Supporting Information

Department of Polymer Science and Engineering, University of Science and Technology of China, Hefei, China.

Table of Contents

1. Basic Formulas

Branch density (BD) was analyzed using ^{1}H NMR spectroscopy:

BD = 1000 x (2/3) x (I_{CH3})/ ($I_{CH2\ and\ CH} + I_{CH3}$).

Incorporation of Methyl 10-undecenoate[1]

$$= \frac{\frac{I_{(COOCH_3)}}{3}}{\frac{I_{(COOCH_3)}}{3} + \frac{I_{(CH2)} + I_{(CH3)} - 15}{4}} * 100\%$$

2. Spectra Data

2.1 ^{1}H and ^{13}C NMR of Ligands

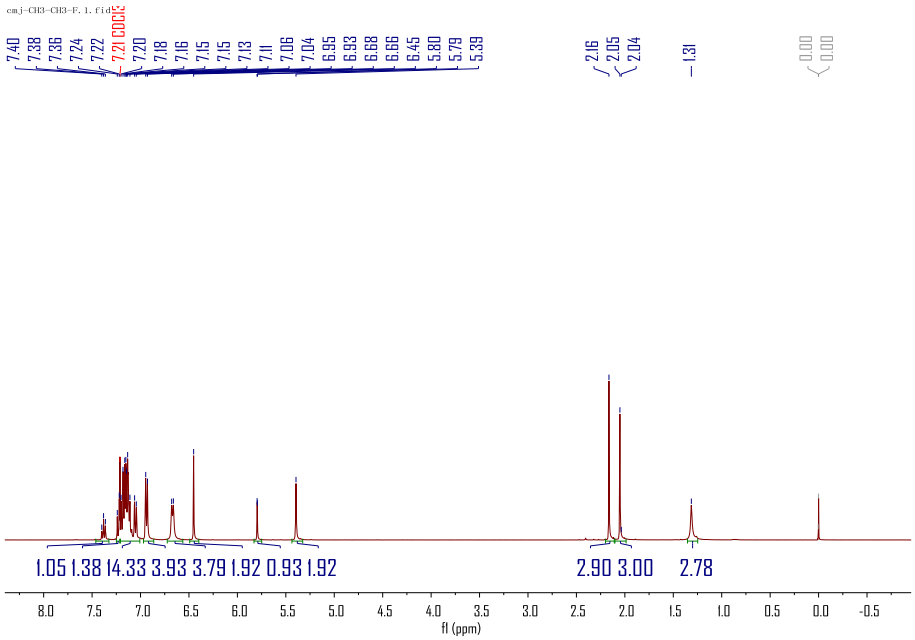


Figure S1. ^{1}H NMR spectrum of **L-1**in $CDCl_3$.

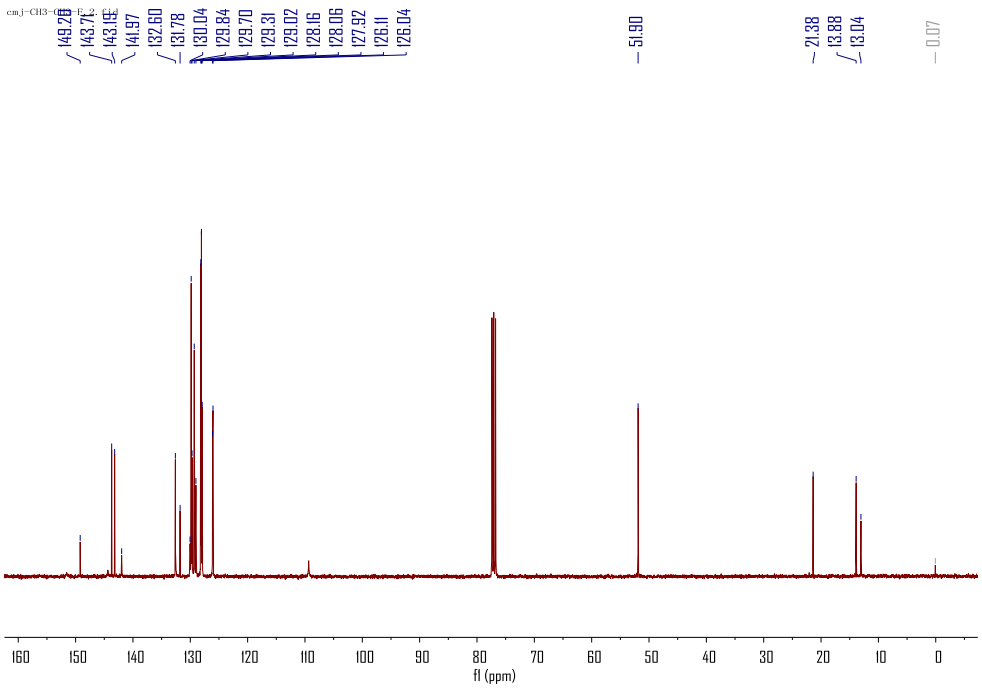


Figure S2. ^{13}C NMR spectrum of **L-1**in $CDCl_3$.

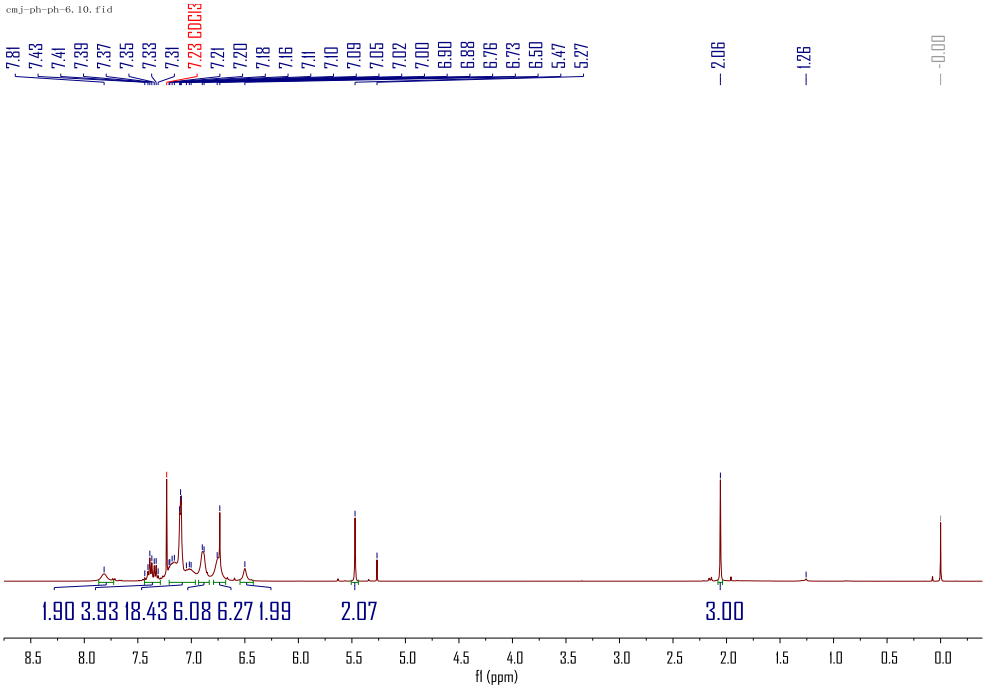


Figure S3. ^{1}H NMR spectrum of **L-2** in $CDCl_3$.

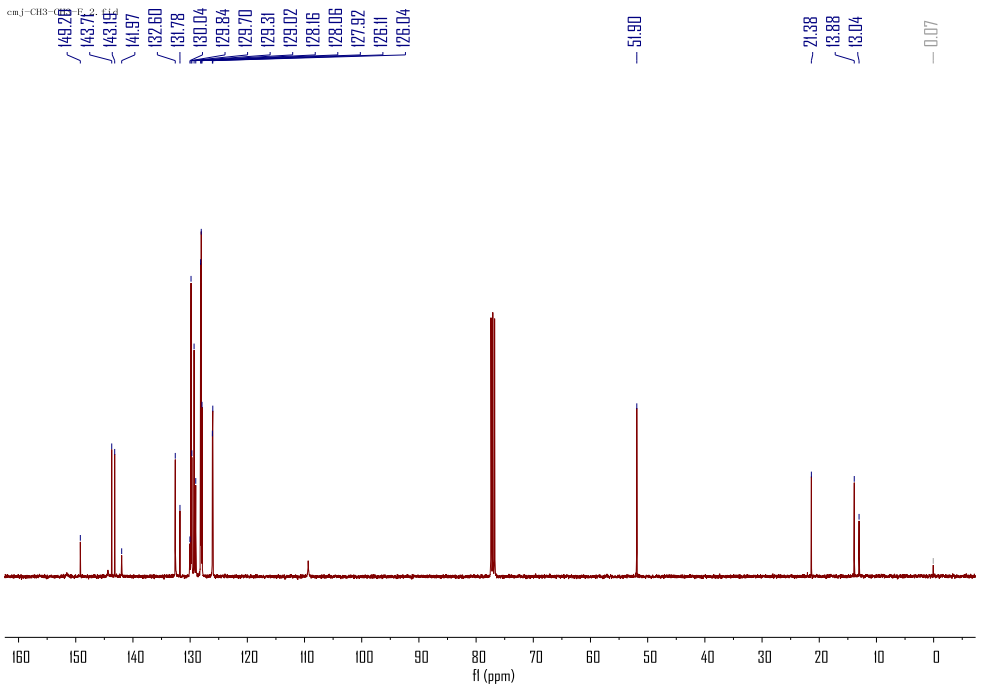


Figure S4. ^{13}C NMR spectrum of **L-2**in $CDCl_3$.

2.2 ESI for ligand

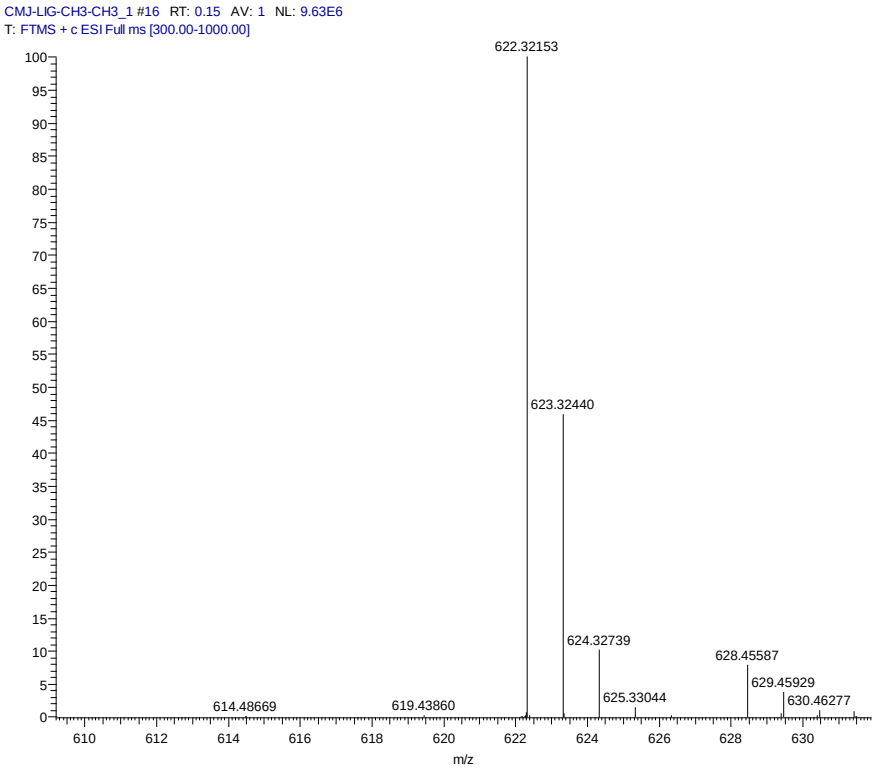


Figure S5. ESI of Ligand of **L-1.**

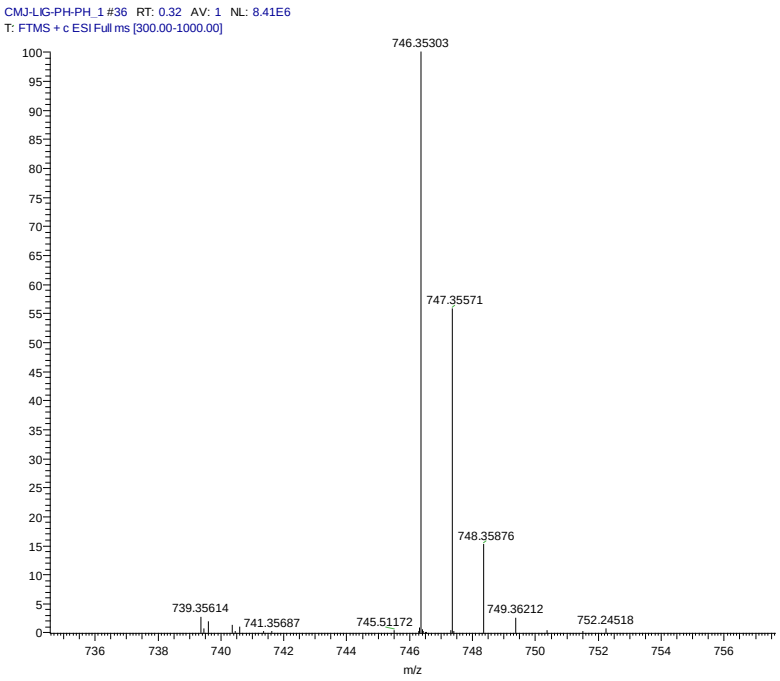


Figure S6. ESI of Ligand **L-2.**

2.3 MALDI-TOF of Complexes.

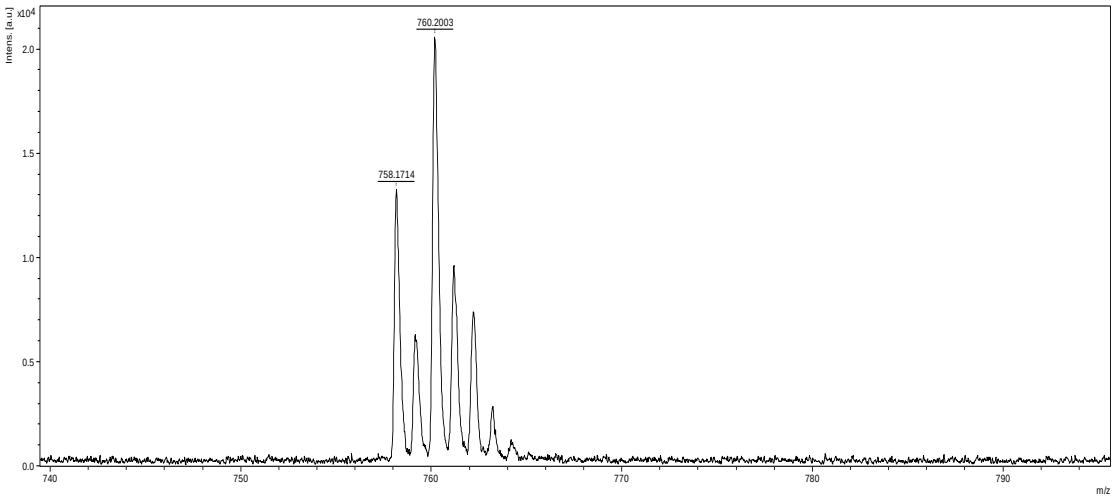


Figure S7. MALDI-TOF of Complexes **Ni-1**.

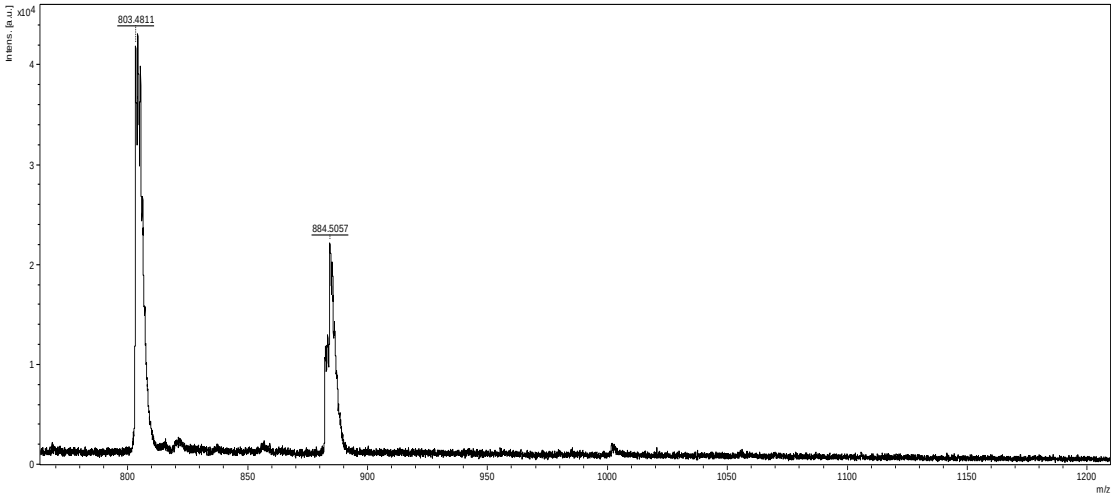


Figure S8. MALDI-TOF of Complexes **Ni-2**.

2.4 ^{1}H of polymer.

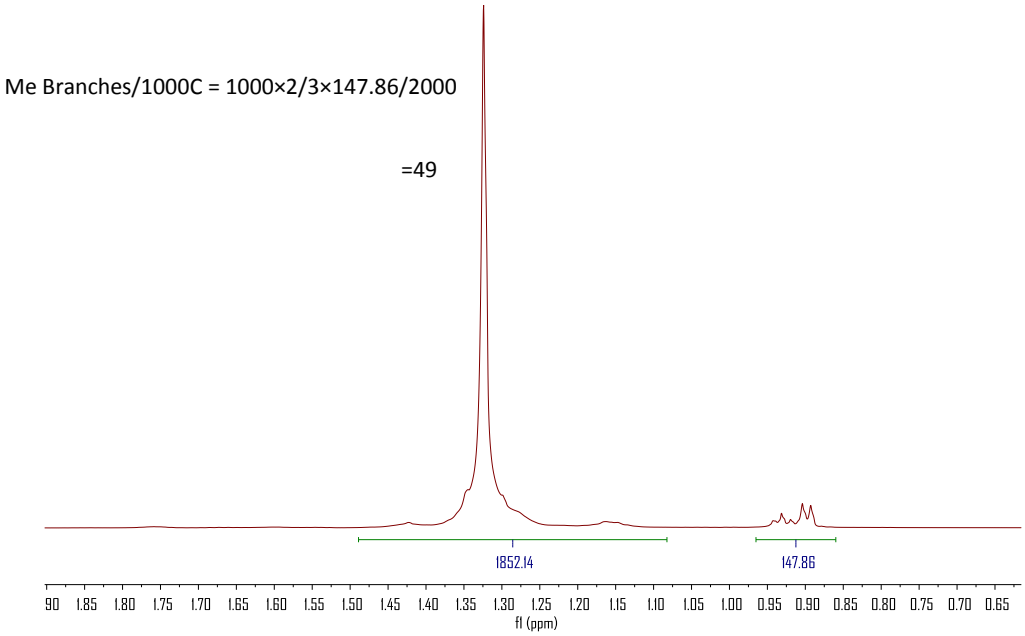


Figure S9. ^{1}H NMR spectrum of the polymer from table 1, entry 1 ($C_2D_2Cl_4$, 120^{o}C).

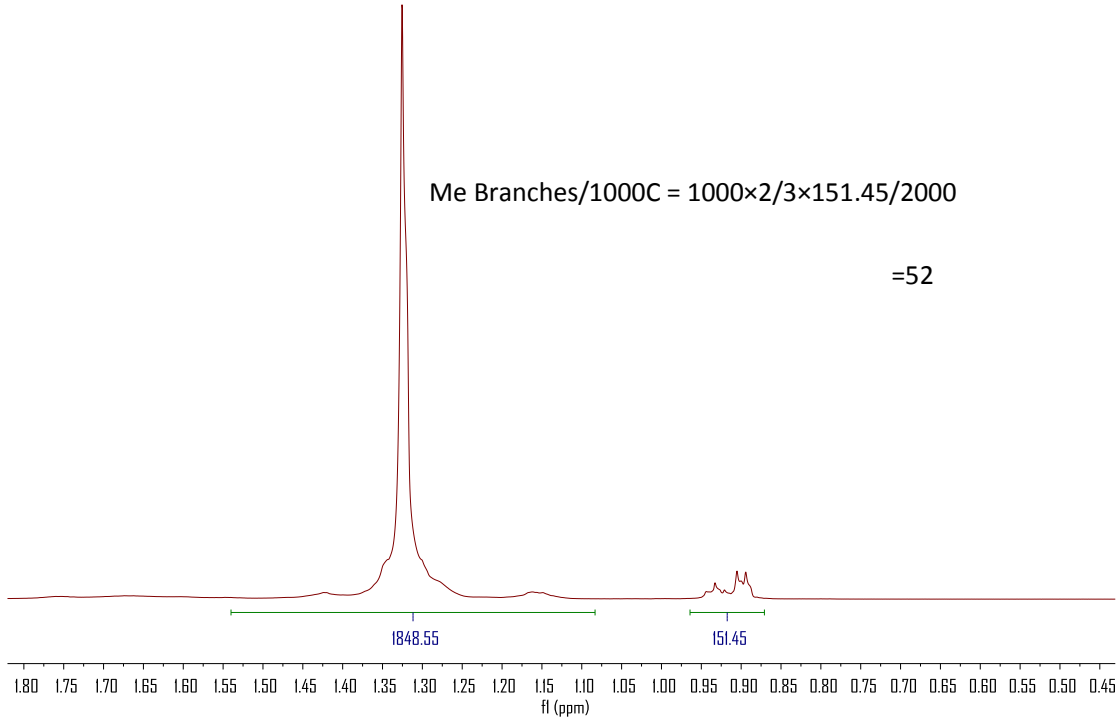


Figure S10. ^{1}H NMR spectrum of the polymer from table 1, entry 2 ($C_2D_2Cl_4$, 120^{o}C)

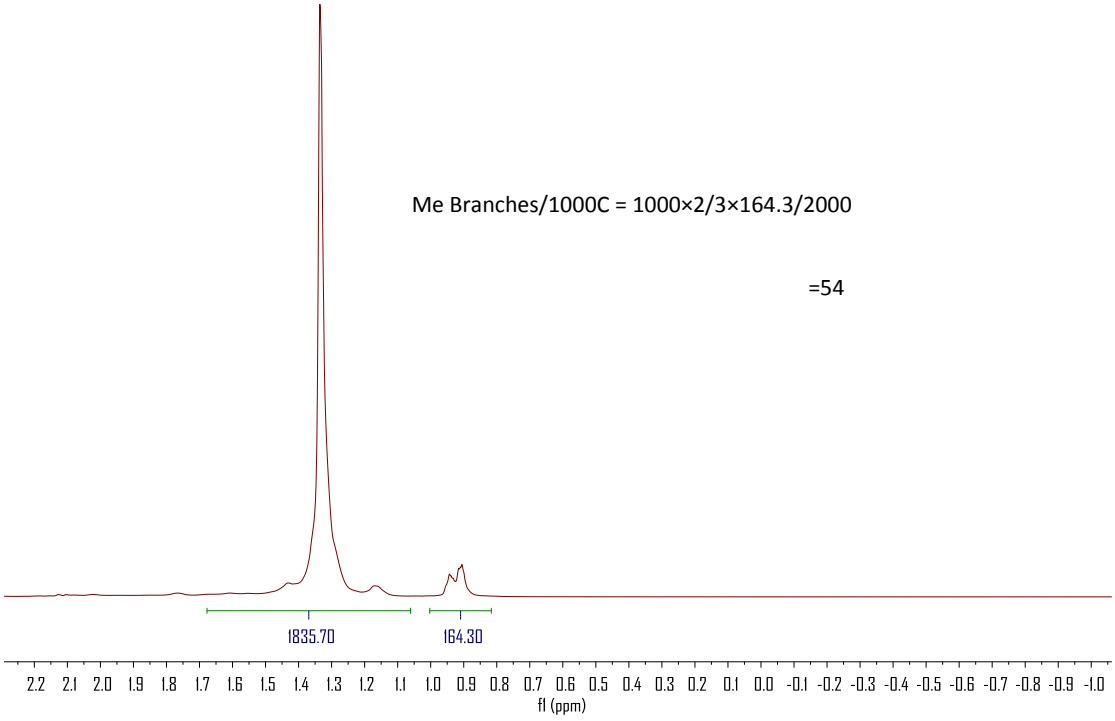


Figure S11. ^{1}H NMR spectrum of the polymer from table 1, entry 3 ($C_2D_2Cl_4$, 120^{o}C)

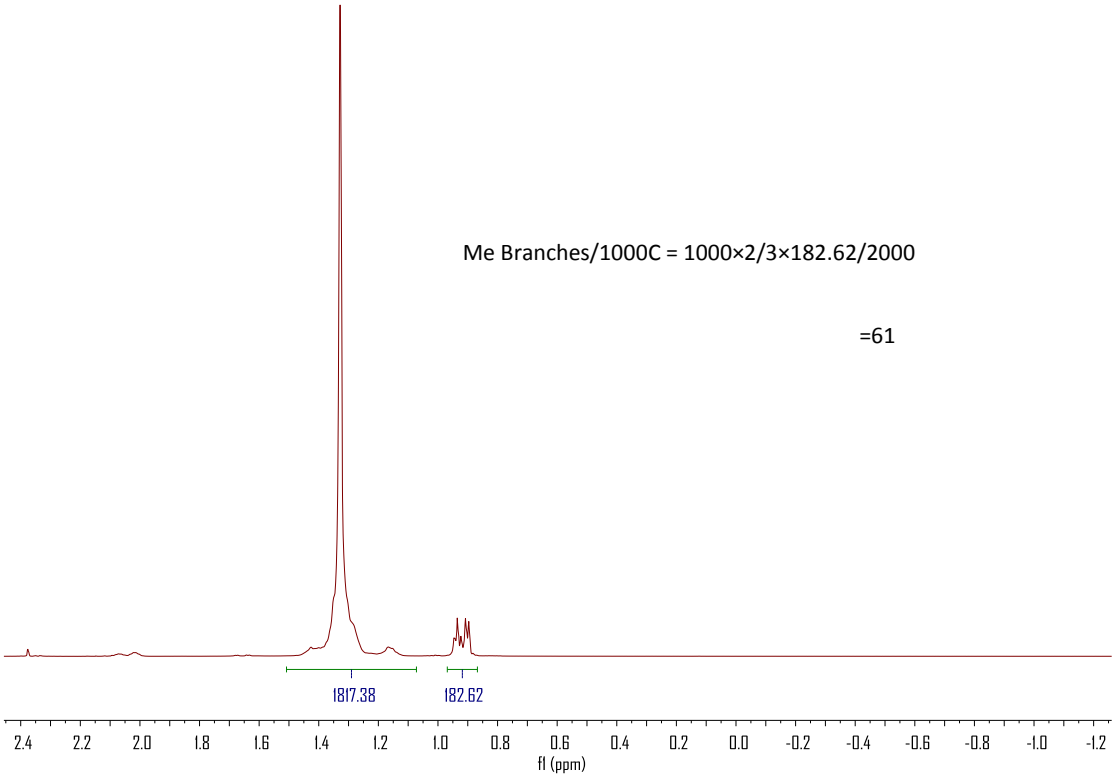


Figure S12. ^{1}H NMR spectrum of the polymer from table 1, entry 4 ($C_2D_2Cl_4$, 120^{o}C)

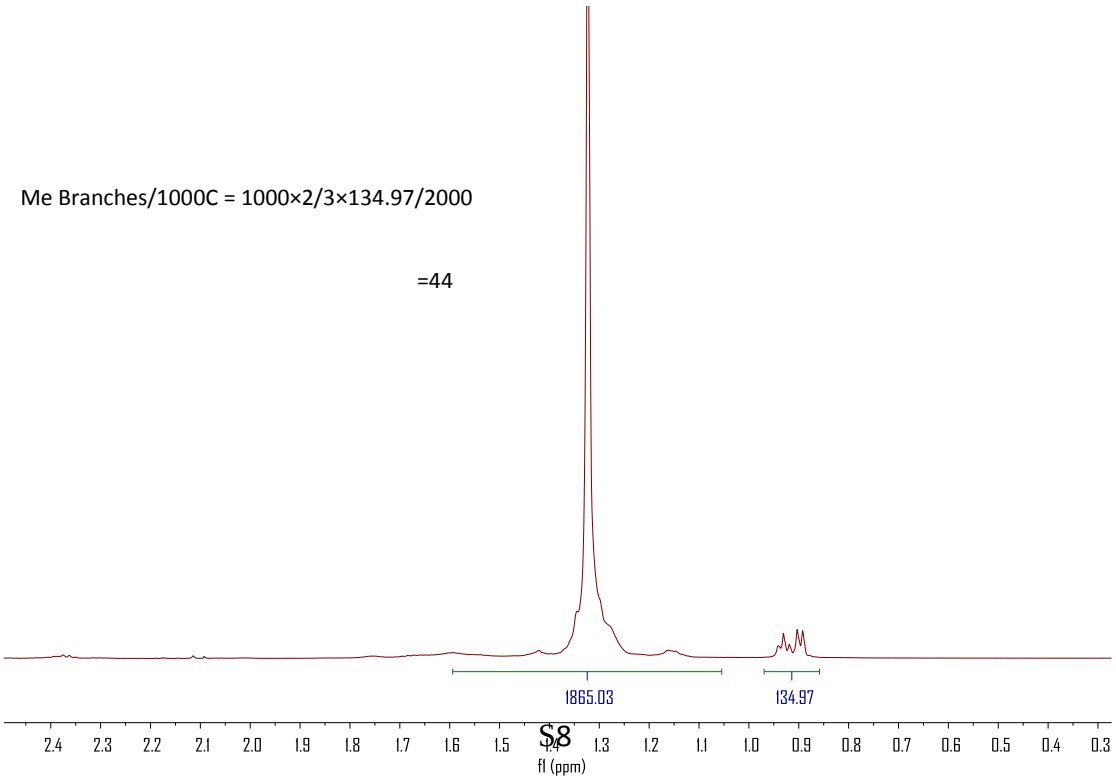


Figure S13. ^{1}H NMR spectrum of the polymer from table 1, entry 5 ($C_2D_2Cl_4$, 120^{o}C)

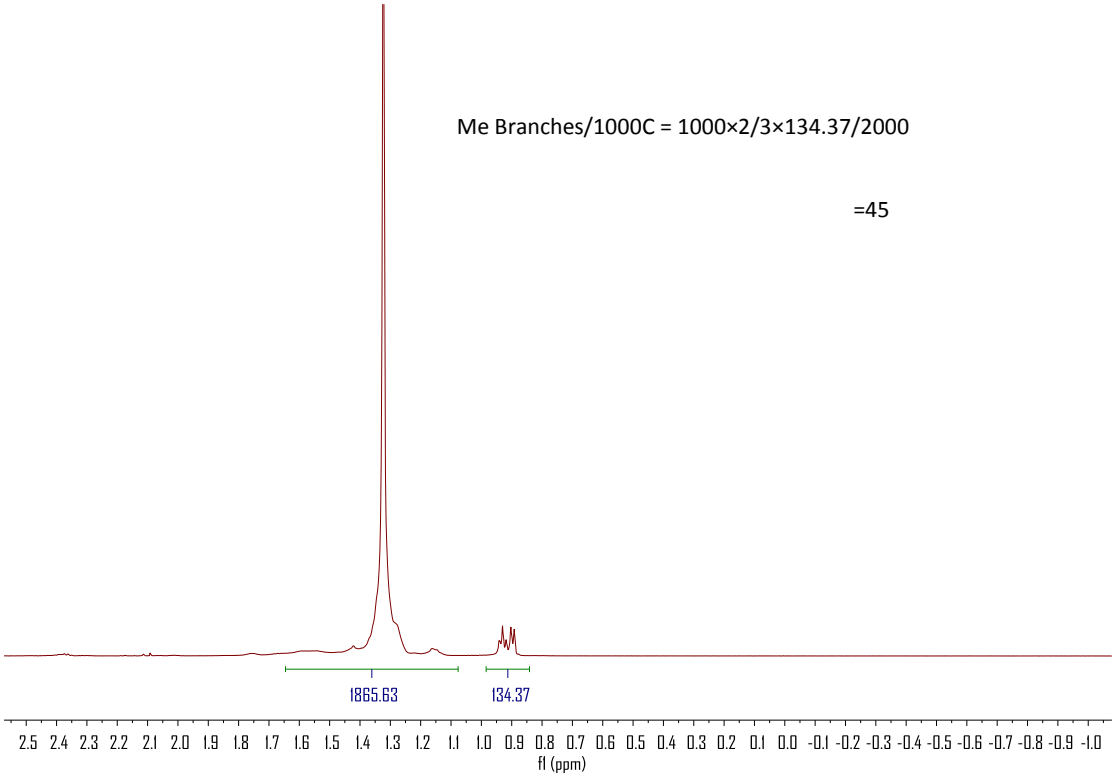


Figure S14. ^{1}H NMR spectrum of the polymer from table 1, entry 6 ($C_2D_2Cl_4$, 120^{o}C)

Me Branches/1000C = 1000×2/3×135.46/2000

=45

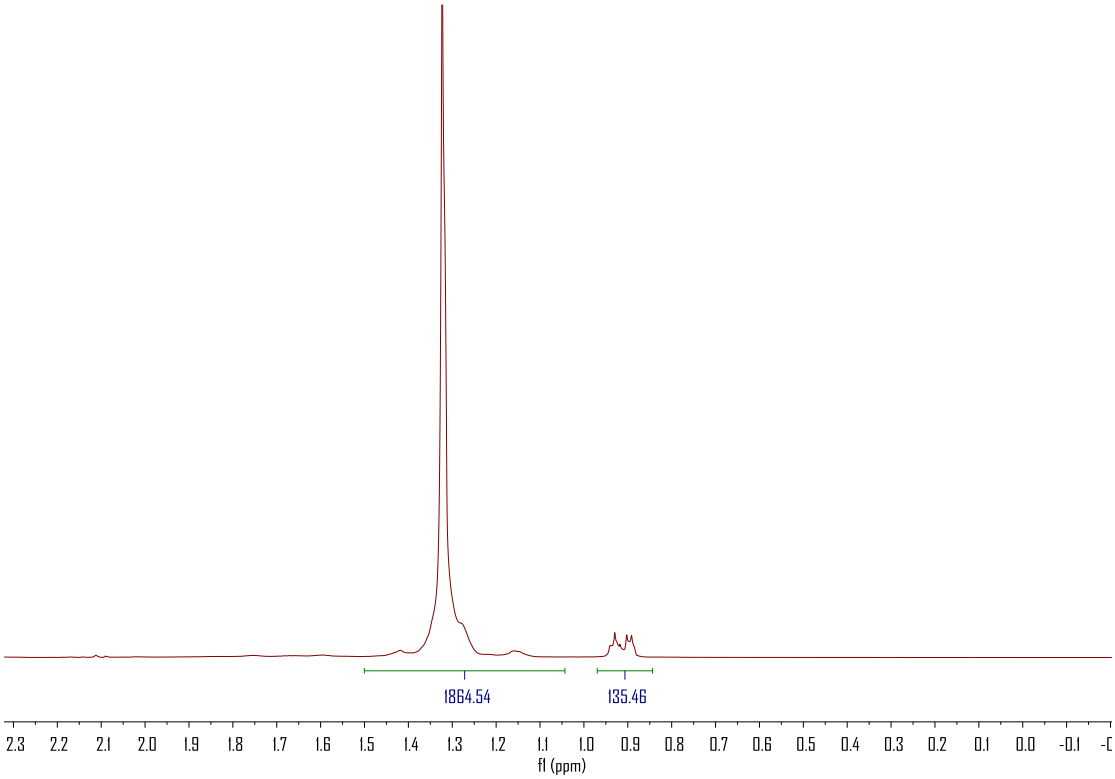


Figure S15. ^{1}H NMR spectrum of the polymer from table 1, entry 7 ($C_2D_2Cl_4$, 120^{o}C)

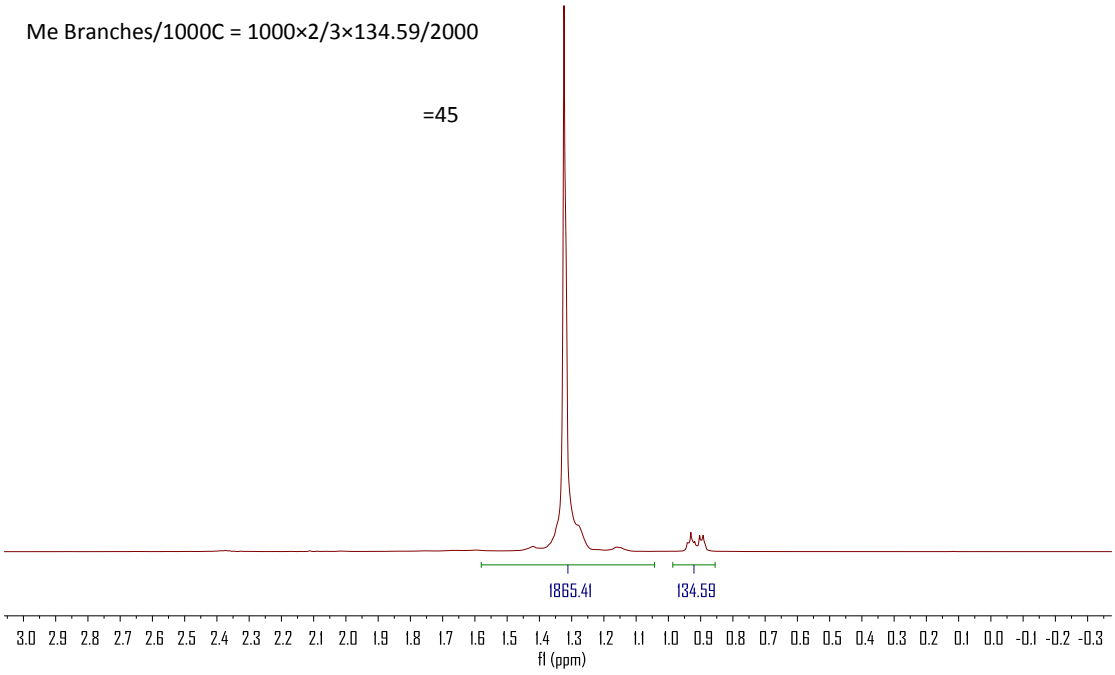


Figure S16. ^{1}H NMR spectrum of the polymer from table 1, entry 8 ($C_2D_2Cl_4$, 120^{o}C)

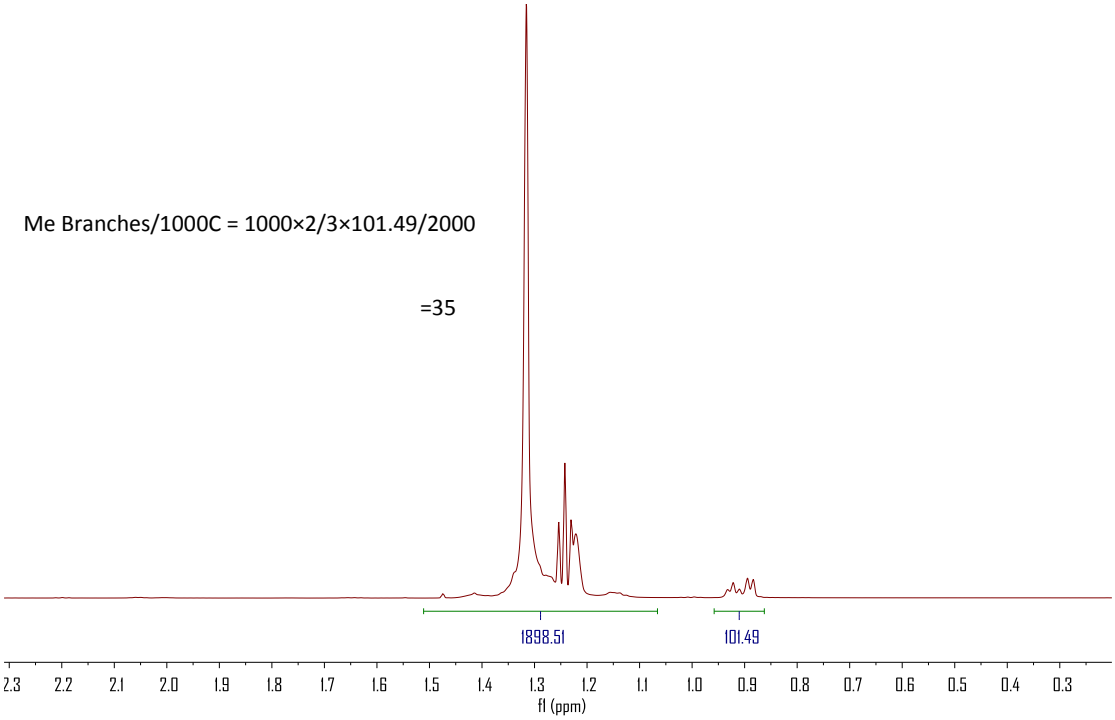


Figure S17. ^{1}H NMR spectrum of the polymer from table 2, entry 1 ($C_2D_2Cl_4$, 120^{o}C)

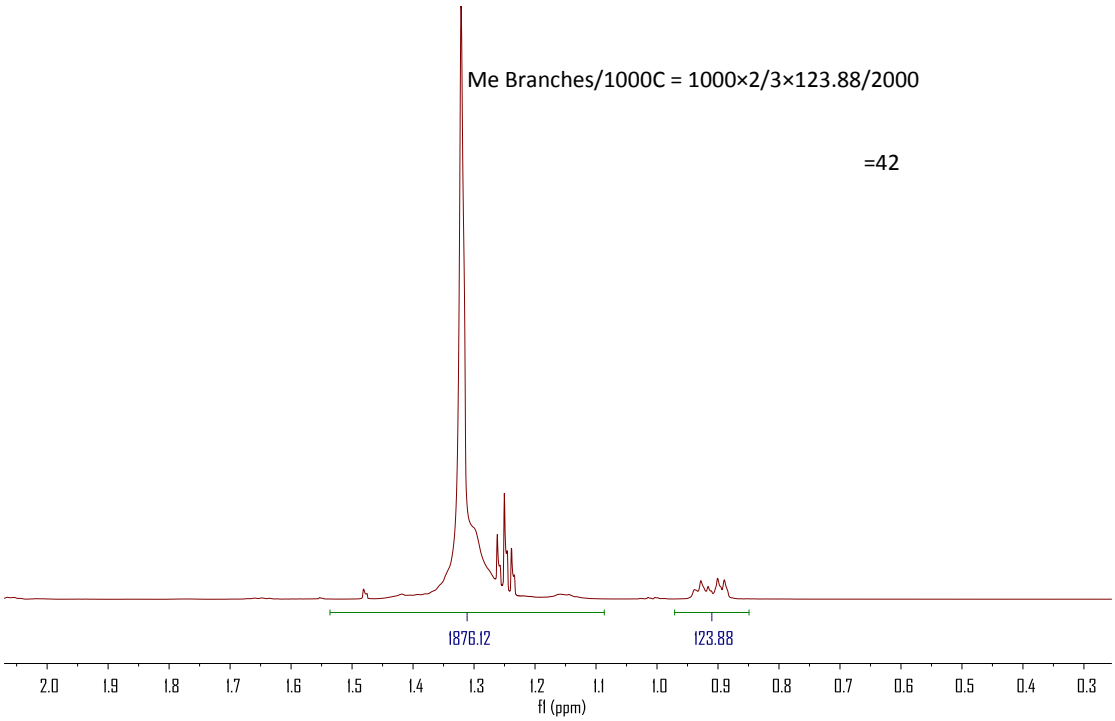


Figure S18. ^{1}H NMR spectrum of the polymer from table 2, entry 2 ($C_2D_2Cl_4$, 120^{o}C)

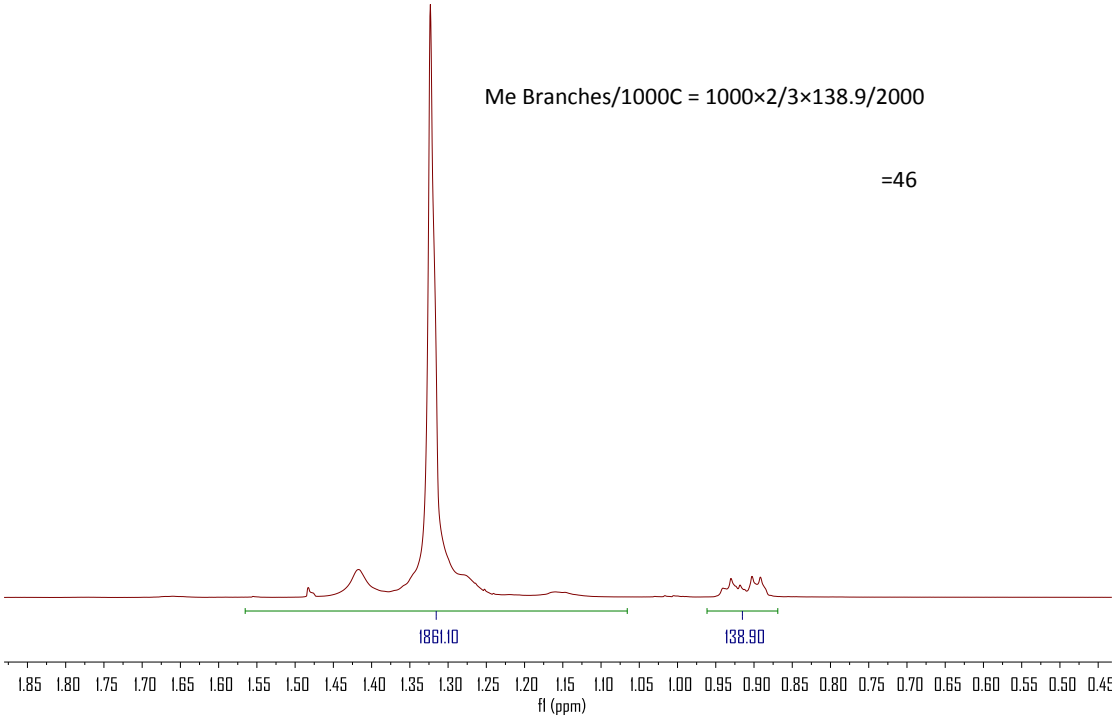


Figure S19. ^{1}H NMR spectrum of the polymer from table 2, entry 4 ($C_2D_2Cl_4$, 120^{o}C)

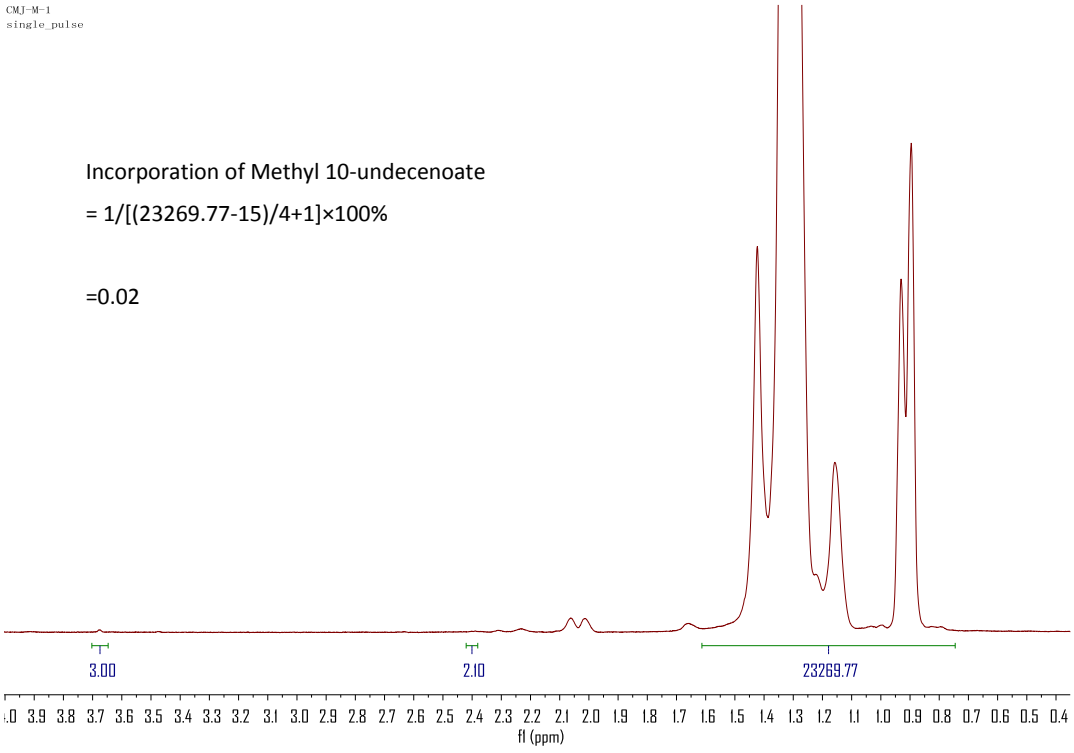


Figure S20. ^{1}H NMR spectrum of the polymer from table 3, entry 1 ($C_2D_2Cl_4$, 120^{o}C)

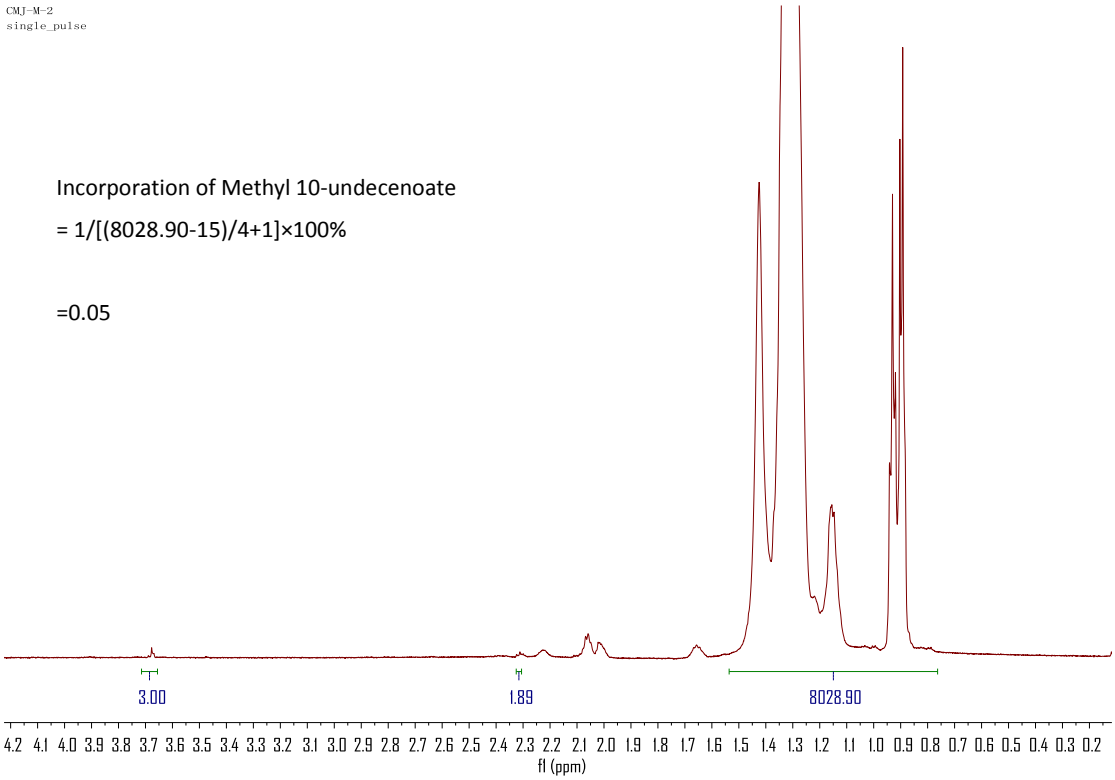


Figure S21. ^{1}H NMR spectrum of the polymer from table 3, entry 2 ($C_2D_2Cl_4$, 120^{o}C)

Incorporation of Methyl 10-undecenoate
= 1/[(5144.9-15)/4+1]×100%

=0.08

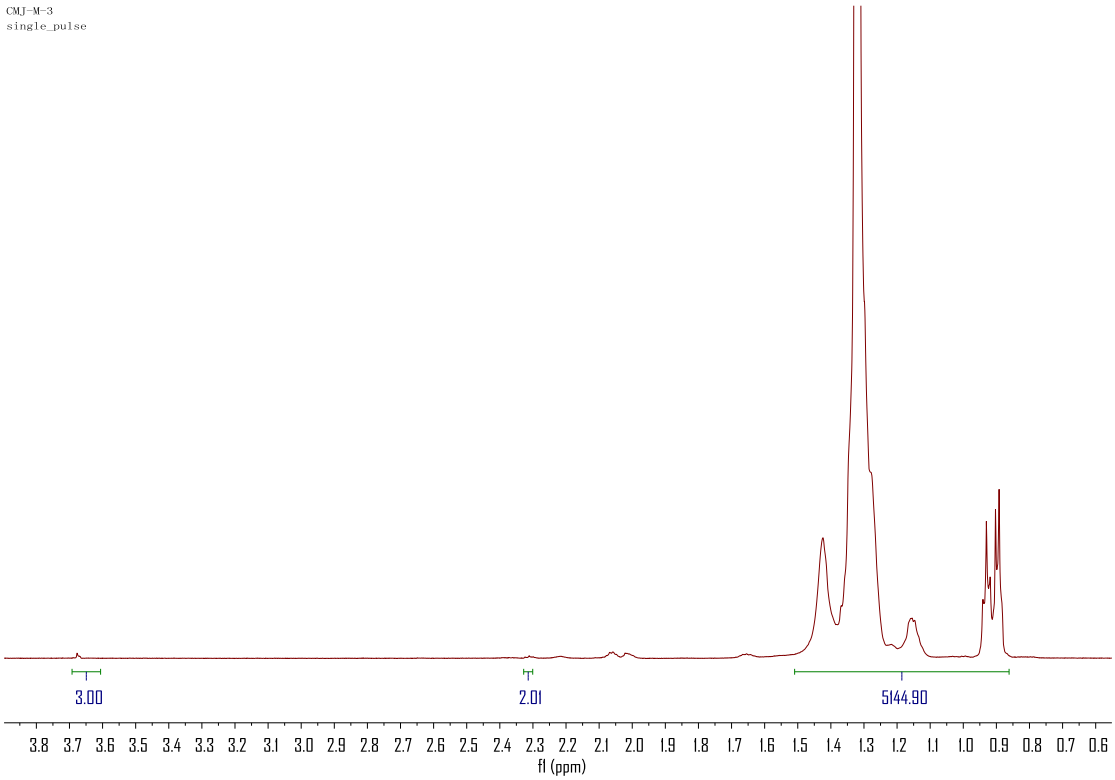


Figure S22. ^{1}H NMR spectrum of the polymer from table 3, entry 3 ($C_2D_2Cl_4$, 120^{o}C)

2.5 DSC of polymer.

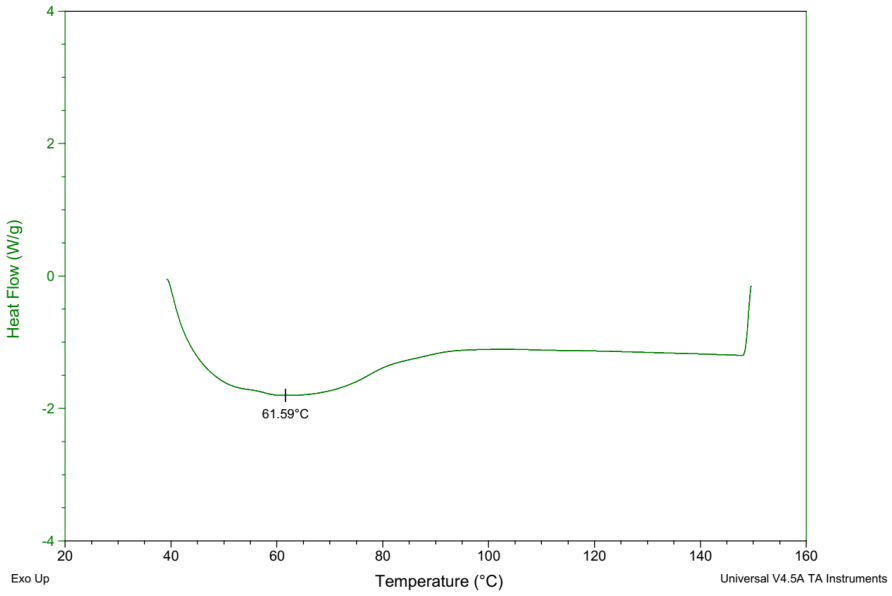


Figure S23. DSC of the polymer from table 1, entry 1

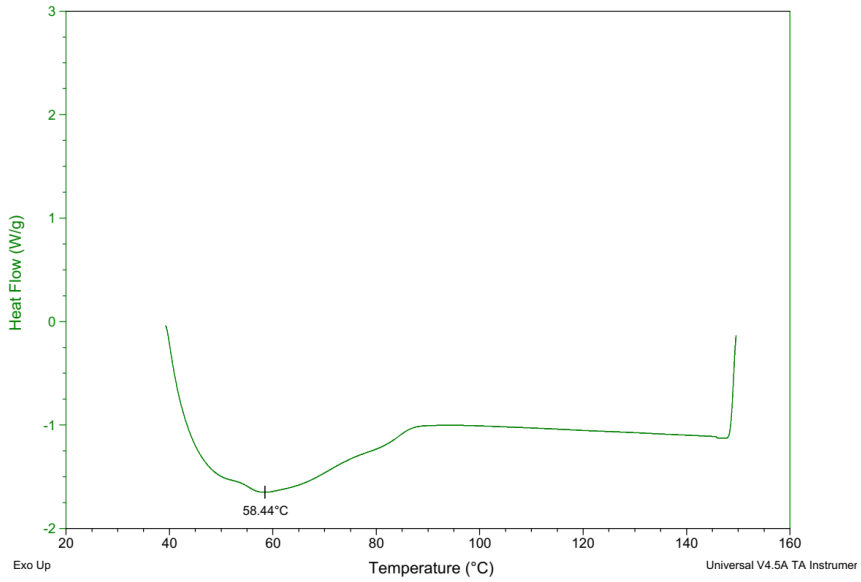


Figure S24. DSC of the polymer table 1, entry 2

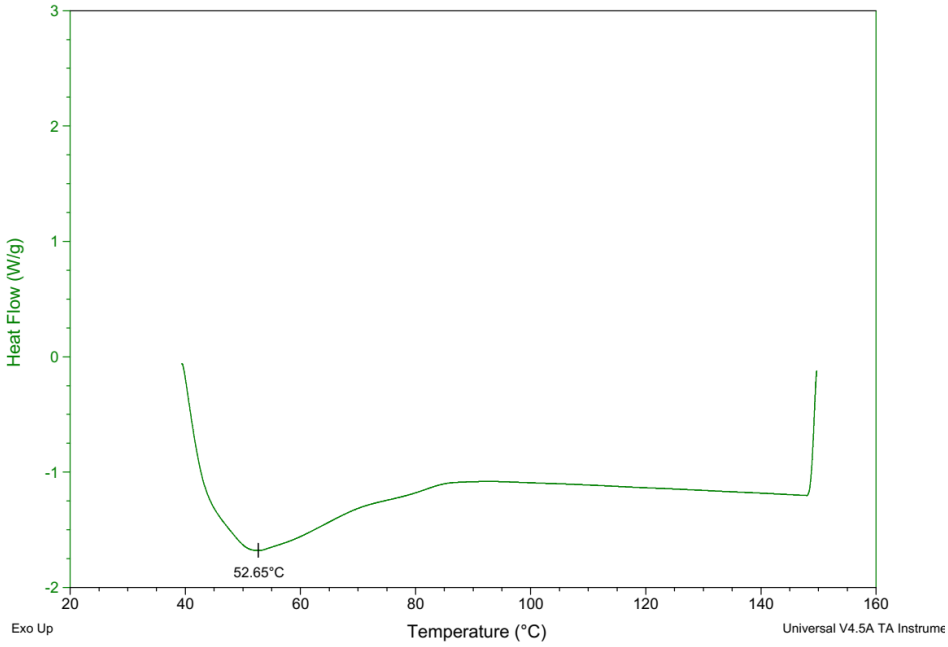


Figure S25. DSC of the polymer table 1, entry 3

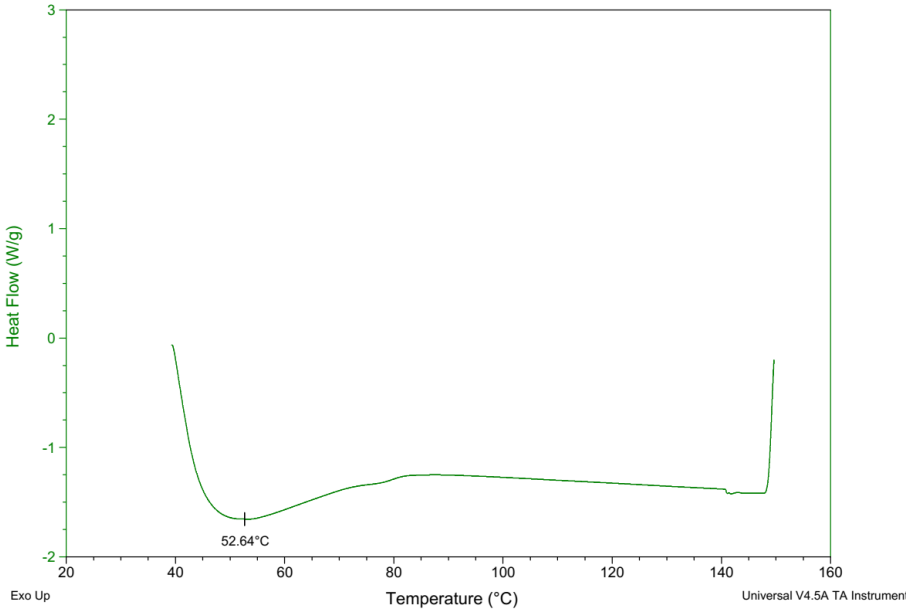


Figure S26. DSC of the polymer table 1, entry 4

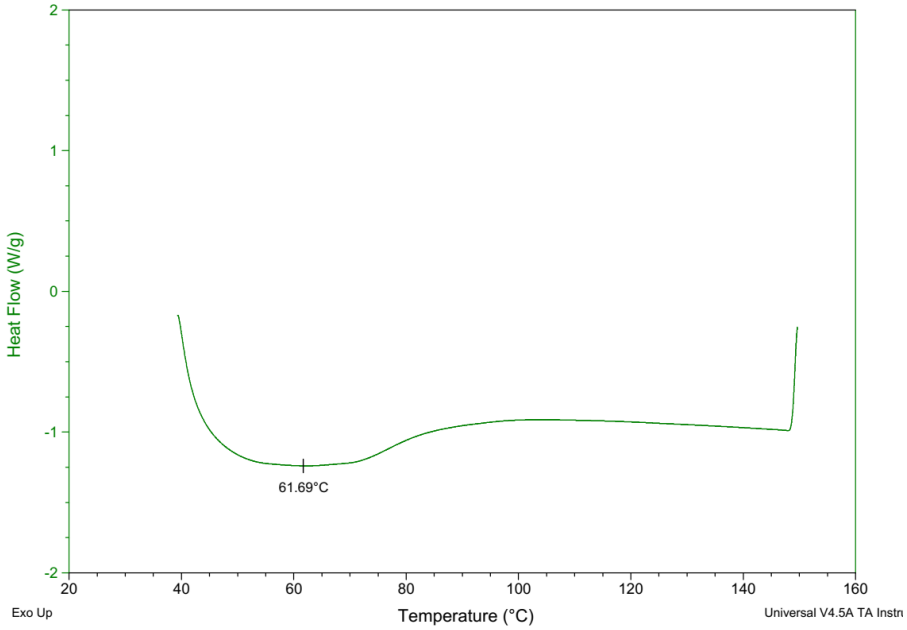


Figure S27. DSC of the polymer table 1, entry 5

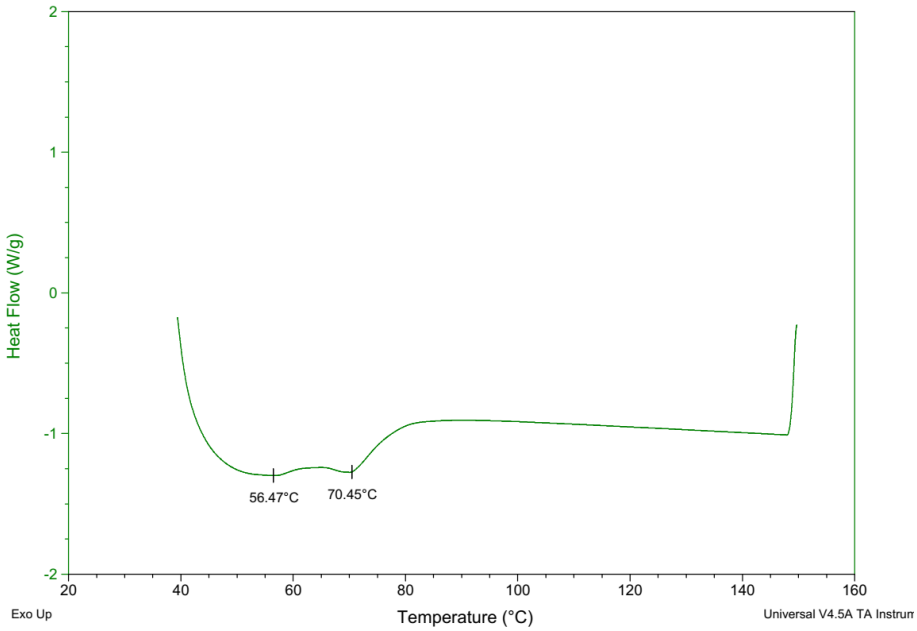


Figure S28. DSC of the polymer table 1, entry 6

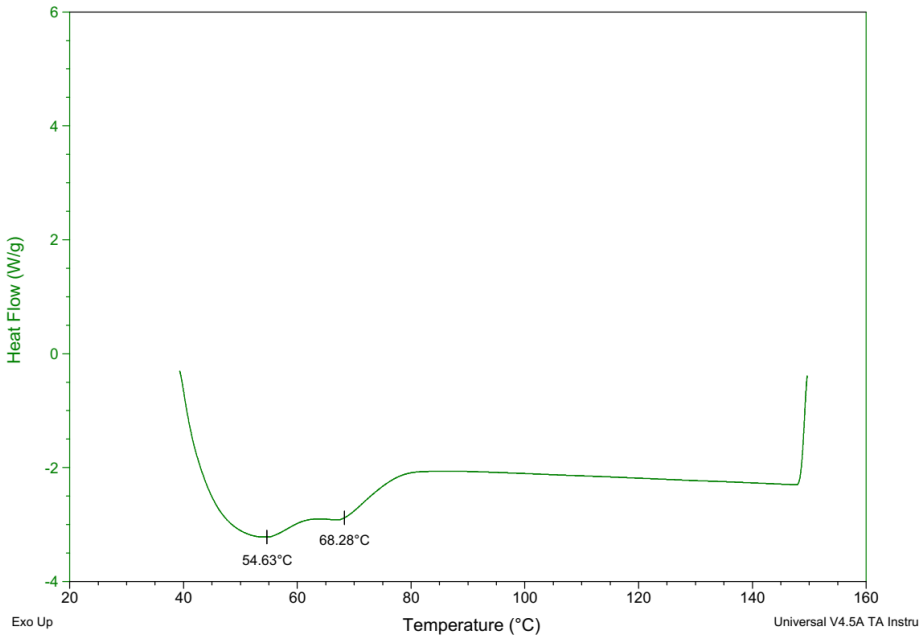


Figure S29. DSC of the polymer table 1, entry 7

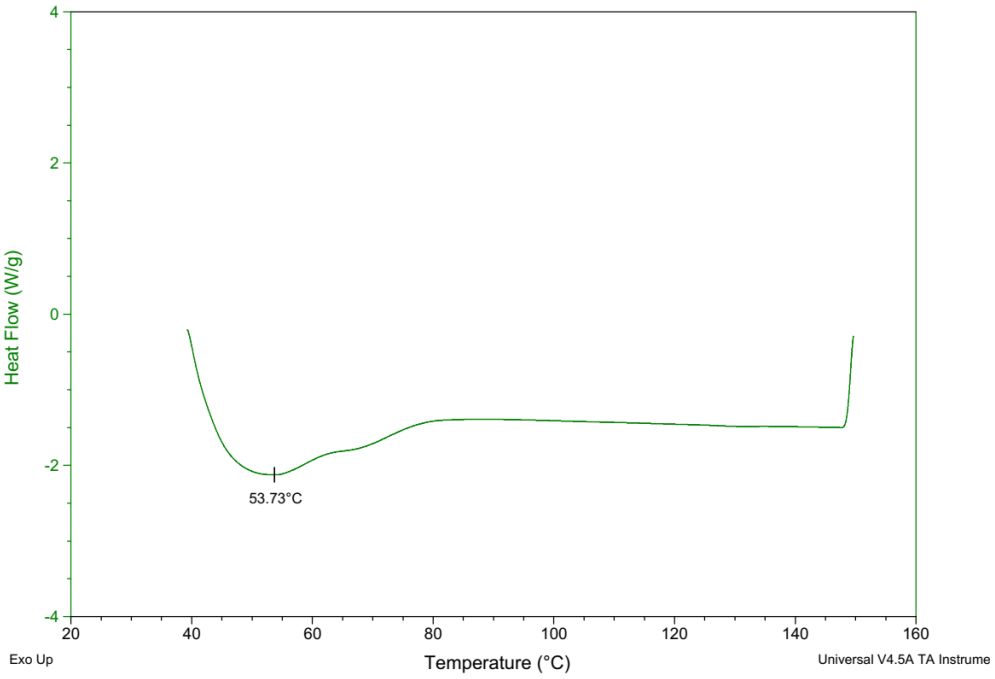


Figure S30. DSC of the polymer table 1, entry 8

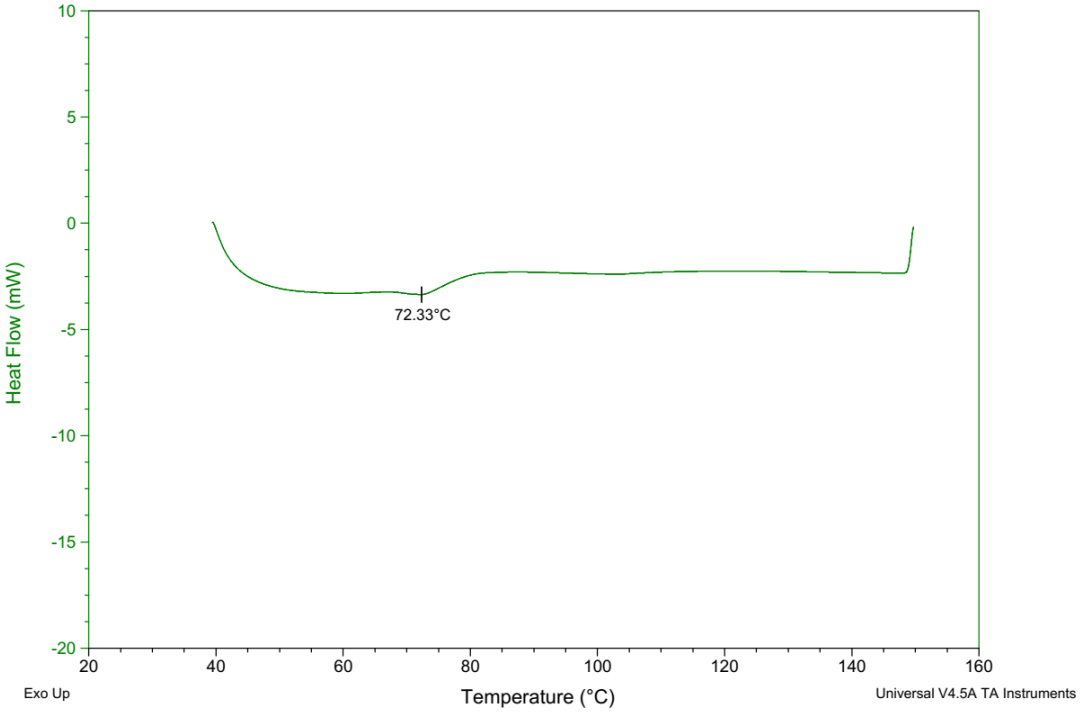


Figure S31. DSC of the polymer table 2, entry 1

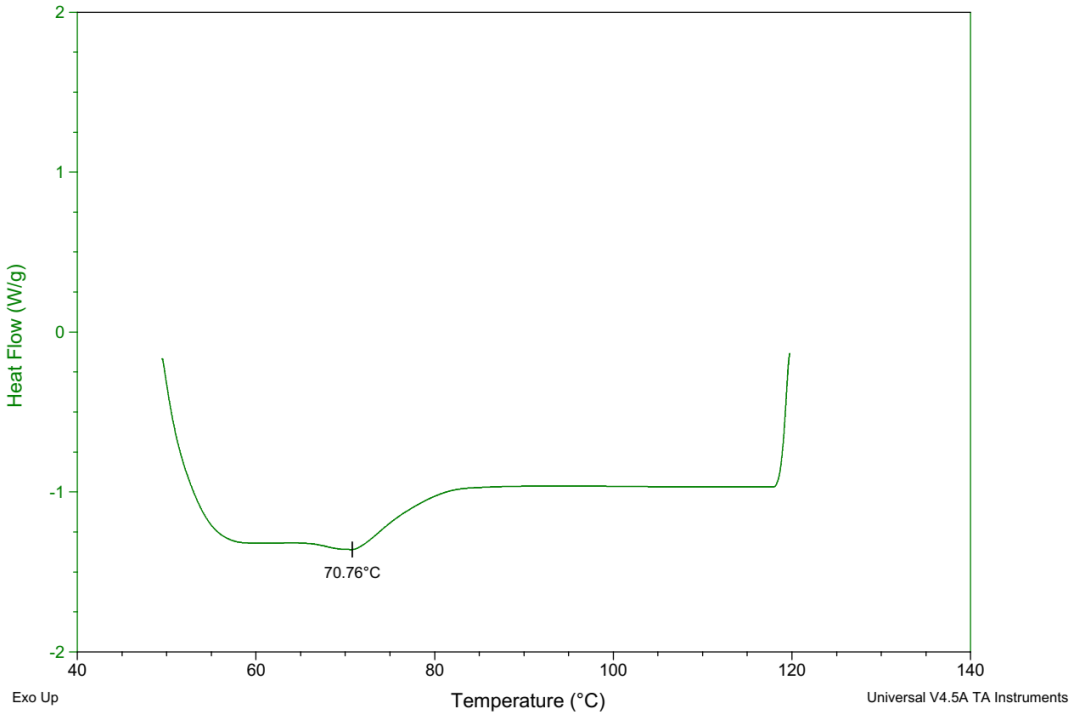


Figure S32. DSC of the polymer table 2, entry 2

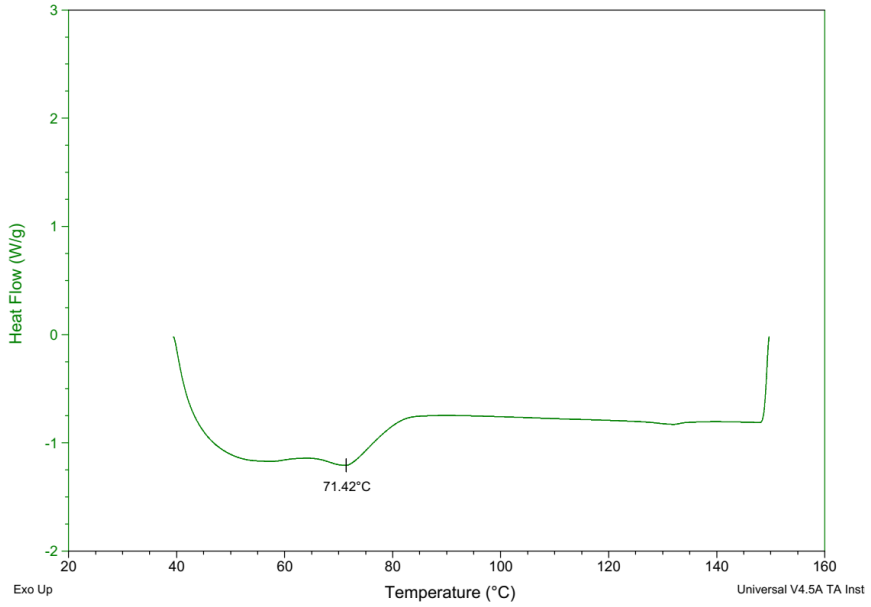


Figure S33. DSC of the polymer table 2, entry 3

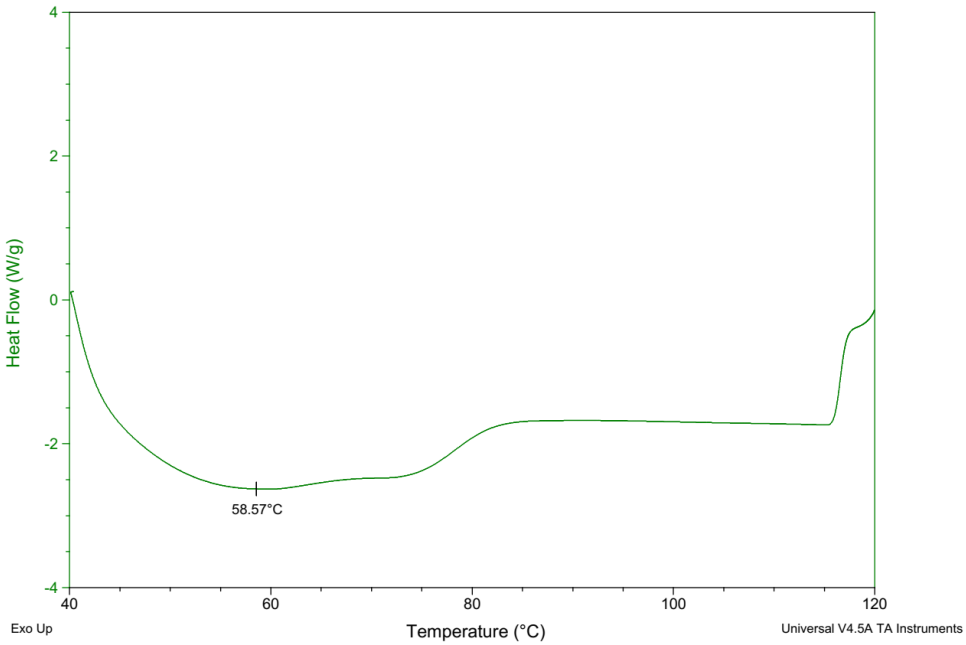


Figure S34. DSC of the Copolymer table 3, entry 1

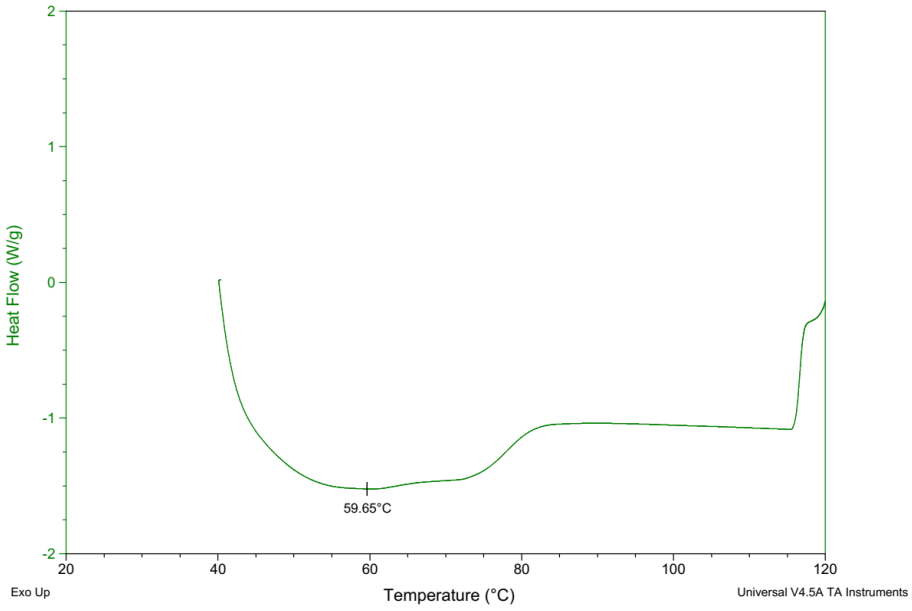


Figure S35. DSC of the Copolymer table 3, entry 2

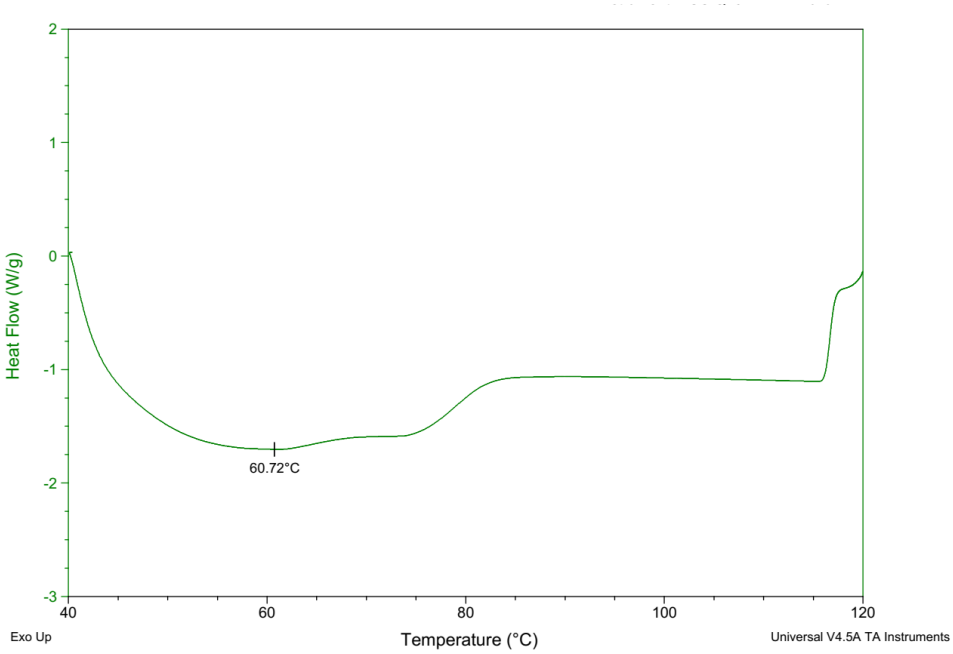
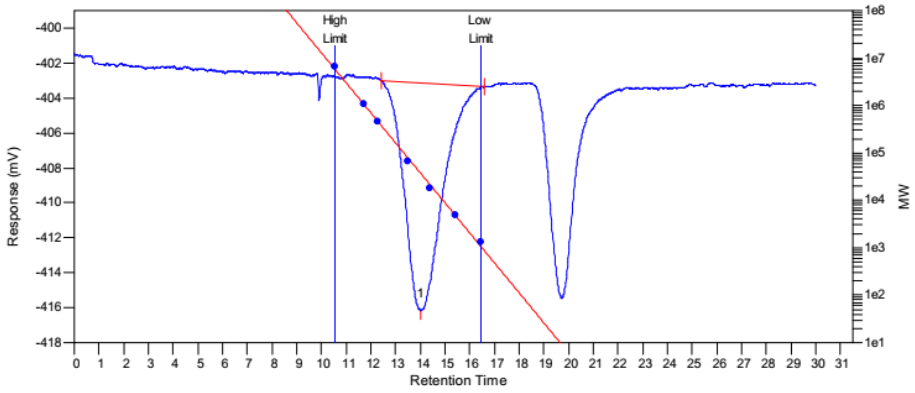
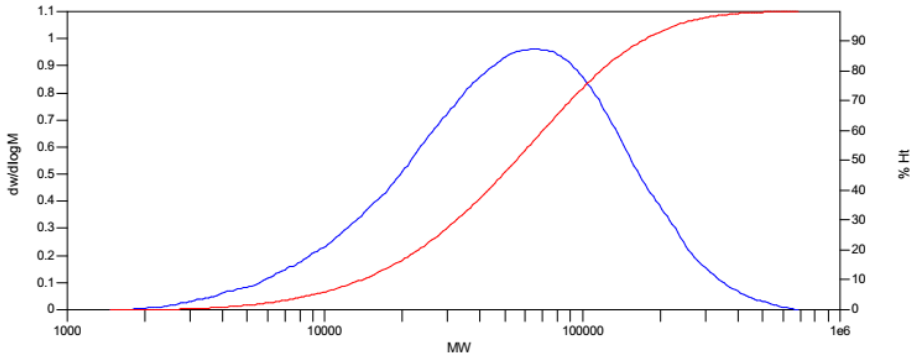


Figure S36. DSC of the Copolymer table 3, entry 3

2.6 GPC of polymer.



Distribution Plots



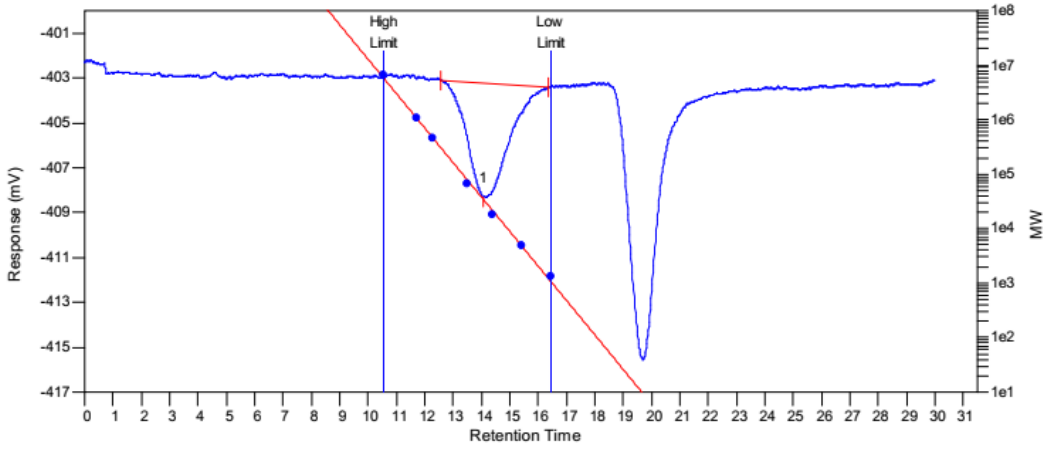
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	64329	30228	76605	146640	228712	68091	2.53424

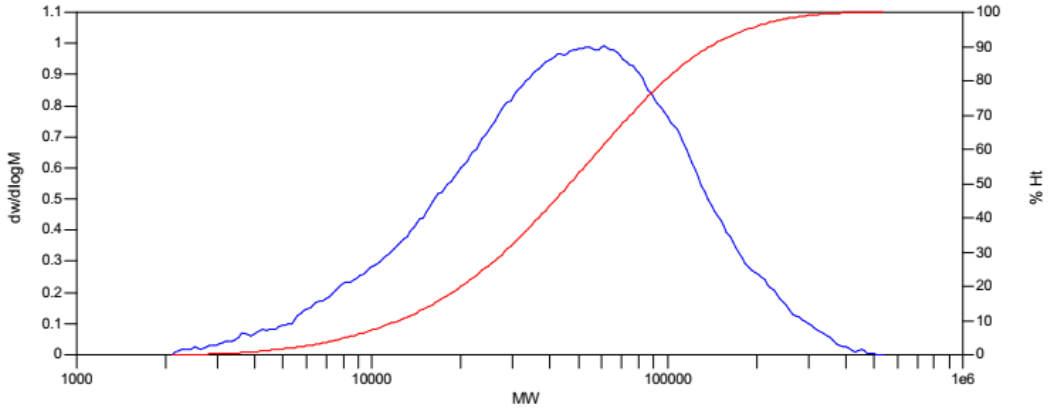
Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.42	14.03	16.62	-13.0112	0	1276	100

Figure S37. GPC of the polymer table 1, entry 1



Distribution Plots



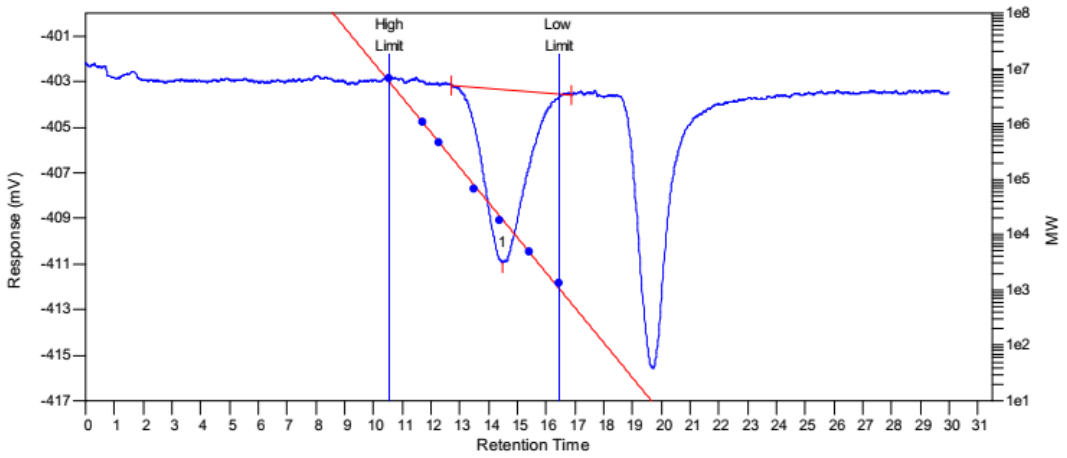
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	61263	26935	63972	118818	180889	57195	2.37505

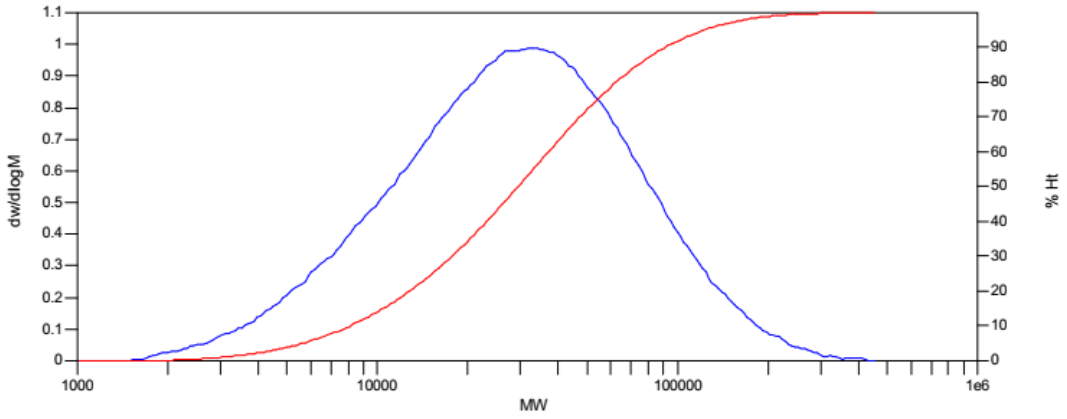
Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.58	14.07	16.37	-5.09971	0	484.901	100

Figure S38. GPC of the polymer table 1, entry 2



Distribution Plots



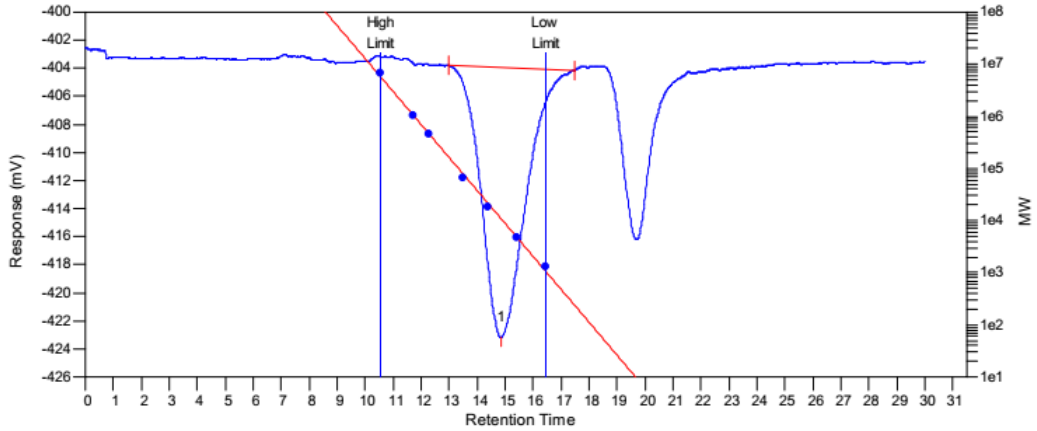
MW Averages

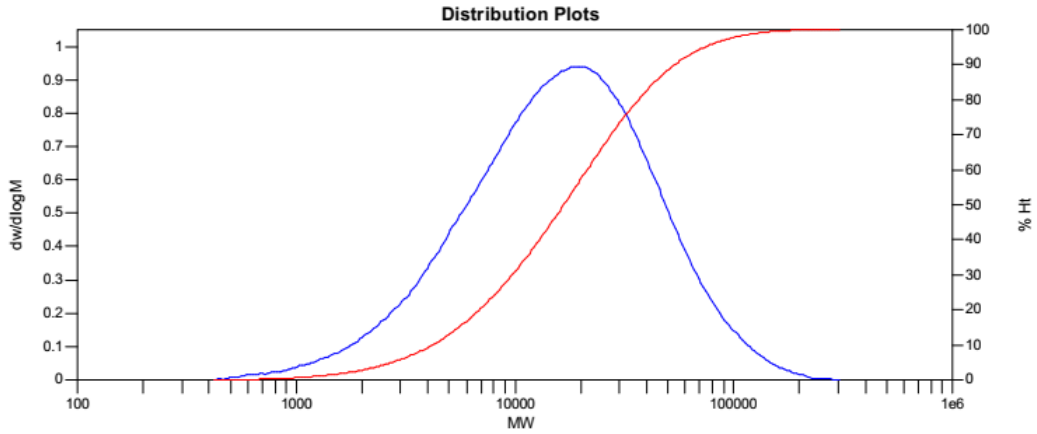
Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	33274	17795	41520	81891	135309	36902	2.33324

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.70	14.48	16.87	-7.5994	0	724.097	100

Figure S39. GPC of the polymer table 1, entry 3





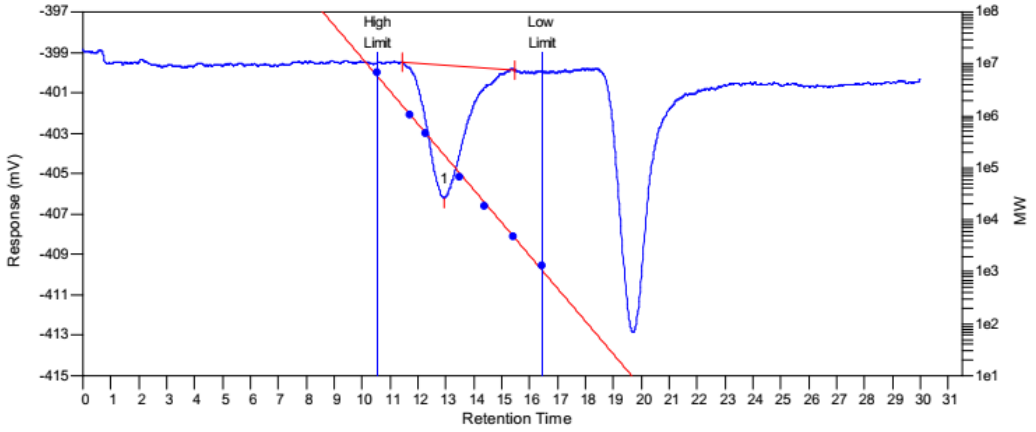
MW Averages

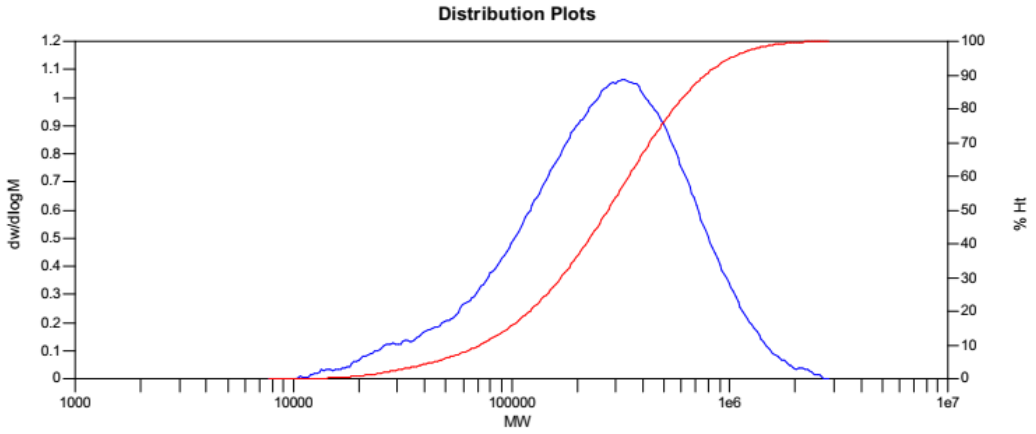
Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	19446	9028	24259	50210	84240	21327	2.68708

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.97	14.85	17.47	-19.2169	0	1927.59	100

Figure S40. GPC of the polymer table 1, entry 4





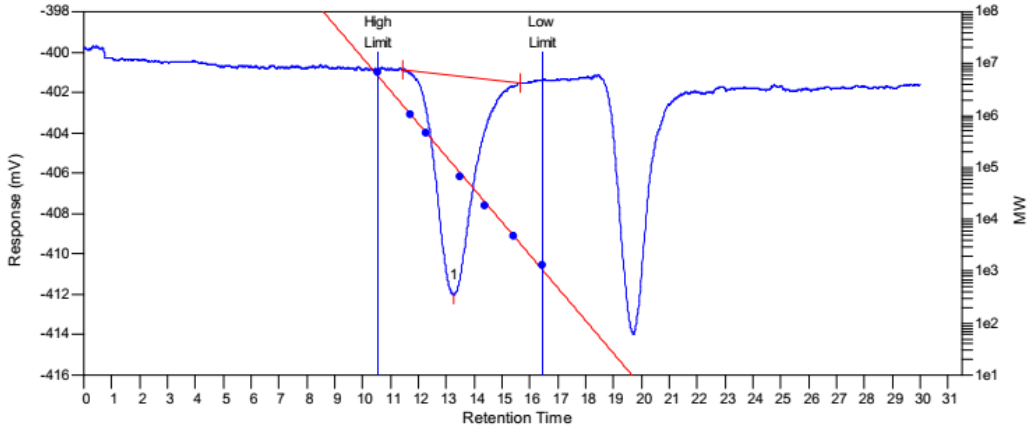
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	330251	152576	363009	647222	973629	326849	2.3792

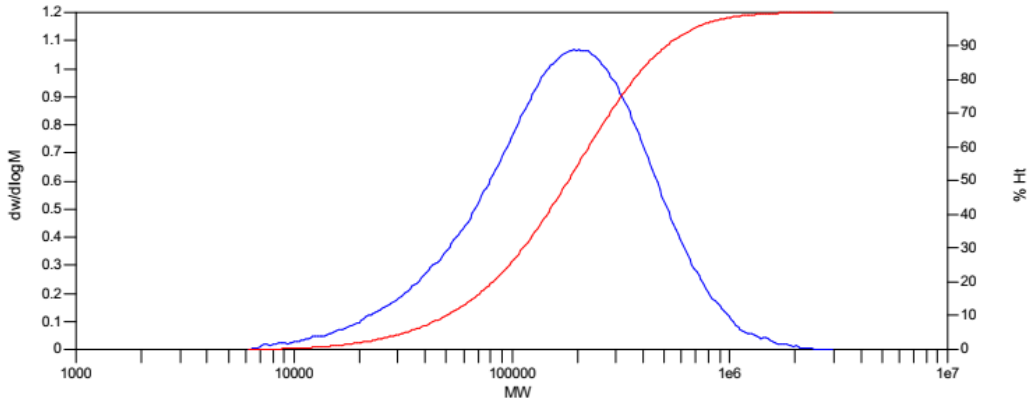
Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.45	12.92	15.48	-6.5435	0	580.646	100

Figure S41. GPC of the polymer table 1, entry 5



Distribution Plots



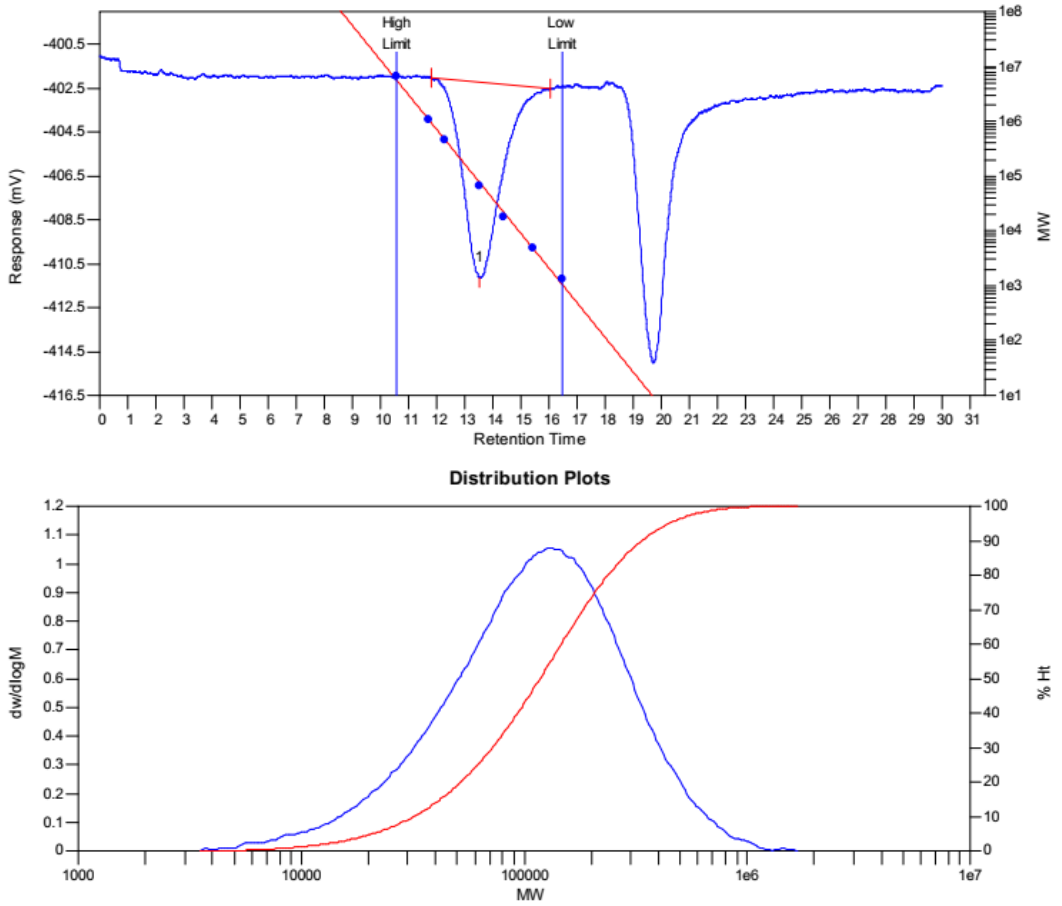
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	202663	104290	241816	448724	730771	217287	2.31869

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.42	13.28	15.63	-10.8392	0	958.602	100

Figure S42. GPC of the polymer table 1, entry 6



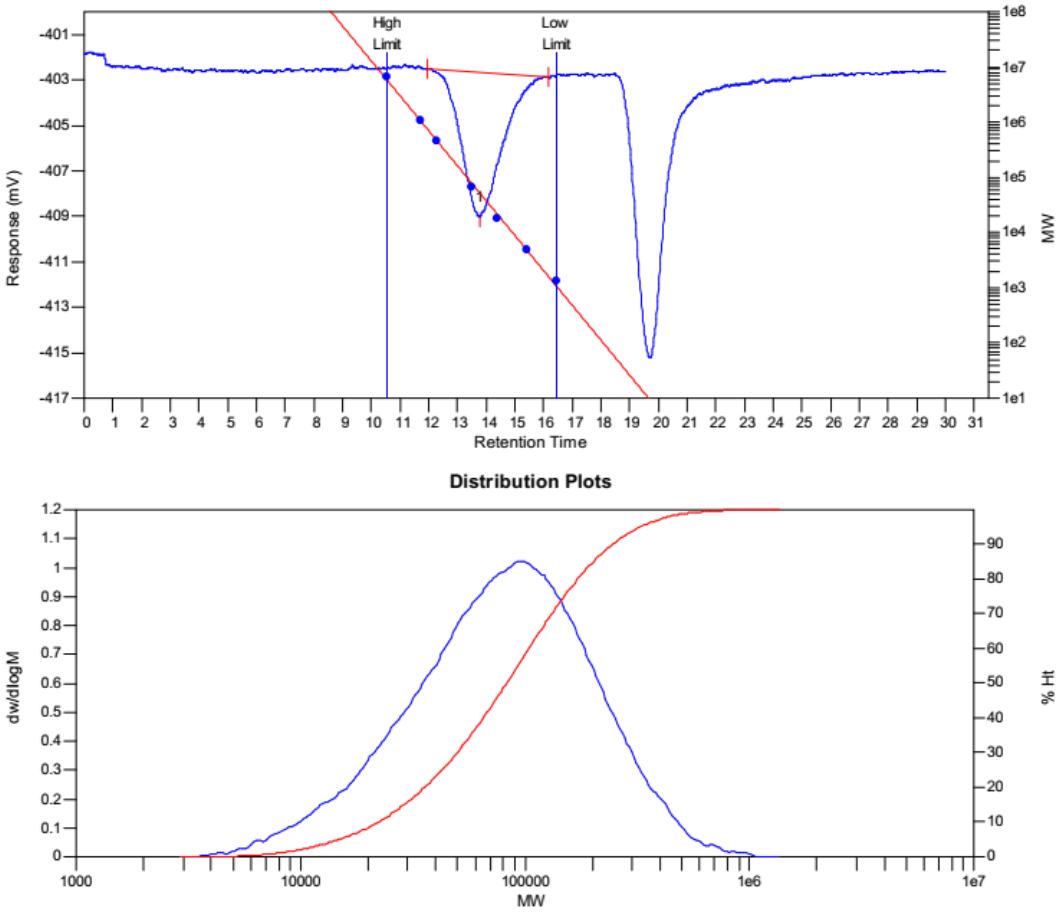
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	133818	66949	158138	294165	471517	141834	2.36207

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.80	13.53	16.02	-8.90883	0	798.235	100

Figure S43. GPC of the polymer table 1, entry 7



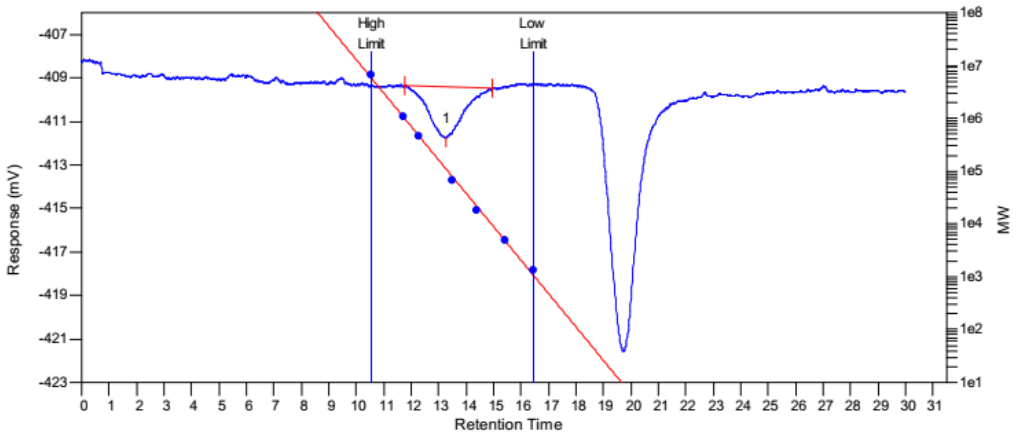
MW Averages

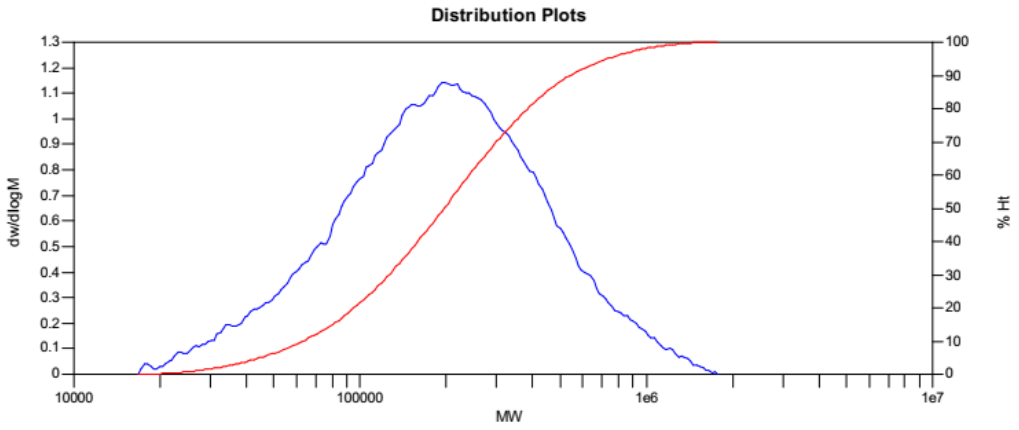
Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	92781	48580	113468	215090	344524	101379	2.33569

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.95	13.78	16.15	-6.33366	0	584.365	100

Figure S44. GPC of the polymer table 1, entry 8





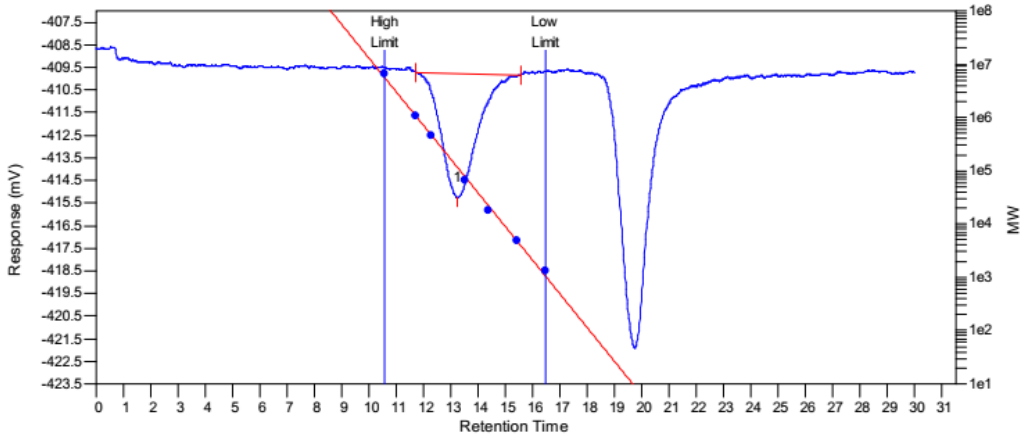
MW Averages

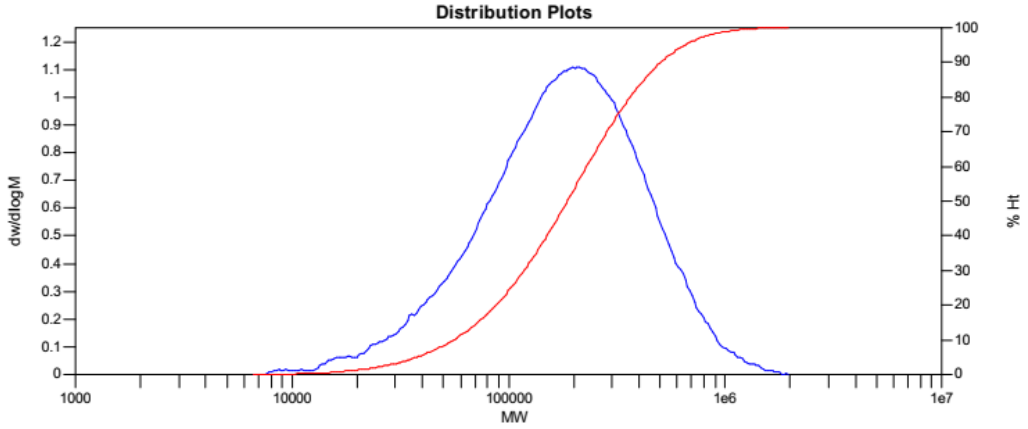
Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	197774	132714	260393	456280	688253	236505	1.96206

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.77	13.27	14.95	-2.34408	0	193.345	100

Figure S45. GPC of the polymer table 2, entry 1





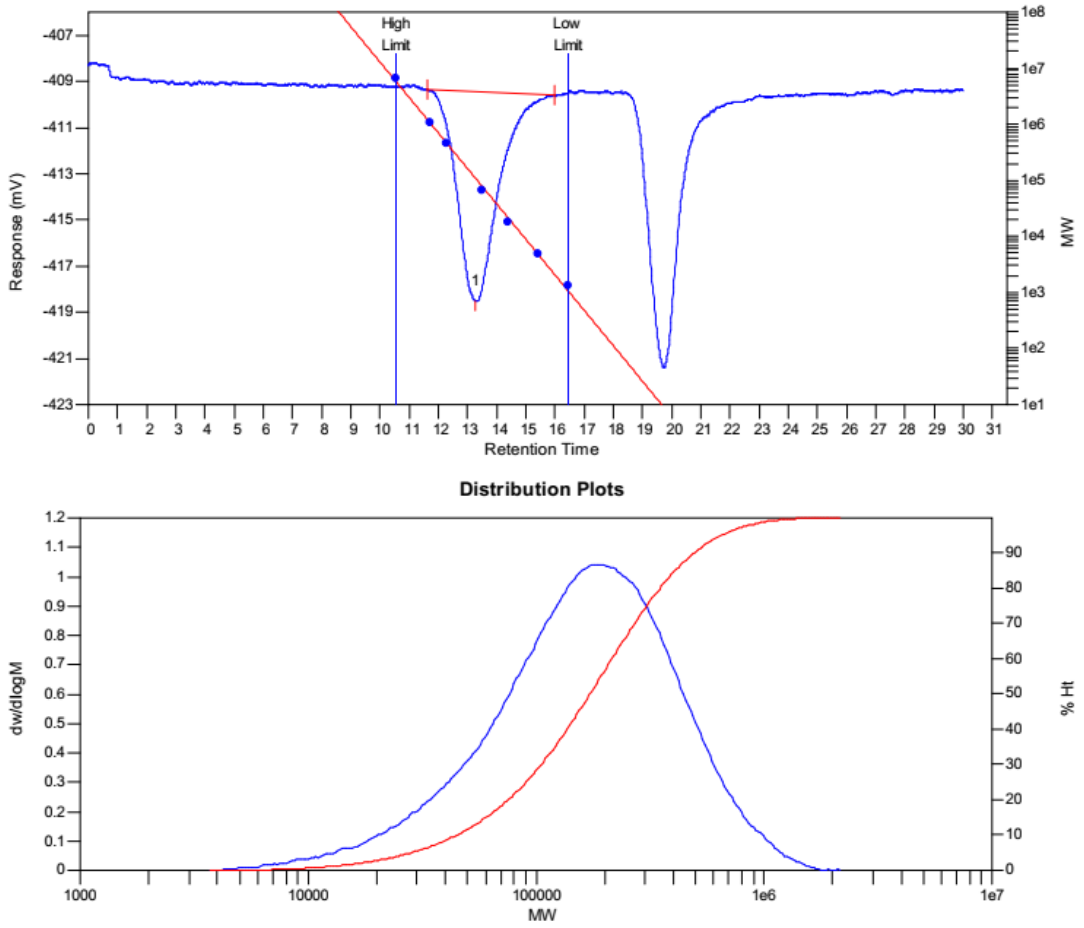
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	207672	114908	241835	417222	627195	219746	2.1046

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.70	13.23	15.58	-5.48456	0	467.208	100

Figure S46. GPC of the polymer table 2, entry 2



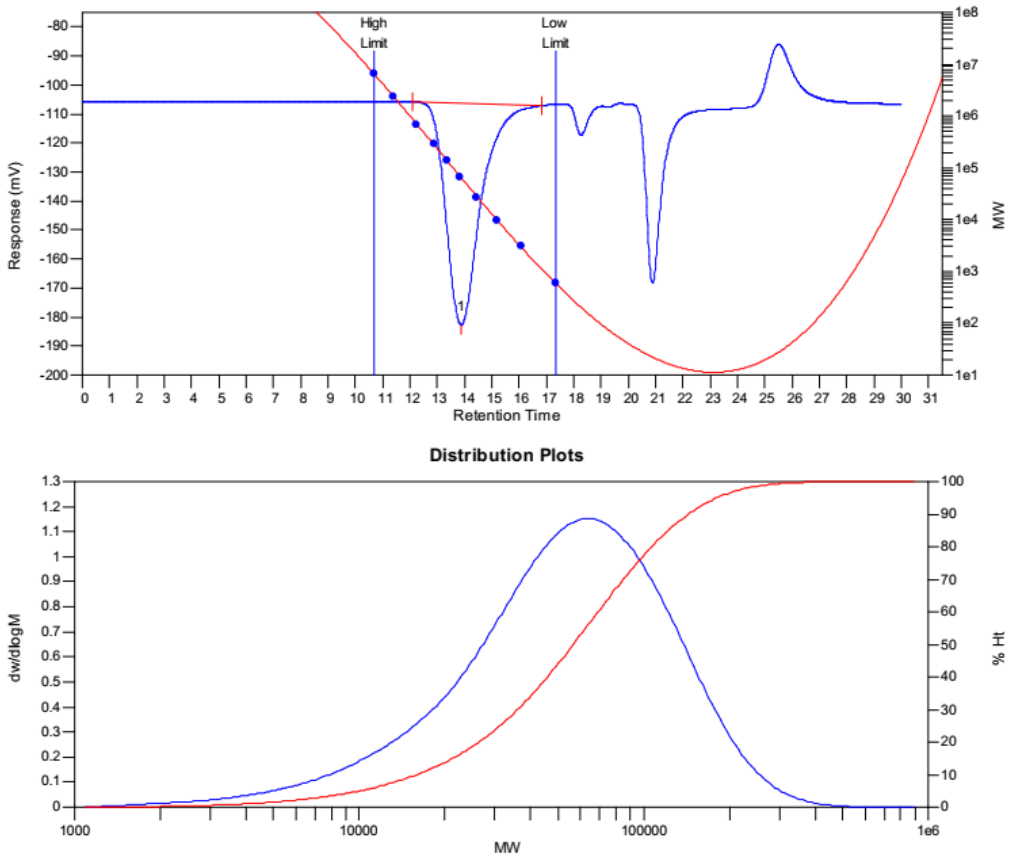
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	193004	93343	229776	417840	636818	206249	2.46163

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.63	13.28	15.98	-9.06945	0	821.784	100

Figure S47. GPC of the polymer table 2, entry 4



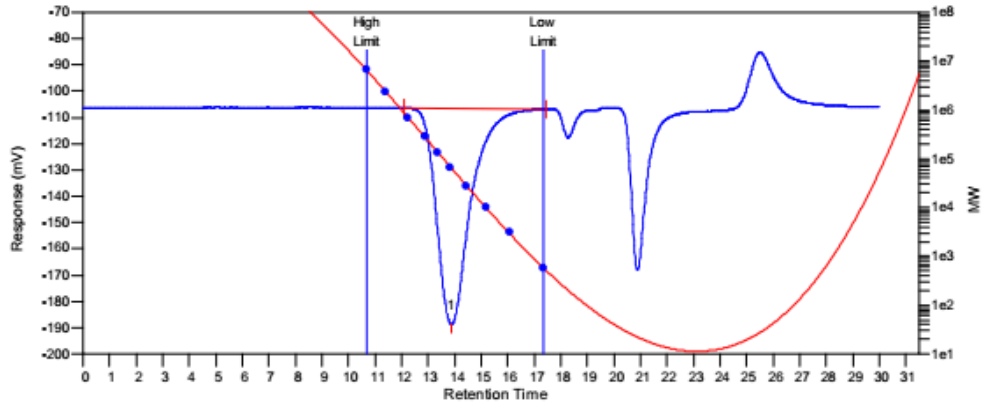
MW Averages

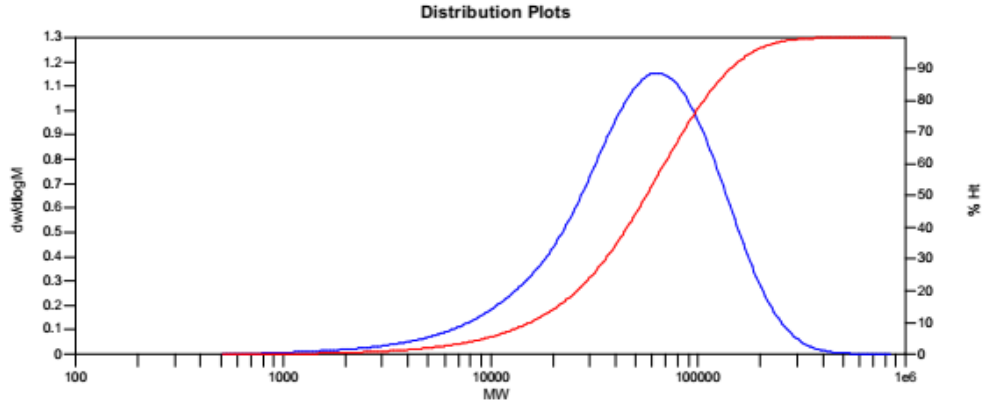
Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	63808	30646	69550	114386	164633	63707	2.26946

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.08	13.88	16.83	-76.3366	0	6278.78	100

Figure S48. GPC of the copolymer table 3, entry 1





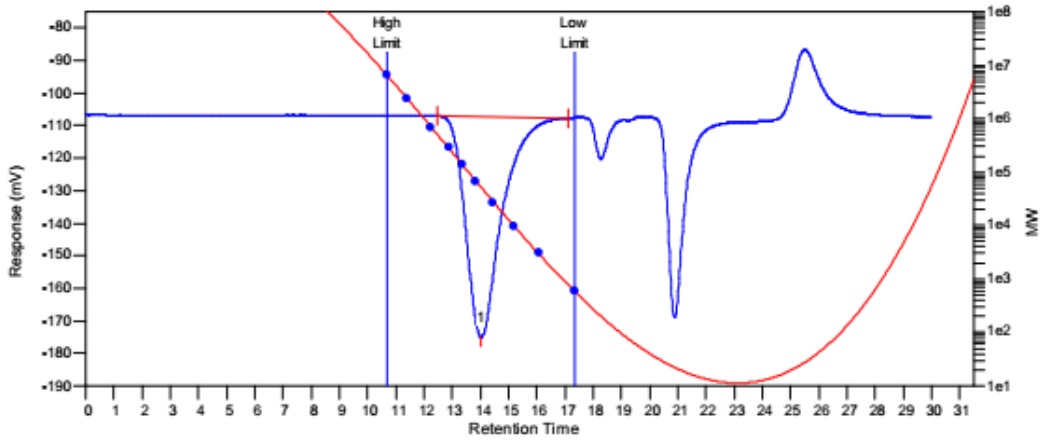
MW Averages

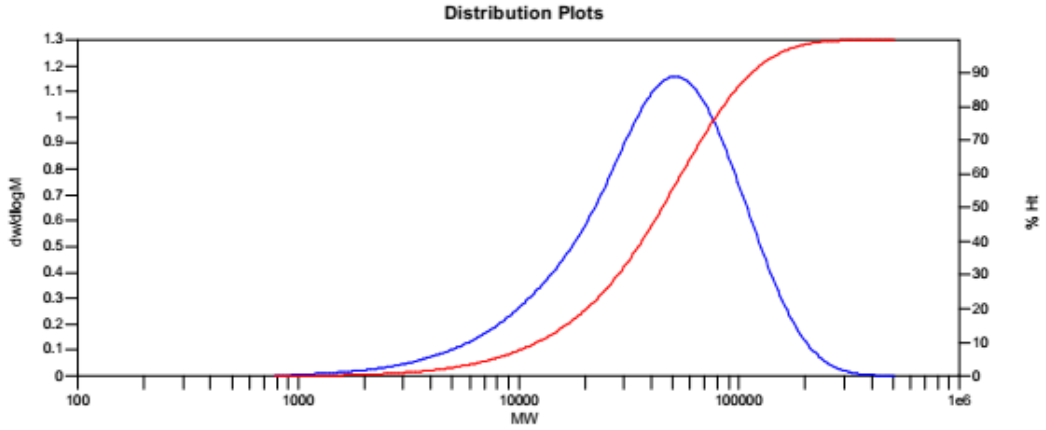
Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	63808	28240	68962	113713	164489	63106	2.442

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.12	13.88	17.45	-82.1455	0	6744.97	100

Figure S49. GPC of the copolymer table 3, entry 2





MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	52548	23702	54701	89997	128372	50056	2.30786

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.47	14.03	17.10	-67.8691	0	5568.72	100

Figure S50. GPC of the copolymer table 3, entry 3

3. X-ray Crystallography

Table S1 Crystal data and structure refinement for 0925CMJCH3CH3_0m.	
Identification code	0925CMJCH3CH3_0m
Empirical formula	$C_{46}H_{41}Br_2Cl_2N_3Ni$
Formula weight	925.25
Temperature/K	170
Crystal system	triclinic
Space group	P-1
a/Å	9.6967(5)
b/Å	11.2561(7)
c/Å	21.1250(12)
α/°	76.356(2)
β/°	77.471(2)
γ/°	67.677(2)
Volume/Å^3	2051.8(2)
Z	2
ρ_{calc}g/cm^3	1.498
μ/mm^{-1}	2.587
F(000)	940
Crystal size/mm^3	0.15 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)

2Θ range for data collection/°	3.97 to 53.016
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 14, -26 ≤ l ≤ 26
Reflections collected	23740
Independent reflections	8403 [R_{int} = 0.0662, R_{sigma} = 0.0779]
Data/restraints/parameters	8403/0/499
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0534, wR_2 = 0.1131
Final R indexes [all data]	R_1 = 0.0888, wR_2 = 0.1353
Largest diff. peak/hole / e Å^{-3}	1.43/-1.43

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2\times 10^3$) for 0925CMJCH3CH3_0m. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br1	4154.5(7)	9415.4(5)	7787.2(3)	46.85(17)
Ni1	4385.6(6)	7317.1(5)	8413.6(3)	24.68(15)
Br2	2413.5(6)	7143.3(6)	9227.5(3)	53.88(19)
Cl1	6765(2)	3267(2)	5373.8(9)	80.0(5)
Cl2	6345(2)	1083.4(17)	6359.4(10)	83.9(6)
N1	5589(3)	5921(3)	7850.4(15)	17.4(7)

N2	7504(3)	6086(3)	8241.3(15)	19.2(7)
N3	6391(4)	6834(3)	8664.3(16)	20.7(7)
C34	7017(4)	5460(4)	7870.7(18)	18.7(8)
C14	4519(4)	6103(4)	6873.8(19)	18.2(8)
C19	4910(4)	5393(4)	7492.1(18)	16.4(8)
C21	4749(4)	3575(4)	8475.7(19)	19.2(8)
C17	3907(4)	3812(4)	7381.2(19)	19.3(8)
C16	3592(4)	4456(4)	6751.6(19)	19.4(8)
C18	4539(4)	4265(4)	7767.2(18)	17.5(8)
C35	8195(4)	4333(4)	7598.4(19)	19.4(8)
C7	4794(4)	7392(4)	6596.1(19)	21.4(9)
C15	3881(4)	5599(4)	6518.9(19)	20.8(9)
C44	7037(5)	7418(4)	8924(2)	22.4(9)
C22	3431(4)	3109(4)	8823.7(19)	19.7(8)
C23	3466(5)	1863(4)	8839.1(19)	22.9(9)
C42	8861(4)	6246(4)	8231(2)	20.9(9)
C6	3491(5)	8423(4)	6251(2)	22.7(9)
C8	6333(5)	7177(4)	6185(2)	23.4(9)
C27	2151(5)	3964(4)	9143(2)	26.8(10)
C28	6235(4)	2436(4)	8551(2)	23.7(9)
C40	9208(4)	3409(4)	8006(2)	23.3(9)

C43	8590(5)	7043(4)	8671(2)	25.7(9)
C24	2277(5)	1457(4)	9170(2)	25.8(9)
C13	6758(5)	6583(4)	5631(2)	25.0(9)
C29	6933(5)	1626(4)	8087(2)	29.0(10)
C25	1023(5)	2306(5)	9491(2)	29.7(10)
C33	6836(5)	2139(5)	9133(2)	30.7(10)
C45	6144(5)	8330(4)	9386(2)	28.4(10)
C38	10450(5)	2186(4)	7129(2)	27.8(10)
C36	8305(5)	4165(4)	6954(2)	25.3(9)
C41	10279(5)	5722(4)	7781(2)	29.3(10)
C9	7391(5)	7525(4)	6378(2)	29.7(10)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 0925CMJCH3CH3_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}
Br1	69.9(4)	25.7(3)	38.2(3)	-11.1(2)	-17.9(3)
Ni1	16.1(3)	30.2(3)	28.3(3)	-14.4(3)	-2.3(2)
Br2	37.1(3)	57.1(4)	69.4(4)	-29.1(3)	22.8(3)
Cl1	67.9(11)	97.0(14)	65.0(11)	5.2(10)	4.0(9)
Cl2	92.3(14)	49.0(10)	90.1(14)	-2.8(9)	-2.9(11)
N1	15.5(16)	20.1(18)	15.2(16)	-1.2(14)	-4.5(13)
N2	17.2(16)	21.4(18)	19.8(17)	-6.8(15)	-1.8(13)

N3	20.4(17)	22.7(19)	19.4(17)	-7.8(15)	-3.6(13)
C34	23(2)	20(2)	14.9(19)	-2.4(17)	-4.2(15)
C14	14.5(18)	18(2)	19.1(19)	-2.6(17)	-4.4(15)
C19	12.7(18)	17(2)	17.2(19)	-4.6(16)	-1.1(14)
C21	23(2)	17(2)	18(2)	-0.7(17)	-4.3(16)
C17	15.4(19)	20(2)	23(2)	-4.2(17)	-1.6(16)
C16	15.1(19)	22(2)	21(2)	-6.2(18)	0.1(15)
C18	12.8(18)	17(2)	19.8(19)	-5.5(17)	-0.8(15)
C35	17.7(19)	19(2)	22(2)	-3.4(17)	-4.1(16)
C7	21(2)	23(2)	21(2)	-4.9(18)	-5.1(16)
C15	19(2)	22(2)	20(2)	-2.3(17)	-5.6(16)
C44	26(2)	21(2)	21(2)	-1.0(18)	-5.1(17)
C22	23(2)	22(2)	16.1(19)	-2.1(17)	-3.0(16)
C23	24(2)	27(2)	17(2)	-5.7(18)	-1.3(16)
C42	18(2)	23(2)	25(2)	-3.6(18)	-4.9(16)
C6	27(2)	13(2)	26(2)	-3.5(18)	-8.3(17)
C8	24(2)	17(2)	26(2)	5.0(18)	-8.2(17)
C27	29(2)	21(2)	29(2)	-4.4(19)	-1.7(18)
C28	21(2)	22(2)	27(2)	6.3(18)	-4.9(17)
C40	21(2)	24(2)	24(2)	-1.8(19)	-4.2(17)
C43	23(2)	27(2)	32(2)	-3(2)	-11.0(18)

C24	34(2)	27(2)	24(2)	-5.4(19)	-2.2(18)
C13	23(2)	26(2)	25(2)	-2.3(19)	-5.3(17)
C29	25(2)	26(2)	31(2)	1(2)	-4.2(18)
C25	26(2)	42(3)	23(2)	-5(2)	0.3(18)
C33	29(2)	33(3)	32(2)	6(2)	-9.0(19)
C45	32(2)	31(3)	23(2)	-6(2)	-6.2(18)
C38	20(2)	20(2)	42(3)	-11(2)	-0.3(19)
C36	27(2)	22(2)	24(2)	-1.3(19)	-4.3(17)
C41	20(2)	33(3)	36(3)	-8(2)	-0.1(18)
C9	35(2)	25(2)	32(2)	-2(2)	-8(2)
C20	37(3)	38(3)	27(2)	-9(2)	-7.1(19)
C39	18(2)	24(2)	37(3)	-2(2)	-7.6(18)
C26	23(2)	38(3)	29(2)	-11(2)	2.9(18)
C37	34(2)	26(2)	26(2)	-10(2)	-4.2(19)
C12	33(3)	26(2)	31(2)	-2(2)	-1(2)
C10	30(2)	30(3)	45(3)	8(2)	-15(2)
C11	24(2)	34(3)	43(3)	-1(2)	0(2)
C32	37(3)	42(3)	44(3)	19(3)	-24(2)
C30	31(3)	29(3)	53(3)	-4(2)	-1(2)
C31	31(3)	31(3)	73(4)	17(3)	-24(3)
C2	23(2)	32(3)	65(4)	-6(3)	-7(2)

C1	27(2)	31(3)	48(3)	9(2)	-4(2)
C3	41(3)	42(3)	44(3)	4(3)	-13(2)
C5	34(3)	57(4)	66(4)	39(3)	7(3)
C4	50(4)	90(5)	67(4)	57(4)	13(3)

Table S4 Bond Lengths for 0925CMJCH3CH3_0m.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Br1	Ni1	2.3732(8)		C44	C45	1.480(6)
Ni1	Br2	2.3130(7)		C22	C23	1.383(6)
Ni1	N1	2.033(3)		C22	C27	1.399(6)
Ni1	N3	1.966(3)		C23	C24	1.388(6)
Cl1	C47	1.722(12)		C42	C43	1.358(6)
Cl1	C46	1.656(18)		C42	C41	1.492(6)
Cl2	C47	1.659(12)		C6	C1	1.383(6)
Cl2	C46	1.709(18)		C6	C5	1.361(7)
N1	C34	1.287(5)		C8	C13	1.392(6)
N1	C19	1.444(5)		C8	C9	1.391(6)
N2	N3	1.385(4)		C27	C26	1.394(6)
N2	C34	1.417(5)		C28	C29	1.384(6)
N2	C42	1.389(5)		C28	C33	1.390(6)
N3	C44	1.326(5)		C40	C39	1.383(6)

C34	C35	1.485(5)		C24	C25	1.384(6)
C14	C19	1.407(5)		C13	C12	1.390(6)
C14	C7	1.532(6)		C29	C30	1.395(6)
C14	C15	1.391(6)		C25	C26	1.378(7)
C19	C18	1.410(6)		C33	C32	1.382(7)
C21	C18	1.532(5)		C38	C39	1.387(6)
C21	C22	1.538(5)		C38	C37	1.389(6)
C21	C28	1.531(5)		C36	C37	1.384(6)
C17	C16	1.393(6)		C9	C10	1.394(6)
C17	C18	1.397(5)		C12	C11	1.375(7)
C16	C15	1.375(6)		C10	C11	1.375(7)
C16	C20	1.507(6)		C32	C31	1.387(8)
C35	C40	1.399(5)		C30	C31	1.382(7)
C35	C36	1.393(6)		C2	C1	1.391(6)
C7	C6	1.537(5)		C2	C3	1.371(7)
C7	C8	1.517(6)		C3	C4	1.361(8)
C44	C43	1.417(6)		C5	C4	1.381(8)

Table S5 Bond Angles for 0925CMJCH3CH3_0m.

Atom	Atom	Atom	Angle/˚		Atom	Atom	Atom	Angle/˚
Br2	Ni1	Br1	117.37(3)		C23	C22	C21	122.4(3)
N1	Ni1	Br1	110.22(9)		C23	C22	C27	118.2(4)

N1	Ni1	Br2	123.11(10)		C27	C22	C21	119.4(4)
N3	Ni1	Br1	99.24(10)		C22	C23	C24	121.2(4)
N3	Ni1	Br2	118.80(10)		N2	C42	C41	125.6(4)
N3	Ni1	N1	80.20(13)		C43	C42	N2	106.3(3)
C34	N1	Ni1	115.0(3)		C43	C42	C41	127.9(4)
C34	N1	C19	121.3(3)		C1	C6	C7	119.3(4)
C19	N1	Ni1	123.5(2)		C5	C6	C7	122.9(4)
N3	N2	C34	115.9(3)		C5	C6	C1	117.7(4)
N3	N2	C42	109.7(3)		C13	C8	C7	122.2(4)
C42	N2	C34	134.0(3)		C9	C8	C7	119.7(4)
N2	N3	Ni1	111.5(2)		C9	C8	C13	118.1(4)
C44	N3	Ni1	134.4(3)		C26	C27	C22	120.6(4)
C44	N3	N2	107.0(3)		C29	C28	C21	122.5(4)
N1	C34	N2	114.3(3)		C29	C28	C33	118.7(4)
N1	C34	C35	129.6(4)		C33	C28	C21	118.6(4)
N2	C34	C35	116.0(3)		C39	C40	C35	120.7(4)
C19	C14	C7	121.0(3)		C42	C43	C44	107.8(4)
C15	C14	C19	118.2(4)		C25	C24	C23	120.1(4)
C15	C14	C7	120.8(3)		C12	C13	C8	120.8(4)
C14	C19	N1	117.5(3)		C28	C29	C30	120.6(4)
C14	C19	C18	120.6(4)		C26	C25	C24	119.7(4)

C18	C19	N1	121.8(3)		C32	C33	C28	121.0(5)
C18	C21	C22	112.0(3)		C39	C38	C37	119.2(4)
C28	C21	C18	115.1(3)		C37	C36	C35	119.3(4)
C28	C21	C22	109.1(3)		C8	C9	C10	120.8(4)
C16	C17	C18	122.4(4)		C40	C39	C38	120.0(4)
C17	C16	C20	121.7(4)		C25	C26	C27	120.2(4)
C15	C16	C17	117.8(4)		C36	C37	C38	121.4(4)
C15	C16	C20	120.5(4)		C11	C12	C13	120.2(4)
C19	C18	C21	122.0(3)		C11	C10	C9	120.1(4)
C17	C18	C19	117.9(4)		C12	C11	C10	119.9(4)
C17	C18	C21	120.1(4)		C33	C32	C31	120.1(5)
C40	C35	C34	118.7(3)		C31	C30	C29	120.2(5)
C36	C35	C34	121.9(4)		C30	C31	C32	119.4(4)
C36	C35	C40	119.4(4)		C3	C2	C1	120.0(5)
C14	C7	C6	112.6(3)		C6	C1	C2	121.2(5)
C8	C7	C14	111.4(3)		C4	C3	C2	118.6(5)
C8	C7	C6	114.1(3)		C6	C5	C4	121.1(5)
C16	C15	C14	122.9(4)		C3	C4	C5	121.4(5)
N3	C44	C43	109.2(4)		Cl2	C47	Cl1	119.4(7)
N3	C44	C45	121.0(4)		Cl1	C46	Cl2	120.3(8)
C43	C44	C45	129.8(4)					

Table S6 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 0925CMJCH3CH3_0m.

Atom	*x*	*y*	*z*	U(eq)
H21	4741	4238	8720.1	23
H17	3684	3036	7554.23	23
H7	4820	7743	6984.98	26
H15	3633	6066	6097.37	25
H23	4320	1273	8619.02	27
H27	2096	4828	9134.02	32
H40	9129	3514	8447.03	28
H43	9313	7303	8787.35	31
H24	2325	596	9176.94	31
H13	6050	6348	5486.06	30
H29	6540	1819	7685.84	35
H25	212.6	2027	9720.82	36
H33	6369	2689	9454.98	37
H45A	6231	9189	9206.51	43
H45B	6525	8002	9810.79	43
H45C	5085	8405	9448.21	43
H38	11223	1462	6964.87	33
H36	7613	4775	6674.37	30

H41A	10751	4785	7932.03	44
H41B	10972	6168	7781.24	44
H41C	10047	5867	7334.01	44
H9	7120	7948	6749.24	36
H20A	3124	3023	6487.04	47
H20B	3286	4145	5880.8	47
H20C	1792	4405	6409.43	47
H39	11001	1718	8055.22	32
H26	90.28	4147	9689	38
H37	9516	2988	6286.63	34
H12	8478	5931	4907.17	39
H10	9558	7498	6172.59	41
H11	10240	6469	5261.16	44
H32	8503	867.5	9649.96	48
H30	8679	-22.5	7883.27	48
H31	9659	-510	8867.56	56
H2	-189	9645	6467.96	51
H1	1841	8085	6960.99	47
H3	242.8	10987	5479.4	61
H5	4708	9151	5471.72	85
H4	2694	10732	4997.96	118

H47A	8046	1985	6186.88	84
H47B	6442	2919	6470.54	84
H46A	7646	1191	5359.93	83
H46B	5885	1789	5328.99	83

Table S7 Atomic Occupancy for 0925CMJCH3CH3_0m.

Atom	*Occupancy*		Atom	*Occupancy*		Atom	*Occupancy*
C47	0.6		H47A	0.6		H47B	0.6
C46	0.4		H46A	0.4		H46B	0.4

Reference

[1] N. Y. Na, S. Y. Dai, C. L. Chen *Macromolecules,* 2018, **51**, 4040-4048