

Supporting information for:

Zinc complexes supported by methyl salicylato ligands: synthesis, structure, and application in ring-opening polymerization of L-lactide

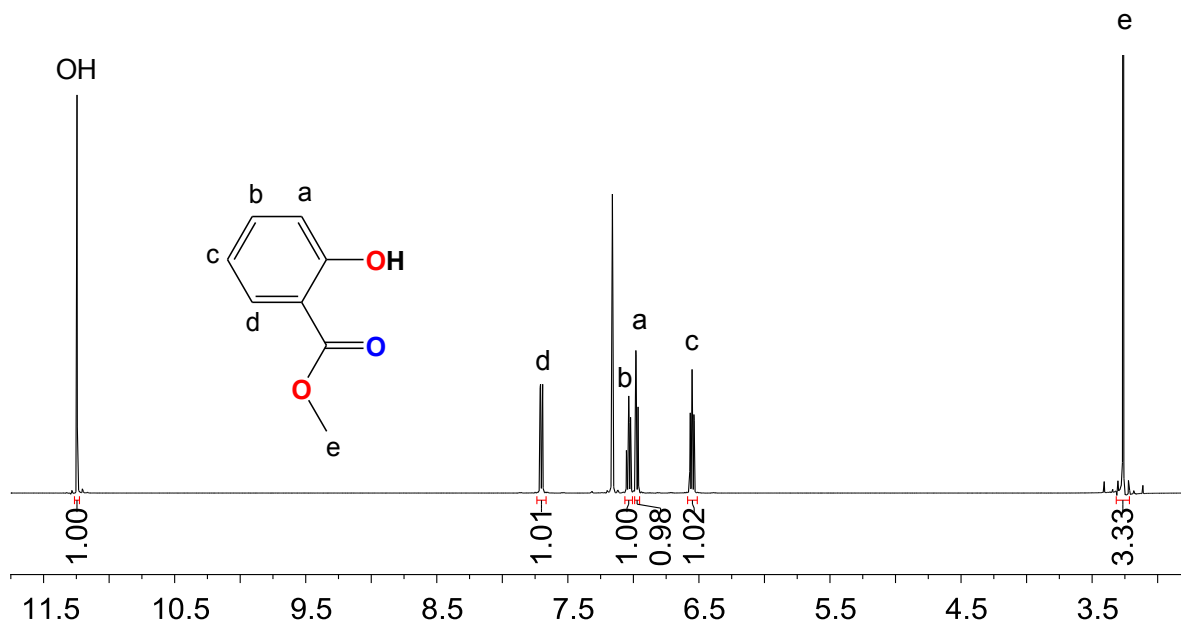
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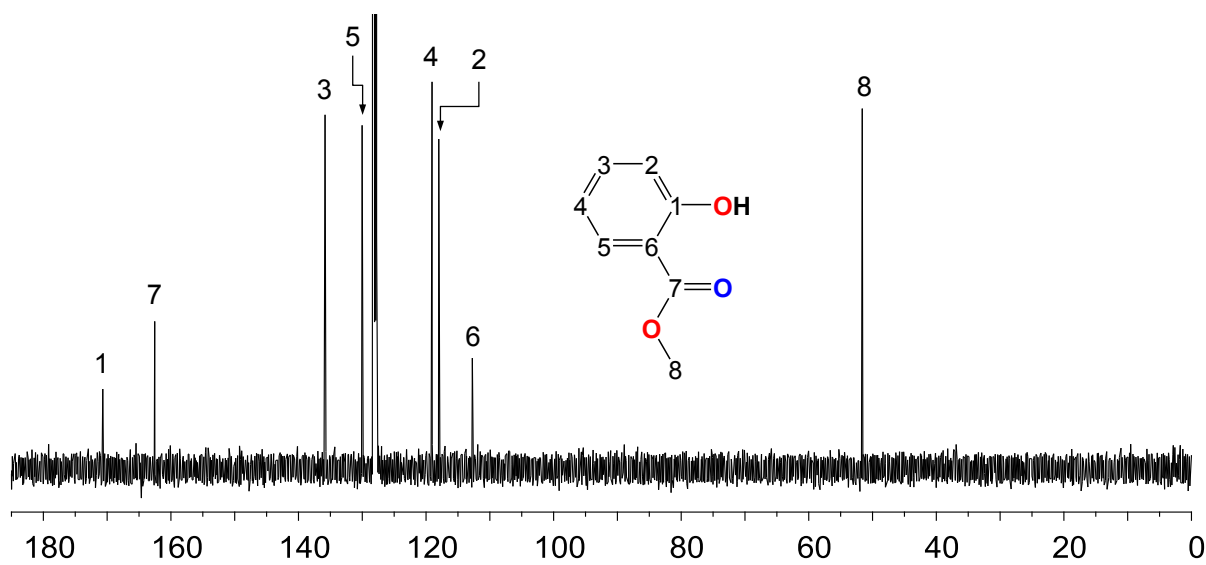
Crystallographic Data for Compounds 1-2.

Table S1. Crystal and Data Collection Parameters for Compounds 1-2.

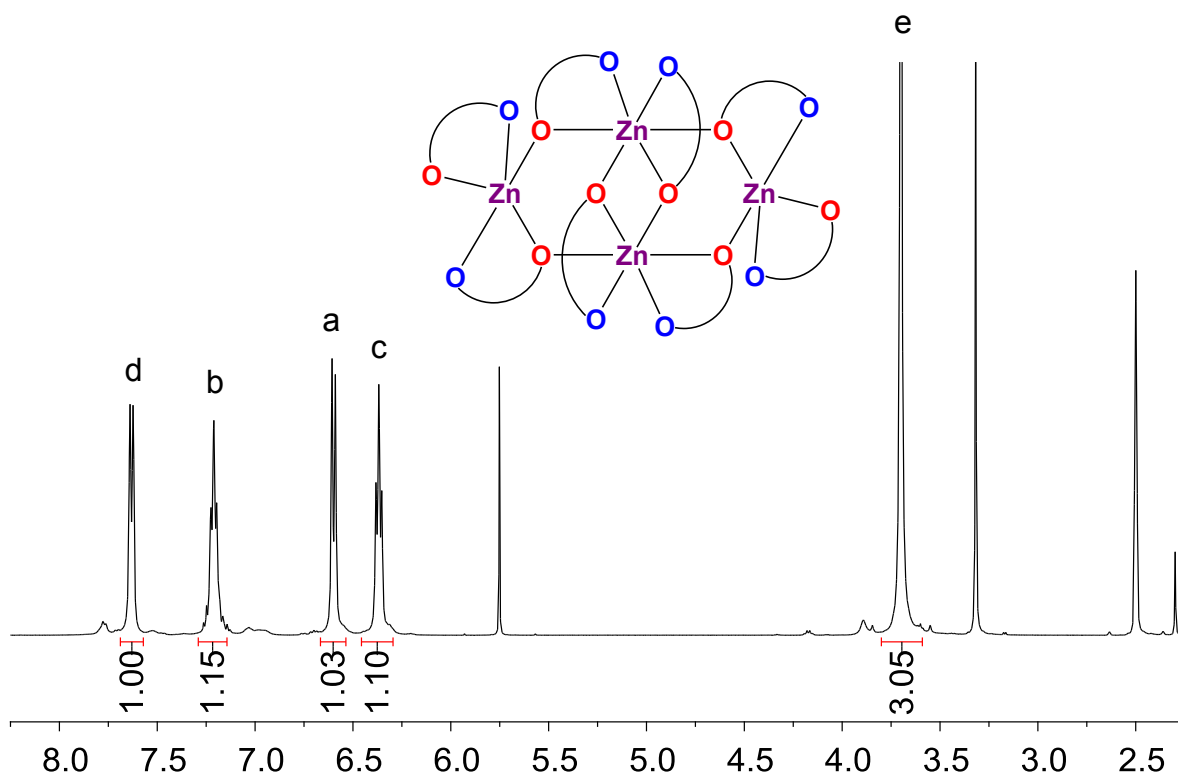
	1·CH ₂ Cl ₂	2·0.5C ₇ H ₈
Chemical formula	C ₆₄ H ₅₆ O ₂₄ Zn ₄ ·CH ₂ Cl ₂	2(C ₂₆ H ₂₄ N ₂ O ₆ Zn)·C ₇ H ₈
Formula Mass	1555.57	1143.86
Crystal system	Triclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> /Å	11.260(3)	27.674(4)
<i>b</i> /Å	12.517(4)	12.210(2)
<i>c</i> /Å	12.752(4)	15.867(3)
α /°	66.13(3)	
β /°	75.17(3)	92.47(2)
γ /°	76.07(3)	
Unit cell volume/Å ³	1569.6(8)	5356.5(15)
Temperature/K	100(2)	100(2)
<i>Z</i>	1	4
Radiation type	MoK α	MoK α
Absorption coefficient, μ /mm ⁻¹	1.679	0.963
No. of reflections measured	17541	58176
No. of independent reflections	6833	11695
<i>R</i> _{int}	0.0318	0.0547
Final <i>R</i> _{<i>I</i>} values (<i>I</i> > 2 σ (<i>I</i>))	0.0336	0.0333
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2 σ (<i>I</i>))	0.0800	0.0737
Final <i>R</i> _{<i>I</i>} values (all data)	0.0500	0.0621
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.0844	0.0796
Goodness of fit on <i>F</i> ²	0.975	0.0871
$\Delta\rho$ _{max} /eÅ ⁻³	0.67	0.69
$\Delta\rho$ _{min} /eÅ ⁻³	-0.45	-0.34



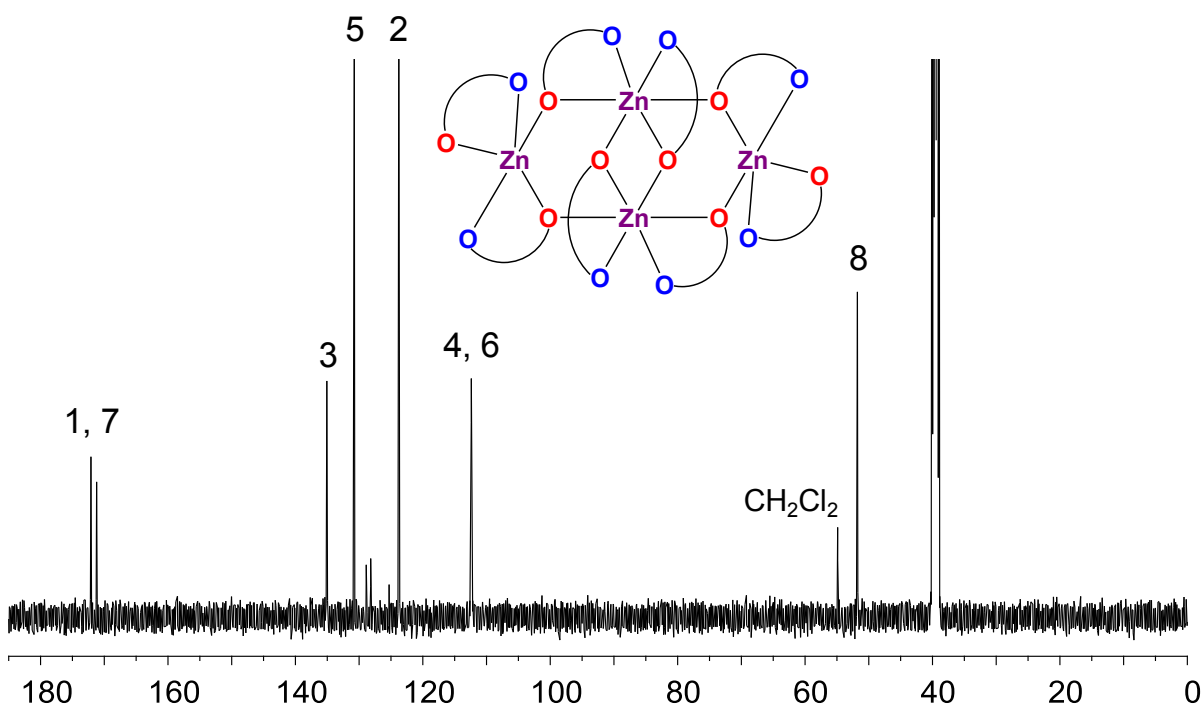
S1. ^1H NMR spectrum of MesalOH ligand in C_6D_6 .



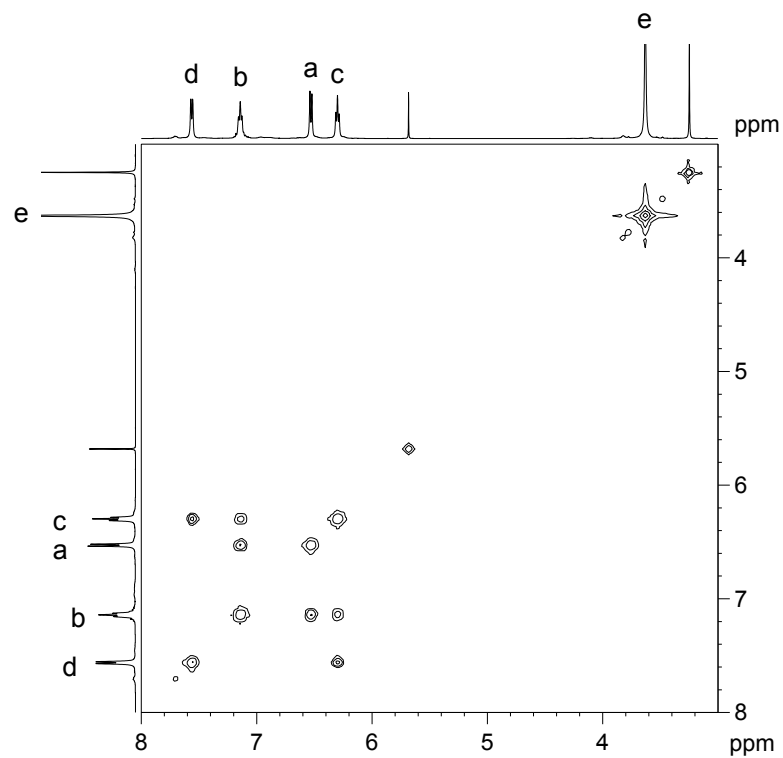
S2. ^{13}C NMR spectrum of MesalOH ligand in C_6D_6 .



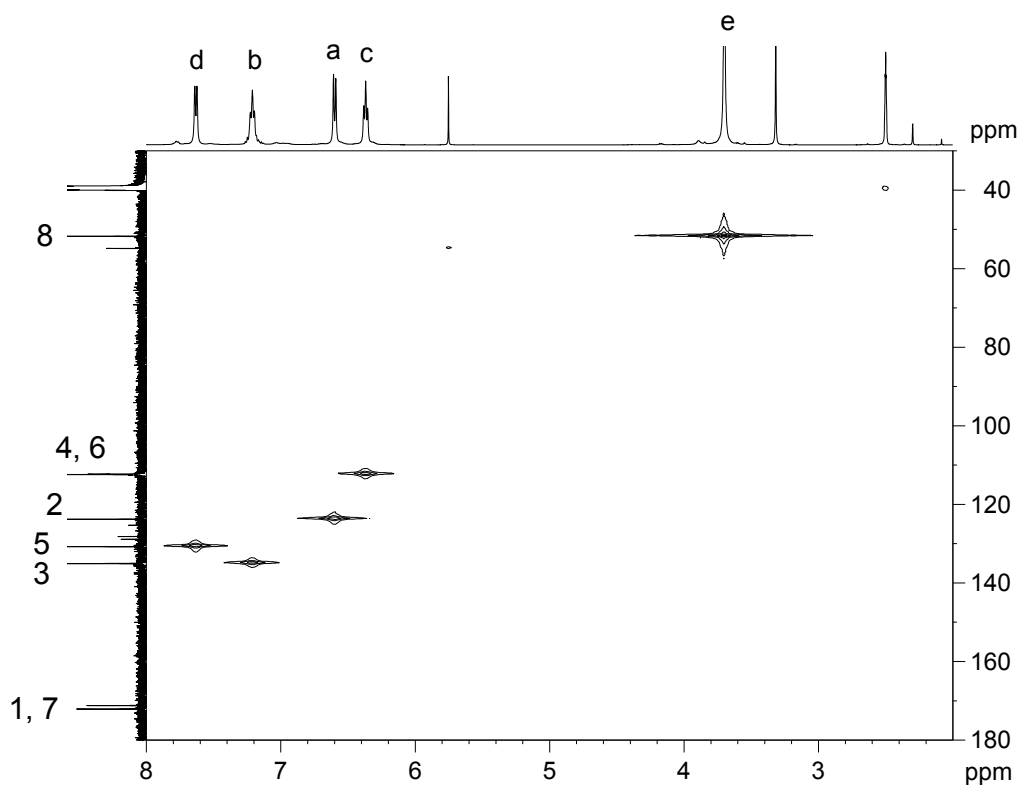
S3. ^1H NMR spectrum of **1** in $\text{DMSO-}D_6$.



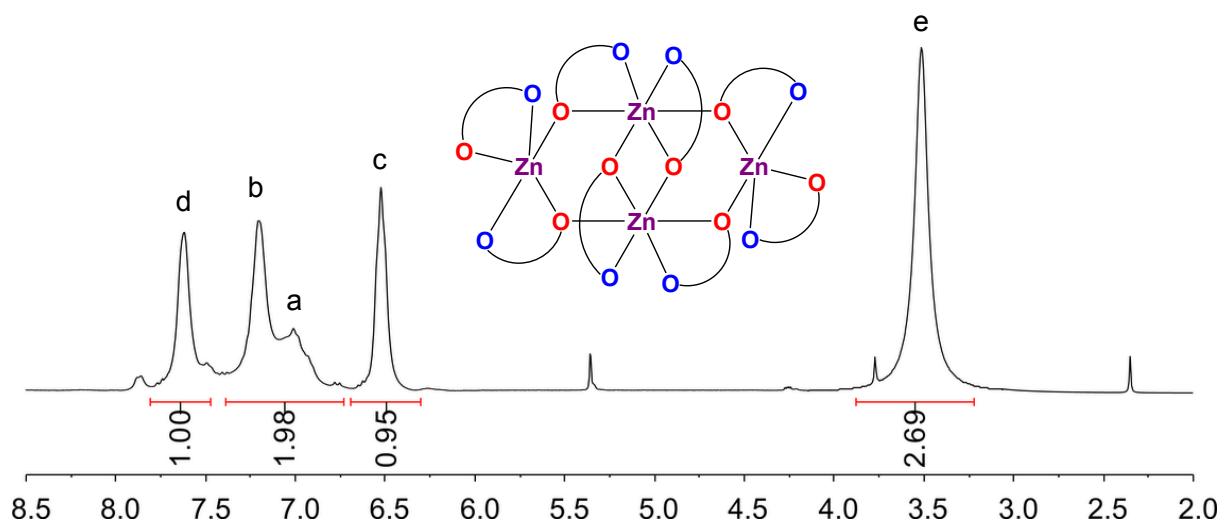
S4. ^{13}C NMR spectrum of **1** in $\text{DMSO-}D_6$.



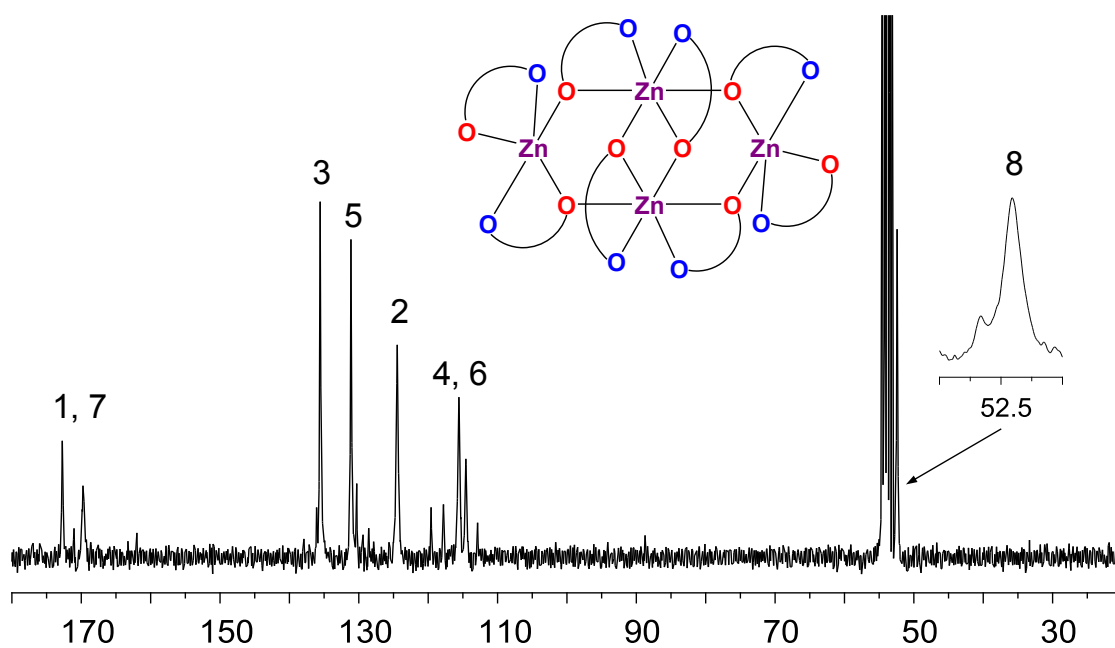
S5. COSY NMR spectrum of **1** in DMSO-D₆.



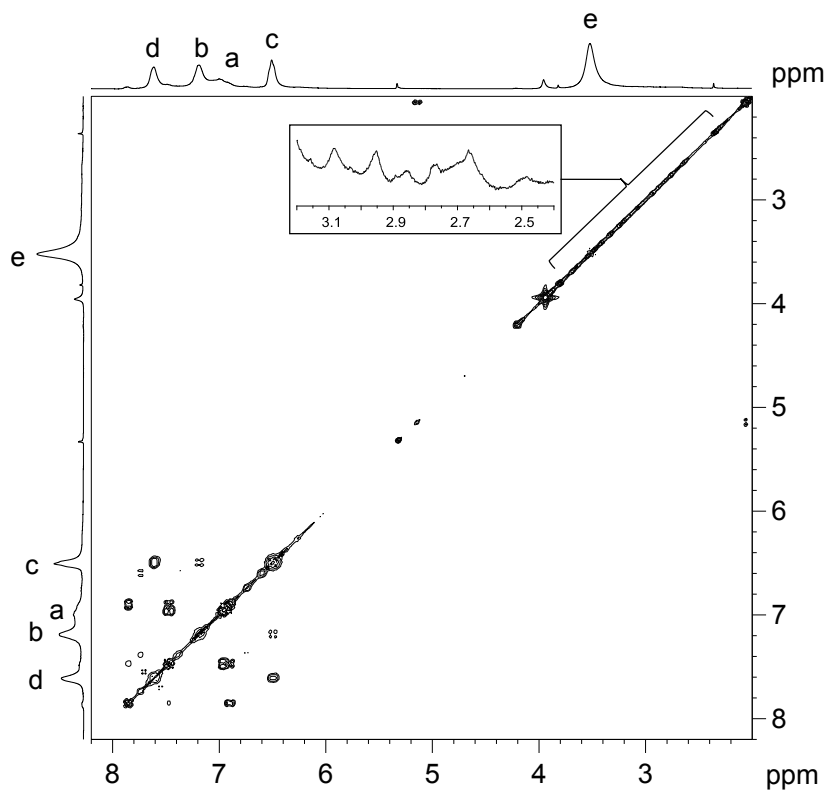
S6. HMQC NMR spectrum of **1** in DMSO-D₆.



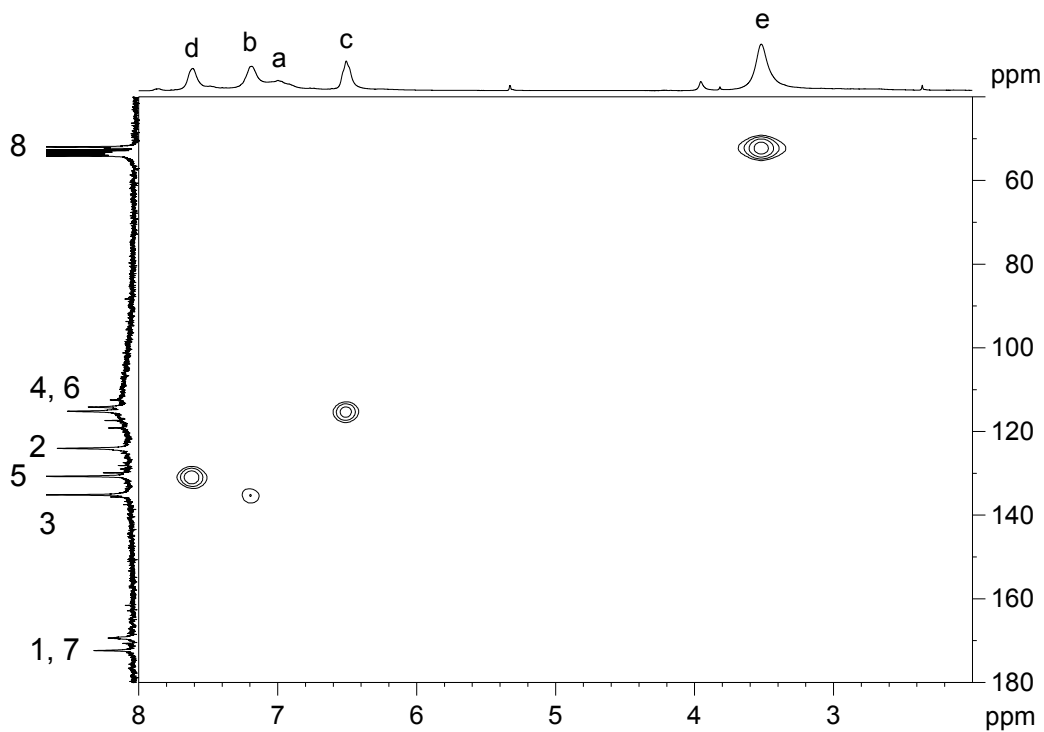
S7. ^1H NMR spectrum of **1** in CD_2Cl_2 .



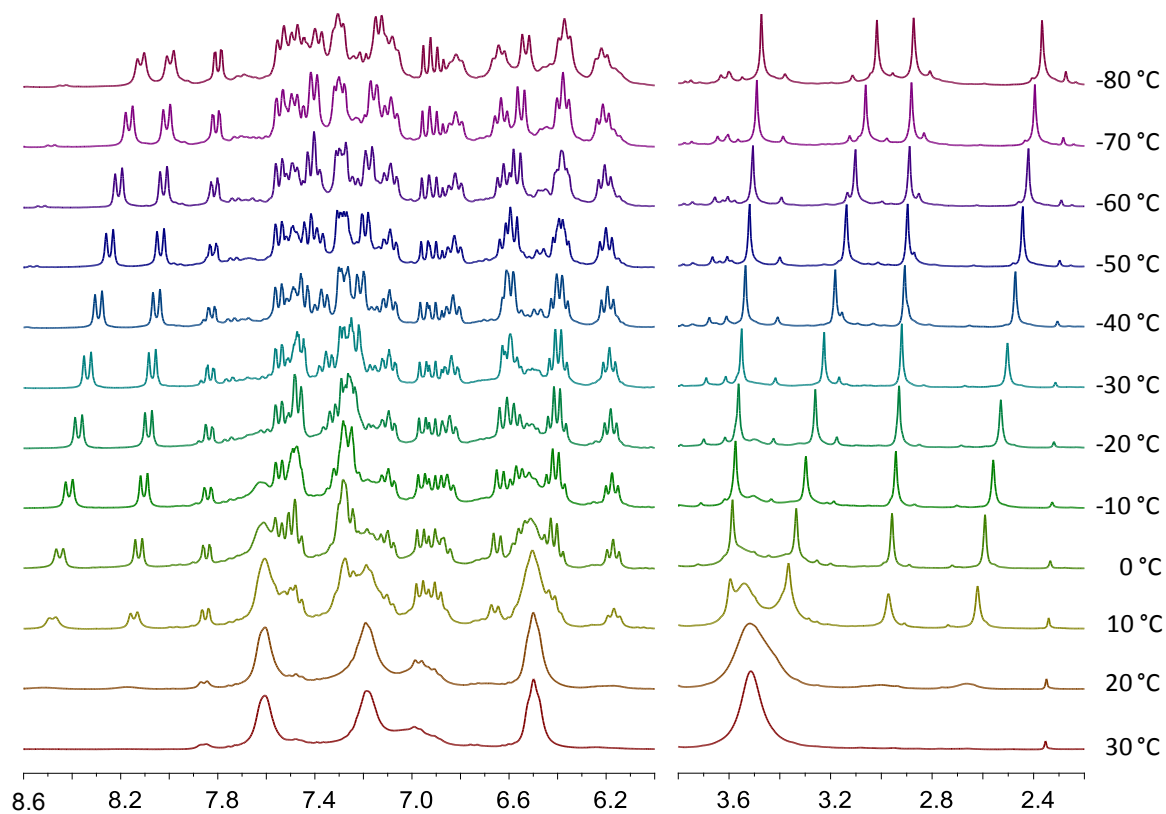
S8. ^{13}C NMR spectrum of **1** in CD_2Cl_2 .



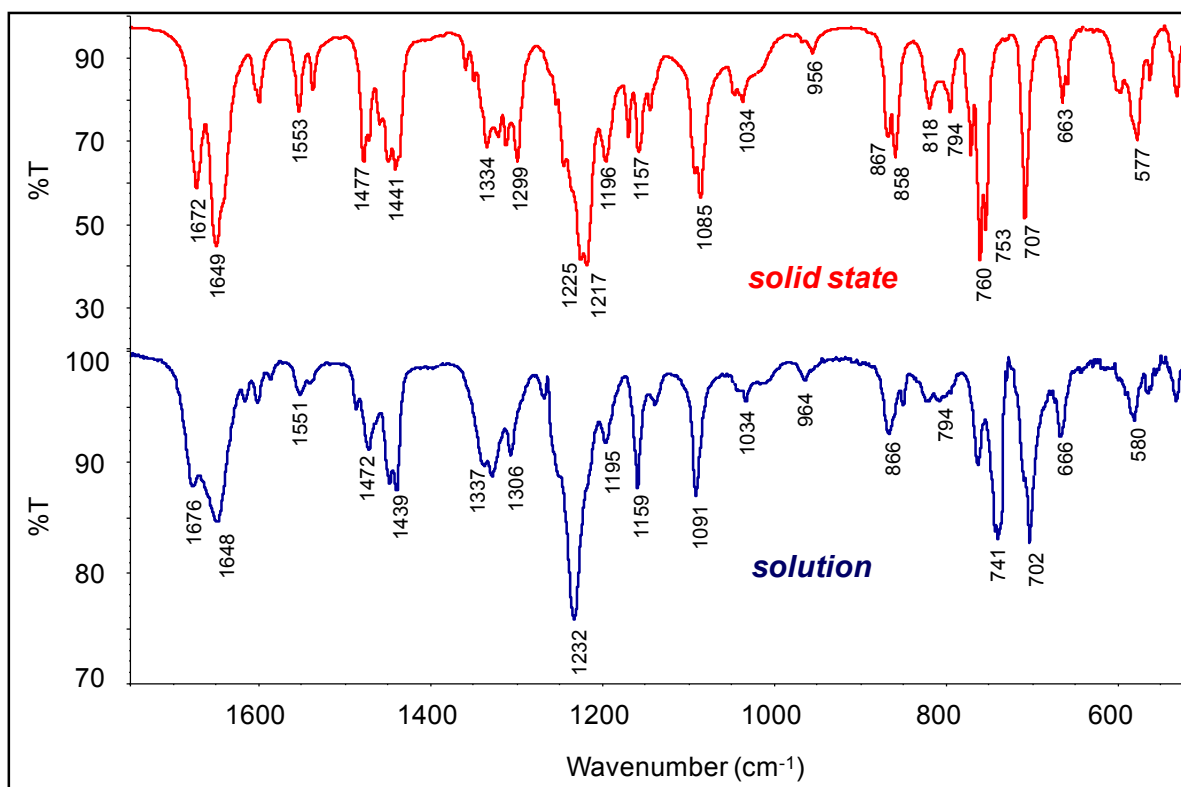
S9. COSY NMR spectrum of **1** in CD₂Cl₂.



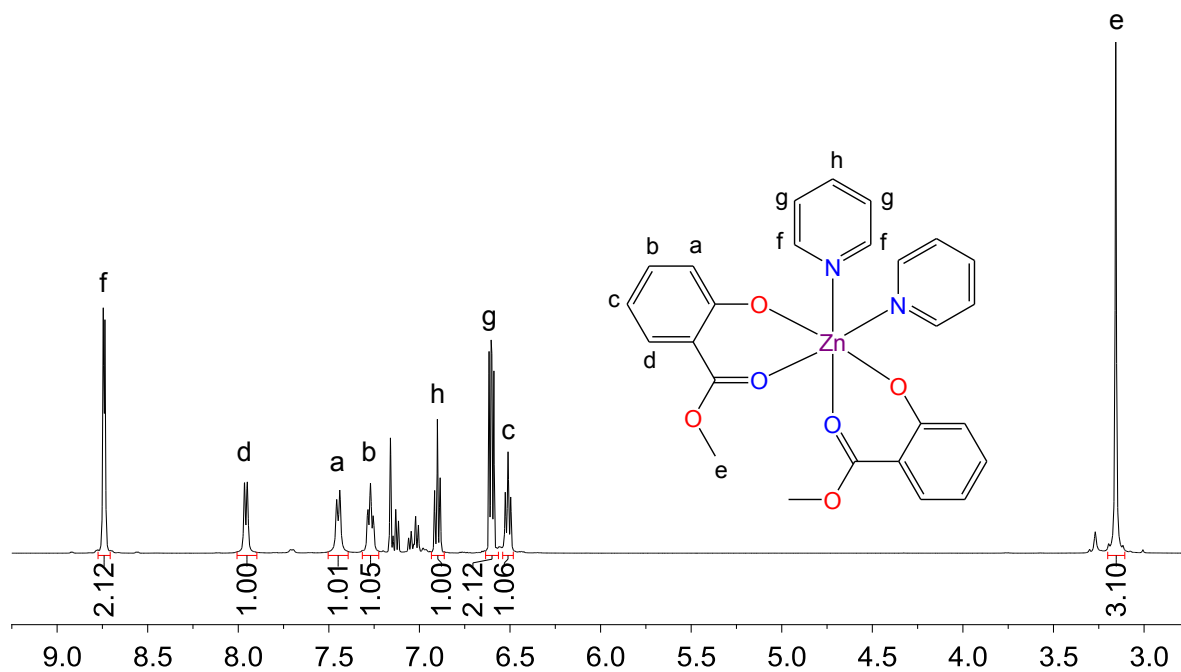
S10. HMQC NMR spectrum of **1** in CD₂Cl₂.



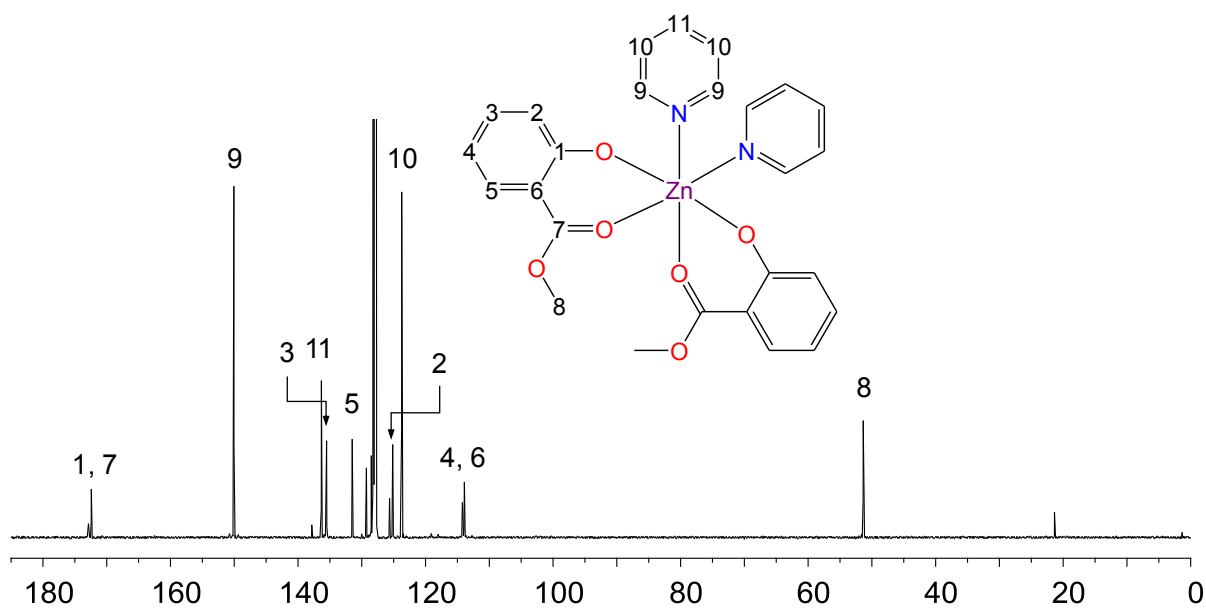
S11. VT ^1H NMR spectra of **1** in CD_2Cl_2 .



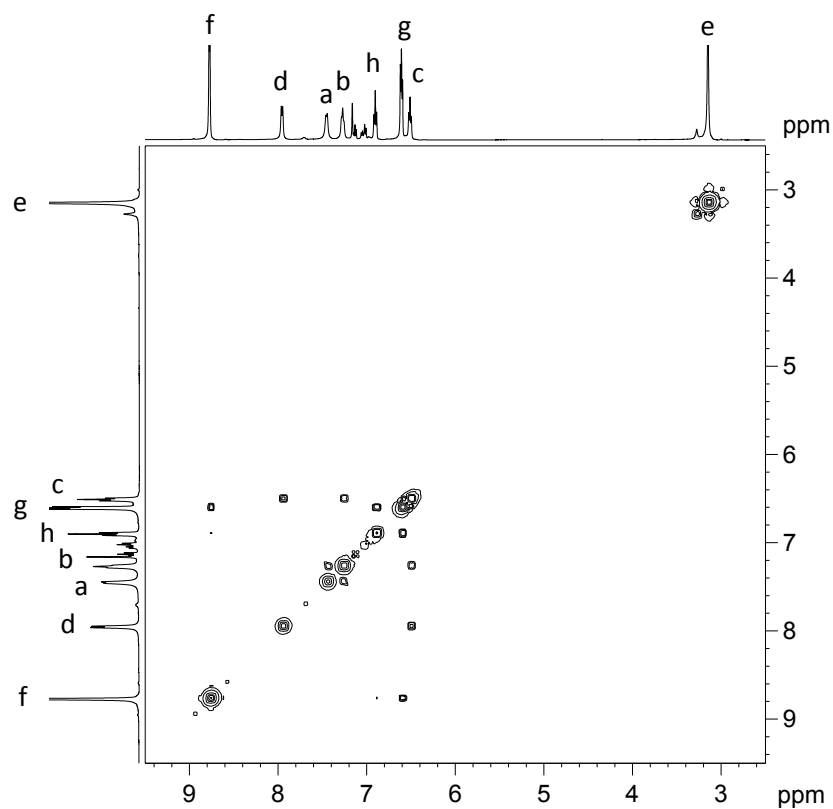
S12. FTIR-ATR spectra of **1** in solid state and in CH_2Cl_2 solution.



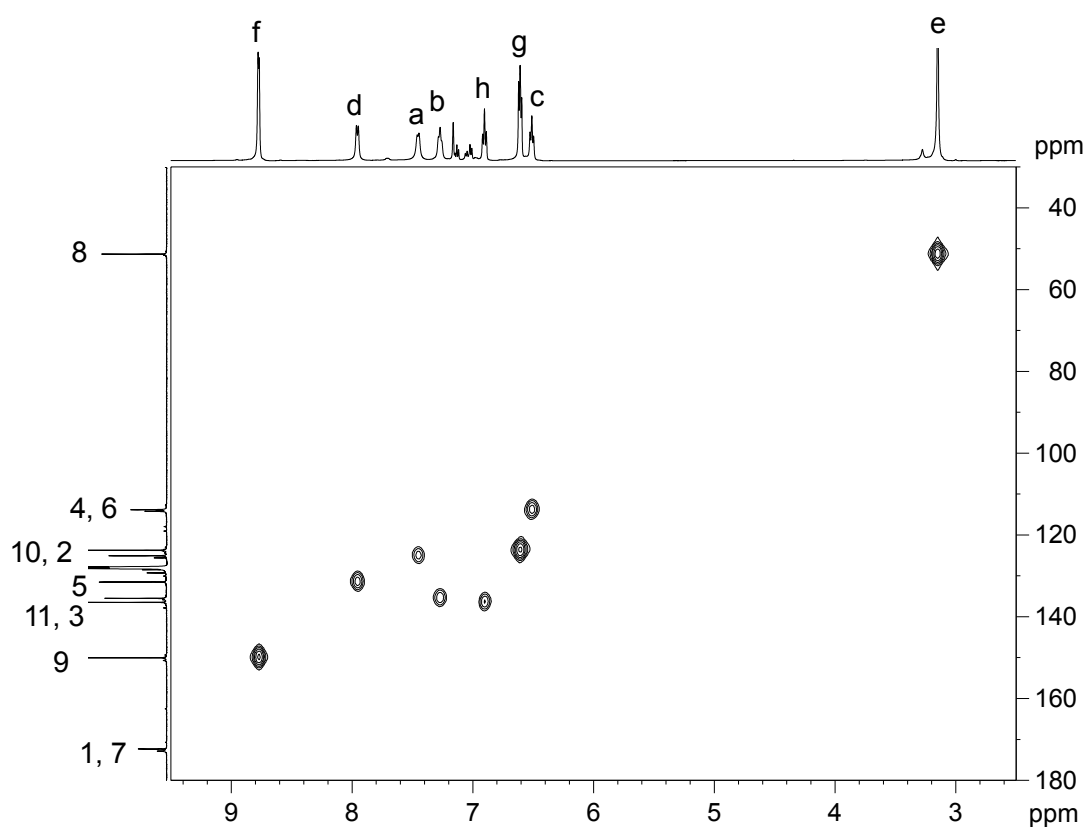
S13. ^1H NMR spectrum of **2** in C_6D_6 .



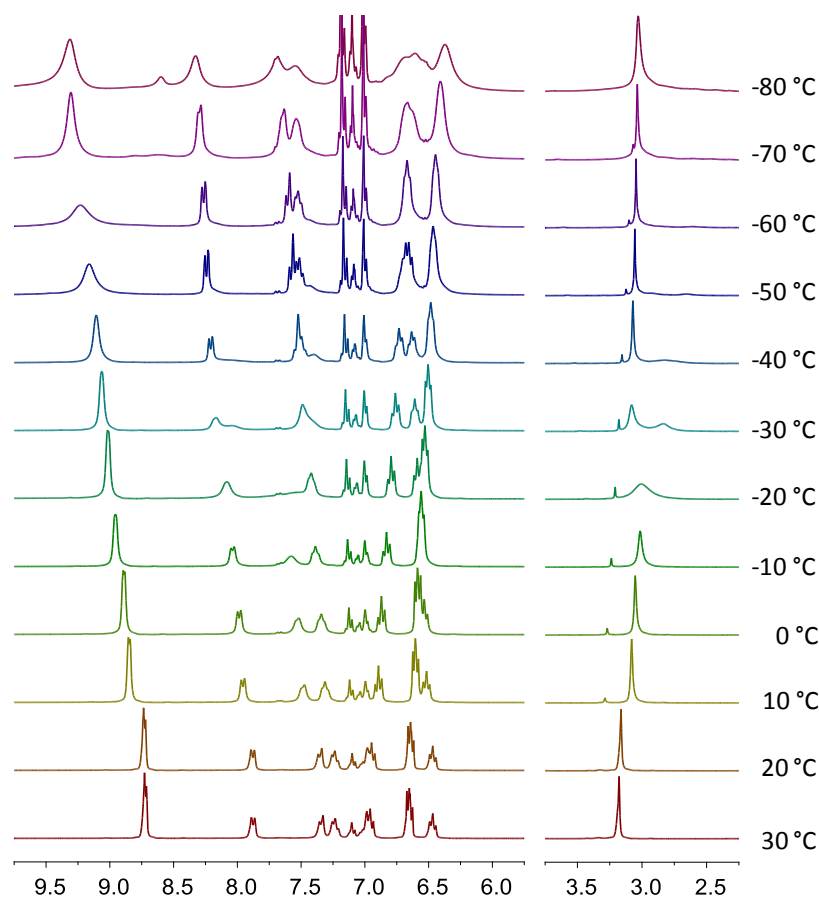
S14. ^{13}C NMR spectrum of **2** in C_6D_6 .



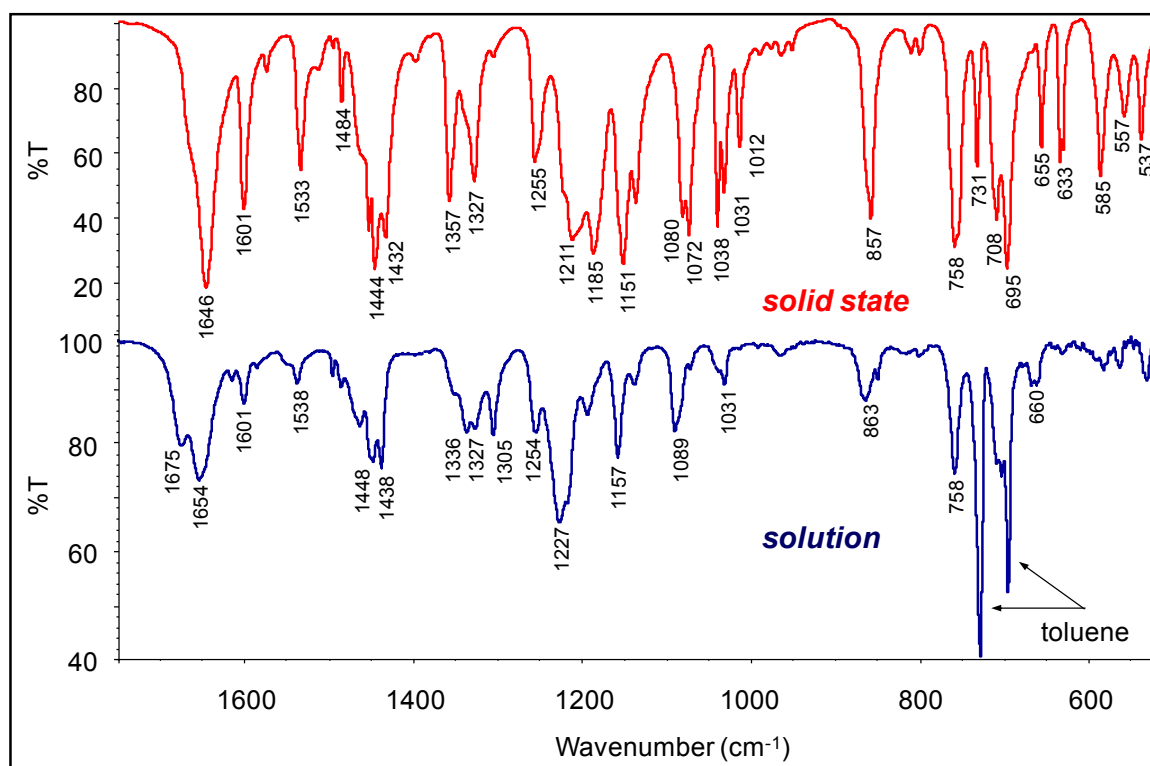
S15. COSY NMR spectrum of **2** in C₆D₆.



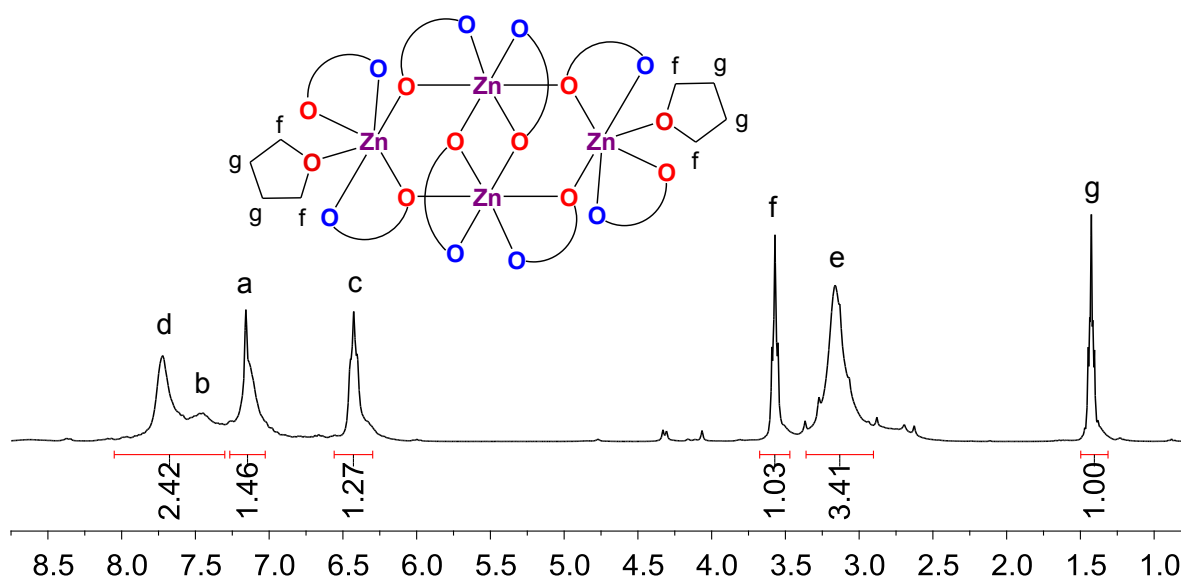
S16. HMQC NMR spectrum of **2** in C₆D₆.



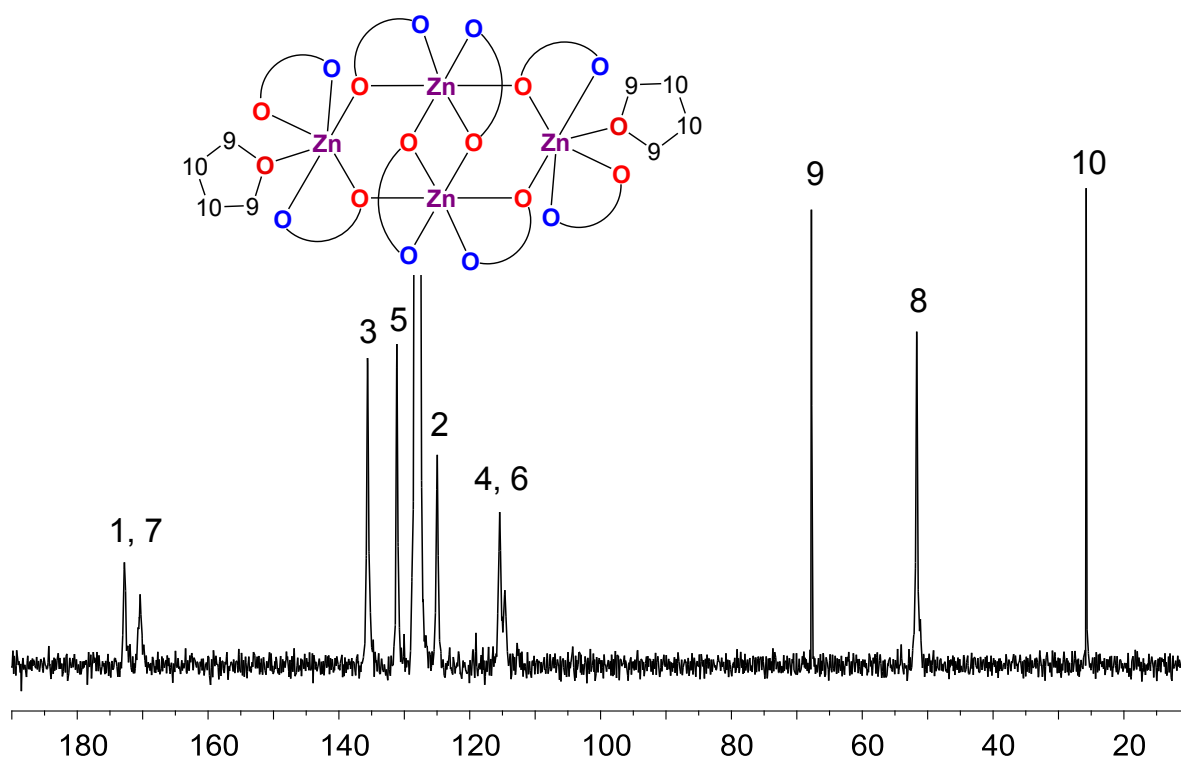
S17. VT ¹H NMR spectra of **2** in C₇D₈.



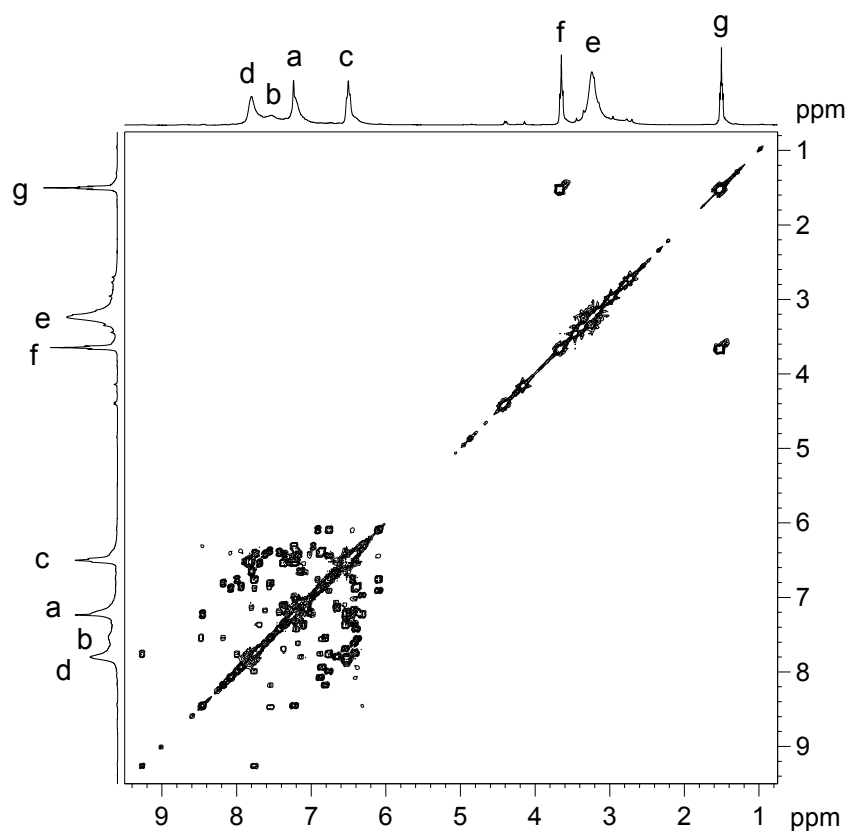
S18. FTIR-ATR spectra of **2** in solid state and in toluene solution.



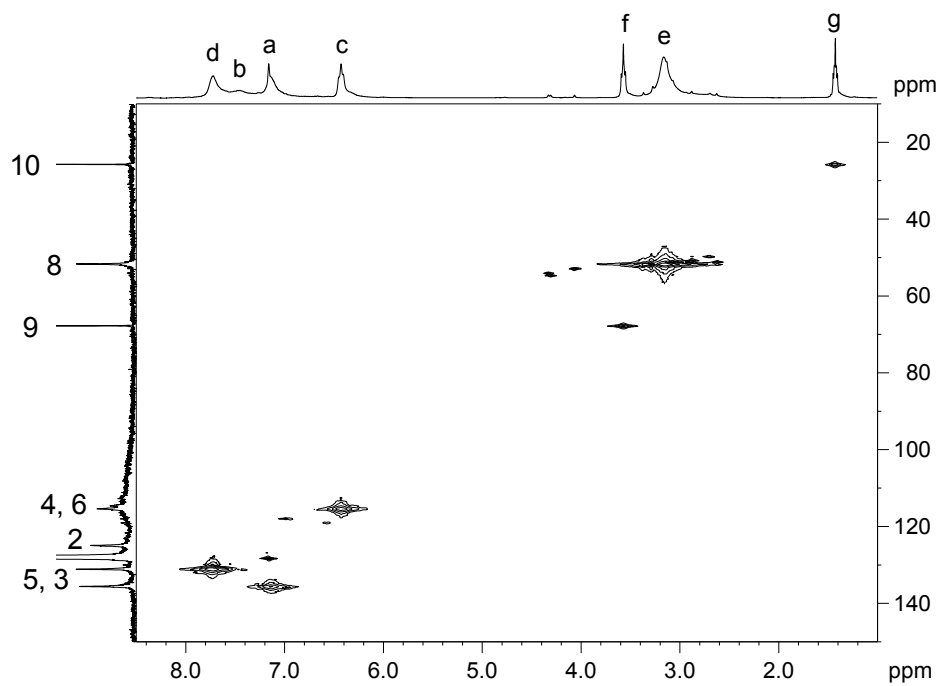
S19. ¹H NMR spectrum of **1**·2THF in C₆D₆.



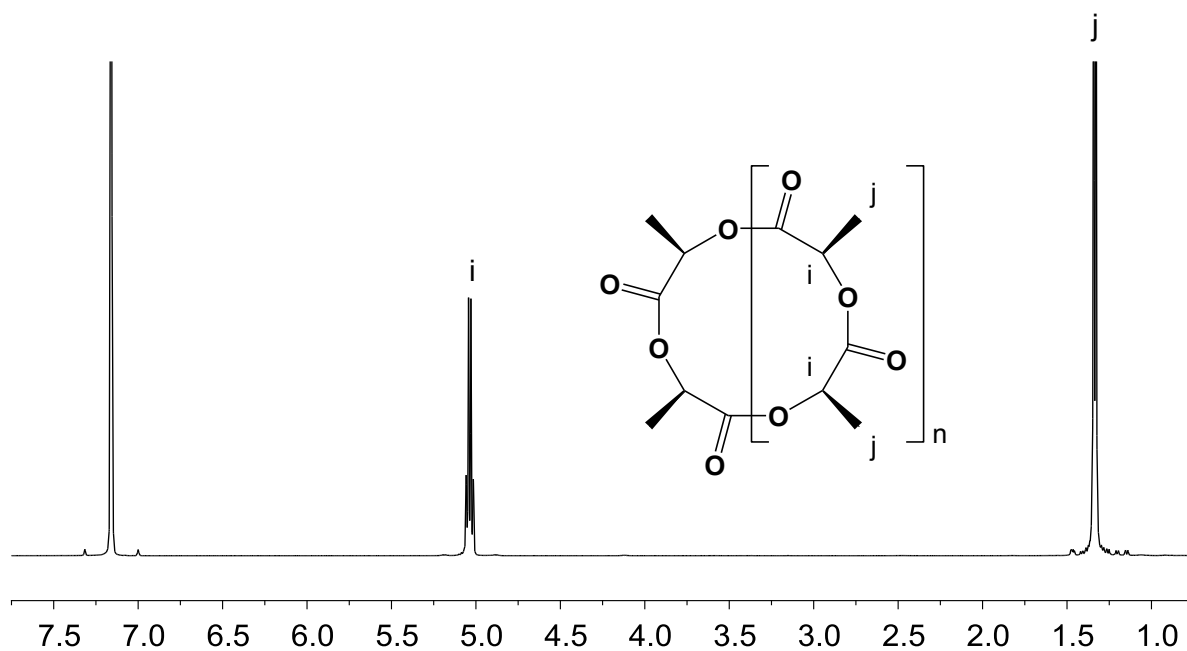
S20. ¹³C NMR spectrum of **1**·2THF in C₆D₆.



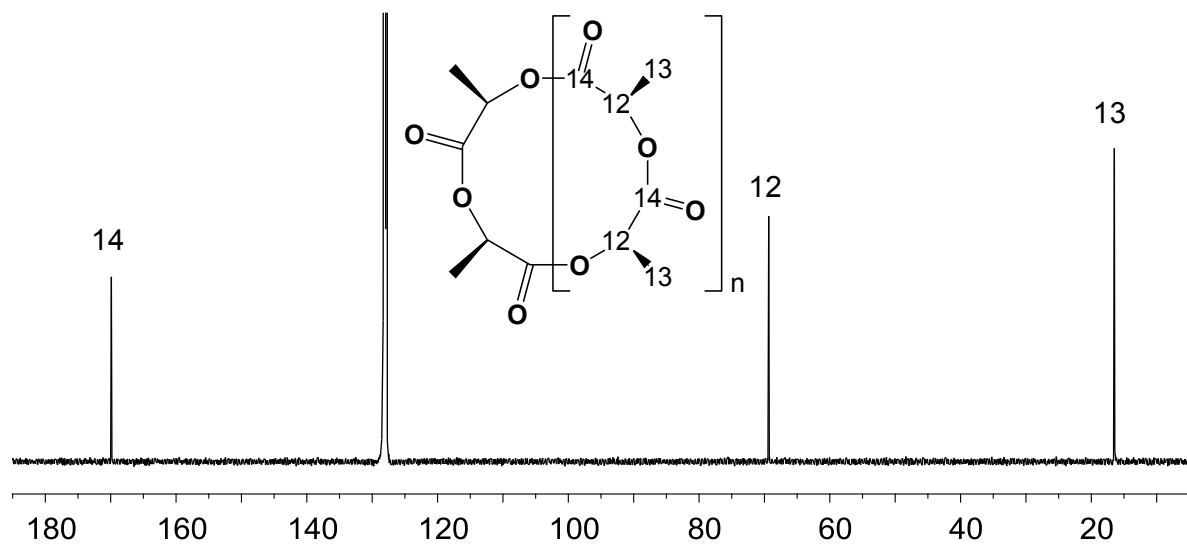
S21. COSY NMR spectrum of **1·2THF** in C_6D_6 .



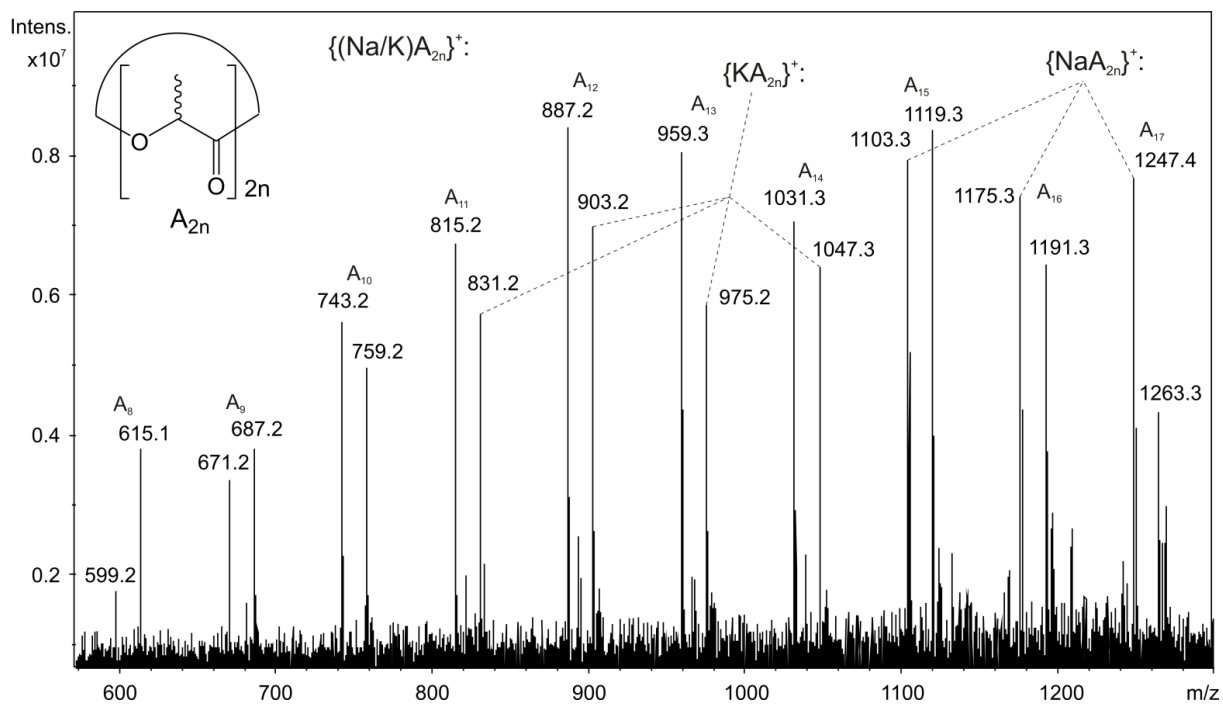
S22. HMQC NMR spectrum of **1·2THF** in C_6D_6 .



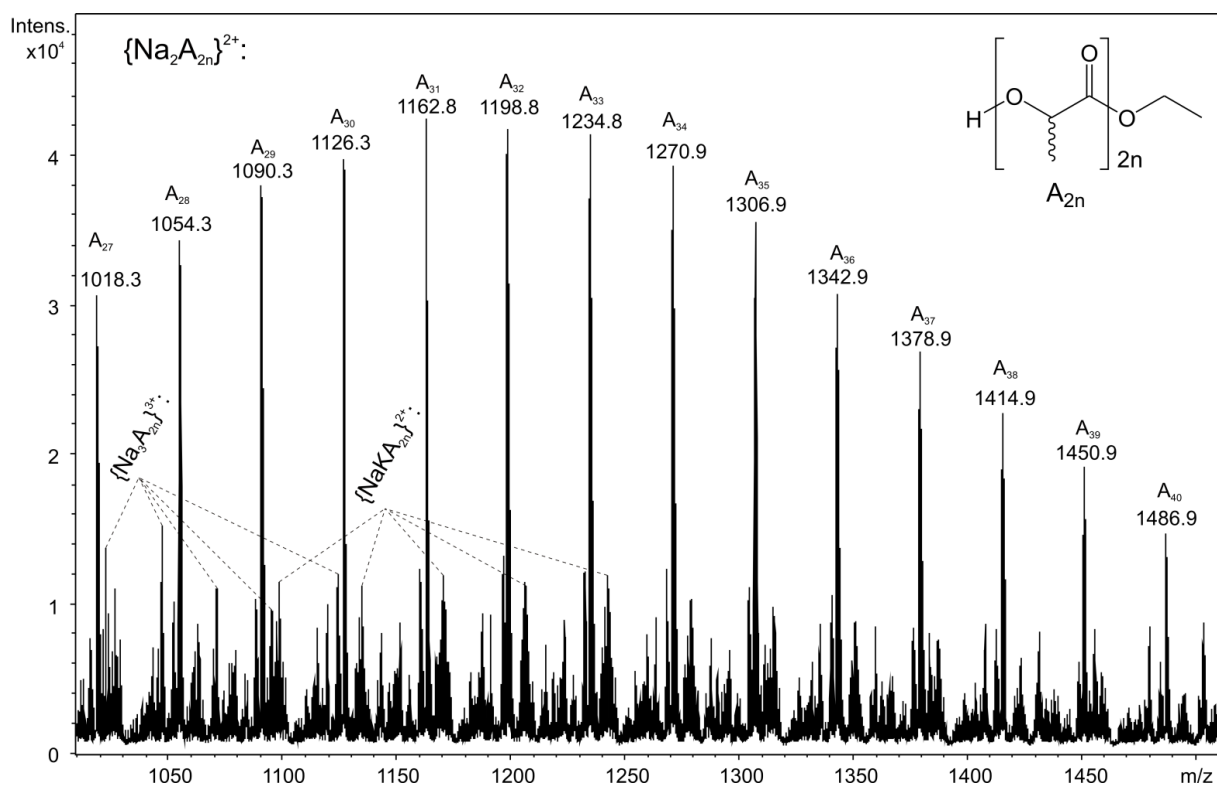
S23. ^1H NMR spectrum of cPLLA in C_6D_6 .



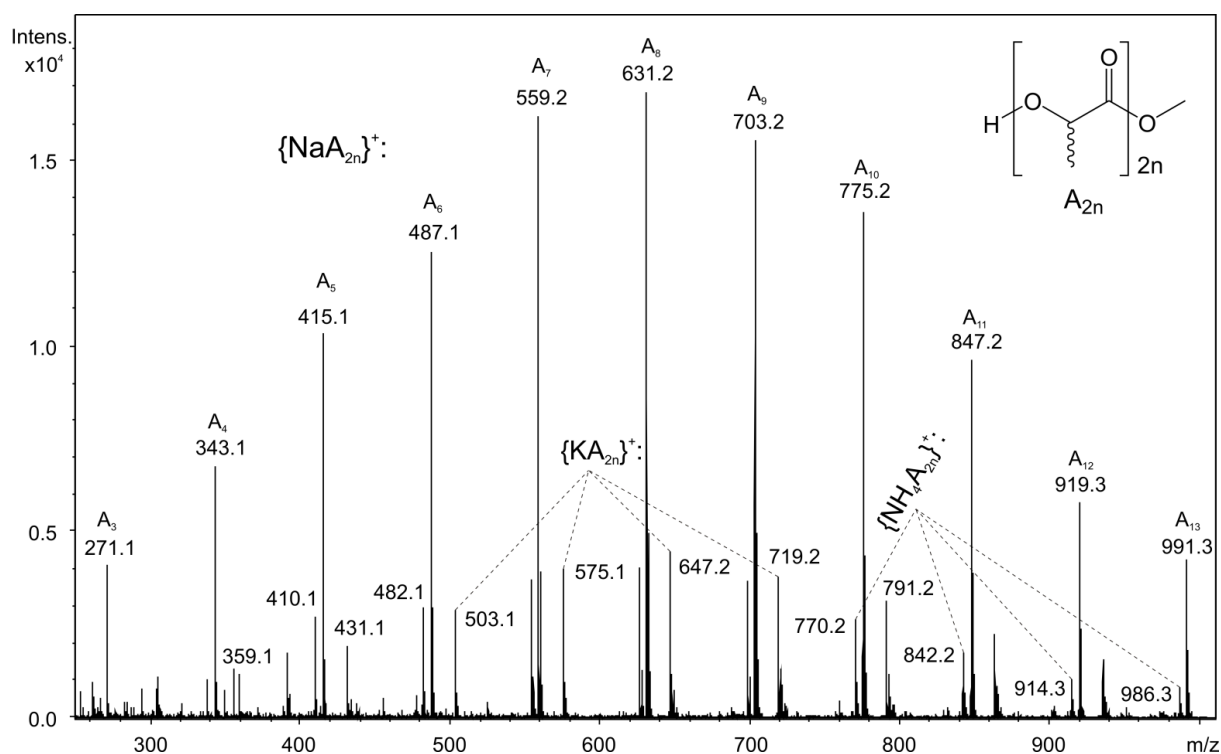
S24. ^{13}C NMR spectrum of cPLLA in C_6D_6 .



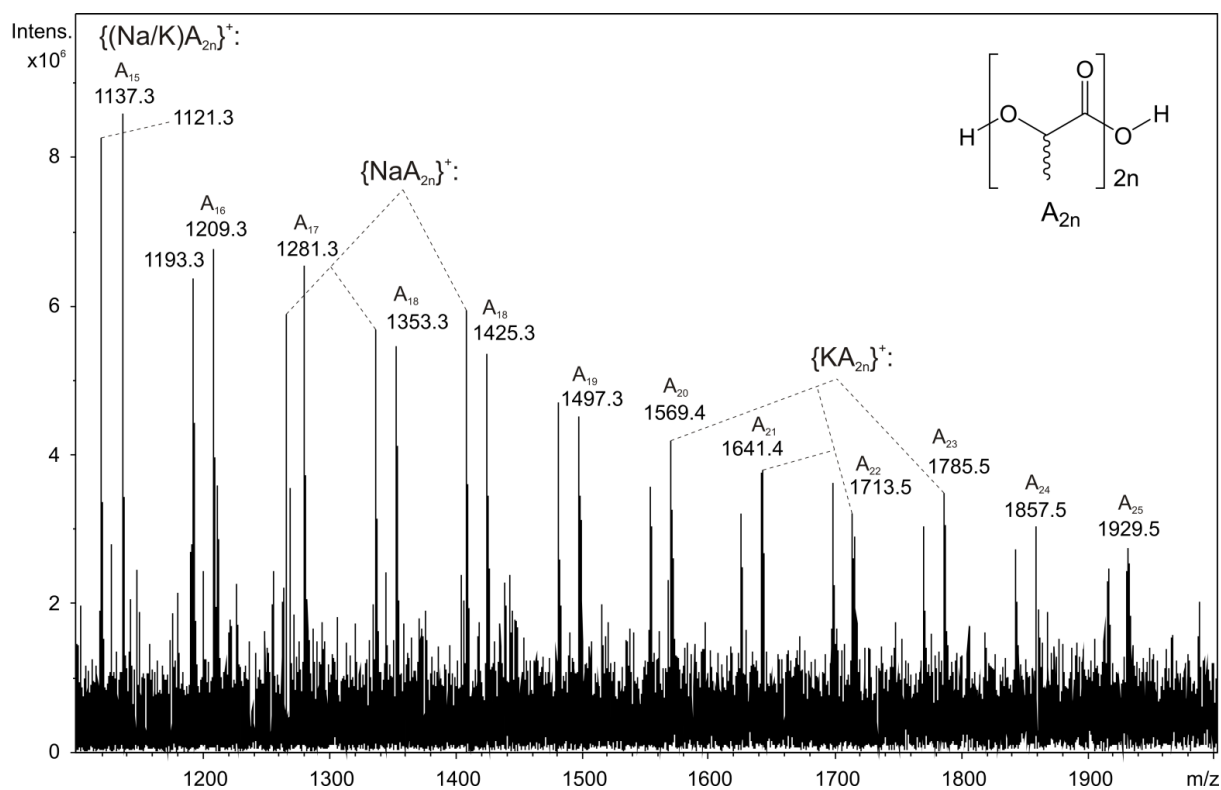
S25. ESI-MS spectrum of cPLLA.



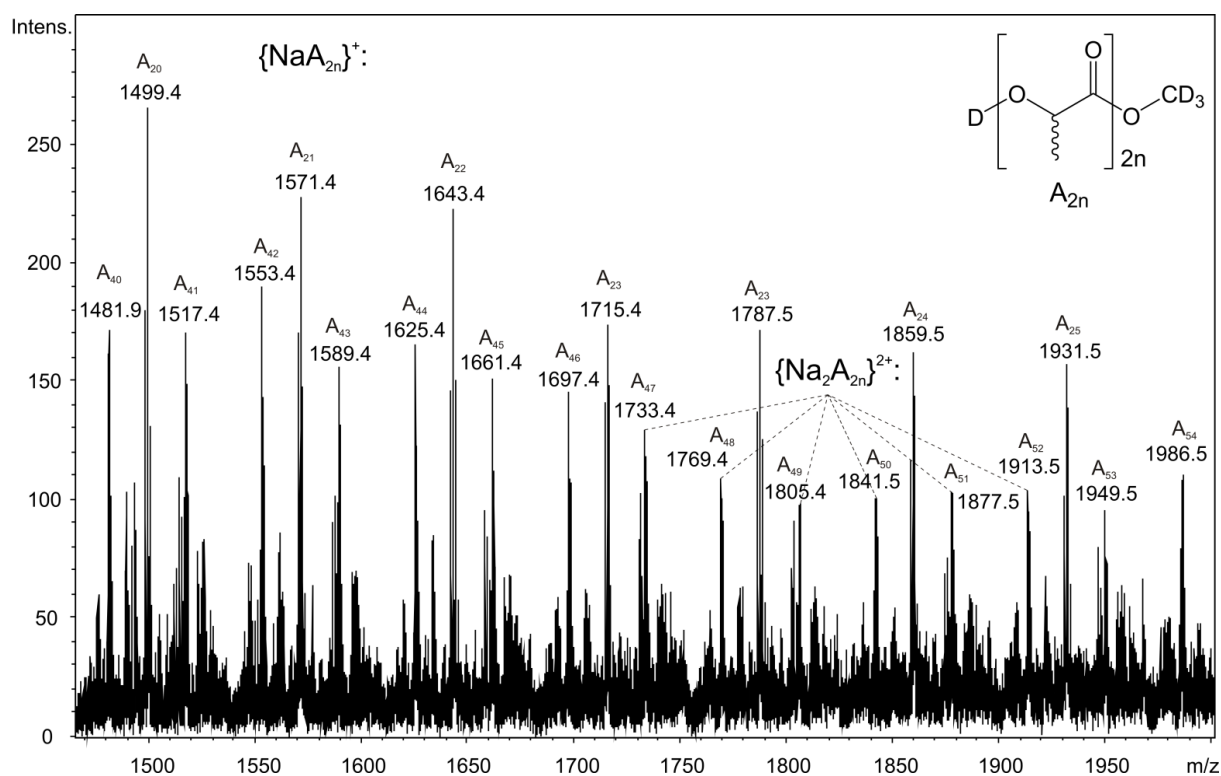
S26. ESI-MS spectrum of PLLA-OEt, obtained by quenching polymerization with EtOH.



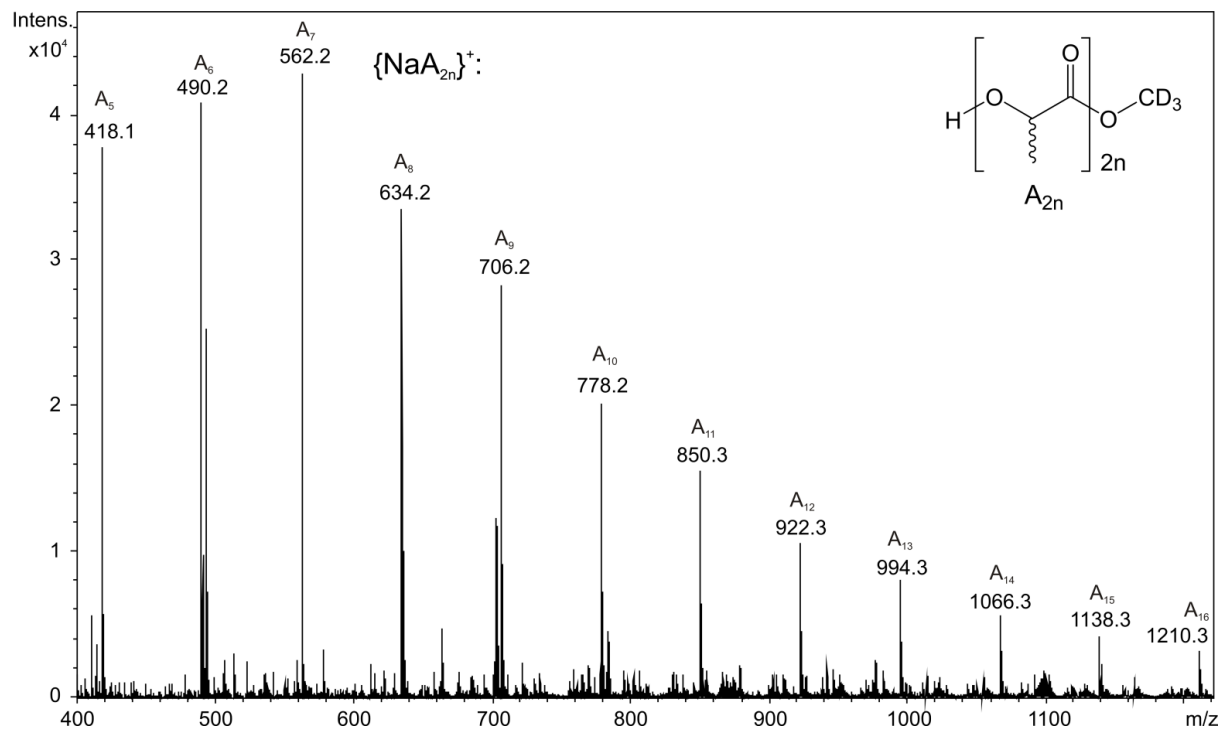
S27. ESI-MS spectrum of PLLA-OMe, obtained by quenching polymerization with MeOH.



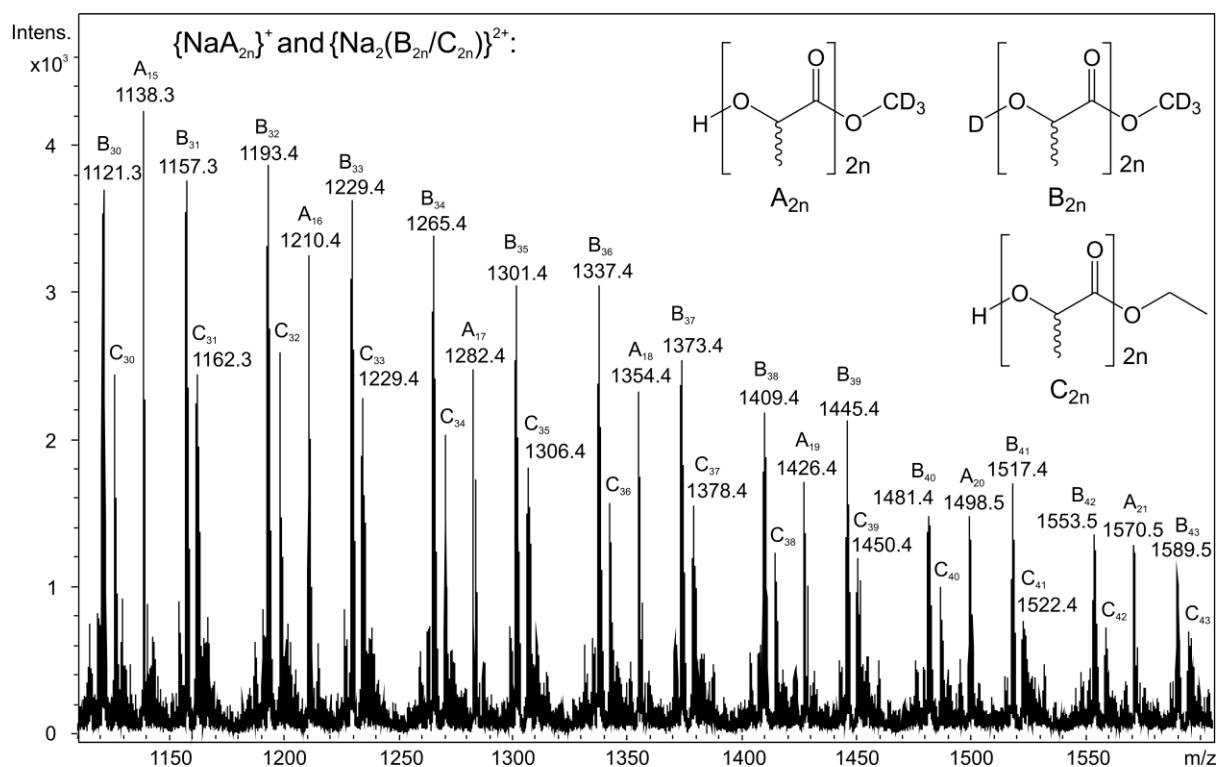
S28. ESI-MS spectrum of PLLA-OH, obtained by quenching polymerization with H_2O .



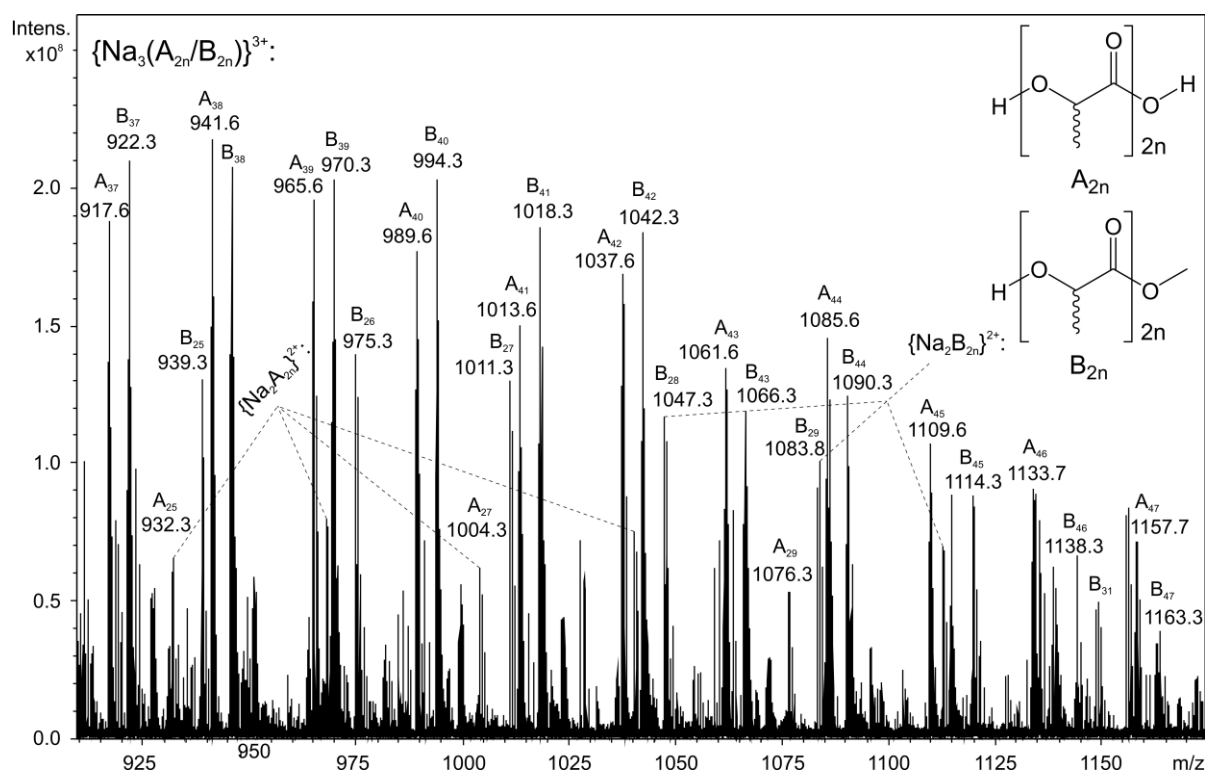
S29. ESI-MS spectrum of DO-PLLA-OCD₃, obtained by quenching polymerization with CD₃OD.



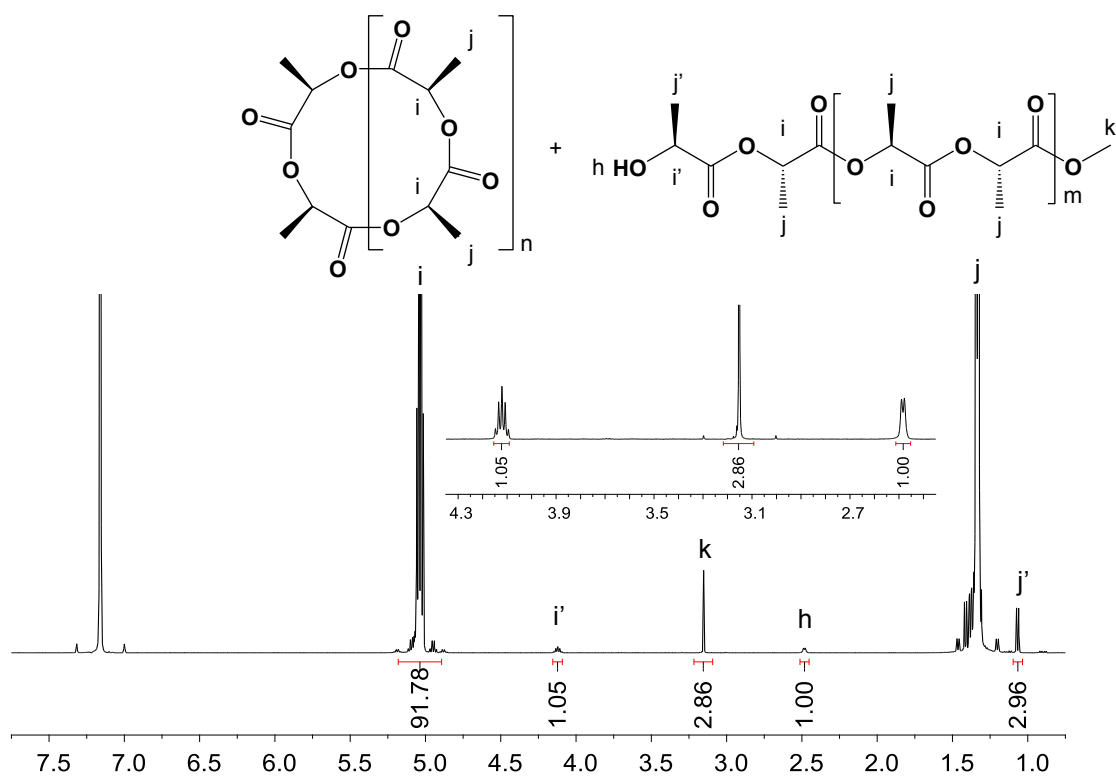
S30. ESI-MS spectrum of PLLA-OCD₃, obtained by dissolving DO-PLLA-OCD₃ in EtOH.



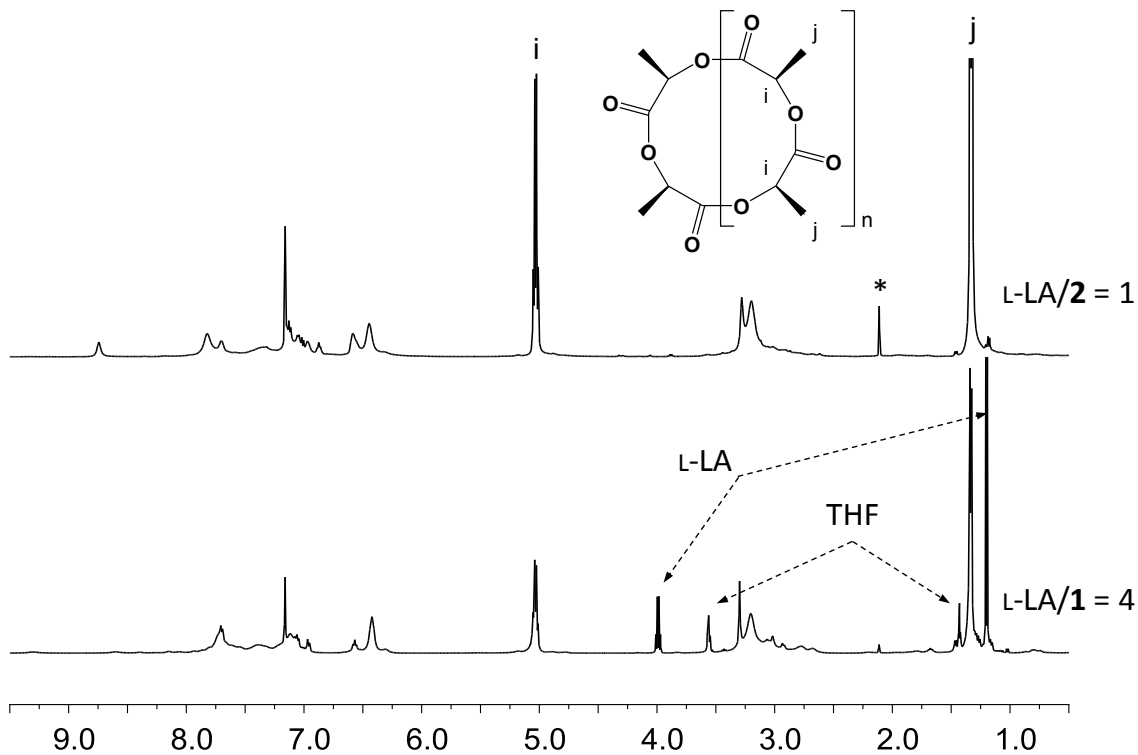
S31. ESI-MS spectrum of DO-PLLA-OCD₃, PLLA-OCD₃ and PLLA-OEt, obtained by dissolving DO-PLLA-OCD₃ in EtOH.



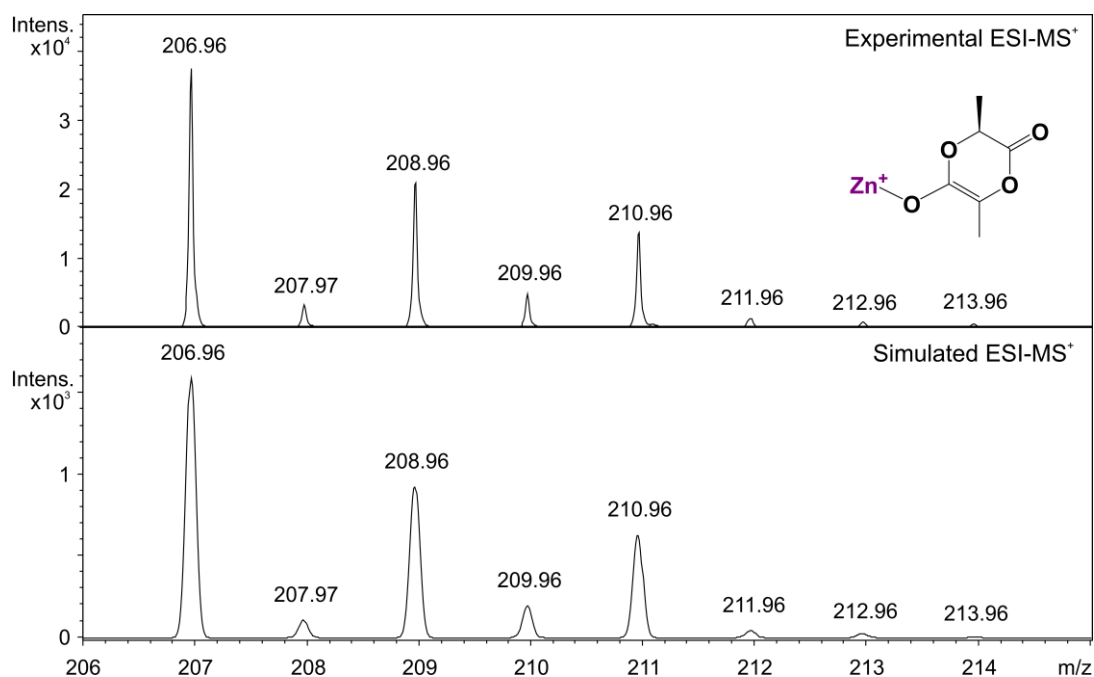
S32. ESI-MS spectrum of PLLA-OMe and PLLA-OH, obtained by quenching polymerization with mixture of MeOH/H₂O.



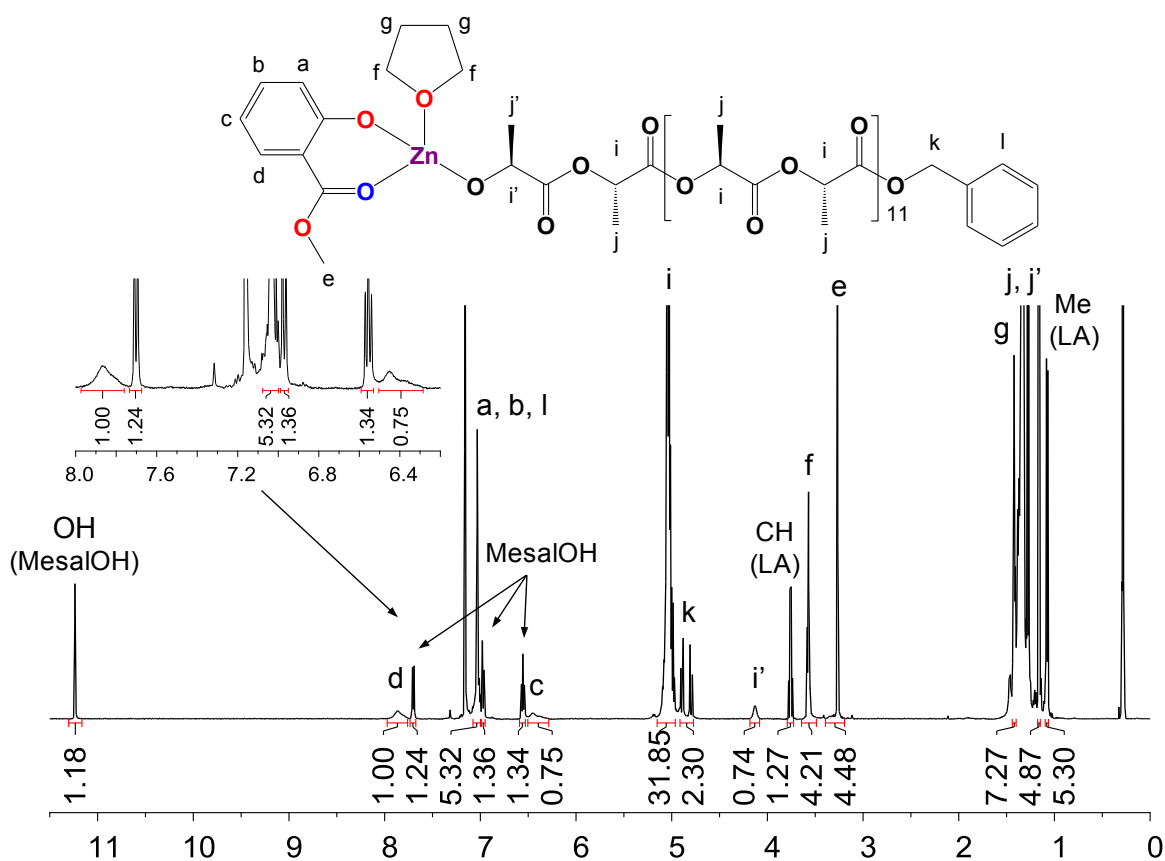
S33. ^1H NMR spectrum in C_6D_6 of mixture of cPLLA and PLLA-OMe obtained in reaction of **2** with L-LA in a L-LA/Zn = 25 ratio, and quenched with MeOH.



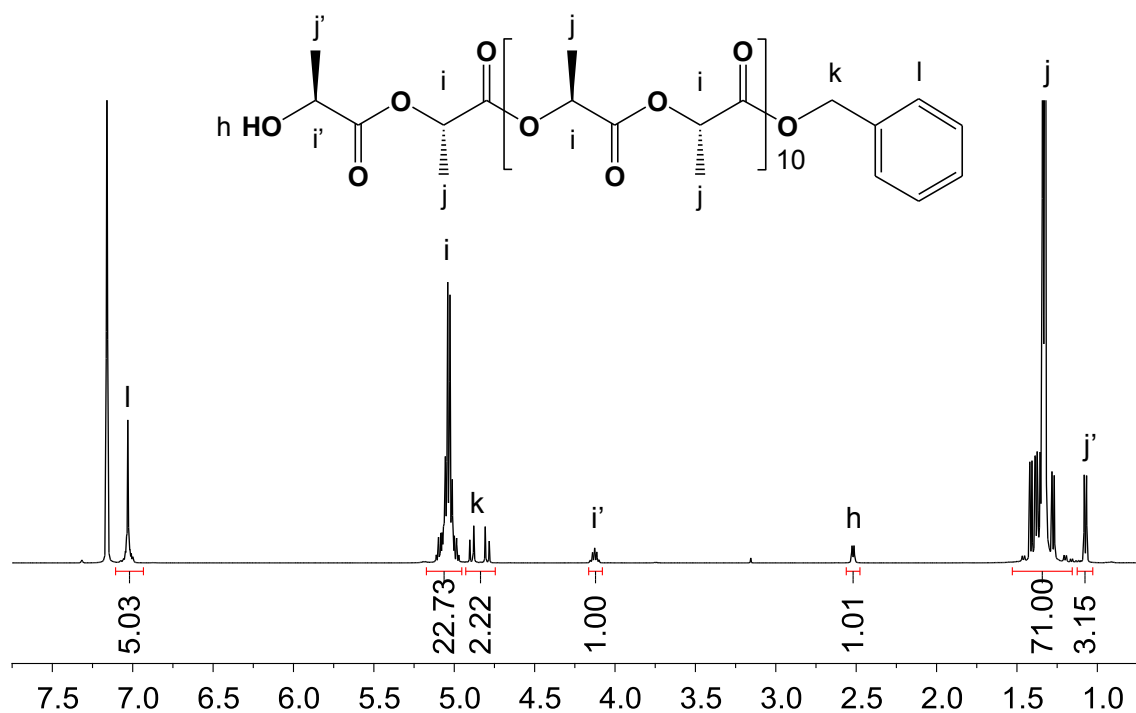
S34. ^1H NMR spectra in C_6D_6 of reaction products of **1** and **2** with L-LA conducted at a molar ratio of L-LA/Zn= 1. * - denotes methyl of toluene.



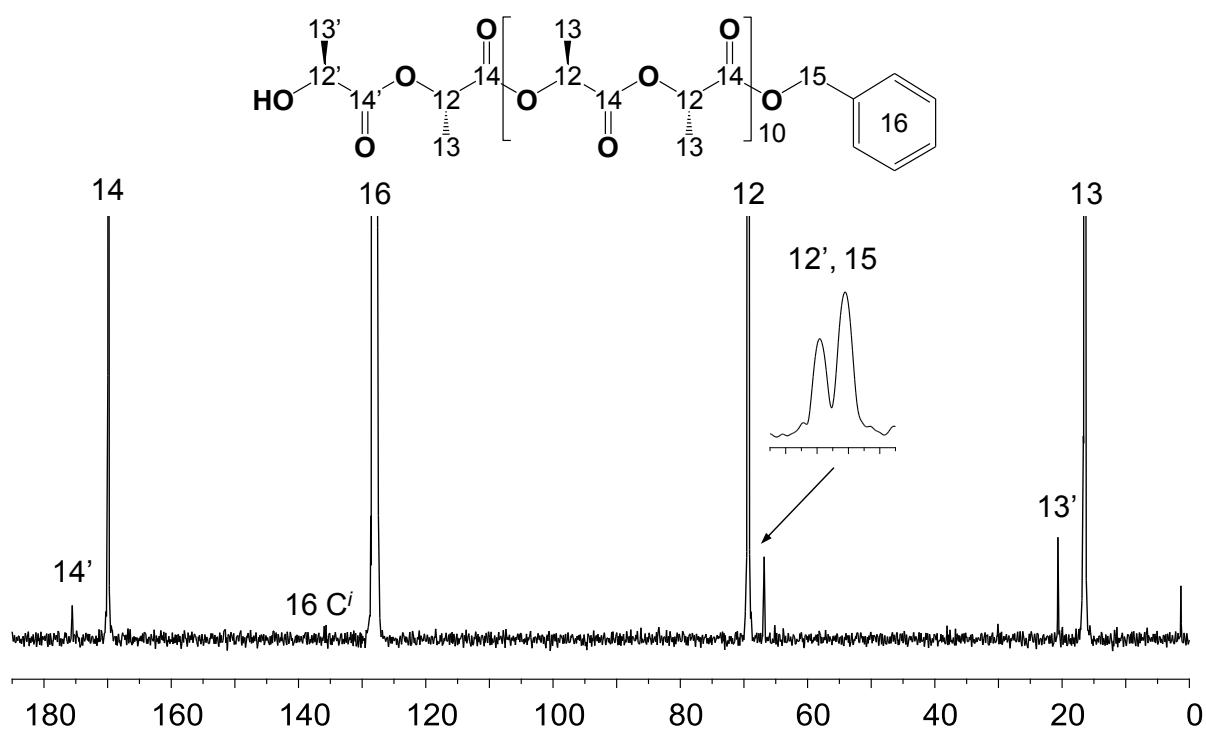
S35. Comparison of the 206-215 *m/z* fragment of the ESI-MS⁺ spectrum with the isotopic distribution computed for the {[Zn(OLA)]⁺} moieties.



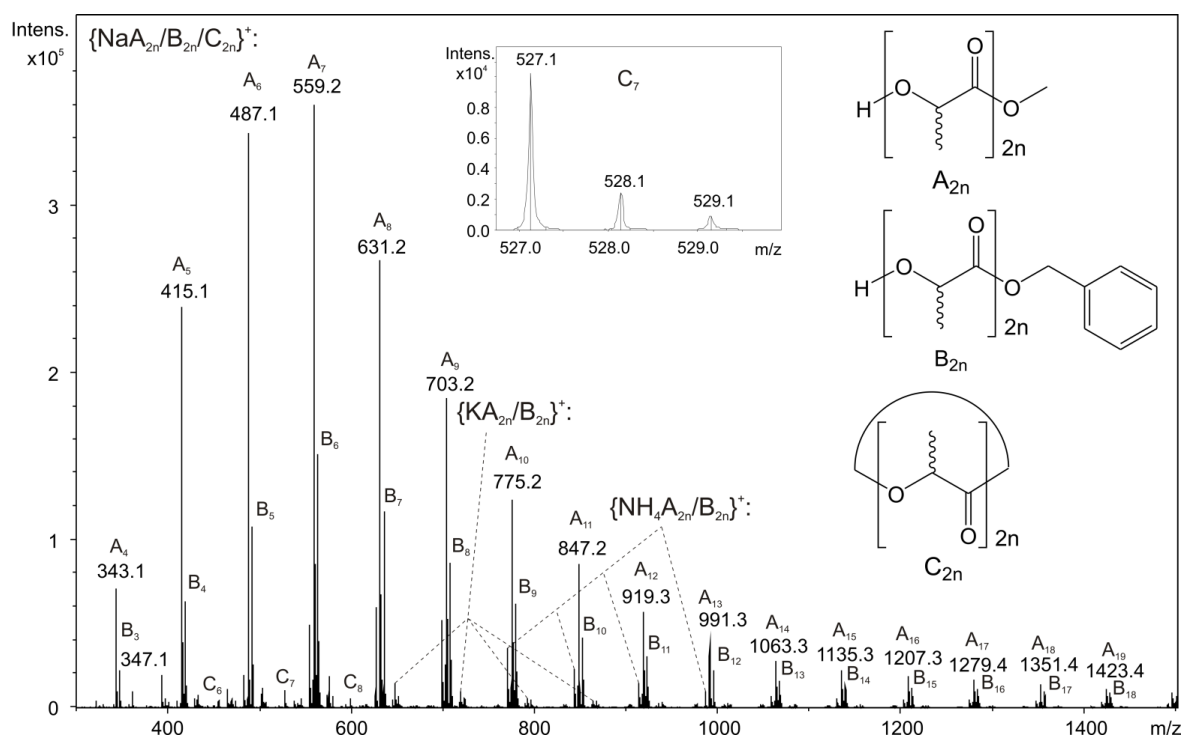
S36. ¹H NMR spectrum in C₆D₆ of reaction products of **1** with 4 equiv of BnOH and L-LA conducted at a molar ratio of L-LA/Zn/BnOH = 10/1/1.



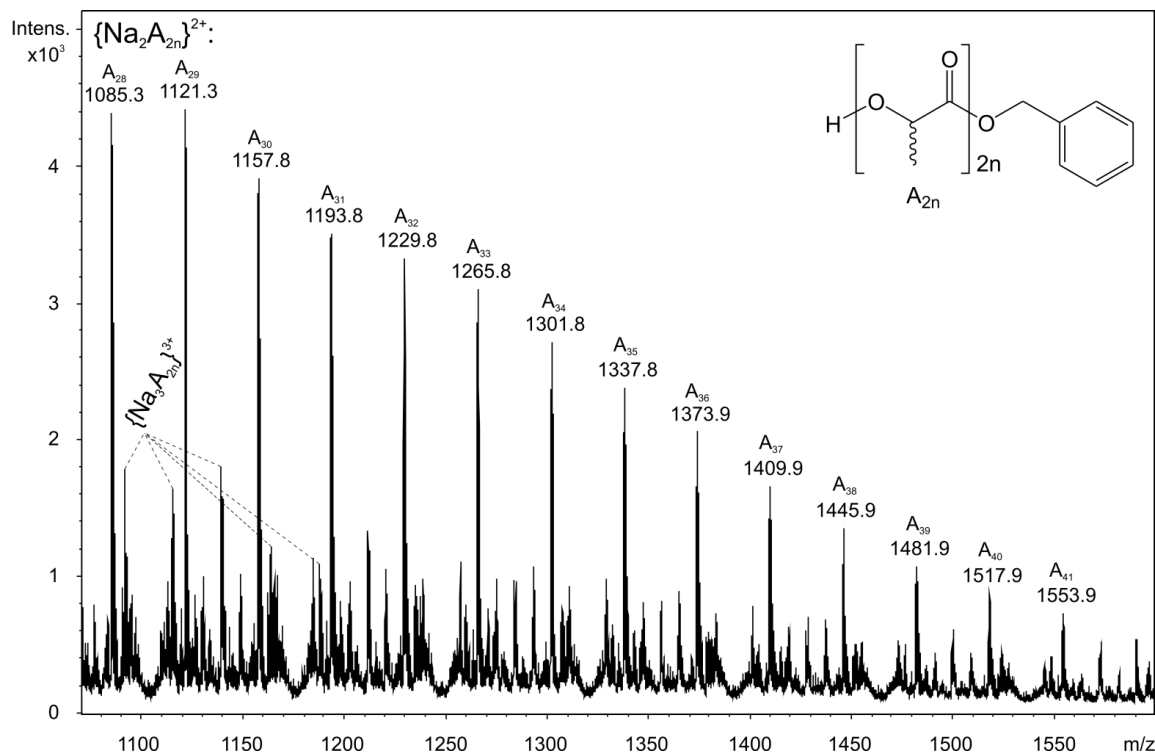
S37. ¹H NMR spectrum of PLLA-OBn in C₆D₆, obtained in reaction of **1** with L-LA in a L-LA/Zn = 10 ratio in the presence of BnOH, and quenched with MeOH.



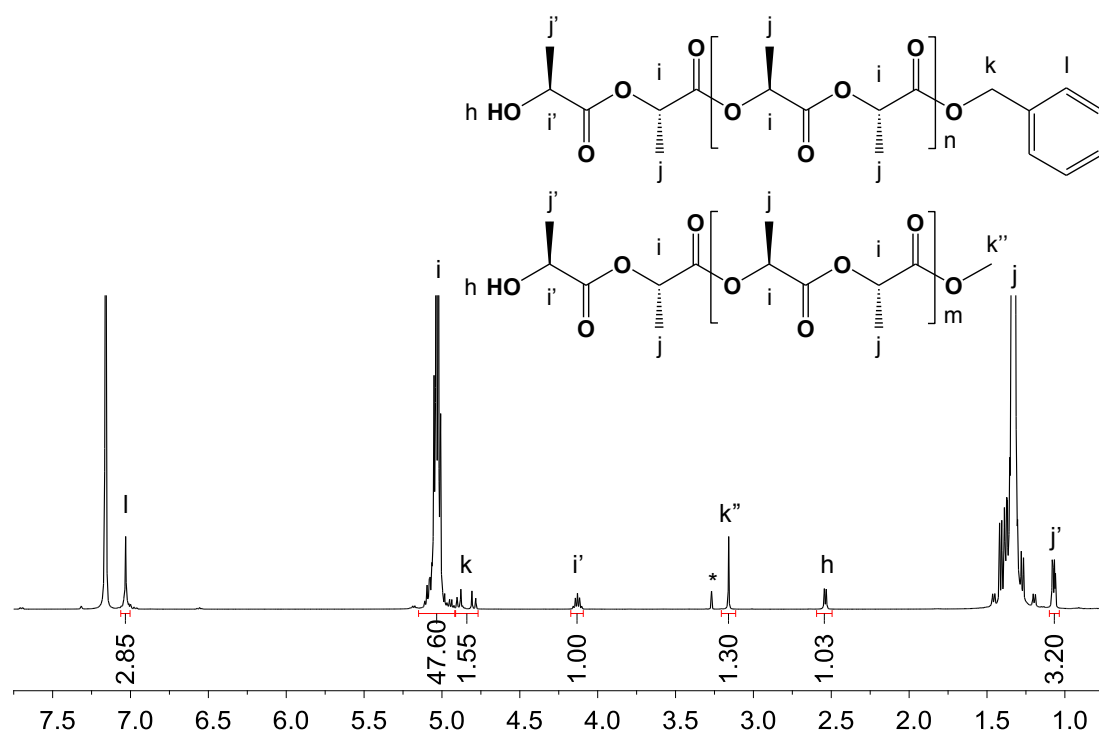
S38. ¹³C NMR spectrum of PLLA-OBn in C₆D₆, obtained in reaction of **1** with L-LA in a L-LA/Zn = 10 ratio in the presence of BnOH, and quenched with MeOH.



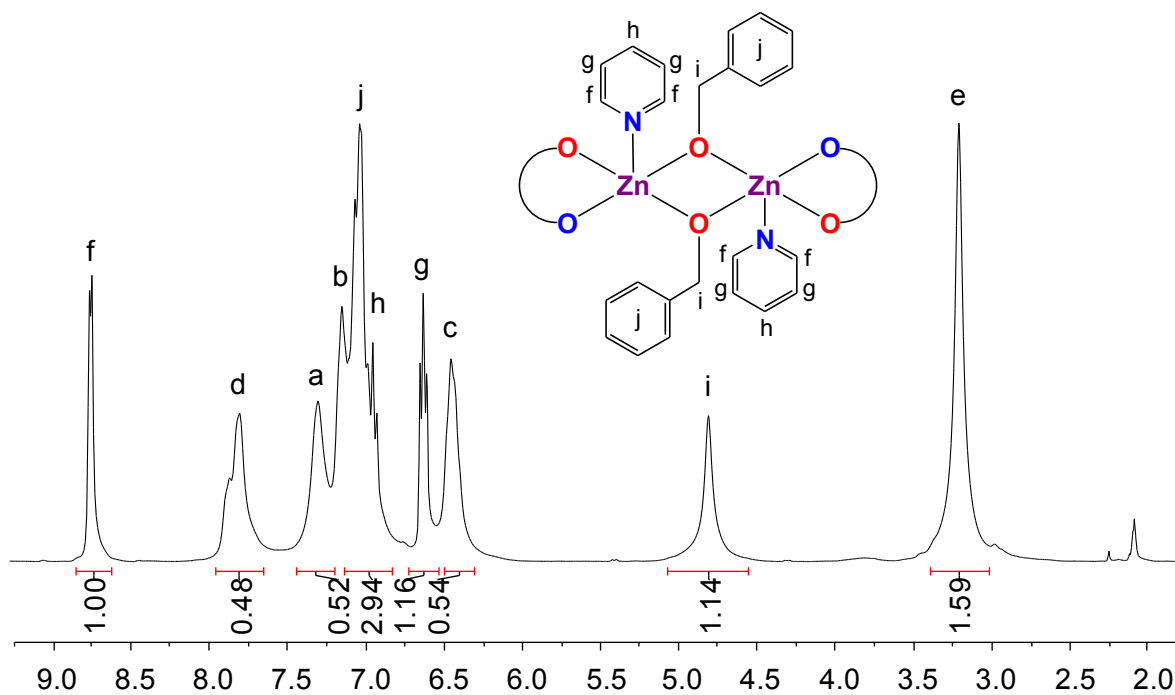
S39. ESI-MS spectrum of mixture of PLLA-OMe, PLLA-OBn and cPLLA, obtained in reaction of **1** with L-LA in L-LA/Zn = 10 ratio in the presence of BnOH, and quenched with MeOH.



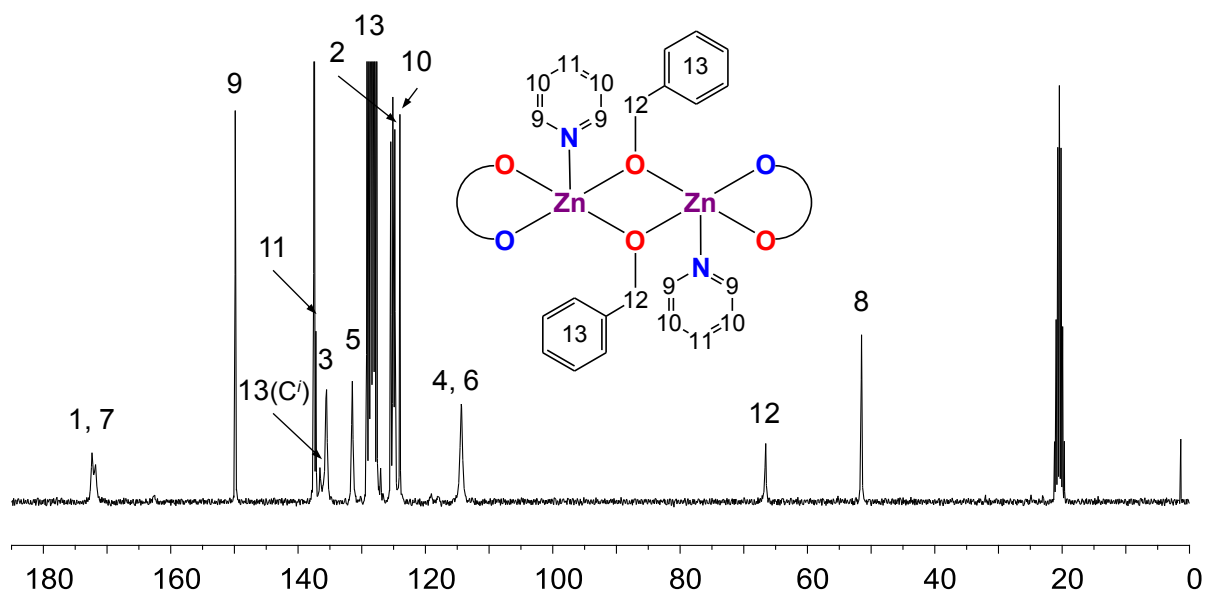
S40. ESI-MS spectrum of PLLA-OBn, obtained in reaction of **2** with L-LA in L-LA/Zn = 10 ratio in the presence of BnOH, and quenched with MeOH.



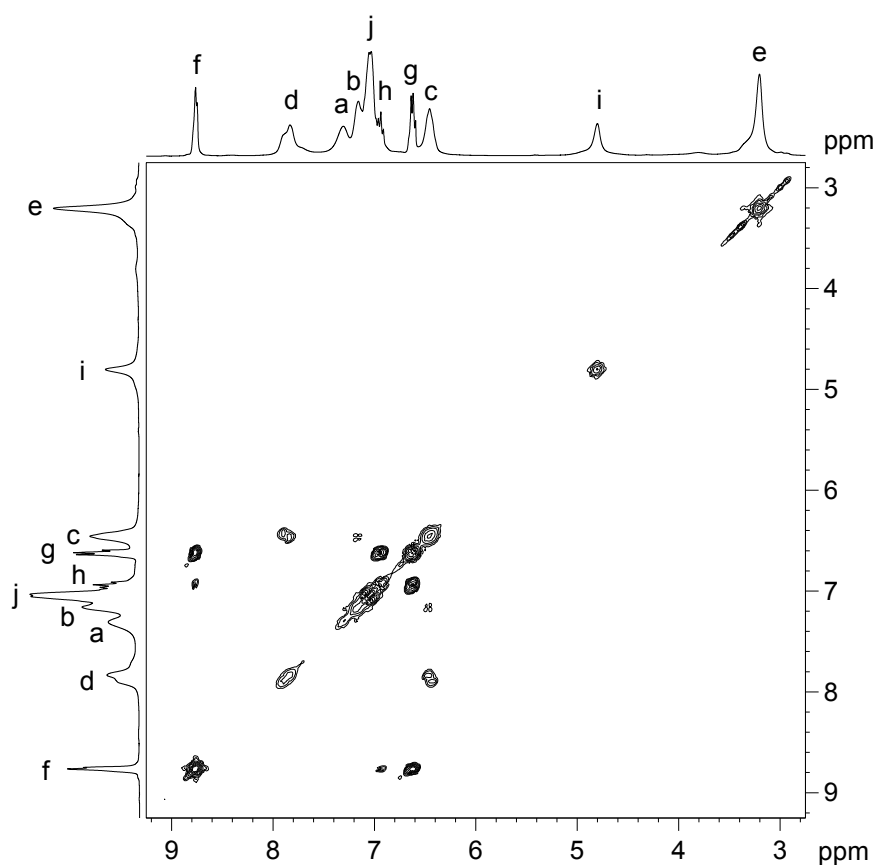
S41. ¹H NMR spectrum in C₆D₆ of mixture of PLLA-OBn and PLLA-OMe obtained in reaction of **1** with L-LA in L-LA/Zn = 25 ratio in the presence of BnOH, and quenched with MeOH. * - denotes free MesalOH.



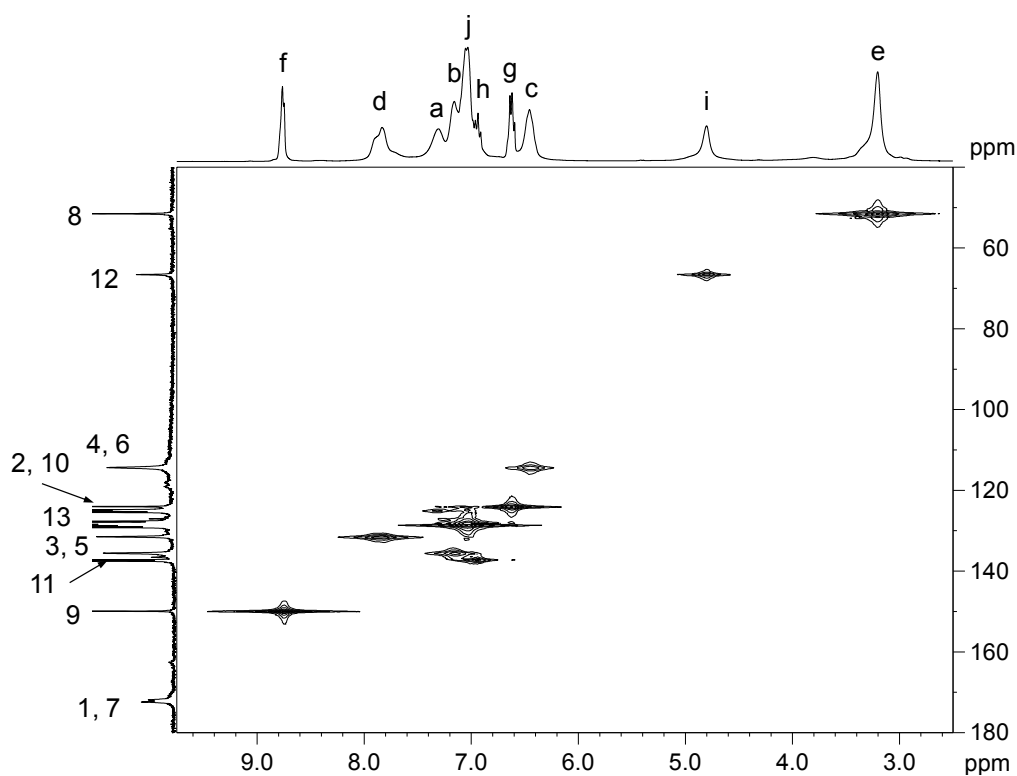
S42. ¹H NMR spectrum of **3** in C₇D₈.



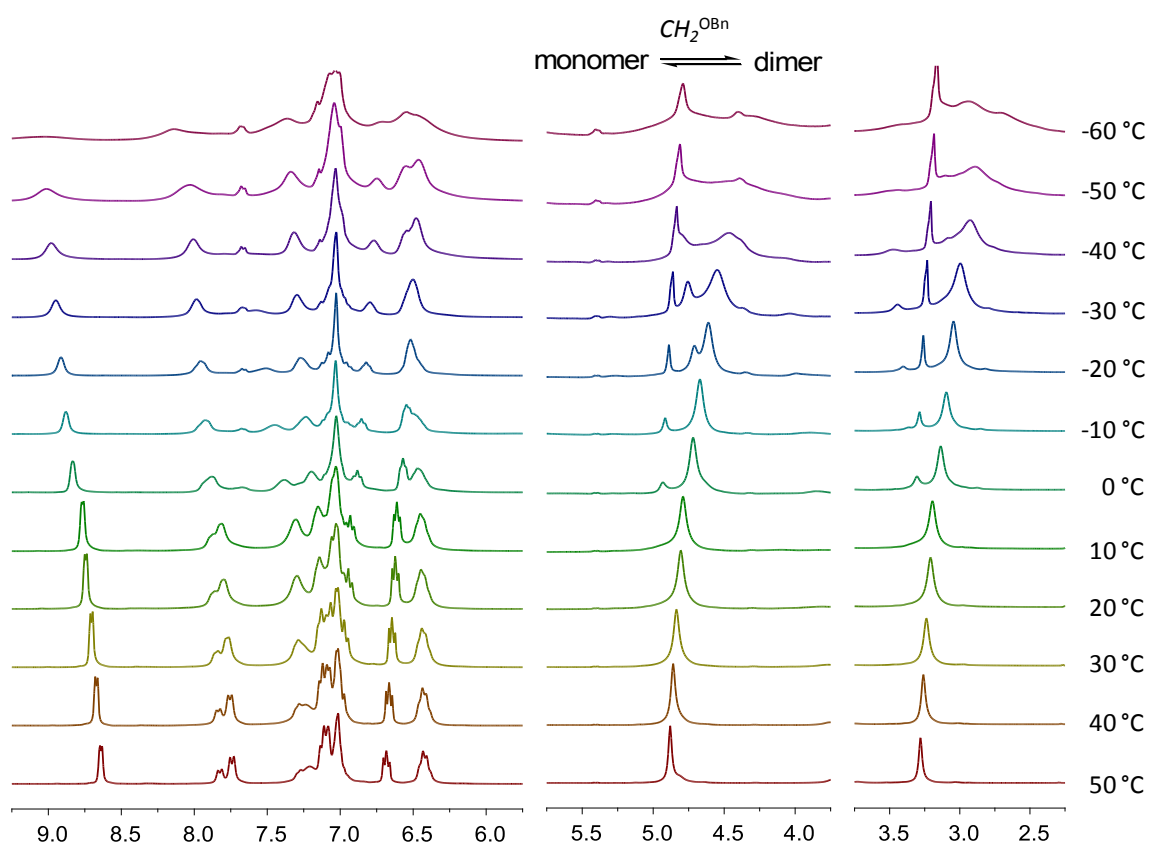
S43. ^{13}C NMR spectrum of **3** in C_7D_8 .



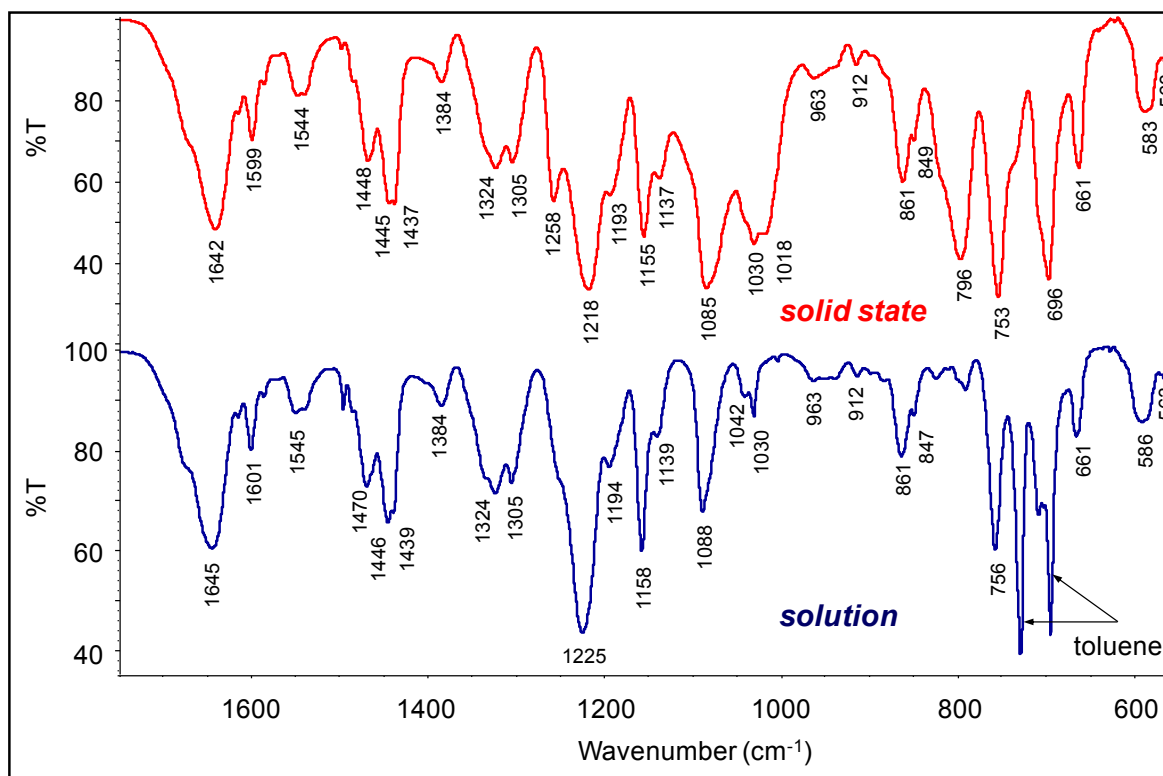
S44. COSY NMR spectrum of **3** in C_7D_8 .



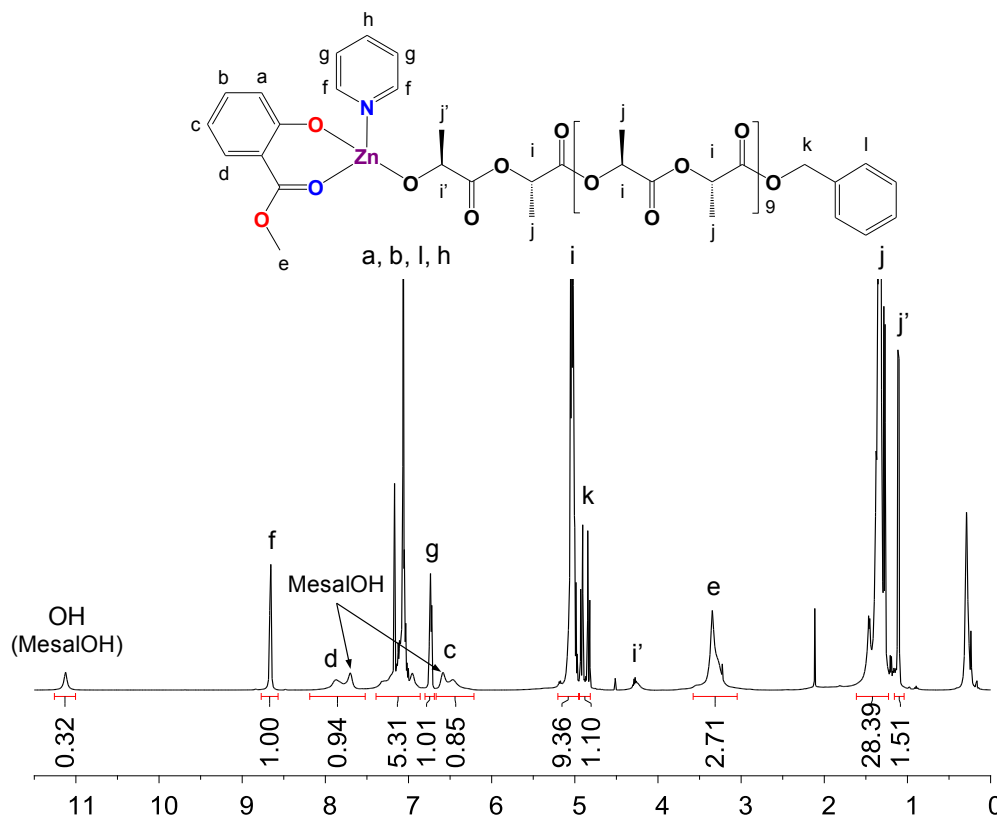
S45. HMQC NMR spectrum of **3** in C_7D_8 .



S46. VT 1H NMR spectra of **3** in C_7D_8 .



S47. FTIR-ATR spectra of **3** in solid state and in toluene solution.



S48. ¹H NMR spectrum in C₆D₆ of reaction products of **2** with BnOH and L-LA conducted at a molar ratio of L-LA/Zn/BnOH = 10/1/1.