Electronic Supplementary Information

Synthesis, structure and catalytic potential of two yttrium diphenylglycinate complexes

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Contents:

Crystallographic section

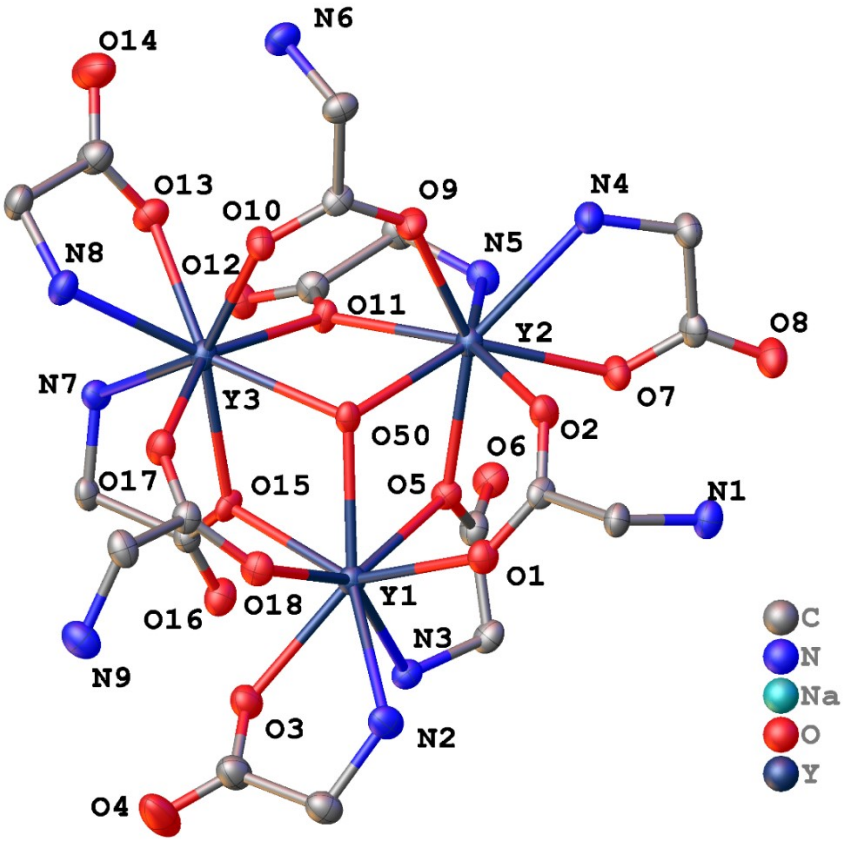

Figure S1. Alternative view of the core of **1**.

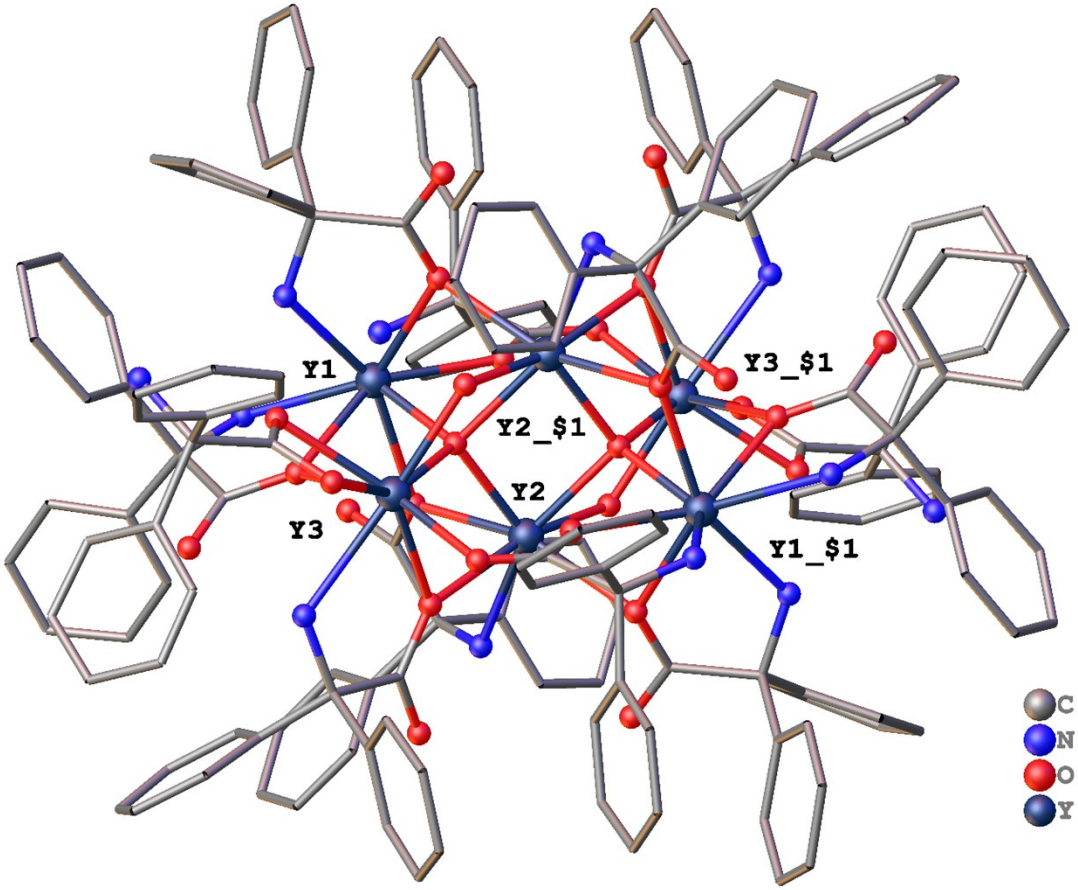

Figure S2. Complete Y_6 cluster with atoms drawn as spheres of arbitrary radius. For clarity, hydrogen atoms and carbon atoms are not shown. Symmetry operation used to generate equivalent atoms: \$1 = 1−*x*, 1−*y*, 1−*z*.

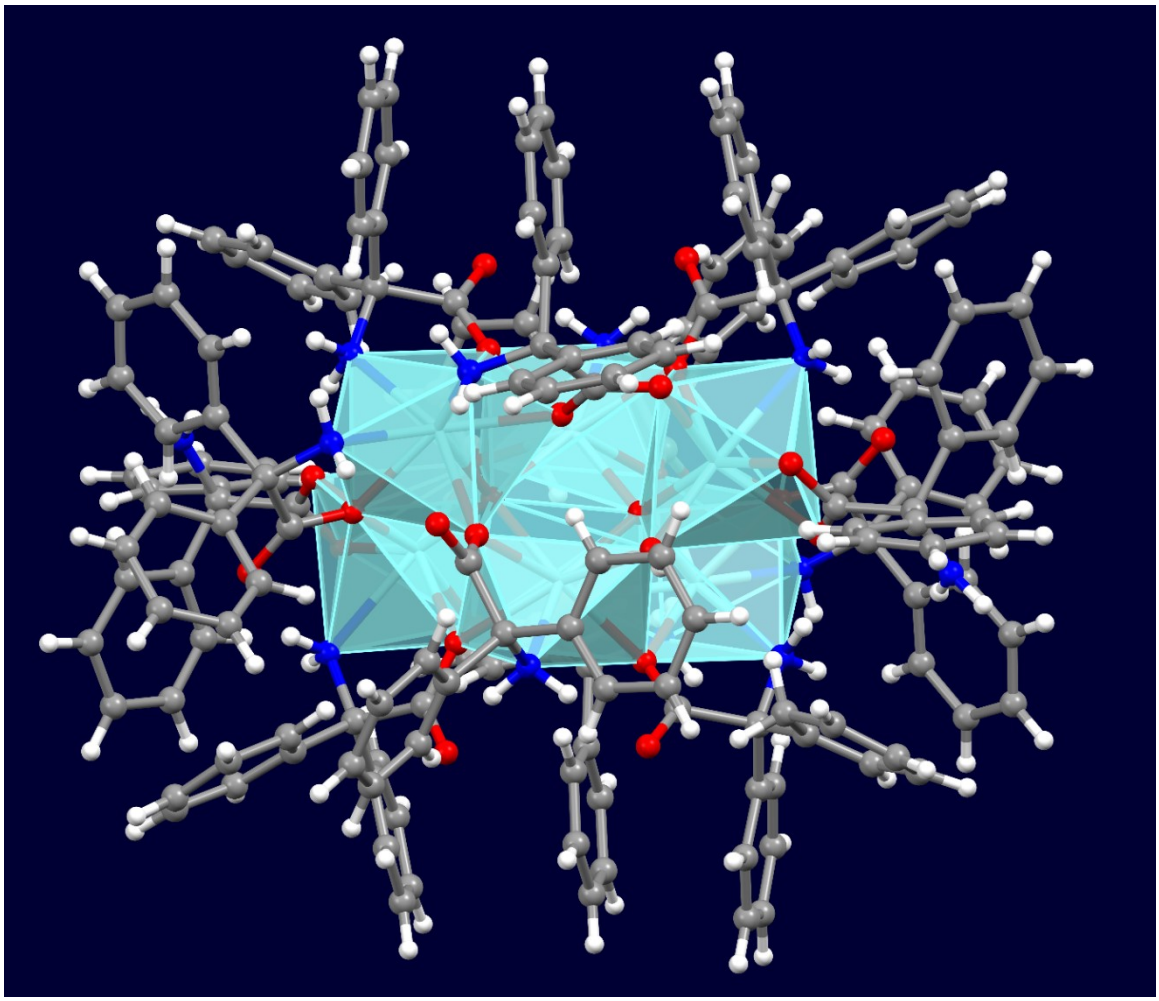

Figure S3. Complete Y_6 cluster with atoms drawn as spheres of arbitrary radius. The coordination environments of each Y atoms are drawn as partially-transparent polyhedral.

Summary by Sample

Dataset Name: D:\icpms\Date\2026\202604\20260410

	Net Intensity				Concentration			
	Value	SD	RSD	Units	Value	SD	RSD	Units
Sample ID : Y(OiPr)3								
Method File : na.mth								
Calibration File :								
Na23	2.18e-03	7.64e-05	3.51	cps	1.61e+04	952	5.92	ppb
Sc -1 (IS) -1	7.24e+05	9.3e+03	1.28	cps				
Sample ID : LH3								
Method File : na.mth								
Calibration File :								
Na23	1.65e-02	4.26e-04	2.58	cps	2.13e+05	5.8e+03	2.72	ppb
Sc -1 (IS) -1	7.e+05	1.04e+04	1.48	cps				

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Table S1. ICP data for LH_3 and [Y(O*i*Pr)$_3$].

The inductively coupled plasma (ICP) analysis was conducted following the microwave digestion pretreatment of samples. Specifically, 0.05g of sample was accurately weighed and transferred into a digestion vessel, followed by the addition of 5 mL of nitric acid (HNO_3) and 2 mL of hydrogen peroxide (H_2O_2) as digestion reagents. The microwave digestion was performed at 220 °C for 30 min. After digestion and cooling to room temperature, the digestate was transferred to a volumetric flask and diluted to a final volume of 50 mL with deionized water. The solution was thoroughly mixed, and the supernatant was carefully collected by standing. Finally, the collected supernatant was subjected to instrumental analysis using a PerkinElmer NexION 5000G ICP instrument.

Catalysis section

Copolymerization of propylene oxide with CO_2

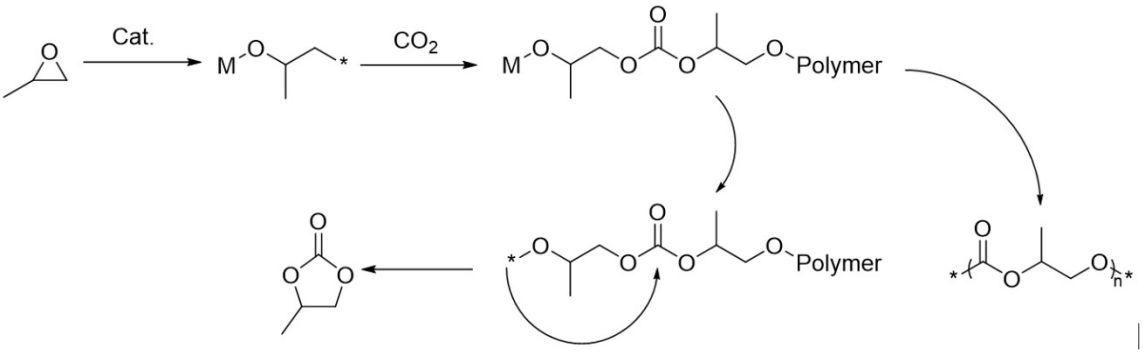


Figure S4. Proposed mechanism for the copolymerization of propylene oxide and CO_2.

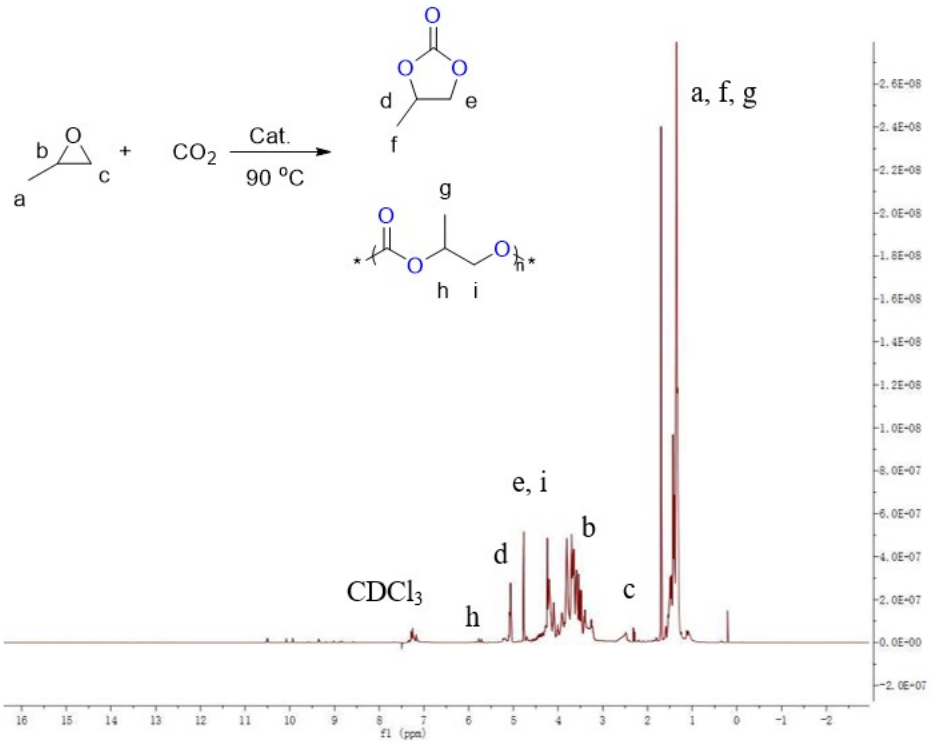
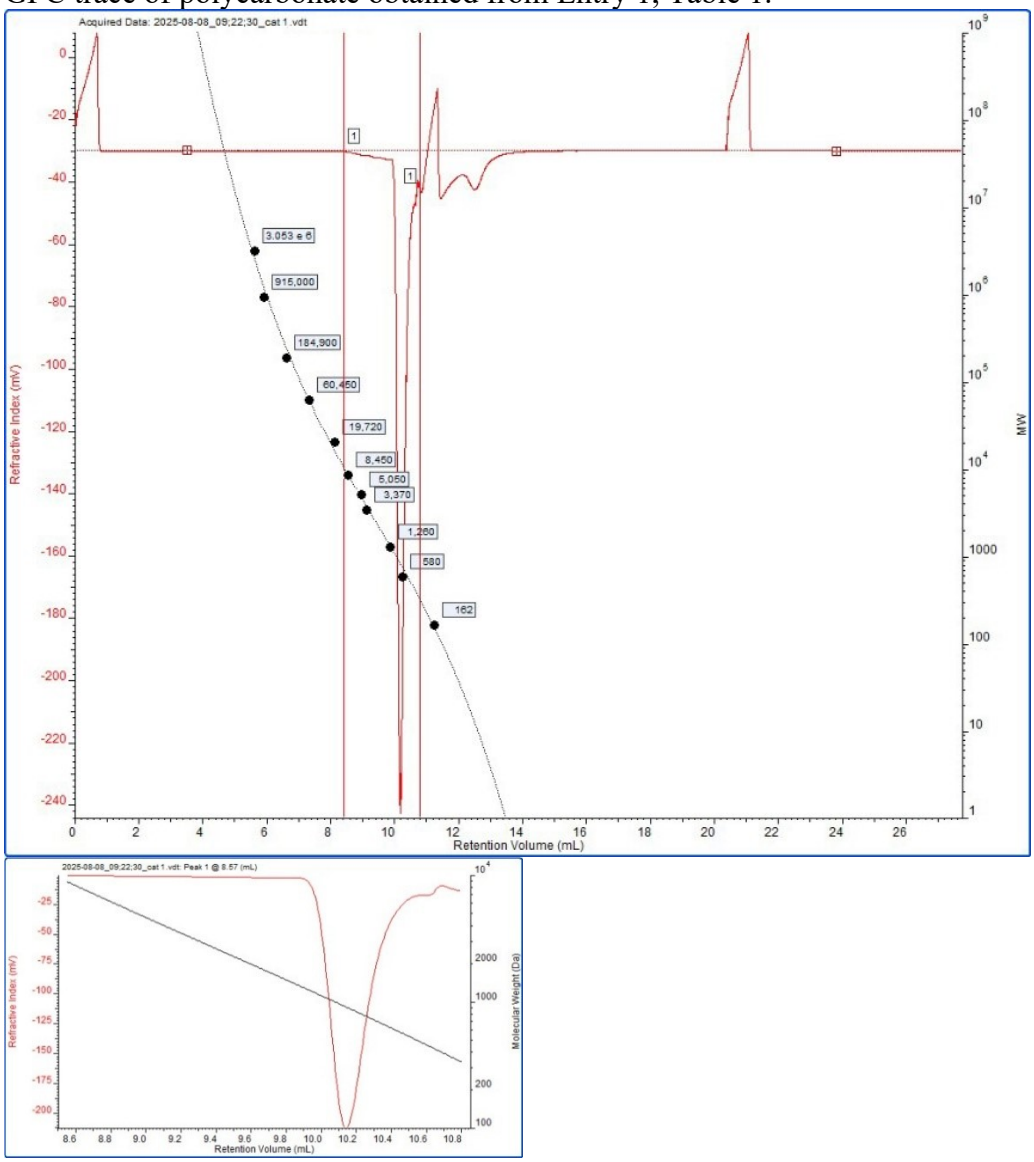


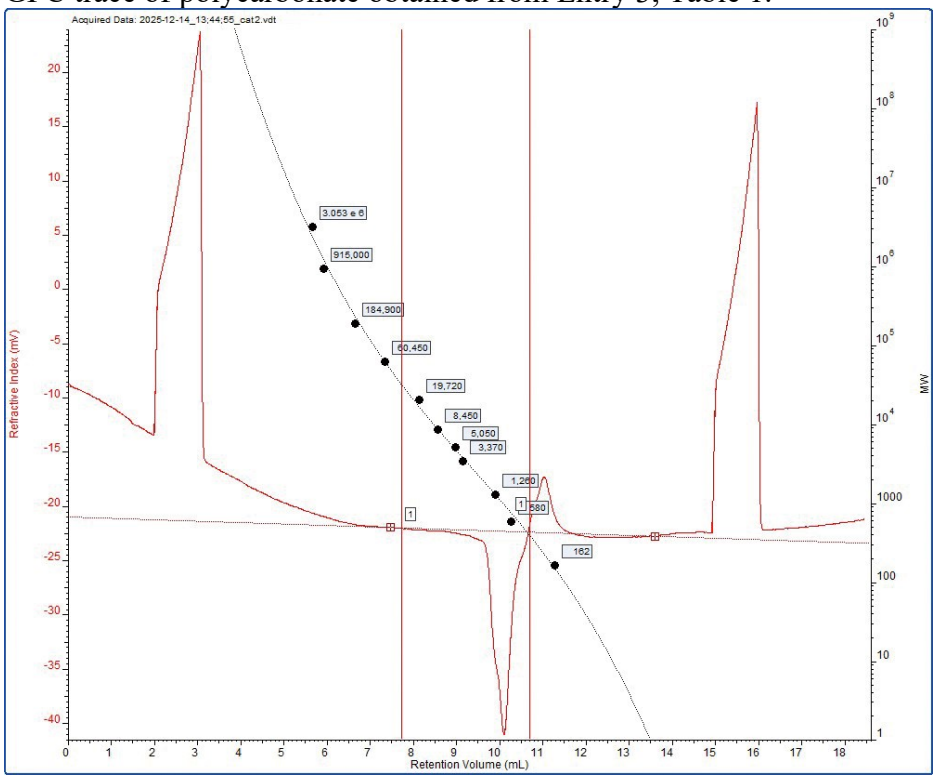
Figure S5. ^1H NMR of the spectrum ($CDCl_3$, 400 MHz, 298 K) of the cyclic/poly(propylene carbonate) synthesized with **1** (Entry 1, Table 2).

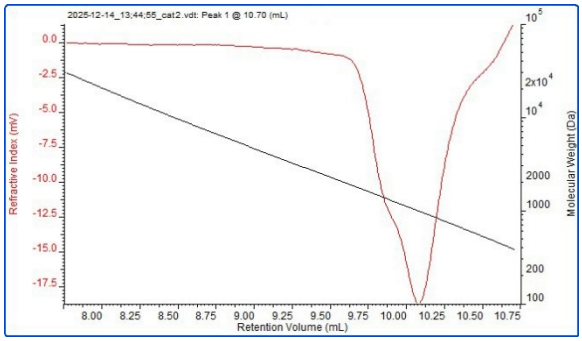
GPC trace of polycarbonate obtained from Entry 1, Table 1.



Peak	1
Ret Vol (mL)	8.571
*M*n (Da)	755
*M*w (Da)	966
*M*z (Da)	1,177
*M*p (Da)	8,978
*M*w/*M*n	1.280

GPC trace of polycarbonate obtained from Entry 3, Table 1.





Peak	1
Ret Vol (mL)	10.704
*M*n (Da)	1,253
*M*w (Da)	1,441
*M*z (Da)	3,401
*M*w/*M*n	1.150

Figure S6. Selected GPC traces for copolymerization of propylene oxide with CO_2.

Ring opening polymerization of ε-CL and δ-VL

MALDI-ToF spectra

PCL

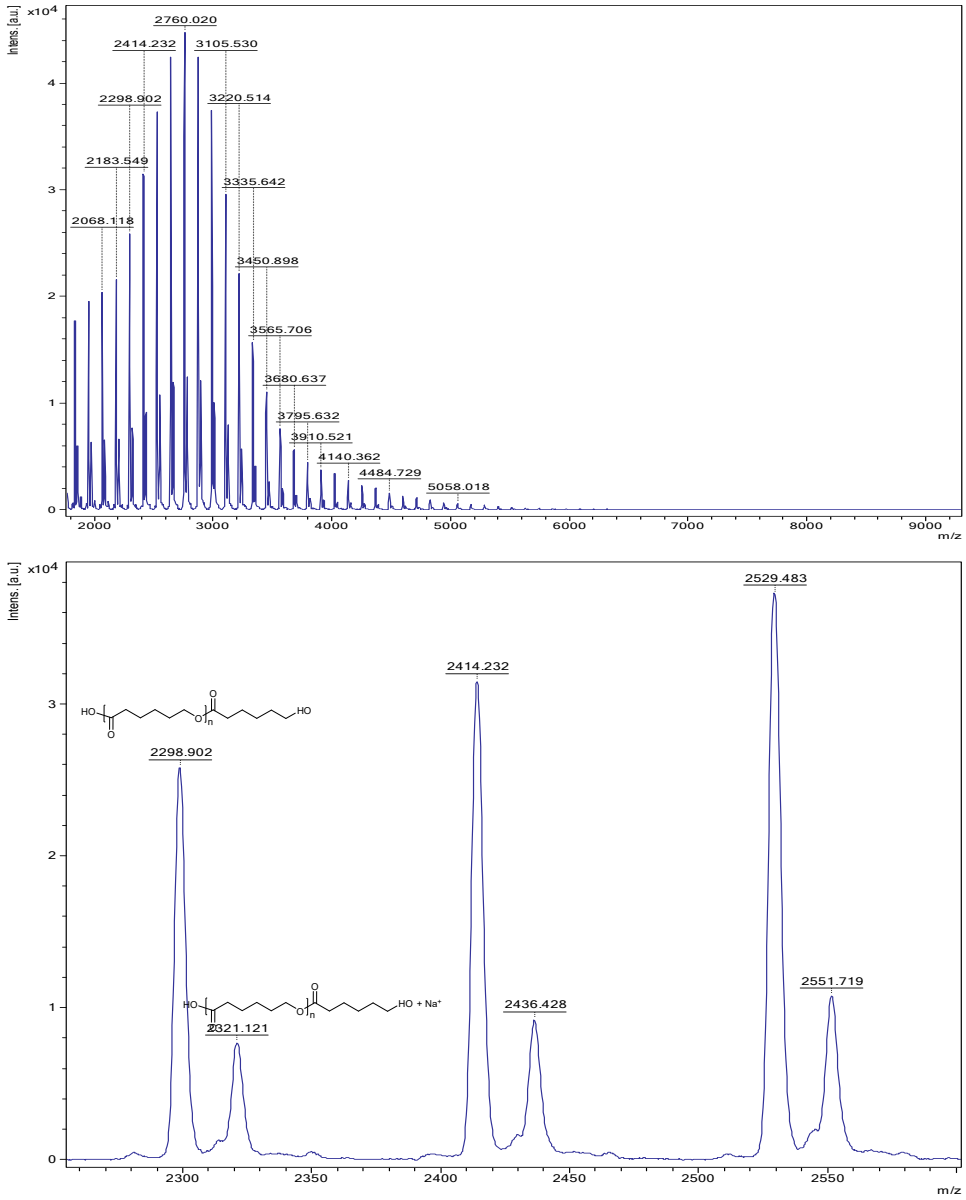


Figure S7. MALDI-ToF spectrum of PCL obtained from entry 1, Table 3 (**1**, 500: 1, at 110 ºC in toluene, N_2). The main family is linear polymers with H/OH end groups, [M = n × 114.14 (ε-CL) + 18 (H/OH)] e.g., n = 20, calc. 2299.4, obsv. 2298.9. Minor family is linear polymers with H/OH end groups as sodium adducts, e.g for n = 20, calc = 2322.4, obsr. = 2321.1.

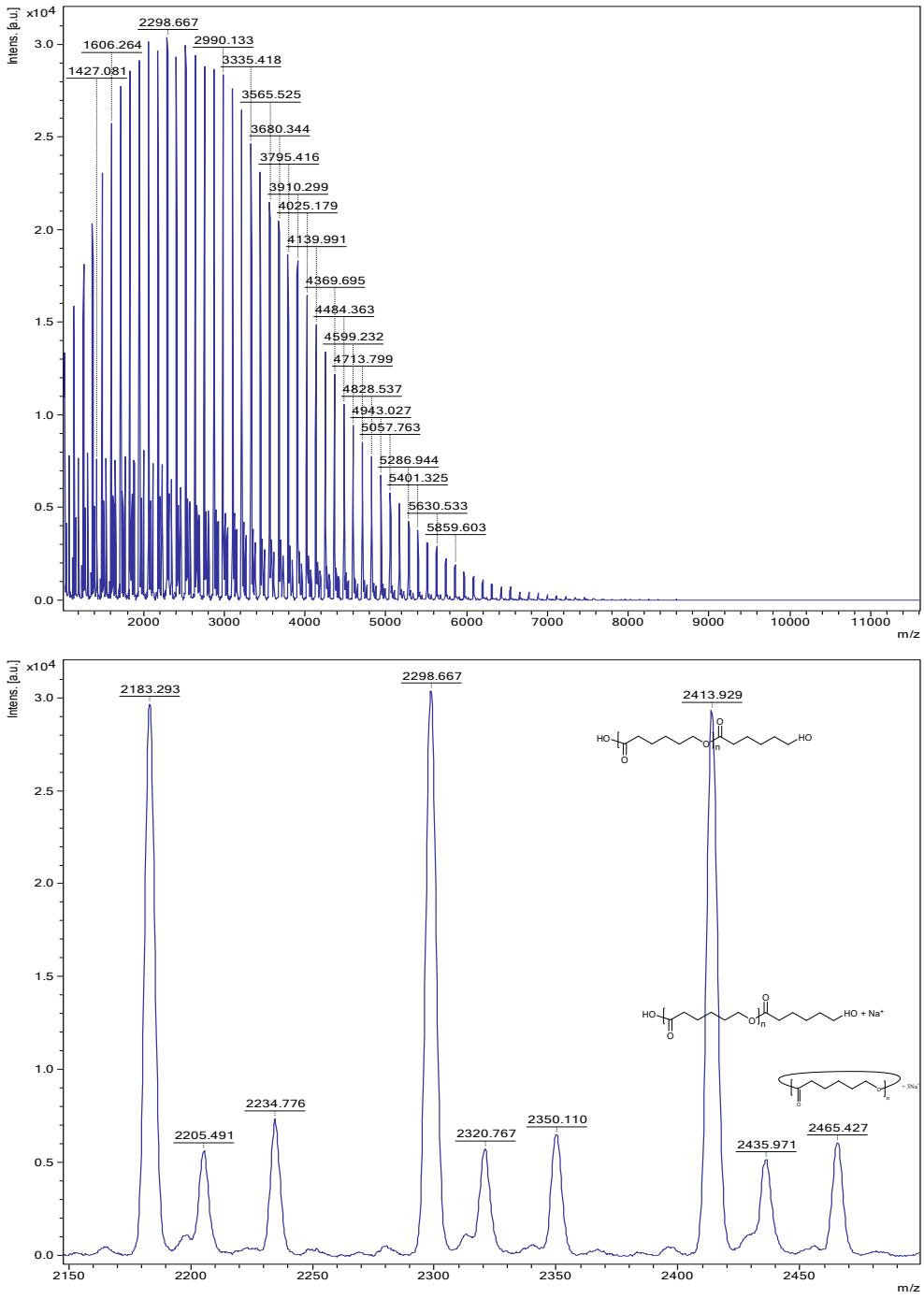


Figure S8. MALDI-ToF spectrum of PCL obtained from entry 2, Table 3 (**1**, 500: 1, melt, N_2). The main family are linear polymers with H/OH end groups [M = n × 114.14 (ε-CL) + 18 (H/OH)] e.g., n = 21, calc. 2414.9, obsv. 2413.9. Minor families include cyclic polymers as sodium adducts, e.g. for n = 21, calc. = 2,436.5, obsr. = 2436.0.

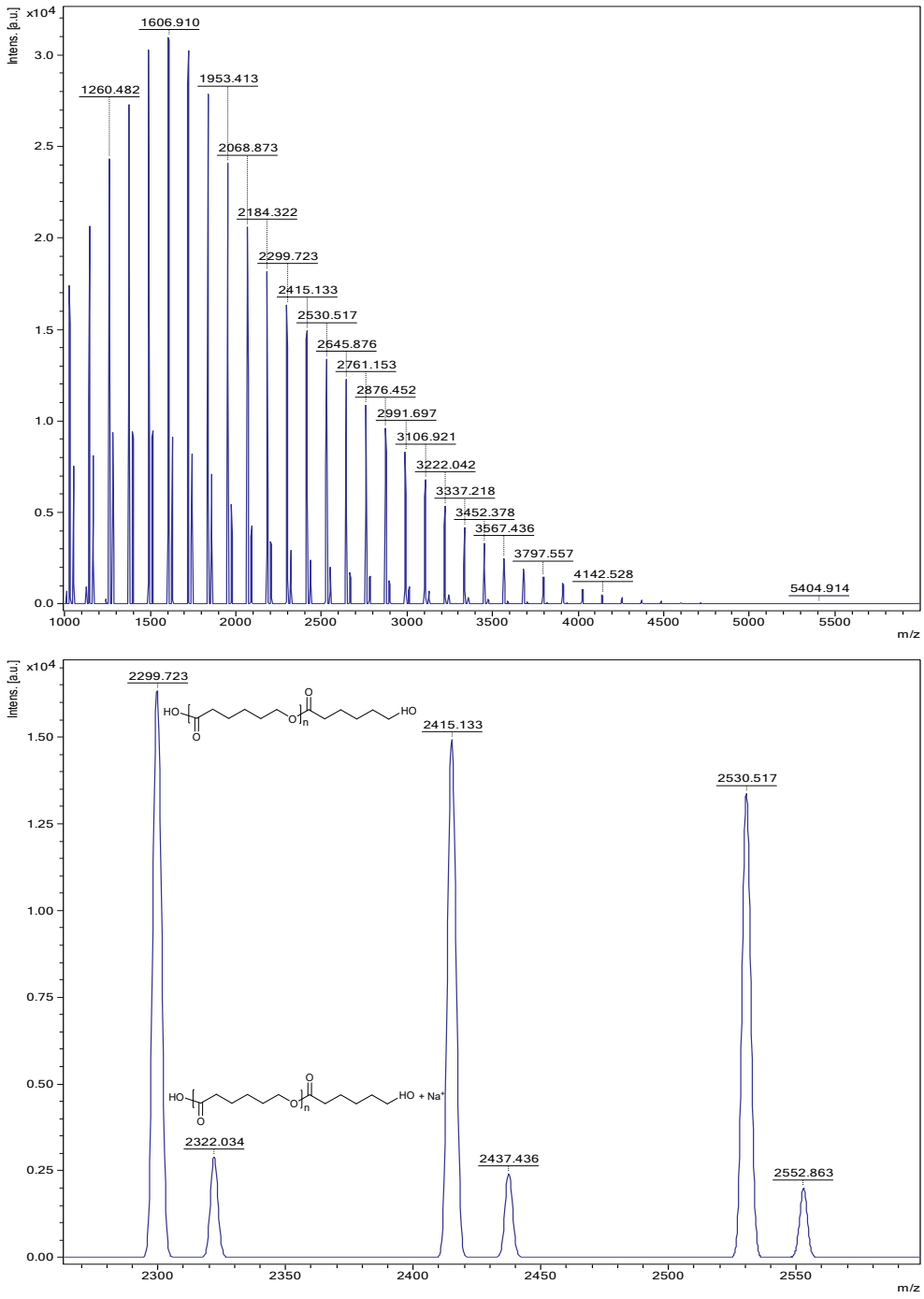


Figure S9. MALDI-ToF spectrum of PCL obtained from entry 9, Table 3 ([$Y(OiPr_3)$], 500: 1, melt, N_2). Present is a family of linear polymers as the sodium adducts [M = 17 (OH) + 1(H) + n × 114.14 (ε-CL) +22.99 (Na^+)] e.g., calc. 2322.8, n = 20, obsv. 2322.0.

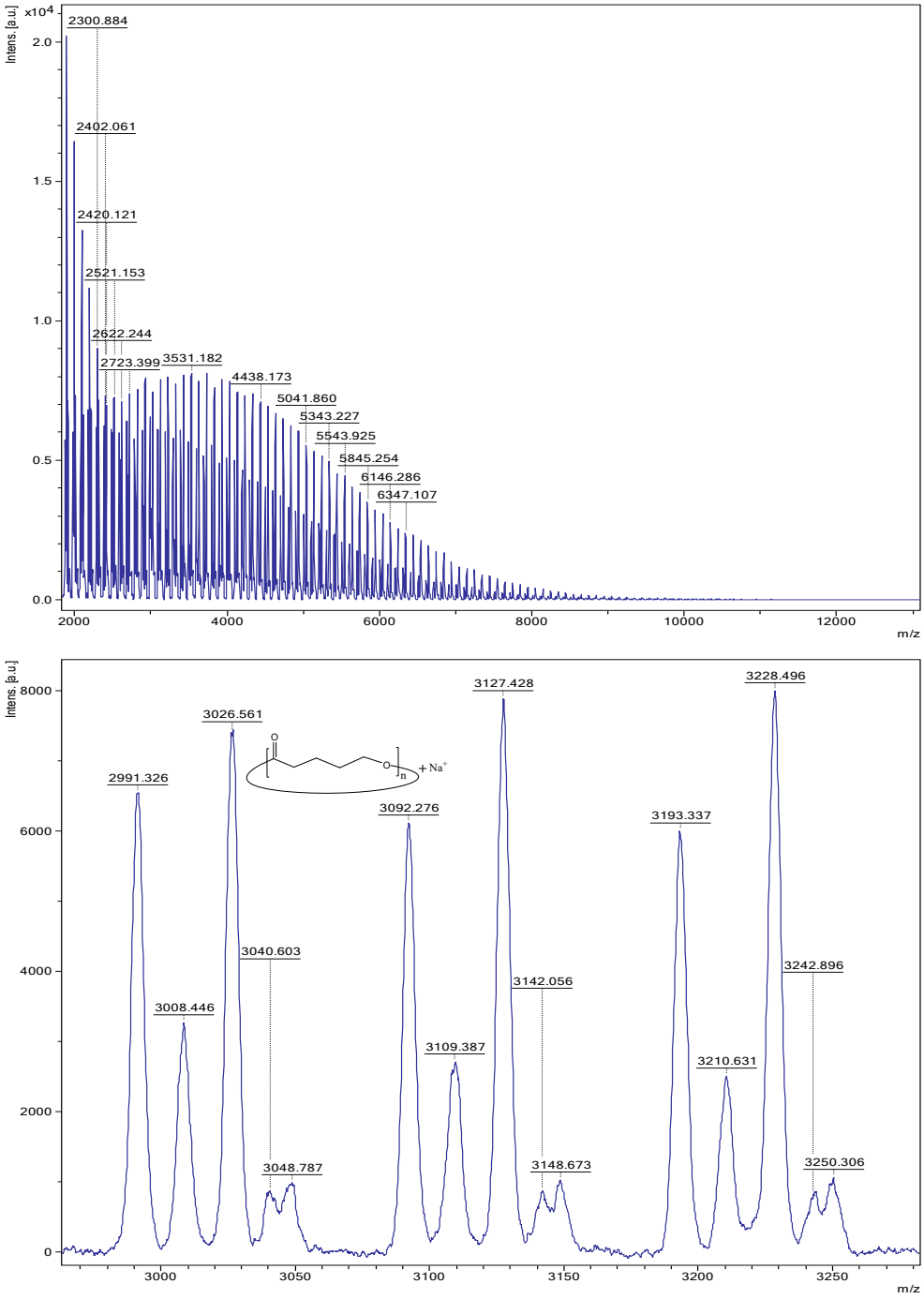


Figure S10. MALDI-ToF spectrum of PVL obtained from entry 11, Table 3 (**1**, 500: 1, at 110 ^{o}C in toluene, N_2). The main family is cyclic polymers as the sodium adducts [M = n × 100.12 (VL) + 22.99 (Na^+)] e.g., calc. 3026.6, n = 30, obsv. 3026.6.

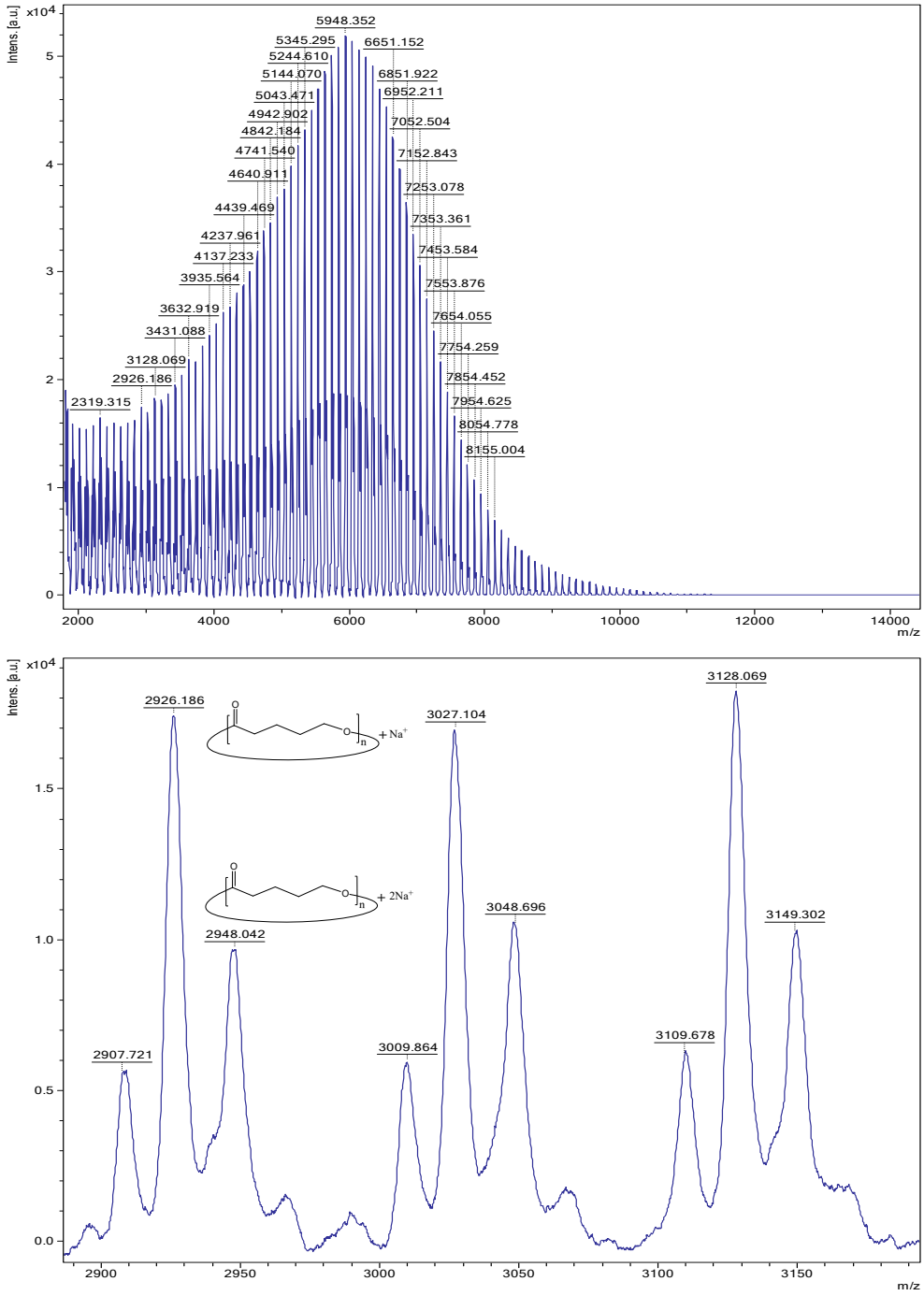


Figure S11. MALDI-ToF spectrum of PVL obtained from entry 19, Table 3 ([Y(O*i*Pr)$_3$], 500:1, melt, N_2). The main family is cyclic polymers as the sodium adducts [M = n × 100.12 (VL) + 22.99 (Na^+)] e.g., calc. 2926.5, n = 29, obsv. 2926.2.

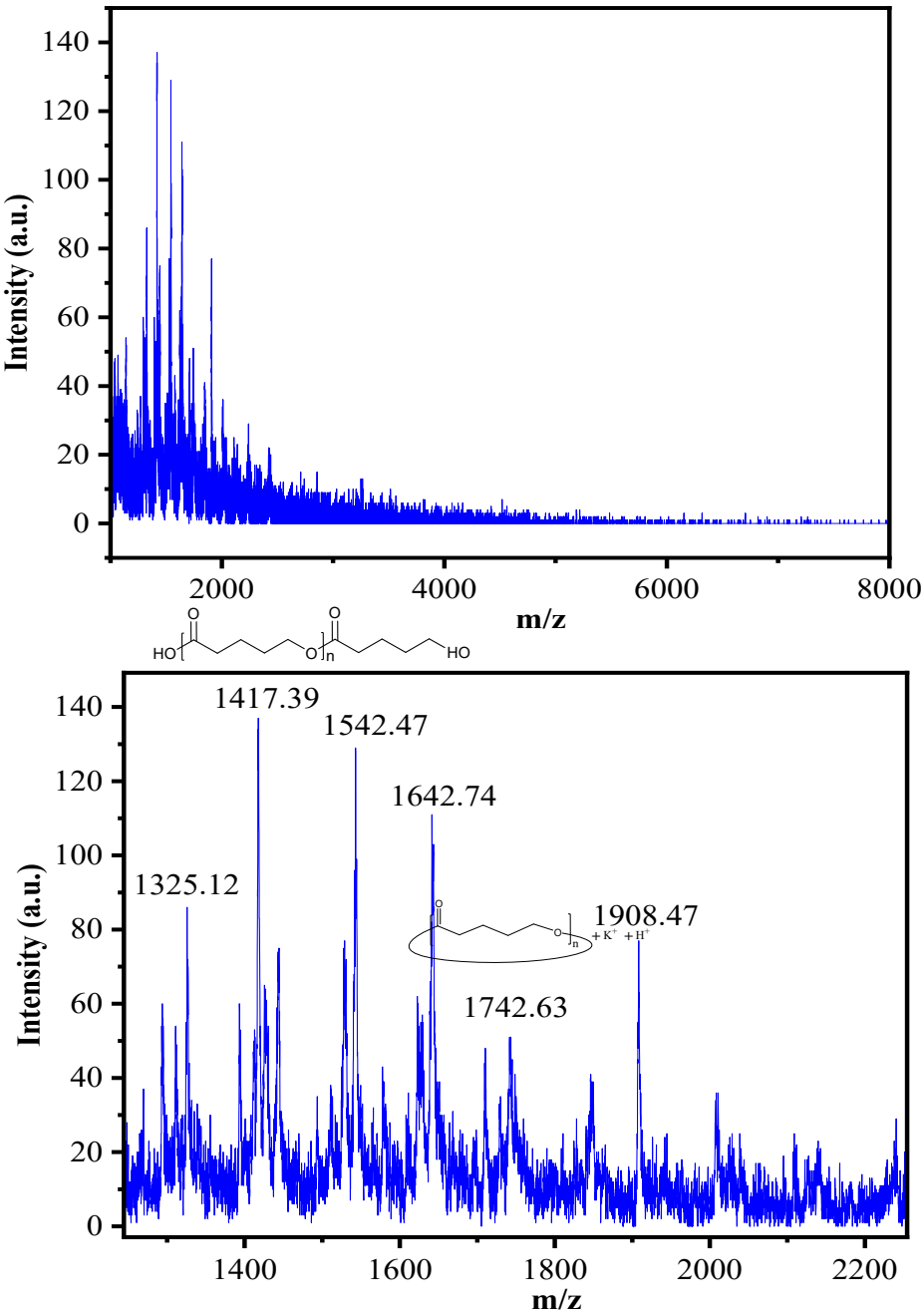


Figure S12. MALDI-ToF spectrum of PVL obtained from entry 14, Table 3 (**2**, 500: 1, at 110 °C in toluene, N_2). The main family is linear polymers as the sodium adducts [M = n × 100.12 (VL) + 17 (OH) + 1(H)] e.g., calc. 1418.7, n = 14, obsv. 1417.4. Minor families include cyclic polymers as proton/potassium adducts is a family of cyclic polymers as the potassium adducts [M = n × 100.12 (VL) + 1 (H^+) + 39.09 (K^+)] e.g., calc. 2360.8, n = 20, obsv. 2359.3.

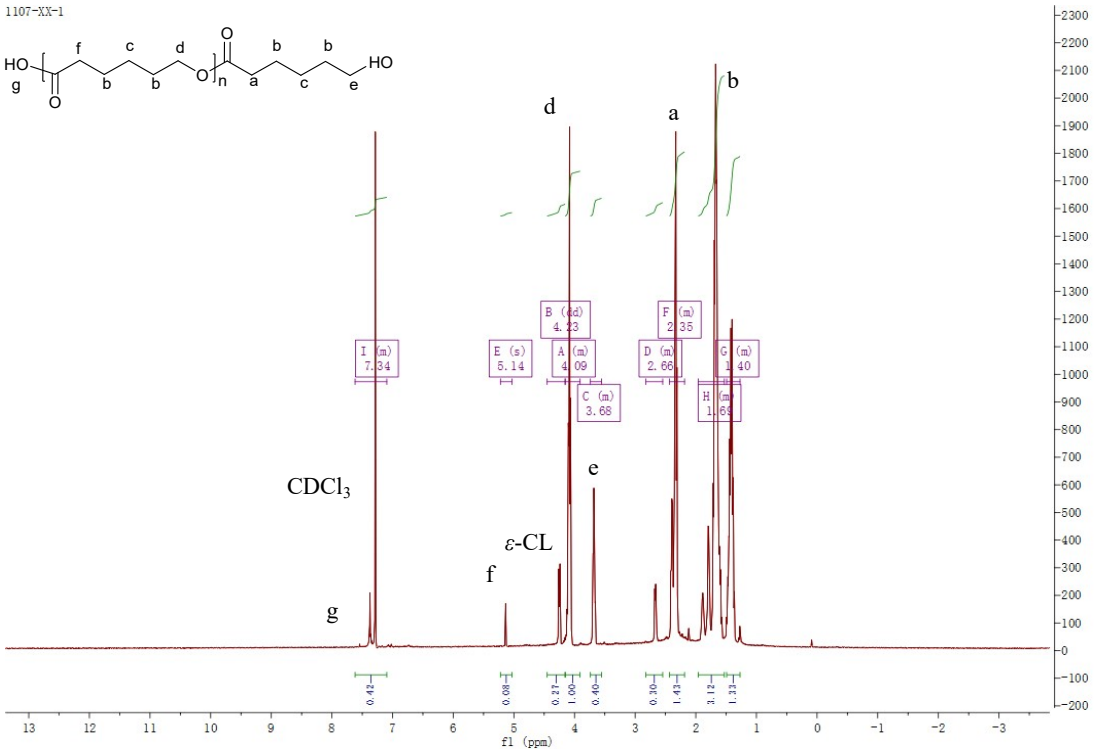


Figure S13. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz, 298 K) of the PCL synthesized with **2** (run 4, Table 3).

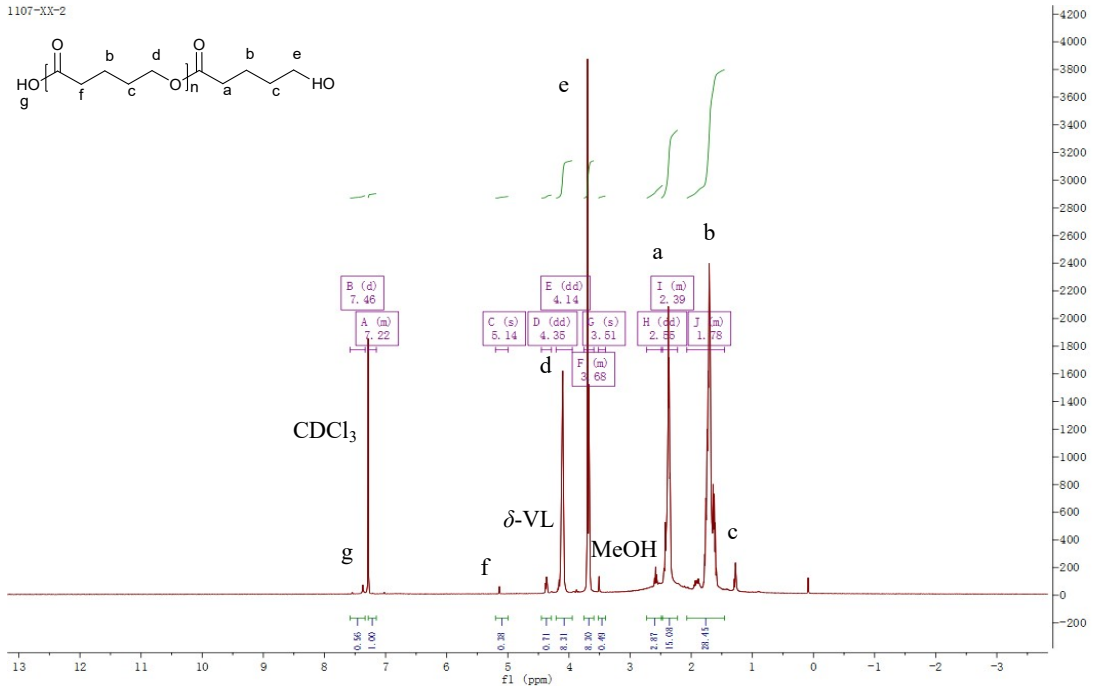
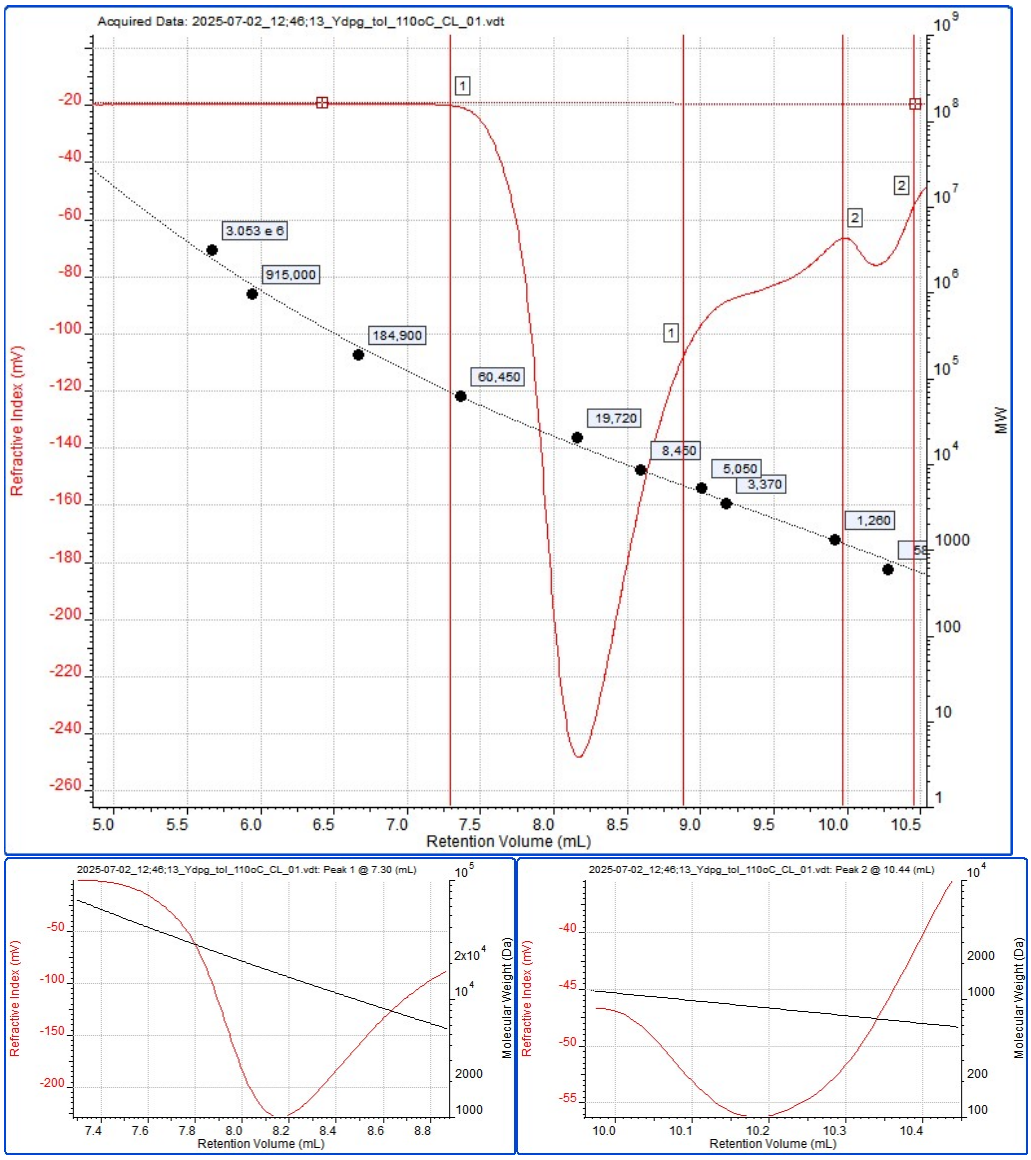


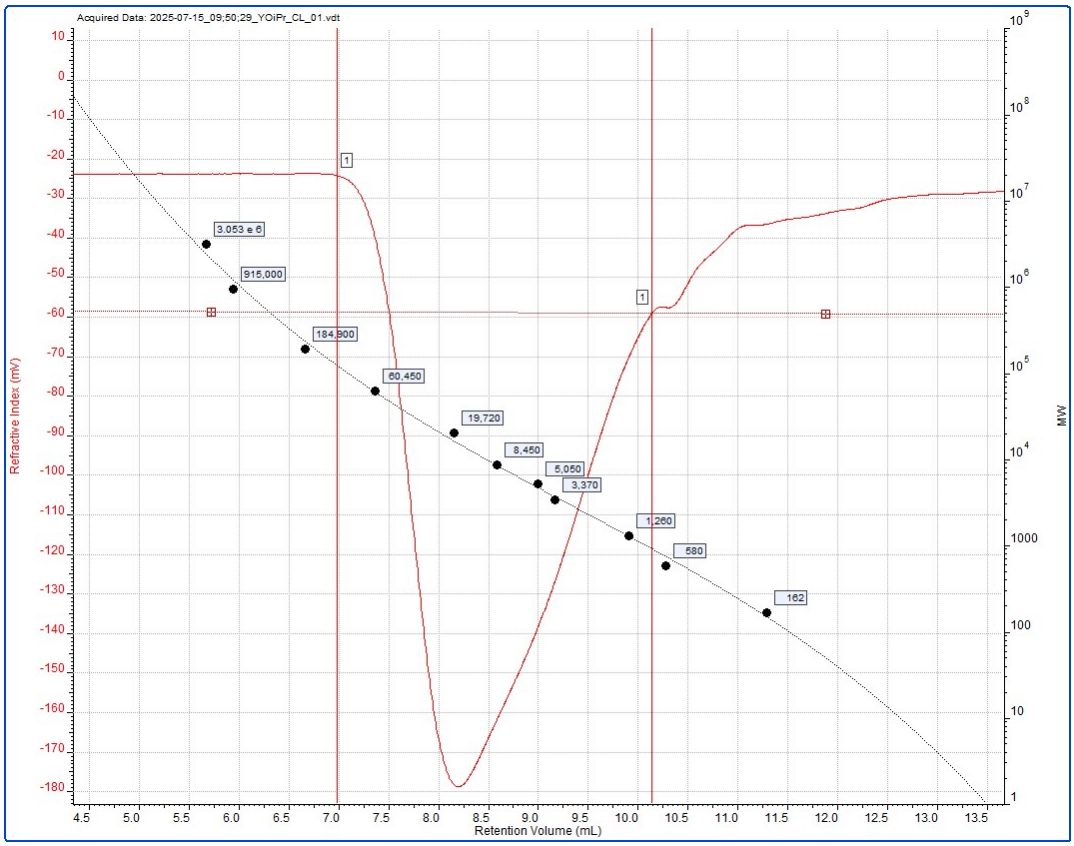
Figure S14. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz, 298 K) of the PVL synthesized with **2** (run 14, Table 3).

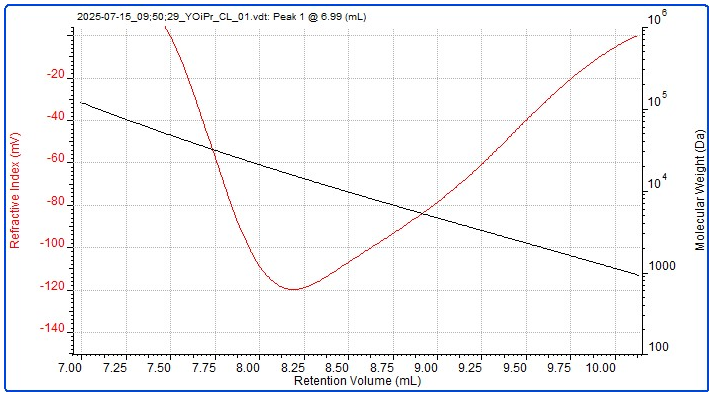
GPC trace for PCL using **1** (entry 1, Table 3)



Peak	1	2
Ret Vol (mL)	7.298	10.438
*M*n (Da)	12,211	826
*M*w (Da)	14,965	858
*M*z (Da)	18,346	889
*M*p (Da)	66,791	581
*M*w/*M*n	1.226	1.039

GPC trace for PCL using [Y(O*i*Pr)$_3$] (entry 9, Table 3).





Peak 1

Ret Vol (mL) 6.994

*M*n (Da) 5,815

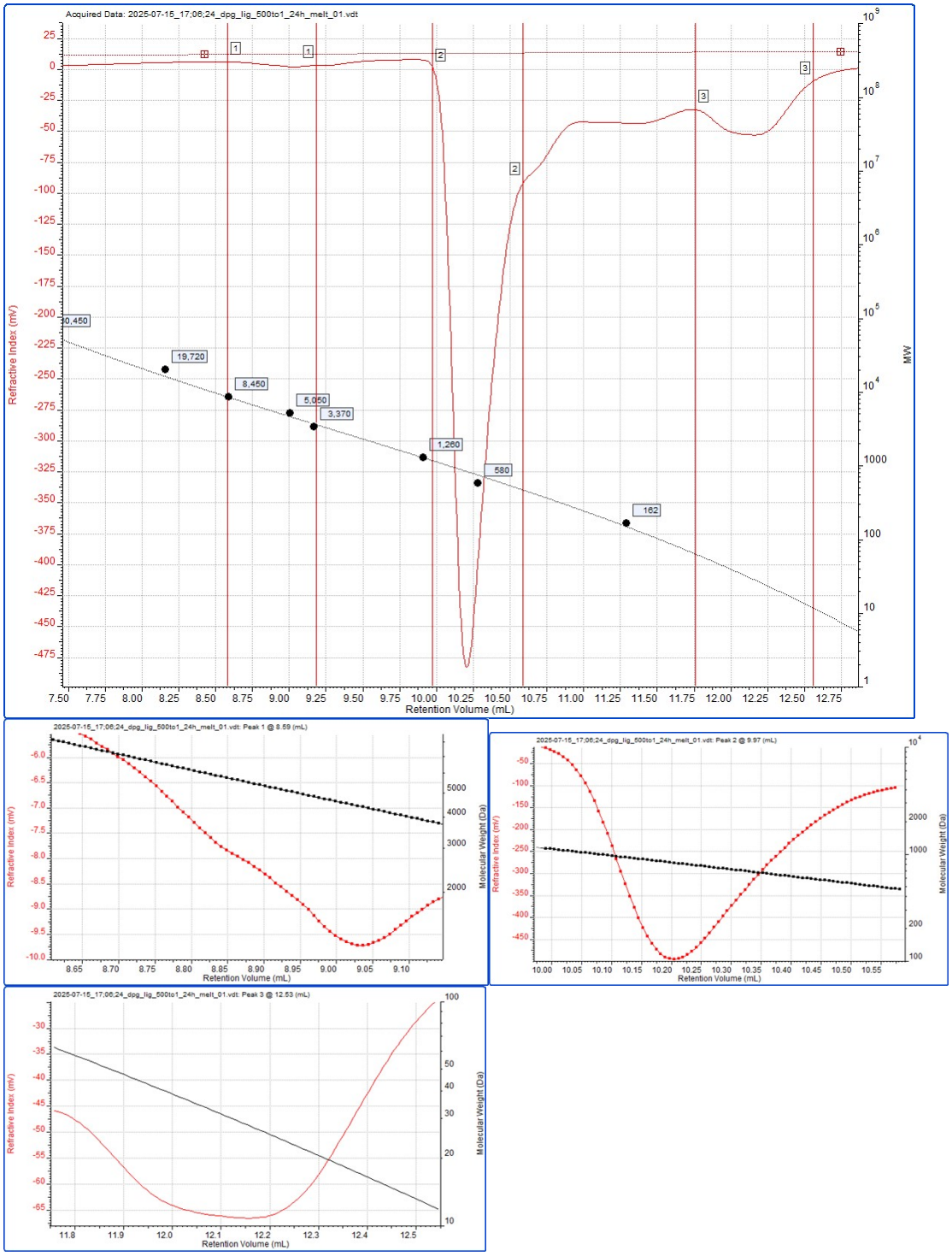
*M*w (Da) 6,349

*M*z (Da) -52088

*M*p (Da) 117,875

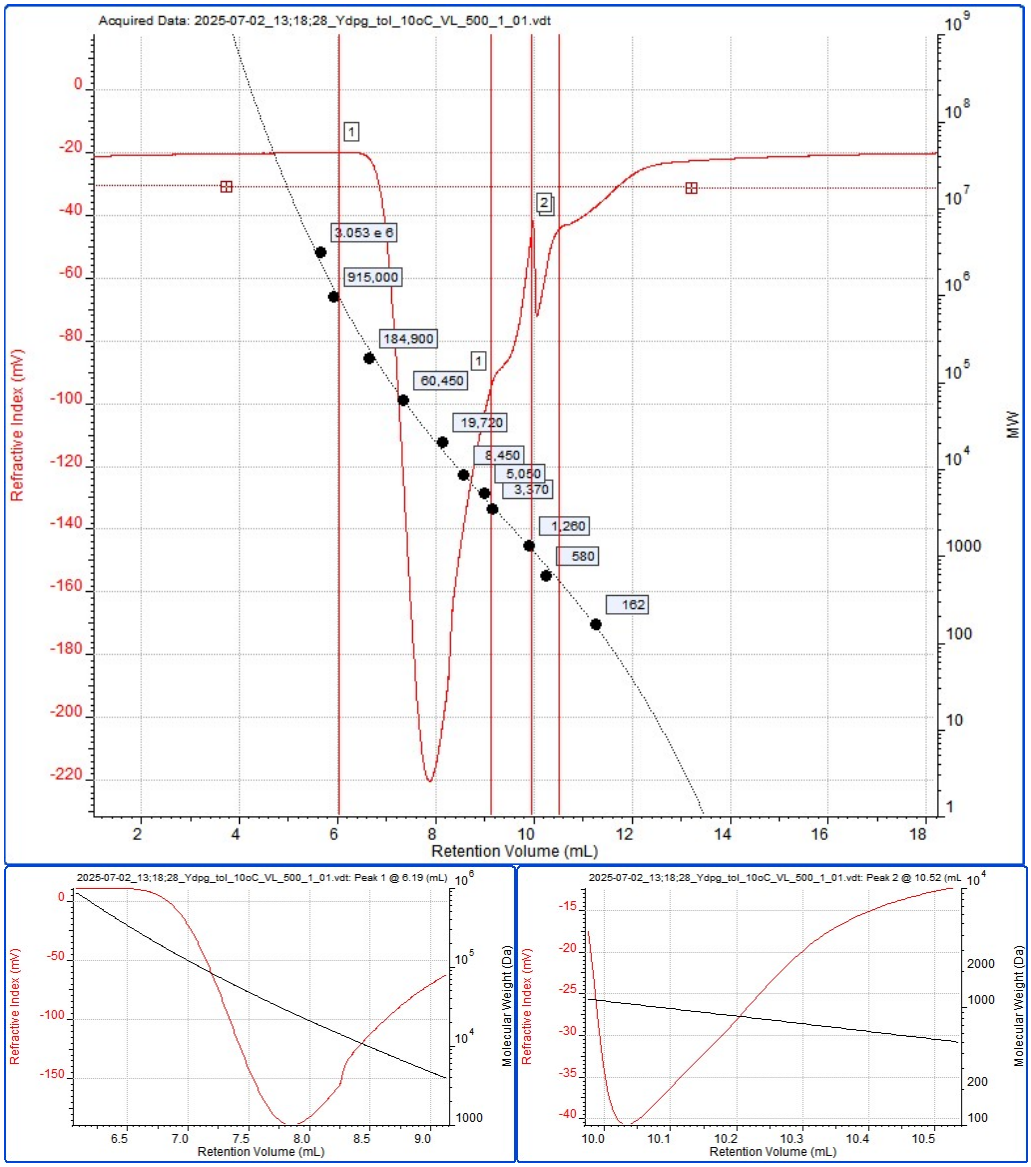
*M*w/*M*n 1.092

GPC trace for PCL using LH_3 (entry 10, Table 3).



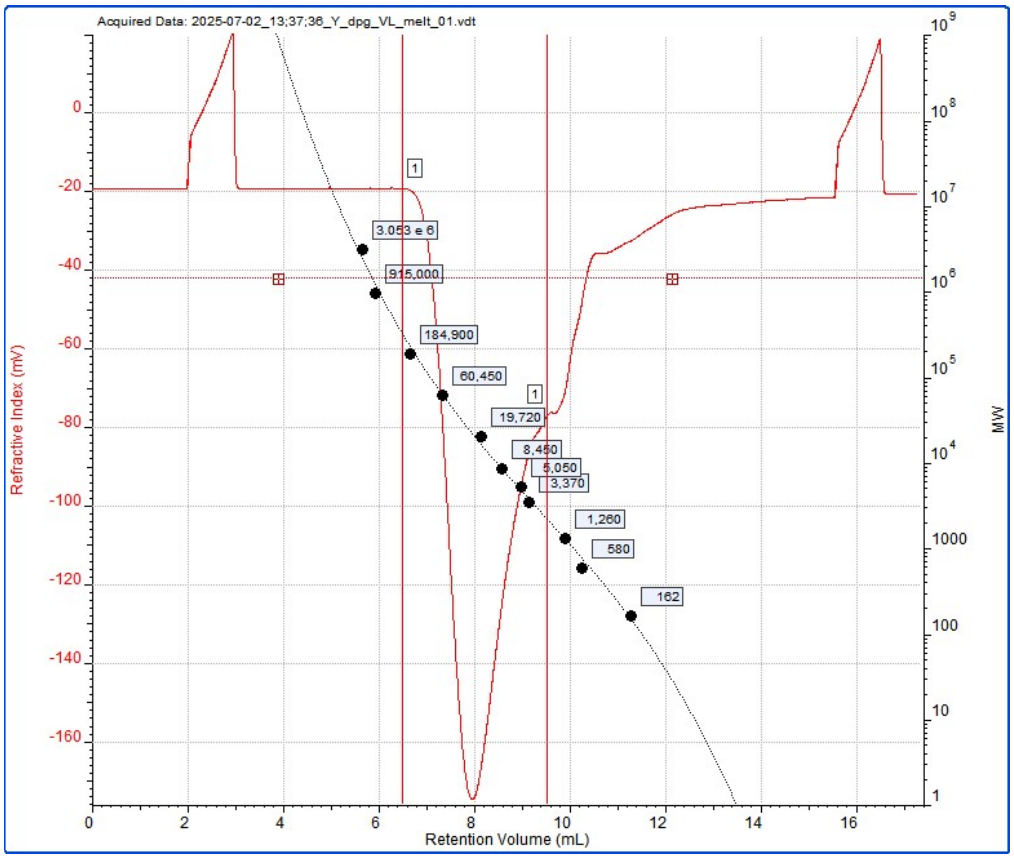
Peak	1	2	3
Ret Vol (mL)	8.587	9.968	12.531
*M*n (Da)	5,123	861	28
*M*w (Da)	5,413	902	34
*M*z (Da)	5,726	936	40
*M*p (Da)	8,305	1,151	12
*M*w/*M*n	1.057	1.047	1.211

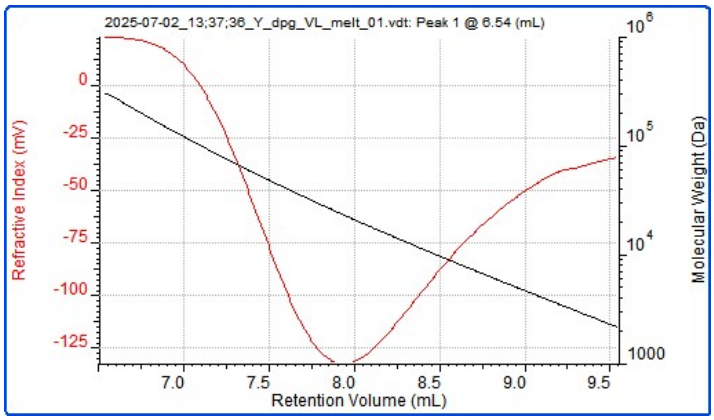
GPC trace for PVL using **1** (entry 11, Table 3).



Peak	1	2
Ret Vol (mL)	6.190	10.522
*M*n (Da)	14,253	841
*M*w (Da)	15,628	885
*M*z (Da)	-356906	924
*M*p (Da)	663,864	506
*M*w/*M*n	1.096	1.052

GPC trace for PVL using **1** (entry 12, Table 3).





Peak 1

Ret Vol (mL) 6.539

*M*n (Da) 9,667

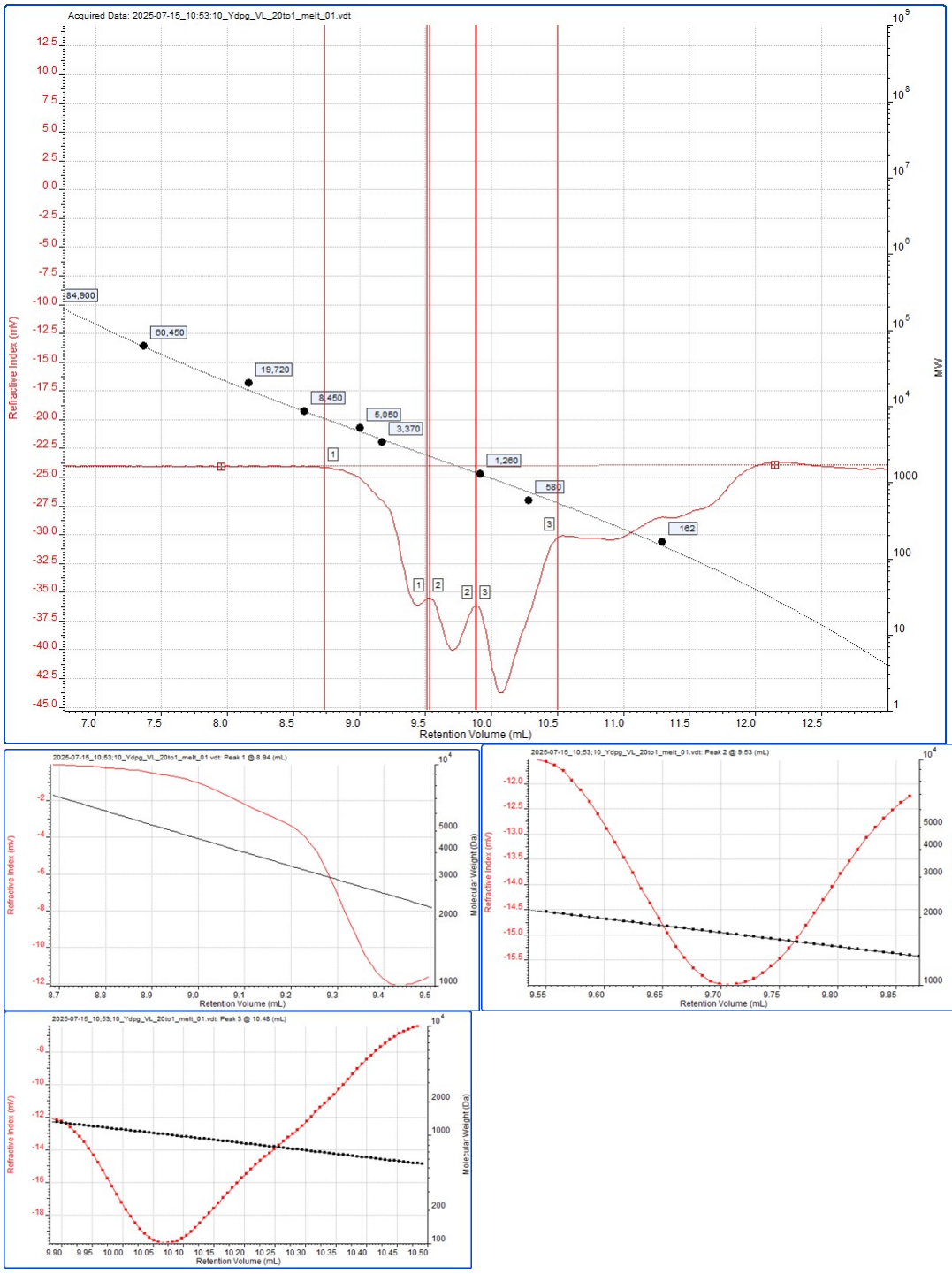
*M*w (Da) 11,119

*M*z (Da) -142581

*M*p (Da) 303,102

*M*w/*M*n 1.150

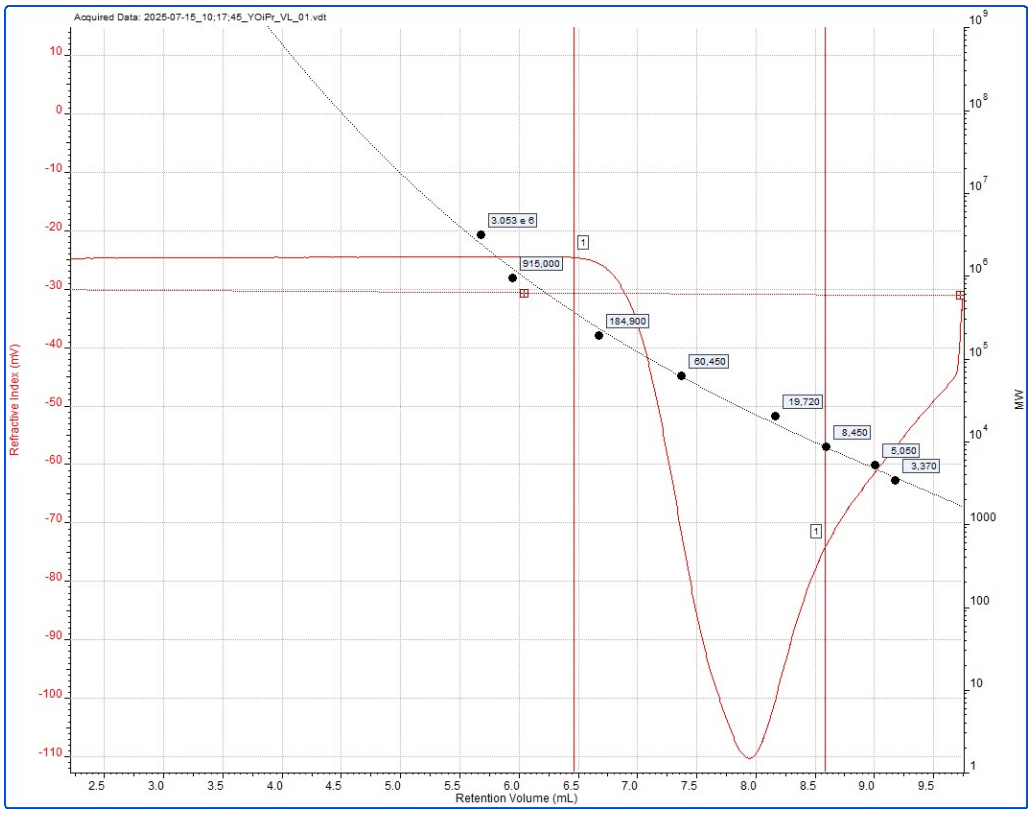
GPC trace for PVL using **1** (entry 13, Table 3).

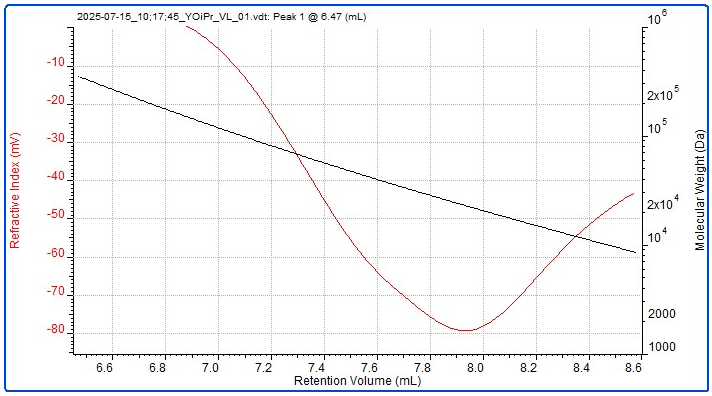


Peak	1	2	3
Ret Vol (mL)	8.944	9.528	10.476
*M*n (Da)	2,845	1,708	920

*M*w (Da)	2,966	1,738	974
*M*z (Da)	3,129	1,768	1,022
*M*p (Da)	5,000	2,157	542
*M*w/*M*n	1.042	1.018	1.059

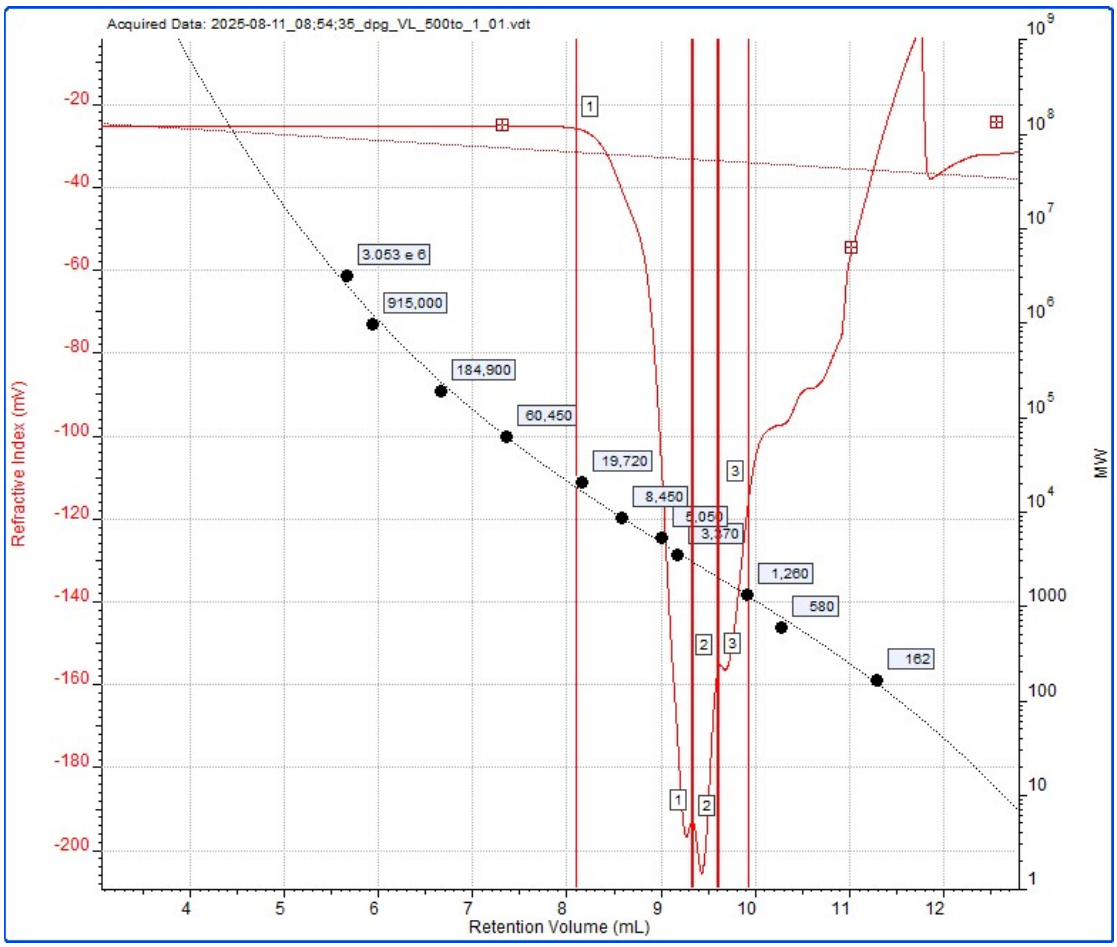
GPC trace for PVL using [Y(O*i*Pr)$_3$] (entry 19, Table 3).





Peak	1
Ret Vol (mL)	6.471
*M*n (Da)	20,706
*M*w (Da)	25,758
*M*z (Da)	-2052
*M*p (Da)	345,542
*M*w/*M*n	1.244

GPC trace for PVL using LH_3 (entry 20, Table 3).



Peak	1	2	3
Ret Vol (mL)	8.117	9.581	9.907
*M*n (Da)	3,849	2,422	1,575

*M*w (Da)	3,949	2,445	1,600
*M*z (Da)	3,765	2,468	1,623
*M*p (Da)	16,926	2,022	1,256
*M*w/*M*n	1.026	1.010	1.015

Figure S15. Selected GPC traces for PCL and PVL.

Depolymerization of PET

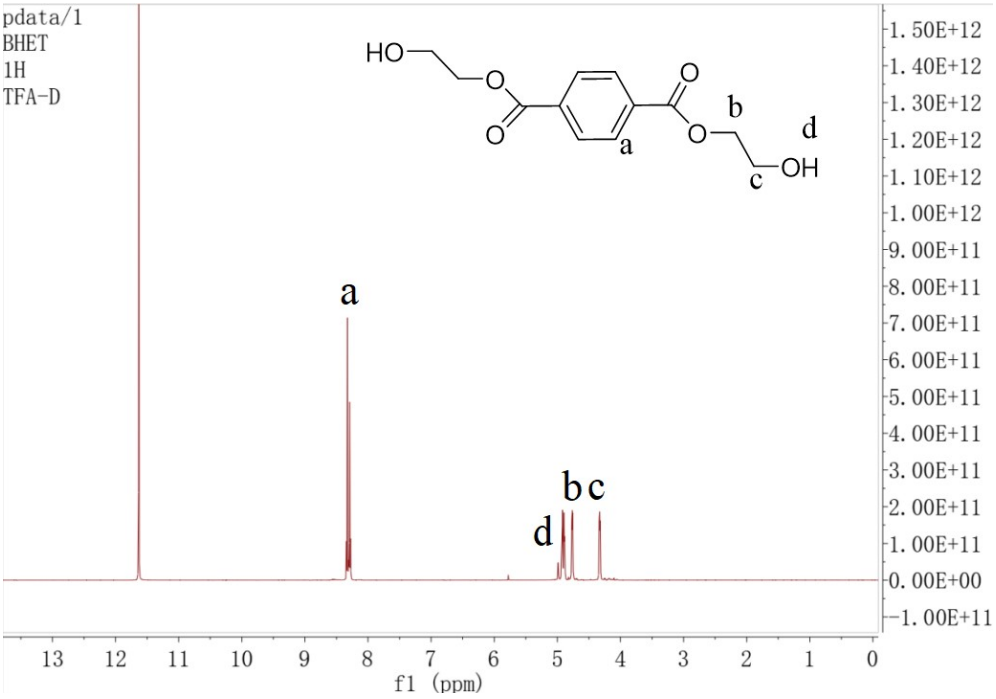


Figure S16. ^{1}H NMR spectrum of BHET.

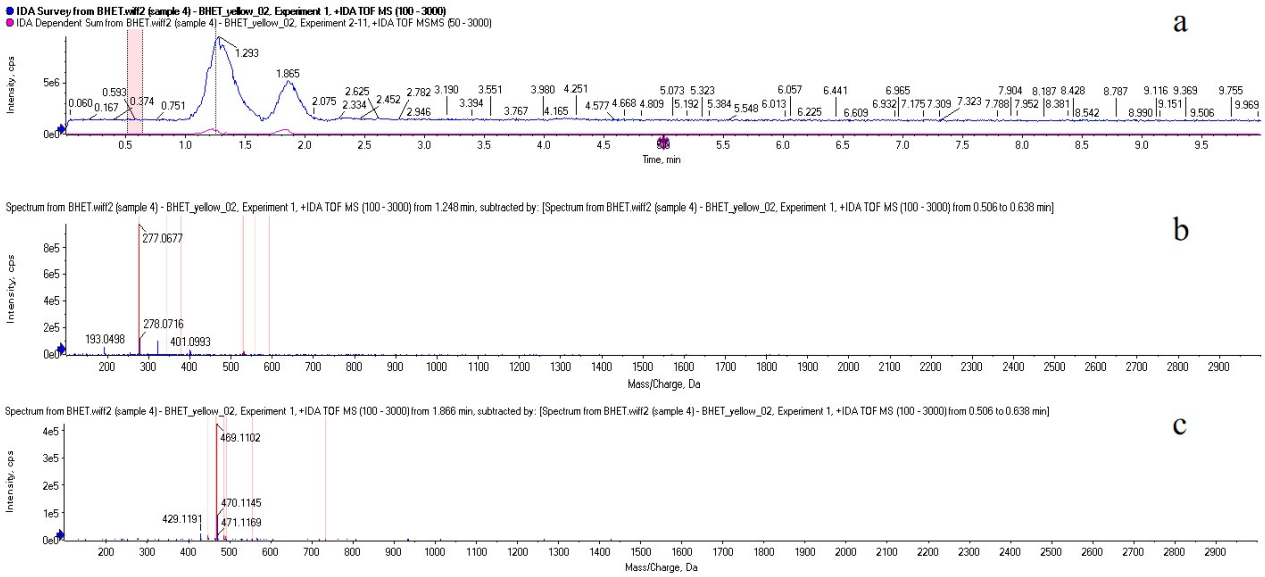


Figure S17. HPLC-MS analysis of run 1: (a) Total ion chromatogram; (b) Mass spectrum at t_R = 1.248 min; (c) Mass spectrum at t_R = 1.866 min.

Ethylene polymerization procedure

Ethylene polymerization experiments were performed in a steel 500 mL autoclave. The reactor was evacuated at 80 °C, cooled down to 20 °C and then charged with the freshly prepared solution of the co-catalyst (Me_2AlCl) in heptane/toluene. Pre-catalysts were introduced into the reactor in sealed glass ampoules, containing 0.5 or 1.0 μmol of appropriate Y-complex in 0.5 mL of solvent. After setting up the desired temperature and ethylene pressure, the reaction started by breaking the ampoule with the pre-catalyst. During the polymerization, ethylene pressure (2 bar), temperature (70 °C) and stirring speed (2000 rpm) remained constant. After 30 min (during which time the ethylene consumption rate declined to nearly zero level), the reactor was opened to the atmosphere, and the polymeric product (if any) was dried in a fume-hood to a constant weight.