Efficient and controlled polymerization of lactide under mild conditions with a sodium-based catalyst

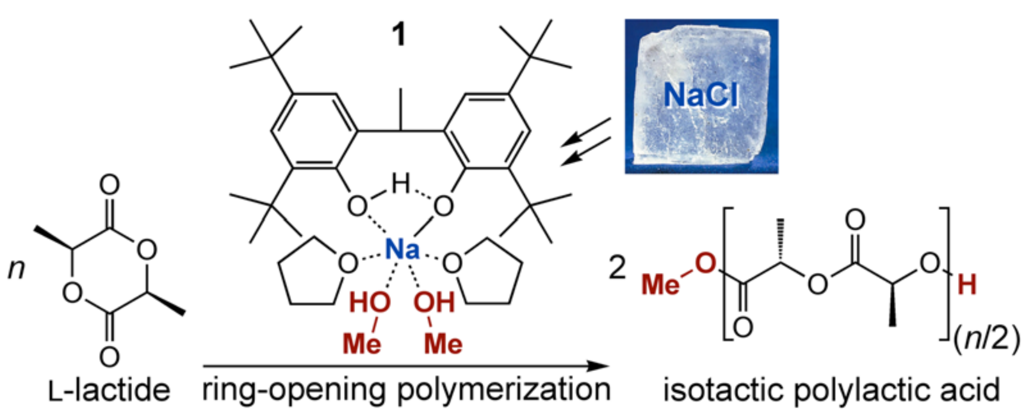
Hsuan-Ying Chen, Jubo Zhang, Chu-Chieh Lin,* Joseph H. Reibenspies, and Stephen A. Miller*

Department of Chemistry, Texas A&M University, College Station, Texas 77843-3255 and Department of Chemistry, National Chung-Hsing University, Taichung 402, Taiwan, R.O.C.

Electronic Supplementary Information
Green Chemistry

Electronic supplementary information available: Catalyst synthesis and characterization data (including X-ray crystallography for **2**), polymer characterization data, and details of the kinetic study.

Table of Contents



General Considerations and Instrumentation. All air sensitive procedures were performed under a purified atmosphere of nitrogen in a glove box or by using standard Schlenk line and vacuum line techniques. Tetrahydrofuran and toluene were purified by a nitrogen sparge and passage through an MBraun cold filtration drying system that employs activated alumina. Methanol was distilled from magnesium sulfate. 1,2-dichloroethane was distilled from CaH_2. Benzene-d_6 was dried over CaH_2 and stored in a Straus flask. $CDCl_3$ was stored over 4Å molecular sieves. 2,2'-ethylidene-bis(4,6-di-*tert*-butylphenol) ($EDBPH_2$) (Aldrich, 99%) and sodium methoxide (Alfa Aesar, 98%) were used as received. L-lactide (PURASORB®) was purified by sublimation and stored in the glovebox before use.

X-ray crystallographic data were obtained on a Bruker SMART 1000 three-circle diffractometer operating at 50 kV and 40 mA, Mo Kα (λ = 0.71073 Å) with a graphite monochromator, and a CCD-PXL-KAF2 detector.

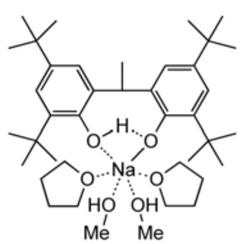
All NMR chemical shifts are given in ppm and were recorded on a Mercury-300BB spectrometer (^{1}H, 299.91 MHz; ^{13}C {^{1}H} 75.41 MHz) using the solvent peak (or residual protonated solvent peak) as an internal standard ($CDCl_3$: ^{1}H 7.27 ppm; ^{13}C 77.2 ppm. C_6D_6: ^{1}H 7.16 ppm; ^{13}C 128.4 ppm.).

Gel permeation chromatography (GPC) measurements were performed on a Hitachi L-7100 system equipped with a differential Bischoff 8120 RI detector using tetrahydrofuran (HPLC grade) as the eluent. Molecular weight and molecular weight distributions were calculated using polystyrene as the standard.

Differential scanning calorimetry (DSC) was performed with a TA Instruments Q600 SDT equipped with DSC-TGA, interfaced via the Thermal Advantage for Q Series Software suite version 2.1.0.240. Polylactic acid melting points were determined using a heating/cooling ramp of 10°C/min. from 25°C to 200°C. In each case the results of the second run are reported and the maximum of the melting endotherm taken as the melting point.

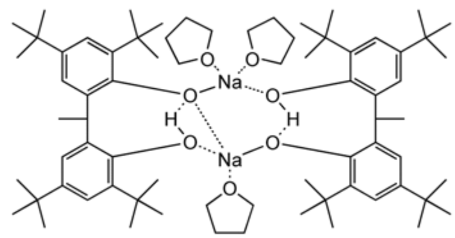
Elemental analysis was performed by Atlantic Microlab in Norcross, Georgia (www.atlanticmicrolab.com).

Preparation of Sodium Complexes 1 and 2.
(EDBPH)Na(MeOH)$_2$(THF)$_2$ (1).



A mixture of 2,2'-ethylidene-bis(4,6-di-*tert*-butylphenol) (13.14 g, 30 mmol, $EDBPH_2$) and NaOMe (4.00 g, 74 mmol) was stirred in a mixed solvent of tetrahydrofuran (30 mL) and MeOH (10 mL) at 70°C for 24 hours. Residual NaOMe was removed by filtration and the solvent was removed under vacuum. The obtained white powder was washed with pentane (3 x 15 mL) and dried *in vacuo*. Yield: 12.42 g (62.0 %). ^{1}H NMR (C_6D_6): δ 1.32 (m, 8H, OCH_2CH_2), 1.40 (s, 18H, $C(CH_3)_3$), 1.50 (s, 18H, $C(CH_3)_3$), 1.94 (d, $^3J_{HH}$ = 7.5 Hz, 3H, $CH(CH_3)$), 3.26 (s, 6H, CH_3OH), 3.40 (m, 8H, OCH_2CH_2), 5.30 (q, $^3J_{HH}$ = 7.5 Hz, 1H, $CH(CH_3)$), 7.31 (s, 2H, Ar-*H*), 7.57 (s, 2H, Ar-*H*), 8.98 (br s, 3H, CH_3OH and ArO-*H*). ^{13}C NMR (C_6D_6): δ 20.2 ($CH(CH_3)$), 25.6 (OCH_2CH_2), 31.3 ($CH(CH_3)$), 30.4, 32.1 ($C(CH_3)$), 35.3, 34.5 ($C(CH_3)_3$), 50.5 (CH_3OH), 68.0 (OCH_2CH_2), 120.5, 120.7, 136.3, 136.6, 138.9, 156.2 (aromatic *C*). Anal. Calc for $C_{40}H_{69}O_6Na$: C, 71.82; H, 10.40. Found: C, 72.21; H, 10.19.

[(EDBPH)Na(THF)$_2$][Na(THF)(EDBPH)] (2).



In the glove box, approximately 200 mg of **1** were dissolved in approximately 4 mL toluene. Crystals suitable for an X-ray diffraction study were obtained by storing the solution in a -35°C freezer within the glove box for three days. XRD data confirms the structure of **2** as a dimeric complex with loss of all MeOH and some THF from **1**. The ^{1}H and ^{13}C NMR data featuring some broad resonances are consistent with an asymmetric dimeric structure. ^{1}H NMR (C_6D_6): δ 1.23 (m, 12H, OCH_2CH_2), 1.40 (s, 36H, $C(CH_3)_3$), 1.51 (s, 36H, $C(CH_3)_3$), 1.94 (br, 6H, $CH(CH_3)$), 3.20 (m, 12H, OCH_2CH_2), 5.27 (br, 2H, $CH(CH_3)$), 7.32 (s, 4H, Ar-*H*), 7.57 (br, 4H, Ar-*H*). ^{13}C NMR (C_6D_6): δ 20.9 ($CH(CH_3)$), 25.8 (OCH_2CH_2), 32.0 ($CH(CH_3)$), 31.0, 32.5 ($C(CH_3)$), 35.7, 34.9 ($C(CH_3)_3$), 68.3 (OCH_2CH_2), 121.4, 126.1, 136.3, 136.5, 139.5, 156.5 (aromatic *C*). Anal. Calc for $C_{79}H_{122}O_7Na_2$ (**2**·C_7H_8): C, 77.16; H, 10.00. Found: C, 77.34; H, 9.93.

Polymerization Procedure. A typical polymerization procedure is provided here that corresponds to Table 1, entry 1. A solution of **1** (0.034 g, 0.05 mmol) and L-lactide (0.446 g, 3.1 mmol) in toluene (20 mL) was stirred at room temperature (20°C) for 8 minutes. At this time, an aliquot of the reaction was taken and the solvent was removed. The obtained residue was analyzed by ^{1}H NMR to determine the percent conversion. The volatile components were removed from the bulk reaction under reduced pressure. The obtained solids were dissolved in tetrahydrofuran (10 mL). The solution was then quenched by the addition of an aqueous acetic acid solution (0.35N, 10 mL) and the polymer was precipitated upon pouring into *n*-hexane (60 mL) to give a white crystalline powder. Isolated yield: 0.25 g (56%). Characterization of the poly(L-lactide) using ^{1}H and ^{13}C NMR spectroscopy (see spectra below) suggest highly isotactic PLA with [*m*] > 98%.

Polymer Synthesis and Characterization Summary

entry[a]	solvent	[L-lactide]$_0$/ [**1**]$_0$	time (min.)	conv. (%)[b]	isolated yield (%)	isotacticity [*m*][c]	T_m (°C)[d]
1	toluene	62	8	>99	56	> 0.98	159.70
2	toluene	134	8	99	70	> 0.98	167.36
3	toluene	200	3	81	80	not deter.	not deter.
4	toluene	200	8	98	80	> 0.99	171.01
5	toluene	230	8	95	81	> 0.99	170.51
6	THF	200	8	11	not deter.	not deter.	not deter.
7	THF	200	240	53	not deter.	not deter.	not deter.
8	THF	100	1320	96	70	> 0.95	155.41
9	$ClCH_2CH_2Cl$	200	8	13	not deter.	not deter.	not deter.
10	$ClCH_2CH_2Cl$	200	240	51	not deter.	not deter.	not deter.
11	$ClCH_2CH_2Cl$	100	1320	96	72	> 0.95	158.93

entry[a]	M_n GPC[e]		M_w GPC[e]		M_w/M_n[e]		M_n calc.[f]	M_n NMR[b]
	measured	rounded	measured	rounded	measured	rounded		
1	11,149	11,100	15,362	15,400	1.37795	1.38	4,400	5,500
2	25,013	25,000	33,233	33,200	1.32863	1.33	9,600	10,100
3	35,037	35,000	43,739	43,700	1.24836	1.25	11,700	11,800
4	39,844	39,800	44,039	44,000	1.10529	1.11	14,100	15,300
5	45,667	45,700	57,852	57,900	1.26682	1.27	15,700	16,000
6	2,686	2,700	2,941	2,900	1.09475	1.10	1,600	2,600
7	9,452	9,500	10,720	10,700	1.13418	1.13	7,700	7,700
8	15,355	15,400	17,814	17,800	1.16014	1.16	6,900	8,000
9	2,735	2,700	3,001	3,000	1.09759	1.10	1,900	3,800
10	12,642	12,600	13,662	13,700	1.08068	1.08	7,400	8,500
11	16,484	16,500	17,719	17,700	1.07493	1.08	6,900	7,700

[a]In 20 mL solvent at 20°C; 0.034 g **1**; quenched with acetic acid in hexane.
[b]By ^{1}H NMR analysis.
[c]By ^{1}H NMR analysis (homonuclear decoupled) of the polylactic acid methine carbon.
[d]By differential scanning calorimetry (DSC). The second scan is reported.
[e]Gel permeation chromatography (GPC) vs. calibrated PS standards.
[f]By (F.W.$_{\text{lactide}}$[L-lactide]$_0$/2[**1**]$_0$)(% conversion).

When using polystyrene standards for GPC analysis of polylactic acid, the PLA molecular weights suggested by GPC are typically larger than the actual molecular weights. Multiplication of the GPC data by a factor of 0.58 has been suggested to arrive at more accurate number average molecular weights. See:

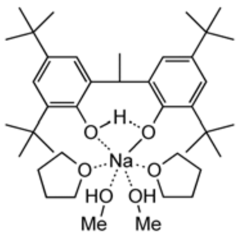
(a) A. Kowalski, A. Duda and S. Penczek, *Macromolecules* 1998, **31**, 2114-2122. (middle of page 2115)
(b) H. Ma and J. Okuda, *Macromolecules* 2005, **38**, 2665-2673. (bottom of page 2666)

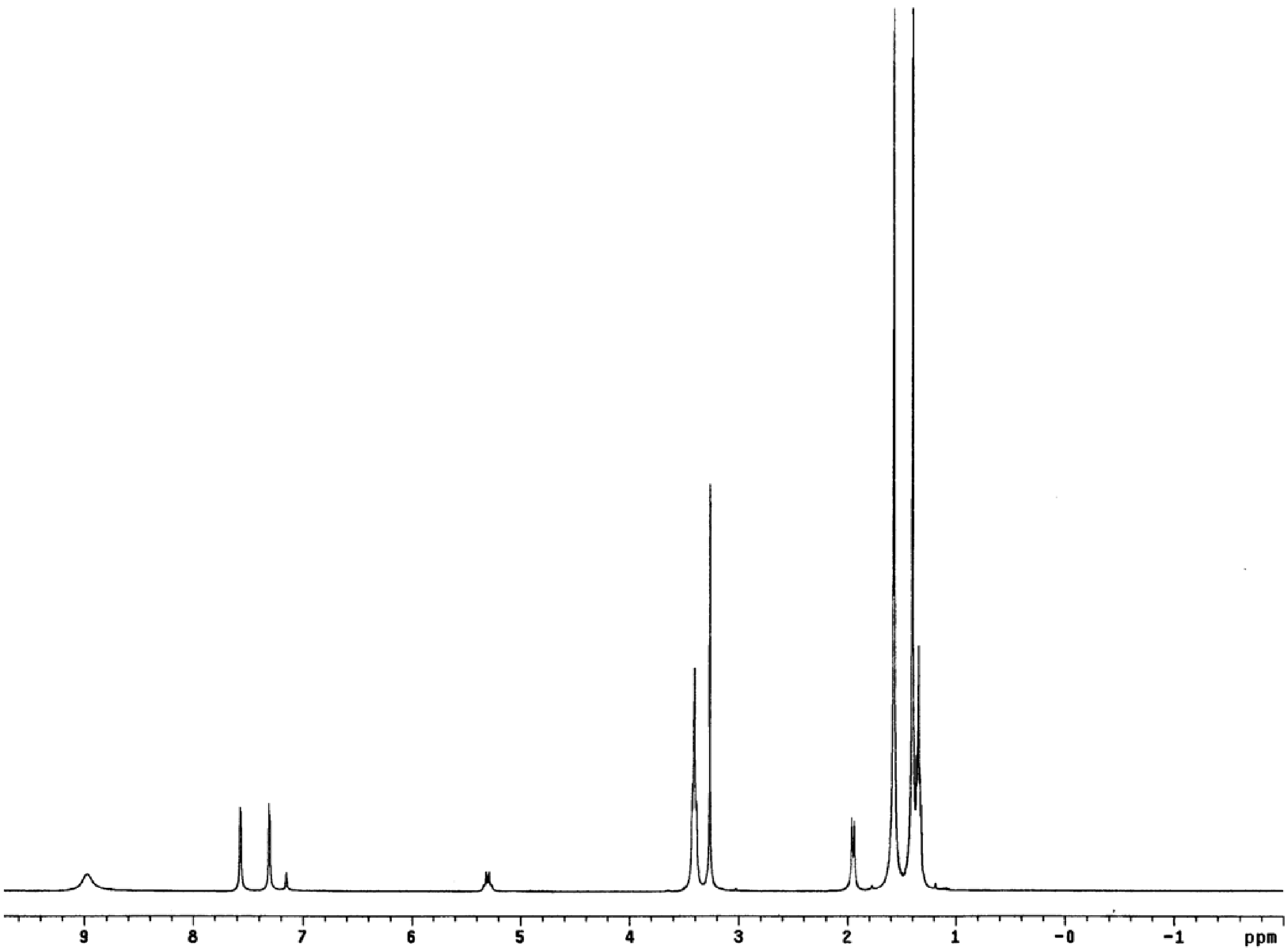
The following table considers this multiplication factor and compares the adjusted GPC data with the NMR molecular weight data. A markedly improved agreement is obtained.

entry[a]	M_n GPC	adjusted M_n GPC (x 0.58)		M_n NMR[b]
	measured	adjusted	rounded	
1	11,149	6,466	6,500	5,500
2	25,013	14,508	14,500	10,100
3	35,037	20,321	20,300	11,800
4	39,844	23,110	23,100	15,300
5	45,667	26,487	26,500	16,000
6	2,686	1,558	1,600	2,600
7	9,452	5,482	5,500	7,700
8	15,355	8,906	8,900	8,000
9	2,735	1,586	1,600	3,800
10	12,642	7,332	7,300	8,500
11	16,484	9,561	9,600	7,700

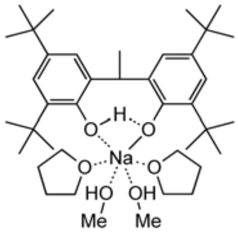
NMR Characterization of 1 and 2

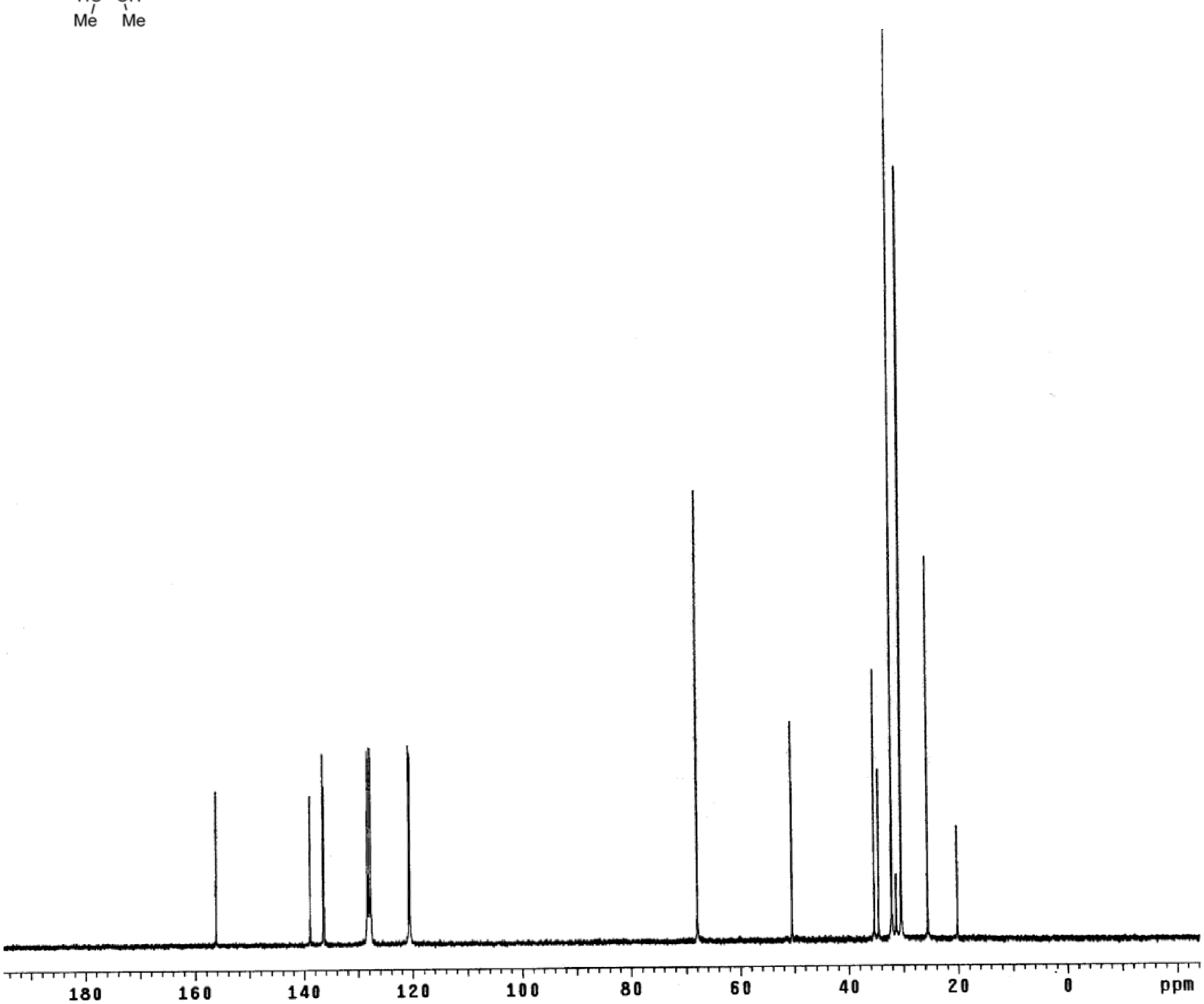
^{1}H NMR of (EDBPH)Na$(MeOH)_2(THF)_2$ (**1**)



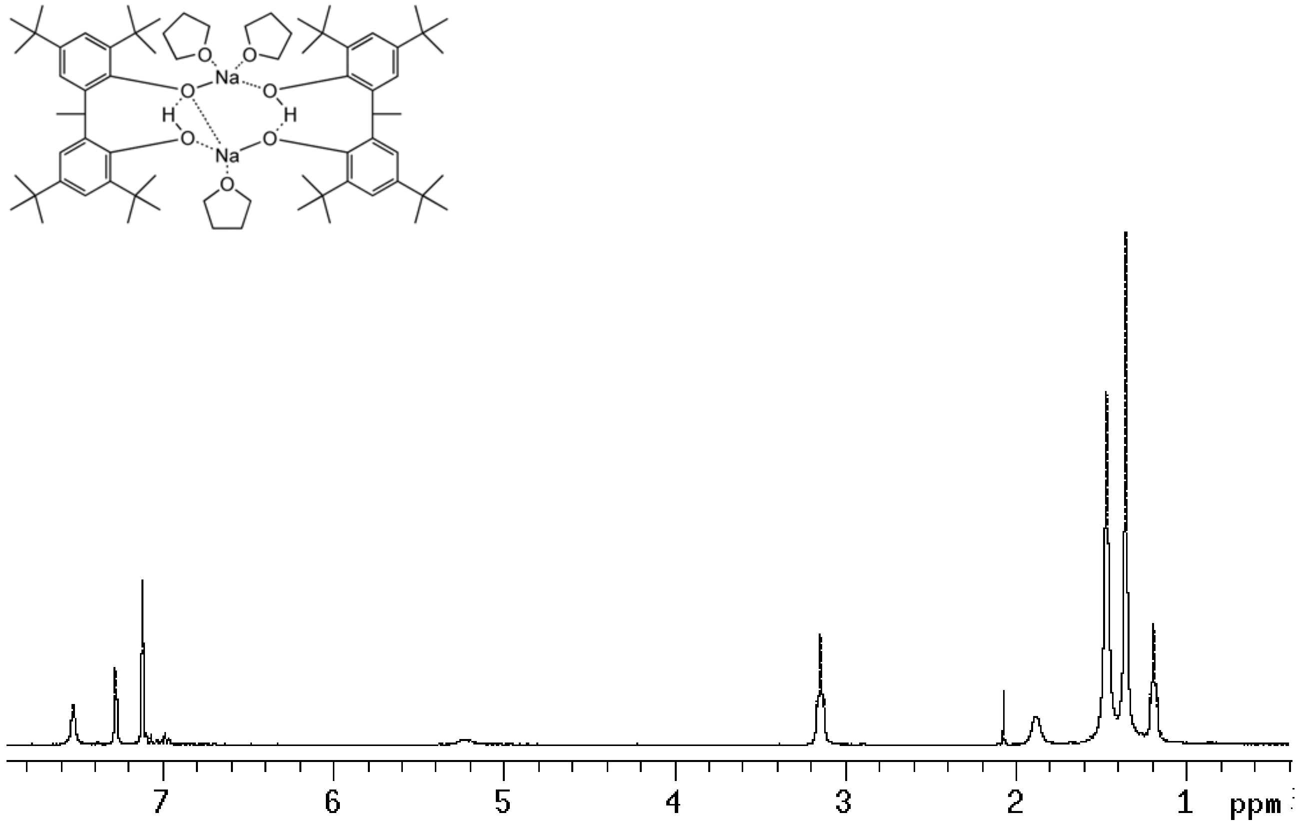


^{13}C NMR of (EDBPH)Na$(MeOH)_2(THF)_2$ (**1**)

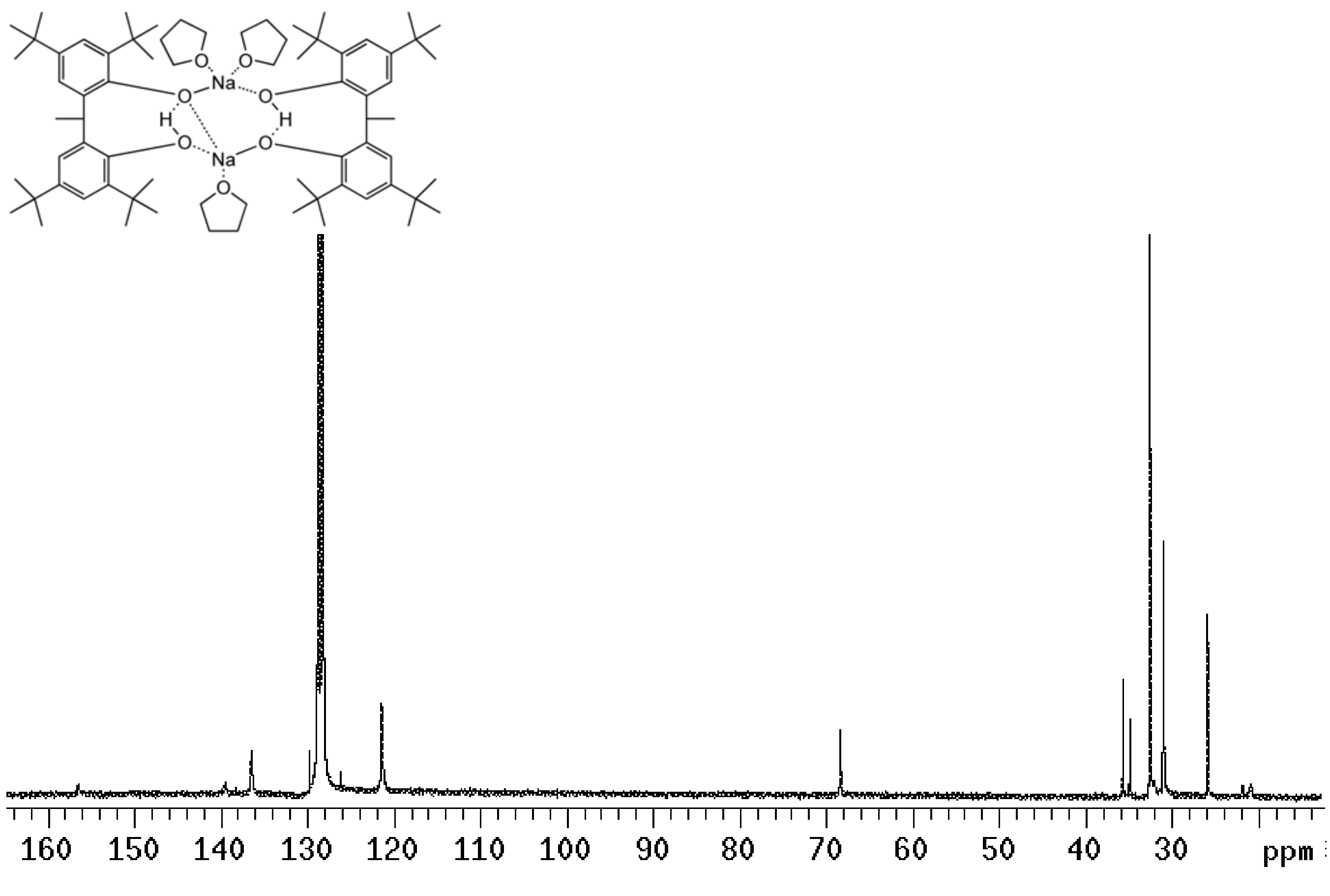




^{1}H NMR of [(EDBPH)Na(THF)$_2$][Na(THF)(EDBPH)] (**2**)

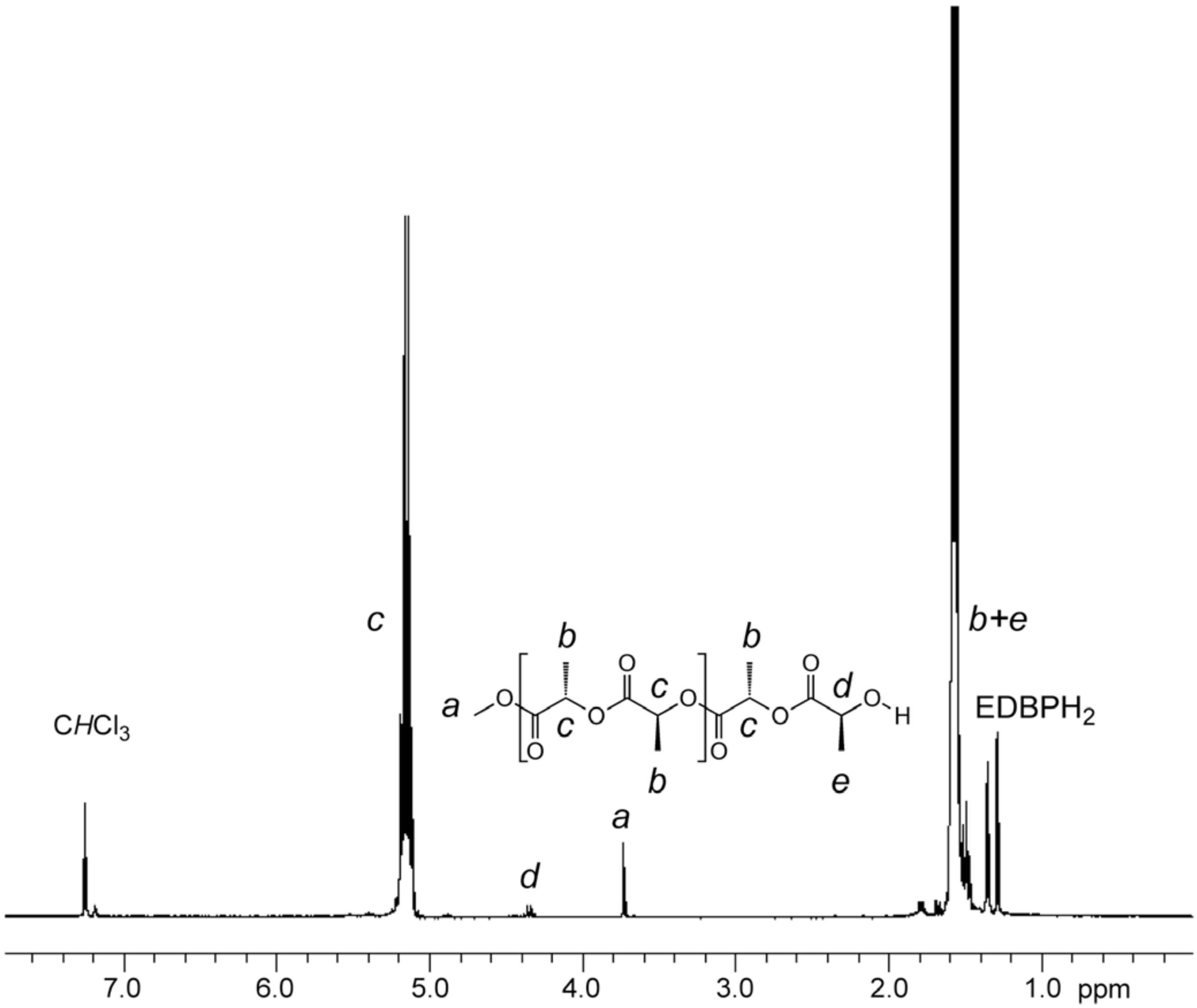


^{13}C NMR of [(EDBPH)Na(THF)$_2$][Na(THF)(EDBPH)] (**2**)

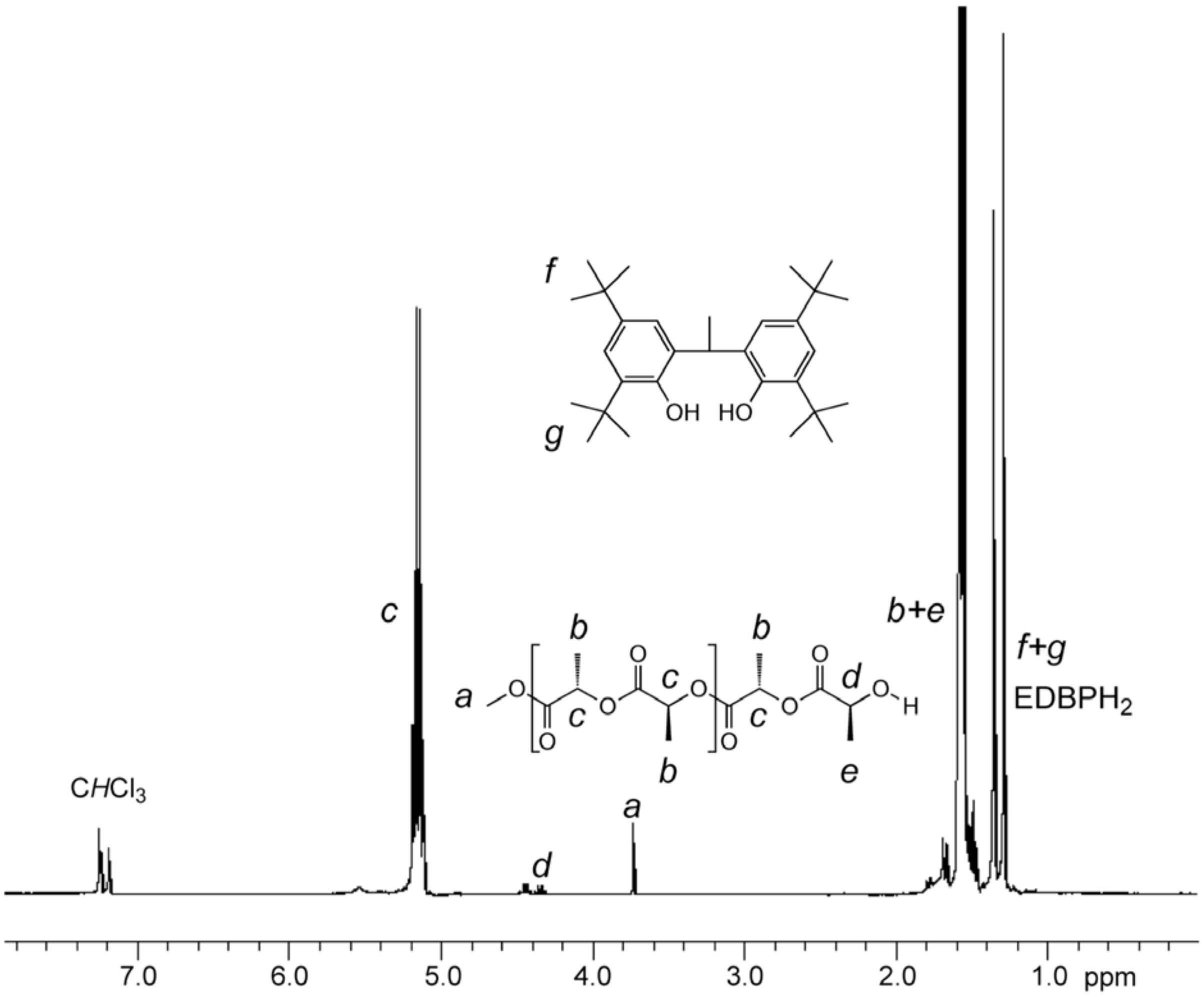


Polymer Characterization by NMR

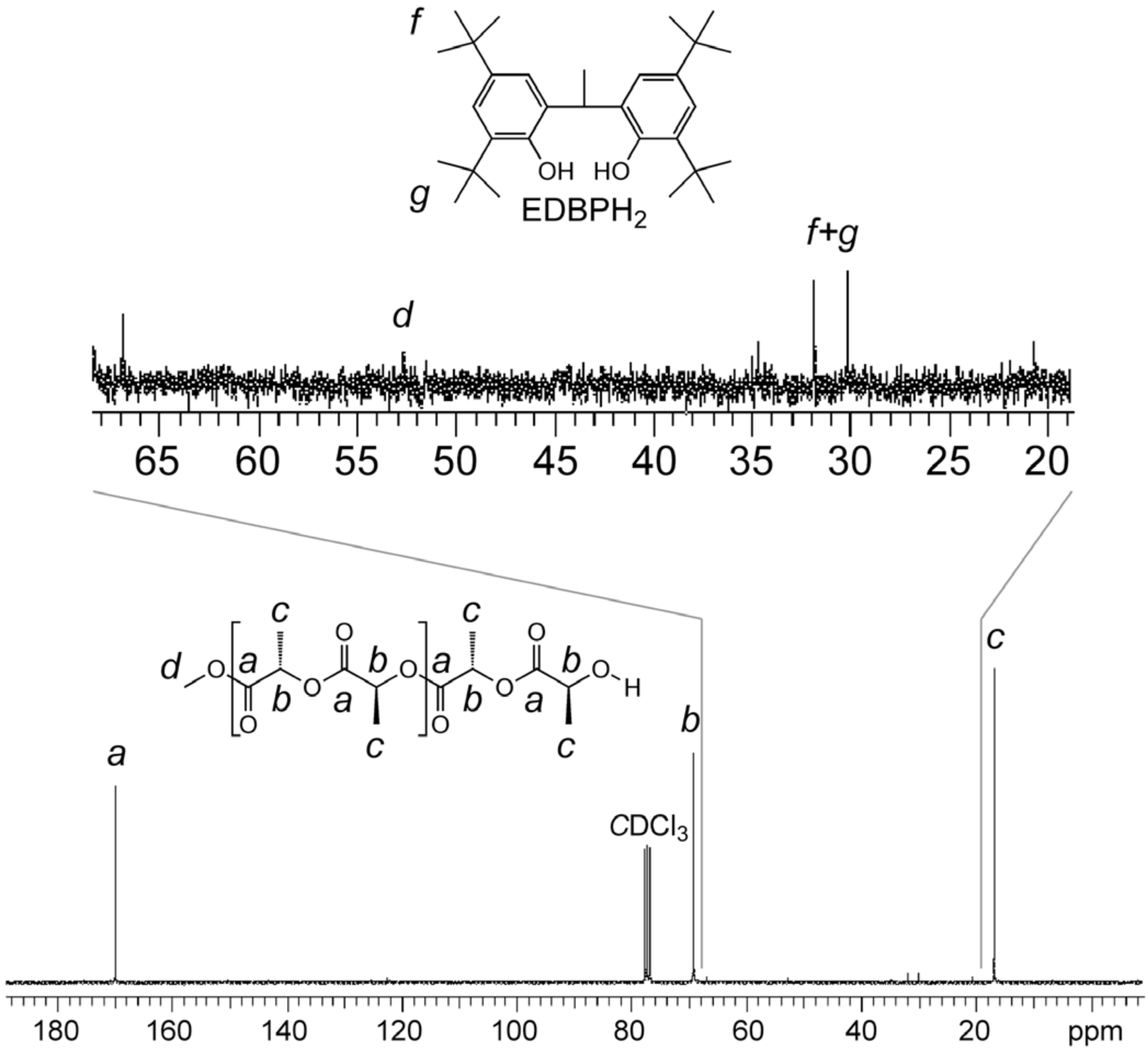
^{1}H NMR of PLA from Table 1, entry 1 (in $CDCl_3$)
The *tert*-butyl group protons of $EDBPH_2$ appear as an impurity and resonate at 1.28 and 1.36 ppm.
The assignments for **a**, **b**, **c**, **d**, and **e** match those from a report that produced low molecular weight polylactic acid via the ring opening polymerization of lactide with potassium methoxide as the initiator: Z. Jedlinski, W. Walach, P. Kurcok and G. Adamus, *Makromol. Chem*. 1991, **192**, 2051-2057.



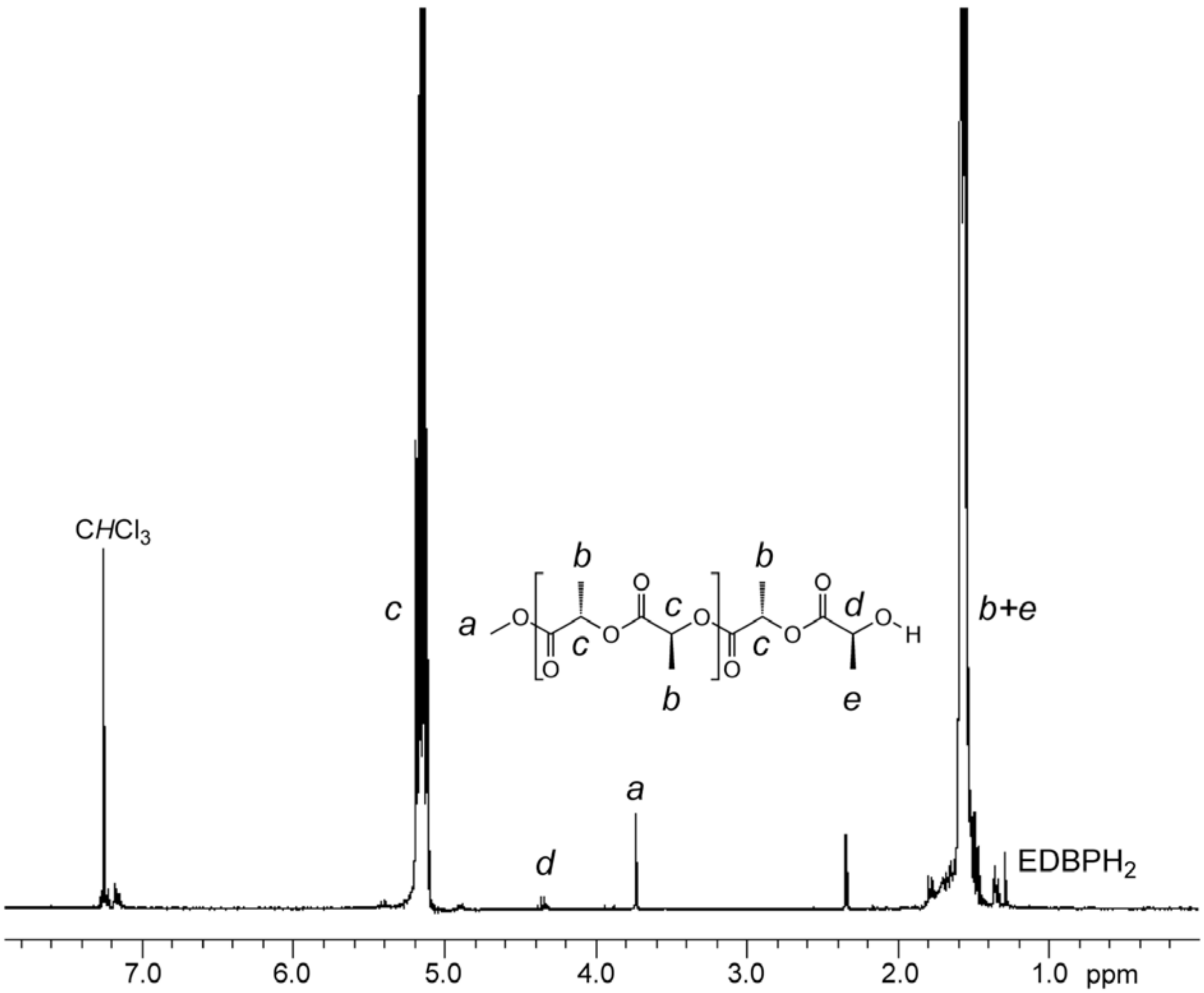
^{1}H NMR of PLA from Table 1, entry 1 + added $EDBPH_2$ (in $CDCl_3$)



^{13}C NMR of PLA from Table 1, entry 1 (in $CDCl_3$)
The methyl carbon of the methyl ester chain end has been located at 52.7 ppm.
The *tert*-butyl group methyl carbons of $EDBPH_2$ appear as an impurity and resonate at 30.3 and 32.0 ppm.

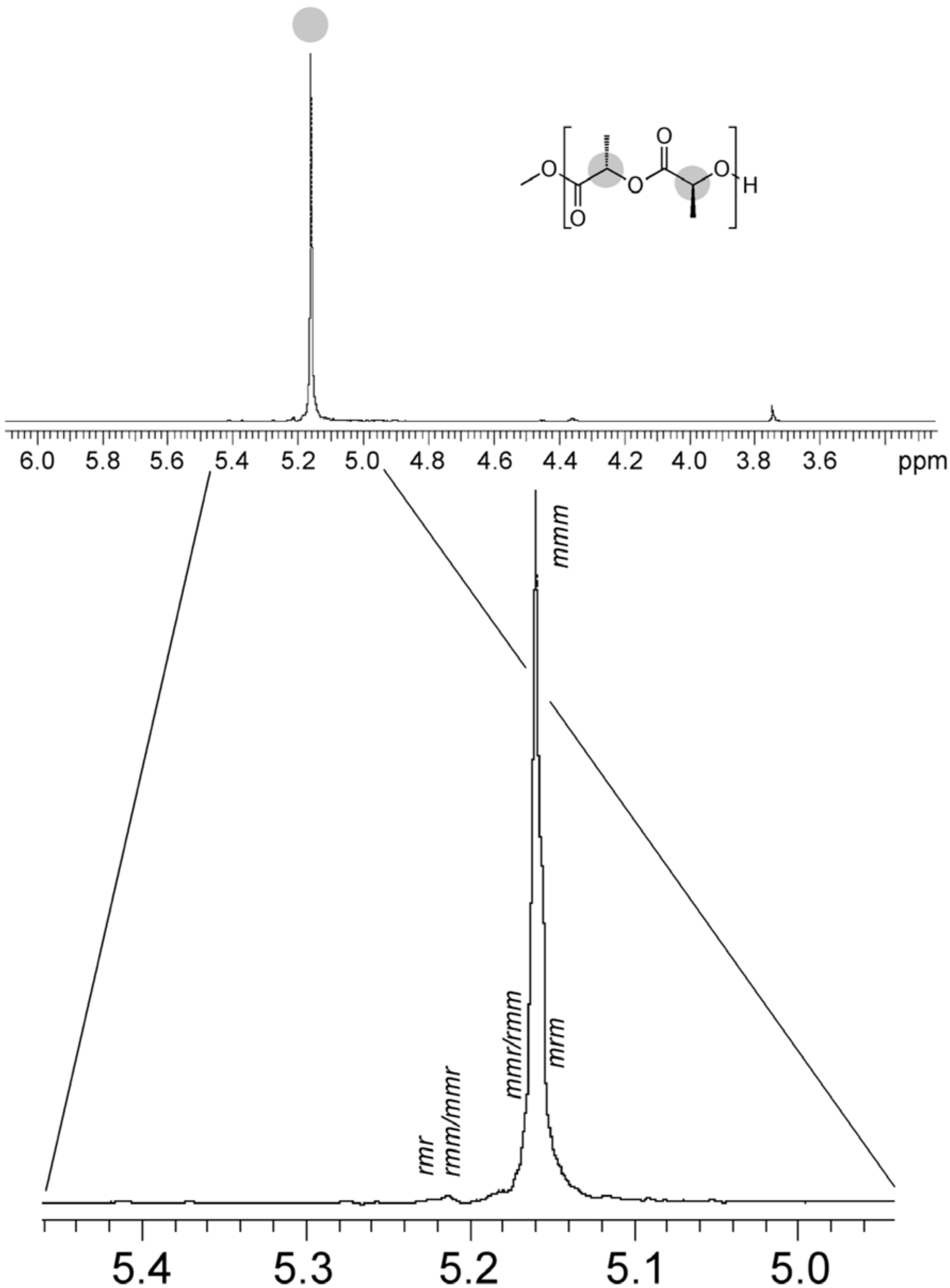


^{1}H NMR of PLA from Table 1, entry 4 (in $CDCl_3$)

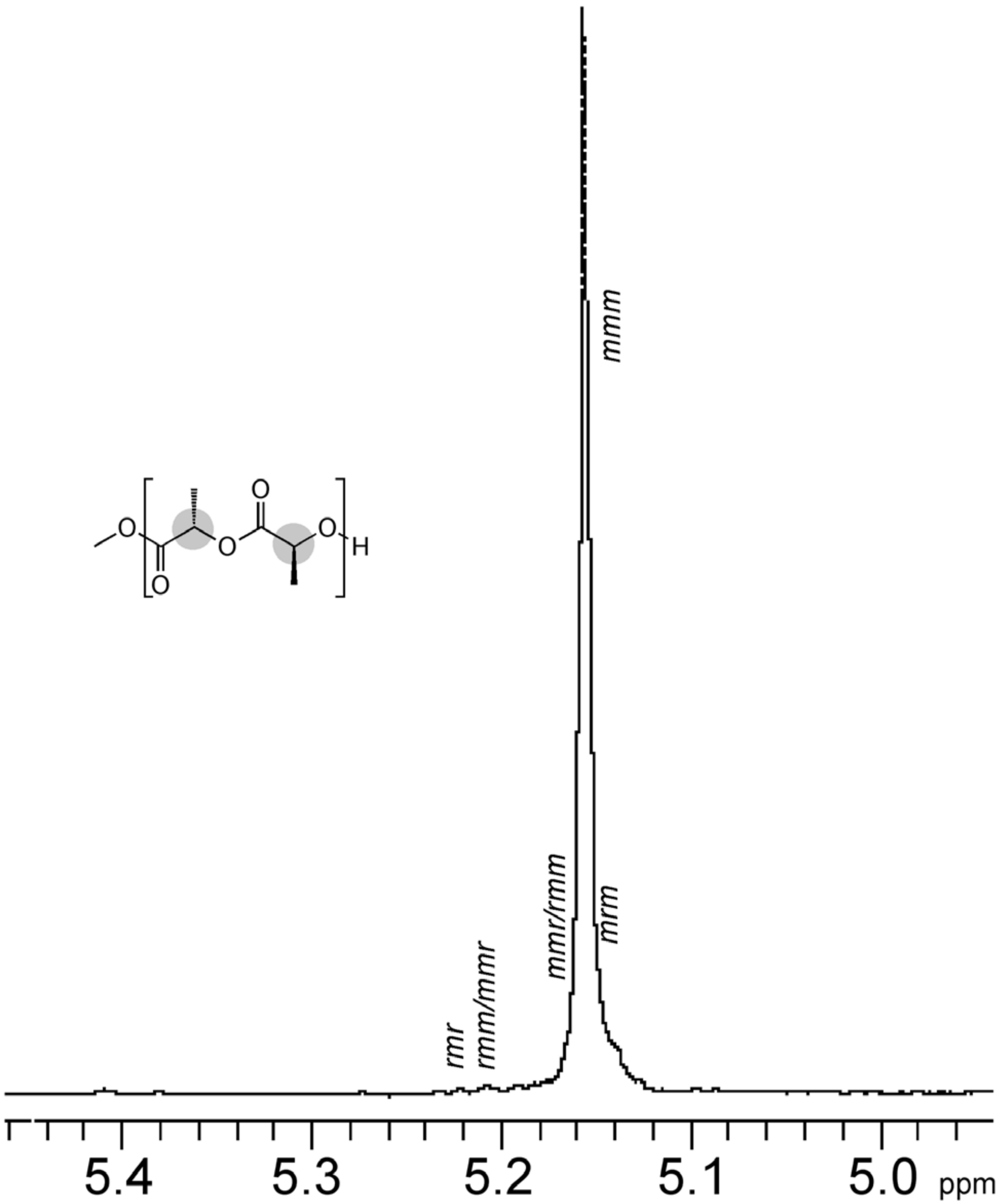


For tetrad peak assignments, see: (a) K. A. M. Thakur, R. T. Kean, E. S. Hall, J. J. Kolstad, T. A. Lindgren, M. A. Doscotch, J. I. Siepmann and E. J. Munson, *Macromolecules* 1997, **30**, 2422-2428. (b) K. A. M. Thakur, R. T. Kean, E. S. Hall, J. J. Kolstad and E. J. Munson, *Macromolecules* 1998, **31**, 1487-1494. (c) K. A. M. Thakur, R. T. Kean, M. T. Zell, B. E. Padden and E. J. Munson, *Chem. Commun.* 1998, 1913-1914. (d) M. H. Chisholm, S. S. Iyer, D. G. McCollum, M. Pagel and U. Werner-Zwanziger, *Macromolecules* 1999, **32**, 963-973. (e) B. M. Chamberlain, M. Cheng, E. B. Lobkovsky and G. W. Coates, *J. Am. Chem. Soc.* 2001, **123**, 3229-3238.

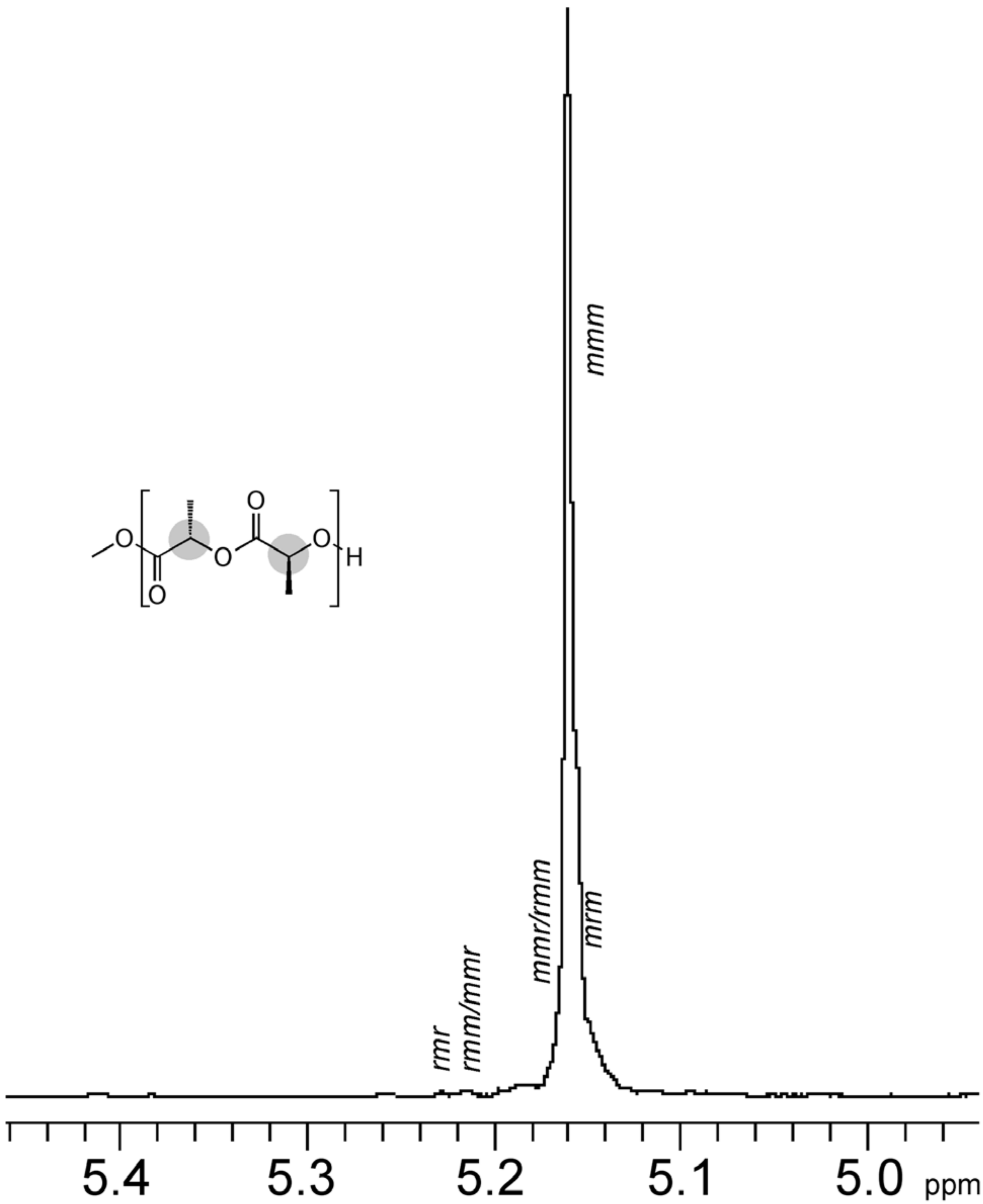
Homonuclear decoupled ^{1}H NMR spectrum of the methine region of PLA from Table 1, entry 1 (in $CDCl_3$)



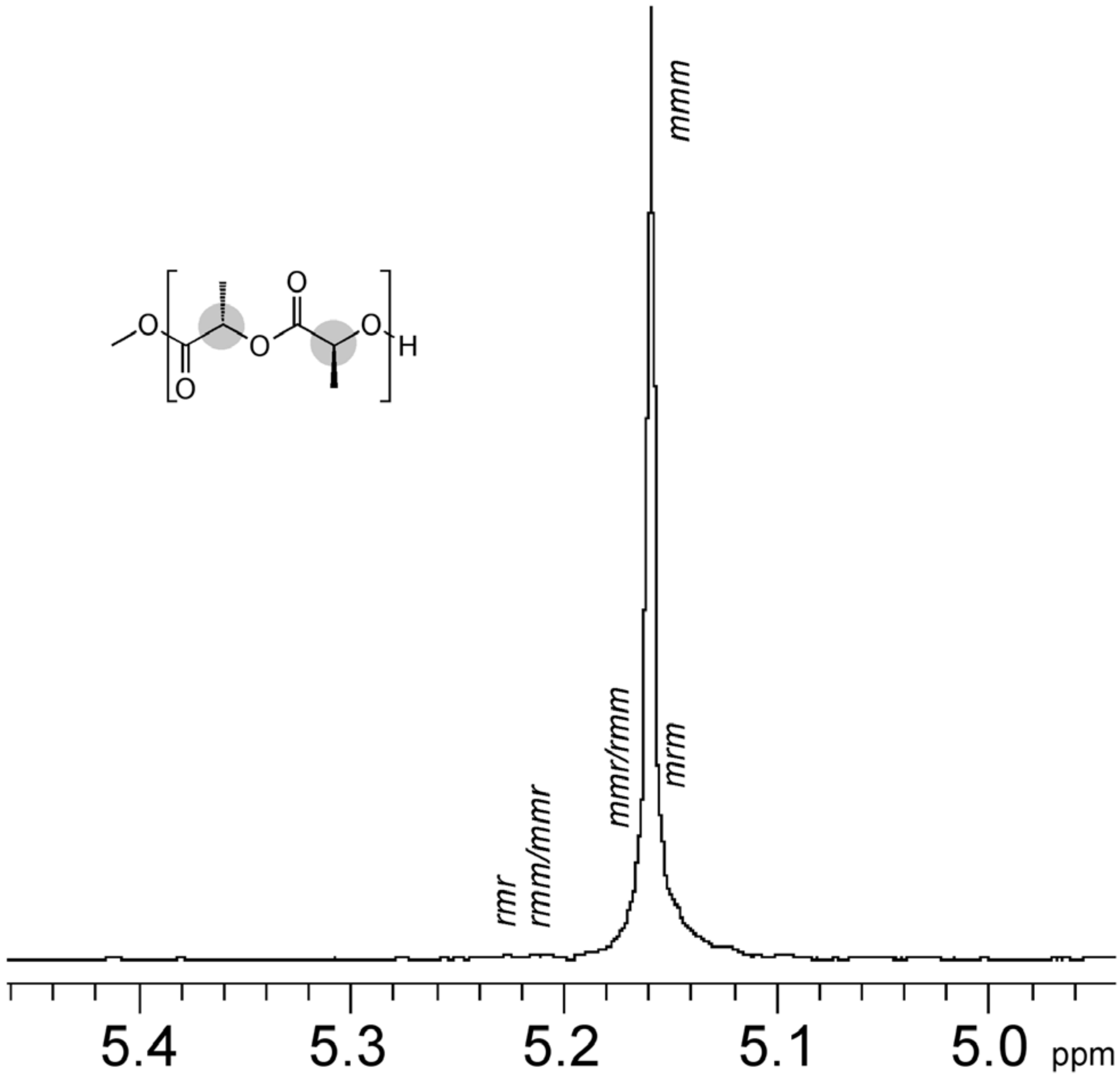
Homonuclear decoupled ^{1}H NMR spectrum of the methine region of PLA from Table 1, entry 2 (in $CDCl_3$)



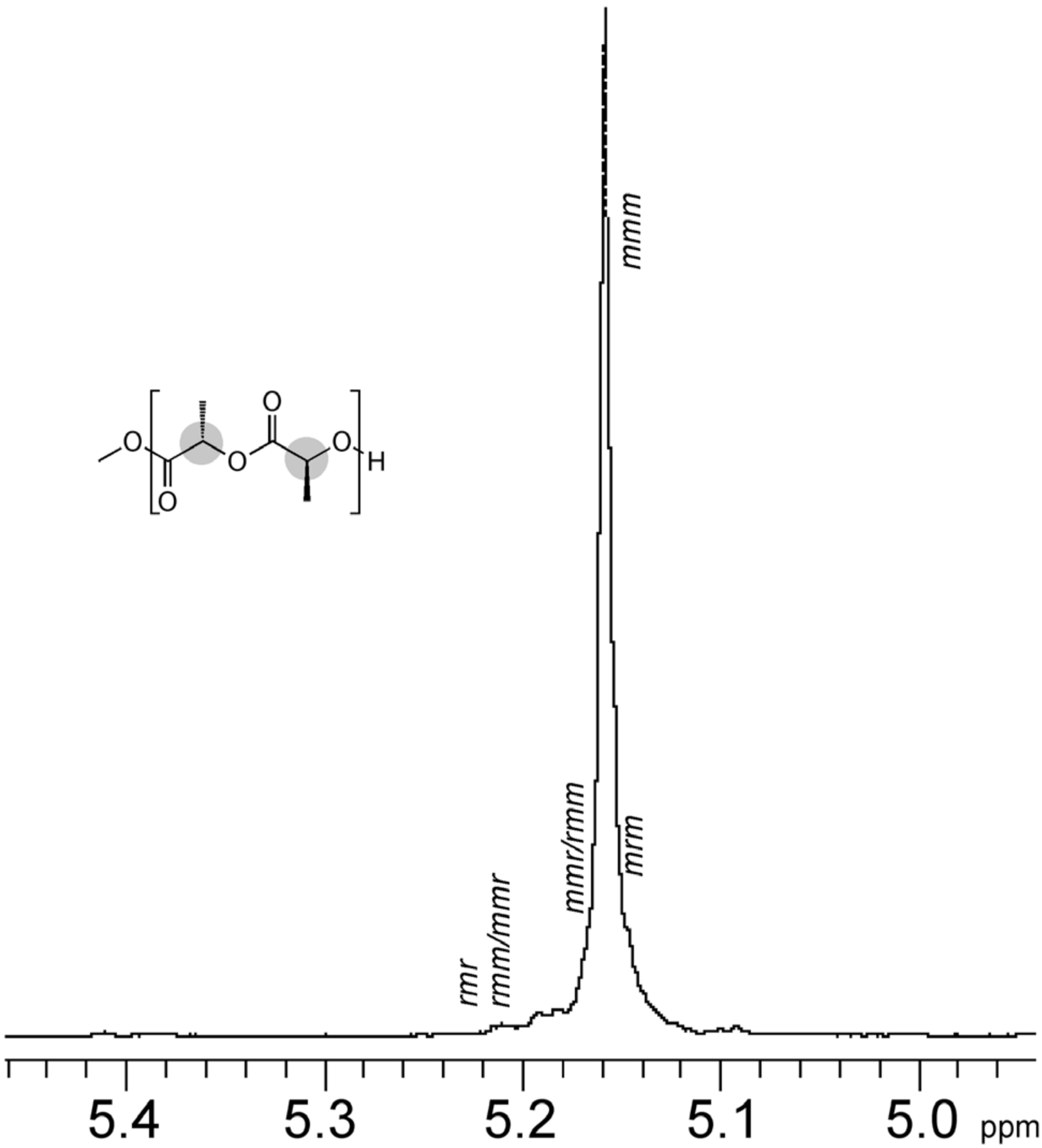
Homonuclear decoupled ^{1}H NMR spectrum of the methine region of PLA from Table 1, entry 4 (in $CDCl_3$)



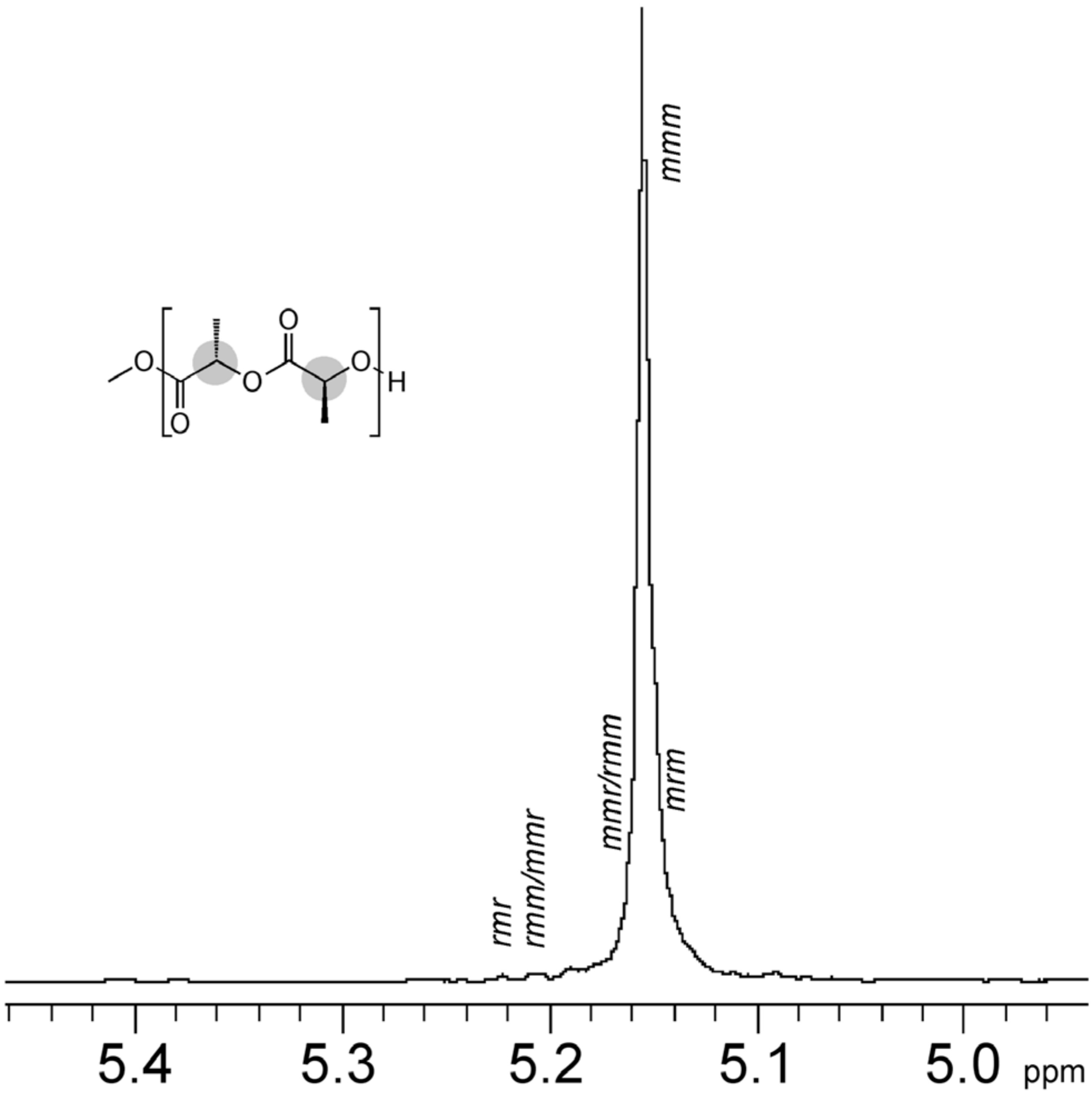
Homonuclear decoupled ^{1}H NMR spectrum of the methine region of PLA from Table 1, entry 5 (in $CDCl_3$)



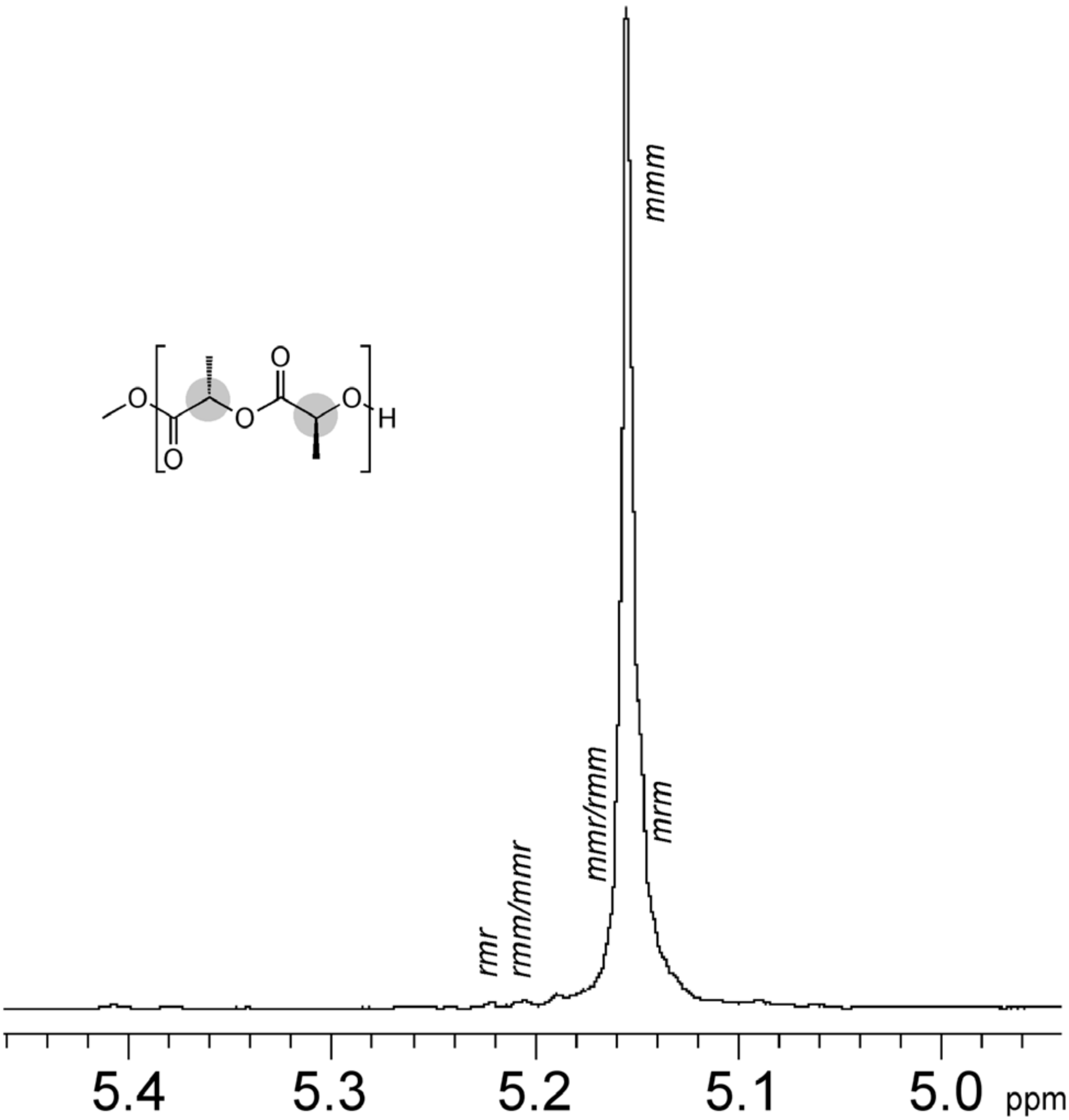
Homonuclear decoupled ^{1}H NMR spectrum of the methine region of PLA from Table 1, entry 8 (in $CDCl_3$)



Homonuclear decoupled ^{1}H NMR spectrum of the methine region of PLA from Table 1, entry 11 (in $CDCl_3$)

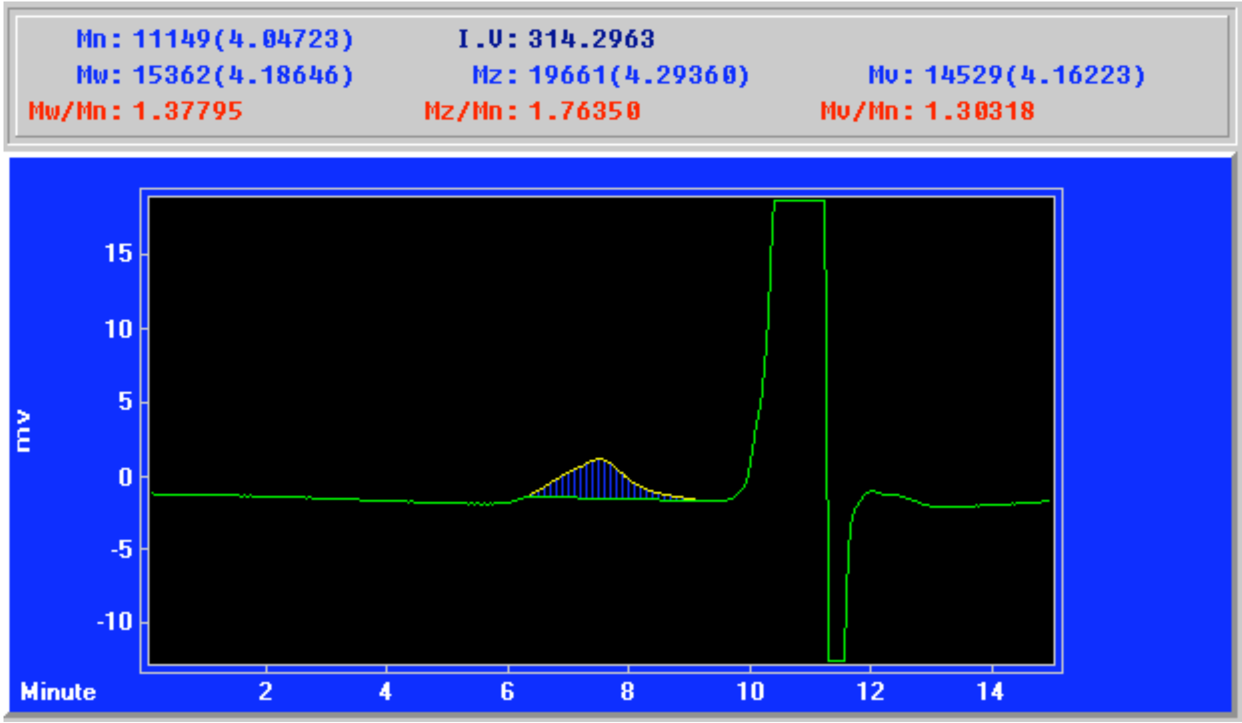


Homonuclear decoupled ^{1}H NMR spectrum of the methine region of PLA from the initiator NaOMe under the conditions of Table 1, entry 8 (in $CDCl_3$)

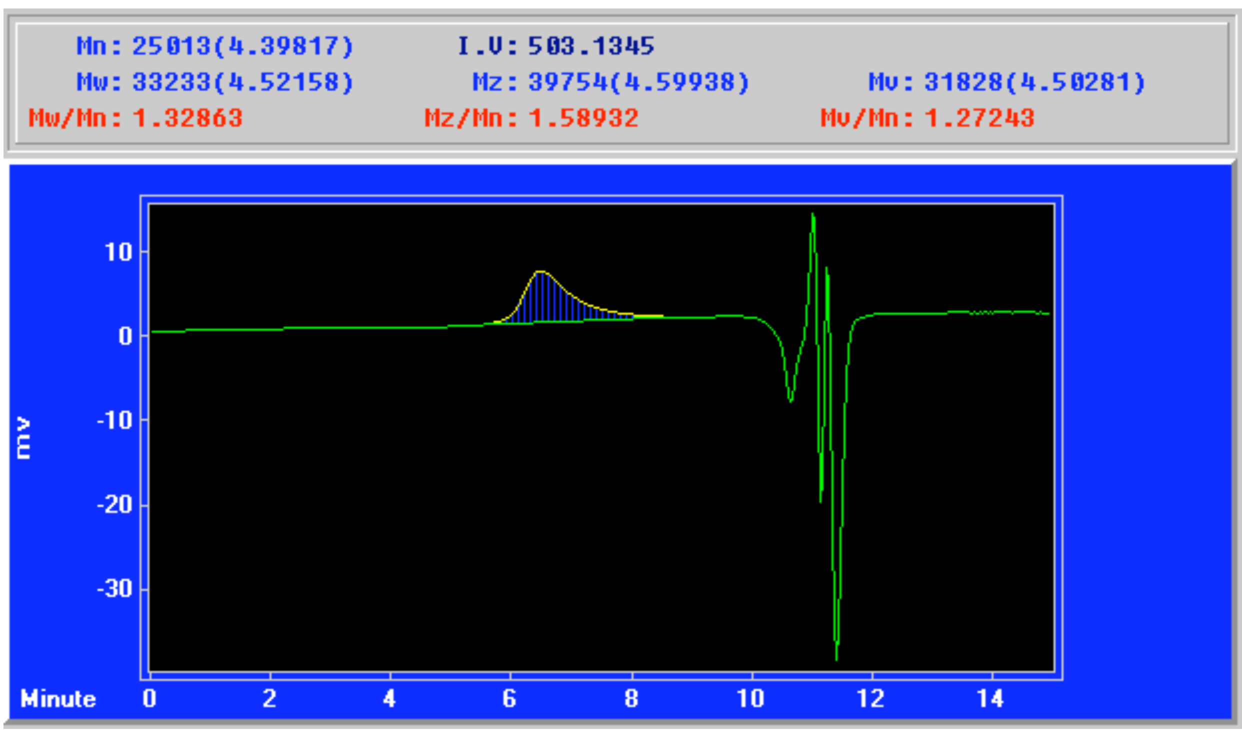


Polymer Characterization by GPC

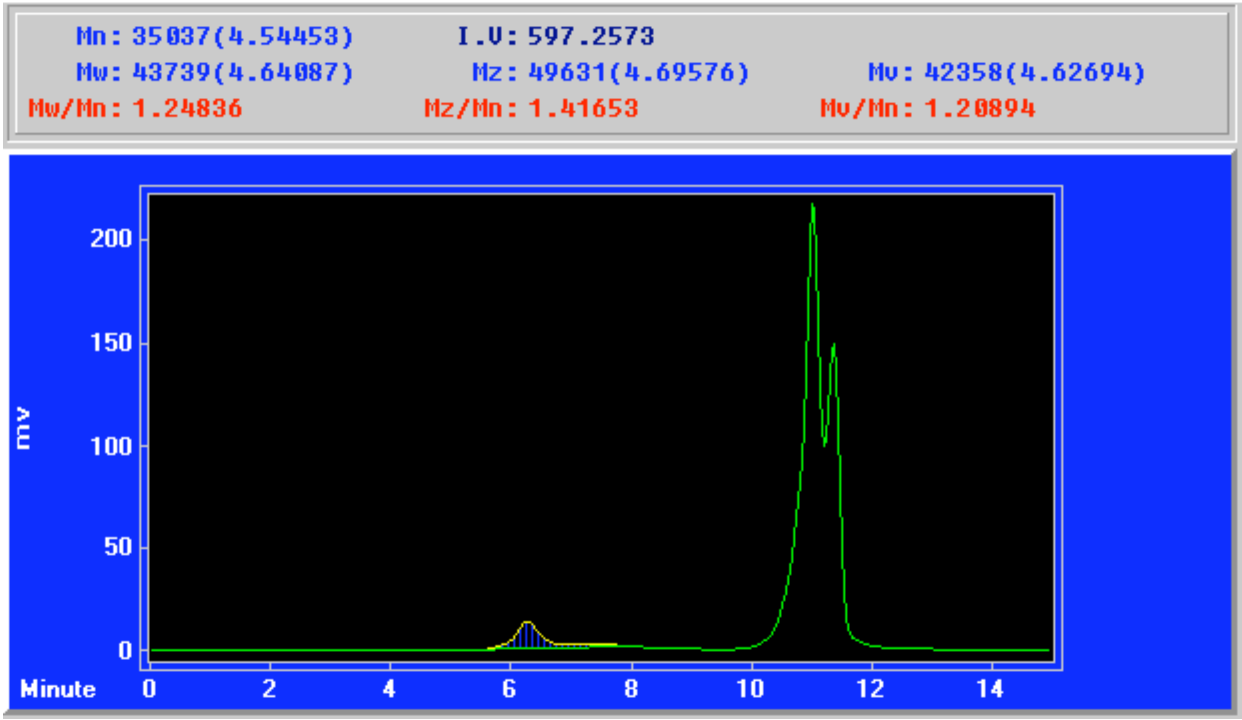
GPC of PLA from Table 1, entry 1



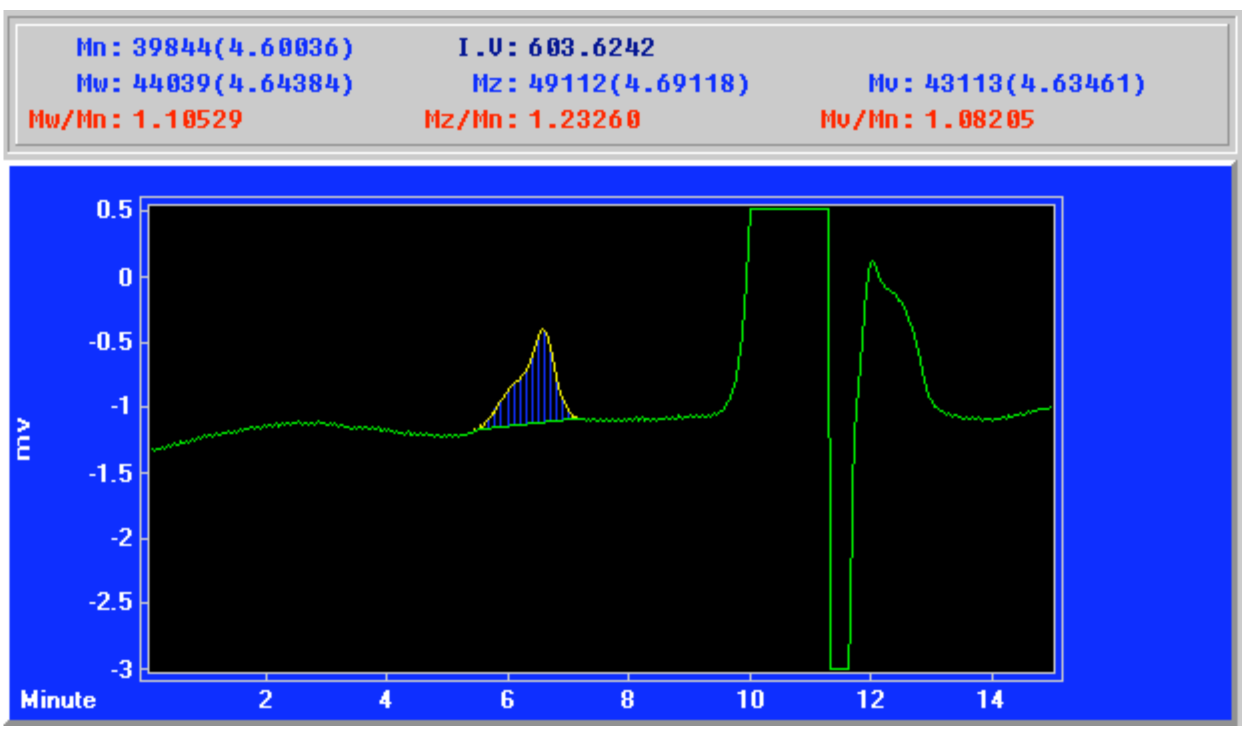
GPC of PLA from Table 1, entry 2



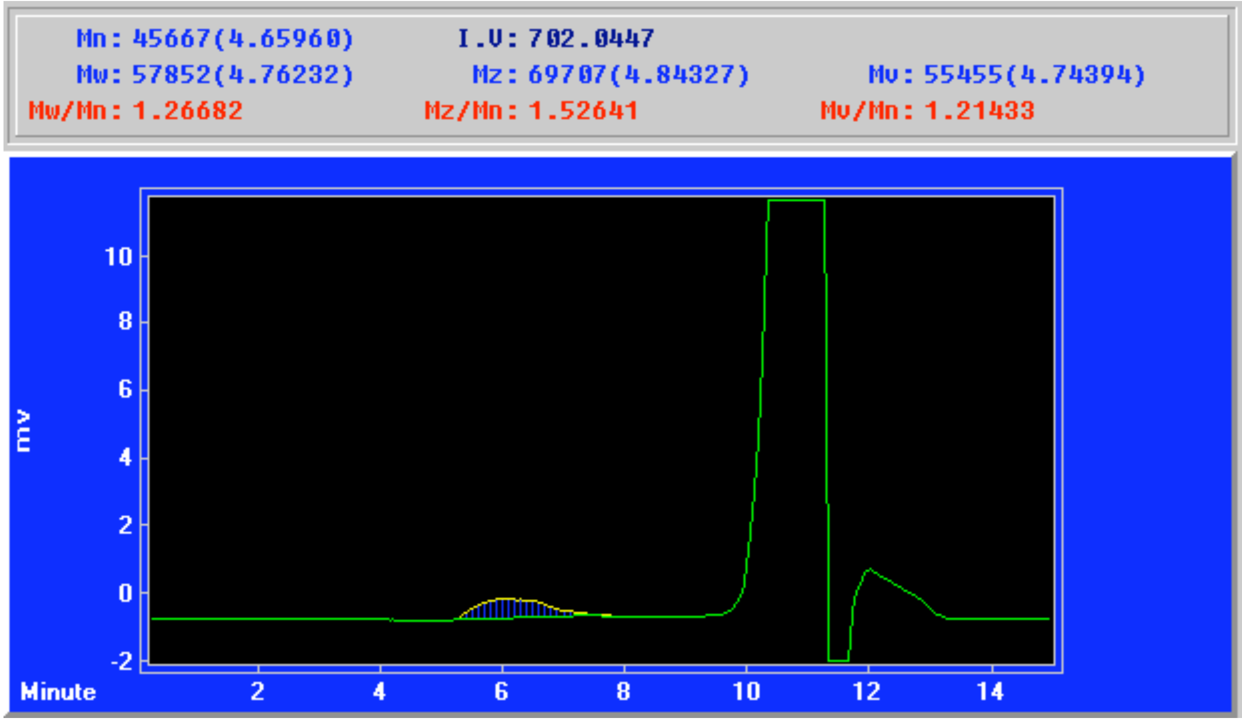
GPC of PLA from Table 1, entry 3



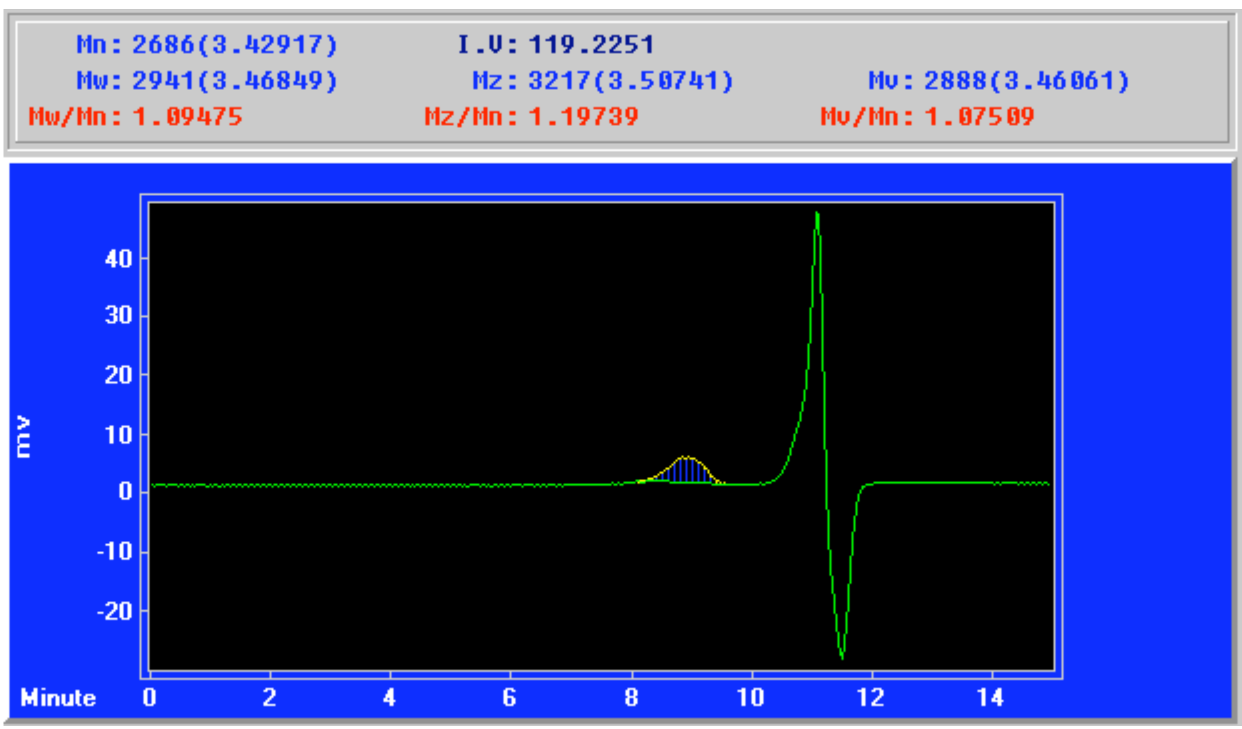
GPC of PLA from Table 1, entry 4



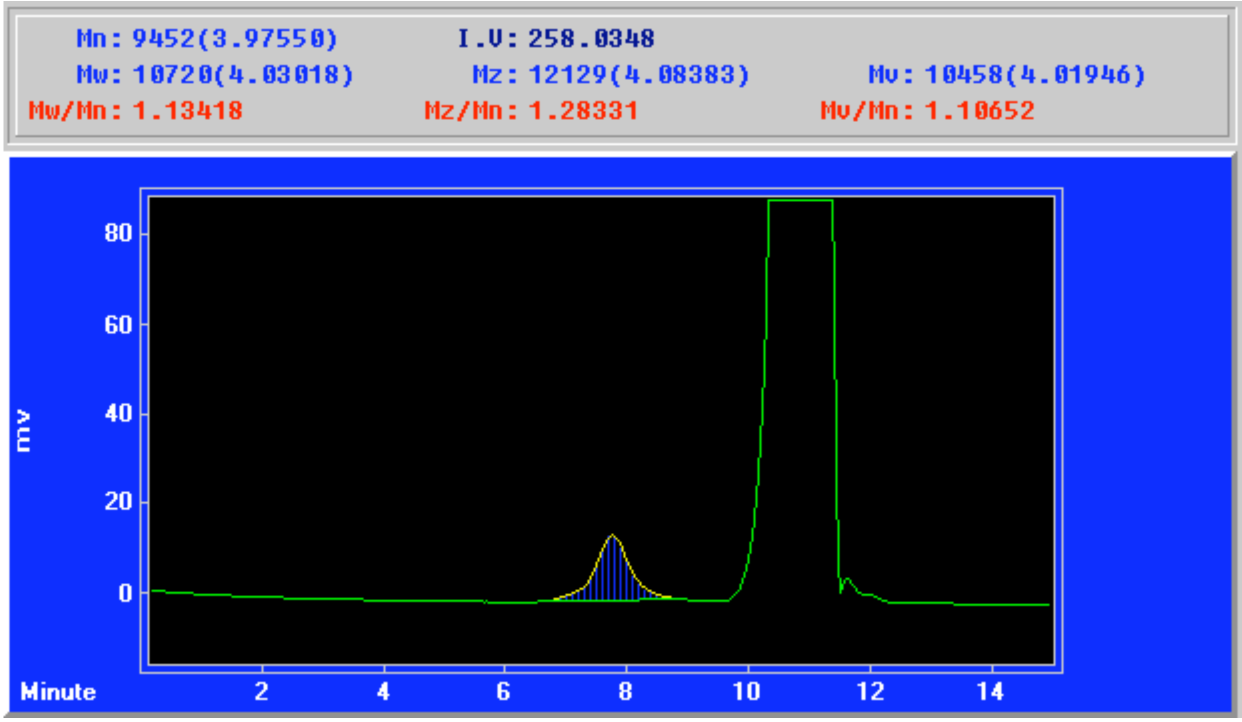
GPC of PLA from Table 1, entry 5



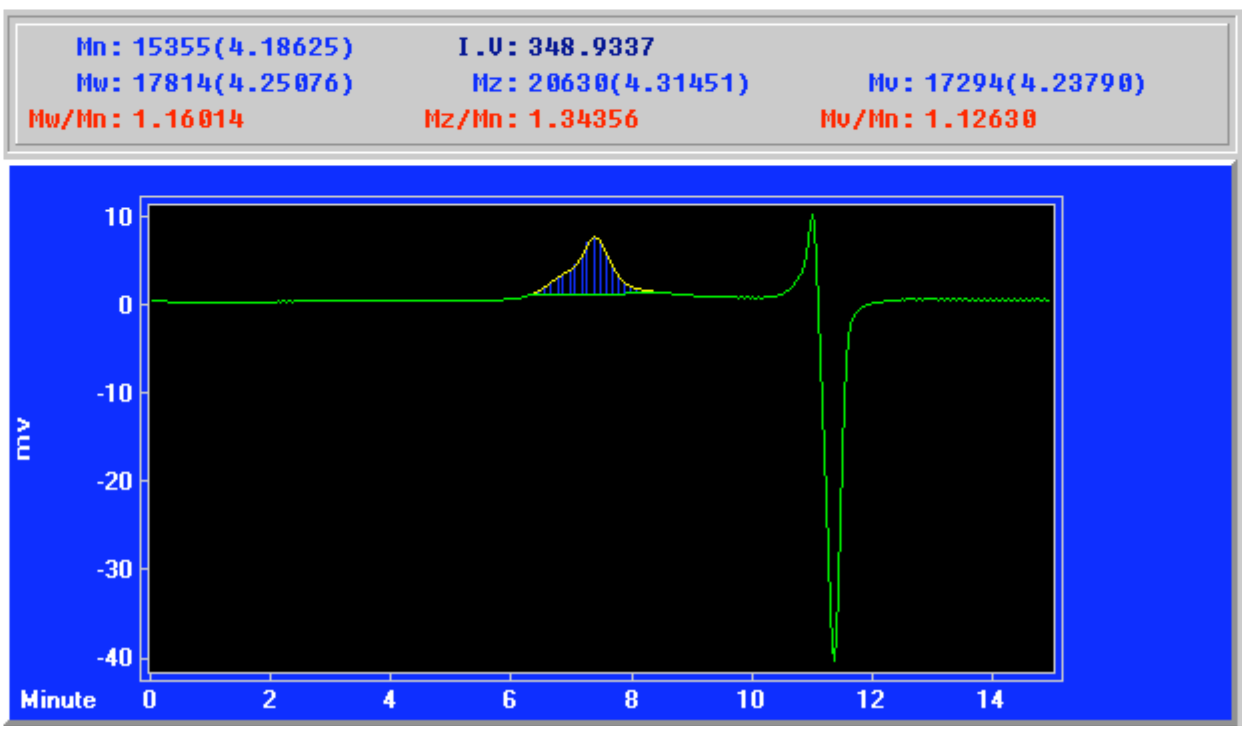
GPC of PLA from Table 1, entry 6



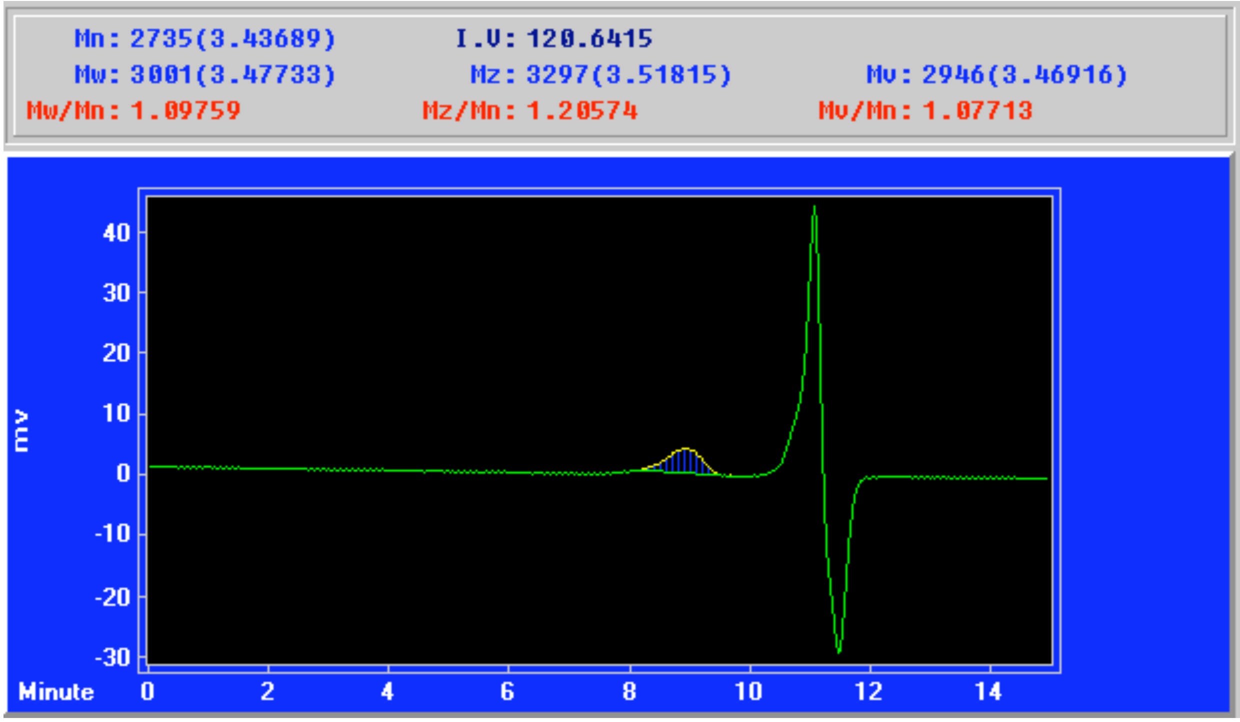
GPC of PLA from Table 1, entry 7



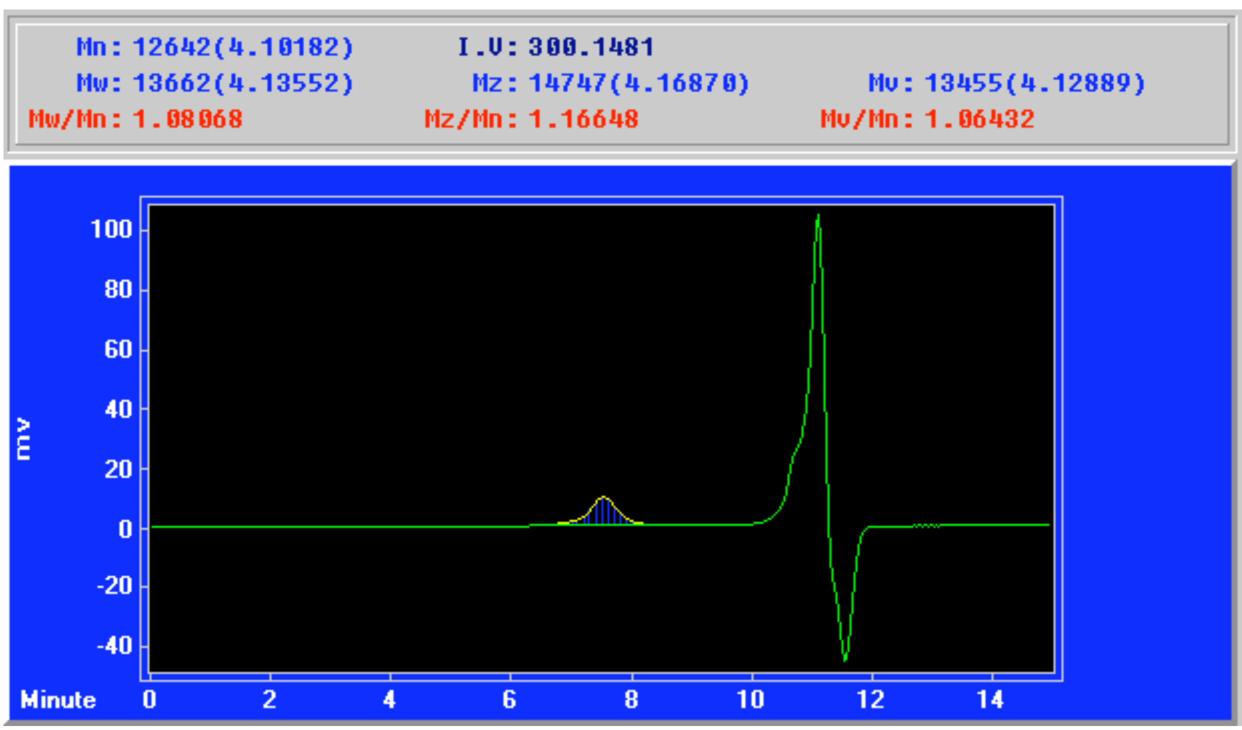
GPC of PLA from Table 1, entry 8



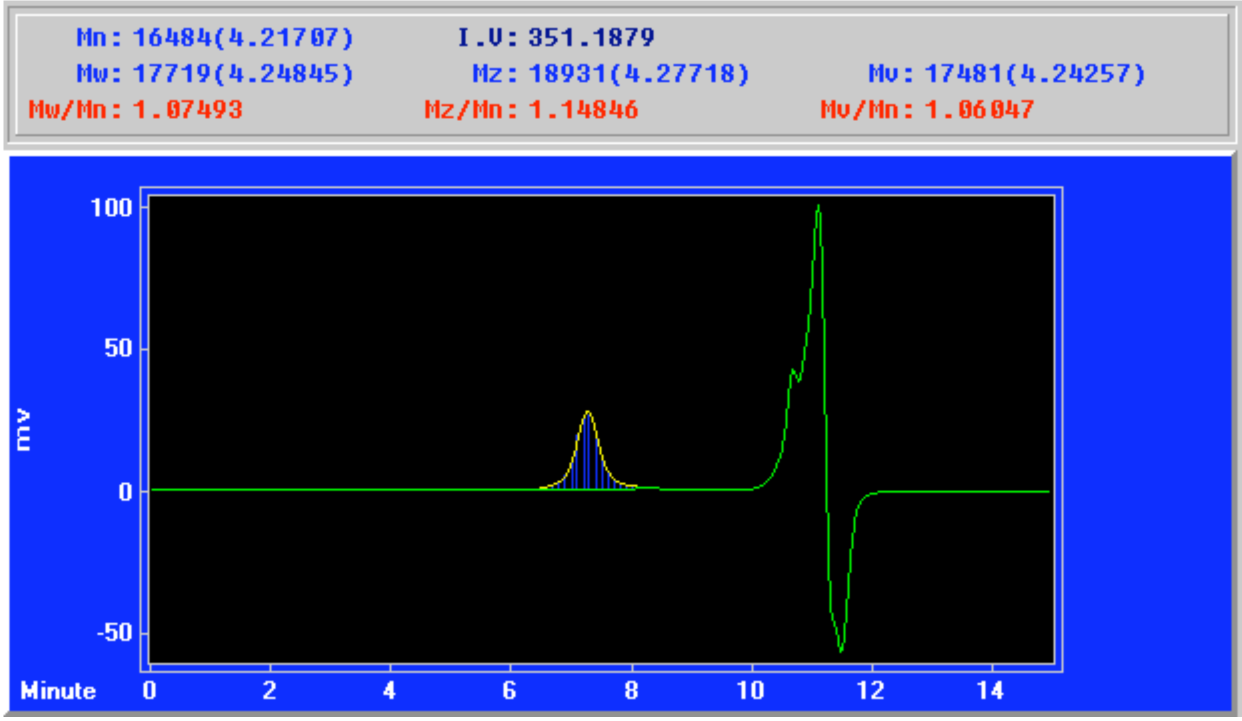
GPC of PLA from Table 1, entry 9



GPC of PLA from Table 1, entry 10



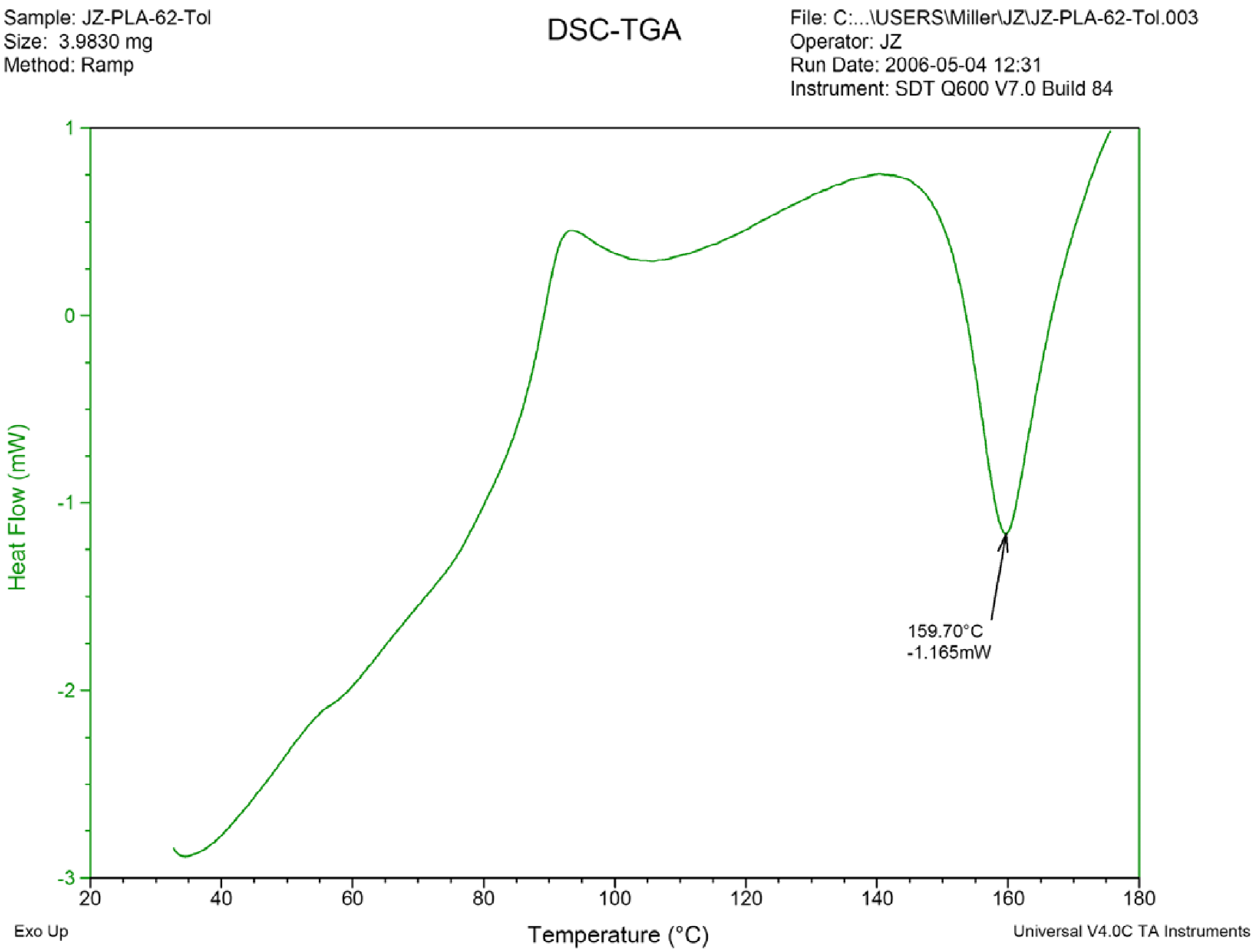
GPC of PLA from Table 1, entry 11



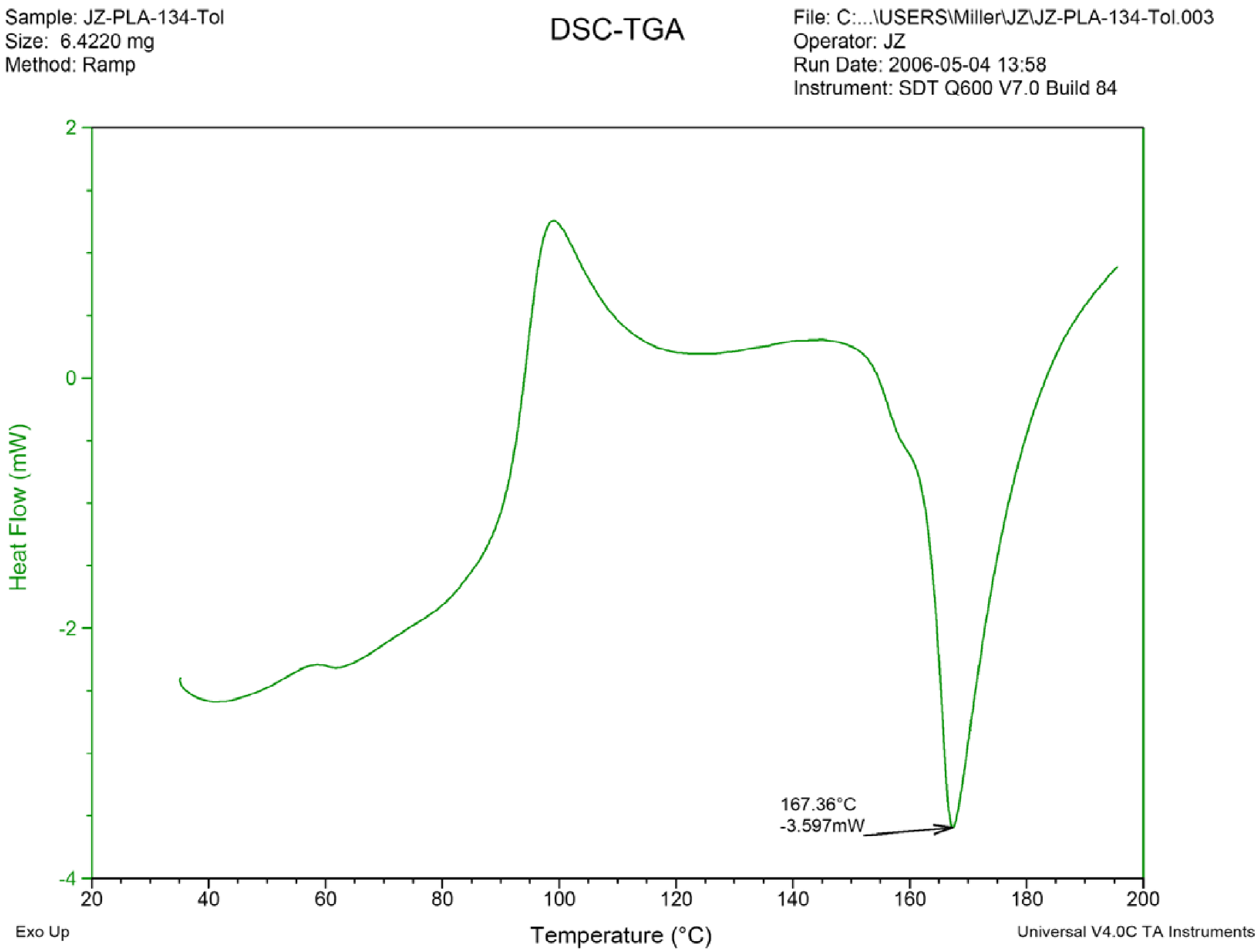
Polymer Characterization by DSC

The second DSC scans are provided below.

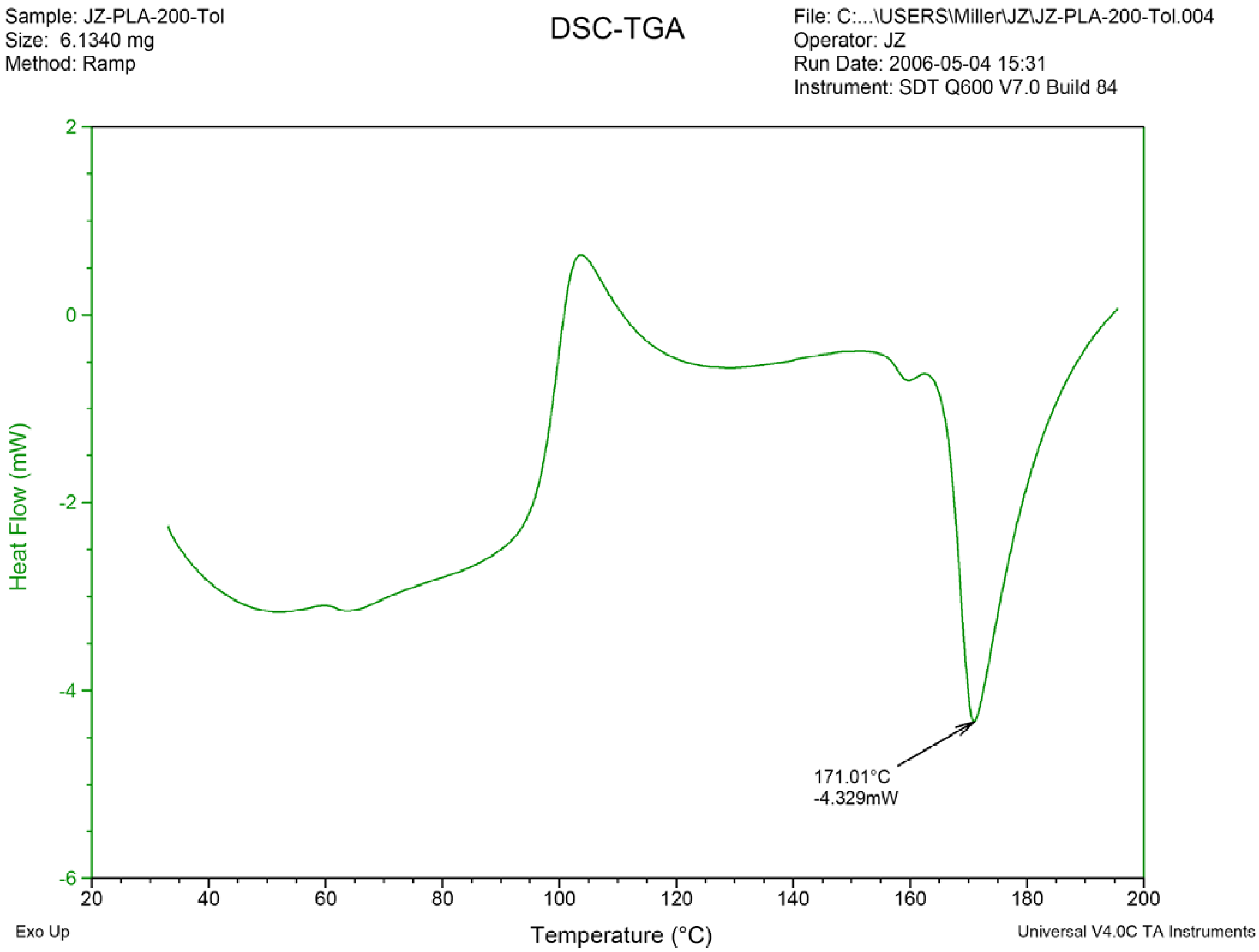
DSC of PLA from Table 1, entry 1



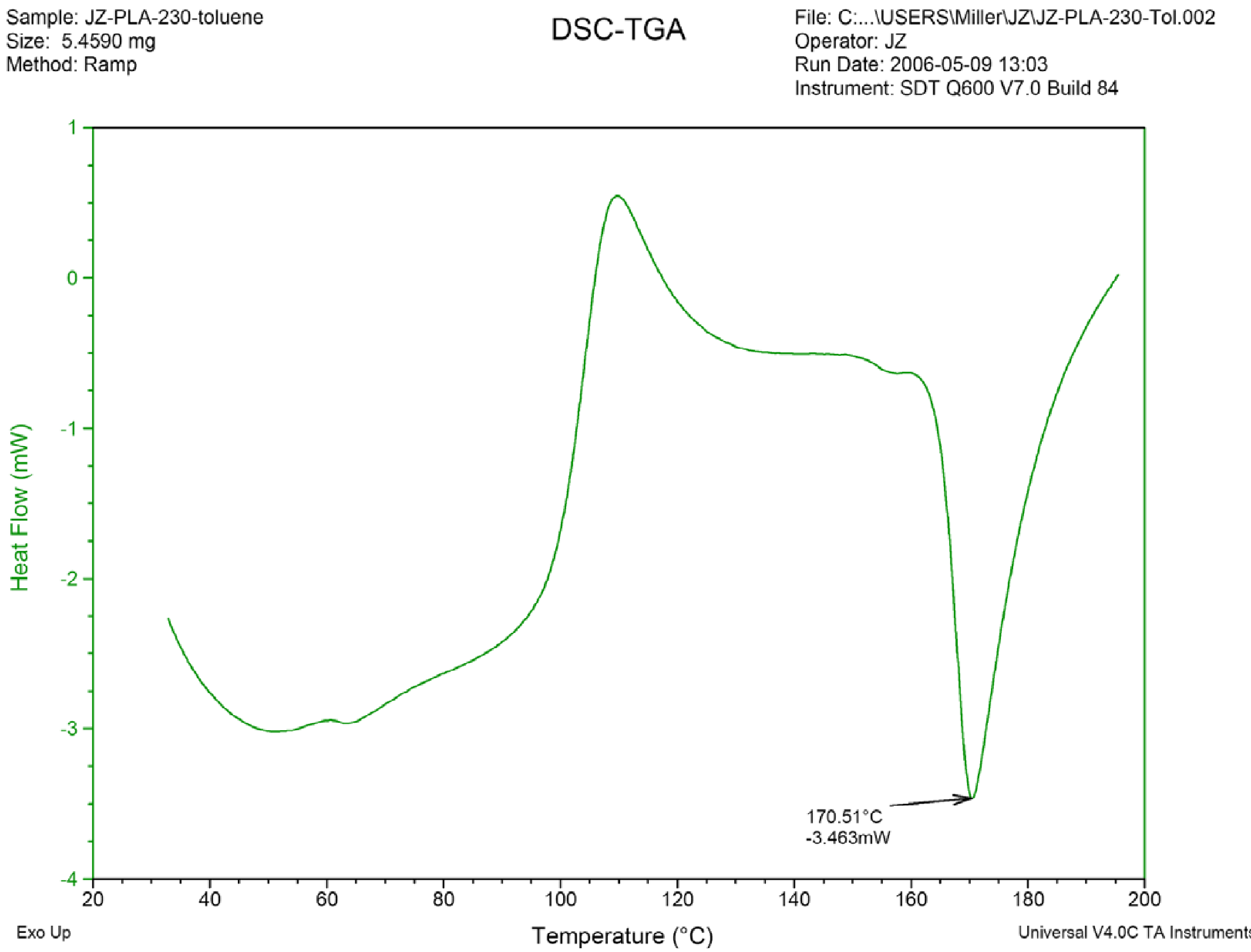
DSC of PLA from Table 1, entry 2



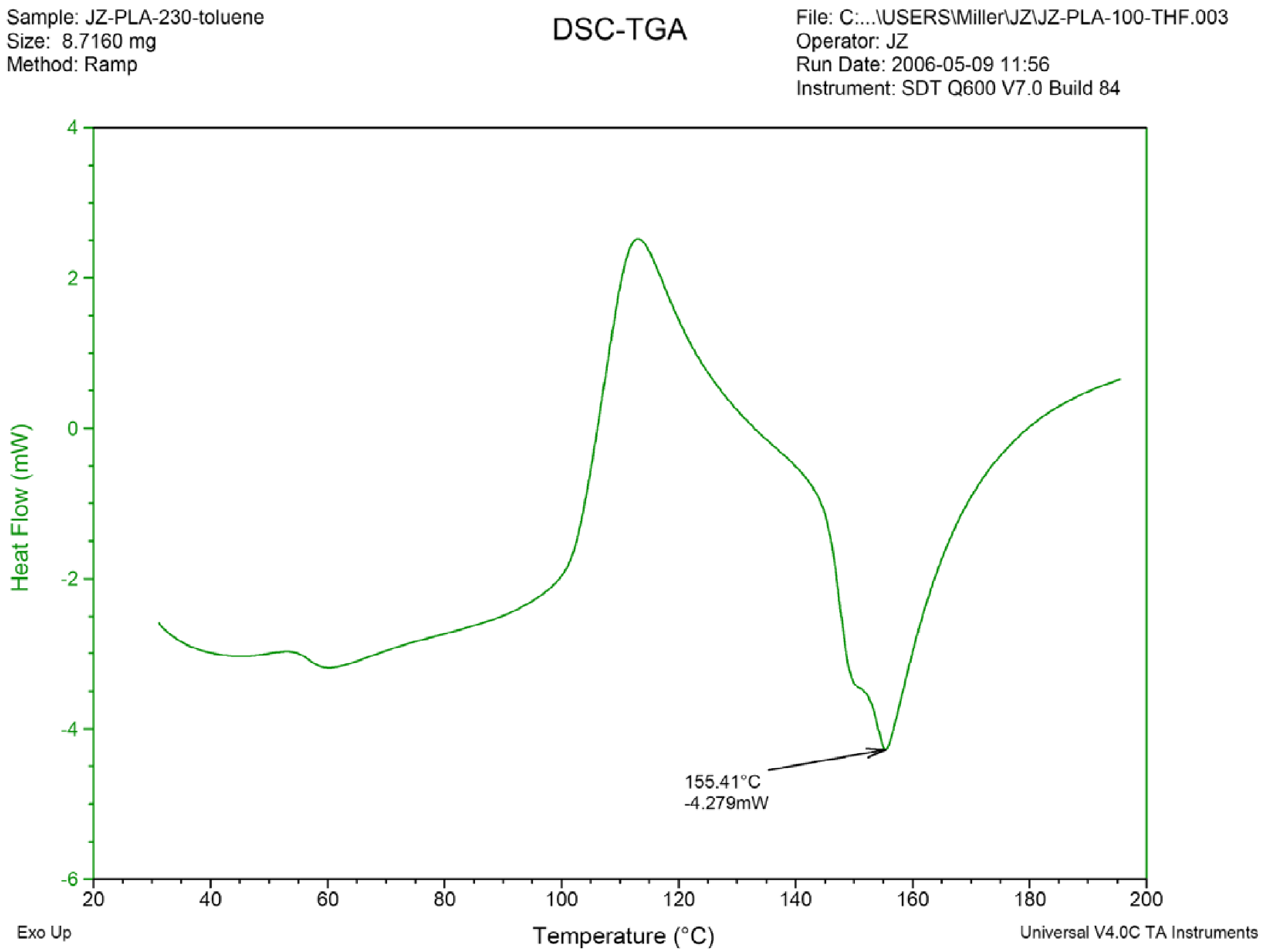
DSC of PLA from Table 1, entry 4



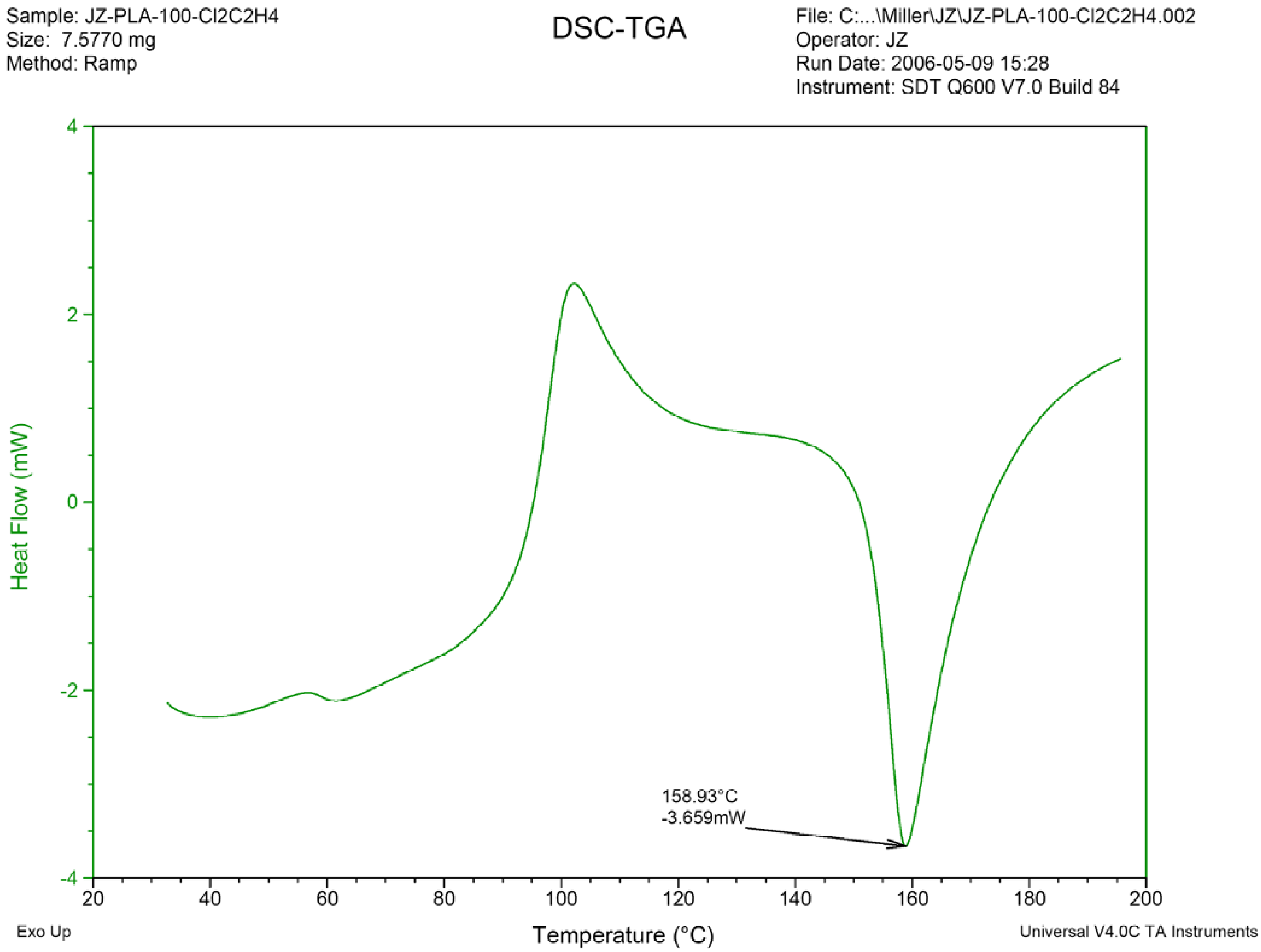
DSC of PLA from Table 1, entry 5



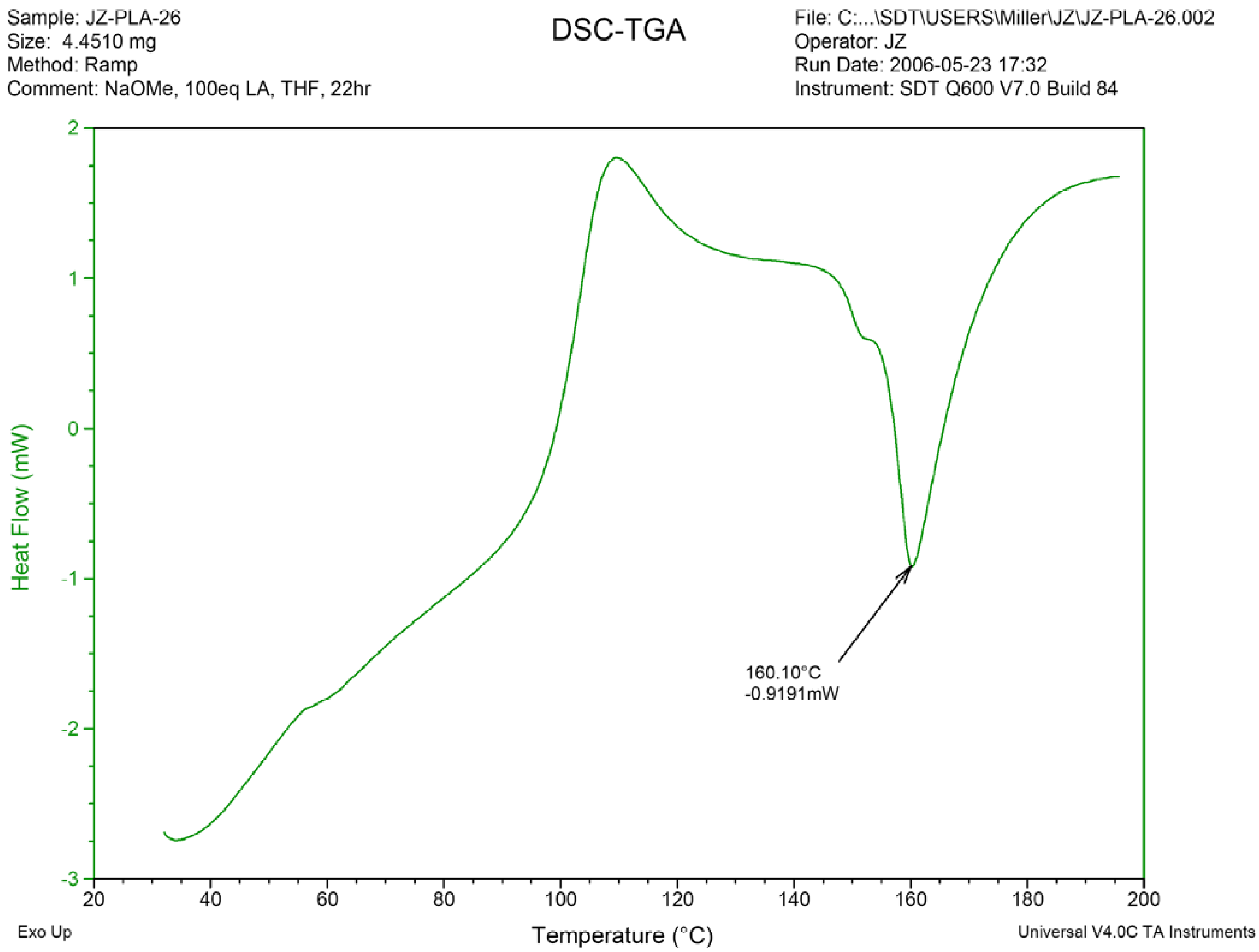
DSC of PLA from Table 1, entry 8



DSC of PLA from Table 1, entry 11

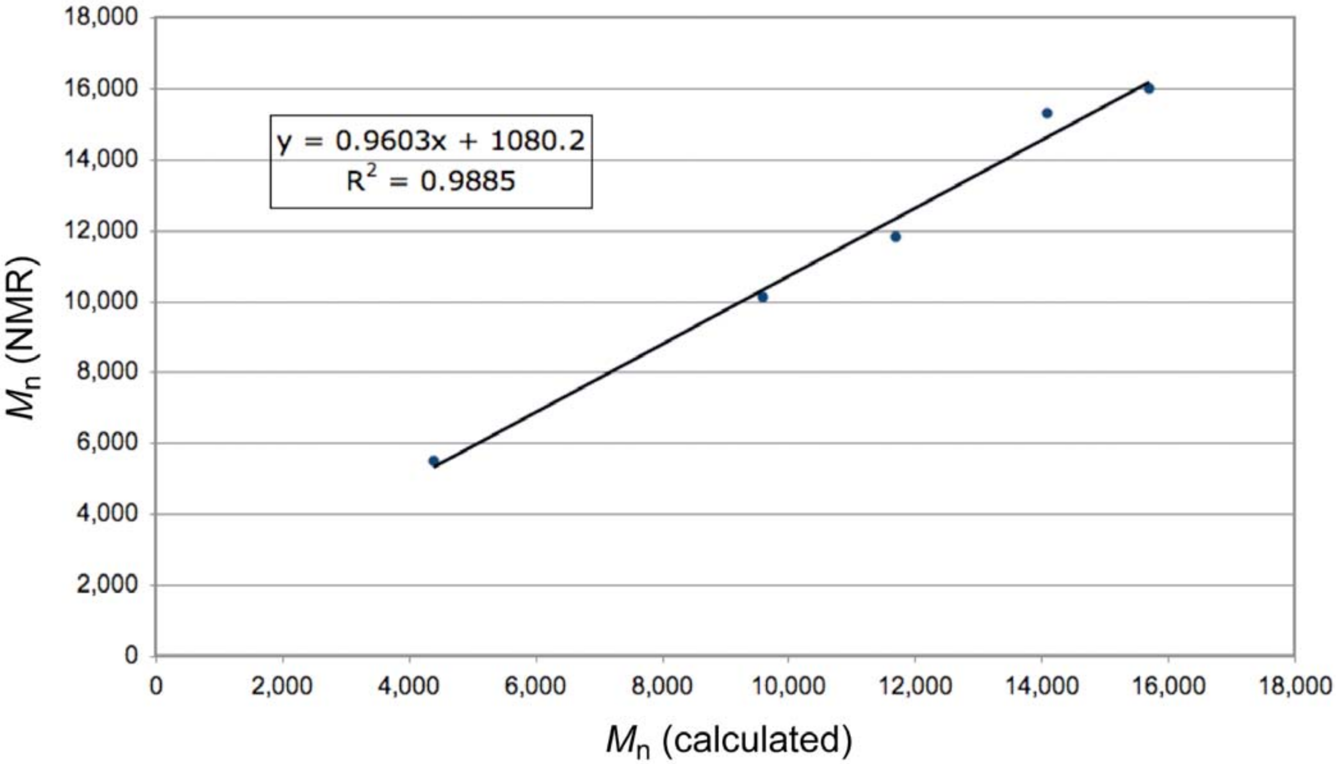


DSC of PLA from the initiator NaOMe under the conditions of Table 1, entry 8



M_n (NMR) vs. M_n (calculated)

entry	M_n calculated	M_n NMR[b]
1	4,400	5,500
2	9,600	10,100
3	11,700	11,800
4	14,100	15,300
5	15,700	16,000

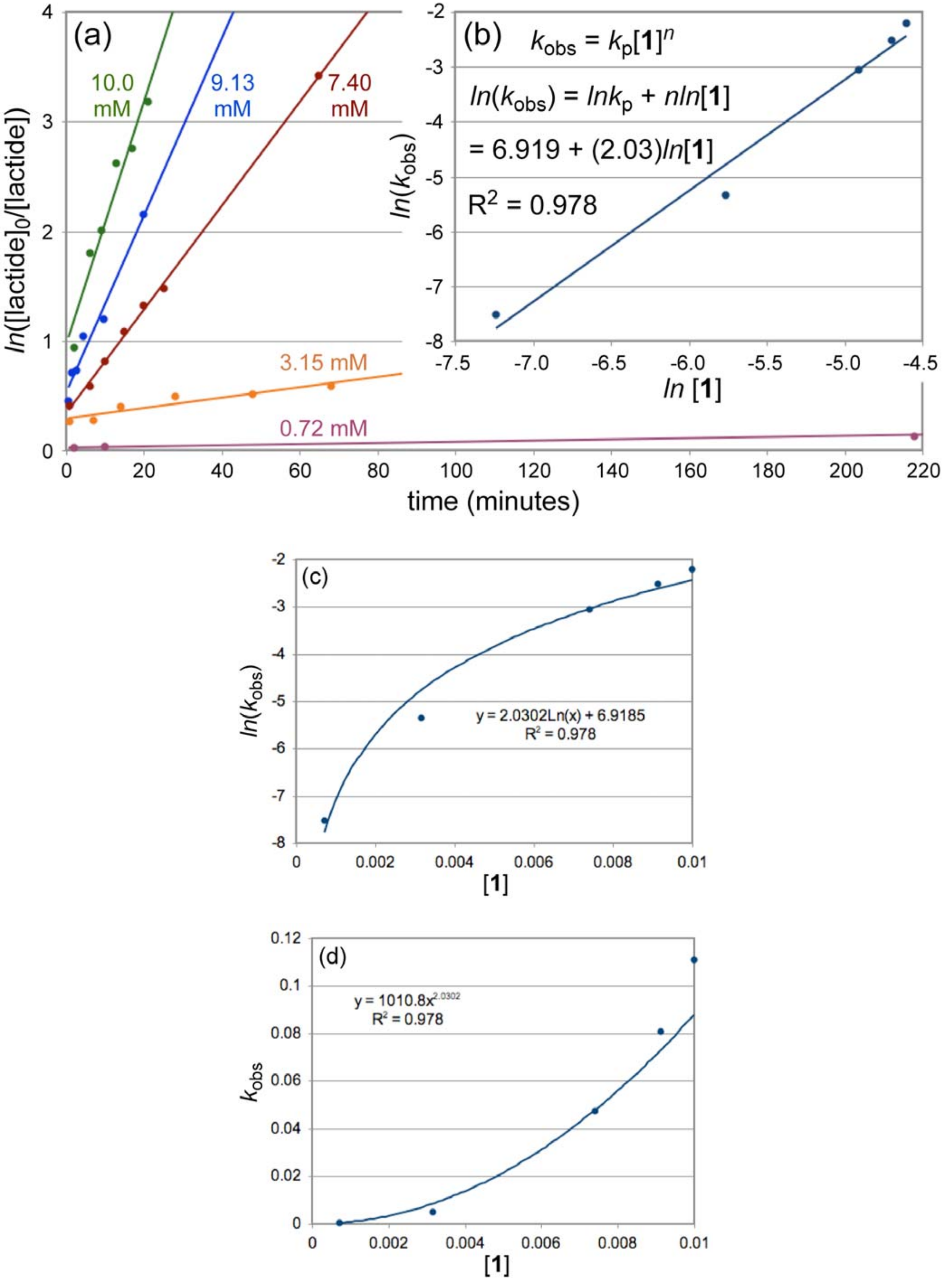


Details of the Kinetic Study of L-Lactide Polymerization with 1

A kinetic study was conducted to establish the reaction order with respect to monomer and catalyst **1**. L-Lactide (0.288 g, 2.00 mmol) was added to a solution of **1** (0.72, 3.15, 7.40, 9.13, or 10.0 mM) in tetrahydrofuran (10 mL). The solution was then stirred at 20°C under an atmosphere of nitrogen. At the indicated time intervals, 0.05 mL aliquots were removed, trapped with liquid N_2, stripped of solvent, and analyzed by ^1H NMR in $CDCl_3$. The lactide concentration [LA] was determined by integrating the quartet methine peak of lactide at 5.00 ppm and the quartet methine peak of polylactic acid at 5.20 ppm.

As expected, plots of *ln*($[lactide]_0/[lactide]$) vs. time for a wide range of [**1**] are linear, indicating the usual first order dependence on monomer concentration (see graph (a) below). Thus, the rate expression can be written as $d[lactide]/dt = k_p[lactide]^1[\mathbf{1}]^n = k_{obs}[lactide]^1$, where $k_{obs} = k_p[\mathbf{1}]^n$. A plot of $ln(k_{obs})$ vs. *ln*[**1**] (see graph (b) below) allows the determination of k_p and *n*. The *y*-intercept of the best fit line (6.919) equals lnk_p and thus the polymerization rate constant, k_p, is 1011 $M^{-2}min^{-1}$ or 16.9 $M^{-2}s^{-1}$. The slope of the best fit line (2.03) equals *n* and thus the reaction is *second order* in catalyst, **1**. Graph (c) below shows the result of plotting $ln(k_{obs})$ vs. [**1**]; the best fit logarithmic curve indicates that $n = 2.03$. Graph (d) below shows the result of plotting k_{obs} vs. [**1**]; the best fit power curve indicates that $n = 2.03$. The overall rate expression is $d[lactide]/dt = k_p[lactide]^1[\mathbf{1}]^2$.

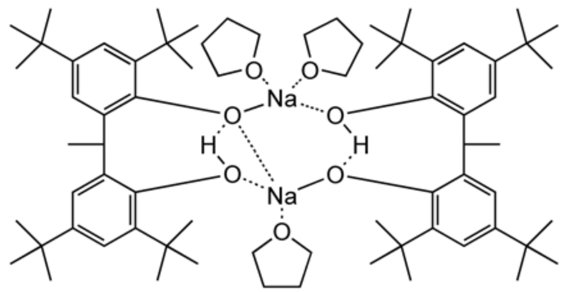
time (min.)	[**1**] = 10.0 mM		[**1**] = 9.13 mM		[**1**] = 7.40 mM		[**1**] = 3.15 mM		[**1**] = 0.72 mM	
	[LA]	*ln*($[LA]_0$/[LA])	[LA]	*ln*($[LA]_0$/[LA])	[LA]	*ln*($[LA]_0$/[LA])	[LA]	*ln*($[LA]_0$/[LA])	[LA]	*ln*($[LA]_0$/[LA])
0	0.20000	0.0000	0.20000	0.0000	0.20000	0.0000	0.20000	0.0000	0.20000	0.0000
0.6			0.12850	0.44238						
1					0.13286	0.40902	0.15370	0.26331		
1.5			0.09892	0.70400						
2	0.07862	0.93369							0.19536	0.02347
2.5			0.09672	0.72649						
4.5			0.07108	1.03451						
6	0.03304	1.80059			0.11148	0.58447				
7							0.15278	0.26931		
9	0.02682	2.00916								
9.5			0.06030	1.19898						
10					0.08888	0.81103			0.19456	0.02757
13	0.01462	2.61592								
14							0.13418	0.39913		
15					0.06818	1.07616				
17	0.01278	2.75043								
20			0.02334	2.14814	0.05372	1.31453				
21	0.00836	3.17485								
25					0.04554	1.47972				
28							0.12222	0.49249		
48							0.12046	0.50699		
65					0.00654	3.42038				
68							0.11144	0.58483		
218									0.17620	0.12669
436									0.15410	0.26071
y=mx+b										
m=k_{obs}		0.11082		0.08083		0.04733		0.00476		0.00054
b		0.95819		0.52239		0.33926		0.28766		0.01955
R^2		0.94954		0.97222		0.99912		0.86961		0.99573
[**1**], mM		0.01000		0.00913		0.00740		0.00315		0.00072
ln[**1**]		-4.60517		-4.69618		-4.90627		-5.76035		-7.23625
$ln(k_{obs})$		-2.19984		-2.51541		-3.05061		-5.34751		-7.52425

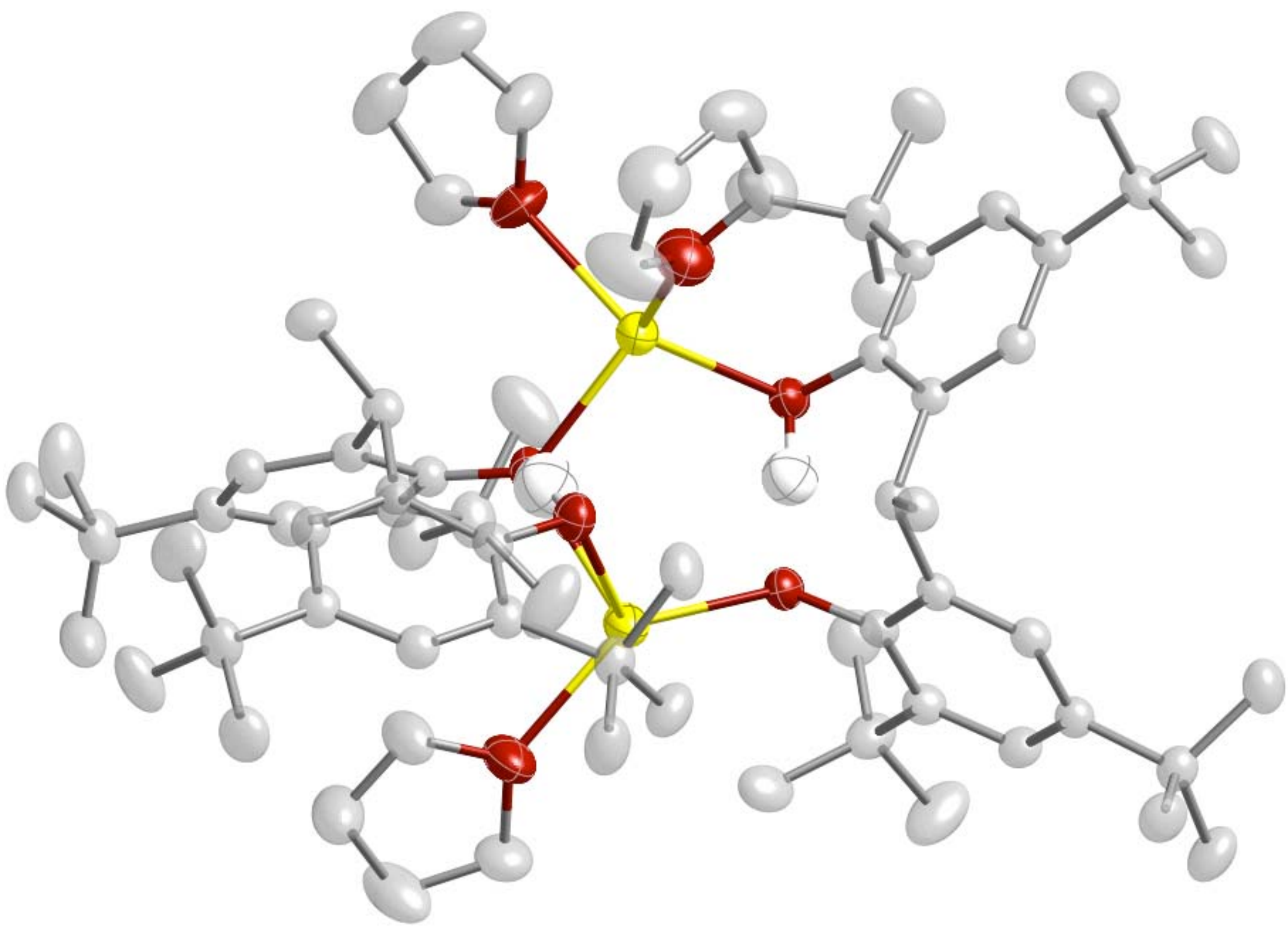

(a)
10.0 mM
9.13 mM
7.40 mM
3.15 mM
0.72 mM
ln([lactide]0/[lactide])
time (minutes)
(b)
kobs = kp[1]^n
ln(kobs) = lnkp + nln[1]
= 6.919 + (2.03)ln[1]
R2 = 0.978
ln(kobs)
ln [1]
(c)
y = 2.0302Ln(x) + 6.9185
R2 = 0.978
ln(kobs)
[1]
(d)
y = 1010.8x^2.0302
R2 = 0.978
kobs
[1]

X-ray Crystallographic Data for 2

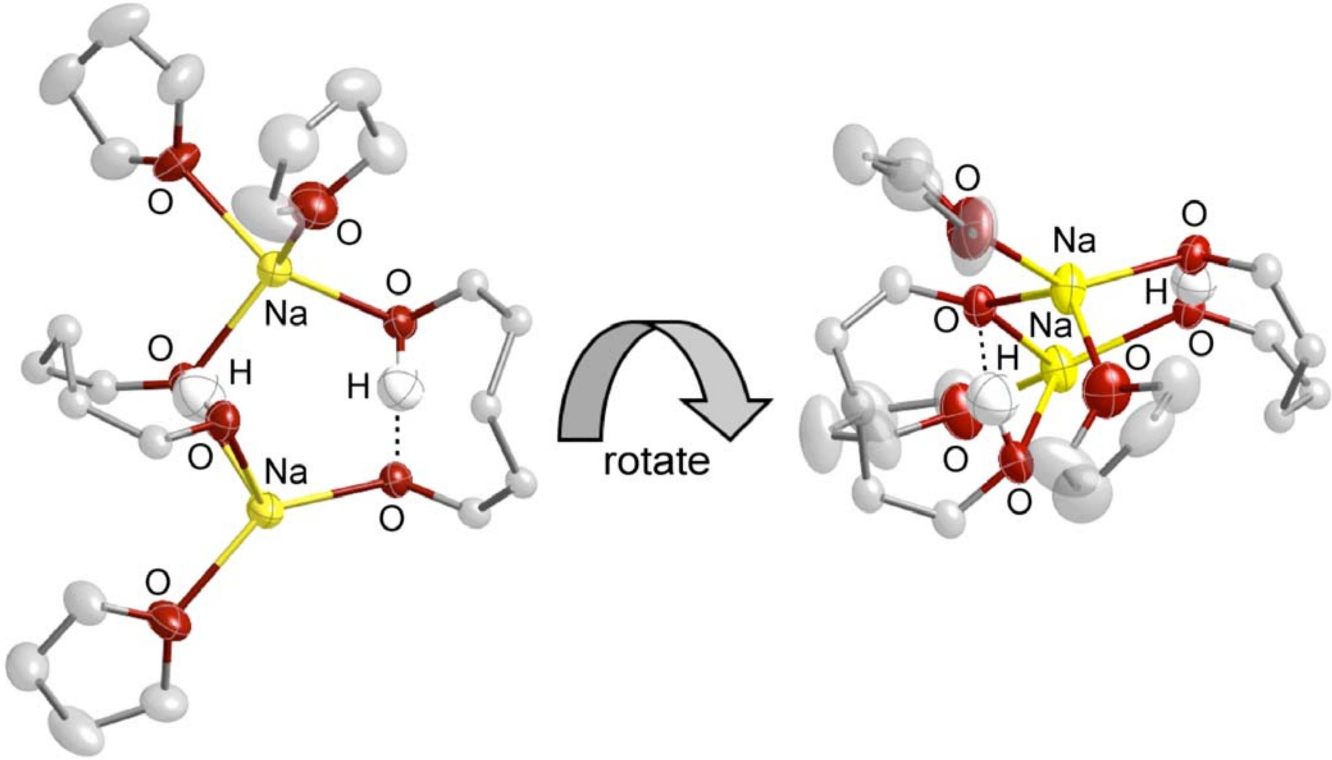
$C_{79}H_{122}Na_2O_7$ (SM114)

CCDC 615697

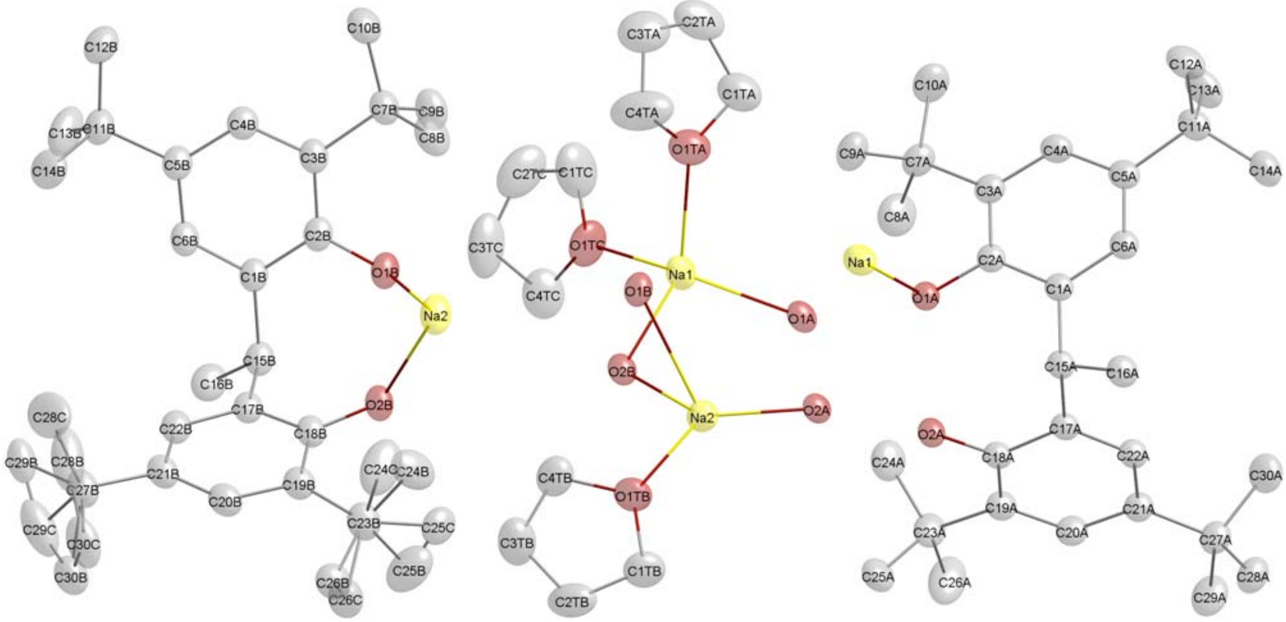




View with 50% probability ellipsoids



View of the core structure with 50% probability ellipsoids



Labeled view of 3 sections (Na2+ligand, core, Na1+ligand) with 50% probability ellipsoids

Data Collection

A Bausch and Lomb 10x microscope was used to identify a suitable colorless parallelpiped 0.3mm x 0.2mm x 0.1mm from a representative sample of crystals of the same habit. The crystal was coated in a cryogenic protectant (mineral oil), and was then fixed to a glass fiber which in turn was fashioned to a copper mounting pin. The mounted crystal was then placed in a cold nitrogen stream (Oxford) maintained at 110K.

A BRUKER SMART 1000 X-ray three-circle diffractometer was employed for crystal screening, unit cell determination and data collection. The goniometer was controlled using the SMART software suite, version 5.056, (Microsoft NT operating system). The sample was optically centered with the aid of a video camera such that no translations were observed as the crystal was rotated through all positions. The detector was set at 5.0 cm from the crystal sample (CCD-PXL-KAF2, SMART 1000, 512x512 pixel). The X-ray radiation employed was generated from a Mo sealed X-ray tube (K_{α} = 0.70173Å with a potential of 50 kV and a current of 40 mA) and filtered with a graphite monochromator in the parallel mode (175 mm collimator with 0.5 mm pinholes).

Dark currents were obtained for the appropriate exposure time 30 sec and a rotation exposure was taken to determine crystal quality and the X-ray beam intersection with the detector. The beam intersection coordinates were compared to the configured coordinates and changes were made accordingly. The rotation exposure indicated acceptable crystal quality and the unit cell determination was undertaken. Sixty data frames were taken at widths of 0.3° with an exposure time of 10 seconds. Over 200 reflections were centered and their positions were determined. These reflections were used in the auto-indexing procedure to determine the unit cell. A suitable cell was found and refined by nonlinear least squares and Bravais lattice procedures and reported here in Table 1. The unit cell was verified by examination of the hkl overlays on several frames of data, including zone photographs. No super-cell or erroneous reflections were observed.

After careful examination of the unit cell, a standard data collection procedure was initiated. This procedure consists of collection of one hemisphere of data collected using omega scans, involving the collection 1201 0.3° frames at fixed angles for ϕ, 2θ, and χ (2θ = -28°, χ = 54.73°), while varying omega. Each frame was exposed for 30 sec and contrasted against a 30 sec. dark current exposure. The total data collection was performed for duration of approximately 13 hours at 110 K. No significant intensity fluctuations of equivalent reflections were observed.

After data collection, the crystal was measured carefully for size, morphology and color. These measurements are reported in Table 1.

Table 1. Crystal data and structure refinement for sm114.

Identification code	sm114	
Empirical formula	C79 H122 Na2 O7	
Formula weight	1229.75	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.035(5) Å	α = 90.000(5)°
	b = 19.797(5) Å	β = 104.979(5)°
	c = 24.936(5) Å	γ = 90.000(5)°
Volume	7647(3) $Å^3$	
Z	4	
Density (calculated)	1.068 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	2696	
Crystal size	0.50 x 0.40 x 0.20 mm^3	
Theta range for data collection	1.33 to 25.00°.	
Index ranges	-19<=h<=19, -23<=k<=23, -29<=l<=29	
Reflections collected	69791	
Independent reflections	13244 [R(int) = 0.0242]	
Completeness to theta = 25.00°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9851 and 0.9632	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13244 / 0 / 821	
Goodness-of-fit on F^2	1.099	
Final R indices [I>2sigma(I)]	R1 = 0.0631, wR2 = 0.1693	
R indices (all data)	R1 = 0.0806, wR2 = 0.1963	
Largest diff. peak and hole	0.357 and -0.542 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for sm114. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Na(1)	8127(1)	1958(1)	6885(1)	64(1)
Na(2)	9215(1)	946(1)	5993(1)	60(1)
O(1A)	7833(1)	832(1)	6957(1)	49(1)
O(2A)	8515(1)	173(1)	6361(1)	47(1)
C(1A)	6414(1)	529(1)	6413(1)	41(1)
C(2A)	6990(1)	694(1)	6925(1)	43(1)
C(3A)	6696(1)	730(1)	7412(1)	49(1)
C(4A)	5816(1)	646(1)	7355(1)	51(1)
C(5A)	5227(1)	496(1)	6856(1)	48(1)
C(6A)	5546(1)	432(1)	6391(1)	44(1)
C(7A)	7325(2)	826(1)	7989(1)	61(1)
C(8A)	7940(2)	221(2)	8116(1)	90(1)
C(9A)	7855(2)	1478(2)	8029(1)	79(1)
C(10A)	6847(2)	867(2)	8447(1)	86(1)
C(11A)	4261(1)	445(1)	6826(1)	57(1)
C(12A)	3914(2)	1165(1)	6863(1)	78(1)
C(13A)	4096(2)	28(2)	7303(1)	80(1)
C(14A)	3751(2)	125(2)	6285(1)	73(1)
C(15A)	6747(1)	453(1)	5891(1)	41(1)
C(16A)	6065(1)	631(1)	5355(1)	51(1)
C(17A)	7135(1)	-249(1)	5871(1)	40(1)
C(18A)	8018(1)	-358(1)	6141(1)	42(1)
C(19A)	8350(1)	-1018(1)	6180(1)	48(1)
C(20A)	7815(1)	-1539(1)	5912(1)	49(1)
C(21A)	6961(1)	-1438(1)	5614(1)	46(1)
C(22A)	6637(1)	-786(1)	5611(1)	44(1)
C(23A)	9275(1)	-1168(1)	6534(1)	61(1)
C(24A)	9366(2)	-926(2)	7132(1)	73(1)
C(25A)	9945(2)	-814(2)	6291(1)	75(1)
C(26A)	9477(2)	-1926(1)	6555(2)	98(1)
C(27A)	6391(1)	-2007(1)	5298(1)	53(1)
C(28A)	6104(2)	-1821(1)	4681(1)	65(1)
C(29A)	6863(2)	-2682(1)	5350(1)	75(1)
C(30A)	5586(2)	-2091(2)	5515(1)	75(1)
O(1B)	8340(1)	2010(1)	5645(1)	57(1)
O(2B)	9354(1)	1875(1)	6591(1)	54(1)
C(1B)	9027(1)	3055(1)	5527(1)	48(1)
C(2B)	8570(1)	2471(1)	5299(1)	49(1)
C(3B)	8350(1)	2359(1)	4722(1)	51(1)
C(4B)	8675(1)	2811(1)	4396(1)	54(1)
C(5B)	9181(1)	3365(1)	4613(1)	53(1)
C(6B)	9331(1)	3484(1)	5180(1)	52(1)
C(7B)	7751(2)	1776(1)	4449(1)	59(1)
C(8B)	8079(2)	1088(1)	4696(1)	73(1)
C(9B)	6853(2)	1904(1)	4538(1)	75(1)
C(10B)	7664(2)	1734(2)	3823(1)	83(1)
C(11B)	9560(2)	3846(1)	4254(1)	65(1)
C(12B)	9384(2)	3612(2)	3652(1)	79(1)
C(13B)	9170(3)	4550(2)	4267(2)	104(1)
C(14B)	10539(2)	3880(2)	4490(1)	98(1)
C(15B)	9208(1)	3200(1)	6146(1)	50(1)
C(16B)	9123(2)	3954(1)	6275(1)	65(1)
C(17B)	10066(1)	2899(1)	6471(1)	49(1)
C(18B)	10083(1)	2249(1)	6711(1)	50(1)
C(19B)	10871(1)	2015(1)	7060(1)	54(1)

C(20B)	11613(1)	2396(1)	7090(1)	59(1)
C(21B)	11621(1)	3004(1)	6817(1)	60(1)
C(22B)	10829(2)	3252(1)	6522(1)	56(1)
C(23B)	10948(2)	1360(1)	7407(1)	68(1)
C(24B)	10714(9)	744(4)	7077(4)	103(4)
C(25B)	10375(7)	1450(7)	7823(5)	113(4)
C(26B)	11868(8)	1280(6)	7795(5)	75(2)
C(23C)	10948(2)	1360(1)	7407(1)	68(1)
C(24C)	11174(11)	765(6)	7016(6)	110(4)
C(25C)	10113(5)	1128(5)	7539(5)	72(3)
C(26C)	11639(13)	1376(12)	7938(8)	126(7)
C(27B)	12467(2)	3381(1)	6836(1)	72(1)
C(28B)	12996(7)	3040(5)	6590(7)	120(6)
C(29B)	12255(5)	4140(3)	6576(5)	79(3)
C(30B)	12858(6)	3588(5)	7460(3)	99(4)
C(27C)	12467(2)	3381(1)	6836(1)	72(1)
C(28C)	12595(6)	3368(8)	6254(3)	152(5)
C(29C)	12488(4)	4035(3)	7087(5)	115(4)
C(30C)	13287(3)	2986(3)	7213(4)	103(3)
O(1TA)	6813(1)	2449(1)	6435(1)	93(1)
C(1TA)	6009(2)	2365(2)	6564(2)	106(1)
C(2TA)	5545(2)	3011(2)	6431(2)	107(1)
C(3TA)	5914(3)	3301(2)	5977(2)	130(1)
C(4TA)	6678(3)	2926(3)	5999(2)	151(2)
O(1TB)	10308(1)	1017(1)	5561(1)	81(1)
C(1TB)	10938(2)	545(2)	5479(2)	94(1)
C(2TB)	11646(2)	920(2)	5371(2)	114(1)
C(3TB)	11419(3)	1633(2)	5369(2)	134(2)
C(4TB)	10584(2)	1681(2)	5452(2)	97(1)
O(1TC)	8502(2)	2891(1)	7433(1)	97(1)
C(1TC)	7893(3)	3358(2)	7542(2)	148(2)
C(2TC)	8301(4)	3825(2)	7941(2)	118(1)
C(3TC)	9228(4)	3734(2)	8016(2)	126(2)
C(4TC)	9306(3)	3031(2)	7801(2)	102(1)
C(1)	6124(5)	4298(3)	4439(3)	154(3)
C(2)	5807(5)	4944(4)	4293(4)	154(3)
C(3)	6291(6)	5492(4)	4499(4)	154(3)
C(4)	7100(6)	5423(5)	4855(4)	154(3)
C(5)	7411(6)	4797(4)	4997(5)	154(3)
C(6)	6927(6)	4246(4)	4791(4)	154(3)
C(7)	5606(7)	3692(5)	4207(5)	154(3)
C(1')	6833(9)	4787(6)	4836(4)	314(8)
C(2')	6852(9)	4136(6)	4718(5)	314(8)
C(3')	6144(11)	3815(7)	4500(6)	314(8)
C(4')	5394(10)	4124(9)	4394(5)	314(8)
C(5')	5372(10)	4755(9)	4508(5)	314(8)
C(6')	6082(9)	5078(7)	4725(5)	314(8)
C(7')	7608(12)	5147(9)	5065(7)	314(8)

Table 3. Bond lengths [Å] and angles [°] for sm114.

Na(1)-O(2B)	2.2758(17)	Na(2)-O(1TB)	2.2858(19)
Na(1)-O(1TC)	2.283(2)	Na(2)-O(2B)	2.3426(18)
Na(1)-O(1A)	2.2950(18)	Na(2)-O(1B)	2.5548(18)
Na(1)-O(1TA)	2.328(2)	Na(2)-H(2O2)	2.36(3)
Na(1)-C(2A)	3.113(2)	O(1A)-C(2A)	1.361(2)
Na(1)-Na(2)	3.7440(13)	O(1A)-H(1O1)	1.01(3)
Na(1)-H(2O2)	2.53(4)	O(2A)-C(18A)	1.348(2)
Na(2)-O(2A)	2.2305(16)	O(2A)-H(1O1)	1.44(3)

C(1A)-C(6A)	1.392(3)
C(1A)-C(2A)	1.408(3)
C(1A)-C(15A)	1.536(3)
C(2A)-C(3A)	1.413(3)
C(3A)-C(4A)	1.391(3)
C(3A)-C(7A)	1.540(3)
C(4A)-C(5A)	1.387(3)
C(4A)-H(4AA)	0.9500
C(5A)-C(6A)	1.390(3)
C(5A)-C(11A)	1.534(3)
C(6A)-H(6AA)	0.9500
C(7A)-C(10A)	1.532(3)
C(7A)-C(8A)	1.531(4)
C(7A)-C(9A)	1.536(4)
C(8A)-H(8AA)	0.9800
C(8A)-H(8AB)	0.9800
C(8A)-H(8AC)	0.9800
C(9A)-H(9AA)	0.9800
C(9A)-H(9AB)	0.9800
C(9A)-H(9AC)	0.9800
C(10A)-H(10A)	0.9800
C(10A)-H(10B)	0.9800
C(10A)-H(10C)	0.9800
C(11A)-C(14A)	1.524(4)
C(11A)-C(13A)	1.527(3)
C(11A)-C(12A)	1.540(3)
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(13A)-H(13A)	0.9800
C(13A)-H(13B)	0.9800
C(13A)-H(13C)	0.9800
C(14A)-H(14A)	0.9800
C(14A)-H(14B)	0.9800
C(14A)-H(14C)	0.9800
C(15A)-C(17A)	1.528(3)
C(15A)-C(16A)	1.533(3)
C(15A)-H(15A)	1.0000
C(16A)-H(16A)	0.9800
C(16A)-H(16B)	0.9800
C(16A)-H(16C)	0.9800
C(17A)-C(22A)	1.386(3)
C(17A)-C(18A)	1.417(3)
C(18A)-C(19A)	1.405(3)
C(19A)-C(20A)	1.397(3)
C(19A)-C(23A)	1.544(3)
C(20A)-C(21A)	1.394(3)
C(20A)-H(20A)	0.9500
C(21A)-C(22A)	1.390(3)
C(21A)-C(27A)	1.535(3)
C(22A)-H(22A)	0.9500
C(23A)-C(25A)	1.532(4)
C(23A)-C(26A)	1.535(4)
C(23A)-C(24A)	1.538(4)
C(24A)-H(24A)	0.9800
C(24A)-H(24B)	0.9800
C(24A)-H(24C)	0.9800
C(25A)-H(25A)	0.9800
C(25A)-H(25B)	0.9800
C(25A)-H(25C)	0.9800
C(26A)-H(26A)	0.9800
C(26A)-H(26B)	0.9800
C(26A)-H(26C)	0.9800
C(27A)-C(29A)	1.525(3)
C(27A)-C(28A)	1.531(3)
C(27A)-C(30A)	1.531(3)
C(28A)-H(28A)	0.9800
C(28A)-H(28B)	0.9800
C(28A)-H(28C)	0.9800
C(29A)-H(29A)	0.9800
C(29A)-H(29B)	0.9800
C(29A)-H(29C)	0.9800
C(30A)-H(30A)	0.9800
C(30A)-H(30B)	0.9800
C(30A)-H(30C)	0.9800
O(1B)-C(2B)	1.369(2)
O(1B)-H(2O2)	1.06(4)
O(2B)-C(18B)	1.349(2)
C(1B)-C(6B)	1.389(3)
C(1B)-C(2B)	1.409(3)
C(1B)-C(15B)	1.522(3)
C(2B)-C(3B)	1.409(3)
C(3B)-C(4B)	1.397(3)
C(3B)-C(7B)	1.544(3)
C(4B)-C(5B)	1.389(3)
C(4B)-H(4BA)	0.9500
C(5B)-C(6B)	1.391(3)
C(5B)-C(11B)	1.535(3)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.530(3)
C(7B)-C(10B)	1.531(4)
C(7B)-C(9B)	1.535(3)
C(8B)-H(8BA)	0.9800
C(8B)-H(8BB)	0.9800
C(8B)-H(8BC)	0.9800
C(9B)-H(9BA)	0.9800
C(9B)-H(9BB)	0.9800
C(9B)-H(9BC)	0.9800
C(10B)-H(10D)	0.9800
C(10B)-H(10E)	0.9800
C(10B)-H(10F)	0.9800
C(11B)-C(12B)	1.526(4)
C(11B)-C(14B)	1.529(4)
C(11B)-C(13B)	1.532(4)
C(12B)-H(12D)	0.9800
C(12B)-H(12E)	0.9800
C(12B)-H(12F)	0.9800
C(13B)-H(13D)	0.9800
C(13B)-H(13E)	0.9800
C(13B)-H(13F)	0.9800
C(14B)-H(14D)	0.9800
C(14B)-H(14E)	0.9800
C(14B)-H(14F)	0.9800
C(15B)-C(17B)	1.526(3)
C(15B)-C(16B)	1.539(3)
C(15B)-H(15B)	1.0000
C(16B)-H(16D)	0.9800
C(16B)-H(16E)	0.9800
C(16B)-H(16F)	0.9800
C(17B)-C(22B)	1.387(3)
C(17B)-C(18B)	1.416(3)
C(18B)-C(19B)	1.415(3)

C(19B)-C(20B)	1.395(3)	C(4TA)-H(4TB)	0.9900
C(19B)-C(23B)	1.547(3)	O(1TB)-C(1TB)	1.430(3)
C(20B)-C(21B)	1.384(3)	O(1TB)-C(4TB)	1.435(4)
C(20B)-H(20B)	0.9500	C(1TB)-C(2TB)	1.438(5)
C(21B)-C(22B)	1.383(3)	C(1TB)-H(1TC)	0.9900
C(21B)-C(27B)	1.538(3)	C(1TB)-H(1TD)	0.9900
C(22B)-H(22B)	0.9500	C(2TB)-C(3TB)	1.458(5)
C(23B)-C(24B)	1.465(8)	C(2TB)-H(2TC)	0.9900
C(23B)-C(26B)	1.548(12)	C(2TB)-H(2TD)	0.9900
C(23B)-C(25B)	1.565(8)	C(3TB)-C(4TB)	1.410(4)
C(24B)-H(24G)	0.9800	C(3TB)-H(3TC)	0.9900
C(24B)-H(24H)	0.9800	C(3TB)-H(3TD)	0.9900
C(24B)-H(24I)	0.9800	C(4TB)-H(4TC)	0.9900
C(25B)-H(25D)	0.9800	C(4TB)-H(4TD)	0.9900
C(25B)-H(25E)	0.9800	O(1TC)-C(4TC)	1.404(4)
C(25B)-H(25F)	0.9800	O(1TC)-C(1TC)	1.421(4)
C(26B)-H(26D)	0.9800	C(1TC)-C(2TC)	1.392(6)
C(26B)-H(26E)	0.9800	C(1TC)-H(1TE)	0.9900
C(26B)-H(26F)	0.9800	C(1TC)-H(1TF)	0.9900
C(24C)-H(24D)	0.9800	C(2TC)-C(3TC)	1.461(6)
C(24C)-H(24E)	0.9800	C(2TC)-H(2TE)	0.9900
C(24C)-H(24F)	0.9800	C(2TC)-H(2TF)	0.9900
C(25C)-H(25G)	0.9800	C(3TC)-C(4TC)	1.509(5)
C(25C)-H(25H)	0.9800	C(3TC)-H(3TE)	0.9900
C(25C)-H(25I)	0.9800	C(3TC)-H(3TF)	0.9900
C(26C)-H(26G)	0.9800	C(4TC)-H(4TE)	0.9900
C(26C)-H(26H)	0.9800	C(4TC)-H(4TF)	0.9900
C(26C)-H(26I)	0.9800	C(1)-C(6)	1.362(5)
C(27B)-C(28B)	1.348(9)	C(1)-C(2)	1.391(5)
C(27B)-C(30B)	1.575(8)	C(1)-C(7)	1.487(5)
C(27B)-C(29B)	1.637(8)	C(2)-C(3)	1.354(5)
C(28B)-H(28D)	0.9800	C(2)-H(2A)	0.9500
C(28B)-H(28E)	0.9800	C(3)-C(4)	1.378(5)
C(28B)-H(28F)	0.9800	C(3)-H(3A)	0.9500
C(29B)-H(29D)	0.9800	C(4)-C(5)	1.347(5)
C(29B)-H(29E)	0.9800	C(4)-H(4A)	0.9500
C(29B)-H(29F)	0.9800	C(5)-C(6)	1.360(5)
C(30B)-H(30D)	0.9800	C(5)-H(5A)	0.9500
C(30B)-H(30E)	0.9800	C(6)-H(6A)	0.9500
C(30B)-H(30F)	0.9800	C(7)-H(7A)	0.9800
C(28C)-H(28G)	0.9800	C(7)-H(7B)	0.9800
C(28C)-H(28H)	0.9800	C(7)-H(7C)	0.9800
C(28C)-H(28I)	0.9800	C(1')-C(6')	1.298(7)
C(29C)-H(29G)	0.9800	C(1')-C(2')	1.326(7)
C(29C)-H(29H)	0.9800	C(1')-C(7')	1.417(8)
C(29C)-H(29I)	0.9800	C(2')-C(3')	1.291(7)
C(30C)-H(30G)	0.9800	C(2')-H(2'A)	0.9500
C(30C)-H(30H)	0.9800	C(3')-C(4')	1.313(7)
C(30C)-H(30I)	0.9800	C(3')-H(3'A)	0.9500
O(1TA)-C(4TA)	1.414(5)	C(4')-C(5')	1.284(7)
O(1TA)-C(1TA)	1.417(4)	C(4')-H(4'A)	0.9500
C(1TA)-C(2TA)	1.473(5)	C(5')-C(6')	1.297(7)
C(1TA)-H(1TA)	0.9900	C(5')-H(5'A)	0.9500
C(1TA)-H(1TB)	0.9900	C(6')-H(6'A)	0.9500
C(2TA)-C(3TA)	1.520(6)	C(7')-H(7'C)	0.9800
C(2TA)-H(2TA)	0.9900	C(7')-H(7'D)	0.9800
C(2TA)-H(2TB)	0.9900	C(7')-H(7'A)	0.9800
C(3TA)-C(4TA)	1.422(6)		
C(3TA)-H(3TA)	0.9900	O(2B)-Na(1)-O(1TC)	97.78(7)
C(3TA)-H(3TB)	0.9900	O(2B)-Na(1)-O(1A)	99.62(6)
C(4TA)-H(4TA)	0.9900	O(1TC)-Na(1)-O(1A)	140.00(9)

O(2B)-Na(1)-O(1TA)	128.68(8)
O(1TC)-Na(1)-O(1TA)	90.99(9)
O(1A)-Na(1)-O(1TA)	105.30(7)
O(2B)-Na(1)-C(2A)	120.96(6)
O(1TC)-Na(1)-C(2A)	134.15(8)
O(1A)-Na(1)-C(2A)	23.49(5)
O(1TA)-Na(1)-C(2A)	83.44(7)
O(2B)-Na(1)-Na(2)	36.44(4)
O(1TC)-Na(1)-Na(2)	134.22(7)
O(1A)-Na(1)-Na(2)	70.32(4)
O(1TA)-Na(1)-Na(2)	116.07(7)
C(2A)-Na(1)-Na(2)	87.45(4)
O(2B)-Na(1)-H(2O2)	35.7(8)
O(1TC)-Na(1)-H(2O2)	109.0(8)
O(1A)-Na(1)-H(2O2)	106.1(8)
O(1TA)-Na(1)-H(2O2)	93.8(8)
C(2A)-Na(1)-H(2O2)	116.7(8)
Na(2)-Na(1)-H(2O2)	38.3(8)
O(2A)-Na(2)-O(1TB)	139.86(7)
O(2A)-Na(2)-O(2B)	104.60(6)
O(1TB)-Na(2)-O(2B)	107.04(7)
O(2A)-Na(2)-O(1B)	114.52(6)
O(1TB)-Na(2)-O(1B)	102.11(7)
O(2B)-Na(2)-O(1B)	61.43(6)
O(2A)-Na(2)-Na(1)	76.21(5)
O(1TB)-Na(2)-Na(1)	141.12(6)
O(2B)-Na(2)-Na(1)	35.24(4)
O(1B)-Na(2)-Na(1)	57.37(4)
O(2A)-Na(2)-H(2O2)	114.5(8)
O(1TB)-Na(2)-H(2O2)	105.7(8)
O(2B)-Na(2)-H(2O2)	37.0(9)
O(1B)-Na(2)-H(2O2)	24.5(9)
Na(1)-Na(2)-H(2O2)	41.6(9)
C(2A)-O(1A)-Na(1)	114.31(12)
C(2A)-O(1A)-H(1O1)	113.3(16)
Na(1)-O(1A)-H(1O1)	110.2(16)
C(18A)-O(2A)-Na(2)	132.49(12)
C(18A)-O(2A)-H(1O1)	108.7(11)
Na(2)-O(2A)-H(1O1)	104.1(11)
C(6A)-C(1A)-C(2A)	118.82(17)
C(6A)-C(1A)-C(15A)	121.04(16)
C(2A)-C(1A)-C(15A)	120.15(16)
O(1A)-C(2A)-C(1A)	120.50(17)
O(1A)-C(2A)-C(3A)	119.09(17)
C(1A)-C(2A)-C(3A)	120.40(17)
O(1A)-C(2A)-Na(1)	42.21(9)
C(1A)-C(2A)-Na(1)	114.17(12)
C(3A)-C(2A)-Na(1)	108.38(12)
C(4A)-C(3A)-C(2A)	117.43(19)
C(4A)-C(3A)-C(7A)	120.78(18)
C(2A)-C(3A)-C(7A)	121.73(18)
C(5A)-C(4A)-C(3A)	123.73(19)
C(5A)-C(4A)-H(4AA)	118.1
C(3A)-C(4A)-H(4AA)	118.1
C(4A)-C(5A)-C(6A)	117.15(18)
C(4A)-C(5A)-C(11A)	120.19(18)
C(6A)-C(5A)-C(11A)	122.58(19)
C(5A)-C(6A)-C(1A)	122.32(18)
C(5A)-C(6A)-H(6AA)	118.8
C(1A)-C(6A)-H(6AA)	118.8
C(10A)-C(7A)-C(8A)	107.9(2)
C(10A)-C(7A)-C(9A)	106.4(2)
C(8A)-C(7A)-C(9A)	109.1(2)
C(10A)-C(7A)-C(3A)	111.7(2)
C(8A)-C(7A)-C(3A)	109.13(19)
C(9A)-C(7A)-C(3A)	112.4(2)
C(7A)-C(8A)-H(8AA)	109.5
C(7A)-C(8A)-H(8AB)	109.5
H(8AA)-C(8A)-H(8AB)	109.5
C(7A)-C(8A)-H(8AC)	109.5
H(8AA)-C(8A)-H(8AC)	109.5
H(8AB)-C(8A)-H(8AC)	109.5
C(7A)-C(9A)-H(9AA)	109.5
C(7A)-C(9A)-H(9AB)	109.5
H(9AA)-C(9A)-H(9AB)	109.5
C(7A)-C(9A)-H(9AC)	109.5
H(9AA)-C(9A)-H(9AC)	109.5
H(9AB)-C(9A)-H(9AC)	109.5
C(7A)-C(10A)-H(10A)	109.5
C(7A)-C(10A)-H(10B)	109.5
H(10A)-C(10A)-H(10B)	109.5
C(7A)-C(10A)-H(10C)	109.5
H(10A)-C(10A)-H(10C)	109.5
H(10B)-C(10A)-H(10C)	109.5
C(14A)-C(11A)-C(13A)	107.7(2)
C(14A)-C(11A)-C(5A)	111.98(18)
C(13A)-C(11A)-C(5A)	111.9(2)
C(14A)-C(11A)-C(12A)	108.6(2)
C(13A)-C(11A)-C(12A)	108.5(2)
C(5A)-C(11A)-C(12A)	108.14(18)
C(11A)-C(12A)-H(12A)	109.5
C(11A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5
C(11A)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
C(11A)-C(13A)-H(13A)	109.5
C(11A)-C(13A)-H(13B)	109.5
H(13A)-C(13A)-H(13B)	109.5
C(11A)-C(13A)-H(13C)	109.5
H(13A)-C(13A)-H(13C)	109.5
H(13B)-C(13A)-H(13C)	109.5
C(11A)-C(14A)-H(14A)	109.5
C(11A)-C(14A)-H(14B)	109.5
H(14A)-C(14A)-H(14B)	109.5
C(11A)-C(14A)-H(14C)	109.5
H(14A)-C(14A)-H(14C)	109.5
H(14B)-C(14A)-H(14C)	109.5
C(17A)-C(15A)-C(16A)	112.72(16)
C(17A)-C(15A)-C(1A)	110.49(14)
C(16A)-C(15A)-C(1A)	112.94(16)
C(17A)-C(15A)-H(15A)	106.7
C(16A)-C(15A)-H(15A)	106.7
C(1A)-C(15A)-H(15A)	106.7
C(15A)-C(16A)-H(16A)	109.5
C(15A)-C(16A)-H(16B)	109.5
H(16A)-C(16A)-H(16B)	109.5
C(15A)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.5
H(16B)-C(16A)-H(16C)	109.5
C(22A)-C(17A)-C(18A)	119.27(17)
C(22A)-C(17A)-C(15A)	121.44(16)

C(18A)-C(17A)-C(15A)	119.25(16)
O(2A)-C(18A)-C(19A)	121.51(17)
O(2A)-C(18A)-C(17A)	119.16(16)
C(19A)-C(18A)-C(17A)	119.32(17)
C(20A)-C(19A)-C(18A)	118.54(17)
C(20A)-C(19A)-C(23A)	120.81(18)
C(18A)-C(19A)-C(23A)	120.60(18)
C(21A)-C(20A)-C(19A)	123.09(18)
C(21A)-C(20A)-H(20A)	118.5
C(19A)-C(20A)-H(20A)	118.5
C(22A)-C(21A)-C(20A)	116.80(18)
C(22A)-C(21A)-C(27A)	120.50(18)
C(20A)-C(21A)-C(27A)	122.69(18)
C(17A)-C(22A)-C(21A)	122.71(18)
C(17A)-C(22A)-H(22A)	118.6
C(21A)-C(22A)-H(22A)	118.6
C(25A)-C(23A)-C(26A)	107.3(2)
C(25A)-C(23A)-C(24A)	109.9(2)
C(26A)-C(23A)-C(24A)	107.7(2)
C(25A)-C(23A)-C(19A)	110.8(2)
C(26A)-C(23A)-C(19A)	111.76(19)
C(24A)-C(23A)-C(19A)	109.31(19)
C(23A)-C(24A)-H(24A)	109.5
C(23A)-C(24A)-H(24B)	109.5
H(24A)-C(24A)-H(24B)	109.5
C(23A)-C(24A)-H(24C)	109.5
H(24A)-C(24A)-H(24C)	109.5
H(24B)-C(24A)-H(24C)	109.5
C(23A)-C(25A)-H(25A)	109.5
C(23A)-C(25A)-H(25B)	109.5
H(25A)-C(25A)-H(25B)	109.5
C(23A)-C(25A)-H(25C)	109.5
H(25A)-C(25A)-H(25C)	109.5
H(25B)-C(25A)-H(25C)	109.5
C(23A)-C(26A)-H(26A)	109.5
C(23A)-C(26A)-H(26B)	109.5
H(26A)-C(26A)-H(26B)	109.5
C(23A)-C(26A)-H(26C)	109.5
H(26A)-C(26A)-H(26C)	109.5
H(26B)-C(26A)-H(26C)	109.5
C(29A)-C(27A)-C(28A)	108.1(2)
C(29A)-C(27A)-C(30A)	108.7(2)
C(28A)-C(27A)-C(30A)	108.6(2)
C(29A)-C(27A)-C(21A)	112.52(18)
C(28A)-C(27A)-C(21A)	108.90(17)
C(30A)-C(27A)-C(21A)	110.00(18)
C(27A)-C(28A)-H(28A)	109.5
C(27A)-C(28A)-H(28B)	109.5
H(28A)-C(28A)-H(28B)	109.5
C(27A)-C(28A)-H(28C)	109.5
H(28A)-C(28A)-H(28C)	109.5
H(28B)-C(28A)-H(28C)	109.5
C(27A)-C(29A)-H(29A)	109.5
C(27A)-C(29A)-H(29B)	109.5
H(29A)-C(29A)-H(29B)	109.5
C(27A)-C(29A)-H(29C)	109.5
H(29A)-C(29A)-H(29C)	109.5
H(29B)-C(29A)-H(29C)	109.5
C(27A)-C(30A)-H(30A)	109.5
C(27A)-C(30A)-H(30B)	109.5
H(30A)-C(30A)-H(30B)	109.5
C(27A)-C(30A)-H(30C)	109.5
H(30A)-C(30A)-H(30C)	109.5
H(30B)-C(30A)-H(30C)	109.5
C(2B)-O(1B)-Na(2)	123.34(12)
C(2B)-O(1B)-H(2O2)	110.0(19)
Na(2)-O(1B)-H(2O2)	67.3(18)
C(18B)-O(2B)-Na(1)	131.34(13)
C(18B)-O(2B)-Na(2)	120.34(12)
Na(1)-O(2B)-Na(2)	108.31(6)
C(6B)-C(1B)-C(2B)	118.69(19)
C(6B)-C(1B)-C(15B)	120.82(18)
C(2B)-C(1B)-C(15B)	120.46(17)
O(1B)-C(2B)-C(3B)	120.18(18)
O(1B)-C(2B)-C(1B)	119.27(19)
C(3B)-C(2B)-C(1B)	120.54(18)
C(4B)-C(3B)-C(2B)	117.52(19)
C(4B)-C(3B)-C(7B)	120.4(2)
C(2B)-C(3B)-C(7B)	122.08(18)
C(5B)-C(4B)-C(3B)	123.2(2)
C(5B)-C(4B)-H(4BA)	118.4
C(3B)-C(4B)-H(4BA)	118.4
C(4B)-C(5B)-C(6B)	117.36(19)
C(4B)-C(5B)-C(11B)	122.8(2)
C(6B)-C(5B)-C(11B)	119.83(19)
C(1B)-C(6B)-C(5B)	122.31(19)
C(1B)-C(6B)-H(6BA)	118.8
C(5B)-C(6B)-H(6BA)	118.8
C(8B)-C(7B)-C(10B)	107.1(2)
C(8B)-C(7B)-C(9B)	109.1(2)
C(10B)-C(7B)-C(9B)	108.4(2)
C(8B)-C(7B)-C(3B)	112.18(19)
C(10B)-C(7B)-C(3B)	111.80(19)
C(9B)-C(7B)-C(3B)	108.15(19)
C(7B)-C(8B)-H(8BA)	109.5
C(7B)-C(8B)-H(8BB)	109.5
H(8BA)-C(8B)-H(8BB)	109.5
C(7B)-C(8B)-H(8BC)	109.5
H(8BA)-C(8B)-H(8BC)	109.5
H(8BB)-C(8B)-H(8BC)	109.5
C(7B)-C(9B)-H(9BA)	109.5
C(7B)-C(9B)-H(9BB)	109.5
H(9BA)-C(9B)-H(9BB)	109.5
C(7B)-C(9B)-H(9BC)	109.5
H(9BA)-C(9B)-H(9BC)	109.5
H(9BB)-C(9B)-H(9BC)	109.5
C(7B)-C(10B)-H(10D)	109.5
C(7B)-C(10B)-H(10E)	109.5
H(10D)-C(10B)-H(10E)	109.5
C(7B)-C(10B)-H(10F)	109.5
H(10D)-C(10B)-H(10F)	109.5
H(10E)-C(10B)-H(10F)	109.5
C(12B)-C(11B)-C(14B)	107.6(2)
C(12B)-C(11B)-C(13B)	108.9(2)
C(14B)-C(11B)-C(13B)	109.7(3)
C(12B)-C(11B)-C(5B)	112.7(2)
C(14B)-C(11B)-C(5B)	108.9(2)
C(13B)-C(11B)-C(5B)	109.0(2)
C(11B)-C(12B)-H(12D)	109.5
C(11B)-C(12B)-H(12E)	109.5
H(12D)-C(12B)-H(12E)	109.5
C(11B)-C(12B)-H(12F)	109.5

H(12D)-C(12B)-H(12F)	109.5
H(12E)-C(12B)-H(12F)	109.5
C(11B)-C(13B)-H(13D)	109.5
C(11B)-C(13B)-H(13E)	109.5
H(13D)-C(13B)-H(13E)	109.5
C(11B)-C(13B)-H(13F)	109.5
H(13D)-C(13B)-H(13F)	109.5
H(13E)-C(13B)-H(13F)	109.5
C(11B)-C(14B)-H(14D)	109.5
C(11B)-C(14B)-H(14E)	109.5
H(14D)-C(14B)-H(14E)	109.5
C(11B)-C(14B)-H(14F)	109.5
H(14D)-C(14B)-H(14F)	109.5
H(14E)-C(14B)-H(14F)	109.5
C(1B)-C(15B)-C(17B)	111.93(16)
C(1B)-C(15B)-C(16B)	112.94(18)
C(17B)-C(15B)-C(16B)	112.59(19)
C(1B)-C(15B)-H(15B)	106.3
C(17B)-C(15B)-H(15B)	106.3
C(16B)-C(15B)-H(15B)	106.3
C(15B)-C(16B)-H(16D)	109.5
C(15B)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
C(15B)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5
C(22B)-C(17B)-C(18B)	119.9(2)
C(22B)-C(17B)-C(15B)	120.36(19)
C(18B)-C(17B)-C(15B)	119.69(17)
O(2B)-C(18B)-C(19B)	122.83(19)
O(2B)-C(18B)-C(17B)	118.91(18)
C(19B)-C(18B)-C(17B)	118.25(18)
C(20B)-C(19B)-C(18B)	118.1(2)
C(20B)-C(19B)-C(23B)	118.7(2)
C(18B)-C(19B)-C(23B)	123.26(19)
C(21B)-C(20B)-C(19B)	124.0(2)
C(21B)-C(20B)-H(20B)	118.0
C(19B)-C(20B)-H(20B)	118.0
C(22B)-C(21B)-C(20B)	116.5(2)
C(22B)-C(21B)-C(27B)	121.7(2)
C(20B)-C(21B)-C(27B)	121.8(2)
C(21B)-C(22B)-C(17B)	122.5(2)
C(21B)-C(22B)-H(22B)	118.7
C(17B)-C(22B)-H(22B)	118.7
C(24B)-C(23B)-C(19B)	114.3(4)
C(24B)-C(23B)-C(26B)	109.3(6)
C(19B)-C(23B)-C(26B)	111.1(5)
C(24B)-C(23B)-C(25B)	111.0(6)
C(19B)-C(23B)-C(25B)	107.4(4)
C(26B)-C(23B)-C(25B)	103.1(5)
C(23B)-C(24B)-H(24G)	109.5
C(23B)-C(24B)-H(24H)	109.5
H(24G)-C(24B)-H(24H)	109.5
C(23B)-C(24B)-H(24I)	109.5
H(24G)-C(24B)-H(24I)	109.5
H(24H)-C(24B)-H(24I)	109.5
C(23B)-C(25B)-H(25D)	109.5
C(23B)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25E)	109.5
C(23B)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25F)	109.5

H(25E)-C(25B)-H(25F)	109.5
C(23B)-C(26B)-H(26D)	109.5
C(23B)-C(26B)-H(26E)	109.5
H(26D)-C(26B)-H(26E)	109.5
C(23B)-C(26B)-H(26F)	109.5
H(26D)-C(26B)-H(26F)	109.5
H(26E)-C(26B)-H(26F)	109.5
H(24D)-C(24C)-H(24E)	109.5
H(24D)-C(24C)-H(24F)	109.5
H(24E)-C(24C)-H(24F)	109.5
H(25G)-C(25C)-H(25H)	109.5
H(25G)-C(25C)-H(25I)	109.5
H(25H)-C(25C)-H(25I)	109.5
H(26G)-C(26C)-H(26H)	109.5
H(26G)-C(26C)-H(26I)	109.5
H(26H)-C(26C)-H(26I)	109.5
C(28B)-C(27B)-C(21B)	113.4(5)
C(28B)-C(27B)-C(30B)	116.2(9)
C(21B)-C(27B)-C(30B)	106.3(3)
C(28B)-C(27B)-C(29B)	111.7(7)
C(21B)-C(27B)-C(29B)	110.0(3)
C(30B)-C(27B)-C(29B)	98.1(6)
C(27B)-C(28B)-H(28D)	109.5
C(27B)-C(28B)-H(28E)	109.5
H(28D)-C(28B)-H(28E)	109.5
C(27B)-C(28B)-H(28F)	109.5
H(28D)-C(28B)-H(28F)	109.5
H(28E)-C(28B)-H(28F)	109.5
C(27B)-C(29B)-H(29D)	109.5
C(27B)-C(29B)-H(29E)	109.5
H(29D)-C(29B)-H(29E)	109.5
C(27B)-C(29B)-H(29F)	109.5
H(29D)-C(29B)-H(29F)	109.5
H(29E)-C(29B)-H(29F)	109.5
C(27B)-C(30B)-H(30D)	109.5
C(27B)-C(30B)-H(30E)	109.5
H(30D)-C(30B)-H(30E)	109.5
C(27B)-C(30B)-H(30F)	109.5
H(30D)-C(30B)-H(30F)	109.5
H(30E)-C(30B)-H(30F)	109.5
H(28G)-C(28C)-H(28H)	109.5
H(28G)-C(28C)-H(28I)	109.5
H(28H)-C(28C)-H(28I)	109.5
H(29G)-C(29C)-H(29H)	109.5
H(29G)-C(29C)-H(29I)	109.5
H(29H)-C(29C)-H(29I)	109.5
H(30G)-C(30C)-H(30H)	109.5
H(30G)-C(30C)-H(30I)	109.5
H(30H)-C(30C)-H(30I)	109.5
C(4TA)-O(1TA)-C(1TA)	106.6(3)
C(4TA)-O(1TA)-Na(1)	126.0(2)
C(1TA)-O(1TA)-Na(1)	127.3(2)
O(1TA)-C(1TA)-C(2TA)	106.5(3)
O(1TA)-C(1TA)-H(1TA)	110.4
C(2TA)-C(1TA)-H(1TA)	110.4
O(1TA)-C(1TA)-H(1TB)	110.4
C(2TA)-C(1TA)-H(1TB)	110.4
H(1TA)-C(1TA)-H(1TB)	108.6
C(1TA)-C(2TA)-C(3TA)	103.0(3)
C(1TA)-C(2TA)-H(2TA)	111.2
C(3TA)-C(2TA)-H(2TA)	111.2

C(1TA)-C(2TA)-H(2TB)	111.2
C(3TA)-C(2TA)-H(2TB)	111.2
H(2TA)-C(2TA)-H(2TB)	109.1
C(4TA)-C(3TA)-C(2TA)	105.7(4)
C(4TA)-C(3TA)-H(3TA)	110.6
C(2TA)-C(3TA)-H(3TA)	110.6
C(4TA)-C(3TA)-H(3TB)	110.6
C(2TA)-C(3TA)-H(3TB)	110.6
H(3TA)-C(3TA)-H(3TB)	108.7
O(1TA)-C(4TA)-C(3TA)	109.7(4)
O(1TA)-C(4TA)-H(4TA)	109.7
C(3TA)-C(4TA)-H(4TA)	109.7
O(1TA)-C(4TA)-H(4TB)	109.7
C(3TA)-C(4TA)-H(4TB)	109.7
H(4TA)-C(4TA)-H(4TB)	108.2
C(1TB)-O(1TB)-C(4TB)	107.9(2)
C(1TB)-O(1TB)-Na(2)	133.12(18)
C(4TB)-O(1TB)-Na(2)	117.24(15)
O(1TB)-C(1TB)-C(2TB)	108.1(3)
O(1TB)-C(1TB)-H(1TC)	110.1
C(2TB)-C(1TB)-H(1TC)	110.1
O(1TB)-C(1TB)-H(1TD)	110.1
C(2TB)-C(1TB)-H(1TD)	110.1
H(1TC)-C(1TB)-H(1TD)	108.4
C(1TB)-C(2TB)-C(3TB)	107.0(3)
C(1TB)-C(2TB)-H(2TC)	110.3
C(3TB)-C(2TB)-H(2TC)	110.3
C(1TB)-C(2TB)-H(2TD)	110.3
C(3TB)-C(2TB)-H(2TD)	110.3
H(2TC)-C(2TB)-H(2TD)	108.6
C(4TB)-C(3TB)-C(2TB)	108.0(3)
C(4TB)-C(3TB)-H(3TC)	110.1
C(2TB)-C(3TB)-H(3TC)	110.1
C(4TB)-C(3TB)-H(3TD)	110.1
C(2TB)-C(3TB)-H(3TD)	110.1
H(3TC)-C(3TB)-H(3TD)	108.4
C(3TB)-C(4TB)-O(1TB)	108.5(3)
C(3TB)-C(4TB)-H(4TC)	110.0
O(1TB)-C(4TB)-H(4TC)	110.0
C(3TB)-C(4TB)-H(4TD)	110.0
O(1TB)-C(4TB)-H(4TD)	110.0
H(4TC)-C(4TB)-H(4TD)	108.4
C(4TC)-O(1TC)-C(1TC)	107.9(3)
C(4TC)-O(1TC)-Na(1)	127.4(2)
C(1TC)-O(1TC)-Na(1)	123.5(2)
C(2TC)-C(1TC)-O(1TC)	110.5(4)
C(2TC)-C(1TC)-H(1TE)	109.6
O(1TC)-C(1TC)-H(1TE)	109.6
C(2TC)-C(1TC)-H(1TF)	109.6
O(1TC)-C(1TC)-H(1TF)	109.6
H(1TE)-C(1TC)-H(1TF)	108.1
C(1TC)-C(2TC)-C(3TC)	106.5(3)
C(1TC)-C(2TC)-H(2TE)	110.4
C(3TC)-C(2TC)-H(2TE)	110.4
C(1TC)-C(2TC)-H(2TF)	110.4
C(3TC)-C(2TC)-H(2TF)	110.4
H(2TE)-C(2TC)-H(2TF)	108.6
C(2TC)-C(3TC)-C(4TC)	104.1(3)
C(2TC)-C(3TC)-H(3TE)	110.9
C(4TC)-C(3TC)-H(3TE)	110.9
C(2TC)-C(3TC)-H(3TF)	110.9
C(4TC)-C(3TC)-H(3TF)	110.9
H(3TE)-C(3TC)-H(3TF)	109.0
O(1TC)-C(4TC)-C(3TC)	105.5(3)
O(1TC)-C(4TC)-H(4TE)	110.6
C(3TC)-C(4TC)-H(4TE)	110.6
O(1TC)-C(4TC)-H(4TF)	110.6
C(3TC)-C(4TC)-H(4TF)	110.6
H(4TE)-C(4TC)-H(4TF)	108.8
C(6)-C(1)-C(2)	117.2
C(6)-C(1)-C(7)	122.0
C(2)-C(1)-C(7)	120.7
C(3)-C(2)-C(1)	120.2
C(3)-C(2)-H(2A)	119.9
C(1)-C(2)-H(2A)	119.9
C(2)-C(3)-C(4)	121.1
C(2)-C(3)-H(3A)	119.5
C(4)-C(3)-H(3A)	119.5
C(5)-C(4)-C(3)	119.0
C(5)-C(4)-H(4A)	120.5
C(3)-C(4)-H(4A)	120.5
C(4)-C(5)-C(6)	120.1
C(4)-C(5)-H(5A)	119.9
C(6)-C(5)-H(5A)	119.9
C(5)-C(6)-C(1)	122.4
C(5)-C(6)-H(6A)	118.8
C(1)-C(6)-H(6A)	118.8
C(1)-C(7)-H(7A)	109.5
C(1)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(1)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6')-C(1')-C(2')	117.2
C(6')-C(1')-C(7')	122.1
C(2')-C(1')-C(7')	120.7
C(3')-C(2')-C(1')	120.2
C(3')-C(2')-H(2'A)	119.9
C(1')-C(2')-H(2'A)	119.9
C(2')-C(3')-C(4')	121.1
C(2')-C(3')-H(3'A)	119.5
C(4')-C(3')-H(3'A)	119.5
C(5')-C(4')-C(3')	119.0
C(5')-C(4')-H(4'A)	120.5
C(3')-C(4')-H(4'A)	120.5
C(4')-C(5')-C(6')	120.1
C(4')-C(5')-H(5'A)	120.0
C(6')-C(5')-H(5'A)	120.0
C(5')-C(6')-C(1')	122.4
C(5')-C(6')-H(6'A)	118.8
C(1')-C(6')-H(6'A)	118.8
C(1')-C(7')-H(7'C)	109.5
C(1')-C(7')-H(7'D)	109.5
H(7'C)-C(7')-H(7'D)	109.5
C(1')-C(7')-H(7'A)	109.5
H(7'C)-C(7')-H(7'A)	109.5
H(7'D)-C(7')-H(7'A)	109.5

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for sm114. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Na(1)	59(1)	52(1)	90(1)	-17(1)	34(1)	-10(1)
Na(2)	54(1)	53(1)	82(1)	0(1)	32(1)	-1(1)
O(1A)	41(1)	56(1)	53(1)	-11(1)	16(1)	-7(1)
O(2A)	39(1)	48(1)	55(1)	-7(1)	14(1)	-5(1)
C(1A)	44(1)	35(1)	46(1)	0(1)	16(1)	-1(1)
C(2A)	44(1)	40(1)	48(1)	-3(1)	15(1)	-3(1)
C(3A)	53(1)	48(1)	49(1)	-6(1)	18(1)	-7(1)
C(4A)	56(1)	52(1)	53(1)	-4(1)	26(1)	-5(1)
C(5A)	48(1)	42(1)	58(1)	-1(1)	22(1)	-3(1)
C(6A)	44(1)	40(1)	50(1)	-1(1)	14(1)	-2(1)
C(7A)	65(2)	74(2)	46(1)	-10(1)	16(1)	-12(1)
C(8A)	93(1)	102(1)	64(2)	-3(2)	-1(2)	13(2)
C(9A)	84(2)	95(1)	59(2)	-25(1)	19(1)	-31(2)
C(10A)	88(2)	123(1)	50(2)	-15(2)	25(1)	-30(2)
C(11A)	49(1)	61(1)	69(2)	-2(1)	27(1)	-3(1)
C(12A)	60(2)	78(2)	103(1)	-7(2)	34(2)	10(1)
C(13A)	62(2)	95(1)	91(2)	12(2)	37(2)	-15(1)
C(14A)	45(1)	87(2)	89(2)	-12(2)	23(1)	-11(1)
C(15A)	40(1)	41(1)	45(1)	1(1)	14(1)	-4(1)
C(16A)	49(1)	55(1)	49(1)	5(1)	12(1)	3(1)
C(17A)	40(1)	45(1)	39(1)	1(1)	14(1)	-1(1)
C(18A)	40(1)	47(1)	41(1)	-2(1)	14(1)	-2(1)
C(19A)	45(1)	51(1)	49(1)	-2(1)	11(1)	4(1)
C(20A)	51(1)	43(1)	53(1)	-1(1)	14(1)	5(1)
C(21A)	48(1)	45(1)	45(1)	-1(1)	14(1)	-5(1)
C(22A)	41(1)	48(1)	42(1)	2(1)	12(1)	-1(1)
C(23A)	50(1)	55(1)	70(2)	-7(1)	3(1)	9(1)
C(24A)	63(2)	82(2)	65(2)	7(1)	-2(1)	5(1)
C(25A)	43(1)	96(2)	85(2)	-20(2)	14(1)	9(1)
C(26A)	75(2)	67(2)	123(1)	-9(2)	-24(2)	24(2)
C(27A)	57(1)	49(1)	54(1)	-4(1)	13(1)	-8(1)
C(28A)	69(2)	65(2)	57(1)	-12(1)	7(1)	-9(1)
C(29A)	82(2)	46(1)	88(2)	-9(1)	8(2)	-8(1)
C(30A)	71(2)	76(2)	83(2)	-9(1)	25(1)	-25(1)
O(1B)	57(1)	49(1)	68(1)	6(1)	23(1)	-8(1)
O(2B)	44(1)	52(1)	68(1)	3(1)	17(1)	-6(1)
C(1B)	46(1)	43(1)	59(1)	1(1)	21(1)	1(1)
C(2B)	44(1)	46(1)	62(1)	4(1)	21(1)	1(1)
C(3B)	46(1)	45(1)	64(1)	-1(1)	18(1)	-3(1)
C(4B)	54(1)	52(1)	57(1)	0(1)	18(1)	-2(1)
C(5B)	53(1)	49(1)	61(1)	2(1)	21(1)	-3(1)
C(6B)	53(1)	42(1)	64(1)	-1(1)	21(1)	-6(1)
C(7B)	57(1)	55(1)	65(1)	-2(1)	15(1)	-12(1)
C(8B)	71(2)	50(1)	94(2)	-10(1)	10(1)	-7(1)
C(9B)	55(1)	72(2)	97(2)	2(2)	17(1)	-13(1)
C(10B)	94(1)	81(2)	71(2)	-12(1)	18(2)	-33(2)
C(11B)	75(2)	61(1)	66(2)	2(1)	30(1)	-15(1)
C(12B)	95(2)	80(2)	68(2)	10(1)	32(2)	-13(2)
C(13B)	158(1)	57(2)	116(1)	17(2)	71(1)	-7(2)
C(14B)	78(2)	144(1)	80(2)	5(2)	33(2)	-41(2)
C(15B)	53(1)	43(1)	60(1)	0(1)	23(1)	-2(1)
C(16B)	82(2)	50(1)	71(2)	-5(1)	32(1)	4(1)
C(17B)	50(1)	51(1)	51(1)	-7(1)	21(1)	-5(1)
C(18B)	47(1)	50(1)	54(1)	-6(1)	19(1)	-5(1)
C(19B)	50(1)	57(1)	57(1)	-5(1)	17(1)	-1(1)

C(20B)	47(1)	67(2)	61(1)	-9(1)	13(1)	-5(1)
C(21B)	53(1)	68(2)	61(1)	-13(1)	21(1)	-15(1)
C(22B)	62(1)	53(1)	59(1)	-5(1)	23(1)	-10(1)
C(23B)	52(1)	66(2)	79(2)	10(1)	7(1)	-2(1)
C(24B)	135(1)	57(1)	93(1)	7(1)	-18(1)	-12(1)
C(25B)	97(1)	143(1)	105(1)	60(1)	38(1)	31(1)
C(26B)	72(1)	76(1)	69(1)	13(1)	1(1)	-1(1)
C(23C)	52(1)	66(2)	79(2)	10(1)	7(1)	-2(1)
C(24C)	135(1)	67(1)	151(1)	18(1)	80(1)	20(1)
C(25C)	71(1)	70(1)	73(1)	24(1)	16(1)	-4(1)
C(26C)	95(1)	176(2)	86(1)	33(1)	-15(1)	-69(1)
C(27B)	57(2)	80(2)	81(2)	-7(1)	19(1)	-22(1)
C(28B)	84(1)	91(1)	215(2)	-25(1)	95(1)	-17(1)
C(29B)	65(1)	66(1)	108(1)	0(1)	25(1)	-24(1)
C(30B)	83(1)	115(1)	85(1)	11(1)	-4(1)	-43(1)
C(27C)	57(2)	80(2)	81(2)	-7(1)	19(1)	-22(1)
C(28C)	89(1)	272(2)	110(1)	-21(1)	53(1)	-84(1)
C(29C)	73(1)	84(1)	189(1)	-38(1)	36(1)	-27(1)
C(30C)	52(1)	100(1)	151(1)	4(1)	16(1)	-24(1)
O(1TA)	72(1)	89(2)	123(2)	0(1)	32(1)	10(1)
C(1TA)	71(2)	111(1)	139(1)	5(1)	33(2)	4(2)
C(2TA)	78(1)	127(1)	112(1)	-46(1)	17(2)	14(1)
C(3TA)	108(1)	124(1)	151(1)	14(1)	20(1)	25(1)
C(4TA)	139(1)	175(1)	162(1)	66(1)	78(1)	75(1)
O(1TB)	64(1)	77(1)	119(2)	0(1)	53(1)	4(1)
C(1TB)	79(2)	83(2)	136(1)	-11(2)	54(2)	12(2)
C(2TB)	80(1)	123(1)	161(1)	43(1)	69(1)	33(2)
C(3TB)	100(1)	99(1)	233(1)	-26(1)	98(1)	-19(1)
C(4TB)	93(1)	76(2)	145(1)	10(2)	73(1)	10(2)
O(1TC)	106(2)	72(1)	123(2)	-48(1)	48(2)	-23(1)
C(1TC)	146(1)	93(1)	220(1)	-79(1)	75(1)	-8(1)
C(2TC)	188(1)	80(1)	93(1)	-23(2)	47(1)	12(1)
C(3TC)	192(1)	95(1)	109(1)	-47(1)	69(1)	-66(1)
C(4TC)	118(1)	104(1)	94(1)	-32(2)	48(1)	-21(1)
C(1)	171(1)	136(1)	160(1)	2(1)	48(1)	-17(1)
C(2)	171(1)	136(1)	160(1)	2(1)	48(1)	-17(1)
C(3)	171(1)	136(1)	160(1)	2(1)	48(1)	-17(1)
C(4)	171(1)	136(1)	160(1)	2(1)	48(1)	-17(1)
C(5)	171(1)	136(1)	160(1)	2(1)	48(1)	-17(1)
C(6)	171(1)	136(1)	160(1)	2(1)	48(1)	-17(1)
C(7)	171(1)	136(1)	160(1)	2(1)	48(1)	-17(1)
C(1')	370(2)	351(1)	258(1)	98(1)	148(1)	147(1)
C(2')	370(2)	351(1)	258(1)	98(1)	148(1)	147(1)
C(3')	370(2)	351(1)	258(1)	98(1)	148(1)	147(1)
C(4')	370(2)	351(1)	258(1)	98(1)	148(1)	147(1)
C(5')	370(2)	351(1)	258(1)	98(1)	148(1)	147(1)
C(6')	370(2)	351(1)	258(1)	98(1)	148(1)	147(1)
C(7')	370(2)	351(1)	258(1)	98(1)	148(1)	147(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for sm114.

	x	y	z	U(eq)
H(1O1)	8072(18)	561(15)	6689(12)	82(8)
H(4AA)	5607	694	7677	62
H(6AA)	5158	317	6045	53
H(8AA)	8256	185	7829	135
H(8AB)	7608	-193	8121	135
H(8AC)	8351	285	8479	135
H(9AA)	8178	1474	7744	119
H(9AB)	8260	1509	8397	119
H(9AC)	7466	1869	7970	119
H(10A)	7266	926	8807	129
H(10B)	6522	448	8451	129
H(10C)	6448	1251	8375	129
H(12A)	4237	1377	7210	117
H(12B)	3301	1143	6856	117
H(12C)	3985	1432	6547	117
H(13A)	4309	-433	7284	119
H(13B)	3475	15	7274	119
H(13C)	4399	233	7658	119
H(14A)	3960	-336	6258	109
H(14B)	3826	393	5970	109
H(14C)	3137	111	6278	109
H(15A)	7229	784	5927	50
H(16A)	6312	575	5037	77
H(16B)	5882	1101	5373	77
H(16C)	5566	331	5313	77
H(20A)	8044	-1984	5934	59
H(22A)	6051	-705	5422	52
H(24A)	9951	-1023	7358	110
H(24B)	8945	-1162	7288	110
H(24C)	9260	-438	7132	110
H(25A)	9884	-971	5910	113
H(25B)	10526	-921	6518	113
H(25C)	9854	-324	6290	113
H(26A)	9426	-2094	6178	147
H(26B)	9069	-2167	6719	147
H(26C)	10067	-2002	6783	147
H(28A)	6613	-1770	4536	98
H(28B)	5781	-1395	4637	98
H(28C)	5733	-2180	4476	98
H(29A)	7378	-2636	5211	112
H(29B)	6480	-3025	5133	112
H(29C)	7035	-2819	5741	112
H(30A)	5760	-2212	5909	113
H(30B)	5220	-2449	5305	113
H(30C)	5263	-1665	5468	113
H(2O2)	8740(20)	2064(17)	6052(16)	108(11)
H(4BA)	8543	2735	4007	64
H(6BA)	9652	3873	5334	62
H(8BA)	8138	1094	5097	110
H(8BB)	8642	995	4626	110
H(8BC)	7668	736	4523	110
H(9BA)	6897	1931	4937	113
H(9BB)	6465	1534	4375	113
H(9BC)	6624	2331	4360	113
H(10D)	7456	2168	3650	124
H(10E)	7254	1377	3661	124

H(10F)	8229	1632	3759	124
H(12D)	9637	3164	3639	118
H(12E)	9642	3933	3442	118
H(12F)	8759	3590	3488	118
H(13D)	9279	4704	4652	156
H(13E)	8546	4531	4100	156
H(13F)	9434	4866	4056	156
H(14D)	10786	3428	4483	147
H(14E)	10672	4044	4873	147
H(14F)	10786	4189	4265	147
H(15B)	8748	2960	6278	61
H(16D)	8566	4124	6054	98
H(16E)	9591	4207	6182	98
H(16F)	9158	4009	6671	98
H(20B)	12147	2227	7310	71
H(22B)	10807	3681	6348	68
H(24G)	10776	353	7325	155
H(24H)	11095	690	6829	155
H(24I)	10114	777	6855	155
H(25D)	9771	1512	7616	170
H(25E)	10570	1846	8057	170
H(25F)	10423	1047	8058	170
H(26D)	12282	1218	7570	113
H(26E)	11884	886	8035	113
H(26F)	12019	1686	8024	113
H(24D)	10724	747	6665	165
H(24E)	11202	330	7207	165
H(24F)	11732	860	6940	165
H(25G)	9648	1110	7196	108
H(25H)	9958	1448	7798	108
H(25I)	10198	679	7709	108
H(26G)	11646	946	8134	189
H(26H)	11526	1746	8171	189
H(26I)	12200	1447	7859	189
H(28D)	13089	2583	6744	180
H(28E)	13550	3277	6657	180
H(28F)	12732	3014	6189	180
H(29D)	11900	4107	6193	119
H(29E)	12796	4373	6581	119
H(29F)	11942	4395	6799	119
H(30D)	13042	3181	7684	149
H(30E)	12420	3826	7598	149
H(30F)	13357	3884	7487	149
H(28G)	12118	3608	6001	228
H(28H)	12608	2899	6131	228
H(28I)	13142	3590	6255	228
H(29G)	11993	4302	6882	172
H(29H)	13024	4267	7077	172
H(29I)	12463	3984	7473	172
H(30G)	13318	2533	7061	154
H(30H)	13227	2949	7593	154
H(30I)	13815	3236	7215	154
H(1TA)	6098	2256	6963	128
H(1TB)	5675	1994	6341	128
H(2TA)	5661	3312	6759	129
H(2TB)	4915	2937	6296	129
H(3TA)	5497	3250	5609	157
H(3TB)	6049	3787	6044	157
H(4TA)	6625	2690	5642	182
H(4TB)	7179	3236	6061	182
H(1TC)	10681	246	5160	113

H(1TD)	11144	261	5814	113
H(2TC)	11738	788	5008	137
H(2TD)	12183	829	5663	137
H(3TC)	11840	1874	5669	161
H(3TD)	11430	1841	5009	161
H(4TC)	10180	1872	5117	116
H(4TD)	10592	1983	5770	116
H(1TE)	7604	3597	7195	177
H(1TF)	7447	3112	7674	177
H(2TE)	8145	3743	8295	142
H(2TF)	8127	4290	7815	142
H(3TE)	9543	3773	8412	152
H(3TF)	9459	4074	7800	152
H(4TE)	9771	3011	7607	122
H(4TF)	9437	2701	8110	122
H(2A)	5249	5002	4049	185
H(3A)	6068	5931	4396	185
H(4A)	7435	5809	4998	185
H(5A)	7969	4741	5242	185
H(6A)	7158	3810	4896	185
H(7A)	5929	3283	4354	232
H(7B)	5490	3696	3801	232
H(7C)	5059	3699	4313	232
H(2'A)	7389	3904	4793	377
H(3'A)	6166	3349	4416	377
H(4'A)	4877	3884	4235	377
H(5'A)	4835	4985	4432	377
H(6'A)	6052	5545	4806	377
H(7'C)	7471	5619	5125	471
H(7'D)	7977	5129	4808	471
H(7'A)	7910	4943	5420	471