Supporting Information

for

Yttrium- and Aluminum-Bis(phenolate)pyridine Complexes : Catalysts and Model Compounds of the Intermediates for the Stereoselective Ring-Opening Polymerization of racemic Lactide and β-Butyrolactone

Joice S. Klitzke, Thierry Roisnel, Evgeny Kirillov, Osvaldo Casagrande Jr and Jean-François Carpentier

Figure S10. ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, toluene-d_8, 258 K) of {ONO^{Me,Cumyl}}Y((*R*)-OCH(CH_3)CH_2COOMe) (**2**).

Figure S11. ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of {ONO^{Me,Cumyl}}Y((*S,S*)-OCH(CH_3)OCH(CH_3)COOMe)(THF) (**3**).

Figure S12. ^{13}C-^{1}H HMQC NMR spectrum (500 MHz, THF-d_8, 298 K) of {ONO^{Me,Cumyl}}Y((*S,S*)-OCH(CH_3)OCH(CH_3)COOMe)(THF) (**3**).

Figure S13. ^{13}C-^{1}H HMBC NMR spectrum (500 MHz, THF-d_8, 298 K) of {ONO^{Me,Cumyl}}Y((*S,S*)-OCH(CH_3)OCH(CH_3)COOMe)(THF) (**3**).

Figure S14a. ^{1}H NMR (500 MHz, THF-d_8, 298K) spectrum of the 1:1 reaction mixture of **1** and methyl (*S,S*)-lactyllactate at room temperature after 30 min (bottom spectrum) and after 18 h reaction, evaporation of volatiles and addition of fresh THF-d_8 (bottom spectrum).

Figure S15. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}AlMe (**4**).

Figure S16. ^{13}C{^{1}H} NMR spectrum (125 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}AlMe (**4**)

Figure S17. ^{1}H NMR spectrum (500 MHz, toluene-d_8, 298 K) of {ONO^{Me,Cumyl}}Al(*i*Pr (*S*)-lactate) (**5**).

Figure S18. ^{13}C{^{1}H} NMR spectrum (125 MHz, toluene-d_8, 298 K) of {ONO^{Me,Cumyl}}Al(*i*Pr (*S*)-lactate) (**5**).

Figure S19. ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, toluene-d_8, 298 K) of {ONO^{Me,Cumyl}}Al(*i*Pr (*S*)-lactate) (**5**).

Figure S20. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}Al((*R*)-OCH(CH_3)CH_2COOMe) (**6**).

Figure S21. ^{13}C{^{1}H} NMR spectrum (100 MHz, C_6D_6, 298 K) of {ONO^{Me,Cumyl}}Al((*R*)-OCH(CH_3)CH_2COOMe) (**6**).

Figure S22. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}Al((*rac*)-OCH(CF_3)CH_2COOEt) (**7**).

Figure S23. ^{13}C{^{1}H} NMR spectrum (125 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}Al((*rac*)-OCH(CF_3)CH_2COOEt) (**7**).

Figure S23bis. DEPT 135 NMR spectrum (125 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}Al((*rac*)-OCH(CF_3)CH_2COOEt) (**7**).

Figure S24. $^{19}F\{^{1}H\}$NMR spectrum (185 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}Al((*rac*)-OCH(CF_3)CH_2COOEt) (**7**).

Figure S25. ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}Al((*rac*)-OCH(CF_3)CH_2COOEt) (**7**).

Figure S26. ^{1}H–^{1}H COSY NMR spectrum (500 MHz, $CDCl_3$, 298 K) of a PLA produced from {ONO^{Me,Cumyl}}Y((*R*)-OCH(CH_3)CH_2COOMe) (**2**).

Figure S27. Detail of the MALDI-ToF mass spectrum of a PLA sample produced from **2** using IAA as matrix (Table 1, entry 10).

Figure S28. ^{1}H–^{1}H COSY NMR spectrum (500 MHz, $CDCl_3$, 298 K) of a PHB produced from {ONO^{Me,Cumyl}}Y((*R*)-OCH(CH_3)CH_2COOMe) (**2**).

Figure S29: Methine region of ^{1}H NMR and ^{1}H homo-decoupled NMR spectra of different PLAs.

Figure S30. Carbonyl (left) and methylene (right) regions of the $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$, 298 K) of a PHB produced from {ONO^{Me,Cumyl}}Y((*R*)-OCH(CH_3)CH_2COOMe) (**2**).

Figure S31. Detail of the MALDI-ToF mass spectrum of a PHB sample produced from **2** using IAA as matrix (Table 1, entry 20).

Table S1. Summary of crystal and refinement data for {ONO^{Me,Cumyl}}H_2, **1** and **6**.

Figure S32. Molecular structure of proligand {ONO^{Me,Cumyl}}H_2.

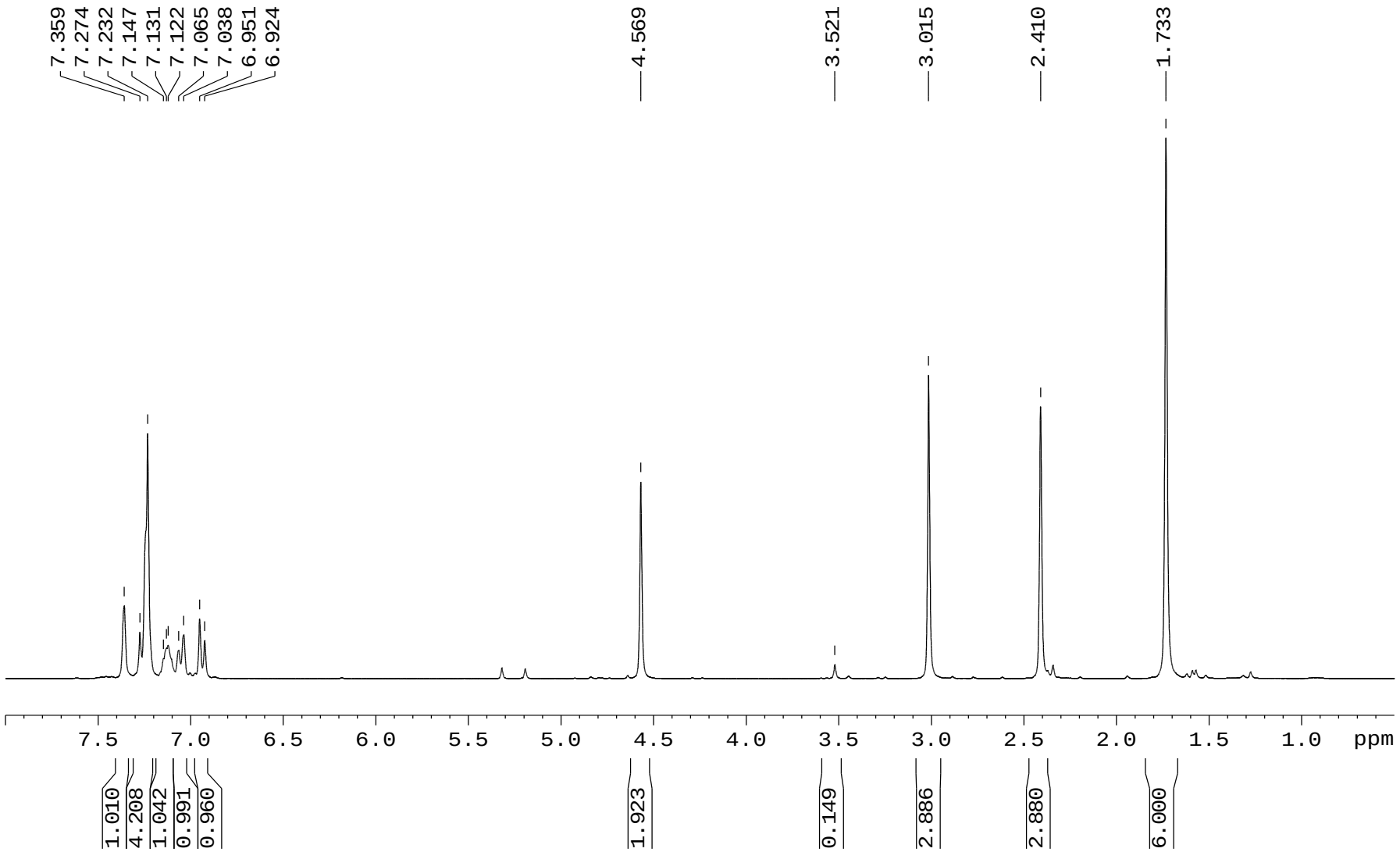


Figure S1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of 1-(methoxymethyl)-4-methyl-2-(2-phenylpropan-2-yl)benzene.

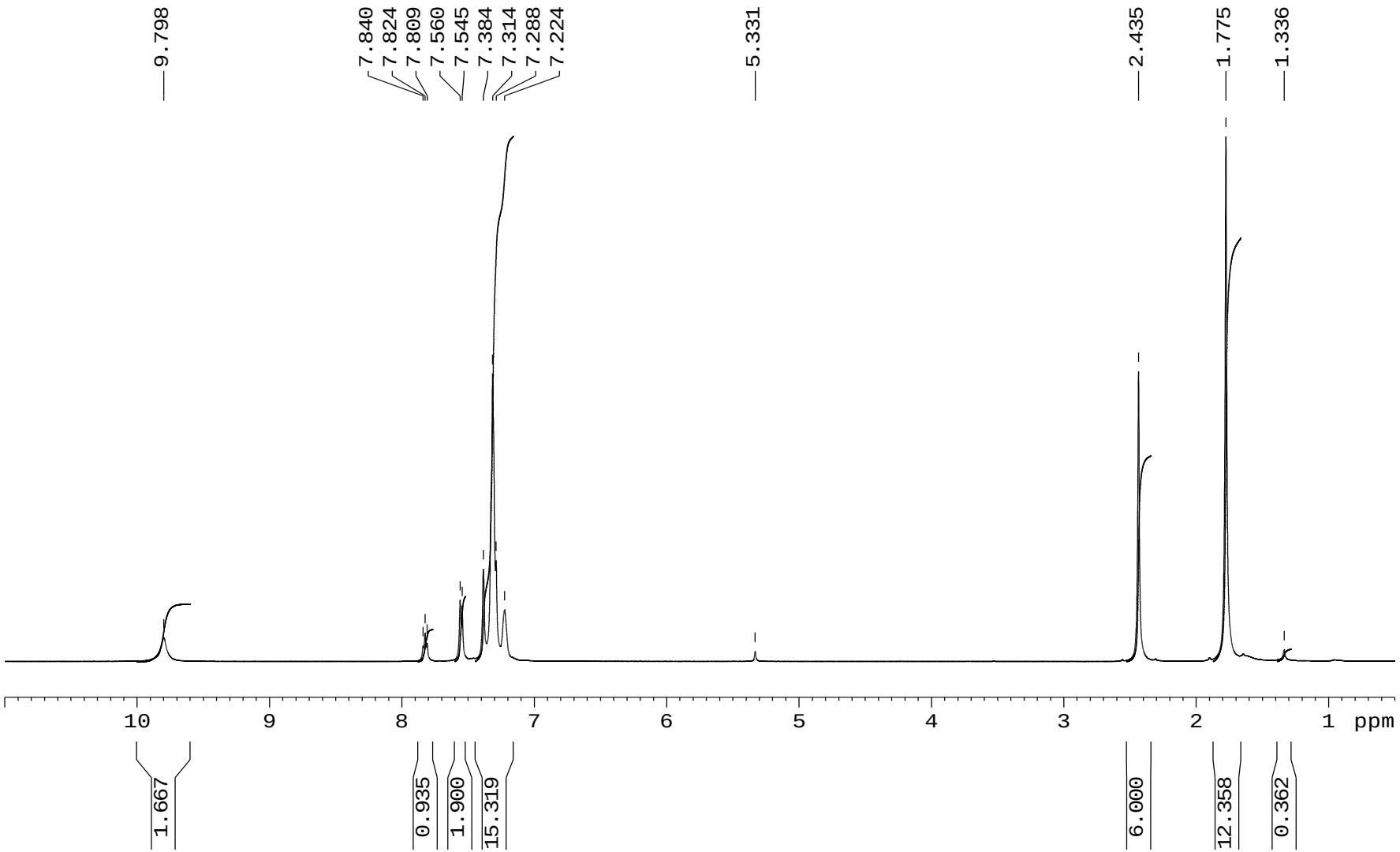


Figure S2. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of $\{ONO^{Me,Cumyl}\}H_2$.

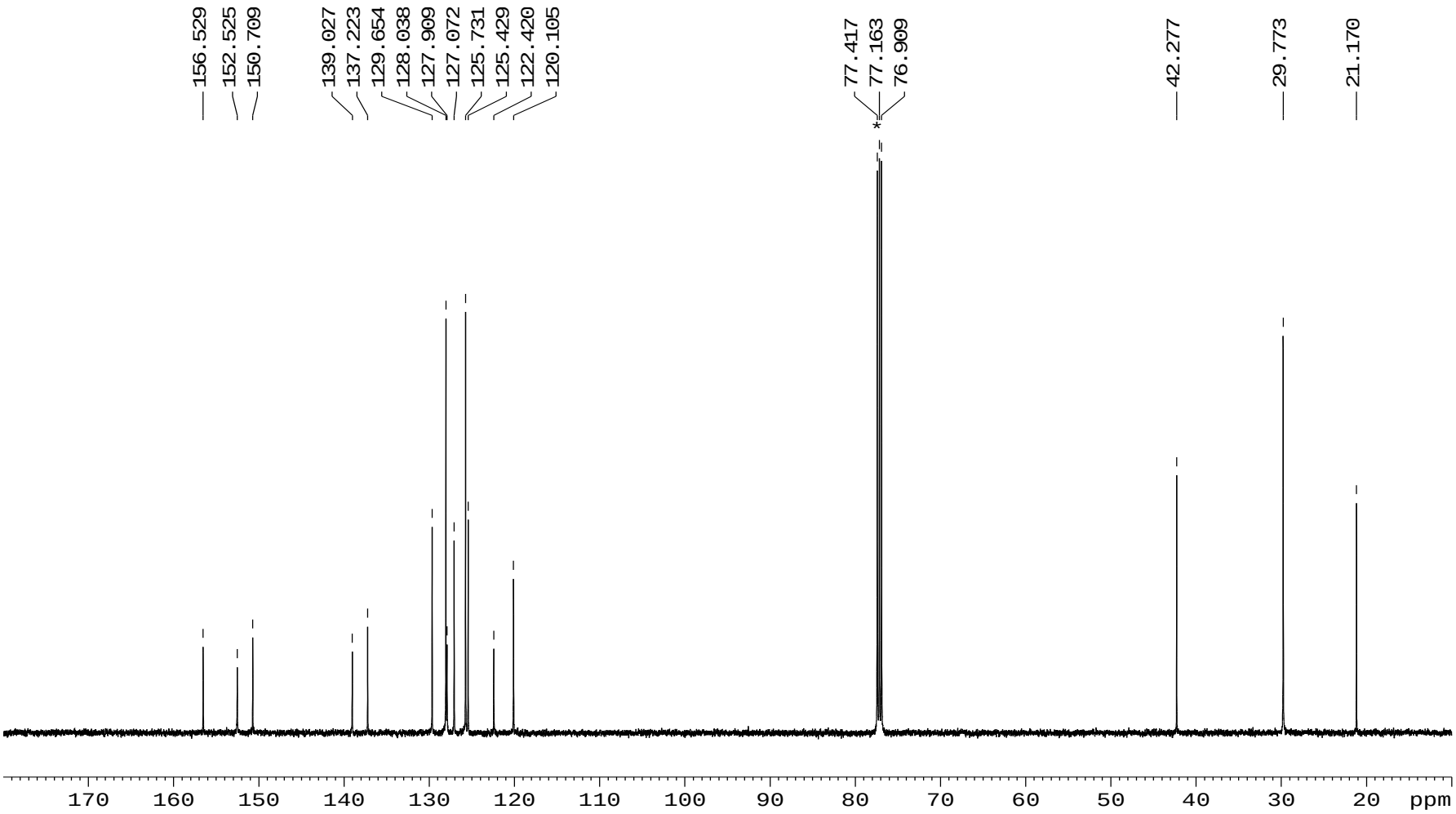


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, $CDCl_3$, 298 K) of $\{ONO^{Me,Cumyl}\}H_2$ (*stands for residual solvent resonances).

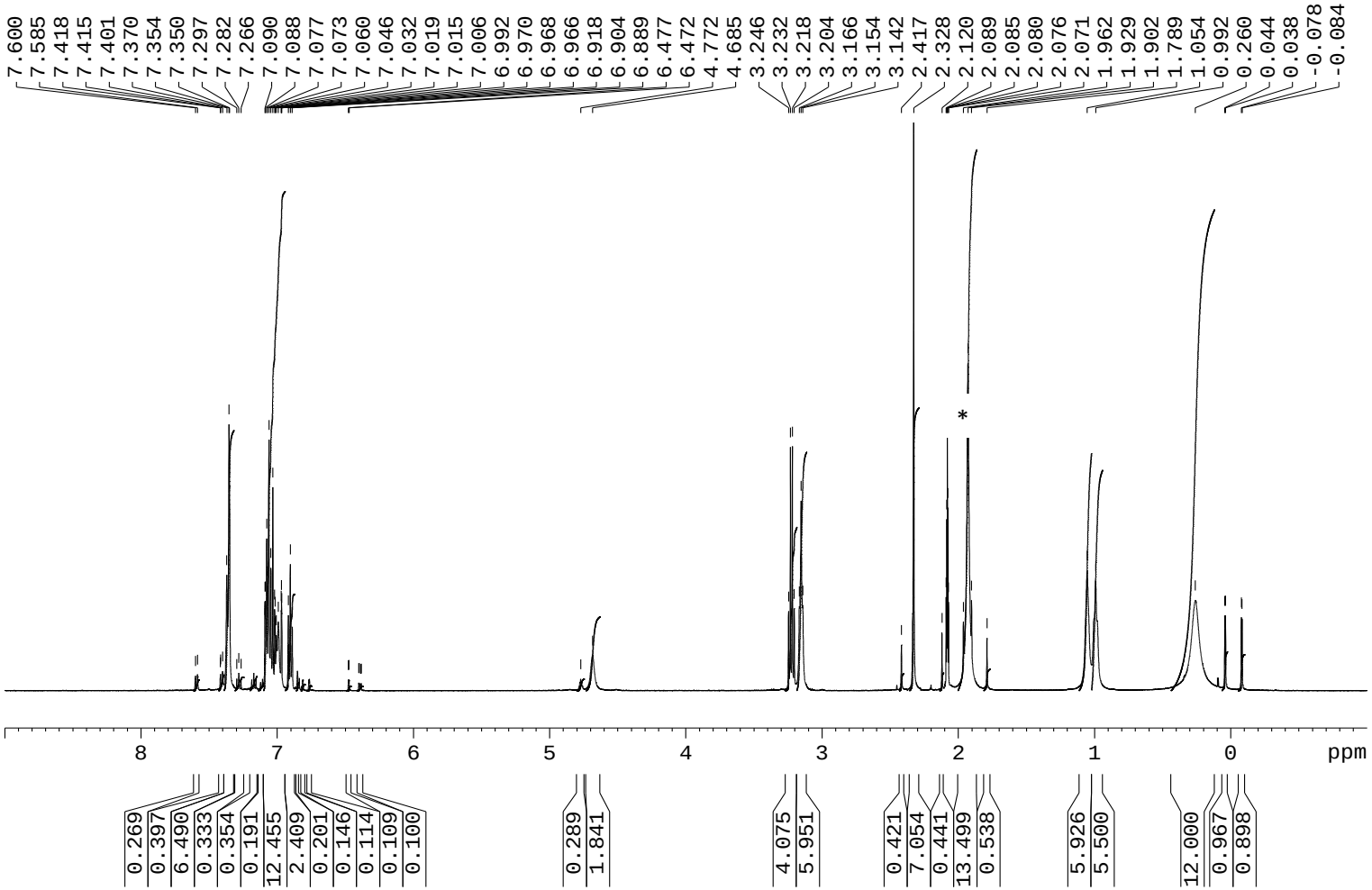


Figure S4. ^{1}H NMR spectrum (500 MHz, toluene-d_8, 298 K) of {ONO^{Me,Cumyl}}Y[N(SiHMe$_2$)$_2$](THF)(Et$_2$O) (**1**) (* stands for residual solvent resonances).

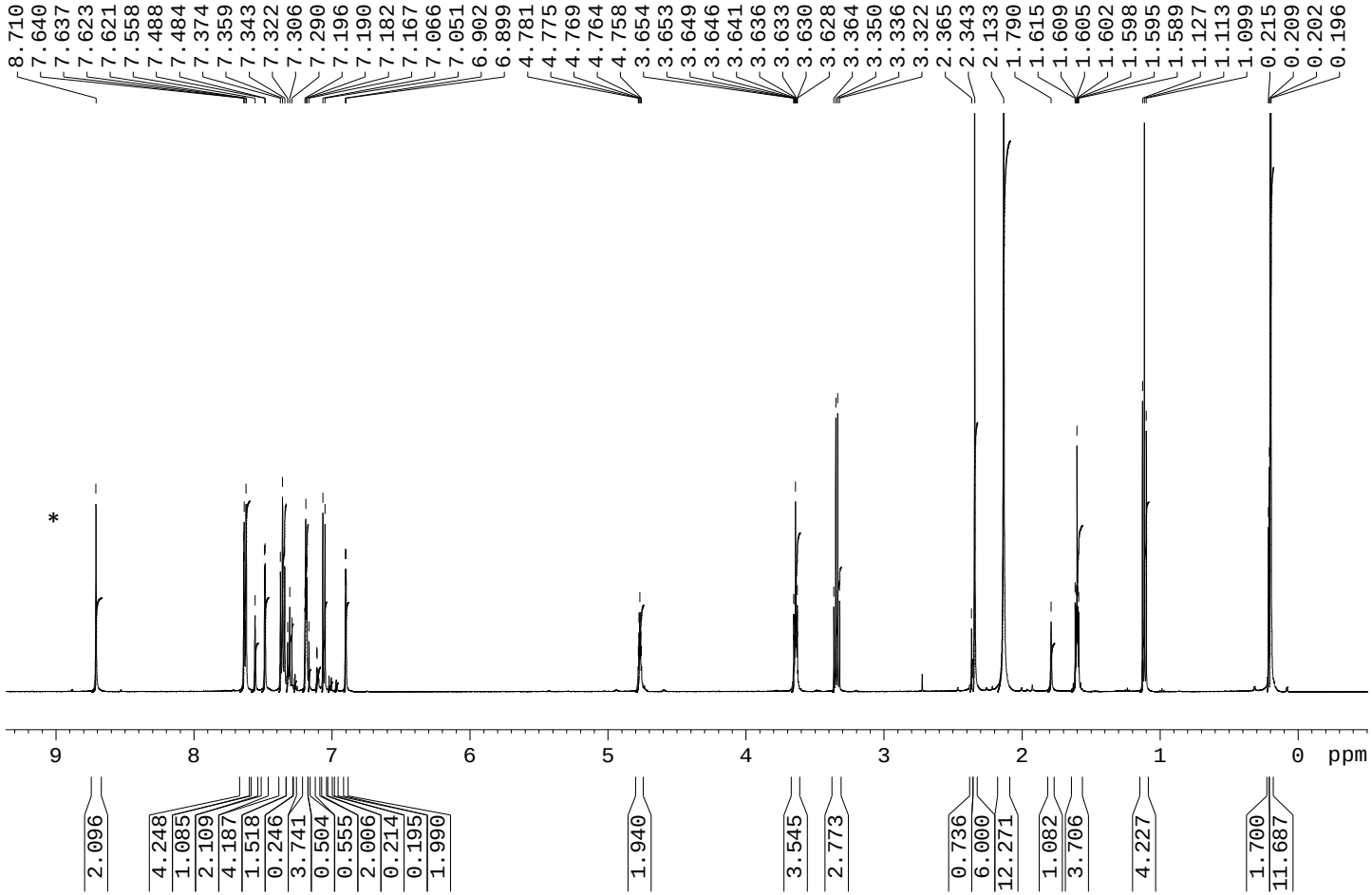


Figure S5. ^{1}H NMR spectrum (500 MHz, pyridine-d_5, 298 K) of {ONO^{Me,Cumyl}}Y[N(SiHMe$_2$)$_2$](THF)(Et$_2$O) (**1**) (* stands for residual solvent resonance).

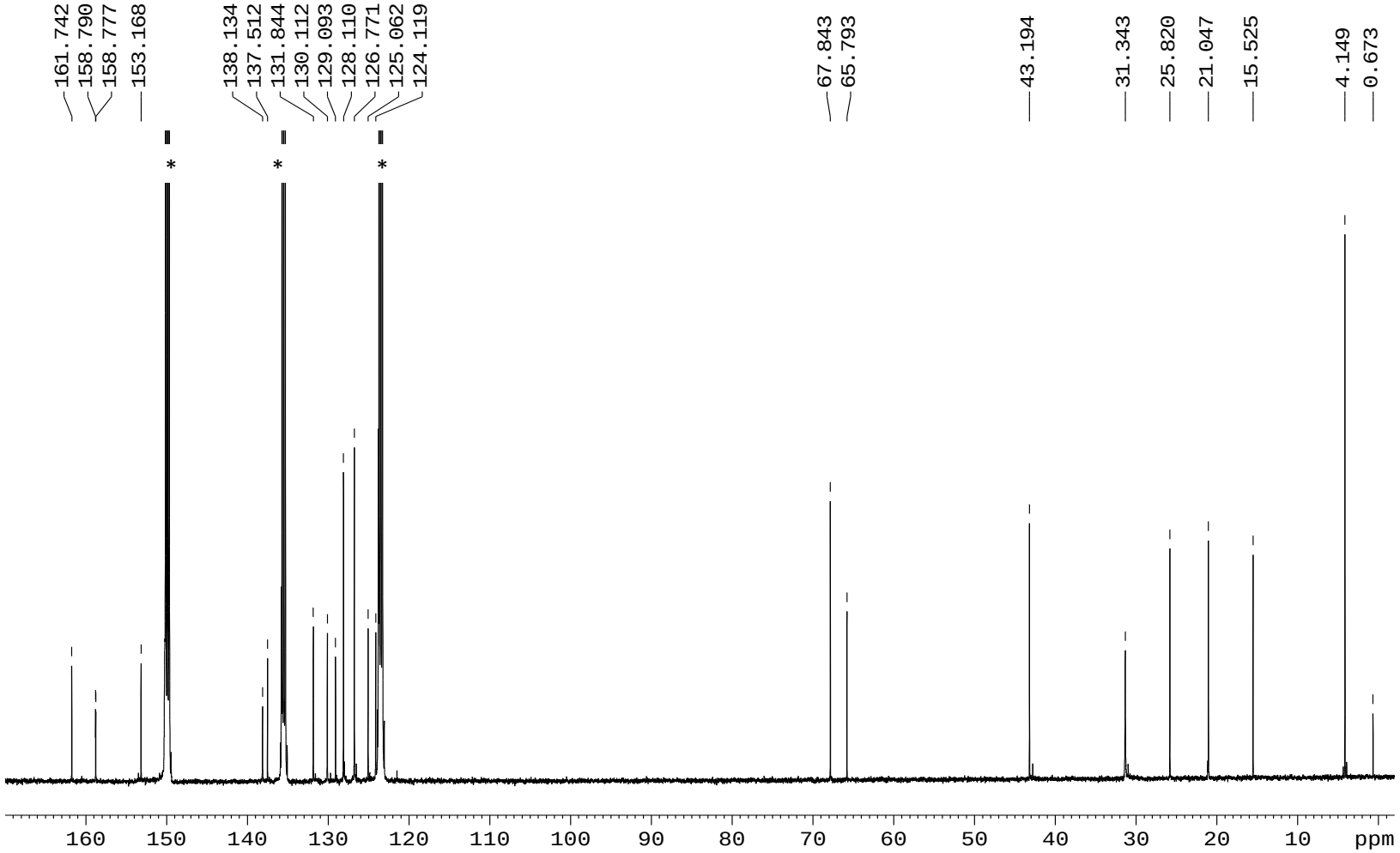


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, pyridine-d_5, 298 K) of {ONO^{Me,Cumyl}}Y[N(SiHMe$_2$)$_2$](THF)(Et$_2$O) (**1**) (* stands for residual solvent resonance).

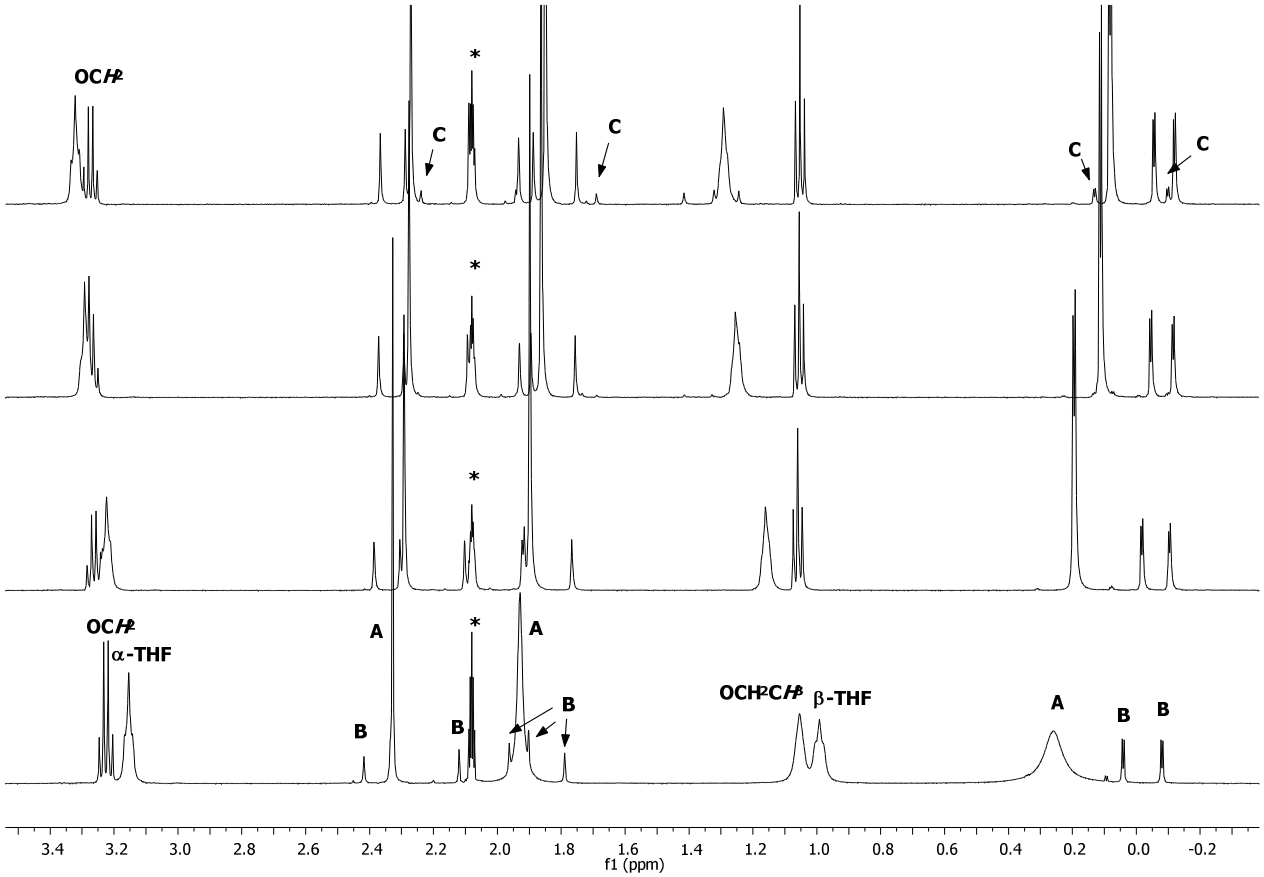


Figure S7. Details of the aliphatic region of the VT-^{1}H NMR spectra (500 MHz, toluene-d_8, 298–363 K) of {ONO^{Me,Cumyl}}Y[N(SiHMe$_2$)$_2$](THF)(Et$_2$O) (**1**); from bottom to top, 298 K, 333 K, 353 K and 363 K. Markers **A** denote genuine compound **1**, and **B** and **C** unidentified species forming upon time and heating (* refers to residual solvent resonances).

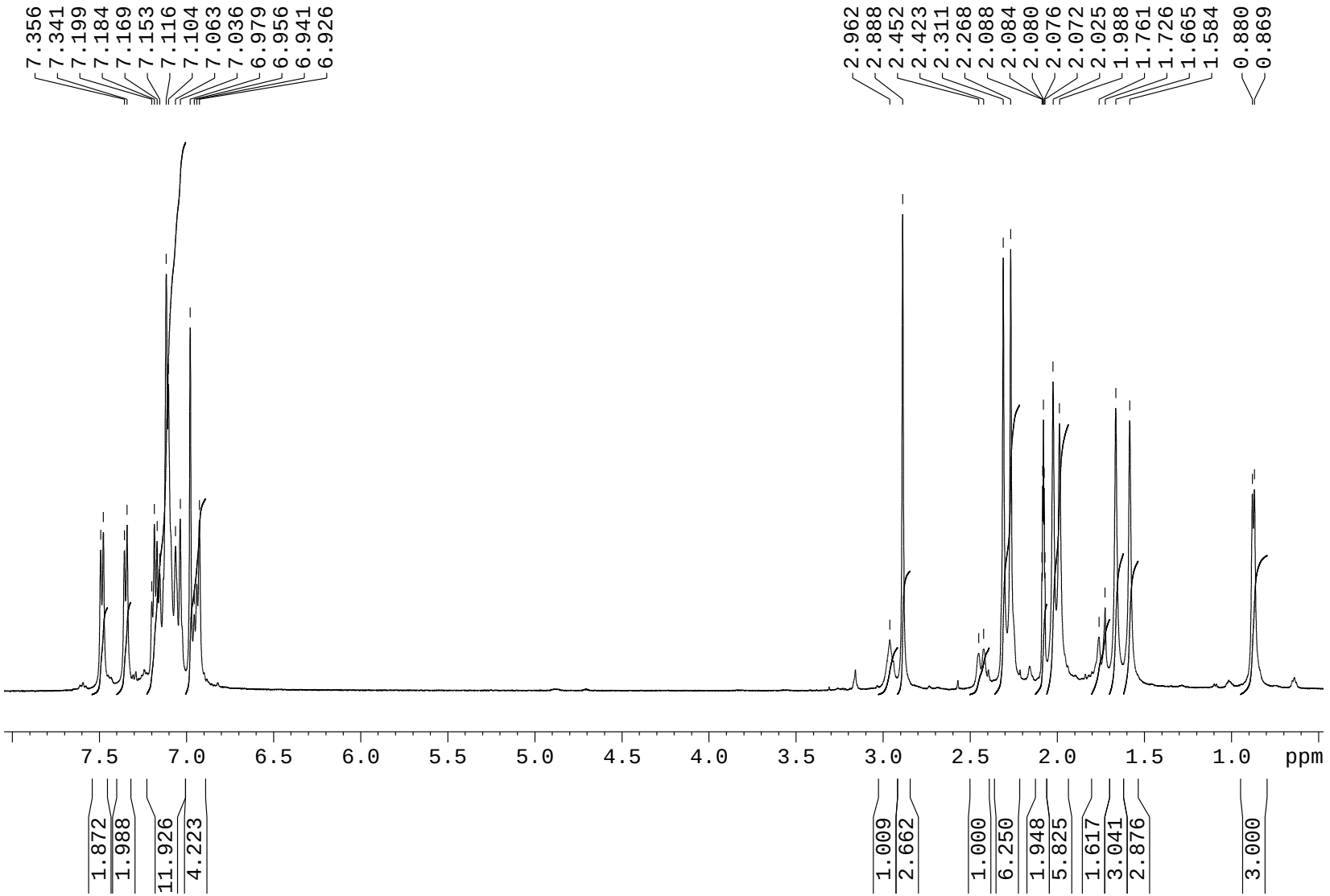


Figure S8. ^{1}H NMR spectrum (500 MHz, toluene-d_8, 258 K) of {ONO^{Me,Cumyl}}Y((*R*)-OCH(CH$_3$)CH$_2$COOMe) (**2**).

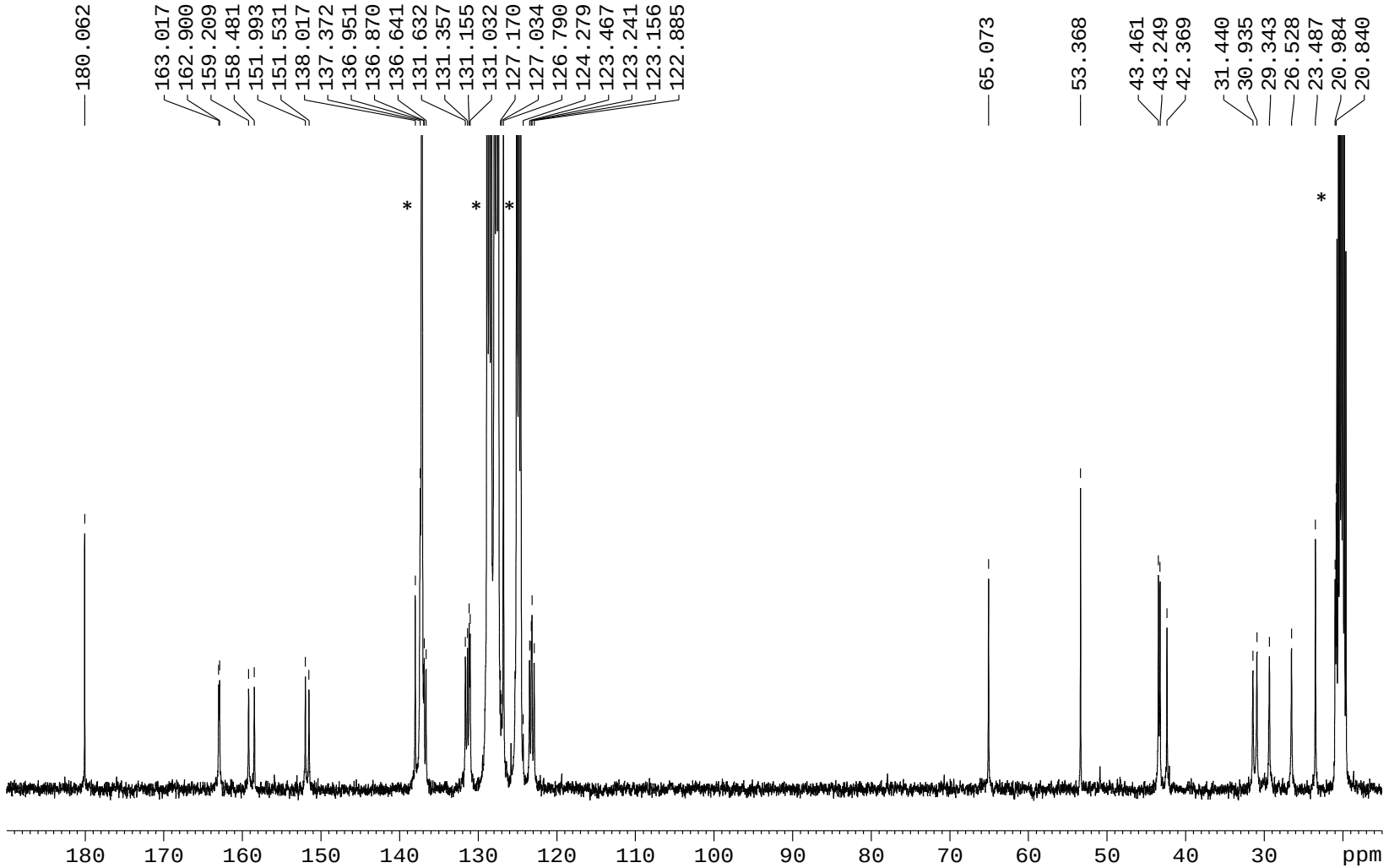


Figure S9. $^{13}C\{^{1}H\}$ NMR (100 MHz, toluene-d_8, 258 K) of {ONO^{Me,Cumyl}}Y((*R*)-OCH(CH_3)CH_2COOMe) (**2**) (* stands for residual solvent resonance).

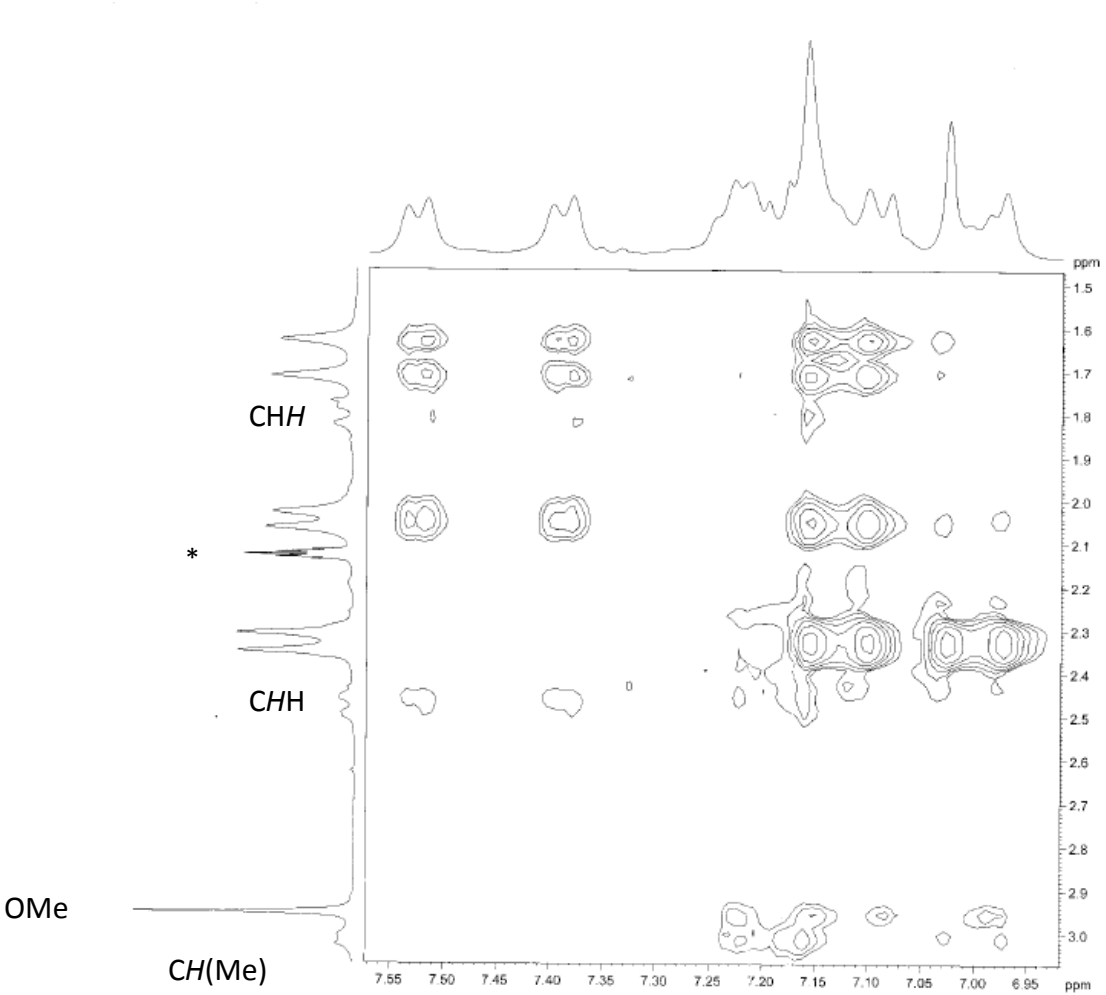


Figure S10. Detail of the $^{1}H–^{1}H$ NOESY NMR spectrum (400 MHz, toluene-d_8, 258 K) of {ONO^{Me,Cumyl}}Y((*R*)-OCH(CH_3)CH_2COOMe) (**2**) (* stands for residual solvent resonance).

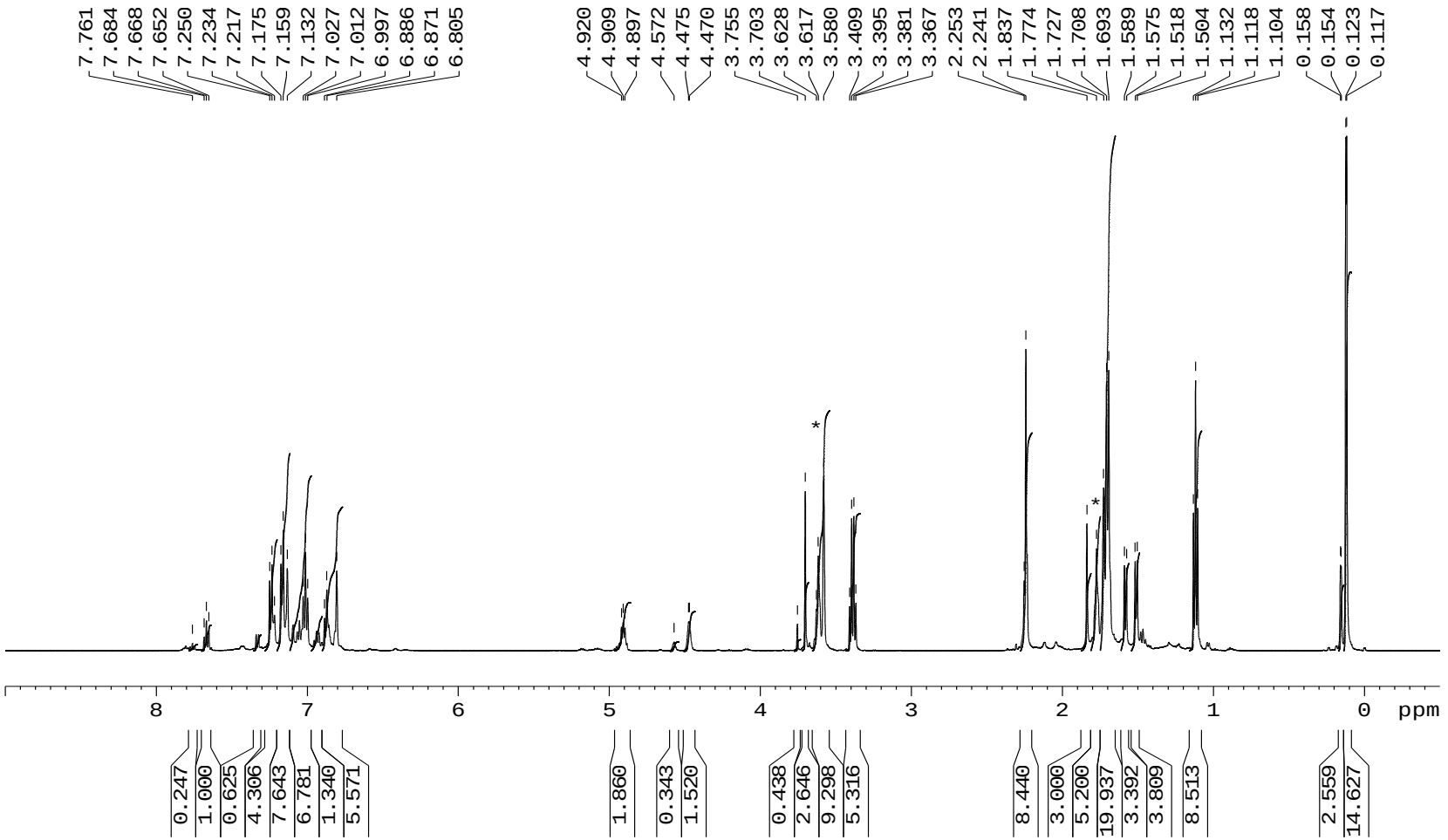


Figure S11. ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of {ONO^{Me,Cumyl}}Y((*S,S*)-OCH(CH$_3$)OCH(CH$_3$)COOMe)(THF) (**3**) *in situ* generated upon addition of one equiv of methyl (S,S)-lactyllactate to **1** (after 30 min at room temperature) (* stands for residual solvent resonance).

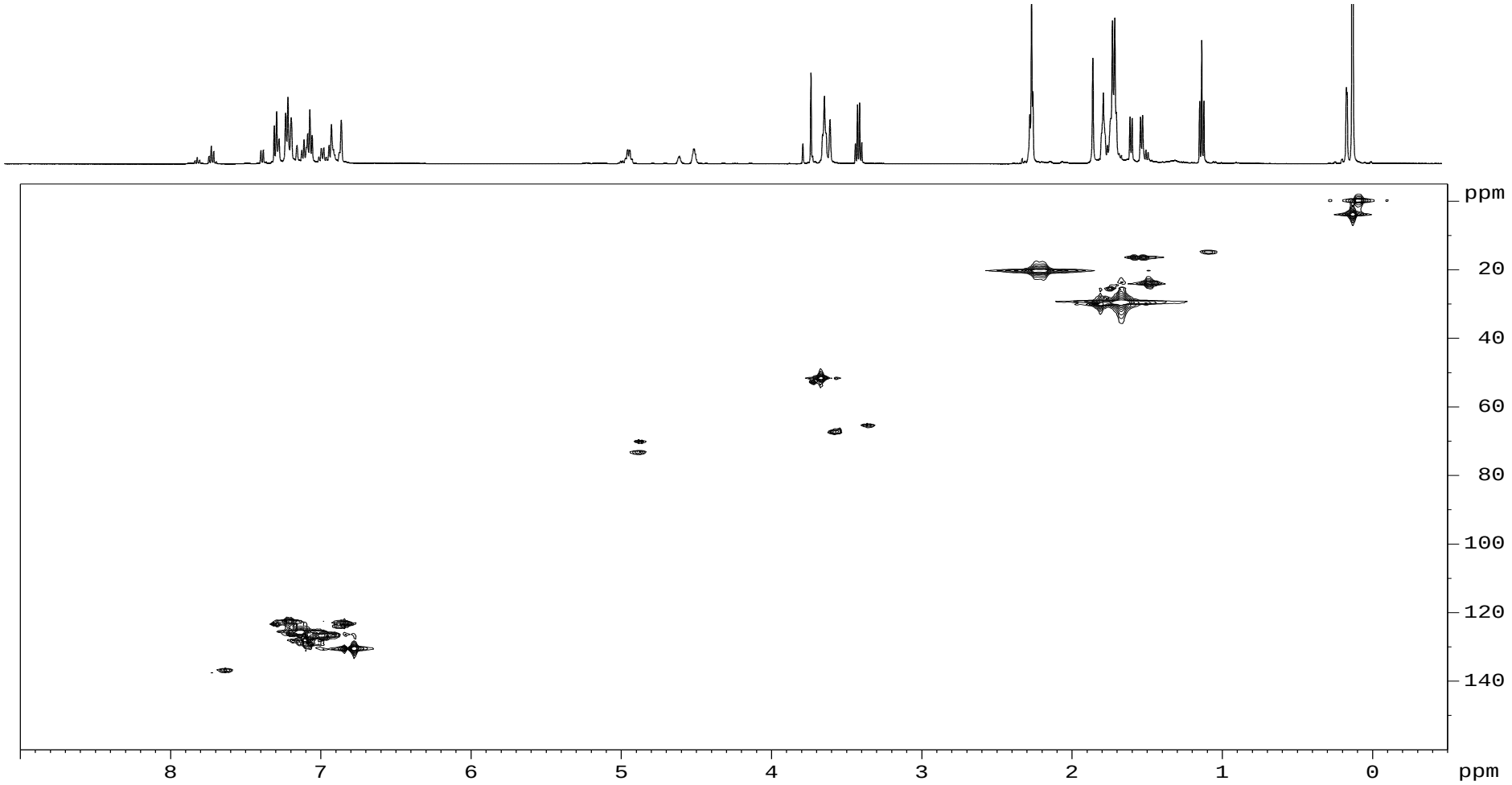


Figure S12. ^{13}C–^{1}H HMQC NMR spectrum (500 MHz, THF-d_8, 298 K) of {ONO^{Me,Cumyl}}Y((*S*,*S*)-OCH(CH_3)OCH(CH_3)COOMe)(THF) (**3**) *in situ* generated upon addition of one equiv of methyl (S,S)-lactyllactate to **1** (after 30 min at room temperature).

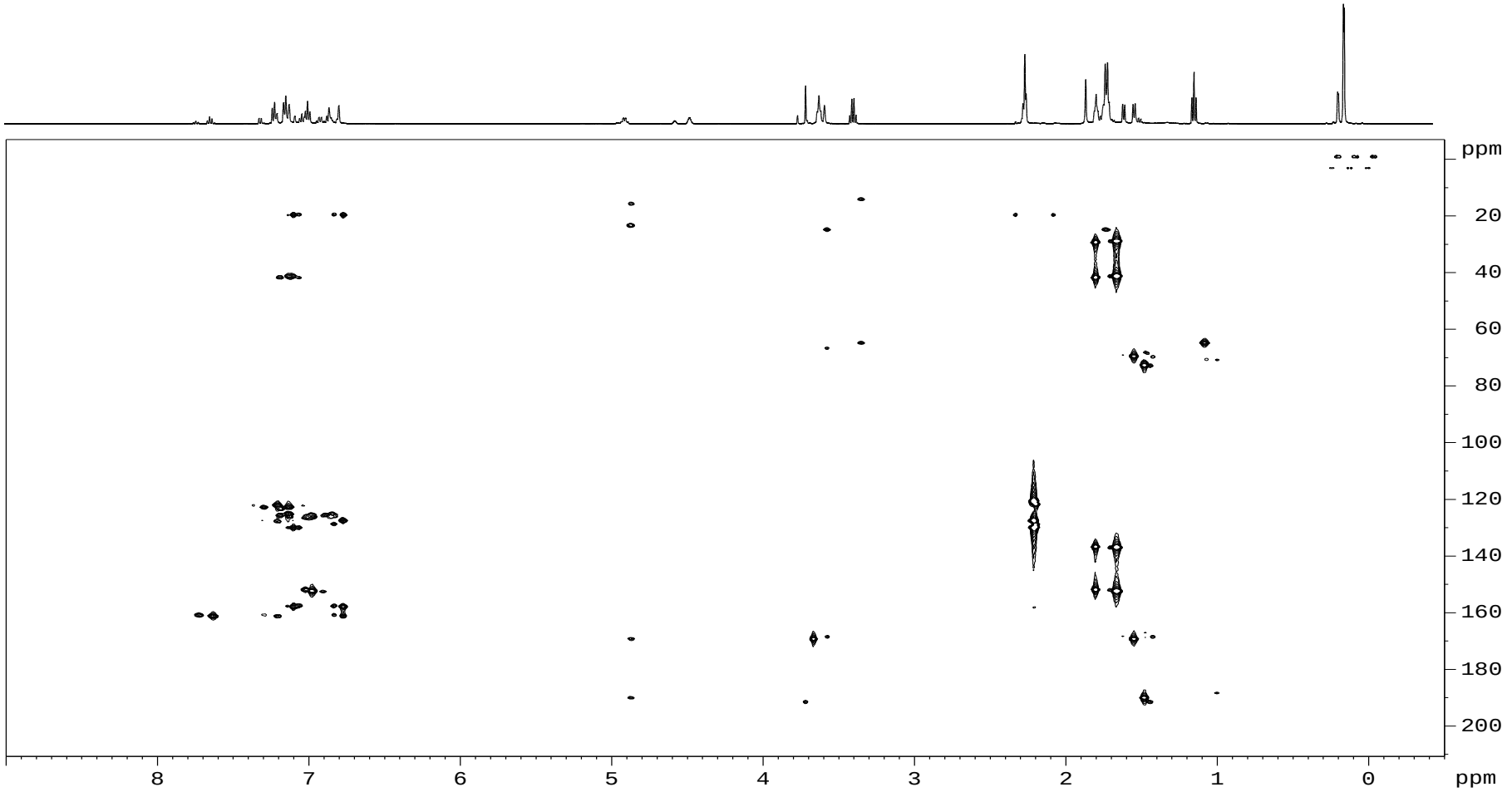


Figure S13. ^{13}C–^{1}H HMBC NMR spectrum (500 MHz, THF-d_8, 298 K) of {ONO^{Me,Cumyl}}Y((*S*,*S*)-OCH(CH_3)OCH(CH_3)COOMe)(THF) (**3**) *in situ* generated upon addition of one equiv of methyl (S,S)-lactyllactate to **1** (after 30 min at room temperature).

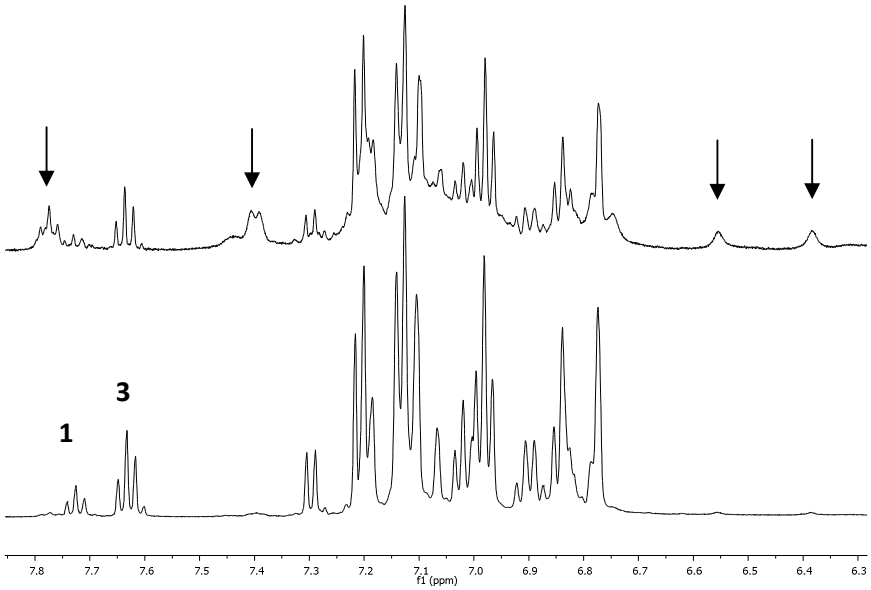


Figure S14a. Details of the aromatic region of the ^{1}H NMR (500 MHz, THF-d_8, 298K) spectrum of the 1:1 reaction mixture of **1** and methyl (*S*,*S*)-lactyllactate at room temperature after 30 min (bottom spectrum) and after 18 h reaction, evaporation of volatiles and addition of fresh THF-d_8 (bottom spectrum).

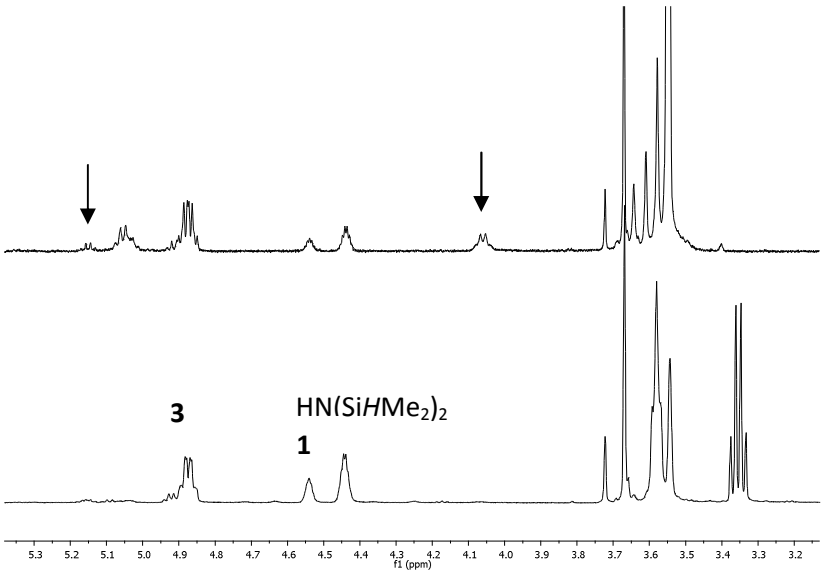


Figure S14b. Details of the SiH region.

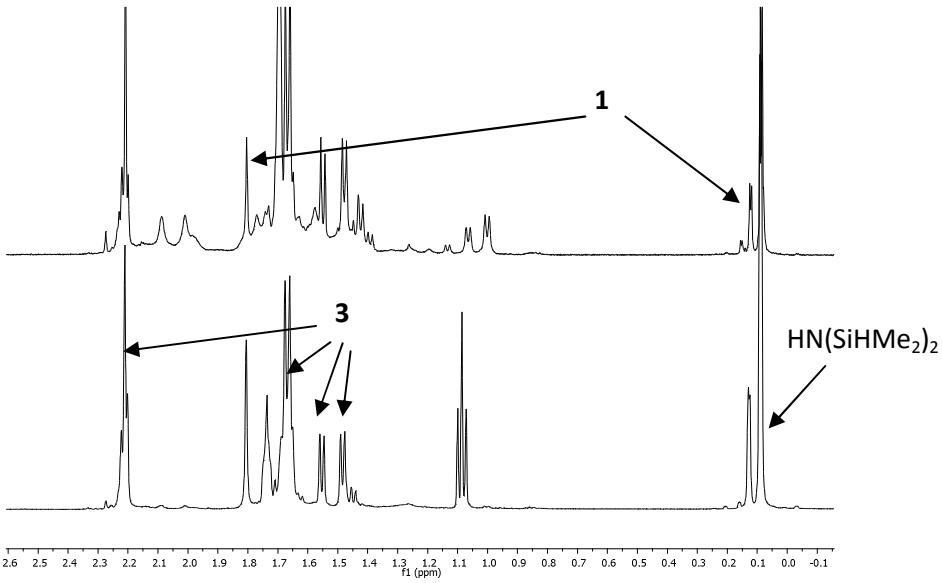


Figure S14c. Details of the aliphatic region.

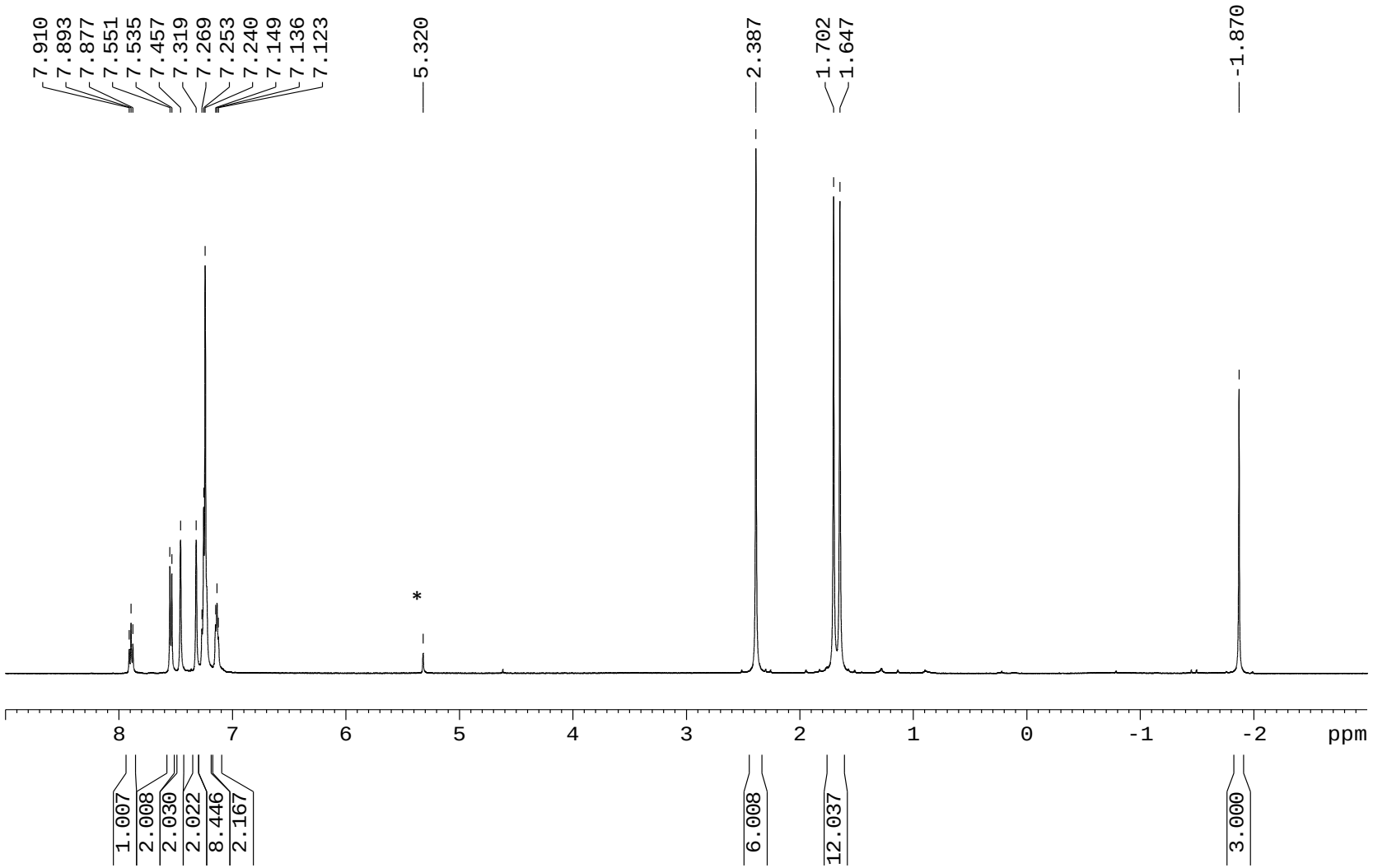


Figure S15. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of {ONO^{Me,Cumyl}}AlMe (**4**) (*stands for residual solvent resonances).

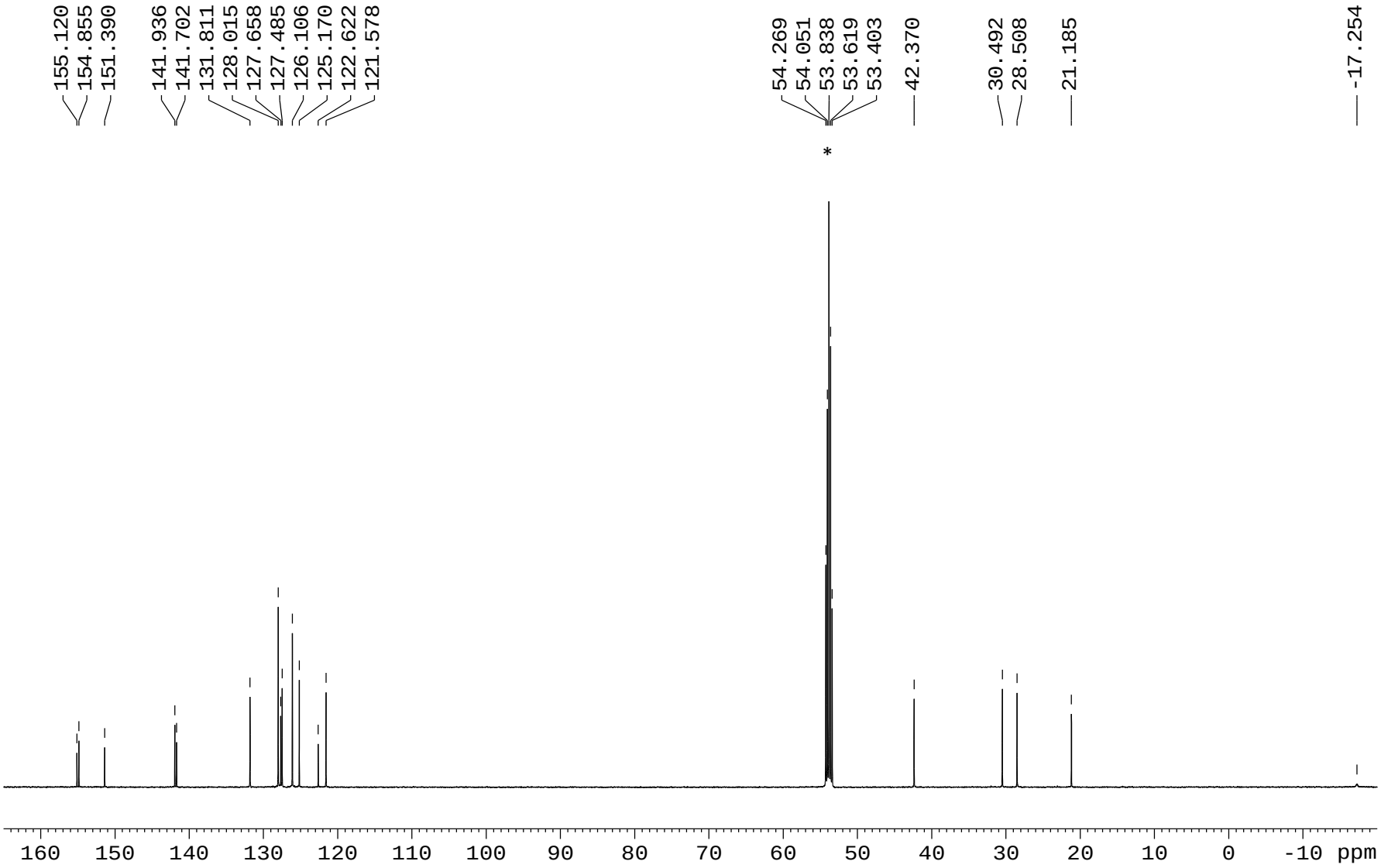


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, CD_2Cl_2, 298 K) of {$ONO^{Me,Cumyl}$}AlMe (**4**) (*stands for residual solvent resonances).

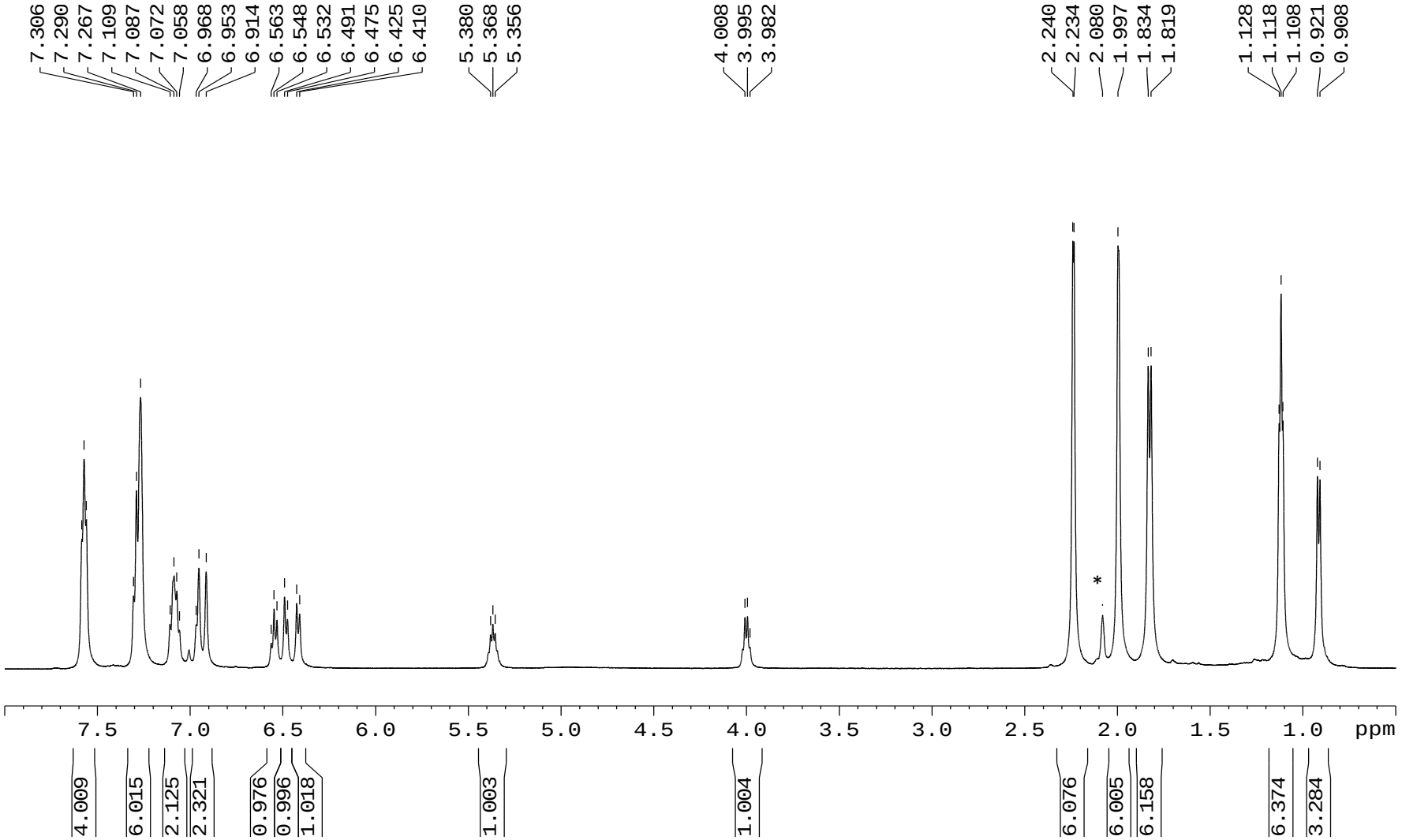


Figure S17. ^{1}H NMR spectrum (500 MHz, toluene-d_8, 298 K) of {ONO^{Me,Cumyl}}Al(*i*Pr (*S*)-lactate) (**5**) (*stands for residual solvent resonances).

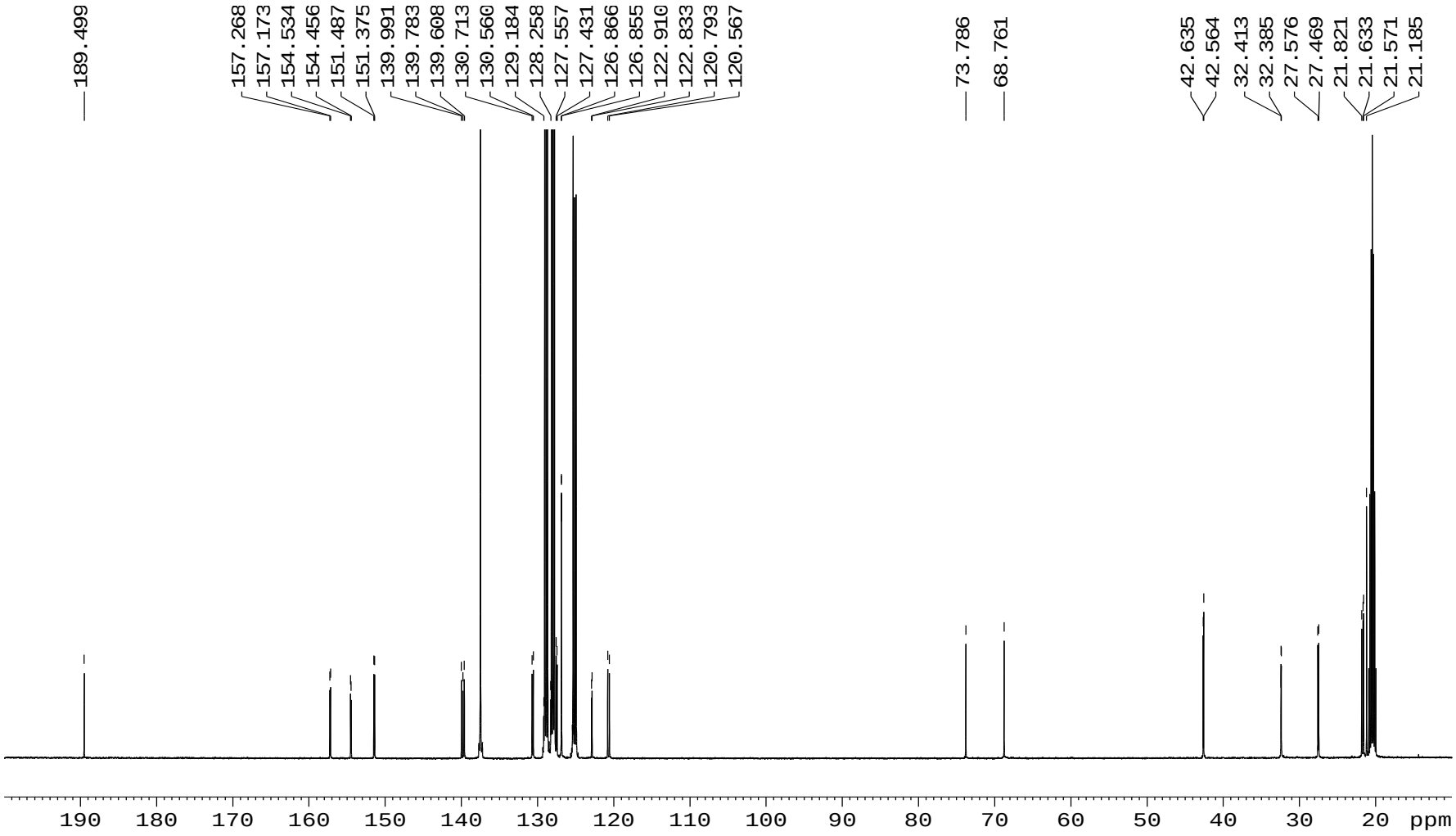


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, toluene-d_8, 298 K) of {ONO^{Me,Cumyl}}Al(*i*Pr (*S*)-lactate) (**5**).

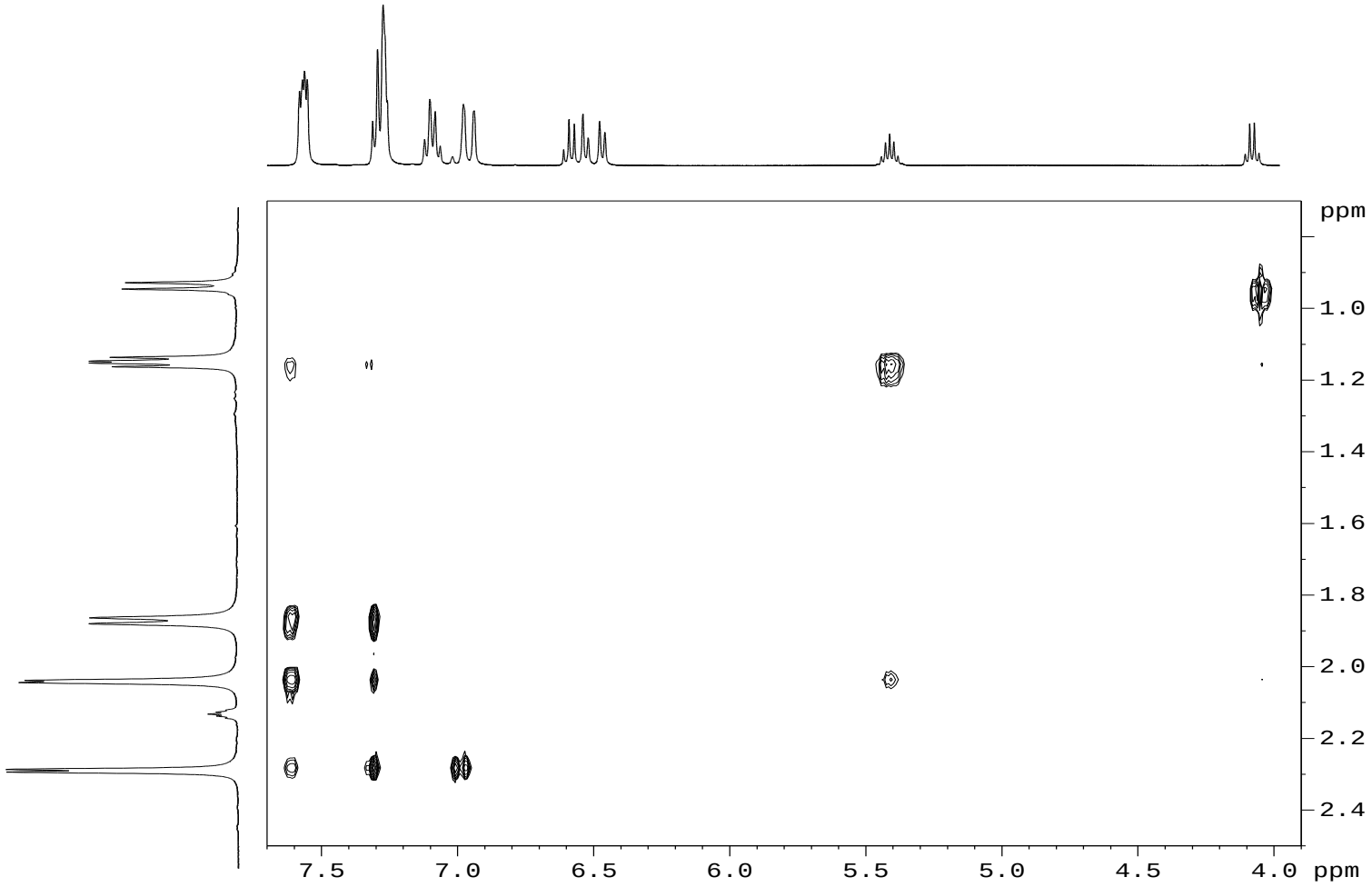


Figure S19. ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, toluene-d_8, 298 K) of {ONO^{Me,Cumyl}}Al(*i*Pr (*S*)-lactate) (**5**).

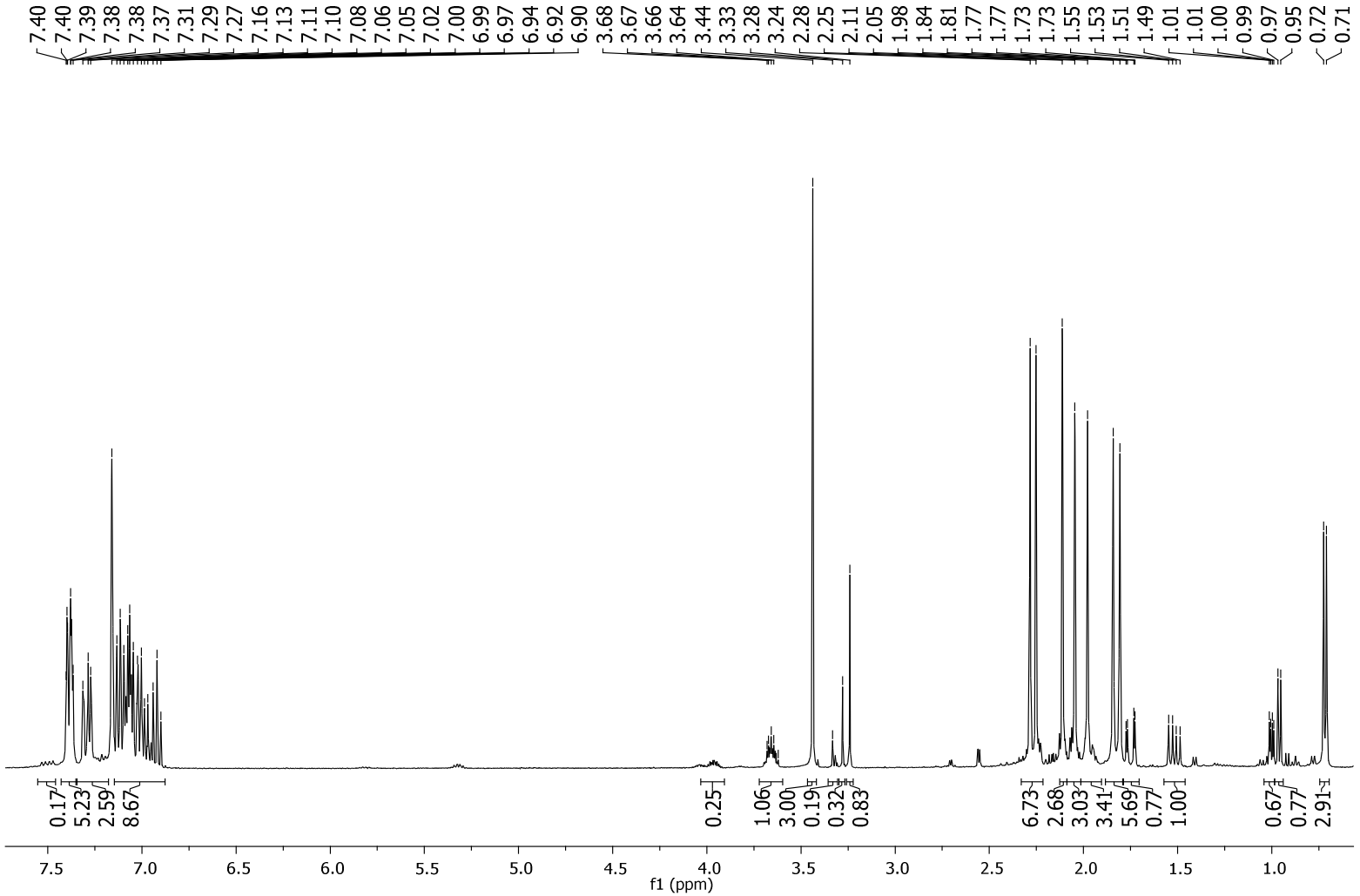


Figure S20. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of {$ONO^{Me,Cumyl}$}Al((*R*)-$OCH(CH_3)CH_2COOMe$) (**6**) (* stands for residual solvent resonances; a small amount of free ligand contaminates the product).

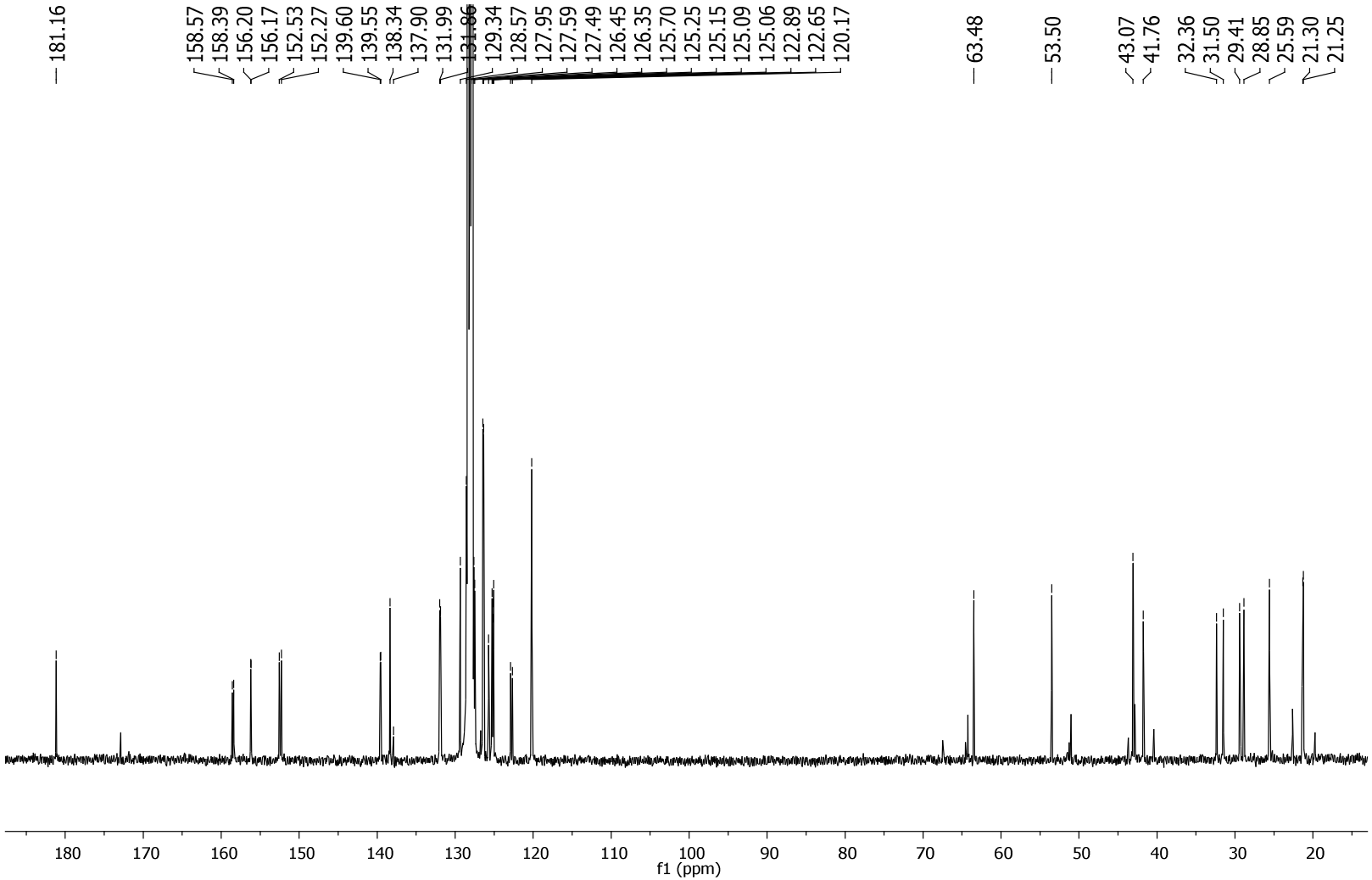


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, C_6D_6, 298 K) of {ONO^{Me,Cumyl}}Al((*R*)-OCH(CH_3)CH_2COOMe) (**6**) (* stands for impurities and residual solvent resonances).

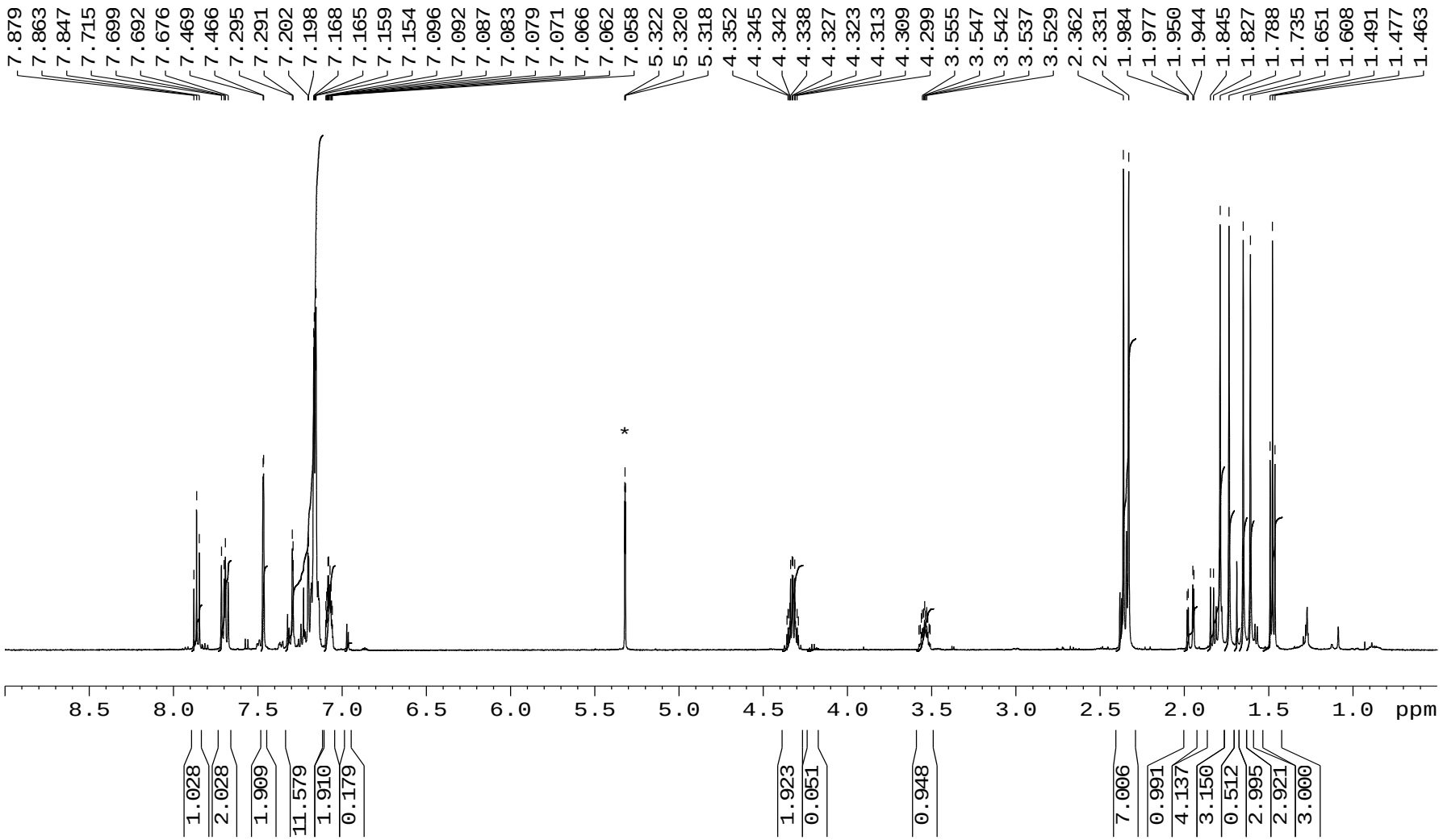


Figure S22. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of {$ONO^{Me,Cumyl}$}Al((*rac*)-$OCH(CF_3)CH_2COOEt$) (**7**) (* stands for residual solvent resonances).

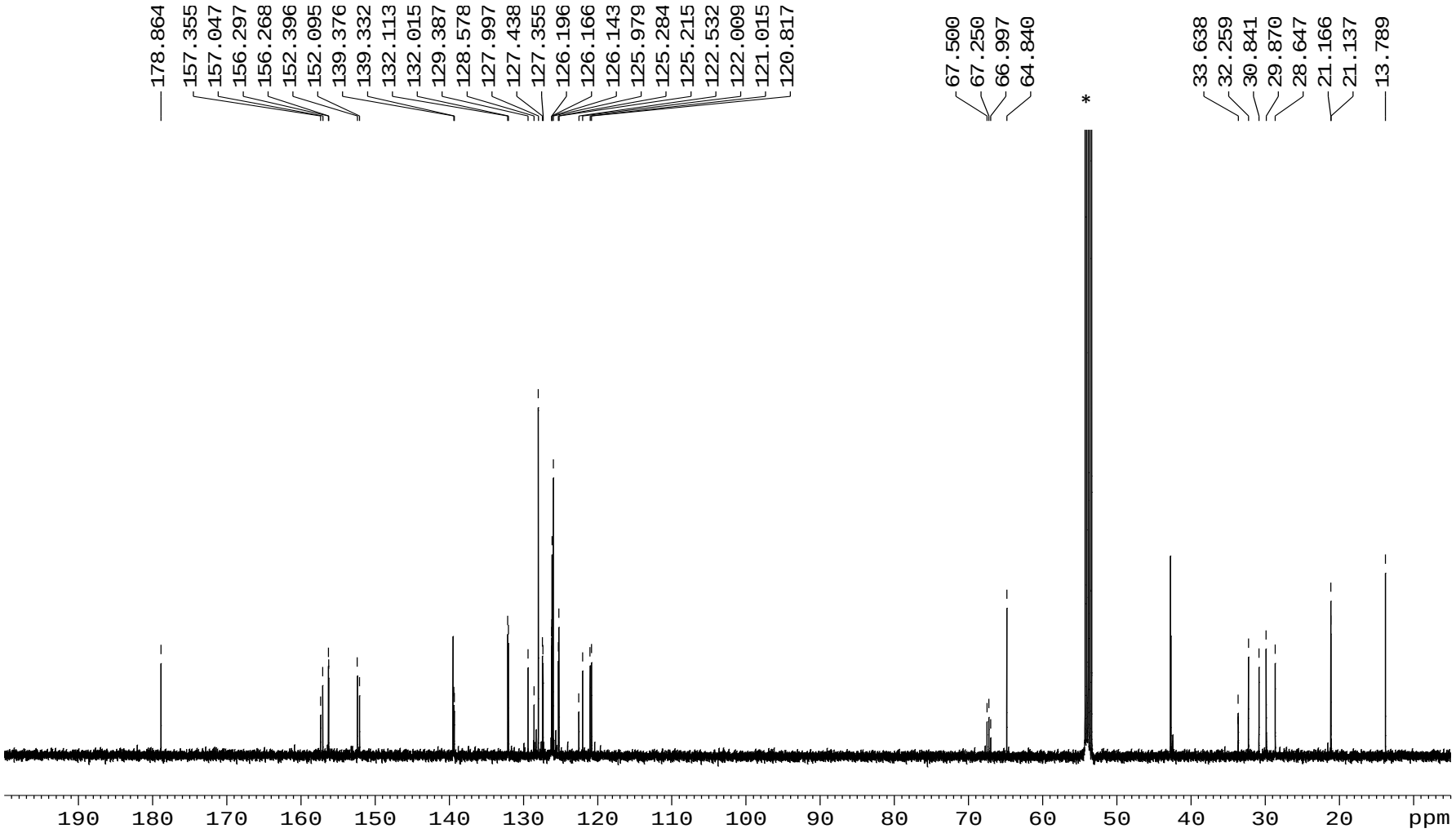


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, CD_2Cl_2, 298 K) of {$ONO^{Me,Cumyl}$}Al((*rac*)-$OCH(CF_3)CH_2COOEt$) (**7**) (*stands for residual solvent resonances).

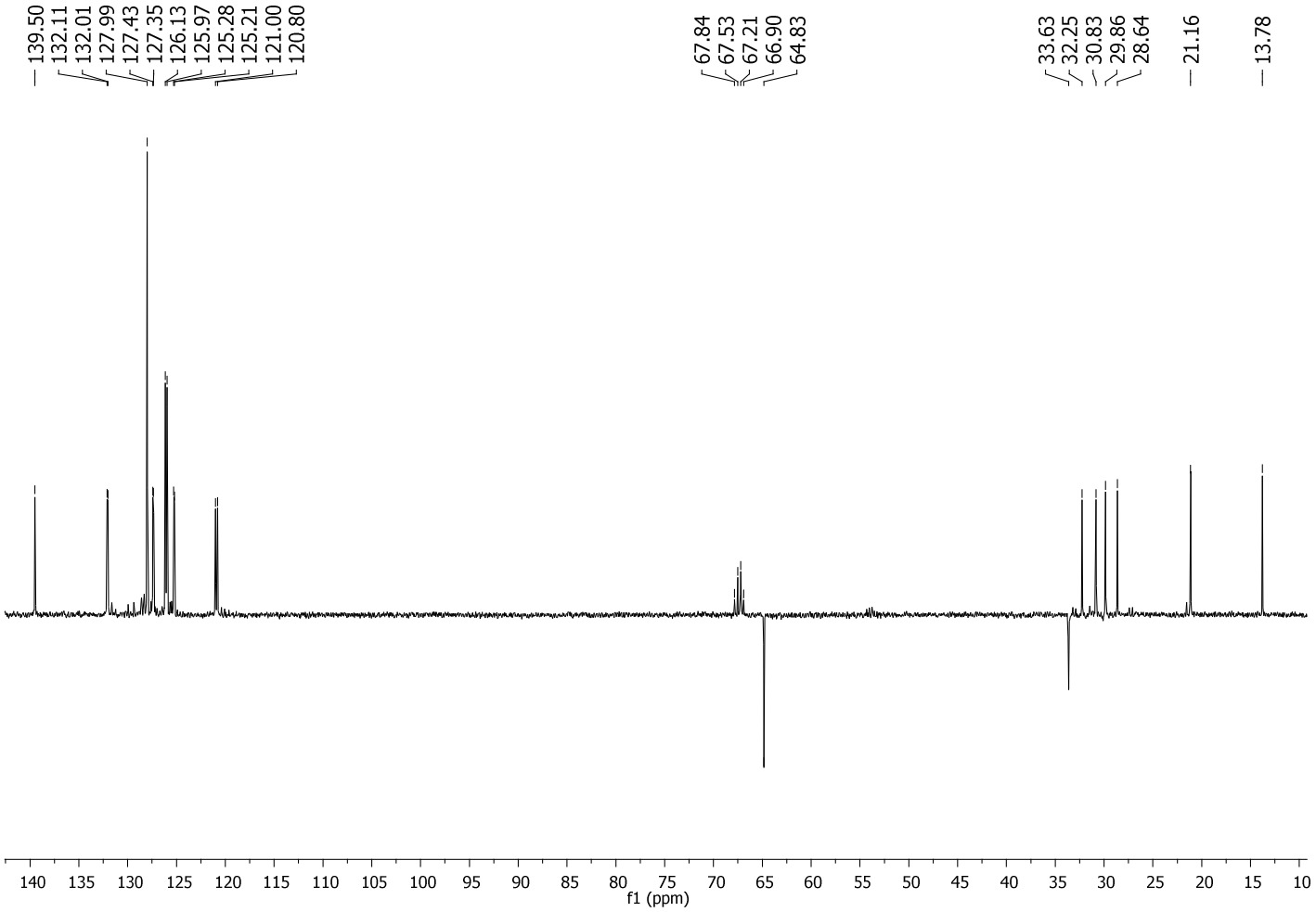


Figure S23bis. DEPT 135 NMR spectrum (125 MHz, CD_2Cl_2, 298 K) of {$ONO^{Me,Cumyl}$}Al((*rac*)-$OCH(CF_3)CH_2COOEt$) (**7**).

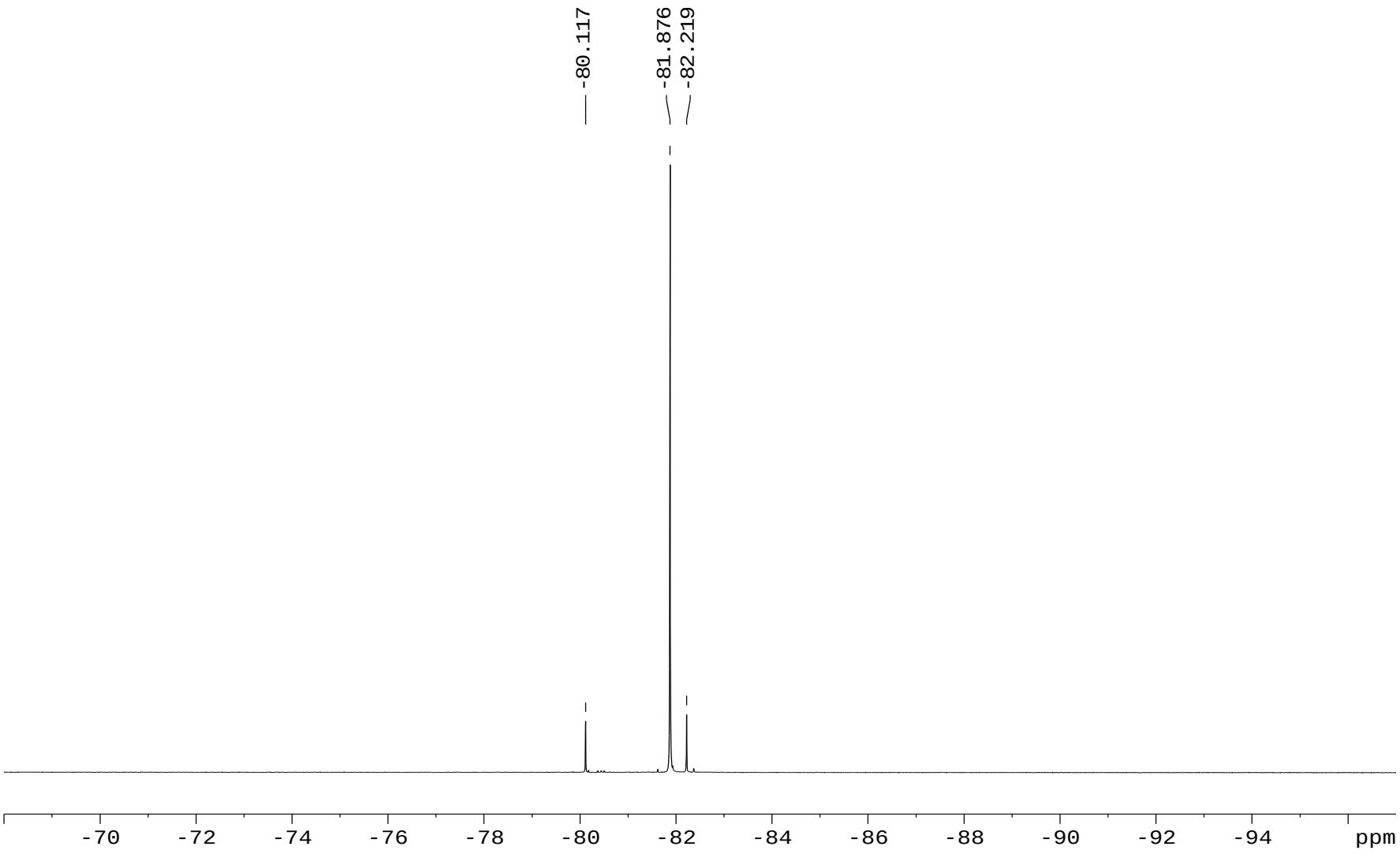


Figure S24. $^{19}F\{^{1}H\}$NMR spectrum (185 MHz, CD_2Cl_2, 298 K) of {$ONO^{Me,Cumyl}$}Al((*rac*)-$OCH(CF_3)CH_2COOEt$) (**7**).

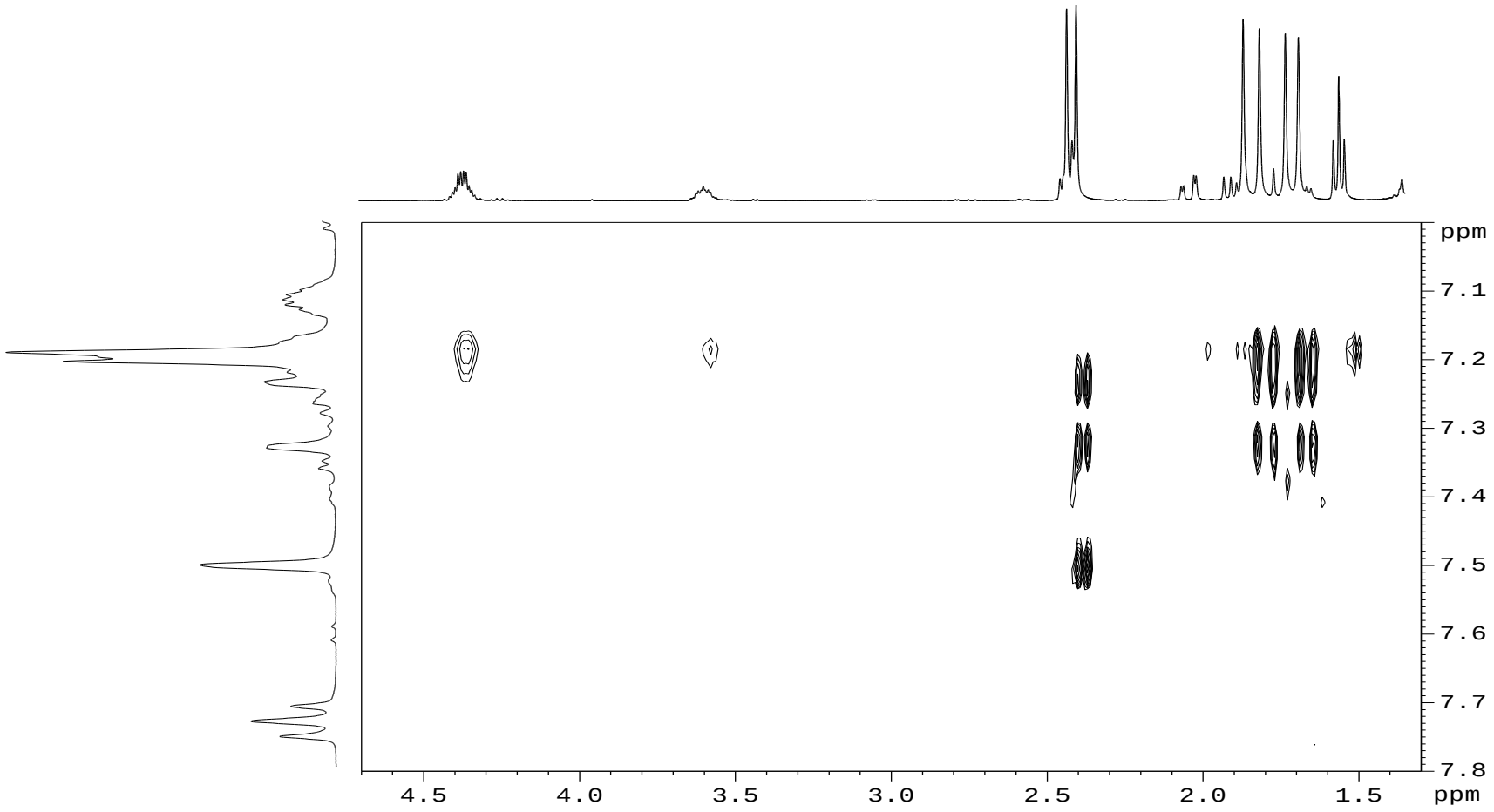


Figure S25. $^{1}H–^{1}H$ NOESY NMR spectrum (400 MHz, CD_2Cl_2, 298 K) of {$ONO^{Me,Cumyl}$}Al((*rac*)-$OCH(CF_3)CH_2COOEt$) (**7**).

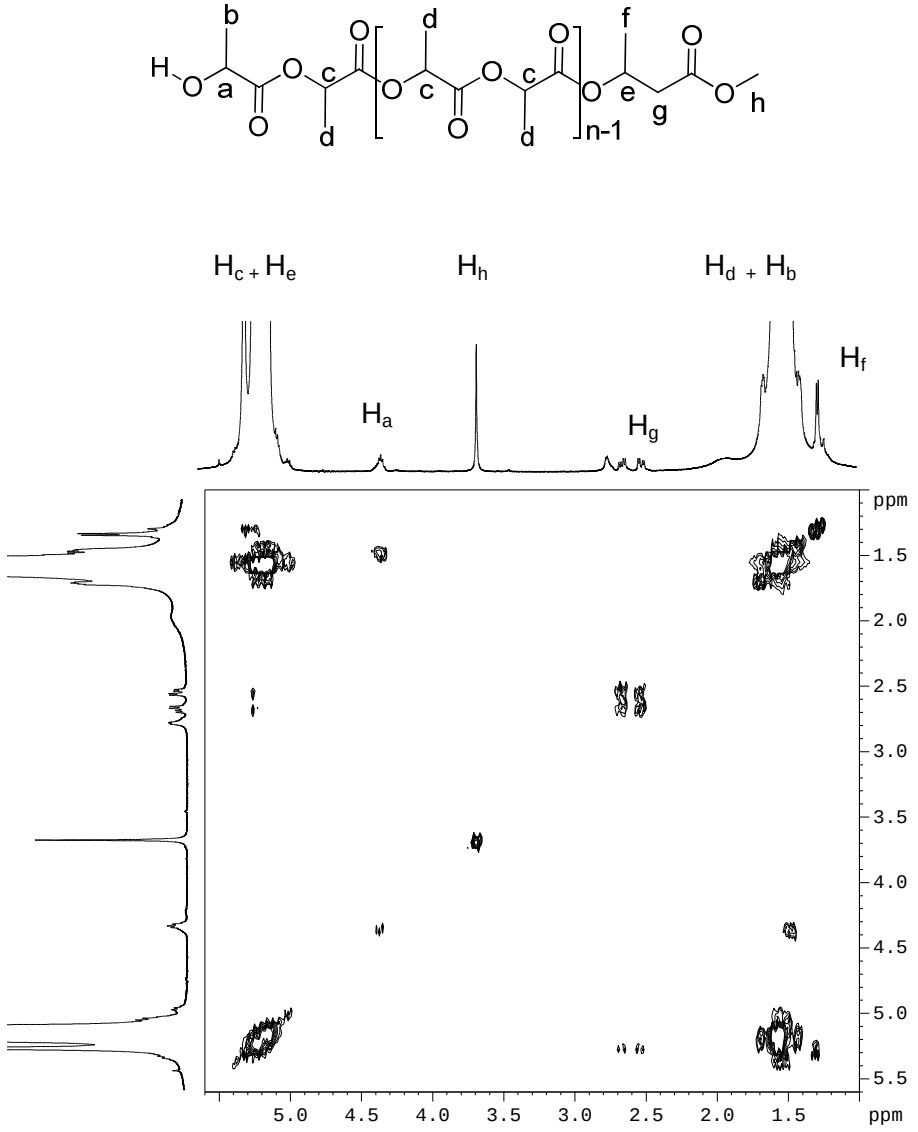


Figure S26. $^{1}H–^{1}H$ COSY NMR spectrum (500 MHz, $CDCl_3$, 298 K) of a PLA produced from {$ONO^{Me,Cumyl}$}Y((*R*)-$OCH(CH_3)CH_2COOMe$) (**2**) (Table 1, entry 10).

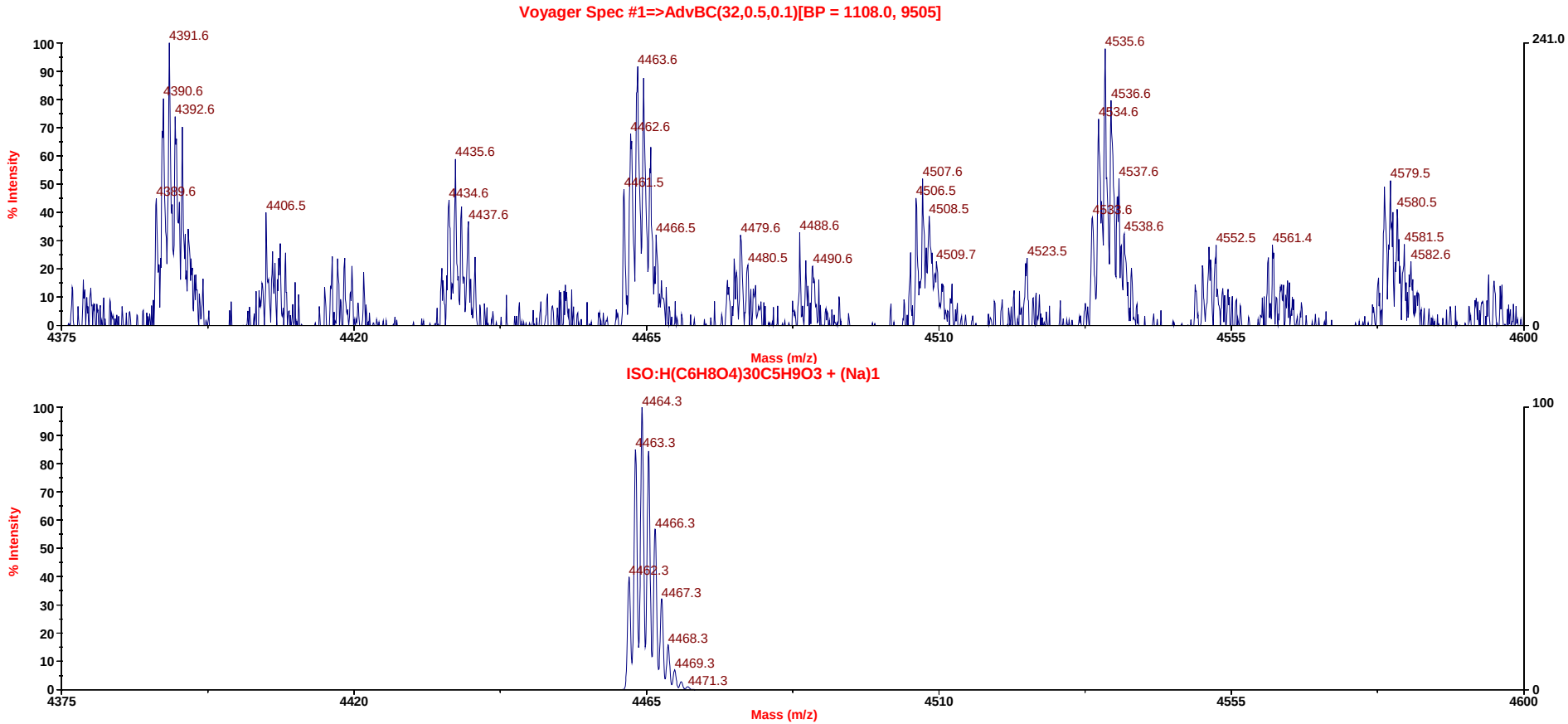


Figure S27. Detail of the MALDI-ToF mass spectrum of a PLA sample produced from **2** using IAA as matrix (Table 1, entry 10). Top: experimental spectrum; the observed two distributions at *m/z* = 4463 and 4479 Da correspond to $MeOC(O)CH_2CH(CH_3)O–(LA)_n–H$ macromolecules ionized by Na^+ and K^+. Bottom: calculated isotopic distribution for macromolecules ionized with Na^+.

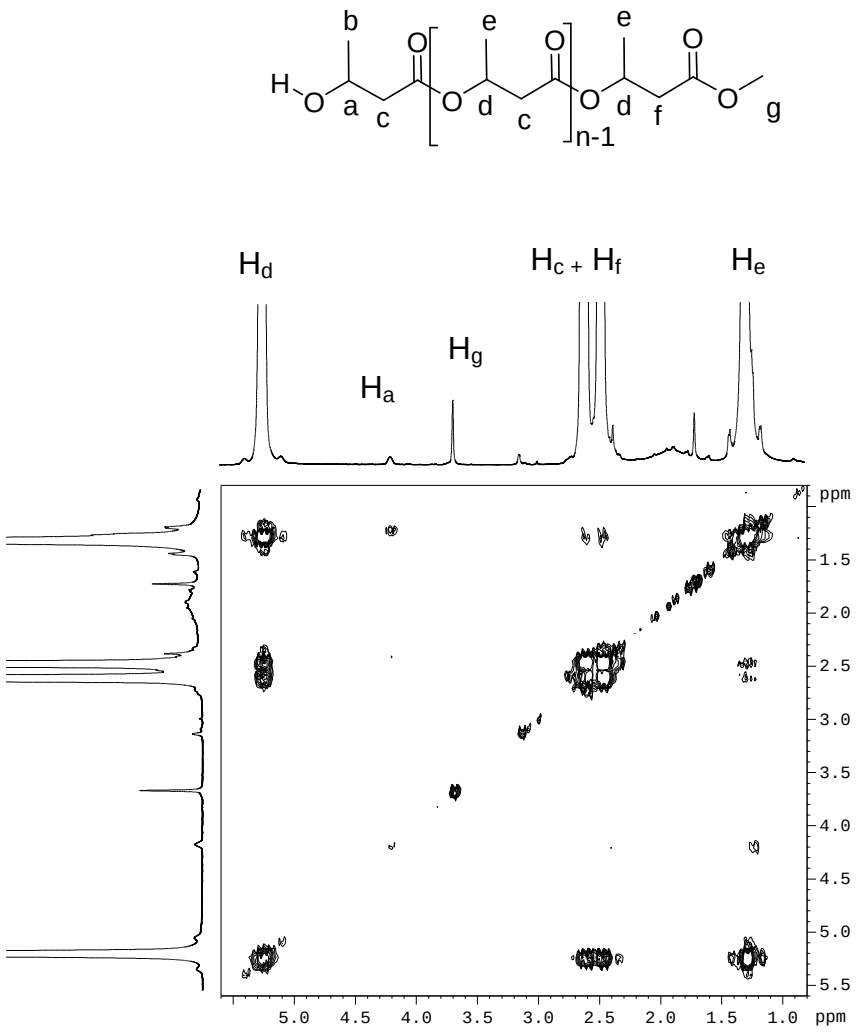


Figure S28. $^{1}H–^{1}H$ COSY NMR spectrum (500 MHz, $CDCl_3$, 298 K) of a PHB produced from {$ONO^{Me,Cumyl}$}Y((*R*)-$OCH(CH_3)CH_2COOMe$) (**2**) (Table 1, entry 21).

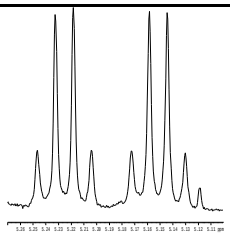
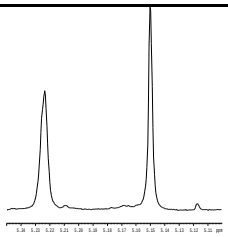
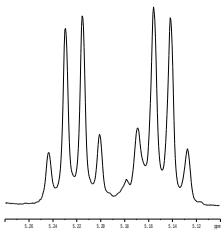
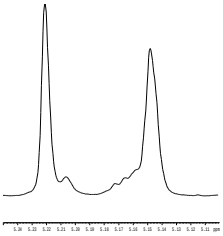
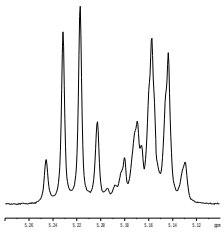
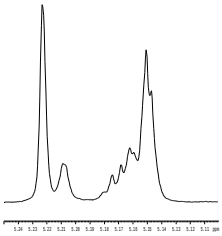
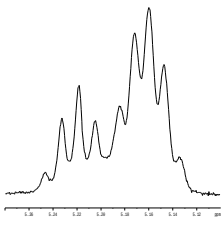
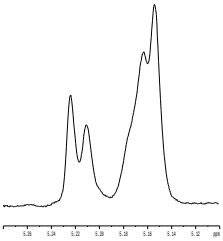
Table 1, Experiment	^{1}H NMR	^{1}H{^{1}H} NMR	P_r
5			0.96
11			0.88
4			0.77
9			0.55

Figure S29. Methine region of ^{1}H NMR and ^{1}H homo-decoupled NMR spectra of different PLAs.

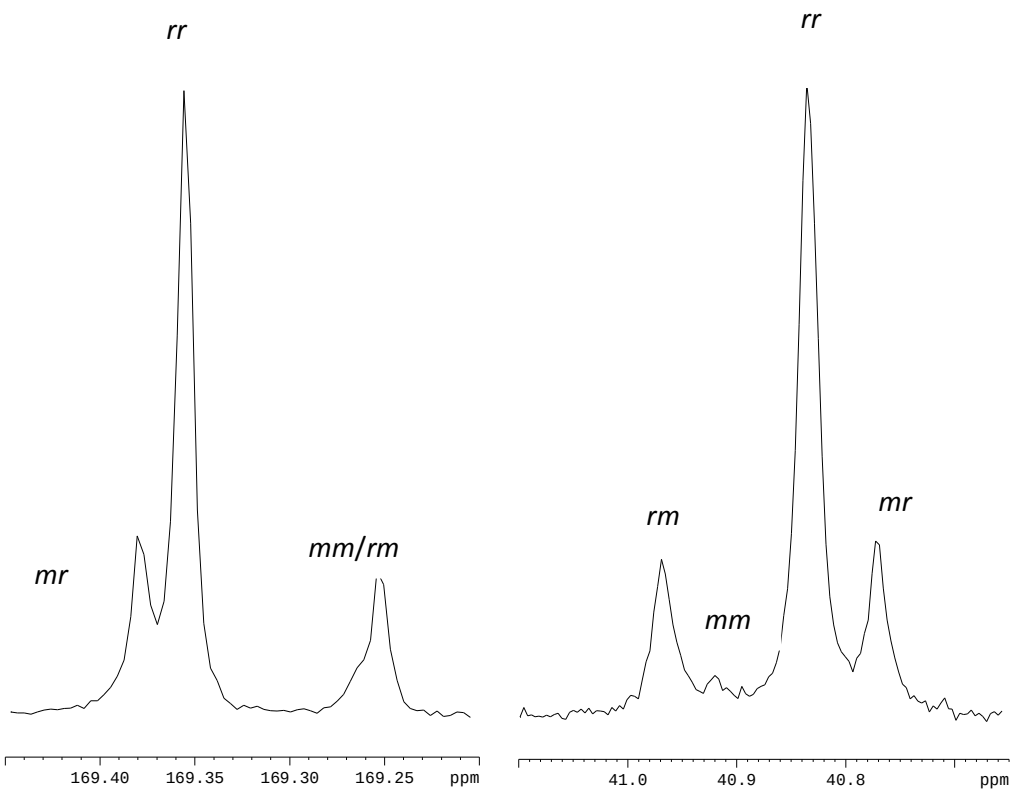


Figure S30. Carbonyl (left) and methylene (right) regions of the $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$, 298 K) of a PHB produced from {$ONO^{Me,Cumyl}$}Y((*R*)-$OCH(CH_3)CH_2COOMe$) (**2**) (Table 1, entry 21).

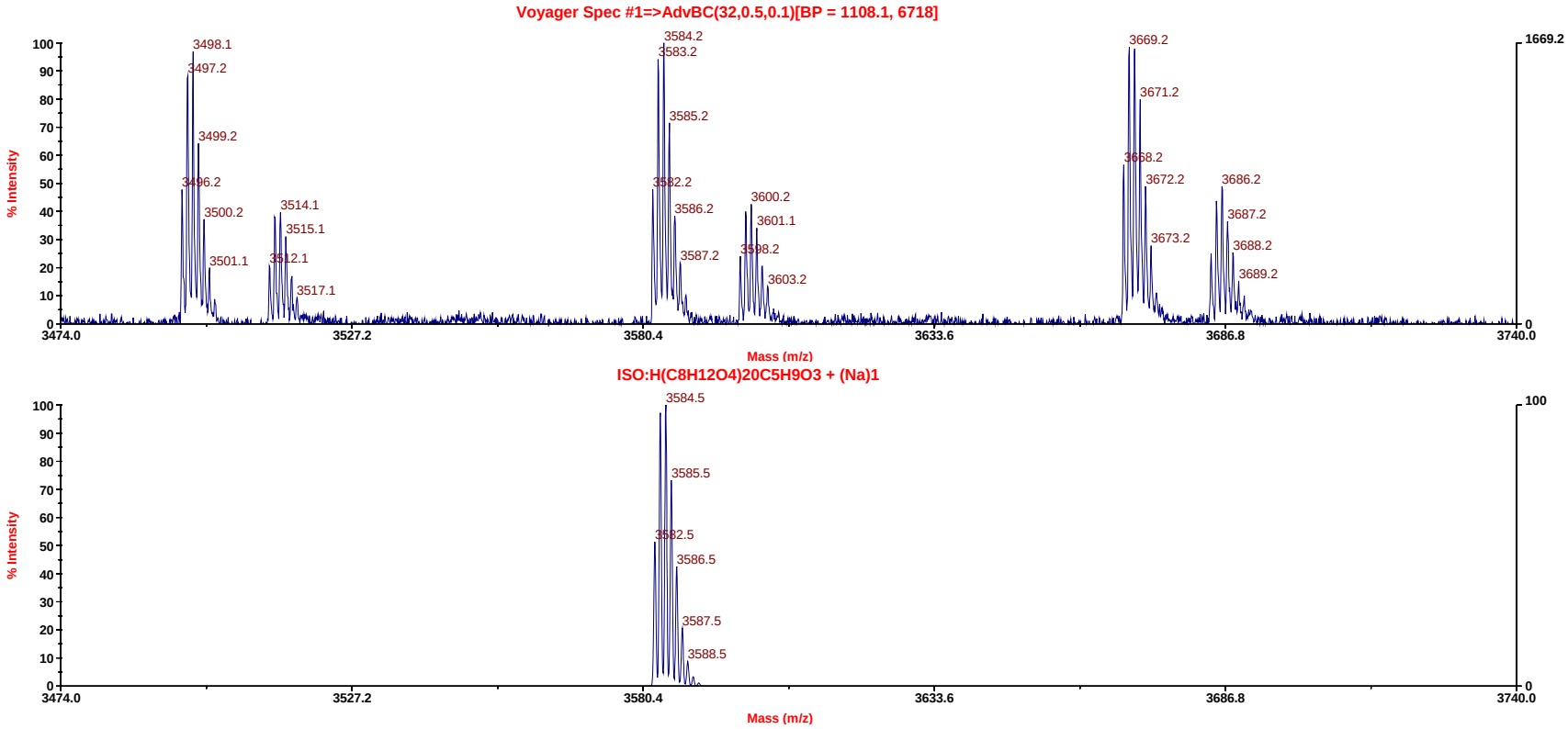


Figure S31. Detail of the MALDI-ToF mass spectrum of a PHB sample produced from **2** using IAA as matrix (Table 1, entry 20). Top: experimental spectrum; the observed two distributions correspond to $MeOC(O)CH_2CH(CH_3)O–(BBL)_n–H$ macromolecules ionized by Na^+ and K^+. Bottom: calculated isotopic distribution for macromolecules ionized with Na^+.

Table S1. Summary of crystal and refinement data for $\{ONO^{Me,Cumyl}\}H_2$**, 1** and **6**.

	$\{ONO^{Me,Cumyl}\}H_2$	**1**	**6**
Empirical formula	$C_{37}H_{37}NO_2$	$C_{49}H_{67}N_2O_4Si_2Y$	$C_{84}H_{88}Al_2N_2O_{10}$
Formula weight	527.68	893.14	1339.52
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	*P 2₁/n*	*P 2₁/n*	P *–1*
a, Å	13.1098(12)	12.896(2)	15.8935(5)
b, Å	8.0072(7)	25.405(3)	16.9816(4)
c, Å	27.619(3)	15.536(2)	18.2728(6)
α (°)	90	90	107.2690(10)
β (°)	90.292(4)	110.122(5)	107.1600(10)
γ (°)	90	90	114.6260(10)
Volume, $Å^3$	2899.2(5)	4779.3(11)	3750.09(19)
Z	4	4	2
Density, $g.m^{-3}$	1.209	1.241	1.186
m, mm^{-1}	0.074	1.314	0.098
F(000)	1128	1896	1424
Crystal size, mm	0.57 × 0.08 × 0.05	0.55 × 0.46 × 0.38	0.6 × 0.3 × 0.23
θ range, deg	2.94 to 27.48	2.94 to 27.48	1.33 to 27.52
Limiting indices	$-16 \le h \le 16$, $-9 \le k \le 10$, $-35 \le l \le 35$	$-16 \le h \le 16$, $-27 \le k \le 32$, $-30 \le l \le 20$	$-20 \le h \le 17$, $-20 \le k \le 22$, $-23 \le l \le 23$
Reflec. Collected	26552	42223	42735
R_{int}	0.07	0.0531	0.044
Unique Refl [I>2σ(I)]	6546	10851	17008
Data/restrains/ param.	6546 / 0 / 369	10851 / 0 / 512	17008 / 0 / 913
Goodness-of-it on F^2	1.012	1.022	1.061
R_1 [I>2σ(I)] (all data)	0.0546 (0.12)	0.0518 (0.0742)	0.078 (0.119)
wR_2 [I>2σ(I)] (all data)	0.1113 (0.144)	0.1261 (0.136)	0.2223 (0.2412)
Largest diff. $e.A^{-3}$	0.255 and –0.243	1.397 and –0.993	0.512 and –0.450

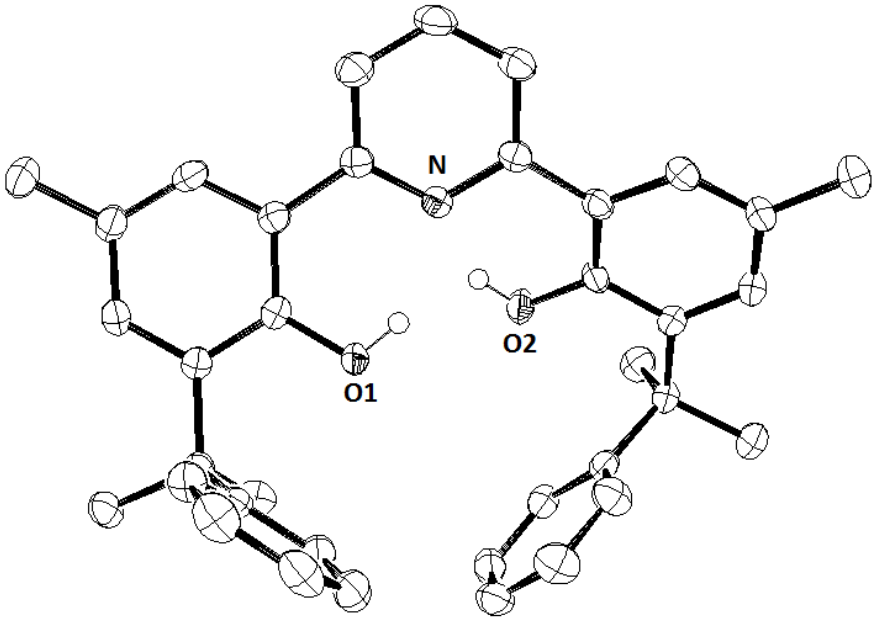


Figure S32. Molecular structure of proligand {ONO^{Me,Cumyl}}H_2 (all hydrogens atoms, except those of the hydroxyl groups, are omitted for clarity; thermal ellipsoids drawn at 50% probability). Selected bond distances (Å) and angles (deg): H(O(1))–N = 1.919; H(O(2))–N = 1.985; ∠Pyr–Ph(1) = 23.55; ∠Pyr–Ph(2) = 23.21.

Computational Details

The geometry optimizations have been performed with the program package TURBOMOLE using density functional theory (DFT).[1] The gradient corrected density functional BP86 in combination with the resolution identity approximation (RI)[2] was applied for the geometry optimizations of stationary points. A triple-ξ zeta valence quality basis set def2-TZVP[3] was used for all atoms. In the calculations have been included solvation effects using COSMO model implemented in the TURBOMOLE program package.[4] The default optimized atomic COSMO radii and the corresponding parameters for solvent toluene (ε = 2.38, radius = 3.48 Å) have been used.

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[1] (a) Ahlrichs, R.; Bar, M.; Haser, M.; Horn, H.; Kolmel, C. *Chem.Phys. Lett.* **1989**, *162*, 165. (b) Treutler, O.; Ahlrichs, R. *J. Chem. Phys.* **1995**, *102*, 346. (c) Eichkorn, K.; Treutler, O.; Ohm, H.; Haser, M.; Ahlrichs, R. *Chem. Phys. Lett.* **1995**, *242*, 652. (d) TURBOMOLE V6.2 2010, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.

[2] (a) Sierka, M.; Hogekamp, A.; Ahlrichs, R. *J. Chem. Phys.* **2003**, *118*, 9136. (b) Deglmann, P.; May, K.; Furche, F.; Ahlrichs, R. *Chem. Phys. Letters* **2004**, *384*, 103.

[3] Weigend, F.; Ahlrichs. R. *Phys. Chem. Chem. Phys.* **2005**, 7, 3297.

[4] (a) Klamt, A.; Eckert, F. *Fluid Phase Equilibria* **2000**, 172, 43. (b) Schafer, A.; Klamt, A.; Sattel, D.; Lohrenz, J. C.; Eckert, F. *Phys. Chem. Chem.Phys.* **2000**, *2*, 2187.

Cartesian coordinates for stationary points

2-I

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Energy = -2097.356473883

Y	0.9827209	-10.7511209	11.6754176
N	-0.0285550	-9.6738647	9.7334433
O	2.7071417	-9.8359767	10.7904770
O	1.8141504	-11.8892817	13.5904832
O	-0.4695819	-9.4695831	12.6263954
O	0.5552253	-12.7221000	11.1730372
O	2.3283733	-13.6349986	14.9014887
C	0.7894324	-14.0032800	11.6628549
H	1.8130599	-14.3375029	11.3853424
C	0.7036653	-14.0281105	13.2196482
H	0.8631761	-15.0394981	13.6154672
H	-0.3147072	-13.7067706	13.4985022
C	1.6518883	-13.0814349	13.8955605
C	3.2259308	-12.7569583	15.6376450
H	4.0036360	-12.3737105	14.9672684
H	3.6576512	-13.3863295	16.4206489
H	2.6552004	-11.9266378	16.0696811
C	-2.0731248	-11.5739340	15.2920934
H	-2.8942386	-11.7512261	14.5945297
C	-1.5257861	-12.6476629	15.9975094
H	-1.9262606	-13.6526099	15.8497237
C	-0.4797975	-12.4368282	16.9017577
H	-0.0582134	-13.2717617	17.4634311
C	0.0140137	-11.1421650	17.0768433
H	0.8265807	-10.9567977	17.7824754
C	-0.5374321	-10.0703256	16.3667215
H	-0.1346358	-9.0707023	16.5283210
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C	-2.3475916	-9.0866920	14.8155775
C	-3.5857837	-8.8378281	15.7166141
H	-4.2246028	-9.7269234	15.8053773
H	-4.1925437	-8.0036713	15.3341757
H	-3.2436239	-8.5762178	16.7276643
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H	-1.3355892	-7.4364299	15.8535358
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H	-0.5803946	-7.8837390	14.2940935
C	-2.7570075	-9.4097751	13.3635868
C	-4.0953440	-9.5897652	13.0134544
H	-4.8552603	-9.5702318	13.7957473
C	-4.5273119	-9.8024431	11.6918810
C	-5.9763938	-10.0909386	11.3856364
H	-6.1887389	-9.9728029	10.3141350
H	-6.6486597	-9.4190093	11.9402333
H	-6.2512862	-11.1214844	11.6638080
C	-3.5689596	-9.7246129	10.6897508
H	-3.8797215	-9.8340487	9.6481343
C	-2.1997846	-9.5291721	10.9688039
C	-1.7630949	-9.4849441	12.3311577
C	-1.3121405	-9.2127985	9.8209970
C	-1.8469603	-8.3853293	8.8153105
H	-2.8535272	-7.9894733	8.9309186
C	-1.0678757	-8.0321313	7.7222654

H	-1.4600653	-7.3611226	6.9562983
C	0.2301833	-8.5160619	7.6367207
H	0.8767262	-8.2216746	6.8131863
C	0.7377824	-9.3564924	8.6464231
C	2.1209200	-9.8665852	8.4652241
C	2.5232767	-10.1568699	7.1437835
H	1.7675200	-10.1576775	6.3554015
C	3.8355146	-10.4688766	6.8154291
C	4.2363481	-10.8415994	5.4090886
H	3.4278231	-10.6314652	4.6955950
H	4.4781888	-11.9137287	5.3277949
H	5.1284563	-10.2861487	5.0820361
C	4.7855509	-10.4260765	7.8504555
H	5.8262224	-10.6185439	7.5876899
C	4.4591130	-10.1696007	9.1822642
C	3.0805392	-9.9630170	9.5225844
C	5.5533173	-10.0938386	10.2654874
C	5.4458357	-8.7336455	11.0003260
H	4.5049693	-8.6498461	11.5534229
H	5.4897461	-7.9207688	10.2612900
H	6.2869609	-8.5888951	11.6927363
C	6.9746784	-10.1451818	9.6448989
H	7.7184634	-10.0403262	10.4467137
H	7.1253540	-9.3227299	8.9299190
H	7.1734352	-11.0978473	9.1350740
C	5.4878960	-11.2973526	11.2268127
C	6.0861370	-11.2452830	12.4970710
H	6.5044424	-10.3075190	12.8641881
C	6.1812466	-12.3835680	13.3024618
H	6.6706814	-12.3136835	14.2761986
C	5.6682267	-13.6068737	12.8615689
H	5.7492548	-14.4986840	13.4850791
C	5.0531376	-13.6714120	11.6088641
H	4.6475284	-14.6180701	11.2467107
C	4.9681418	-12.5315698	10.8042890
H	4.4974204	-12.6021954	9.8224688
C	-0.2088143	-15.0109038	11.0829736
H	-0.0063664	-16.0349802	11.4321115
H	-0.1426511	-14.9954278	9.9868180
H	-1.2350077	-14.7339093	11.3675075

2-II

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Energy = -2097.356995094

Y	0.3540211	-2.0558538	8.5042054
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O	0.7937327	-3.3630313	6.8692681
O	0.1670266	-0.0065147	8.1493584
O	2.5495781	-1.2649090	9.1026515
O	4.1774218	0.2772797	9.2364246
C	2.8915682	-0.0789431	9.2458886
C	5.1508692	-0.7901317	9.0565629
H	5.0466691	-1.5322246	9.8564937
H	6.1246382	-0.2961515	9.1049826
H	5.0045055	-1.2711449	8.0826278
C	-0.4416665	-4.8506599	13.1801104
H	-1.5072910	-4.6510024	13.3097063

C	0.0060978	-6.1712670	13.1245332	C	-1.3947850	-2.4676433	10.9955513
H	-0.7104677	-6.9895708	13.2183528	C	-2.8245651	-2.9466578	8.9165354
C	1.3649416	-6.4467464	12.9445930	C	-4.0176690	-3.6465362	8.6575241
H	1.7184755	-7.4778983	12.8958047	H	-4.7212200	-3.8188806	9.4691807
C	2.2625254	-5.3846265	12.8225556	C	-4.2635792	-4.1516113	7.3876309
H	3.3262348	-5.5822615	12.6762394	H	-5.1724391	-4.7208343	7.1857687
C	1.8074747	-4.0631701	12.8785952	C	-3.3236533	-3.9484858	6.3856585
H	2.5309696	-3.2549850	12.7708751	H	-3.4749584	-4.3596677	5.3898670
C	0.4476834	-3.7707679	13.0535743	C	-2.1368628	-3.2479027	6.6687982
C	-0.0831598	-2.3315702	13.2053893	C	-1.1825890	-3.0383790	5.5494559
C	-0.3137772	-2.1160285	14.7220179	C	-1.7306971	-2.7733306	4.2759725
H	0.6260396	-2.3087361	15.2581257	H	-2.8045033	-2.5884318	4.1969100
H	-1.0743670	-2.7999313	15.1229232	C	-0.9506392	-2.7097749	3.1281233
H	-0.6203315	-1.0824232	14.9413902	C	-1.5437431	-2.3639007	1.7840882
C	0.9434303	-1.2666537	12.7564062	H	-1.2313718	-1.3613515	1.4495183
H	1.8383877	-1.2803499	13.3960970	H	-2.6417489	-2.3720909	1.8191680
H	0.4906593	-0.2686578	12.8417611	H	-1.2253296	-3.0747025	1.0063556
H	1.2544804	-1.4267914	11.7175062	C	0.4235177	-2.9803051	3.2623432
C	-1.3819965	-2.1526038	12.3938781	H	1.0310830	-2.9818374	2.3560000
C	-2.5501451	-1.6723287	12.9829198	C	1.0331776	-3.2368264	4.4889577
H	-2.5426664	-1.4098778	14.0420219	C	0.2317803	-3.2036047	5.6768761
C	-3.7531996	-1.4986644	12.2744711	C	2.5418480	-3.5375899	4.5936190
C	-4.9664014	-0.9005833	12.9440335	C	3.2510382	-2.3427875	5.2717722
H	-4.8336390	0.1767388	13.1347977	H	2.9310199	-2.2248829	6.3136285
H	-5.1674519	-1.3757352	13.9163041	H	3.0117258	-1.4201971	4.7248371
H	-5.8633233	-1.0164441	12.3203131	H	4.3440899	-2.4673182	5.2502635
C	-3.7752487	-1.8951005	10.9432113	C	3.1953751	-3.7088603	3.1994338
H	-4.7025072	-1.7887939	10.3754981	H	4.2533599	-3.9761925	3.3300508
C	-2.6337899	-2.4019648	10.2852598	H	3.1533193	-2.7767751	2.6164312

H	2.7175270	-4.5085996	2.6171099
C	2.7692795	-4.8678090	5.3387734
C	3.7811338	-5.0392689	6.2935315
H	4.4004288	-4.1930871	6.5910589
C	4.0087805	-6.2823611	6.8929484
H	4.7979339	-6.3836428	7.6405386
C	3.2289140	-7.3869523	6.5462571
H	3.4023046	-8.3559818	7.0169331
C	2.2188932	-7.2333618	5.5918529
H	1.5970482	-8.0856241	5.3110037
C	1.9970471	-5.9904558	4.9972697
H	1.1972900	-5.8833359	4.2617285
C	0.8913110	1.1730937	8.2704888
H	0.2224703	2.0009606	8.5847563
C	1.9437288	1.0651849	9.4311274
H	2.5053849	2.0006050	9.5456578
H	1.3818747	0.8780498	10.3594735
C	1.5507424	1.5761609	6.9462304
H	2.0839137	2.5350689	7.0327341
H	0.7785791	1.6762972	6.1718427
H	2.2633371	0.8070134	6.6103929

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Energy = -2301.411647702

Al	0.6953634	-10.8487739	11.2744170
N	-0.1696311	-10.0054909	9.6566144
O	2.2952849	-10.1651391	10.8361823
O	1.5936931	-11.5499800	12.9436758
O	-0.3481446	-9.8980788	12.3807904
O	0.2504495	-12.4658778	10.7486107
O	2.1663195	-13.0884656	14.4656567
C	0.7013315	-13.7088974	11.2142993
H	1.7557738	-13.8730924	10.9031997
C	0.6635482	-13.7800634	12.7607327
H	0.9811848	-14.7599834	13.1404462
H	-0.3759171	-13.6080808	13.0908287
C	1.5023994	-12.7073664	13.3812947
C	2.9690692	-12.0678525	15.1257691
H	3.7472066	-11.7095215	14.4430288
H	3.4093429	-12.5725828	15.9898259
H	2.3233352	-11.2407405	15.4412760
C	-1.9968668	-11.6795048	15.0861932
H	-2.7491479	-11.6912002	14.2961864
C	-1.6948244	-12.8641203	15.7643565
H	-2.2132943	-13.7866487	15.4953922
C	-0.7430944	-12.8694645	16.7869612
H	-0.5088962	-13.7914628	17.3210741
C	-0.0962789	-11.6757681	17.1164189
H	0.6476725	-11.6596629	17.9153092
C	-0.3992796	-10.4945723	16.4326604
H	0.1153798	-9.5763314	16.7178820
C	-1.3589872	-10.4700882	15.4065393
C	-1.8162619	-9.1397625	14.7747482
C	-2.8436902	-8.5442776	15.7754671
H	-3.6729136	-9.2328899	15.9863915
H	-3.2568302	-7.5956755	15.4014723
H	-2.3356068	-8.3441173	16.7287591

C	-0.6694561	-8.1034305	14.6661139	H	3.8092965	-10.9329374	4.8957258
H	-0.3146885	-7.8050600	15.6625038	H	5.0050614	-11.9690009	5.6995223
H	-1.0472403	-7.1967123	14.1719334	H	5.3633351	-10.2566988	5.4319627
H	0.1723786	-8.4898353	14.0841826	C	4.7545522	-10.4220847	8.1670306
C	-2.4509029	-9.3602003	13.3853164	H	5.8345872	-10.4668916	8.0266153
C	-3.8329907	-9.2820044	13.2167405	C	4.2487095	-10.2007139	9.4486910
H	-4.4614987	-9.0925488	14.0870541	C	2.8248035	-10.2031935	9.6164637
C	-4.4763131	-9.4652166	11.9790709	C	5.2102821	-9.9789601	10.6364776
C	-5.9822992	-9.4724867	11.8846860	C	4.7583432	-8.7456740	11.4613155
H	-6.3156526	-9.4849296	10.8380448	H	3.7919027	-8.9148830	11.9437298
H	-6.4216758	-8.5865402	12.3680991	H	4.6685339	-7.8748663	10.7954460
H	-6.4141690	-10.3561002	12.3812088	H	5.5057455	-8.4960475	12.2270517
C	-3.6722689	-9.6292638	10.8622655	C	6.6460622	-9.6610114	10.1360378
H	-4.1502927	-9.7494868	9.8889541	H	7.2808750	-9.4165004	10.9982946
C	-2.2624547	-9.6702384	10.9472780	H	6.6438943	-8.7952126	9.4575714
C	-1.6477643	-9.6586499	12.2356290	H	7.1112064	-10.5125211	9.6214707
C	-1.4767984	-9.5957810	9.7012044	C	5.3429580	-11.2416793	11.5134304
C	-2.0751751	-9.0265790	8.5613126	C	6.0227089	-11.1826452	12.7436091
H	-3.0916005	-8.6477661	8.6185414	H	6.3760939	-10.2231965	13.1243571
C	-1.3475570	-8.8871101	7.3893964	C	6.2764064	-12.3347435	13.4920808
H	-1.8001309	-8.4232859	6.5116226	H	6.8156967	-12.2547971	14.4380389
C	-0.0224457	-9.2953258	7.3617258	C	5.8462218	-13.5834029	13.0334373
H	0.5819304	-9.1285531	6.4744230	H	6.0453554	-14.4851565	13.6144546
C	0.5639791	-9.8633659	8.5074476	C	5.1594293	-13.6586694	11.8200308
C	1.9920576	-10.2295848	8.4563628	H	4.8165410	-14.6250093	11.4451837
C	2.5761718	-10.4934635	7.1981906	C	4.9152035	-12.5025503	11.0712949
H	1.9297031	-10.6200976	6.3282531	H	4.3895373	-12.5828414	10.1191680
C	3.9465018	-10.6237869	7.0337759	C	-0.1479980	-14.8300029	10.6155379
C	4.5601407	-10.9610265	5.6970547	H	0.2103137	-15.8215720	10.9306580

H	-0.1059065	-14.7751703	9.5196201
H	-1.1979561	-14.7171192	10.9245307

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Energy = -2301.410479498

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O	0.6899573	-2.8666511	7.0723067
O	-0.4655085	-0.1505659	7.9807588
O	1.8893713	-1.2641458	8.8134203
O	3.4997088	0.2008448	9.3597909
C	2.2283051	-0.1065530	9.1047539
C	4.4614151	-0.8918936	9.3146237
H	4.1403099	-1.7035277	9.9770786
H	5.4035865	-0.4534748	9.6535948
H	4.5511257	-1.2657969	8.2883640
C	-0.2083351	-4.9819629	12.4797345
H	-1.2526529	-4.7486267	12.6962820
C	0.1584744	-6.3032807	12.2199523
H	-0.5997495	-7.0884672	12.2387089
C	1.4889324	-6.6203755	11.9323703
H	1.7785383	-7.6511742	11.7231511
C	2.4401786	-5.5994824	11.9071757
H	3.4820896	-5.8288983	11.6768343
C	2.0663328	-4.2771765	12.1663295
H	2.8301237	-3.5003427	12.1335559
C	0.7362833	-3.9425626	12.4554018
C	0.3072893	-2.5144035	12.8479525
C	0.2344548	-2.5035553	14.3957482
H	1.2122715	-2.8012147	14.7992985
H	-0.5135421	-3.2111372	14.7788809
H	0.0015744	-1.5000835	14.7827174
C	1.3492780	-1.4471992	12.4450611
H	2.2889932	-1.5807781	13.0008910
H	0.9614795	-0.4482954	12.6911953
H	1.5586116	-1.4947332	11.3718923
C	-1.0533074	-2.1759302	12.2057203
C	-2.1446668	-1.7983850	12.9858307
H	-2.0197354	-1.7150784	14.0660880
C	-3.4122741	-1.5019615	12.4504814
C	-4.5283986	-1.0061408	13.3366191
H	-4.3365103	0.0188417	13.6928159
H	-4.6469188	-1.6388033	14.2293976
H	-5.4875911	-0.9954696	12.8012315
C	-3.5896317	-1.6918522	11.0884317
H	-4.5715685	-1.4944550	10.6546222
C	-2.5358308	-2.1020335	10.2415520
C	-1.2242938	-2.2388986	10.7846716
C	-2.8521968	-2.4864654	8.8535130
C	-4.1463819	-2.9484157	8.5536312
H	-4.8833798	-3.0357485	9.3474898
C	-4.4569299	-3.3503545	7.2623264
H	-5.4505333	-3.7367443	7.0299336
C	-3.4795797	-3.2956273	6.2790307
H	-3.6908032	-3.6570930	5.2762072
C	-2.1906236	-2.8280572	6.5934495
C	-1.1616928	-2.8011806	5.5376507

C	-1.5774601	-2.7285333	4.1889266	C	2.7129416	-4.7720593	5.9667251
H	-2.6262002	-2.5228914	3.9677078	C	3.6461704	-4.8606115	7.0083771
C	-0.6922700	-2.8782006	3.1322848	H	4.2803632	-4.0069674	7.2464425
C	-1.1382766	-2.7485153	1.6965149	C	3.7759458	-6.0281919	7.7668736
H	-0.7003174	-1.8592032	1.2157010	H	4.5063097	-6.0652118	8.5771565
H	-2.2308178	-2.6591229	1.6253985	C	2.9723584	-7.1374615	7.4993503
H	-0.8315481	-3.6198358	1.0977692	H	3.0684456	-8.0464041	8.0950227
C	0.6496782	-3.1649892	3.4464498	C	2.0357838	-7.0649654	6.4643614
H	1.3372974	-3.3403062	2.6182160	H	1.3946348	-7.9209058	6.2448998
C	1.1347436	-3.2176663	4.7514396	C	1.9125261	-5.8976061	5.7094709
C	0.2273204	-2.9466621	5.8263071	H	1.1721296	-5.8535252	4.9082822
C	2.6134271	-3.5427274	5.0415885	C	0.2677540	1.0391086	8.0198919
C	3.3059041	-2.2916413	5.6272630	H	-0.4284977	1.8734075	8.2325561
H	2.8876750	-2.0309729	6.6051117	C	1.2808525	1.0447892	9.1999708
H	3.1620029	-1.4438534	4.9422996	H	1.8369717	1.9885139	9.2662921
H	4.3900544	-2.4528419	5.7264641	H	0.7093158	0.9169819	10.1340279
C	3.3870872	-3.9180725	3.7526691	C	0.9515758	1.3315629	6.6788703
H	4.4177028	-4.1874280	4.0227275	H	1.4608866	2.3073243	6.6908449
H	3.4329746	-3.0736557	3.0486722	H	0.1973160	1.3430469	5.8811252
H	2.9410818	-4.7807749	3.2389752	H	1.6882900	0.5527469	6.4298474