47)-C(28)	1.530(5)
O(13)-C(121)	1.431(5)	C(47)-C(418)	1.535(9)
O(11)-C(11)	1.199(6)	C(415)-C(417)	1.504(11)
C(11)-C(12)	1.510(6)		
C(12)-C(115)	1.542(6)	C(415)-C(416)	1.535(9)
C(12)-C(13)	1.548(6)	C(418)-C(420)	1.499(10)
C(13)-C(14)	1.489(7)	C(418)-C(419)	1.517(10)
C(14)-C(15)	1.3299(8)	C(18)-O(22)	1.470(4)
C(15)-C(16)	1.507(7)	C(18)-C(19)	1.508(5)
C(16)-C(17)	1.540(5)	C(19)-C(110)	1.381(5)
C(17)-C(18)	1.531(7)	C(19)-C(114)	1.382(5)
C(17)-C(118)	1.537(6)	C(110)-C(111)	1.390(5)
C(115)-C(116)	1.505(6)	C(111)-C(112)	1.365(5)
C(115)-C(117)	1.514(7)	C(112)-C(113)	1.381(5)
C(118)-C(119)	1.504(6)	C(113)-C(114)	1.387(5)
C(118)-C(120)	1.514(6)	O(21)-C(21)	1.226(4)
C(22)-C(21)	1.489(6)	O(22)-C(21)	1.330(4)
C(22)-C(23)	1.528(6)	O(23)-C(212)	1.408(4)
C(22)-C(215)	1.541(6)	O(23)-C(221)	1.413(5)
C(23)-C(24)	1.484(8)	C(28)-C(29)	1.494(5)
C(24)-C(25)	1.3284(8)	C(29)-C(214)	1.374(5)
C(25)-C(26)	1.544(7)	C(29)-C(210)	1.396(5)
C(26)-C(27)	1.544(6)	C(210)-C(211)	1.342(5)
C(27)-C(218)	1.521(6)	C(211)-C(212)	1.373(5)
C(27)-C(28)	1.530(5)	C(212)-C(213)	1.384(5)
C(215)-C(217)	1.509(7)	C(213)-C(214)	1.410(5)
C(215)-C(216)	1.526(8)		
C(218)-C(220)	1.497(7)	C(11)-O(12)-C(31)	11.9(11)
C(218)-C(219)	1.512(6)	C(11)-O(12)-C(28)	119.8(4)
O(31)-C(31)	1.200(9)	C(31)-O(12)-C(28)	116.3(6)
C(31)-C(32)	1.513(8)	C(112)-O(13)-C(121)	117.1(4)
C(32)-C(315)	1.540(9)	O(11)-C(11)-O(12)	123.9(5)
C(32)-C(33)	1.548(8)	O(11)-C(11)-C(12)	123.8(6)
C(33)-C(34)	1.493(9)	O(12)-C(11)-C(12)	112.3(5)
C(34)-C(35)	1.3296(8)	C(11)-C(12)-C(115)	112.5(5)
C(35)-C(36)	1.507(9)	C(11)-C(12)-C(13)	110.0(5)
C(36)-C(37)	1.540(8)	C(115)-C(12)-C(13)	111.7(5)
C(37)-C(18)	1.525(11)	C(14)-C(13)-C(12)	113.0(5)
C(37)-C(318)	1.532(9)	C(15)-C(14)-C(13)	124.0(5)
C(315)-C(316)	1.496(9)	C(14)-C(15)-C(16)	121.8(7)
C(315)-C(317)	1.516(9)	C(15)-C(16)-C(17)	113.1(5)
C(318)-C(319)	1.503(9)	C(18)-C(17)-C(118)	116.8(5)
C(318)-C(320)	1.514(9)	C(18)-C(17)-C(16)	110.2(6)
C(42)-C(21)	1.485(10)	C(118)-C(17)-C(16)	111.8(5)
C(42)-C(43)	1.525(8)	C(116)-C(115)-C(117)	110.5(6)
C(42)-C(415)	1.544(9)	C(116)-C(115)-C(12)	110.6(5)
C(43)-C(44)	1.493(10)	C(117)-C(115)-C(12)	114.8(6)

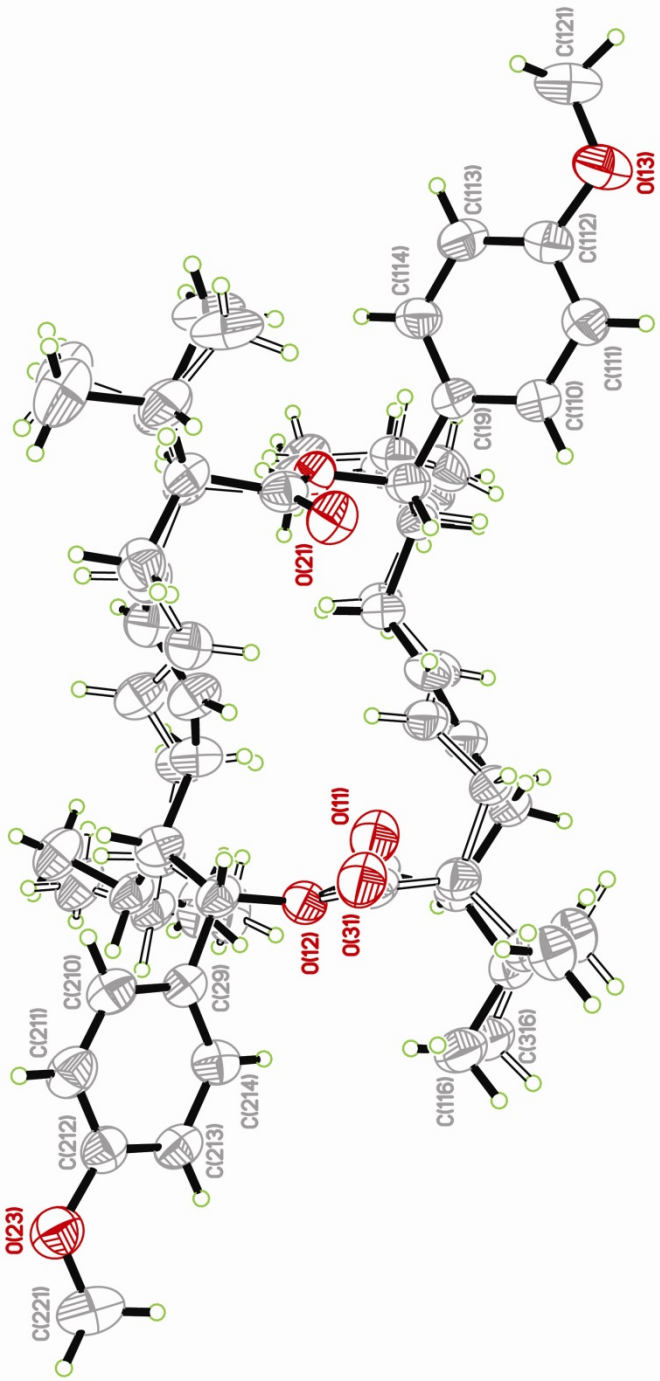
C(119)-C(118)-C(120) 110.0(6)
C(119)-C(118)-C(17) 110.8(6)
C(120)-C(118)-C(17) 113.6(5)
C(21)-C(22)-C(23) 107.4(6)
C(21)-C(22)-C(215) 111.2(5)
C(23)-C(22)-C(215) 110.9(5)
C(24)-C(23)-C(22) 112.1(7)
C(25)-C(24)-C(23) 122.9(10)
C(24)-C(25)-C(26) 124.0(7)
C(27)-C(26)-C(25) 111.2(5)
C(218)-C(27)-C(28) 116.0(5)
C(218)-C(27)-C(26) 114.3(5)
C(28)-C(27)-C(26) 110.3(5)
C(217)-C(215)-C(216) 110.5(6)
C(217)-C(215)-C(22) 111.9(6)
C(216)-C(215)-C(22) 111.5(6)
C(220)-C(218)-C(219) 109.8(6)
C(220)-C(218)-C(27) 115.3(5)
C(219)-C(218)-C(27) 112.7(5)
O(31)-C(31)-O(12) 117.5(10)
O(31)-C(31)-C(32) 128.5(12)
O(12)-C(31)-C(32) 114.0(10)
C(31)-C(32)-C(315) 111.8(10)
C(31)-C(32)-C(33) 106.5(9)
C(315)-C(32)-C(33) 112.9(10)
C(34)-C(33)-C(32) 112.9(10)
C(35)-C(34)-C(33) 121.7(11)
C(34)-C(35)-C(36) 124.5(15)
C(35)-C(36)-C(37) 112.0(11)
C(18)-C(37)-C(318) 118.5(10)
C(18)-C(37)-C(36) 109.8(11)
C(318)-C(37)-C(36) 112.9(10)
C(316)-C(315)-C(317) 111.7(12)
C(316)-C(315)-C(32) 110.7(11)
C(317)-C(315)-C(32) 114.9(12)
C(319)-C(318)-C(320) 109.8(12)
C(319)-C(318)-C(37) 111.5(12)
C(320)-C(318)-C(37) 114.1(12)
C(21)-C(42)-C(43) 107.5(11)
C(21)-C(42)-C(415) 108.4(10)
C(43)-C(42)-C(415) 113.8(10)
C(44)-C(43)-C(42) 112.9(10)
C(45)-C(44)-C(43) 121.3(15)
C(44)-C(45)-C(46) 121.1(13)
C(47)-C(46)-C(45) 114.4(11)
C(28)-C(47)-C(418) 114.7(9)
C(28)-C(47)-C(46) 113.0(10)
C(418)-C(47)-C(46) 113.0(9)
C(417)-C(415)-C(416) 109.4(12)
C(417)-C(415)-C(42) 112.0(12)
C(416)-C(415)-C(42) 109.9(11)
C(420)-C(418)-C(419) 110.6(11)
C(420)-C(418)-C(47) 114.7(12)
C(419)-C(418)-C(47) 111.7(11)
O(22)-C(18)-C(19) 109.1(3)
O(22)-C(18)-C(37) 107.9(8)
C(19)-C(18)-C(37) 113.6(7)
O(22)-C(18)-C(17) 107.5(5)
C(19)-C(18)-C(17) 118.2(4)
C(37)-C(18)-C(17) 5.2(9)
C(110)-C(19)-C(114) 117.9(4)
C(110)-C(19)-C(18) 118.3(3)
C(114)-C(19)-C(18) 123.8(4)
C(19)-C(110)-C(111) 120.5(4)
C(112)-C(111)-C(110) 120.4(4)
C(111)-C(112)-C(113) 120.4(4)
C(111)-C(112)-O(13) 115.3(4)
C(113)-C(112)-O(13) 124.4(4)
C(112)-C(113)-C(114) 118.5(4)
C(19)-C(114)-C(113) 122.2(4)
C(21)-O(22)-C(18) 116.9(3)
C(212)-O(23)-C(221) 116.2(3)
O(21)-C(21)-O(22) 122.9(4)
O(21)-C(21)-C(42) 123.2(8)
O(22)-C(21)-C(42) 113.8(8)
O(21)-C(21)-C(22) 122.8(5)
O(22)-C(21)-C(22) 114.2(5)
C(42)-C(21)-C(22) 5.5(9)
O(12)-C(28)-C(29) 110.4(3)
O(12)-C(28)-C(27) 110.2(4)
C(29)-C(28)-C(27) 114.9(4)
O(12)-C(28)-C(47) 106.8(7)
C(29)-C(28)-C(47) 110.5(6)
C(27)-C(28)-C(47) 8.2(7)
C(214)-C(29)-C(210) 117.6(4)
C(214)-C(29)-C(28) 124.4(4)
C(210)-C(29)-C(28) 117.9(4)
C(211)-C(210)-C(29) 121.7(4)
C(210)-C(211)-C(212) 120.2(4)
C(211)-C(212)-C(213) 121.5(4)
C(211)-C(212)-O(23) 116.0(4)
C(213)-C(212)-O(23) 122.4(4)
C(212)-C(213)-C(214) 116.7(4)
C(29)-C(214)-C(213) 122.2(4)

Table 6. Torsion angles [°] for C42 H60 O6.

C(31)-O(12)-C(11)-O(11) -77(3)
C(28)-O(12)-C(11)-O(11) -0.6(11)
C(31)-O(12)-C(11)-C(12) 101(4)
C(28)-O(12)-C(11)-C(12) 176.7(4)
O(11)-C(11)-C(12)-C(115) 73.4(10)
O(12)-C(11)-C(12)-C(115) -103.9(7)
O(11)-C(11)-C(12)-C(13) -51.8(10)
O(12)-C(11)-C(12)-C(13) 130.9(7)
C(11)-C(12)-C(13)-C(14) -64.8(8)
C(115)-C(12)-C(13)-C(14) 169.5(7)
C(12)-C(13)-C(14)-C(15) 102.7(8)
C(13)-C(14)-C(15)-C(16) -178.5(7)
C(14)-C(15)-C(16)-C(17) -122.3(10)
C(15)-C(16)-C(17)-C(18) -60.3(11)
C(15)-C(16)-C(17)-C(118) 168.1(9)
C(11)-C(12)-C(115)-C(116) 62.4(11)
C(13)-C(12)-C(115)-C(116) -173.3(10)
C(11)-C(12)-C(115)-C(117) -63.4(11)
C(13)-C(12)-C(115)-C(117) 60.9(10)
C(18)-C(17)-C(118)-C(119) 152.2(9)
C(16)-C(17)-C(118)-C(119) -79.6(11)
C(18)-C(17)-C(118)-C(120) -83.3(11)
C(16)-C(17)-C(118)-C(120) 44.9(12)
C(21)-C(22)-C(23)-C(24) -68.0(13)
C(215)-C(22)-C(23)-C(24) 170.2(11)
C(22)-C(23)-C(24)-C(25) 113.3(11)
C(23)-C(24)-C(25)-C(26) 175.9(7)
C(24)-C(25)-C(26)-C(27) -116.8(8)
C(25)-C(26)-C(27)-C(218) 159.9(7)
C(25)-C(26)-C(27)-C(28) -67.2(9)
C(21)-C(22)-C(215)-C(217) -173.5(9)
C(23)-C(22)-C(215)-C(217) -54.0(13)
C(21)-C(22)-C(215)-C(216) 62.1(10)
C(23)-C(22)-C(215)-C(216) -178.4(11)
C(28)-C(27)-C(218)-C(220) -70.9(10)
C(26)-C(27)-C(218)-C(220) 59.3(10)
C(28)-C(27)-C(218)-C(219) 161.9(8)
C(26)-C(27)-C(218)-C(219) -67.9(10)
C(11)-O(12)-C(31)-O(31) 119(5)
C(28)-O(12)-C(31)-O(31) 8.5(19)
C(11)-O(12)-C(31)-C(32) -59(3)
C(28)-O(12)-C(31)-C(32) -169.2(8)
O(31)-C(31)-C(32)-C(315) 63(2)
O(12)-C(31)-C(32)-C(315) -119.8(15)
O(31)-C(31)-C(32)-C(33) -61(2)
O(12)-C(31)-C(32)-C(33) 116.4(14)
C(31)-C(32)-C(33)-C(34) -55.8(16)
C(315)-C(32)-C(33)-C(34) -178.8(15)
C(32)-C(33)-C(34)-C(35) -116.3(18)
C(33)-C(34)-C(35)-C(36) -175.0(13)
C(34)-C(35)-C(36)-C(37) 110(2)
C(35)-C(36)-C(37)-C(18) -80(2)
C(35)-C(36)-C(37)-C(318) 145.7(19)
C(31)-C(32)-C(315)-C(316) 54(3)
C(33)-C(32)-C(315)-C(316) 174(2)
C(31)-C(32)-C(315)-C(317) -73(3)
C(33)-C(32)-C(315)-C(317) 47(3)

C(18)-C(37)-C(318)-C(319) 149(2)
C(36)-C(37)-C(318)-C(319) -81(3)
C(18)-C(37)-C(318)-C(320) -86(2)
C(36)-C(37)-C(318)-C(320) 44(3)
C(21)-C(42)-C(43)-C(44) -46(3)
C(415)-C(42)-C(43)-C(44) -166(2)
C(42)-C(43)-C(44)-C(45) -125(3)
C(43)-C(44)-C(45)-C(46) -179.3(18)
C(44)-C(45)-C(46)-C(47) 113(2)
C(45)-C(46)-C(47)-C(28) -82(2)
C(45)-C(46)-C(47)-C(418) 145.4(15)
C(21)-C(42)-C(415)-C(417) 162(2)
C(43)-C(42)-C(415)-C(417) -78(3)
C(21)-C(42)-C(415)-C(416) 40(2)
C(43)-C(42)-C(415)-C(416) 160(3)
C(28)-C(47)-C(418)-C(420) -72(2)
C(46)-C(47)-C(418)-C(420) 60(2)
C(28)-C(47)-C(418)-C(419) 161.6(18)
C(46)-C(47)-C(418)-C(419) -67(2)
C(318)-C(37)-C(18)-O(22) 66.2(14)
C(36)-C(37)-C(18)-O(22) -65.6(13)
C(318)-C(37)-C(18)-C(19) -54.9(14)
C(36)-C(37)-C(18)-C(19) 173.3(10)
C(318)-C(37)-C(18)-C(17) 153(13)
C(36)-C(37)-C(18)-C(17) 21(12)
C(118)-C(17)-C(18)-O(22) 61.9(7)
C(16)-C(17)-C(18)-O(22) -67.0(7)
C(118)-C(17)-C(18)-C(19) -62.0(7)
C(16)-C(17)-C(18)-C(19) 169.0(5)
C(118)-C(17)-C(18)-C(37) -33(13)
C(16)-C(17)-C(18)-C(37) -162(13)
O(22)-C(18)-C(19)-C(110) 144.8(3)
C(37)-C(18)-C(19)-C(110) -94.7(8)
C(17)-C(18)-C(19)-C(110) -92.0(5)
O(22)-C(18)-C(19)-C(114) -35.7(4)
C(37)-C(18)-C(19)-C(114) 84.8(9)
C(17)-C(18)-C(19)-C(114) 87.5(6)
C(114)-C(19)-C(110)-C(111) -0.8(5)
C(18)-C(19)-C(110)-C(111) 178.8(3)
C(19)-C(110)-C(111)-C(112) 0.1(6)
C(110)-C(111)-C(112)-C(113) 0.6(6)

C(110)-C(111)-C(112)-O(13) -179.5(3)
C(121)-O(13)-C(112)-C(111) 174.4(3)
C(121)-O(13)-C(112)-C(113) -5.7(6)
C(111)-C(112)-C(113)-C(114) -0.6(6)
O(13)-C(112)-C(113)-C(114) 179.6(3)
C(110)-C(19)-C(114)-C(113) 0.8(5)
C(18)-C(19)-C(114)-C(113) -178.7(3)
C(112)-C(113)-C(114)-C(19) -0.1(6)
C(19)-C(18)-O(22)-C(21) -90.6(3)
C(37)-C(18)-O(22)-C(21) 145.5(7)
C(17)-C(18)-O(22)-C(21) 140.1(4)
C(18)-O(22)-C(21)-O(21) 0.0(5)
C(18)-O(22)-C(21)-C(42) -177.2(7)
C(18)-O(22)-C(21)-C(22) 176.8(4)
C(43)-C(42)-C(21)-O(21) -59.6(17)
C(415)-C(42)-C(21)-O(21) 63.8(15)
C(43)-C(42)-C(21)-O(22) 117.5(12)
C(415)-C(42)-C(21)-O(22) -119.1(12)
C(43)-C(42)-C(21)-C(22) -147(11)
C(415)-C(42)-C(21)-C(22) -24(11)
C(23)-C(22)-C(21)-O(21) -65.3(9)
C(215)-C(22)-C(21)-O(21) 56.3(8)
C(23)-C(22)-C(21)-O(22) 117.9(6)
C(215)-C(22)-C(21)-O(22) -120.5(6)
C(23)-C(22)-C(21)-C(42) 30(11)
C(215)-C(22)-C(21)-C(42) 152(11)
C(11)-O(12)-C(28)-C(29) -109.1(5)
C(31)-O(12)-C(28)-C(29) -96.1(9)
C(11)-O(12)-C(28)-C(27) 122.9(6)
C(31)-O(12)-C(28)-C(27) 135.8(10)
C(11)-O(12)-C(28)-C(47) 130.7(7)
C(31)-O(12)-C(28)-C(47) 143.7(10)
C(218)-C(27)-C(28)-O(12) 73.9(6)
C(26)-C(27)-C(28)-O(12) -58.2(6)
C(218)-C(27)-C(28)-C(29) -51.6(7)
C(26)-C(27)-C(28)-C(29) 176.3(4)
C(218)-C(27)-C(28)-C(47) 7(6)
C(26)-C(27)-C(28)-C(47) -125(7)
C(418)-C(47)-C(28)-O(12) 62.4(11)
C(46)-C(47)-C(28)-O(12) -69.1(11)
C(418)-C(47)-C(28)-C(29) -57.8(12)
C(46)-C(47)-C(28)-C(29) 170.7(9)
C(418)-C(47)-C(28)-C(27) 178(10)
C(46)-C(47)-C(28)-C(27) 47(6)
O(12)-C(28)-C(29)-C(214) -21.1(5)
C(27)-C(28)-C(29)-C(214) 104.2(5)
C(47)-C(28)-C(29)-C(214) 96.8(7)
O(12)-C(28)-C(29)-C(210) 162.5(3)
C(27)-C(28)-C(29)-C(210) -72.1(5)
C(47)-C(28)-C(29)-C(210) -79.6(7)
C(214)-C(29)-C(210)-C(211) -1.2(6)
C(28)-C(29)-C(210)-C(211) 175.5(3)
C(29)-C(210)-C(211)-C(212) -0.4(6)
C(210)-C(211)-C(212)-C(213) 2.5(6)
C(210)-C(211)-C(212)-O(23) -179.3(3)
C(221)-O(23)-C(212)-C(211) -180.0(4)
C(221)-O(23)-C(212)-C(213) -1.7(5)
C(211)-C(212)-C(213)-C(214) -2.8(5)
O(23)-C(212)-C(213)-C(214) 179.1(3)
C(210)-C(29)-C(214)-C(213) 0.7(5)
C(28)-C(29)-C(214)-C(213) -175.6(3)
C(212)-C(213)-C(214)-C(29) 1.2(5)


C(121)
O(13)
C(113)
C(112)
C(114)
C(111)
C(110)
C(19)
O(21)
O(11)
O(12)
O(31)
C(210)
C(29)
C(211)
C(214)
C(212)
C(213)
O(23)
C(221)
C(316)
C(116)

ORTEP view of the C42 H60 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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