Synthesis of bifunctional monomers via palladium catalyzed carbonylation of cardanol and its derivatives.

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Supplementary Information

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1 Monomers from Methoxycarbonylation of Cardanol

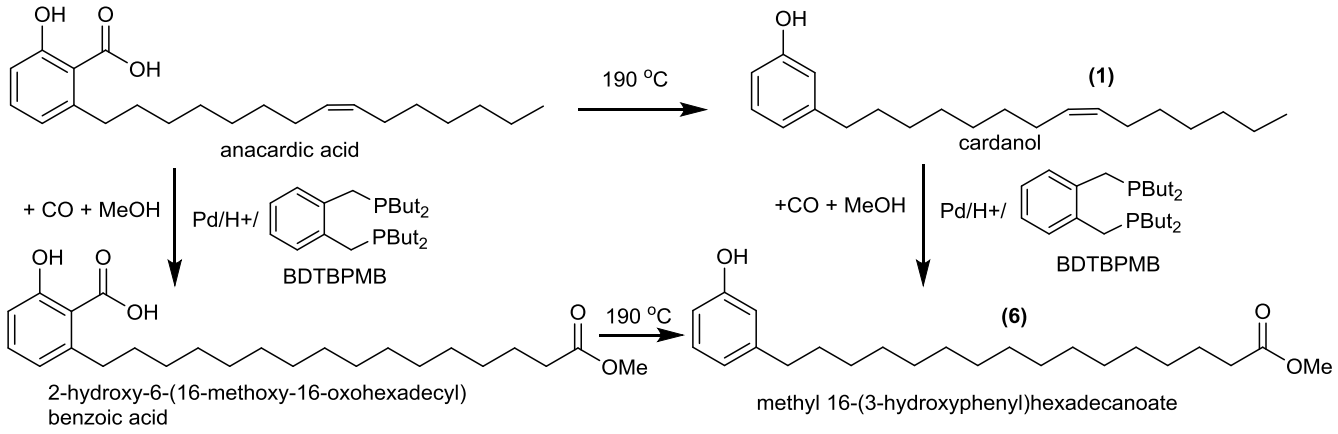


Figure S1. Synthesis of methyl16-(3-hydroxyphenyl)hexadecanoate

2 Monomers from methoxycarbonylation of shorter chain 3-alkenylphenols derived from cardanol

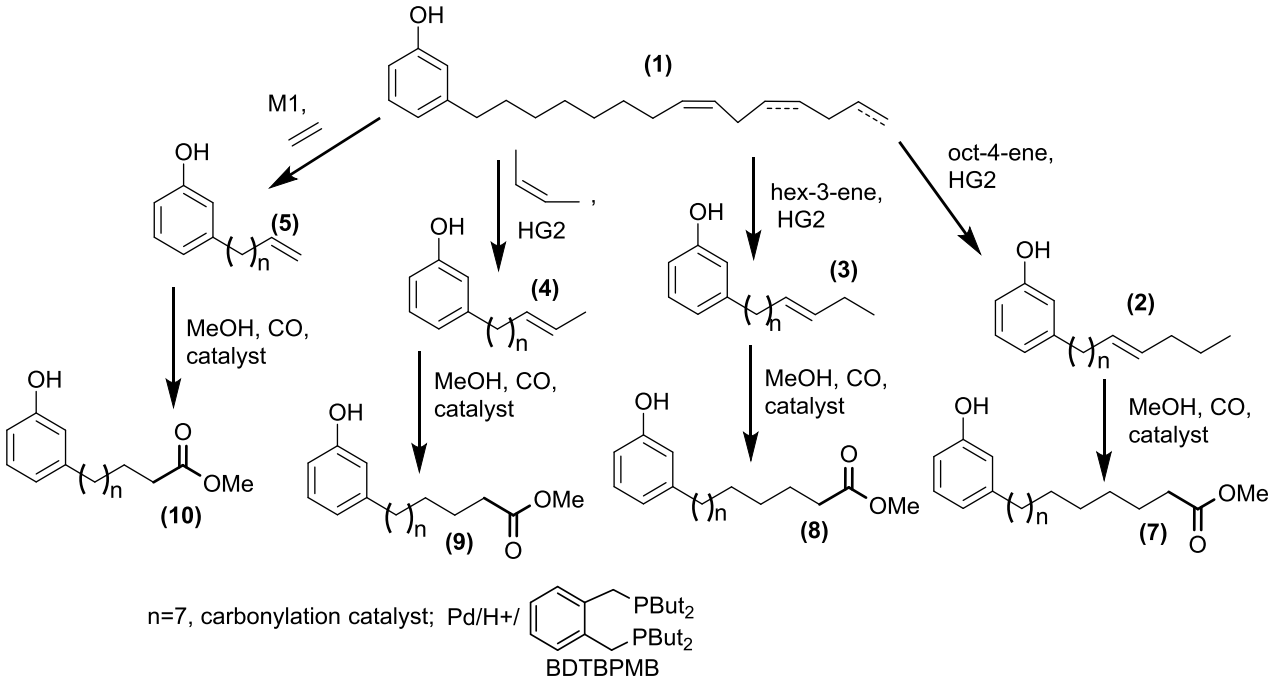


Figure S2. Synthesis of short chain monomers from cardanol

3 Polymerization and Cyclisation Reactions of methyl 16-(3-hydroxyphenyl)hexadecanoate

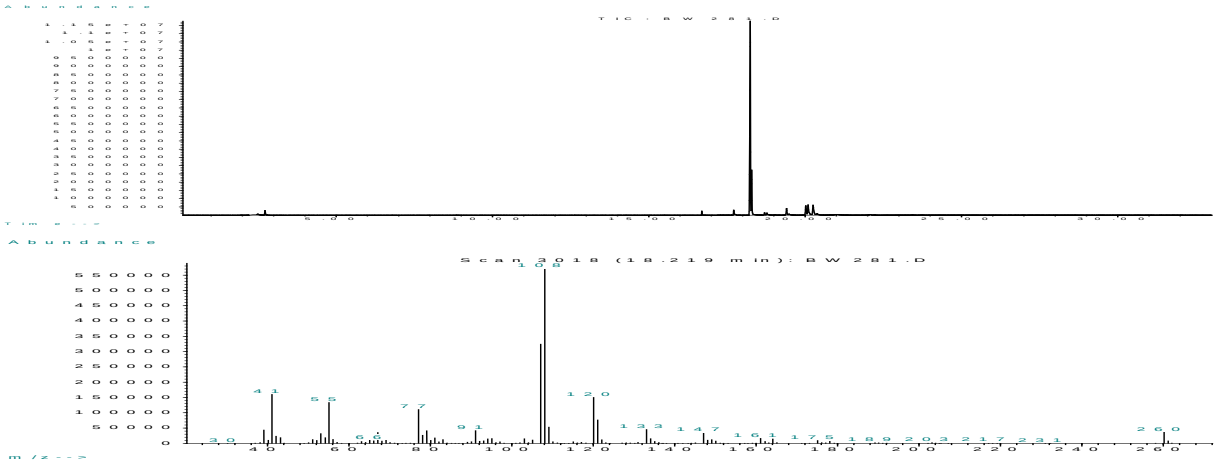
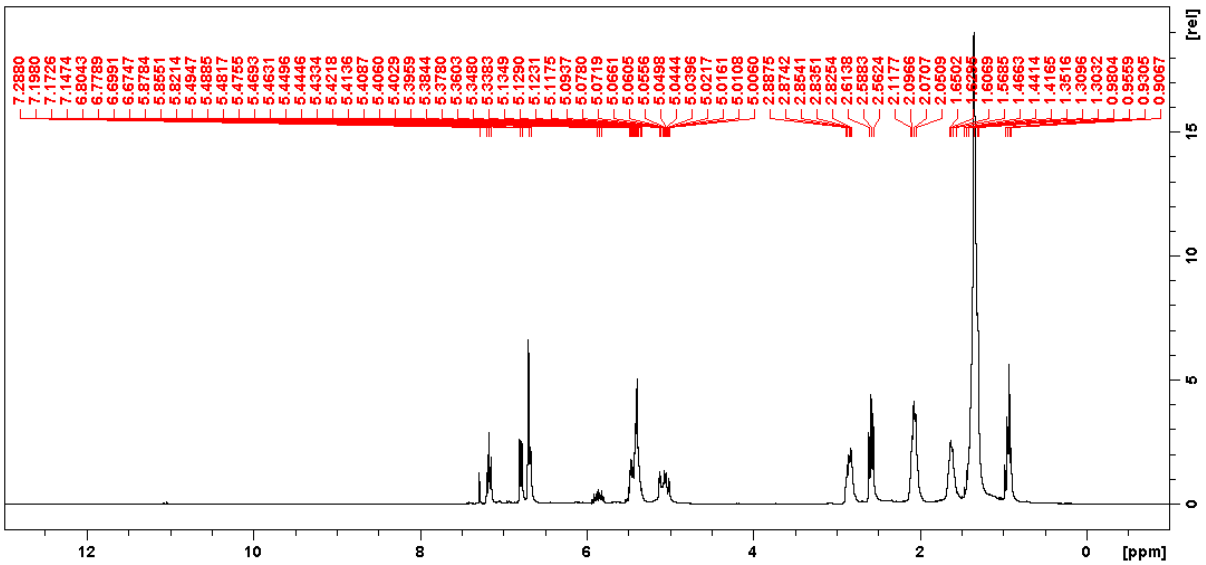


Figure S3. Polymerization of methyl 16-(3-hydroxyphenyl)hexadecanoate and formation of a 20 membered ring lactone

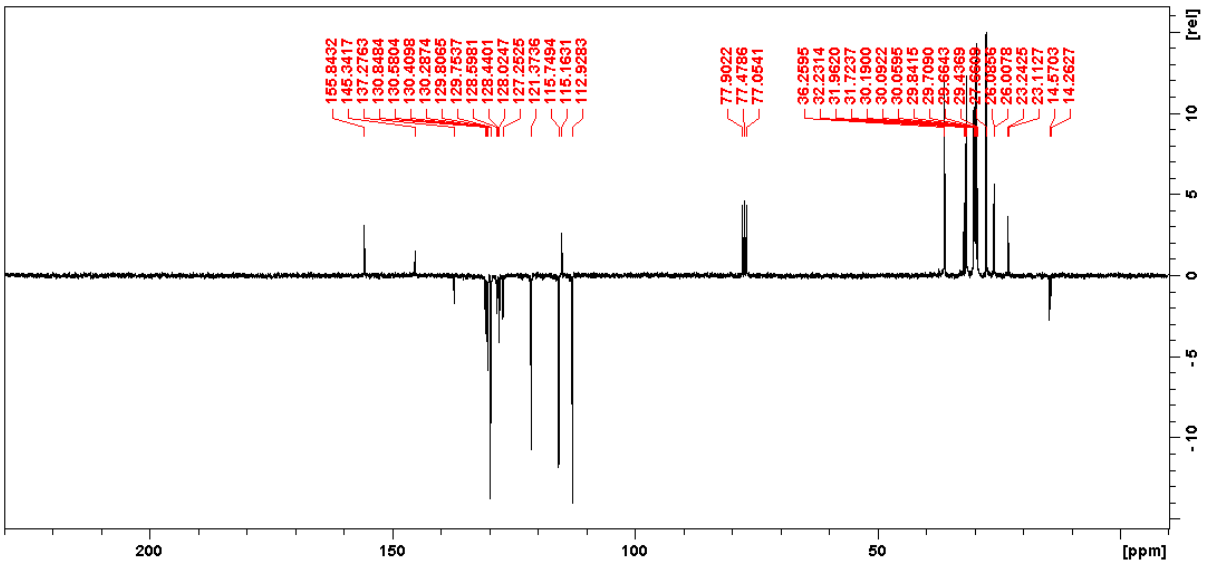
4 NMR Spectra of Cardanol and Short Chain Derivatives of Cardanol

4.1 Cardanol; (E)-3-(pentadec-8-enyl)phenol (1)

^{1}H NMR



^{13}C NMR



4.2 (E)-3-(dodec-8-enyl)phenol (2)

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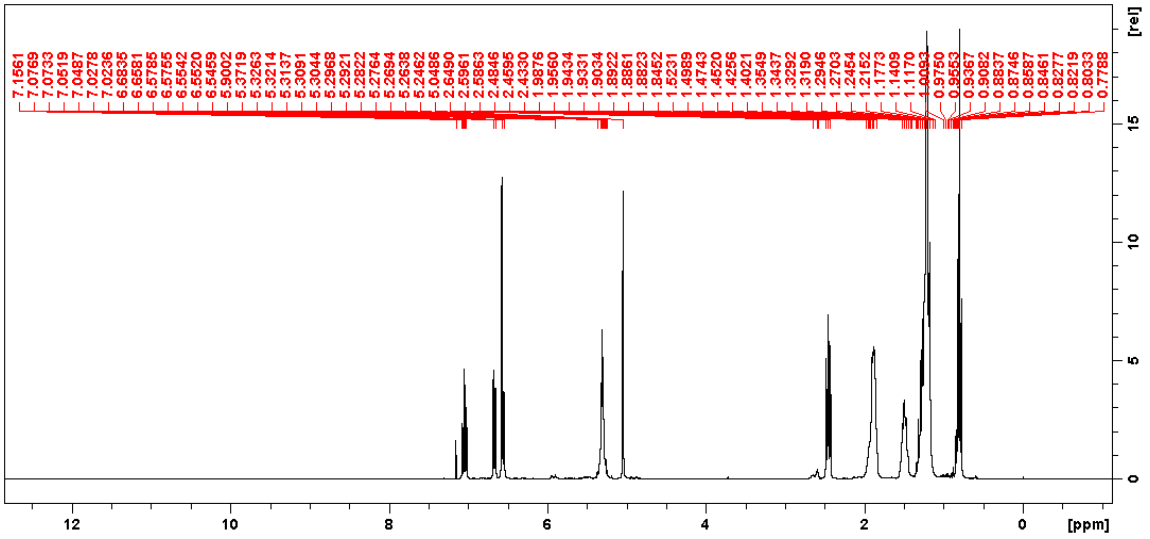

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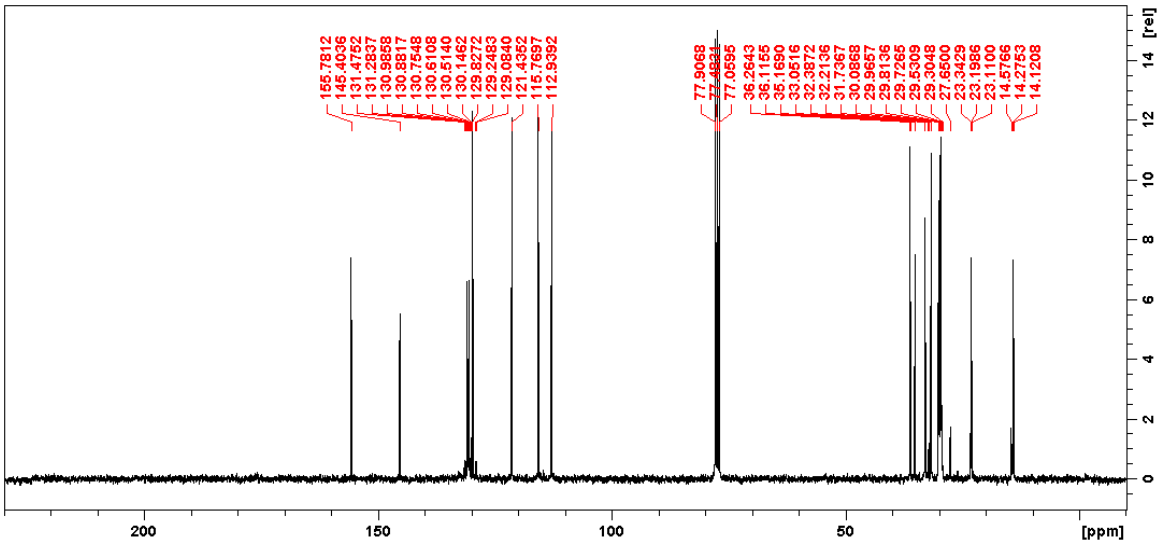

4.3 (E)-3-(undec-8-enyl)phenol (3)

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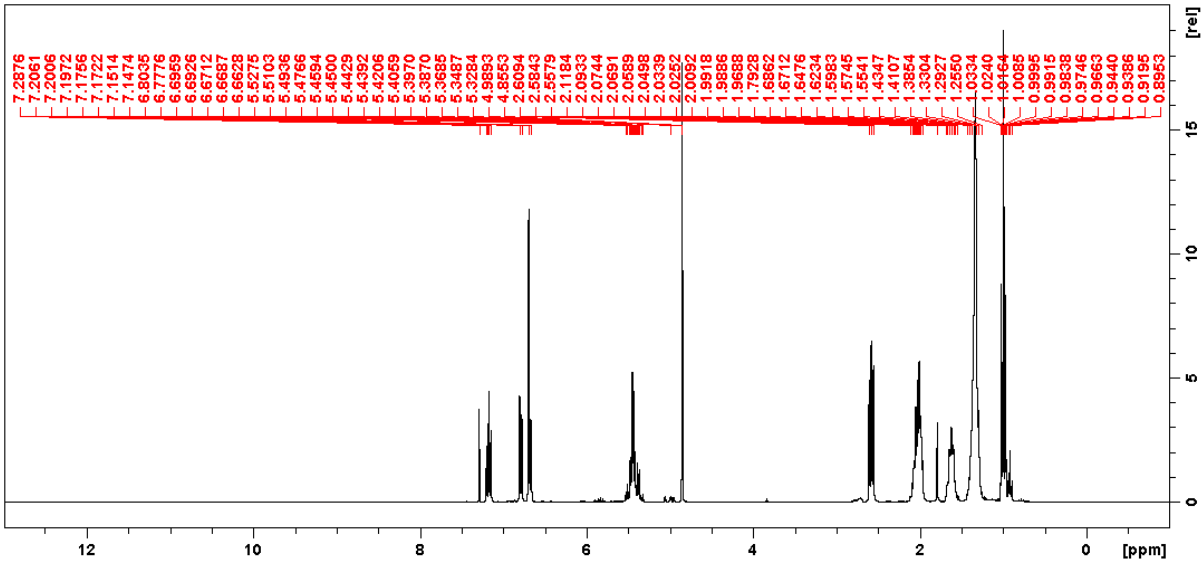

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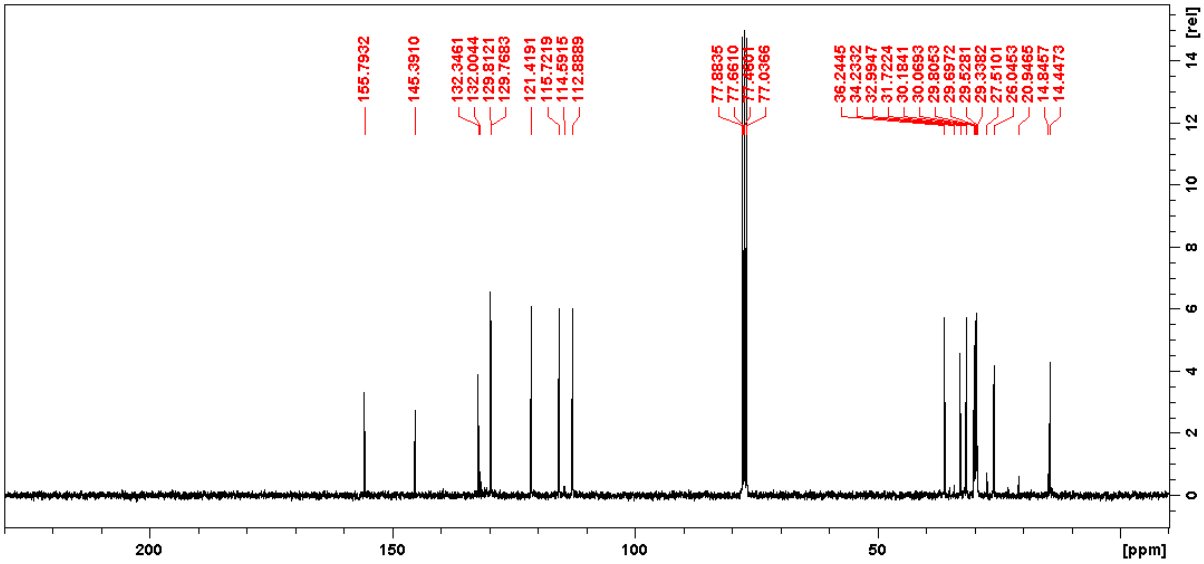

4.4 (E)-3-(dec-8-enyl)phenol (4)

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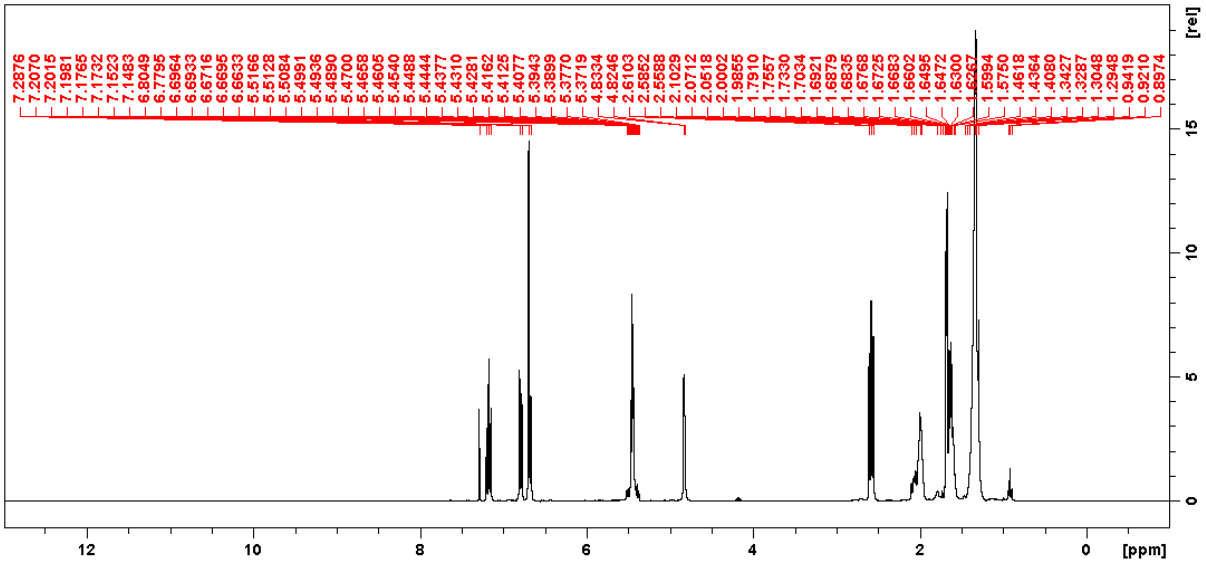

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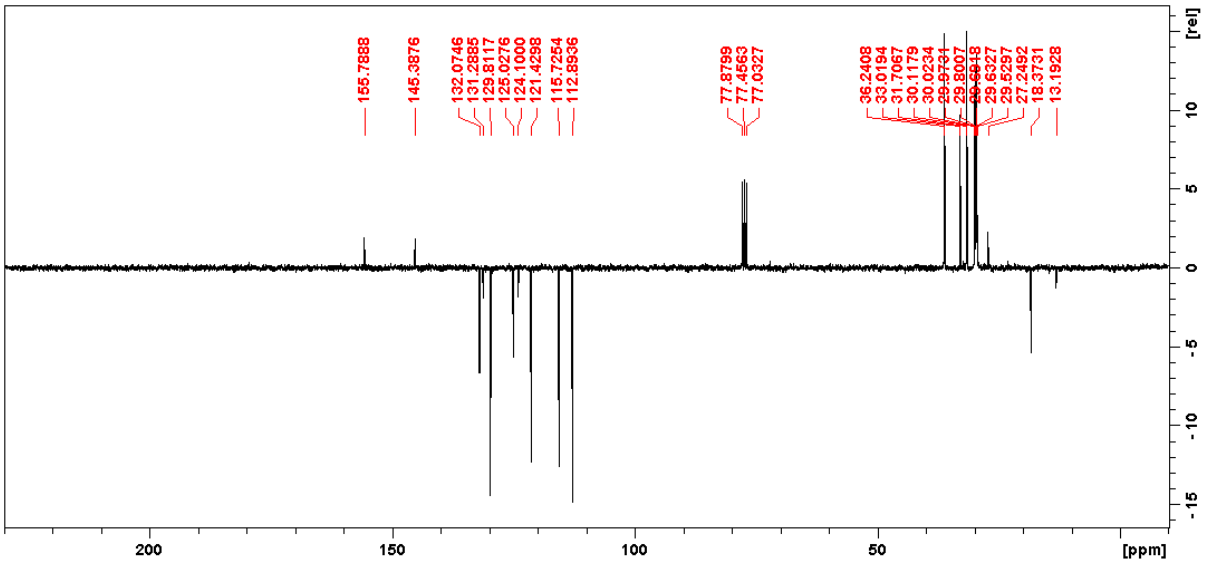
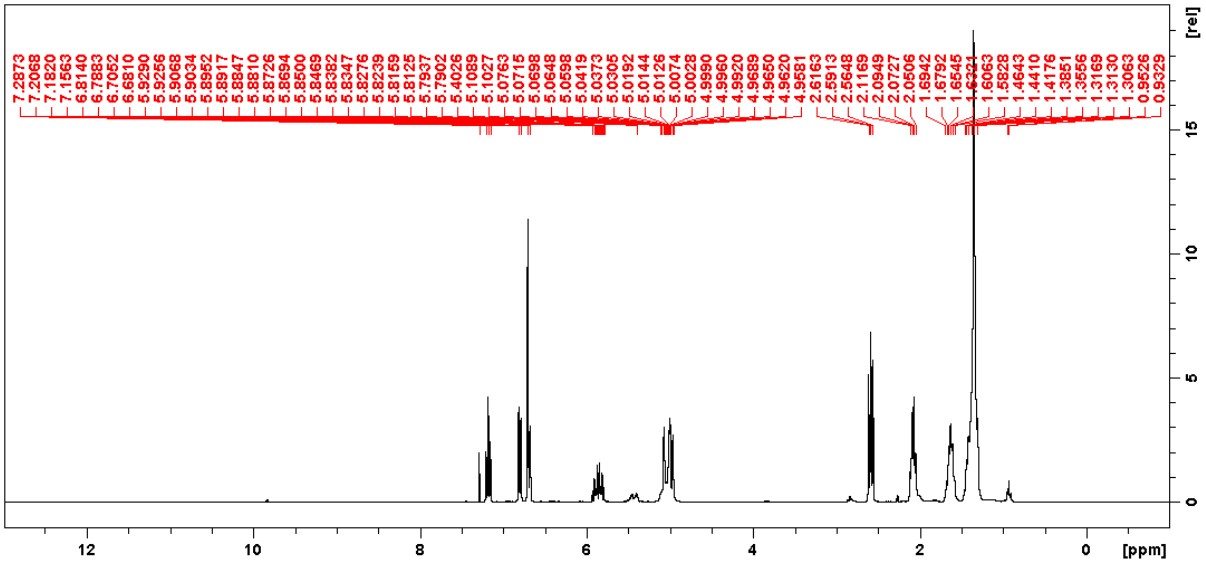


4.53-(non-8-enyl)phenol; HOPhC9-ene (5)

^{1}H NMR



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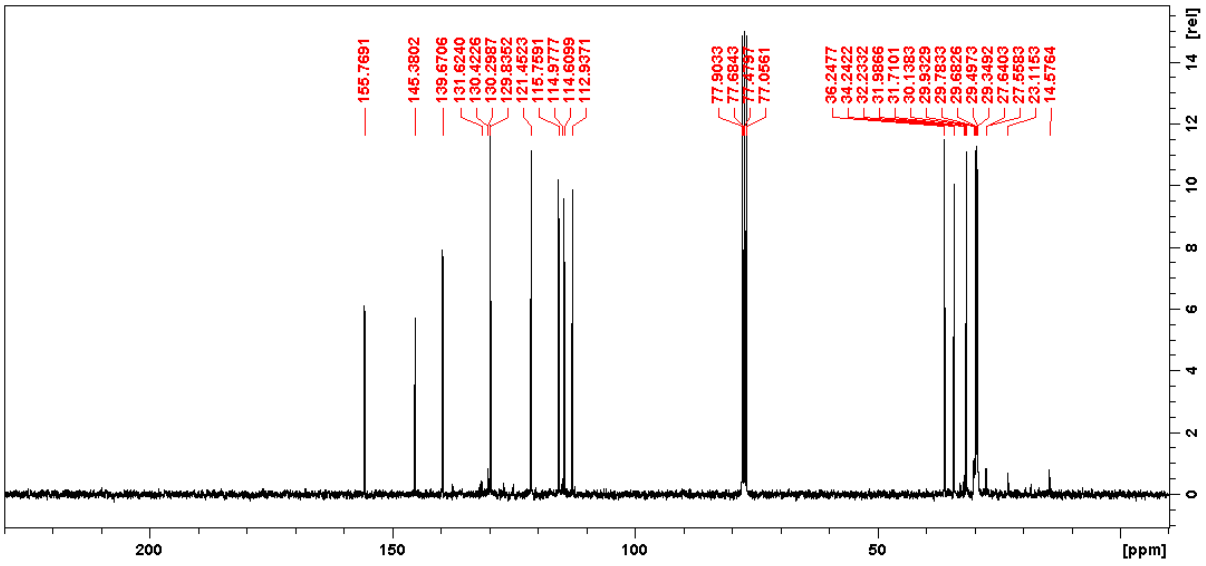
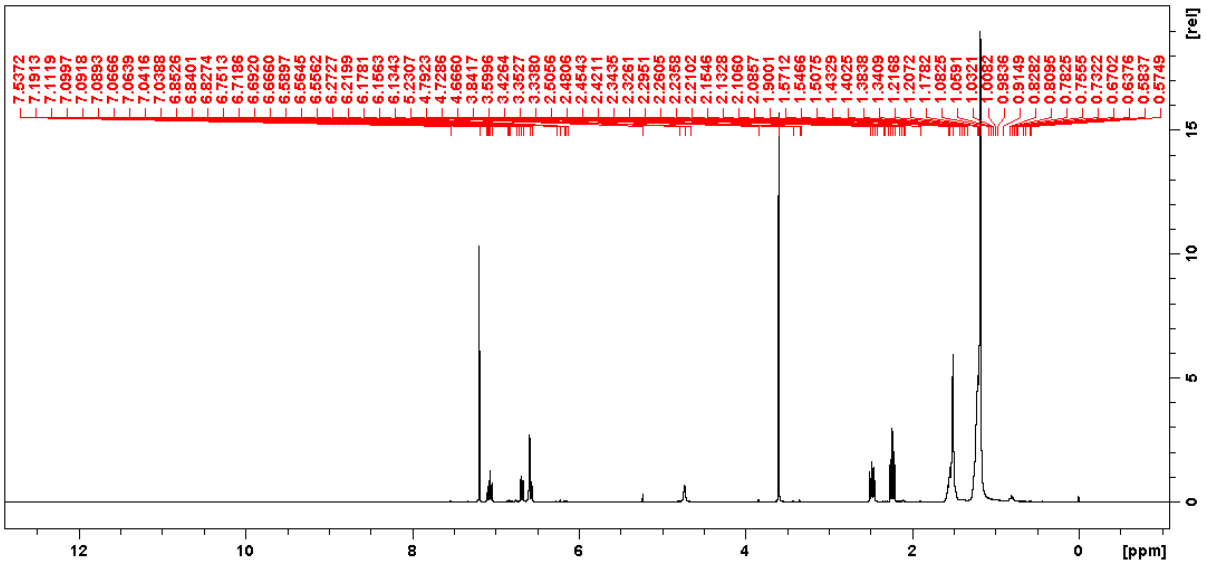


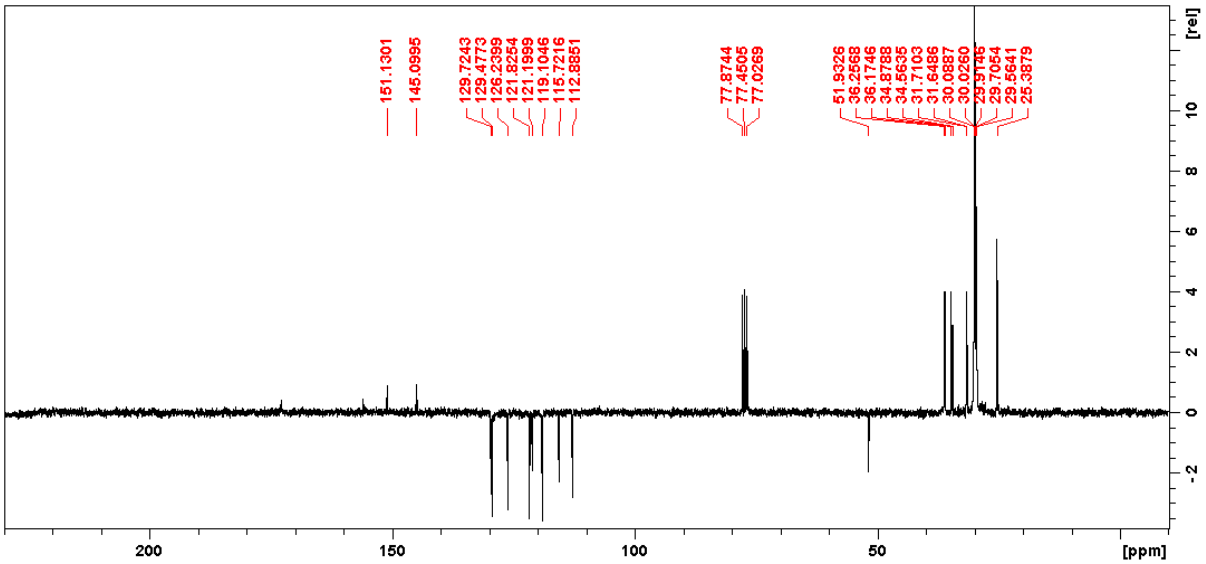
5 NMR Spectra of Monomers from Methoxycarbonylation of Cardanol and its Derivatives

5.1 Methyl 16-(3-hydroxyphenyl)hexadecanoate (6)

^{1}H NMR

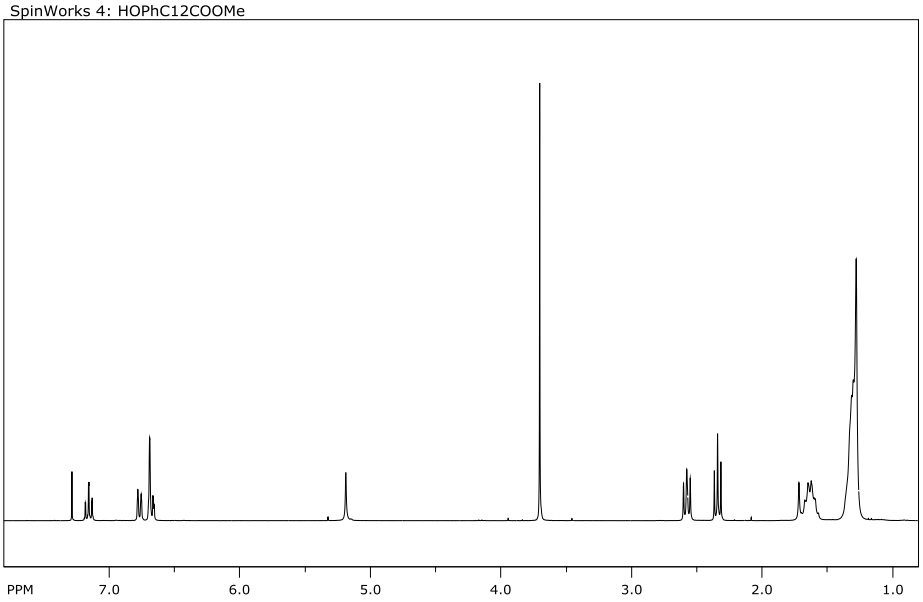


13C NMR



5.2 Methyl 13-(3-hydroxyphenyl)tridecanoate (7)

^{1}H NMR



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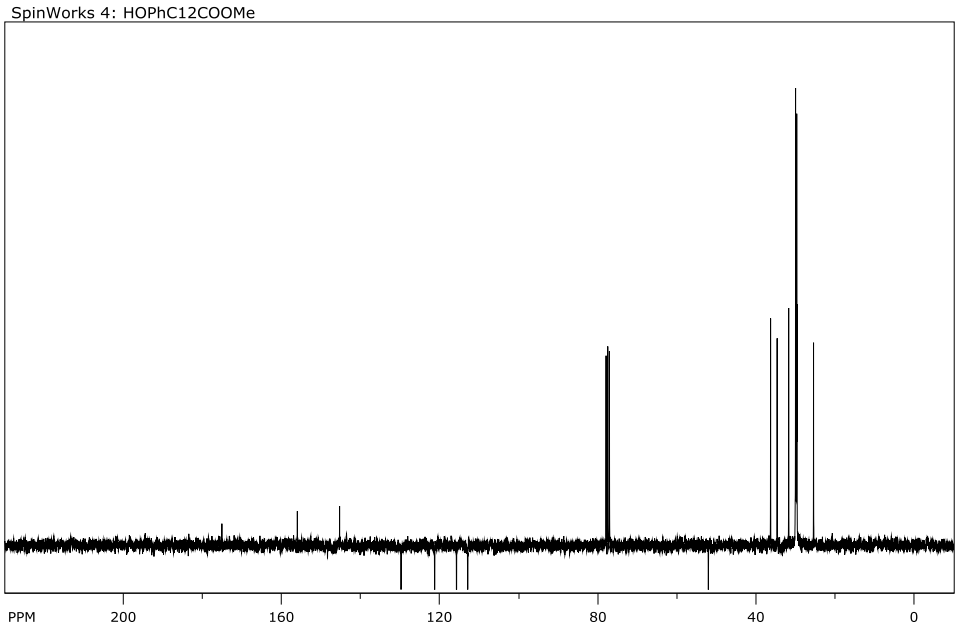

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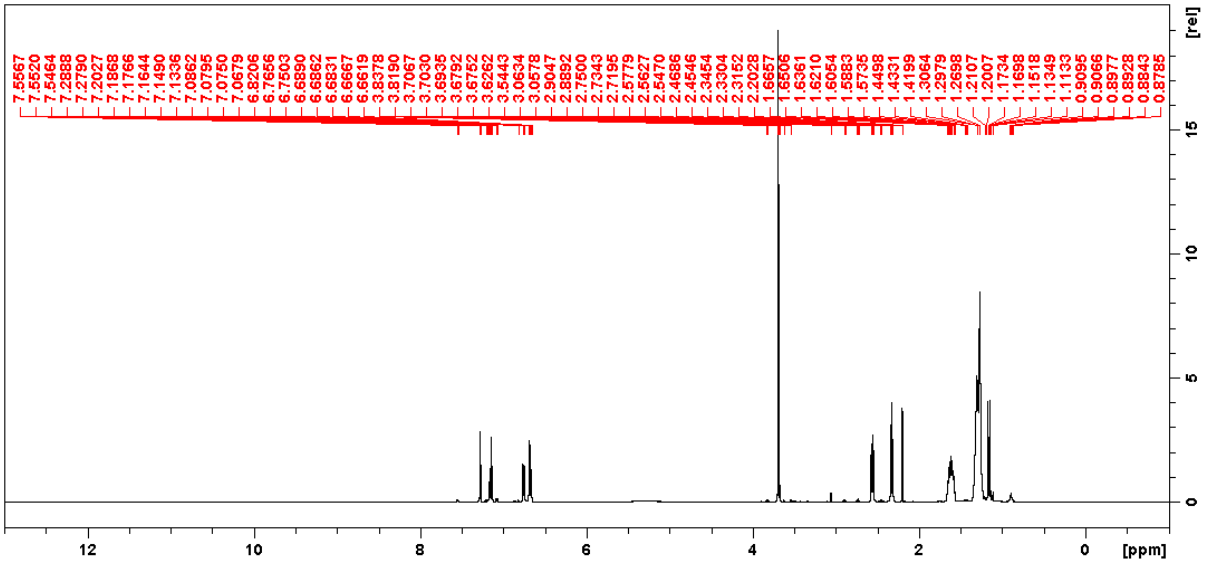
5.3 Methyl 12-(3-hydroxyphenyl)dodecanoate (8)

^{1}H NMR



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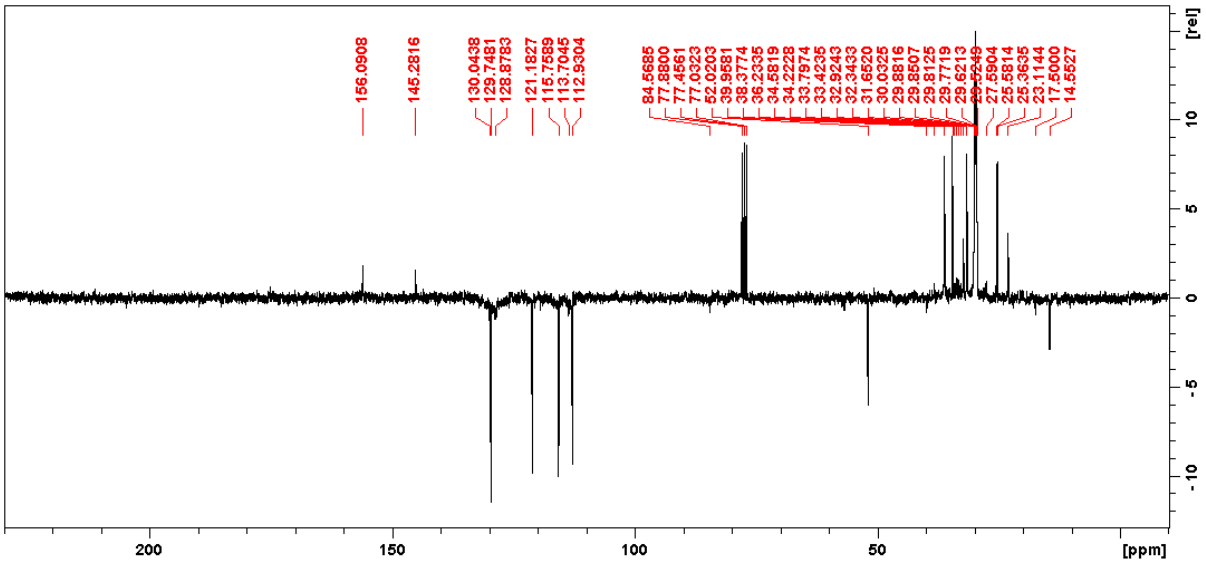
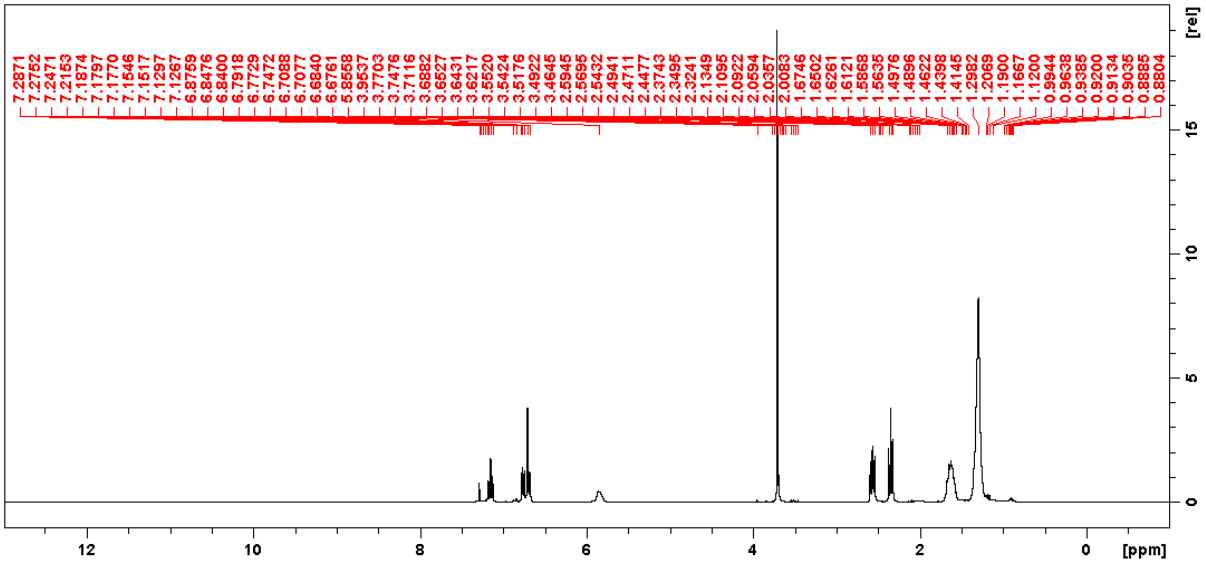


5.4 Methyl 11-(3-hydroxyphenyl)undecanoate (9)

^{1}H NMR



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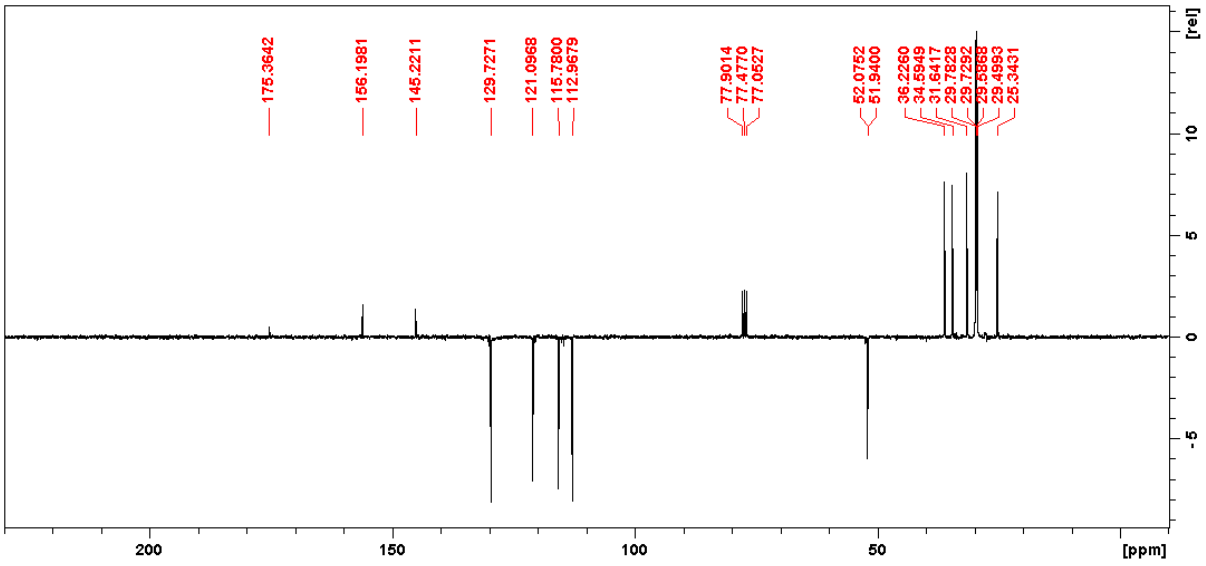
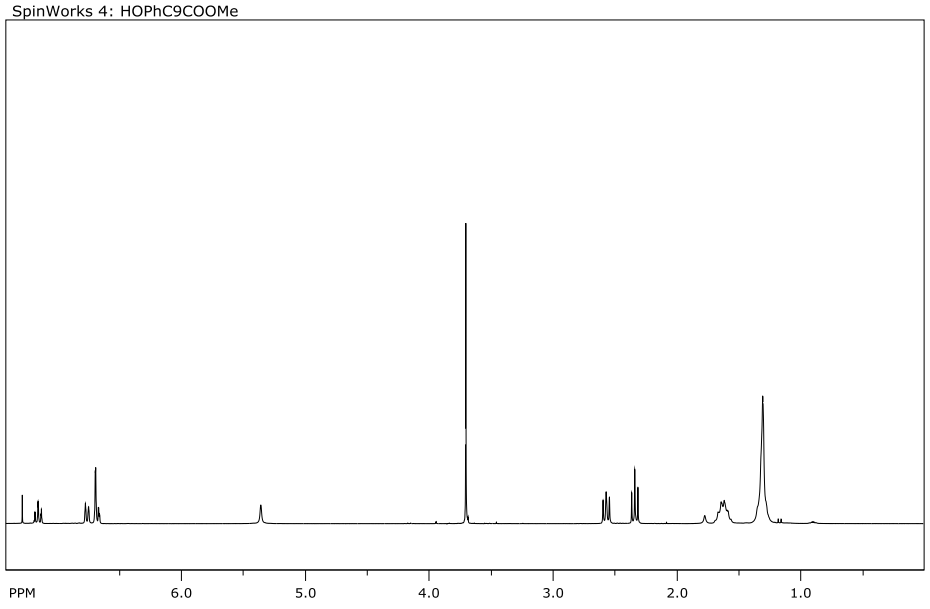


5.5 Methyl 10-(3-hydroxyphenyl)decanoate (10)

^{1}H NMR



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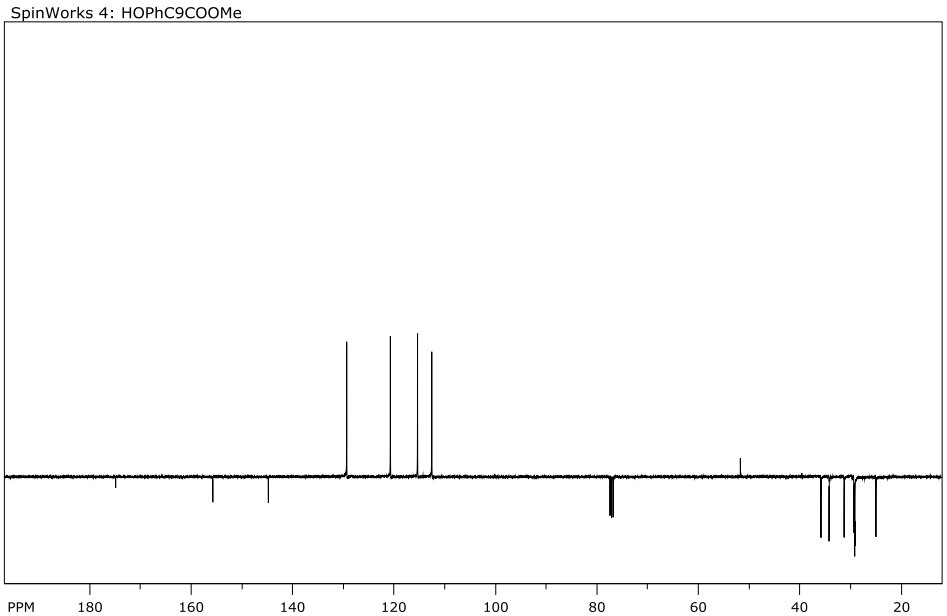

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6 NMR Spectra of Lactones (contaminated with linear monomers)

6.1 Cyclisation of HOPhC15COOMe; Methyl 16-(3-hydroxyphenyl)hexadecanoate

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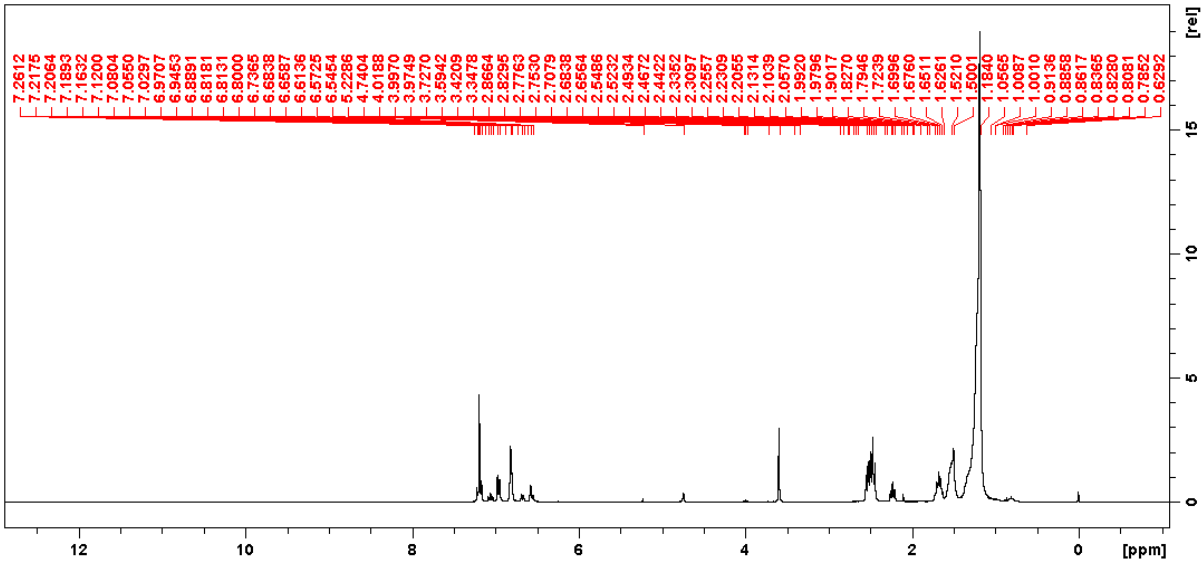

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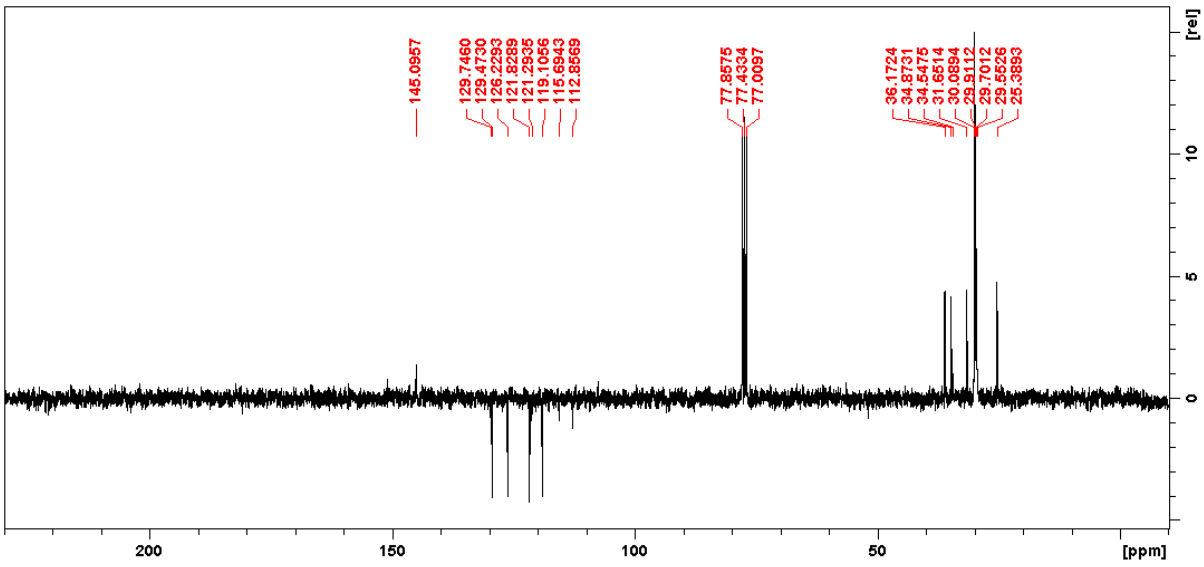
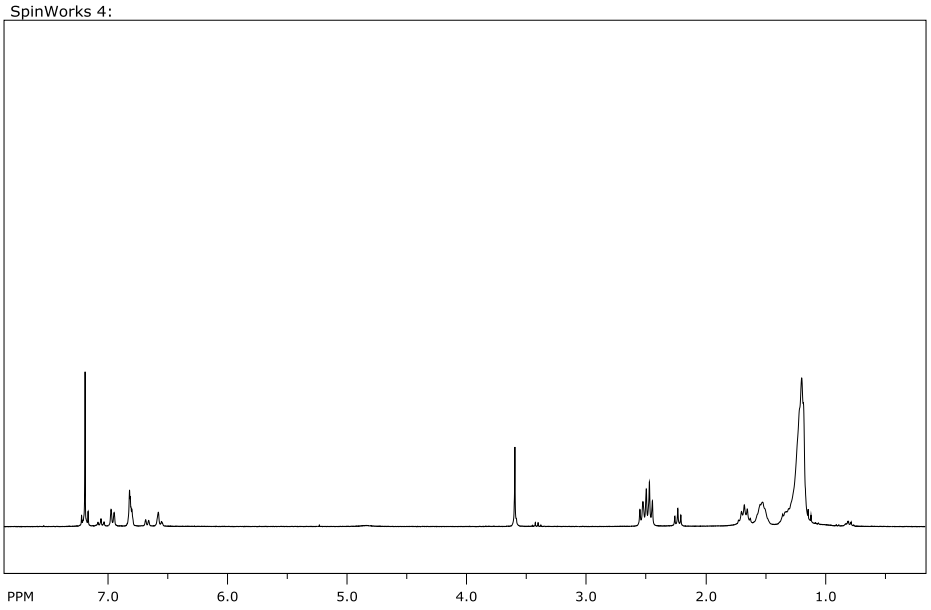


6.2 Cyclisation of HOPhC12COOMe; Methyl 13-(3-hydroxyphenyl)tridecanoate

^{1}H NMR



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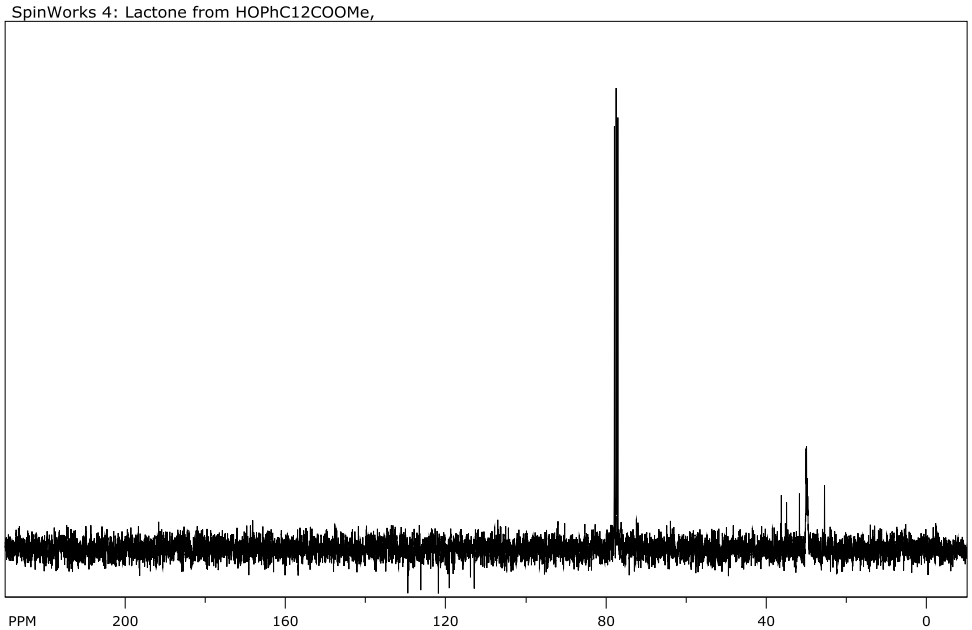
^{13}C NMR



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number of scans: 800

freq. of 0 ppm: 75.450117 MHz
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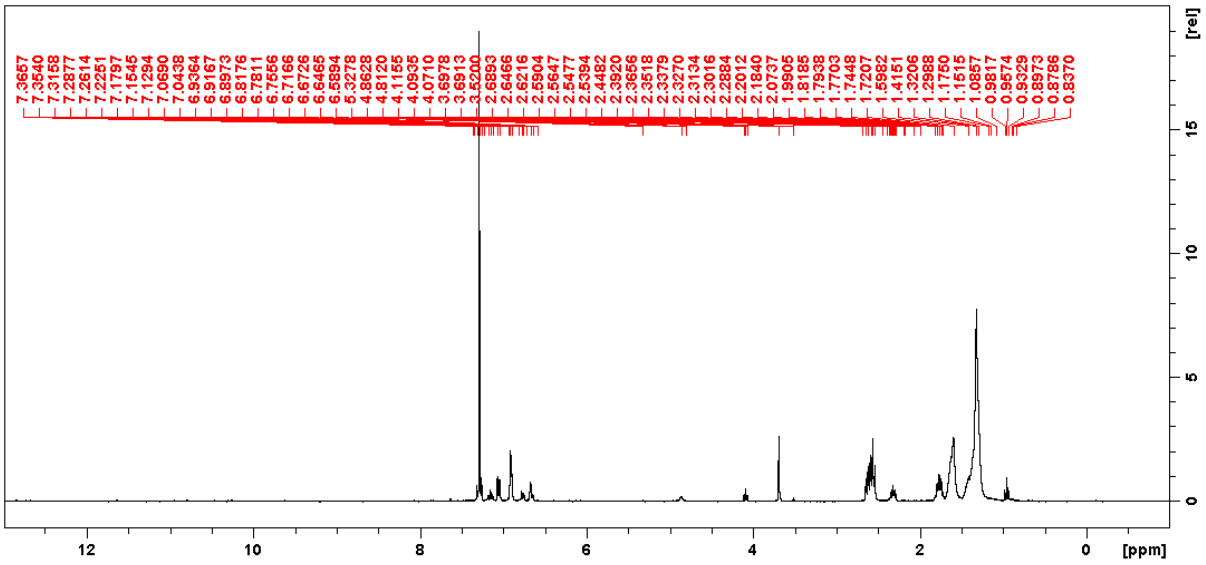
6.3 Cyclisation of HOPhC10COOMe; Methyl 11-(3-hydroxyphenyl)undecanoate

^{1}H NMR



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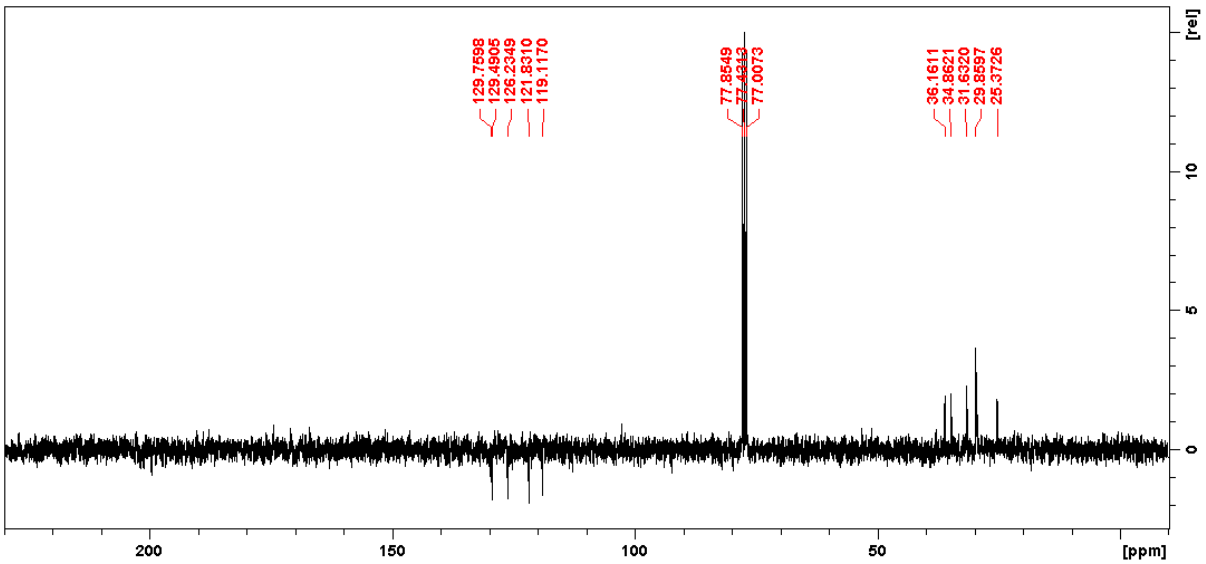
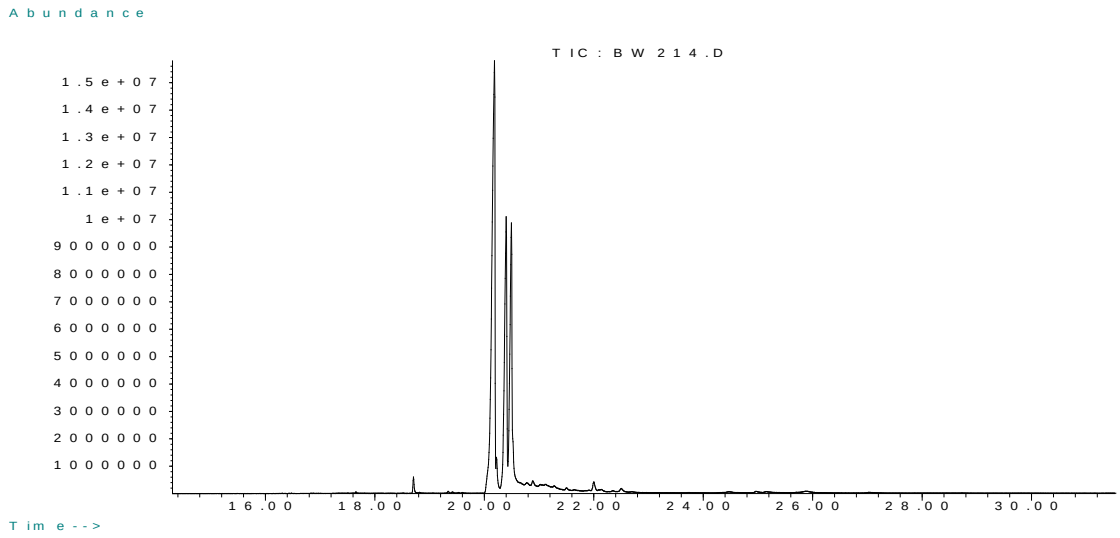
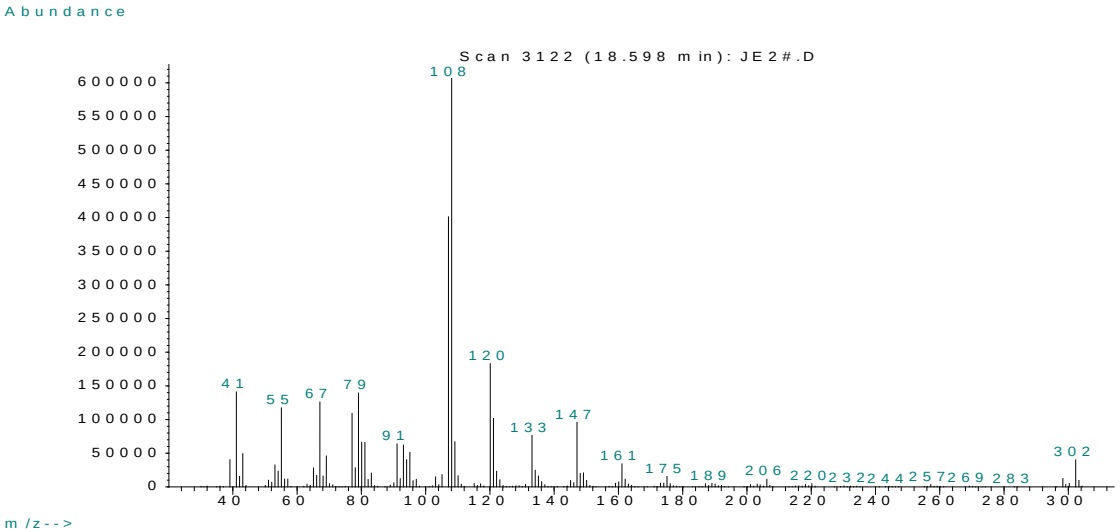


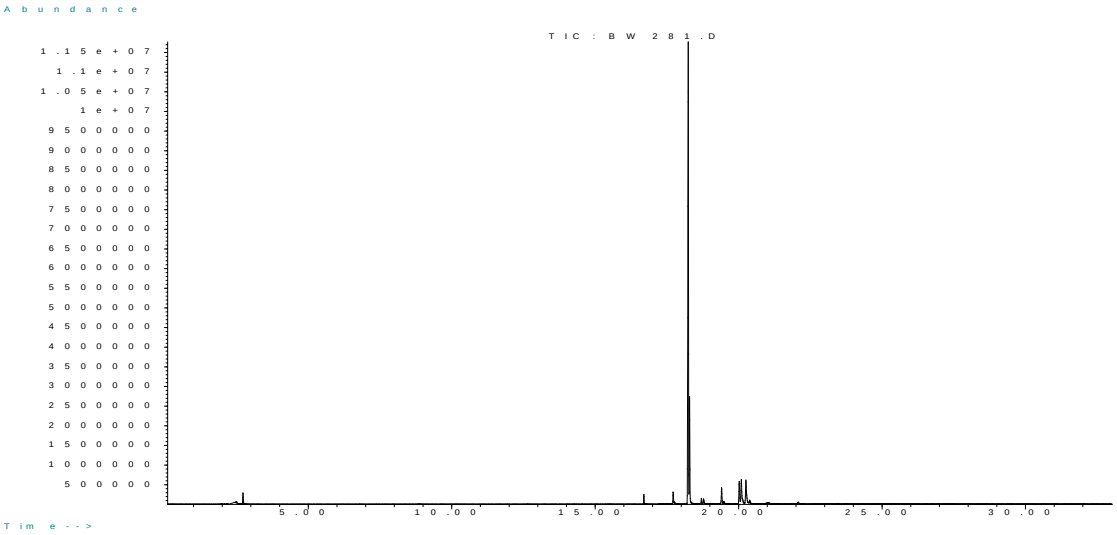
7 GC-MS spectra of cardanol and short chain derivatives of cardanol

7.1 HOPhC15-ene; Cardanol

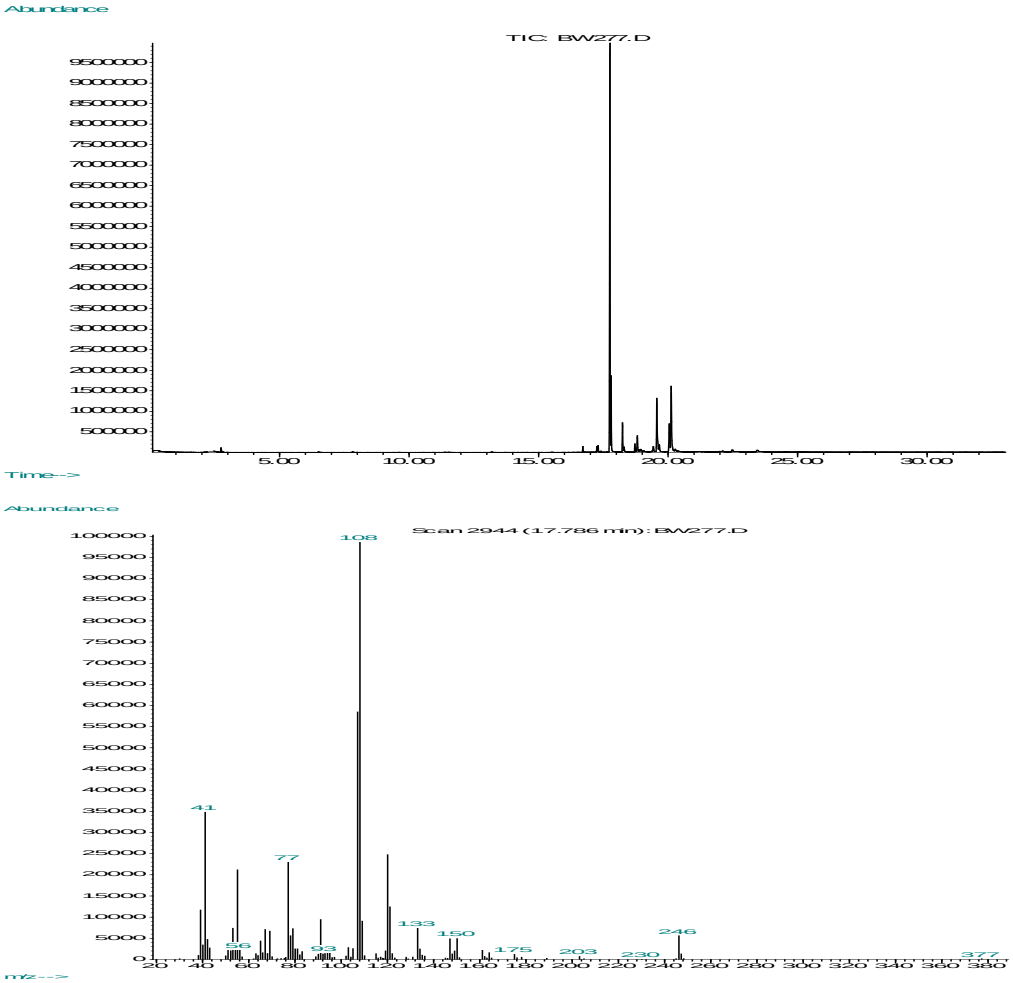




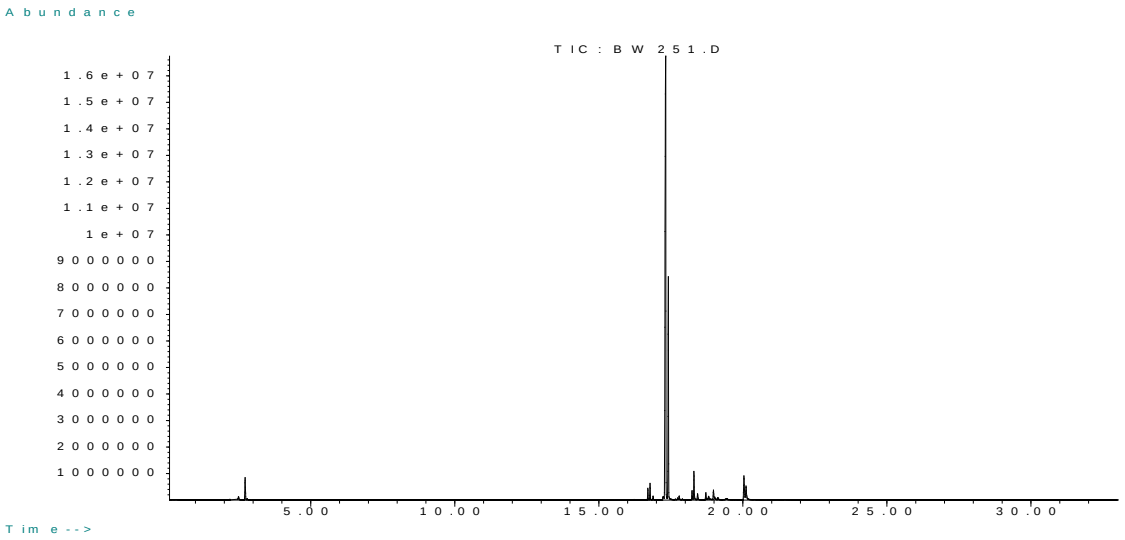
7.2 HOPhC12-ene; (E)-3-(dodec-8-en-1-yl)phenol; (oct-4-enolysis of cardanol)

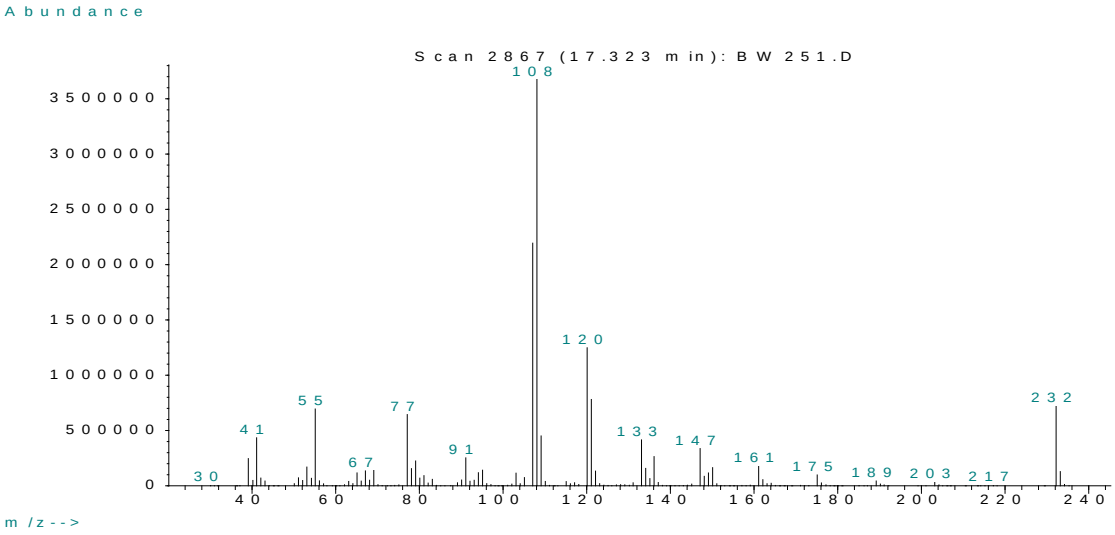


7.3 HOPhC11-ene; (E)-3-(undec-8-en-1-yl)phenol; (hex-3-enolysis of cardanol

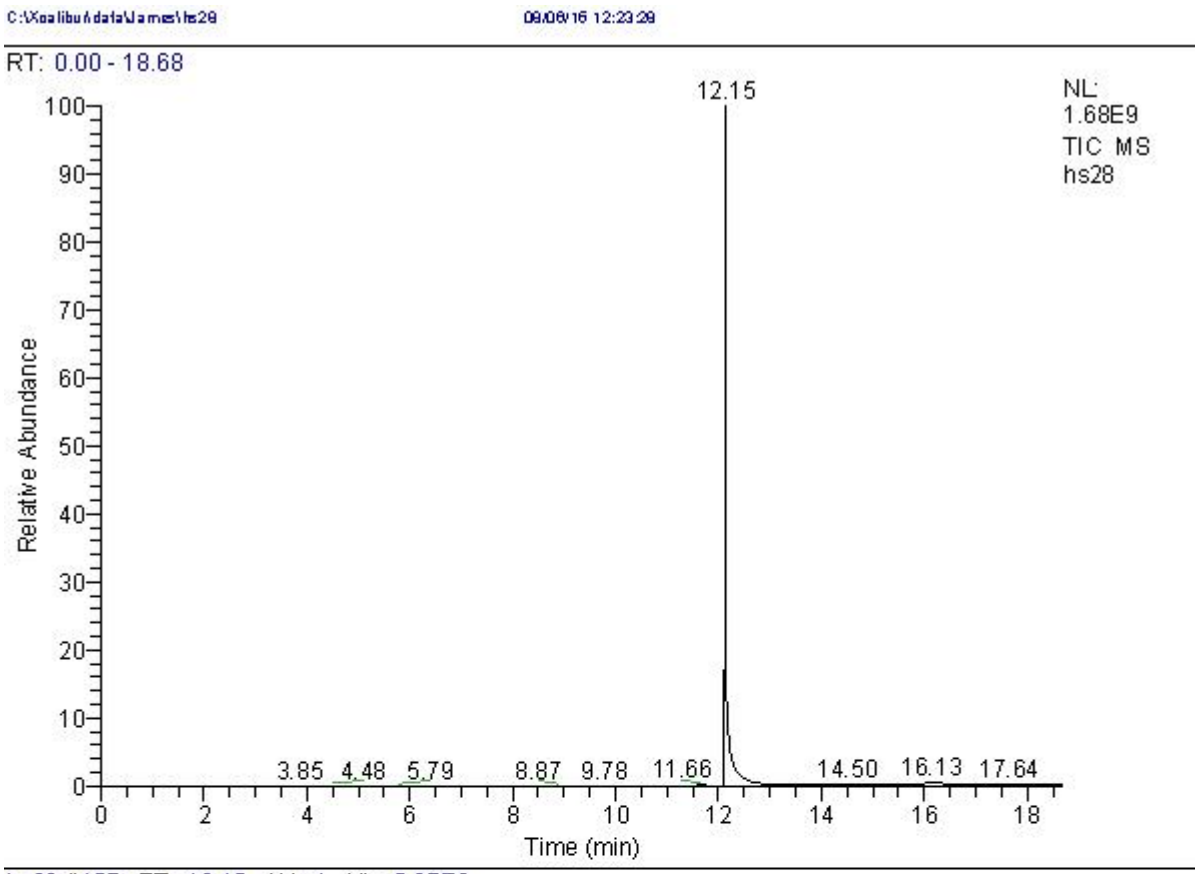


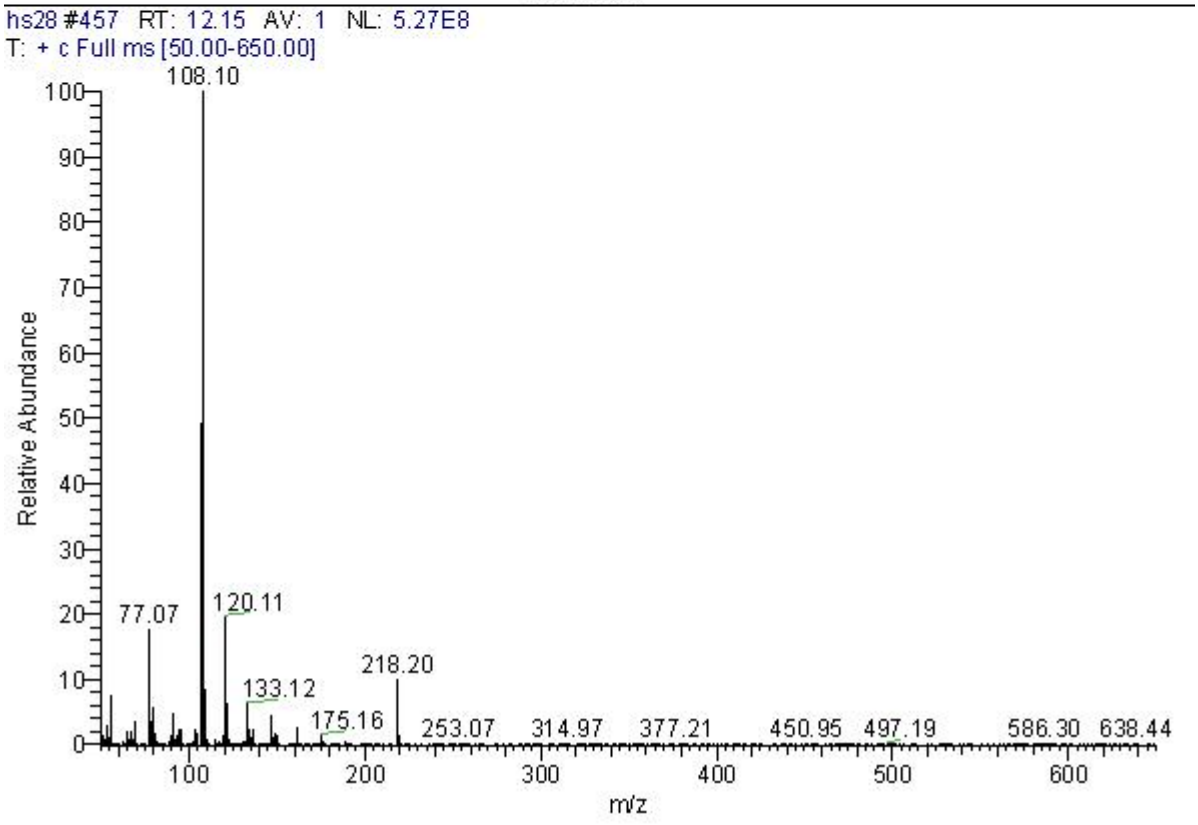
7.4 HOPhC10-ene; (E)-3-(dec-8-en-1-yl)phenol; (but-2-enolysis of cardanol)





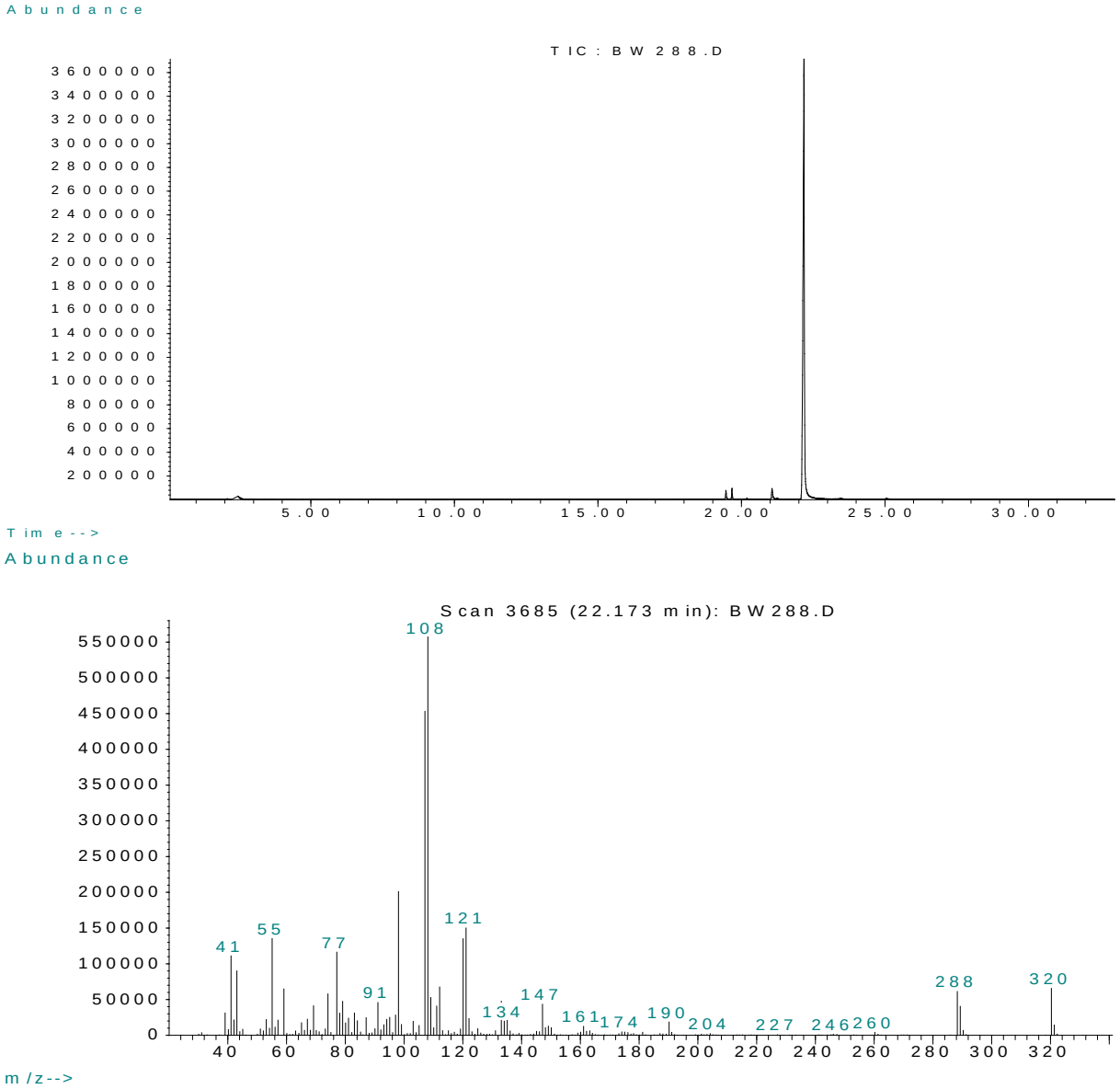
7.5 HOPhC9-ene; 3-(non-8-en-1-yl)phenol; (ethenolysis of cardanol)



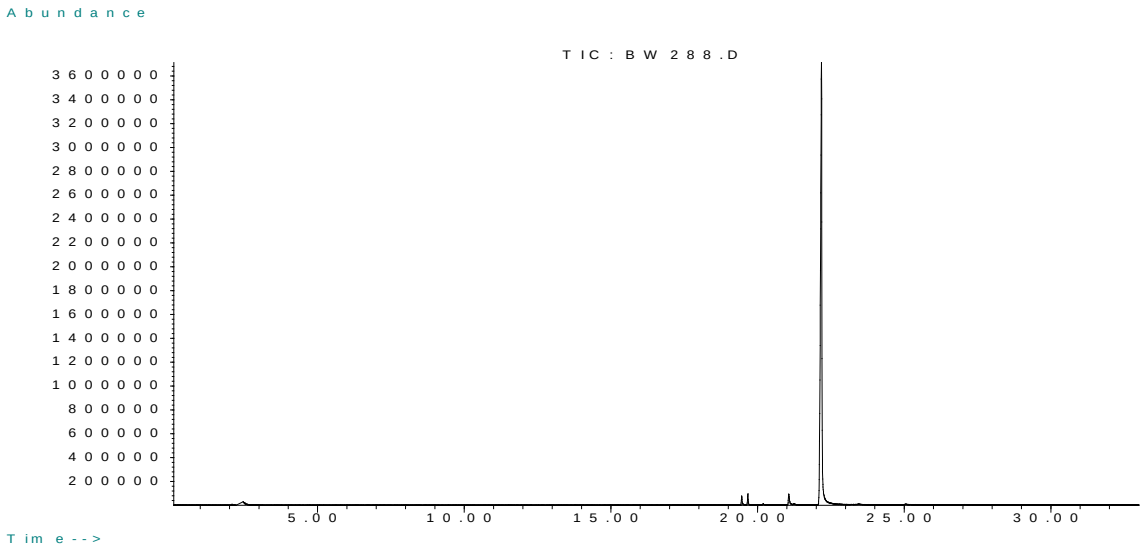


8 GC-MS spectra of Monomers

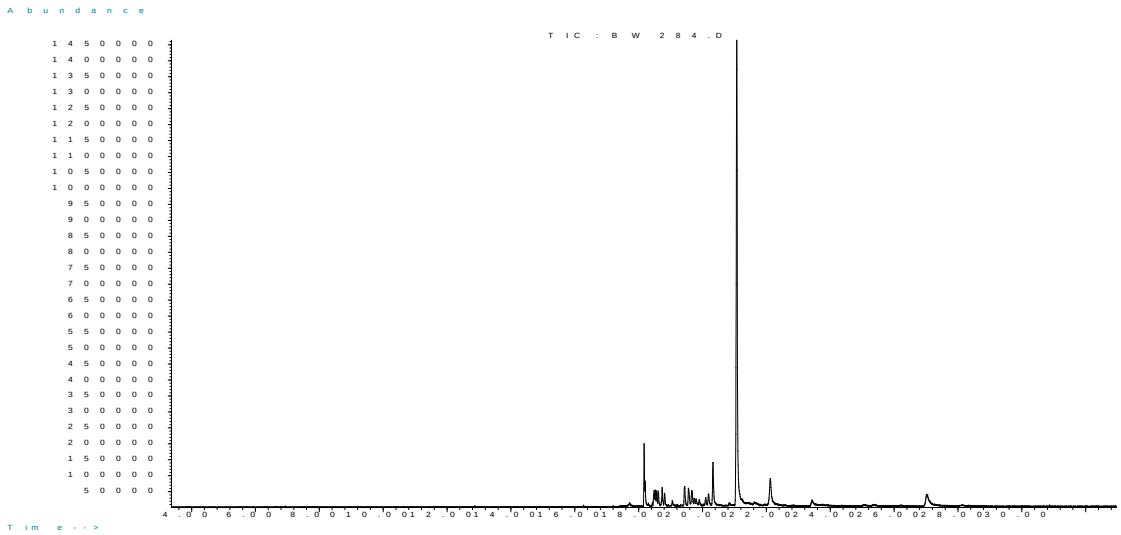
8.1 HOPhC15COOMe; Methyl 16-(3-hydroxyphenyl)hexadecanoate

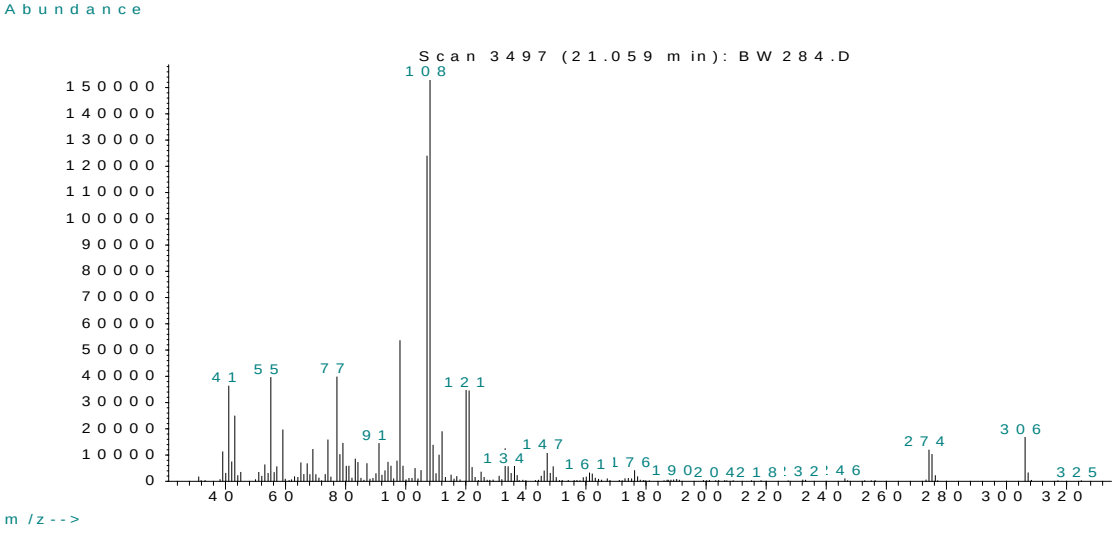


8.2 HOPhC12COOMe; Methyl 13-(3-hydroxyphenyl)tridecanoate

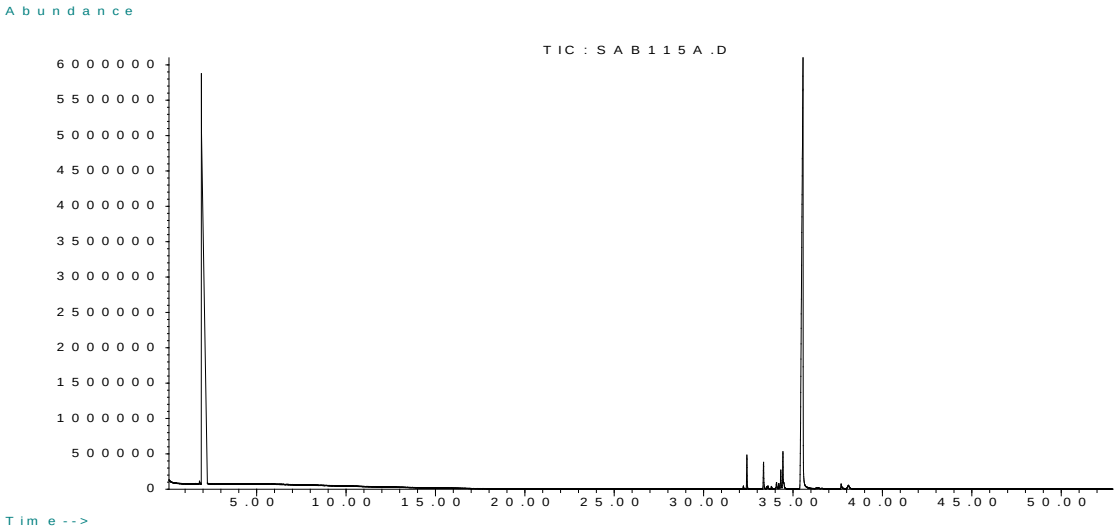


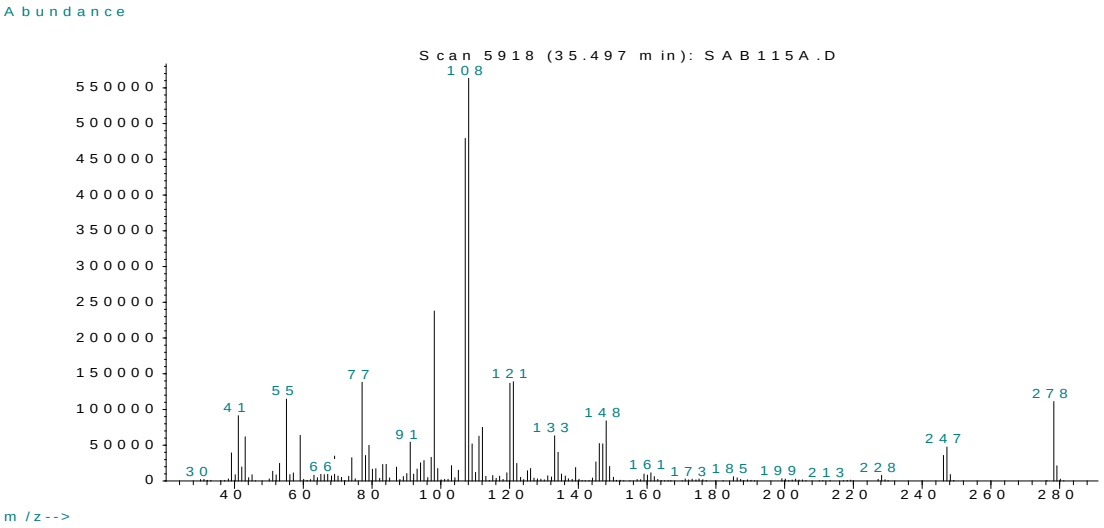
8.3 HOPhC11COOMe; Methyl 12-(3-hydroxyphenyl)dodecanoate



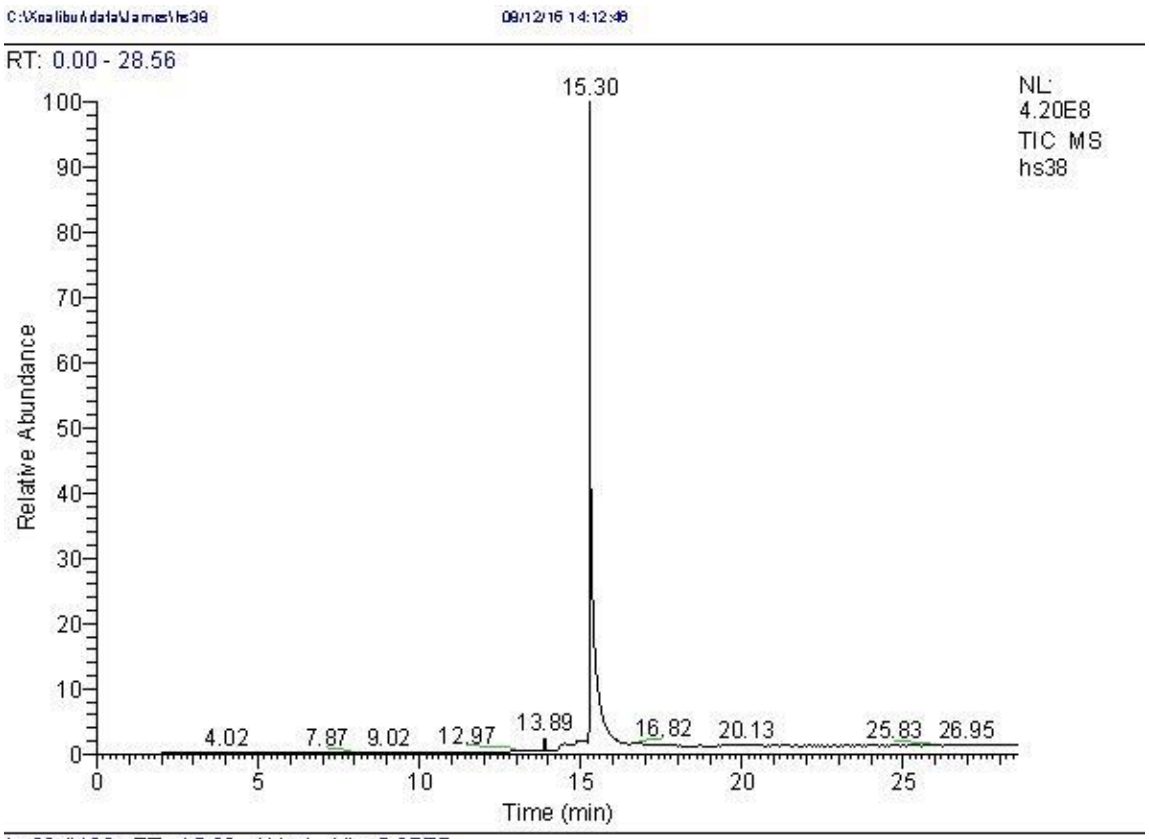


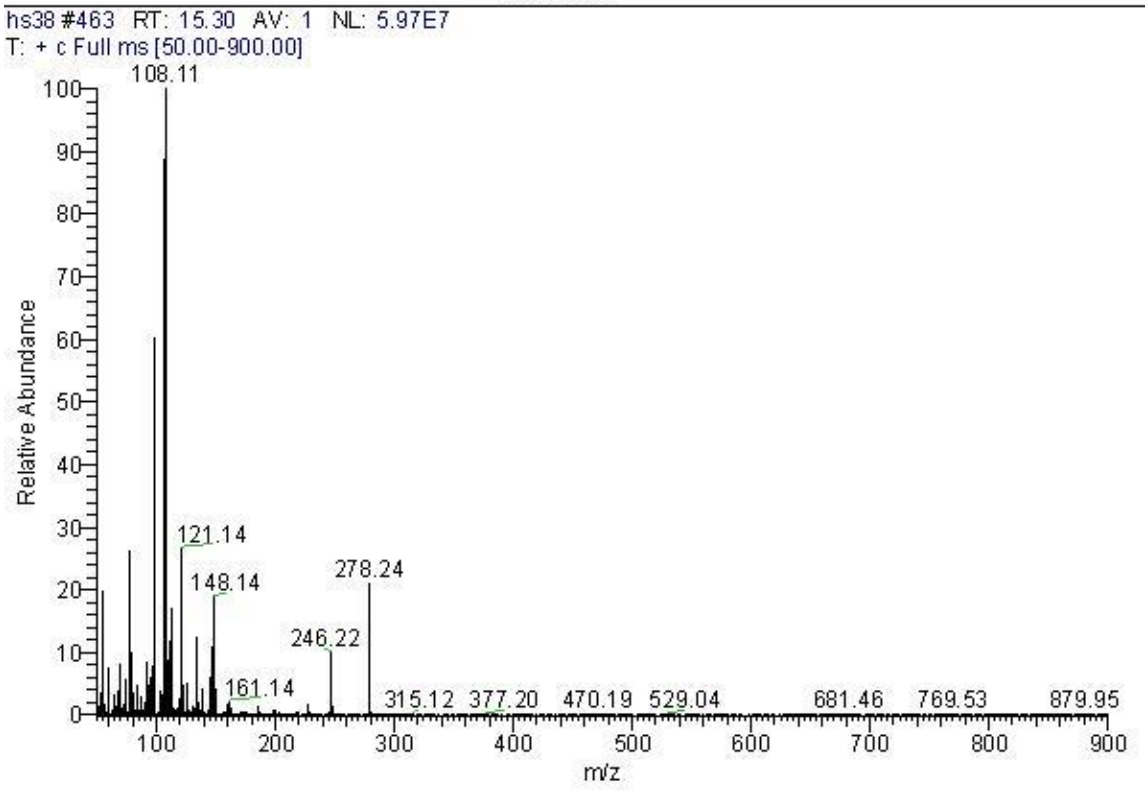
8.4 HOPhC10COOMe; Methyl 11-(3-hydroxyphenyl)undecanoate





8.5 HOPhC9COOMe; Methyl 10-(3-hydroxyphenyl)decanoate

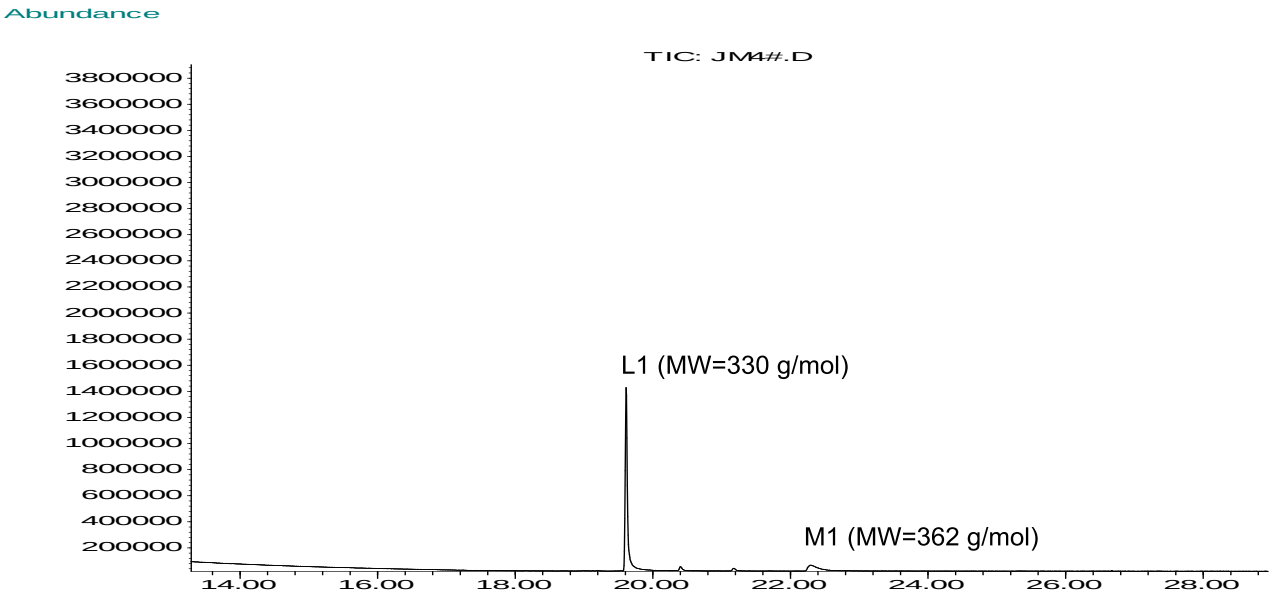




9 Formation of Lactones

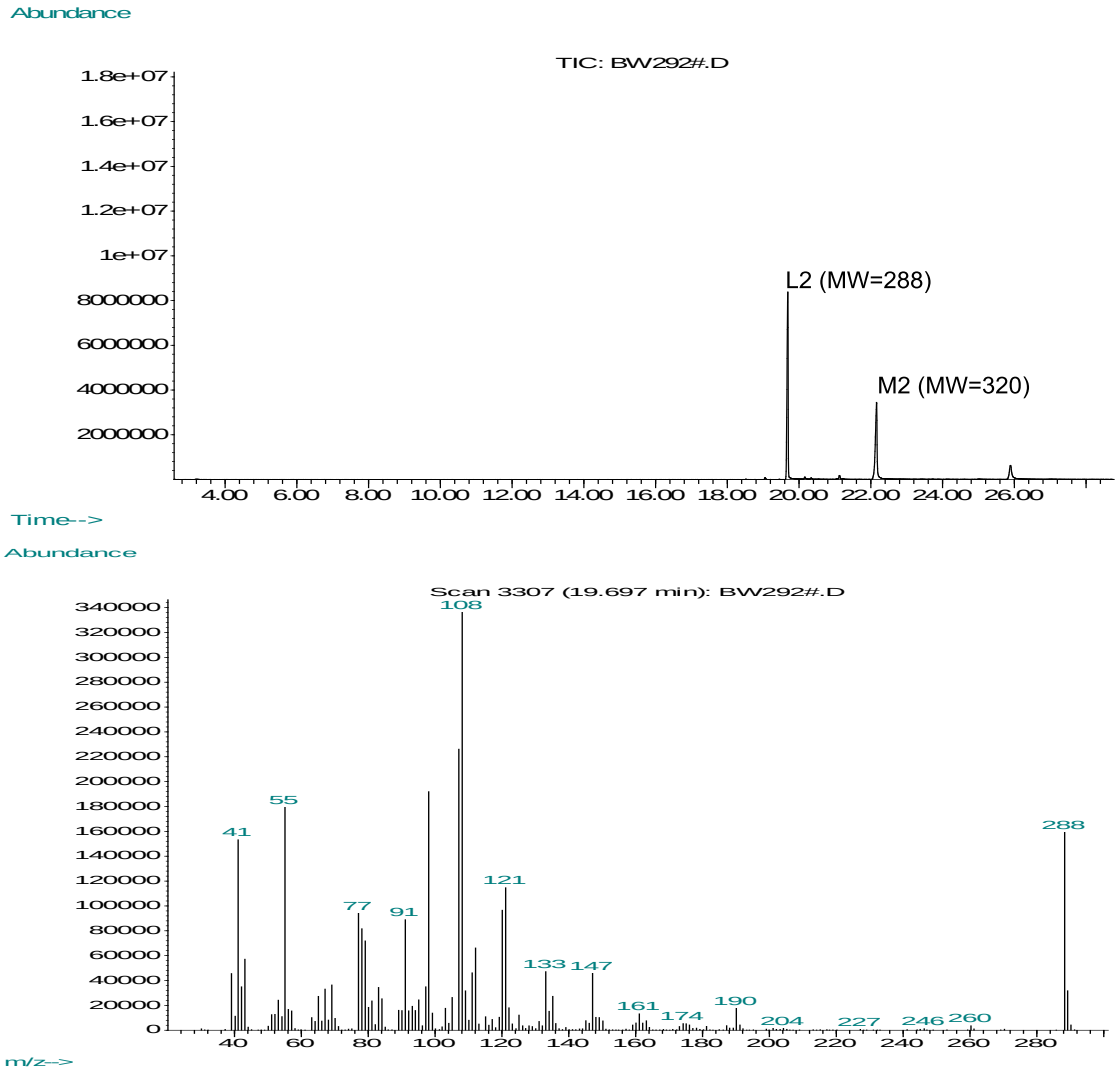
For the GCMS spectra below, L and M are respective peaks for lactones formed and starting monomers during polymerization reactions.

9.1 Cyclisation of HOPhC15COOMe

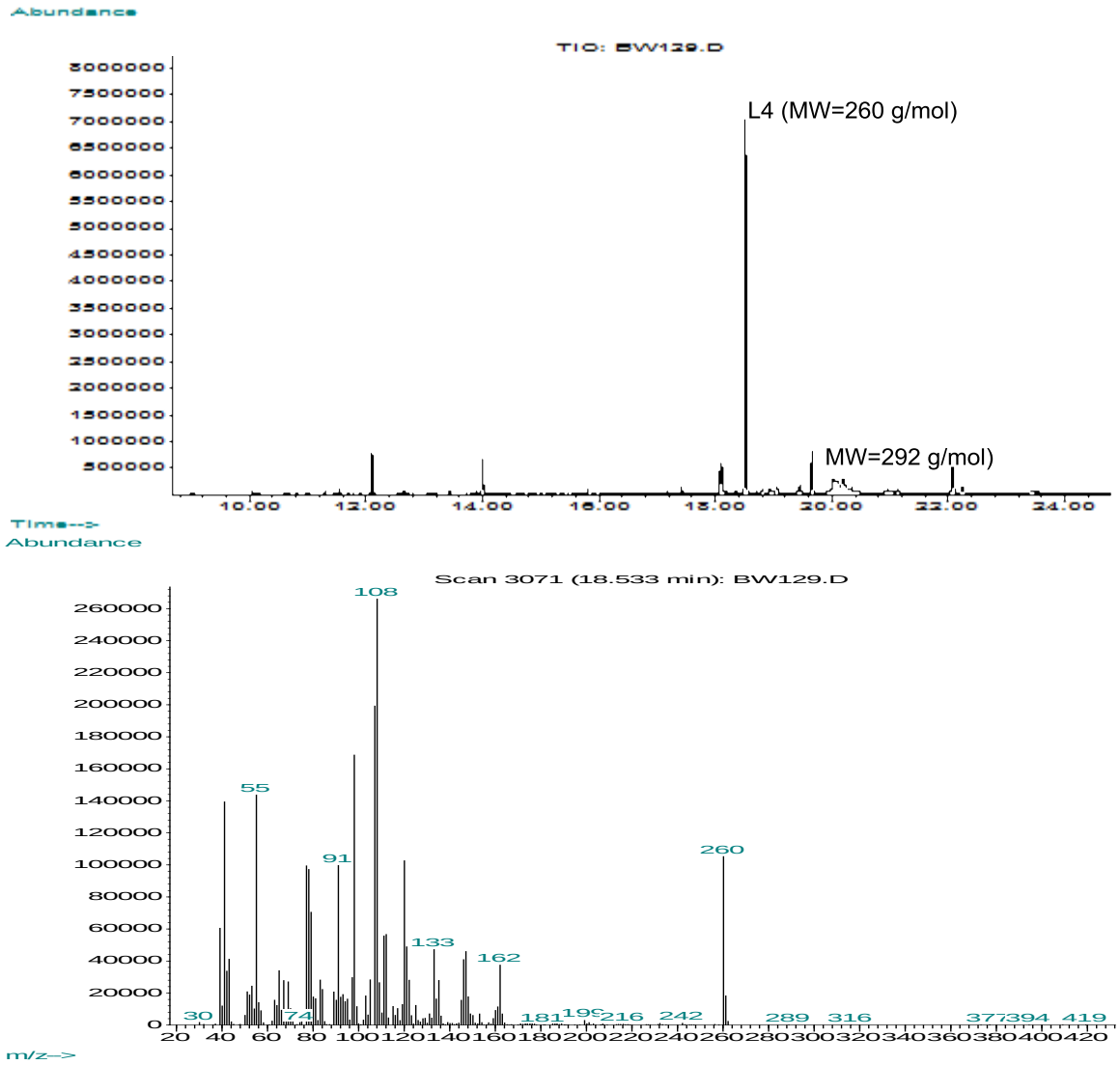


P

9.2 Cyclisation of HOPhC12COOMe



9.3 Cyclisation of HOPhC10COOMe



10 MALDI-TOF MS analysis of oligomers

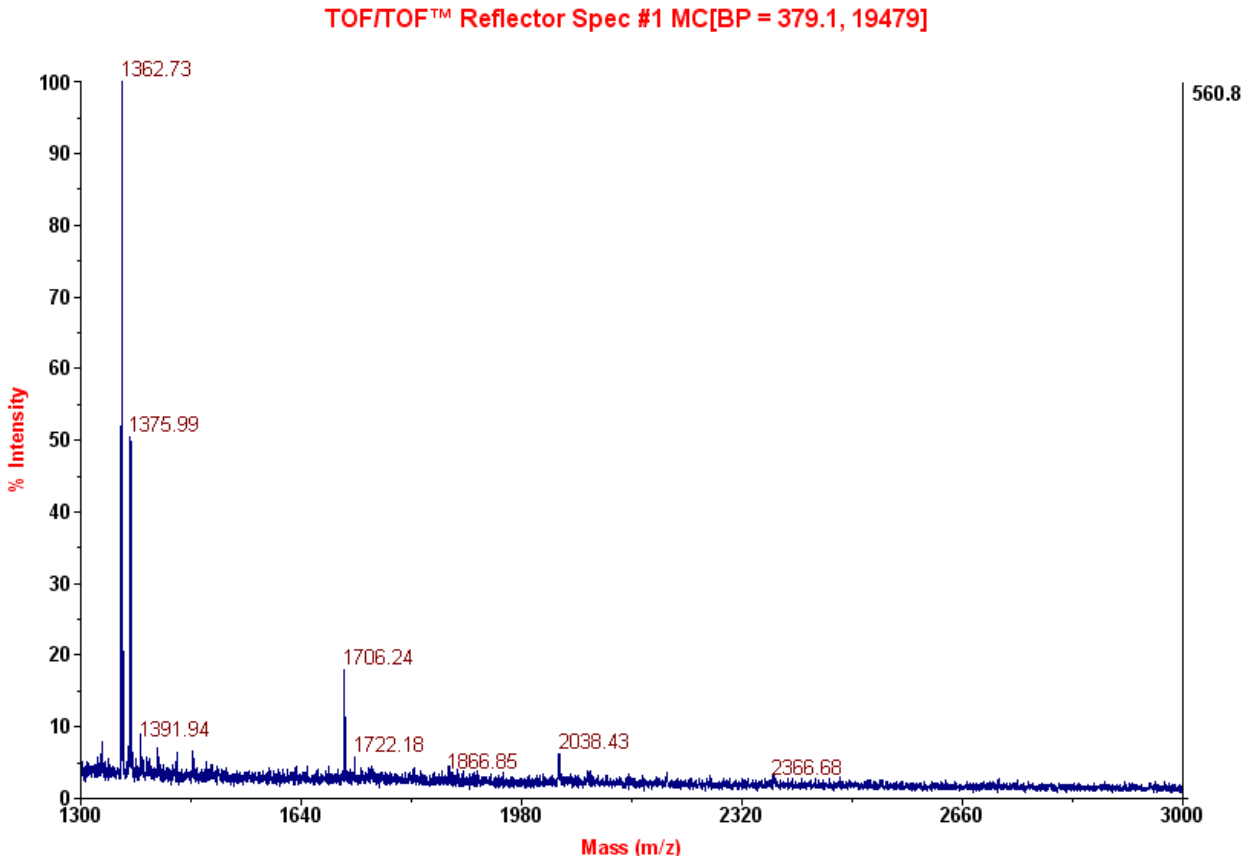


Figure S4. MALDI-TOF MS spectrum of oligomers from condensation reaction 16-(3-hydroxyphenyl) hexadecanoate. The peak 2366.68 corresponds to condensation of 7 monomers (2366.68-23=2343.68; 2343.68-32 = 2311.68; 2311.68/330=7). Other peaks: 2038.43, 1706.24, and 1375.99 correspond to condensation of 6, 5, and 4 monomers respectively.

11 X-ray crystal and molecular structure of Methyl 16-(3-hydroxyphenyl)hexadecanoate (6)

Data Collection

A colorless platelet crystal of $C_{23}H_{38}O_3$ having approximate dimensions of 0.100 x 0.100 x 0.010 mm was mounted in a loop. All measurements were made on a Rigaku Saturn70 diffractometer Cu-Kα radiation.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a = 5.4446(14) Å α = 96.276(11)^o

b = 7.879(2) Å β = 94.390(10)°
c = 25.390(7) Å γ = 98.942(11)°
V = 1064.6(5) Å^3

For Z = 2 and F.W. = 362.55, the calculated density is 1.131 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -100 ± 1°C to a maximum 2θ value of 135.1°.

Data Reduction

Of the 11397 reflections were collected, where 3380 were unique (R_{int} = 0.1278). Data were collected and processed using CrystalClear (Rigaku). [1]

The linear absorption coefficient, μ, for Cu-Kα radiation is 5.655 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically and the rest were refined using the riding model.The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 3380 observed reflections and 240 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.2377$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.5542$$

The goodness of fit[4] was 1.93. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.85 and -0.69 e$^-$/Å^3, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All

calculations were performed using the CrystalStructure[9] crystallographic software package except for refinement, which was performed using SHELXL2013[10].

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998-2014). Tokyo 196-8666, Japan.

(2) SHELXS97: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

(3) Least Squares function minimized: (SHELXL2013)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Goodness of fit is defined as:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 4.1: Crystal Structure Analysis Package, Rigaku Corporation (2000-2014). Tokyo 196-8666, Japan.

(10) SHELXL2013: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{23}H_{38}O_3$
Formula Weight	362.55
Crystal Color, Habit	colorless, platelet
Crystal Dimensions	0.100 X 0.100 X 0.010 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 5.4446(14) Å b = 7.879(2) Å c = 25.390(7) Å α = 96.276(11) ^{o} β = 94.390(10) ^{o} γ = 98.942(11) ^{o} V = 1064.6(5) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.131 g/cm^3
F_{000}	400.00
μ(CuKα)	5.655 cm^{-1}

B. Intensity Measurements

Diffractometer	Saturn70
Radiation	CuKα (λ = 1.54187 Å)
Voltage, Current	40kV, 20mA
Temperature	-100.0^{o}C
Detector Aperture	70.0 x 70.0 mm
Pixel Size	0.034 mm
$2\theta_{max}$	135.1^{o}
No. of Reflections Measured	Total: 11397 Unique: 3380 (R_{int} = 0.1278)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXS97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2(Fo^2) + (0.2000 \cdot P)^2 + 0.0000 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	135.1^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	3380
No. Variables	240
Reflection/Parameter Ratio	14.08
Residuals: R1 ($I>2.00\sigma(I)$)	0.2377
Residuals: R (All reflections)	0.2818
Residuals: wR2 (All reflections)	0.5542
Goodness of Fit Indicator	1.928
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.85 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.69 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O1	1.2280(13)	0.9234(10)	1.4366(2)	4.81(17)
O22	-0.8409(12)	0.3261(9)	0.6132(2)	3.99(15)
O23	-0.6091(12)	0.4031(10)	0.5489(3)	4.66(17)
C1	1.3762(17)	0.9849(12)	1.4009(3)	3.43(19)
C2	1.3176(16)	0.9537(12)	1.3468(3)	3.12(18)
C3	1.4810(17)	1.0163(12)	1.3111(3)	3.15(18)
C4	1.7036(18)	1.1153(13)	1.3323(4)	3.8(2)
C5	1.7655(19)	1.1492(15)	1.3856(4)	4.4(2)
C6	1.6053(19)	1.0848(14)	1.4206(4)	3.9(2)
C7	1.4247(17)	0.9749(13)	1.2520(3)	3.28(18)
C8	1.1567(17)	0.9257(14)	1.2287(4)	3.56(19)
C9	1.1308(18)	0.8977(14)	1.1671(4)	3.8(2)
C10	0.8630(18)	0.8480(14)	1.1421(4)	3.60(19)
C11	0.8449(17)	0.8255(14)	1.0824(4)	3.6(2)
C12	0.5848(18)	0.7849(14)	1.0547(4)	3.9(2)
C13	0.5641(19)	0.7570(16)	0.9948(4)	4.4(2)
C14	0.2965(19)	0.7128(15)	0.9679(4)	4.2(2)
C15	0.2876(19)	0.6868(14)	0.9080(4)	4.1(2)
C16	0.0294(17)	0.6400(14)	0.8793(4)	3.57(19)
C17	0.0201(18)	0.6227(15)	0.8189(4)	3.9(2)
C18	-0.235(2)	0.5642(15)	0.7891(4)	4.4(2)
C19	-0.2227(18)	0.5591(14)	0.7292(4)	3.62(19)
C20	-0.4665(17)	0.4859(13)	0.6953(4)	3.27(18)
C21	-0.4337(18)	0.4930(14)	0.6360(3)	3.43(19)
C22	-0.6485(16)	0.3977(13)	0.5999(4)	3.07(18)
C24	-0.799(2)	0.3144(16)	0.5097(4)	4.9(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1O	1.128(8)	0.813(3)	1.421(2)	0.9(13)
H2	1.16035	0.88710	1.33326	3.746
H4	1.81780	1.16136	1.30894	4.571
H5	1.92131	1.21828	1.39890	5.226
H6	1.65048	1.10823	1.45790	4.654
H7A	1.51307	0.87868	1.24034	3.938
H7B	1.49970	1.07693	1.23573	3.938
H8A	1.06258	1.01817	1.24085	4.270
H8B	1.08138	0.81793	1.24200	4.270
H9A	1.20717	1.00561	1.15393	4.506
H9B	1.22585	0.80560	1.15508	4.506
H10A	0.78700	0.73850	1.15442	4.325
H10B	0.76635	0.93889	1.15443	4.325
H11A	0.93626	0.73105	1.07053	4.368
H11B	0.93100	0.93305	1.07065	4.368
H12A	0.49533	0.88104	1.06580	4.708
H12B	0.49730	0.67939	1.06734	4.708
H13A	0.65525	0.66194	0.98351	5.313
H13B	0.64800	0.86318	0.98194	5.313
H14A	0.21168	0.60587	0.98024	5.022
H14B	0.20414	0.80754	0.97883	5.022
H15A	0.37145	0.79460	0.89601	4.938
H15B	0.38422	0.59403	0.89749	4.938
H16A	-0.06997	0.72956	0.89123	4.287
H16B	-0.05119	0.52887	0.88985	4.287
H17A	0.09059	0.73624	0.80841	4.635
H17B	0.12974	0.53939	0.80730	4.635
H18A	-0.34843	0.64440	0.80088	5.240
H18B	-0.30395	0.44741	0.79739	5.240
H19A	-0.16656	0.67841	0.72120	4.344
H19B	-0.09464	0.48901	0.71863	4.344
H20A	-0.59767	0.55337	0.70577	3.923
H20B	-0.52098	0.36437	0.70143	3.923
H21A	-0.40641	0.61562	0.62931	4.113
H21B	-0.28222	0.44438	0.62758	4.113
H24A	-0.95548	0.35766	0.51494	5.889
H24B	-0.82213	0.19010	0.51269	5.889

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H24C	-0.74956	0.33417	0.47421	5.889

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.065(5)	0.079(6)	0.029(4)	-0.021(4)	0.009(3)	0.005(3)
O22	0.038(4)	0.075(5)	0.030(3)	-0.009(3)	-0.001(3)	-0.000(3)
O23	0.050(4)	0.085(6)	0.035(4)	-0.009(4)	0.000(3)	0.004(3)
C1	0.047(6)	0.048(6)	0.032(5)	-0.007(5)	0.006(4)	0.012(4)
C2	0.038(5)	0.057(6)	0.017(4)	-0.004(4)	-0.008(3)	0.005(4)
C3	0.042(5)	0.051(6)	0.025(5)	0.005(4)	0.004(4)	0.003(4)
C4	0.045(5)	0.053(7)	0.049(6)	-0.000(5)	0.015(4)	0.019(4)
C5	0.043(6)	0.085(8)	0.032(5)	0.001(5)	-0.004(4)	0.000(5)
C6	0.056(6)	0.059(7)	0.033(5)	0.006(5)	0.002(4)	0.014(4)
C7	0.048(6)	0.044(6)	0.030(5)	0.002(4)	0.009(4)	-0.002(4)
C8	0.038(5)	0.056(7)	0.038(5)	-0.005(5)	0.004(4)	0.010(4)
C9	0.049(6)	0.064(7)	0.032(5)	0.006(5)	0.013(4)	0.013(4)
C10	0.050(6)	0.055(7)	0.032(5)	0.012(5)	0.010(4)	-0.005(4)
C11	0.042(5)	0.063(7)	0.035(5)	0.016(5)	-0.009(4)	0.015(4)
C12	0.042(6)	0.064(7)	0.041(6)	0.012(5)	-0.004(4)	-0.003(5)
C13	0.052(6)	0.079(8)	0.036(6)	0.005(6)	-0.000(4)	0.011(5)
C14	0.046(6)	0.062(7)	0.047(6)	-0.003(5)	0.003(5)	0.009(5)
C15	0.048(6)	0.060(7)	0.045(6)	0.004(5)	-0.004(5)	0.003(5)
C16	0.041(5)	0.056(7)	0.037(5)	0.001(5)	0.007(4)	0.008(4)
C17	0.038(5)	0.066(7)	0.043(6)	0.009(5)	0.008(4)	0.001(5)
C18	0.058(7)	0.065(8)	0.041(6)	0.008(5)	0.007(5)	0.005(5)
C19	0.042(5)	0.058(7)	0.034(5)	-0.002(5)	0.002(4)	0.009(4)
C20	0.043(5)	0.040(6)	0.040(5)	0.005(4)	0.003(4)	0.008(4)
C21	0.042(5)	0.057(7)	0.032(5)	0.008(5)	0.012(4)	0.004(4)
C22	0.027(5)	0.051(6)	0.041(5)	0.010(4)	0.006(4)	0.009(4)
C24	0.063(7)	0.088(9)	0.026(5)	-0.012(6)	0.004(5)	0.002(5)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C1	1.338(12)	O22	C22	1.201(11)
O23	C22	1.331(12)	O23	C24	1.420(11)
C1	C2	1.373(11)	C1	C6	1.393(13)
C2	C3	1.393(12)	C3	C4	1.371(12)
C3	C7	1.498(11)	C4	C5	1.357(13)
C5	C6	1.374(14)	C7	C8	1.508(12)
C8	C9	1.547(13)	C9	C10	1.519(13)
C10	C11	1.502(12)	C11	C12	1.503(13)
C12	C13	1.505(13)	C13	C14	1.532(14)
C14	C15	1.509(14)	C15	C16	1.506(13)
C16	C17	1.521(13)	C17	C18	1.509(14)
C18	C19	1.522(14)	C19	C20	1.522(12)
C20	C21	1.534(13)	C21	C22	1.479(12)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
O1	H1O	0.98(3)	C2	H2	0.950
C4	H4	0.950	C5	H5	0.950
C6	H6	0.950	C7	H7A	0.990
C7	H7B	0.990	C8	H8A	0.990
C8	H8B	0.990	C9	H9A	0.990
C9	H9B	0.990	C10	H10A	0.990
C10	H10B	0.990	C11	H11A	0.990
C11	H11B	0.990	C12	H12A	0.990
C12	H12B	0.990	C13	H13A	0.990
C13	H13B	0.990	C14	H14A	0.990
C14	H14B	0.990	C15	H15A	0.990
C15	H15B	0.990	C16	H16A	0.990
C16	H16B	0.990	C17	H17A	0.990
C17	H17B	0.990	C18	H18A	0.990
C18	H18B	0.990	C19	H19A	0.990
C19	H19B	0.990	C20	H20A	0.990
C20	H20B	0.990	C21	H21A	0.990
C21	H21B	0.990	C24	H24A	0.980
C24	H24B	0.980	C24	H24C	0.980

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C22	O23	C24	118.0(7)	O1	C1	C2	124.2(8)
O1	C1	C6	117.1(8)	C2	C1	C6	118.6(9)
C1	C2	C3	122.2(8)	C2	C3	C4	117.1(8)
C2	C3	C7	122.6(7)	C4	C3	C7	120.2(8)
C3	C4	C5	121.9(9)	C4	C5	C6	120.8(9)
C1	C6	C5	119.4(8)	C3	C7	C8	119.3(8)
C7	C8	C9	112.6(8)	C8	C9	C10	114.1(8)
C9	C10	C11	112.6(8)	C10	C11	C12	115.8(8)
C11	C12	C13	116.4(8)	C12	C13	C14	115.0(8)
C13	C14	C15	112.6(8)	C14	C15	C16	115.0(8)
C15	C16	C17	115.0(8)	C16	C17	C18	116.1(8)
C17	C18	C19	111.4(9)	C18	C19	C20	115.4(8)
C19	C20	C21	110.7(8)	C20	C21	C22	113.9(8)
O22	C22	O23	122.2(8)	O22	C22	C21	125.8(8)
O23	C22	C21	111.9(7)				

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	O1	H1O	109(3)	C1	C2	H2	118.9
C3	C2	H2	118.9	C3	C4	H4	119.1
C5	C4	H4	119.1	C4	C5	H5	119.6
C6	C5	H5	119.6	C1	C6	H6	120.3
C5	C6	H6	120.3	C3	C7	H7A	107.5
C3	C7	H7B	107.5	C8	C7	H7A	107.5
C8	C7	H7B	107.5	H7A	C7	H7B	107.0
C7	C8	H8A	109.1	C7	C8	H8B	109.1
C9	C8	H8A	109.1	C9	C8	H8B	109.1
H8A	C8	H8B	107.8	C8	C9	H9A	108.7
C8	C9	H9B	108.7	C10	C9	H9A	108.7
C10	C9	H9B	108.7	H9A	C9	H9B	107.6
C9	C10	H10A	109.1	C9	C10	H10B	109.1
C11	C10	H10A	109.1	C11	C10	H10B	109.1
H10A	C10	H10B	107.8	C10	C11	H11A	108.3
C10	C11	H11B	108.3	C12	C11	H11A	108.3
C12	C11	H11B	108.3	H11A	C11	H11B	107.4
C11	C12	H12A	108.2	C11	C12	H12B	108.2
C13	C12	H12A	108.2	C13	C12	H12B	108.2
H12A	C12	H12B	107.4	C12	C13	H13A	108.5
C12	C13	H13B	108.5	C14	C13	H13A	108.5
C14	C13	H13B	108.5	H13A	C13	H13B	107.5
C13	C14	H14A	109.1	C13	C14	H14B	109.1
C15	C14	H14A	109.1	C15	C14	H14B	109.1
H14A	C14	H14B	107.8	C14	C15	H15A	108.5
C14	C15	H15B	108.5	C16	C15	H15A	108.5
C16	C15	H15B	108.5	H15A	C15	H15B	107.5
C15	C16	H16A	108.5	C15	C16	H16B	108.5
C17	C16	H16A	108.5	C17	C16	H16B	108.5
H16A	C16	H16B	107.5	C16	C17	H17A	108.3
C16	C17	H17B	108.3	C18	C17	H17A	108.3
C18	C17	H17B	108.3	H17A	C17	H17B	107.4
C17	C18	H18A	109.4	C17	C18	H18B	109.4
C19	C18	H18A	109.4	C19	C18	H18B	109.4
H18A	C18	H18B	108.0	C18	C19	H19A	108.4
C18	C19	H19B	108.4	C20	C19	H19A	108.4
C20	C19	H19B	108.4	H19A	C19	H19B	107.5

Table 7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C19	C20	H20A	109.5	C19	C20	H20B	109.5
C21	C20	H20A	109.5	C21	C20	H20B	109.5
H20A	C20	H20B	108.1	C20	C21	H21A	108.8
C20	C21	H21B	108.8	C22	C21	H21A	108.8
C22	C21	H21B	108.8	H21A	C21	H21B	107.7
O23	C24	H24A	109.5	O23	C24	H24B	109.5
O23	C24	H24C	109.5	H24A	C24	H24B	109.5
H24A	C24	H24C	109.5	H24B	C24	H24C	109.5

Table 8. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C24	O23	C22	O22	-2.7(15)	C24	O23	C22	C21	179.0(8)
O1	C1	C2	C3	-178.1(8)	O1	C1	C6	C5	179.2(8)
C2	C1	C6	C5	0.1(15)	C6	C1	C2	C3	1.0(15)
C1	C2	C3	C4	-1.5(14)	C1	C2	C3	C7	176.6(8)
C2	C3	C4	C5	1.0(15)	C2	C3	C7	C8	24.2(14)
C4	C3	C7	C8	-157.8(9)	C7	C3	C4	C5	-177.1(8)
C3	C4	C5	C6	0.0(17)	C4	C5	C6	C1	-0.6(17)
C3	C7	C8	C9	176.6(8)	C7	C8	C9	C10	-180.0(8)
C8	C9	C10	C11	178.8(8)	C9	C10	C11	C12	-177.0(8)
C10	C11	C12	C13	-178.3(8)	C11	C12	C13	C14	179.0(8)
C12	C13	C14	C15	179.8(9)	C13	C14	C15	C16	179.0(8)
C14	C15	C16	C17	177.1(8)	C15	C16	C17	C18	176.1(8)
C16	C17	C18	C19	177.5(8)	C17	C18	C19	C20	174.6(8)
C18	C19	C20	C21	178.1(8)	C19	C20	C21	C22	170.2(8)
C20	C21	C22	O22	3.5(15)	C20	C21	C22	O23	-178.2(8)

Table 9. Possible hydrogen bonds

Donor	H	Acceptor	D...A	D-H	H...A	D-H...A
O1	H1O	O22[1]	2.769(9)	0.98(3)	1.85(4)	154(4)

Symmetry Operators:

(1) -X,-Y+1,-Z+2

Table 10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C5	3.587(13)	O22	C20	2.838(10)
O22	C24	2.650(11)	C1	C4	2.752(14)
C2	C5	2.724(13)	C2	C8	3.035(12)
C3	C6	2.784(12)			

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H2	2.599	O1	H6	2.510
O22	H20A	2.889	O22	H20B	2.689
O22	H21A	2.989	O22	H21B	3.021
O22	H24A	2.574	O22	H24B	2.674
O23	H21A	2.553	O23	H21B	2.529
C1	H5	3.247	C2	H1O	2.49(5)
C2	H4	3.222	C2	H6	3.241
C2	H7A	3.013	C2	H7B	3.257
C2	H8A	3.061	C2	H8B	2.882
C3	H5	3.235	C3	H8A	2.787
C3	H8B	2.831	C4	H2	3.217
C4	H6	3.230	C4	H7A	2.842
C4	H7B	2.579	C6	H1O	3.10(4)
C6	H2	3.235	C6	H4	3.225
C7	H2	2.695	C7	H4	2.629
C7	H9A	2.726	C7	H9B	2.726
C8	H2	2.705	C8	H10A	2.769
C8	H10B	2.753	C9	H7A	2.717
C9	H7B	2.667	C9	H11A	2.706
C9	H11B	2.663	C10	H8A	2.767
C10	H8B	2.767	C10	H12A	2.740
C10	H12B	2.717	C11	H9A	2.688
C11	H9B	2.704	C11	H13A	2.740
C11	H13B	2.754	C12	H10A	2.767
C12	H10B	2.727	C12	H14A	2.762
C12	H14B	2.760	C13	H11A	2.731
C13	H11B	2.755	C13	H15A	2.709
C13	H15B	2.694	C14	H12A	2.744
C14	H12B	2.729	C14	H16A	2.708
C14	H16B	2.749	C15	H13A	2.709
C15	H13B	2.706	C15	H17A	2.762
C15	H17B	2.707	C16	H14A	2.733
C16	H14B	2.747	C16	H18A	2.758
C16	H18B	2.792	C17	H15A	2.715
C17	H15B	2.756	C17	H19A	2.715
C17	H19B	2.635	C18	H16A	2.788
C18	H16B	2.735	C18	H20A	2.766

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C18	H20B	2.792	C19	H17A	2.650
C19	H17B	2.686	C19	H21A	2.762
C19	H21B	2.618	C20	H18A	2.814
C20	H18B	2.739	C21	H19A	2.663
C21	H19B	2.692	C22	H20A	2.805
C22	H20B	2.671	C22	H24A	2.584
C22	H24B	2.622	C22	H24C	3.167
H1O	H2	2.364	H1O	H6	3.383
H2	H7A	3.156	H2	H7B	3.526
H2	H8A	2.714	H2	H8B	2.313
H4	H5	2.288	H4	H7A	2.882
H4	H7B	2.403	H5	H6	2.323
H7A	H8A	2.840	H7A	H8B	2.329
H7A	H9A	3.004	H7A	H9B	2.528
H7B	H8A	2.369	H7B	H8B	2.839
H7B	H9A	2.475	H7B	H9B	2.928
H8A	H9A	2.396	H8A	H9B	2.881
H8A	H10A	3.055	H8A	H10B	2.579
H8B	H9A	2.881	H8B	H9B	2.396
H8B	H10A	2.597	H8B	H10B	3.030
H9A	H10A	2.859	H9A	H10B	2.377
H9A	H11A	2.978	H9A	H11B	2.458
H9B	H10A	2.364	H9B	H10B	2.859
H9B	H11A	2.521	H9B	H11B	2.937
H10A	H11A	2.335	H10A	H11B	2.843
H10A	H12A	3.067	H10A	H12B	2.570
H10B	H11A	2.843	H10B	H11B	2.369
H10B	H12A	2.551	H10B	H12B	2.967
H11A	H12A	2.836	H11A	H12B	2.355
H11A	H13A	2.545	H11A	H13B	3.014
H11B	H12A	2.335	H11B	H12B	2.836
H11B	H13A	3.029	H11B	H13B	2.585
H12A	H13A	2.839	H12A	H13B	2.342
H12A	H14A	3.037	H12A	H14B	2.574
H12B	H13A	2.354	H12B	H13B	2.839
H12B	H14A	2.561	H12B	H14B	3.011
H13A	H14A	2.380	H13A	H14B	2.868

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H13A	H15A	2.983	H13A	H15B	2.498
H13B	H14A	2.868	H13B	H14B	2.382
H13B	H15A	2.511	H13B	H15B	2.957
H14A	H15A	2.849	H14A	H15B	2.365
H14A	H16A	2.971	H14A	H16B	2.570
H14B	H15A	2.353	H14B	H15B	2.849
H14B	H16A	2.542	H14B	H16B	3.057
H15A	H16A	2.369	H15A	H16B	2.842
H15A	H17A	2.556	H15A	H17B	2.929
H15B	H16A	2.842	H15B	H16B	2.335
H15B	H17A	3.080	H15B	H17B	2.542
H16A	H17A	2.341	H16A	H17B	2.852
H16A	H18A	2.613	H16A	H18B	3.121
H16B	H17A	2.852	H16B	H17B	2.387
H16B	H18A	2.983	H16B	H18B	2.592
H17A	H18A	2.374	H17A	H18B	2.850
H17A	H19A	2.485	H17A	H19B	2.842
H17B	H18A	2.850	H17B	H18B	2.345
H17B	H19A	3.019	H17B	H19B	2.440
H18A	H19A	2.343	H18A	H19B	2.860
H18A	H20A	2.647	H18A	H20B	3.147
H18B	H19A	2.860	H18B	H19B	2.404
H18B	H20A	2.989	H18B	H20B	2.594
H19A	H20A	2.385	H19A	H20B	2.862
H19A	H21A	2.544	H19A	H21B	2.810
H19B	H20A	2.863	H19B	H20B	2.363
H19B	H21A	3.074	H19B	H21B	2.421
H20A	H21A	2.335	H20A	H21B	2.870
H20B	H21A	2.871	H20B	H21B	2.445

Table 12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	O22[1]	2.769(9)	O1	O23[2]	3.579(11)
O1	C5[3]	3.546(14)	O1	C24[4]	3.447(14)
O1	C24[1]	3.244(13)	O22	O1[1]	2.769(9)
O22	C1[1]	3.472(11)	O22	C2[1]	3.426(11)
O23	O1[2]	3.579(11)	O23	O23[5]	3.261(10)
O23	C24[5]	3.434(13)	C1	O22[1]	3.472(11)
C1	C22[2]	3.560(15)	C2	O22[1]	3.426(11)
C5	O1[6]	3.546(14)	C22	C1[2]	3.560(15)
C24	O1[7]	3.447(14)	C24	O1[1]	3.244(13)
C24	O23[5]	3.434(13)			

Symmetry Operators:

(1) -X,-Y+1,-Z+2
(2) -X+1,-Y+1,-Z+2
(3) X-1,Y,Z
(4) X+2,Y+1,Z+1
(5) -X-1,-Y+1,-Z+1
(6) X+1,Y,Z
(7) X-2,Y-1,Z-1

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H5[1]	3.248	O1	H6[2]	2.758
O1	H21B[3]	3.232	O1	H24A[4]	2.911
O1	H24B[5]	2.756	O1	H24B[4]	2.723
O1	H24C[5]	3.253	O22	H1O[4]	1.85(4)
O22	H2[4]	2.765	O22	H19B[1]	3.329
O22	H21B[1]	2.744	O23	H1O[4]	3.26(4)
O23	H1O[3]	3.42(4)	O23	H24C[6]	2.762
C1	H5[1]	3.307	C1	H21A[7]	3.303
C1	H21B[3]	3.331	C1	H24B[5]	3.441
C1	H24C[5]	3.341	C2	H4[1]	3.512
C2	H5[1]	3.462	C2	H20B[3]	3.067
C2	H21A[7]	3.334	C2	H21B[3]	3.252
C3	H19A[7]	3.299	C3	H20A[7]	3.431
C3	H20B[3]	3.025	C3	H21A[7]	3.219
C4	H2[8]	3.287	C4	H8A[8]	3.250
C4	H19A[9]	3.251	C4	H20A[7]	3.003
C4	H21A[7]	2.987	C5	H2[8]	3.446
C5	H21A[7]	2.927	C5	H24C[10]	3.367
C6	H21A[7]	3.097	C6	H24A[10]	3.532
C6	H24B[5]	3.547	C6	H24B[3]	3.200
C6	H24C[5]	3.232	C7	H8A[8]	3.473
C7	H10B[8]	3.224	C7	H18A[7]	3.486
C7	H18B[3]	3.370	C7	H19A[7]	3.291
C7	H20B[3]	3.138	C8	H4[1]	3.438
C8	H7A[1]	3.505	C8	H17A[7]	3.356
C8	H18A[7]	3.564	C8	H18B[3]	3.180
C8	H19A[7]	3.228	C9	H10B[8]	3.468
C9	H12A[8]	3.370	C9	H16A[7]	3.479
C9	H16B[3]	3.459	C9	H17A[7]	3.311
C9	H18B[3]	3.210	C10	H7A[1]	3.262
C10	H9B[1]	3.477	C10	H15A[7]	3.467
C10	H15B[3]	3.539	C10	H16A[7]	3.559
C10	H16B[3]	3.328	C10	H17A[7]	3.342
C10	H17B[3]	3.443	C11	H12A[8]	3.563
C11	H14A[3]	3.548	C11	H14B[8]	3.398
C11	H14B[7]	3.465	C11	H15A[7]	3.389
C11	H15B[3]	3.453	C11	H16A[7]	3.503

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C11	H16B^{3}	3.292	C12	H9B^{1}	3.334
C12	H11A^{1}	3.550	C12	H13A^{3}	3.560
C12	H13B^{7}	3.411	C12	H14A^{3}	3.480
C12	H14B^{7}	3.458	C12	H15A^{7}	3.377
C12	H15B^{3}	3.367	C13	H12A^{7}	3.432
C13	H12B^{3}	3.578	C13	H13A^{3}	3.449
C13	H13B^{7}	3.381	C13	H14A^{3}	3.380
C13	H14B^{8}	3.506	C13	H14B^{7}	3.440
C13	H16A^{8}	3.428	C14	H11A^{1}	3.383
C14	H11A^{3}	3.532	C14	H11B^{7}	3.430
C14	H12A^{7}	3.446	C14	H12B^{3}	3.498
C14	H13A^{1}	3.510	C14	H13A^{3}	3.361
C14	H13B^{7}	3.402	C15	H10A^{3}	3.496
C15	H10B^{7}	3.538	C15	H11A^{3}	3.445
C15	H11B^{7}	3.396	C15	H12A^{7}	3.401
C15	H12B^{3}	3.379	C15	H16A^{8}	3.524
C15	H18A^{8}	3.503	C16	H9A^{7}	3.411
C16	H9B^{3}	3.556	C16	H10A^{3}	3.335
C16	H10B^{7}	3.550	C16	H11A^{3}	3.339
C16	H11B^{7}	3.432	C16	H13A^{1}	3.466
C16	H15B^{1}	3.546	C17	H8A^{7}	3.427
C17	H8B^{3}	3.584	C17	H9A^{7}	3.376
C17	H9B^{3}	3.582	C17	H10A^{3}	3.302
C17	H10B^{7}	3.444	C17	H18A^{8}	3.484
C18	H7A^{3}	3.555	C18	H7B^{7}	3.462
C18	H8A^{7}	3.461	C18	H8B^{3}	3.279
C18	H9A^{7}	3.513	C18	H9B^{3}	3.382
C18	H15B^{1}	3.581	C18	H17B^{1}	3.504
C19	H4^{9}	3.152	C19	H7B^{7}	3.504
C19	H8A^{7}	3.297	C19	H8B^{3}	3.324
C19	H20A^{8}	3.506	C20	H7A^{3}	3.442
C20	H19B^{1}	3.519	C21	H1O^{3}	3.39(4)
C21	H5^{9}	3.548	C21	H24C^{6}	3.395
C22	H1O^{4}	2.85(4)	C22	H1O^{3}	3.54(4)
C22	H5^{7}	3.570	C22	H24C^{6}	3.573
C24	H1O^{4}	2.77(5)	C24	H5^{11}	3.053
C24	H6^{11}	3.282	C24	H6^{12}	3.407

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C24	H24A^{13}	3.187	H1O	O22^{4}	1.85(4)
H1O	O23^{4}	3.26(4)	H1O	O23^{3}	3.42(4)
H1O	C21^{3}	3.39(4)	H1O	C22^{4}	2.85(4)
H1O	C22^{3}	3.54(4)	H1O	C24^{4}	2.77(5)
H1O	H6^{2}	3.185	H1O	H21B^{3}	2.540
H1O	H24A^{4}	2.388	H1O	H24B^{5}	3.537
H1O	H24B^{4}	2.467	H2	O22^{4}	2.765
H2	C4^{1}	3.287	H2	C5^{1}	3.446
H2	H4^{1}	3.146	H2	H5^{1}	3.423
H2	H19B^{3}	3.064	H2	H20B^{3}	3.106
H2	H21B^{3}	3.042	H4	C2^{8}	3.512
H4	C8^{8}	3.438	H4	C19^{9}	3.152
H4	H2^{8}	3.146	H4	H8A^{8}	2.536
H4	H8B^{8}	3.584	H4	H17A^{9}	3.226
H4	H19A^{9}	2.340	H4	H19B^{9}	3.105
H4	H20A^{7}	2.753	H4	H21A^{7}	3.424
H4	H21A^{9}	3.563	H5	O1^{8}	3.248
H5	C1^{8}	3.307	H5	C2^{8}	3.462
H5	C21^{9}	3.548	H5	C22^{7}	3.570
H5	C24^{10}	3.053	H5	H2^{8}	3.423
H5	H19A^{9}	3.546	H5	H21A^{7}	3.335
H5	H21A^{9}	2.936	H5	H21B^{9}	3.217
H5	H24A^{10}	3.016	H5	H24B^{10}	3.157
H5	H24C^{10}	2.507	H6	O1^{2}	2.758
H6	C24^{5}	3.407	H6	C24^{10}	3.282
H6	H1O^{2}	3.185	H6	H6^{2}	3.260
H6	H21A^{7}	3.592	H6	H24A^{10}	2.855
H6	H24B^{5}	3.137	H6	H24B^{10}	3.035
H6	H24B^{3}	2.814	H6	H24C^{5}	3.044
H6	H24C^{10}	3.440	H7A	C8^{8}	3.505
H7A	C10^{8}	3.262	H7A	C18^{3}	3.555
H7A	C20^{3}	3.442	H7A	H8A^{8}	3.021
H7A	H8B^{8}	3.202	H7A	H10A^{8}	2.947
H7A	H10B^{8}	2.714	H7A	H18B^{3}	2.683
H7A	H20B^{3}	2.548	H7B	C18^{7}	3.462
H7B	C19^{7}	3.504	H7B	H8A^{8}	3.165
H7B	H10B^{8}	2.830	H7B	H17A^{9}	2.850

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H7B	H18A[7]	2.693	H7B	H19A[7]	3.022
H7B	H20A[7]	3.070	H8A	C4[1]	3.250
H8A	C7[1]	3.473	H8A	C17[7]	3.427
H8A	C18[7]	3.461	H8A	C19[7]	3.297
H8A	H4[1]	2.536	H8A	H7A[1]	3.021
H8A	H7B[1]	3.165	H8A	H17A[7]	2.622
H8A	H18A[7]	3.193	H8A	H19A[7]	2.441
H8B	C17[3]	3.584	H8B	C18[3]	3.279
H8B	C19[3]	3.324	H8B	H4[1]	3.584
H8B	H7A[1]	3.202	H8B	H17B[3]	2.969
H8B	H18B[3]	2.712	H8B	H19B[3]	2.725
H8B	H20B[3]	3.294	H9A	C16[7]	3.411
H9A	C17[7]	3.376	H9A	C18[7]	3.513
H9A	H10B[8]	3.168	H9A	H12A[8]	2.995
H9A	H15A[9]	3.018	H9A	H16A[7]	2.665
H9A	H17A[7]	2.918	H9A	H18A[7]	2.833
H9B	C10[8]	3.477	H9B	C12[8]	3.334
H9B	C16[3]	3.556	H9B	C17[3]	3.582
H9B	C18[3]	3.382	H9B	H10A[8]	3.182
H9B	H10B[8]	2.969	H9B	H12A[8]	2.860
H9B	H12B[8]	2.935	H9B	H16B[3]	2.747
H9B	H17B[3]	3.356	H9B	H18B[3]	2.514
H10A	C15[3]	3.496	H10A	C16[3]	3.335
H10A	C17[3]	3.302	H10A	H7A[1]	2.947
H10A	H9B[1]	3.182	H10A	H15B[3]	2.787
H10A	H16B[3]	2.906	H10A	H17B[3]	2.579
H10A	H18B[4]	3.201	H10A	H18B[3]	3.565
H10B	C7[1]	3.224	H10B	C9[1]	3.468
H10B	C15[7]	3.538	H10B	C16[7]	3.550
H10B	C17[7]	3.444	H10B	H7A[1]	2.714
H10B	H7B[1]	2.830	H10B	H9A[1]	3.168
H10B	H9B[1]	2.969	H10B	H15A[7]	2.746
H10B	H16A[7]	3.243	H10B	H17A[7]	2.605
H11A	C12[8]	3.550	H11A	C14[8]	3.383
H11A	C14[3]	3.532	H11A	C15[3]	3.445
H11A	C16[3]	3.339	H11A	H12A[8]	3.106
H11A	H12B[8]	3.150	H11A	H14A[8]	2.995

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H11A	H14A[3]	2.790	H11A	H14B[8]	2.909
H11A	H15B[3]	3.090	H11A	H16B[3]	2.520
H11B	C14[7]	3.430	H11B	C15[7]	3.396
H11B	C16[7]	3.432	H11B	H12A[8]	3.172
H11B	H13B[9]	3.067	H11B	H14B[8]	3.018
H11B	H14B[7]	2.680	H11B	H15A[7]	2.991
H11B	H16A[7]	2.697	H12A	C9[1]	3.370
H12A	C11[1]	3.563	H12A	C13[7]	3.432
H12A	C14[7]	3.446	H12A	C15[7]	3.401
H12A	H9A[1]	2.995	H12A	H9B[1]	2.860
H12A	H11A[1]	3.106	H12A	H11B[1]	3.172
H12A	H13B[7]	2.649	H12A	H14B[7]	3.103
H12A	H15A[7]	2.602	H12B	C13[3]	3.578
H12B	C14[3]	3.498	H12B	C15[3]	3.379
H12B	H9B[1]	2.935	H12B	H11A[1]	3.150
H12B	H13A[3]	2.823	H12B	H14A[3]	3.135
H12B	H15B[3]	2.573	H12B	H16B[4]	3.054
H13A	C12[3]	3.560	H13A	C13[3]	3.449
H13A	C14[8]	3.510	H13A	C14[3]	3.361
H13A	C16[8]	3.466	H13A	H12B[3]	2.823
H13A	H13A[3]	3.068	H13A	H14A[8]	3.135
H13A	H14A[3]	2.573	H13A	H14B[8]	3.046
H13A	H16A[8]	2.928	H13A	H16B[8]	3.141
H13B	C12[7]	3.411	H13B	C13[7]	3.381
H13B	C14[7]	3.402	H13B	H11B[9]	3.067
H13B	H12A[7]	2.649	H13B	H13B[7]	2.993
H13B	H14B[8]	3.132	H13B	H14B[7]	2.652
H13B	H16A[8]	3.047	H14A	C11[3]	3.548
H14A	C12[3]	3.480	H14A	C13[3]	3.380
H14A	H11A[1]	2.995	H14A	H11A[3]	2.790
H14A	H12B[3]	3.135	H14A	H13A[1]	3.135
H14A	H13A[3]	2.573	H14A	H14A[4]	2.937
H14B	C11[1]	3.398	H14B	C11[7]	3.465
H14B	C12[7]	3.458	H14B	C13[1]	3.506
H14B	C13[7]	3.440	H14B	H11A[1]	2.909
H14B	H11B[1]	3.018	H14B	H11B[7]	2.680
H14B	H12A[7]	3.103	H14B	H13A[1]	3.046

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H14B	H13B[1]	3.132	H14B	H13B[7]	2.652
H15A	C10[7]	3.467	H15A	C11[7]	3.389
H15A	C12[7]	3.377	H15A	H9A[9]	3.018
H15A	H10B[7]	2.746	H15A	H11B[7]	2.991
H15A	H12A[7]	2.602	H15A	H16A[8]	3.171
H15A	H18A[8]	3.172	H15B	C10[3]	3.539
H15B	C11[3]	3.453	H15B	C12[3]	3.367
H15B	C16[8]	3.546	H15B	C18[8]	3.581
H15B	H10A[3]	2.787	H15B	H11A[3]	3.090
H15B	H12B[3]	2.573	H15B	H16A[8]	3.020
H15B	H16B[8]	3.211	H15B	H18A[8]	2.979
H15B	H18B[8]	3.362	H16A	C9[7]	3.479
H16A	C10[7]	3.559	H16A	C11[7]	3.503
H16A	C13[1]	3.428	H16A	C15[1]	3.524
H16A	H9A[7]	2.665	H16A	H10B[7]	3.243
H16A	H11B[7]	2.697	H16A	H13A[1]	2.928
H16A	H13B[1]	3.047	H16A	H15A[1]	3.171
H16A	H15B[1]	3.020	H16B	C9[3]	3.459
H16B	C10[3]	3.328	H16B	C11[3]	3.292
H16B	H9B[3]	2.747	H16B	H10A[3]	2.906
H16B	H11A[3]	2.520	H16B	H12B[4]	3.054
H16B	H13A[1]	3.141	H16B	H15B[1]	3.211
H17A	C8[7]	3.356	H17A	C9[7]	3.311
H17A	C10[7]	3.342	H17A	H4[9]	3.226
H17A	H7B[9]	2.850	H17A	H8A[7]	2.622
H17A	H9A[7]	2.918	H17A	H10B[7]	2.605
H17A	H18A[8]	3.261	H17A	H20A[8]	3.516
H17B	C10[3]	3.443	H17B	C18[8]	3.504
H17B	H8B[3]	2.969	H17B	H9B[3]	3.356
H17B	H10A[3]	2.579	H17B	H18A[8]	2.855
H17B	H18B[8]	3.297	H17B	H20A[8]	3.075
H18A	C7[7]	3.486	H18A	C8[7]	3.564
H18A	C15[1]	3.503	H18A	C17[1]	3.484
H18A	H7B[7]	2.693	H18A	H8A[7]	3.193
H18A	H9A[7]	2.833	H18A	H15A[1]	3.172
H18A	H15B[1]	2.979	H18A	H17A[1]	3.261
H18A	H17B[1]	2.855	H18B	C7[3]	3.370

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H18B	C8[3]	3.180	H18B	C9[3]	3.210
H18B	H7A[3]	2.683	H18B	H8B[3]	2.712
H18B	H9B[3]	2.514	H18B	H10A[4]	3.201
H18B	H10A[3]	3.565	H18B	H15B[1]	3.362
H18B	H17B[1]	3.297	H19A	C3[7]	3.299
H19A	C4[9]	3.251	H19A	C7[7]	3.291
H19A	C8[7]	3.228	H19A	H4[9]	2.340
H19A	H5[9]	3.546	H19A	H7B[7]	3.022
H19A	H8A[7]	2.441	H19A	H20A[8]	3.430
H19B	O22[8]	3.329	H19B	C20[8]	3.519
H19B	H2[3]	3.064	H19B	H4[9]	3.105
H19B	H8B[3]	2.725	H19B	H20A[8]	2.726
H19B	H20B[8]	3.461	H20A	C3[7]	3.431
H20A	C4[7]	3.003	H20A	C19[1]	3.506
H20A	H4[7]	2.753	H20A	H7B[7]	3.070
H20A	H17A[1]	3.516	H20A	H17B[1]	3.075
H20A	H19A[1]	3.430	H20A	H19B[1]	2.726
H20B	C2[3]	3.067	H20B	C3[3]	3.025
H20B	C7[3]	3.138	H20B	H2[3]	3.106
H20B	H7A[3]	2.548	H20B	H8B[3]	3.294
H20B	H19B[1]	3.461	H21A	C1[7]	3.303
H21A	C2[7]	3.334	H21A	C3[7]	3.219
H21A	C4[7]	2.987	H21A	C5[7]	2.927
H21A	C6[7]	3.097	H21A	H4[7]	3.424
H21A	H4[9]	3.563	H21A	H5[7]	3.335
H21A	H5[9]	2.936	H21A	H6[7]	3.592
H21A	H24C[6]	2.872	H21B	O1[3]	3.232
H21B	O22[8]	2.744	H21B	C1[3]	3.331
H21B	C2[3]	3.252	H21B	H1O[3]	2.540
H21B	H2[3]	3.042	H21B	H5[9]	3.217
H21B	H24A[8]	3.541	H21B	H24C[6]	3.273
H24A	O1[4]	2.911	H24A	C6[11]	3.532
H24A	C24[13]	3.187	H24A	H1O[4]	2.388
H24A	H5[11]	3.016	H24A	H6[11]	2.855
H24A	H21B[1]	3.541	H24A	H24A[13]	2.549
H24A	H24C[13]	3.112	H24B	O1[12]	2.756
H24B	O1[4]	2.723	H24B	C1[12]	3.441

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H24B	C6[12]	3.547	H24B	C6[3]	3.200
H24B	H1O[12]	3.537	H24B	H1O[4]	2.467
H24B	H5[11]	3.157	H24B	H6[11]	3.035
H24B	H6[12]	3.137	H24B	H6[3]	2.814
H24B	H24B[14]	3.275	H24C	O1[12]	3.253
H24C	O23[6]	2.762	H24C	C1[12]	3.341
H24C	C5[11]	3.367	H24C	C6[12]	3.232
H24C	C21[6]	3.395	H24C	C22[6]	3.573
H24C	H5[11]	2.507	H24C	H6[11]	3.440
H24C	H6[12]	3.044	H24C	H21A[6]	2.872
H24C	H21B[6]	3.273	H24C	H24A[13]	3.112
H24C	H24C[6]	3.525			

Symmetry Operators:

(1) X-1,Y,Z
(2) -X+3,-Y+2,-Z+3
(3) -X+1,-Y+1,-Z+2
(4) -X,-Y+1,-Z+2
(5) X+2,Y+1,Z+1
(6) -X-1,-Y+1,-Z+1
(7) -X+1,-Y+2,-Z+2
(8) X+1,Y,Z
(9) -X+2,-Y+2,-Z+2
(10) X+3,Y+1,Z+1
(11) X-3,Y-1,Z-1
(12) X-2,Y-1,Z-1
(13) -X-2,-Y+1,-Z+1
(14) -X-2,-Y,-Z+1