

Supporting Information

Bis(pentiptycenyl)-diimine-Nickel Complexes for Ethene Polymerization and Copolymerization with polar Monomers

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General experimental

All chemicals were purchased as reagent grade from commercial suppliers and used without further purification, unless otherwise noted. Diethylaluminium chloride (1 M solution in hexane) was purchased from Acros Organics. Toluene was dried under sodium, distilled under a nitrogen atmosphere and stored over molecular sieves (4 Å). ^1H and ^{13}C NMR spectra were recorded on a Bruker DRX500 spectrometer. The chemical shifts are given in parts per million (ppm) on the delta scale (δ) and are referenced to the residual peak of chloroform (^1H NMR= 7.26, ^{13}C NMR= 77.16 ppm), 1,1,2,2-tetrachloroethane- d_2 (^1H NMR= 6.00, ^{13}C NMR= 73.78 ppm). Abbreviations for NMR: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sep = septet, hept = heptet, m = multiplet, br = broad signal. Thin layer chromatography (tlc) was performed by using silica 60 F 254 (0.2 mm) on aluminum plates. Preparative chromatography was done on Merck silica 60 (0.063 – 0.2 mm).

NMR spectra

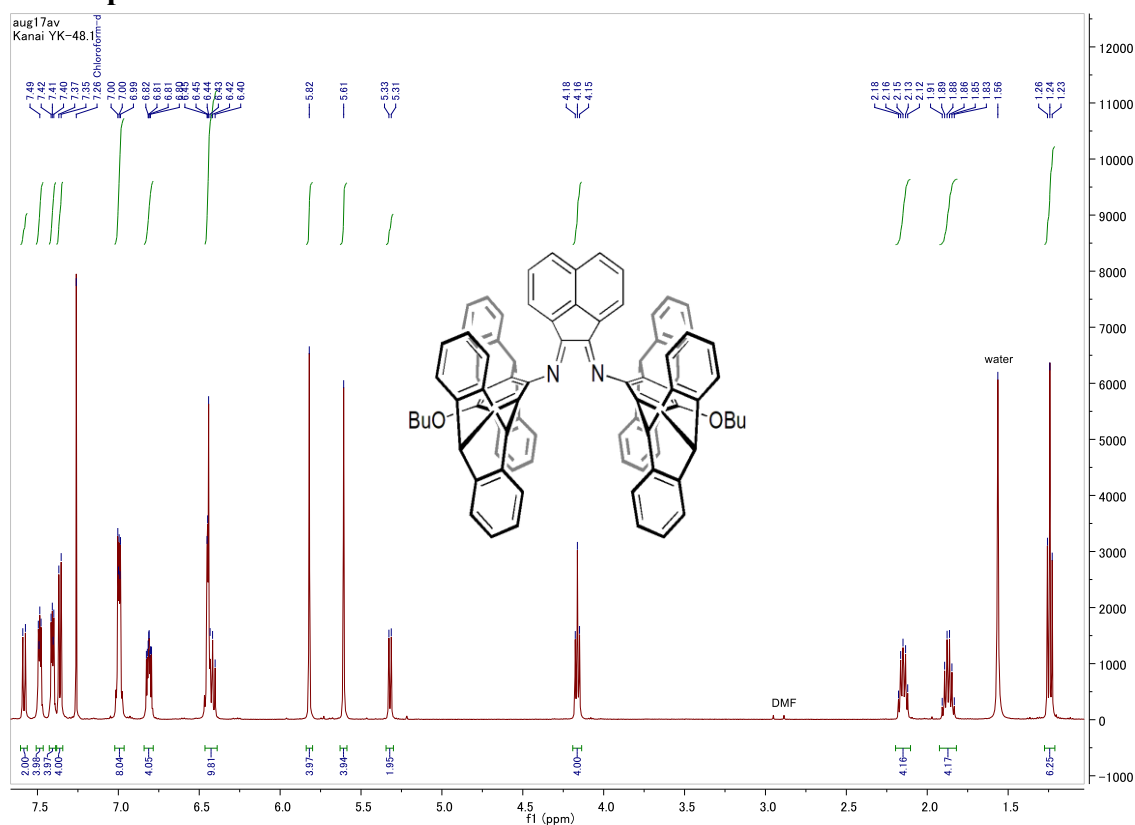


Fig S 1. ^1H NMR spectrum of diimine **2a**.

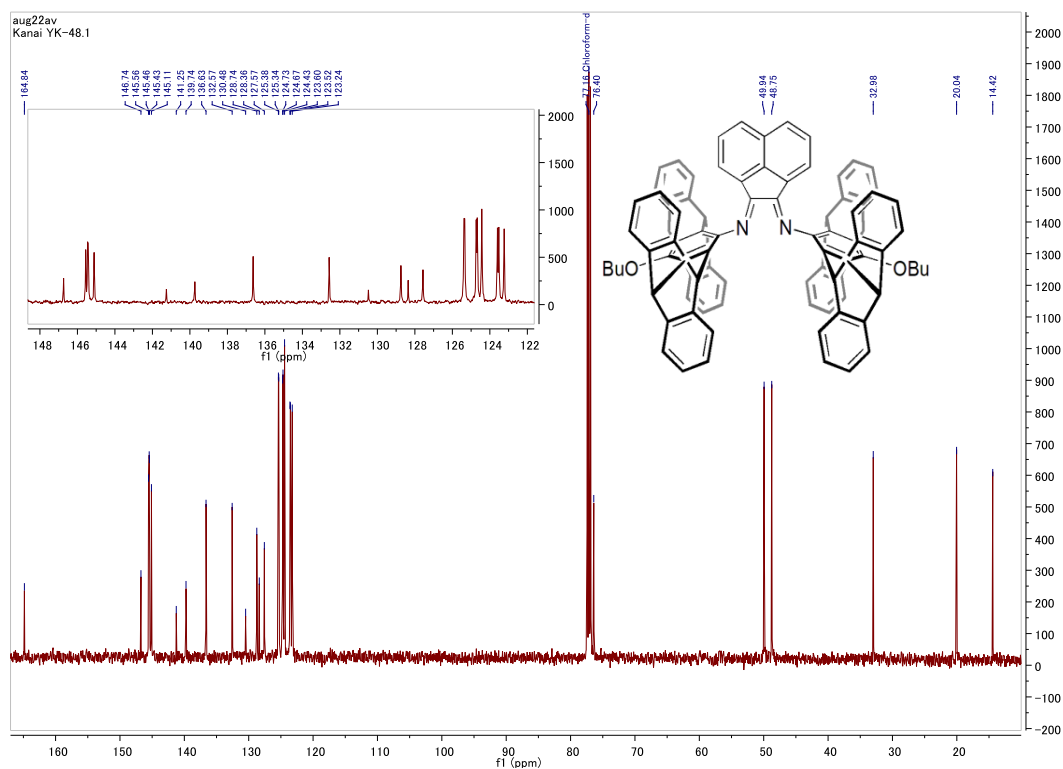


Fig S 2. ^{13}C NMR spectrum of diimine **2a**.

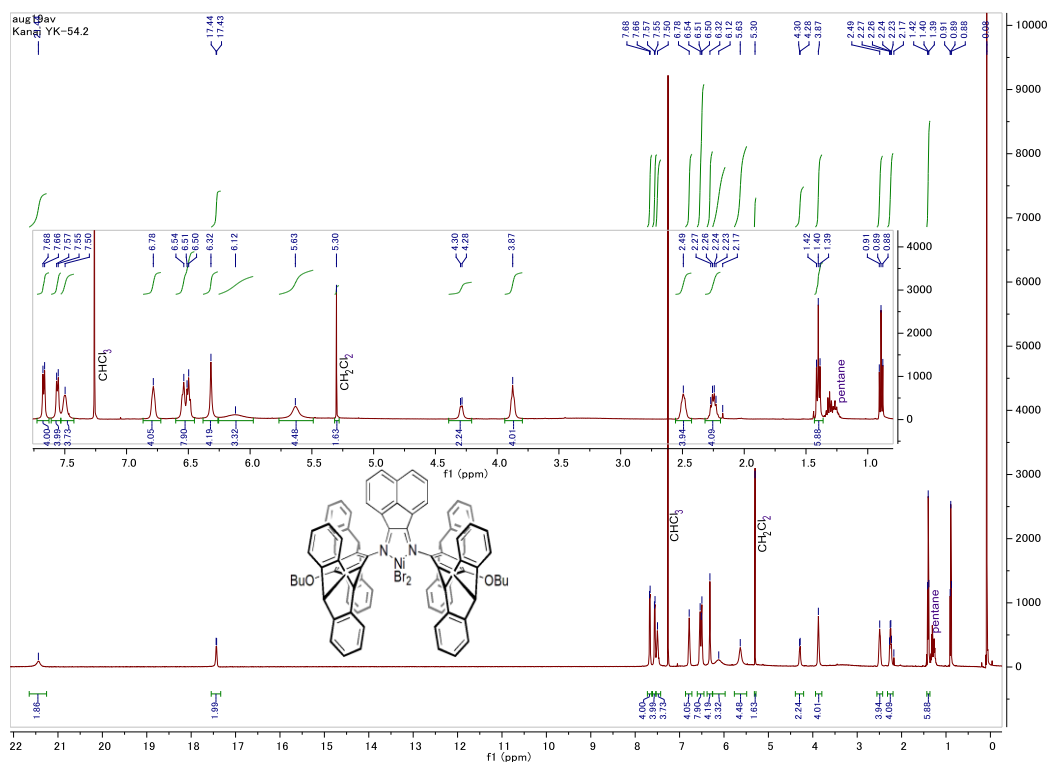


Fig S 3. ^1H NMR spectrum of paramagnetic nickel complex **3a**.

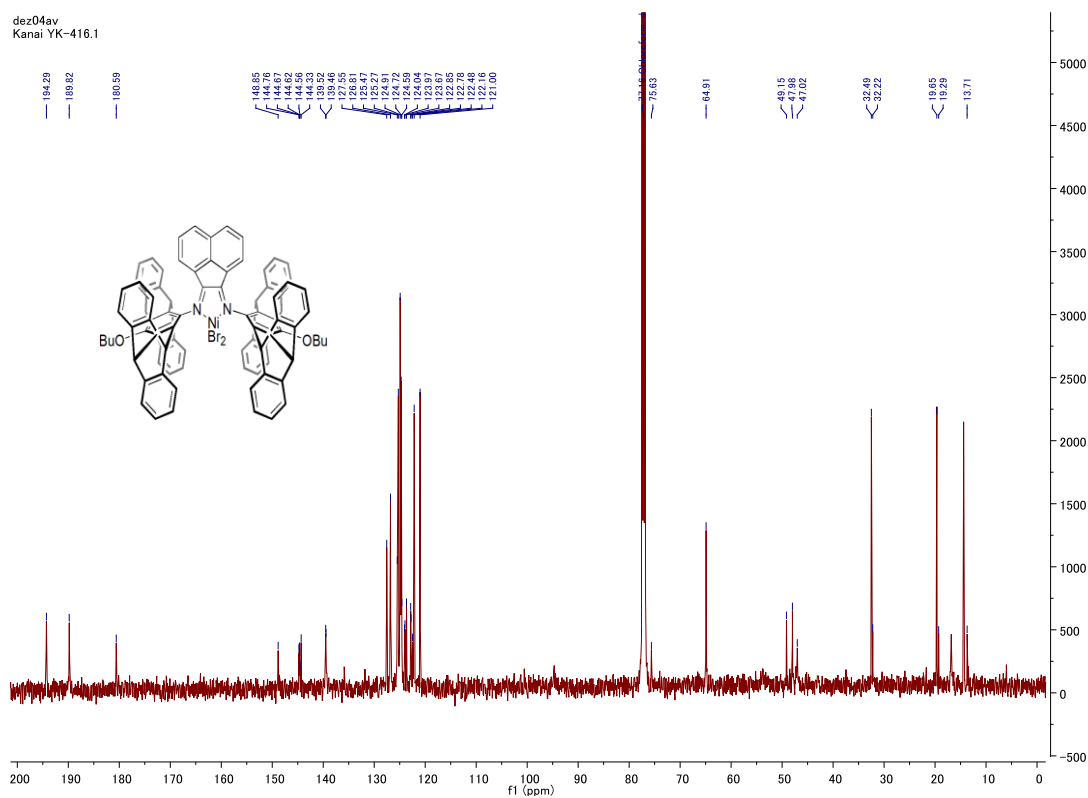


Fig S 4. ^{13}C NMR spectrum of paramagnetic nickel complex **3a**.

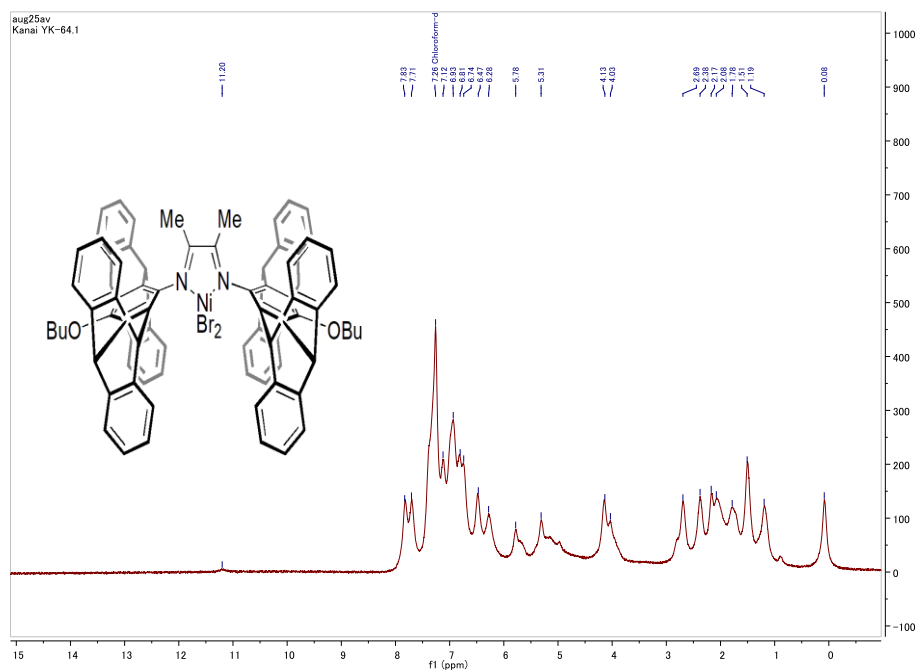


Fig S 5. ^1H NMR spectrum of paramagnetic nickel complex **3b**.

Mass spectra

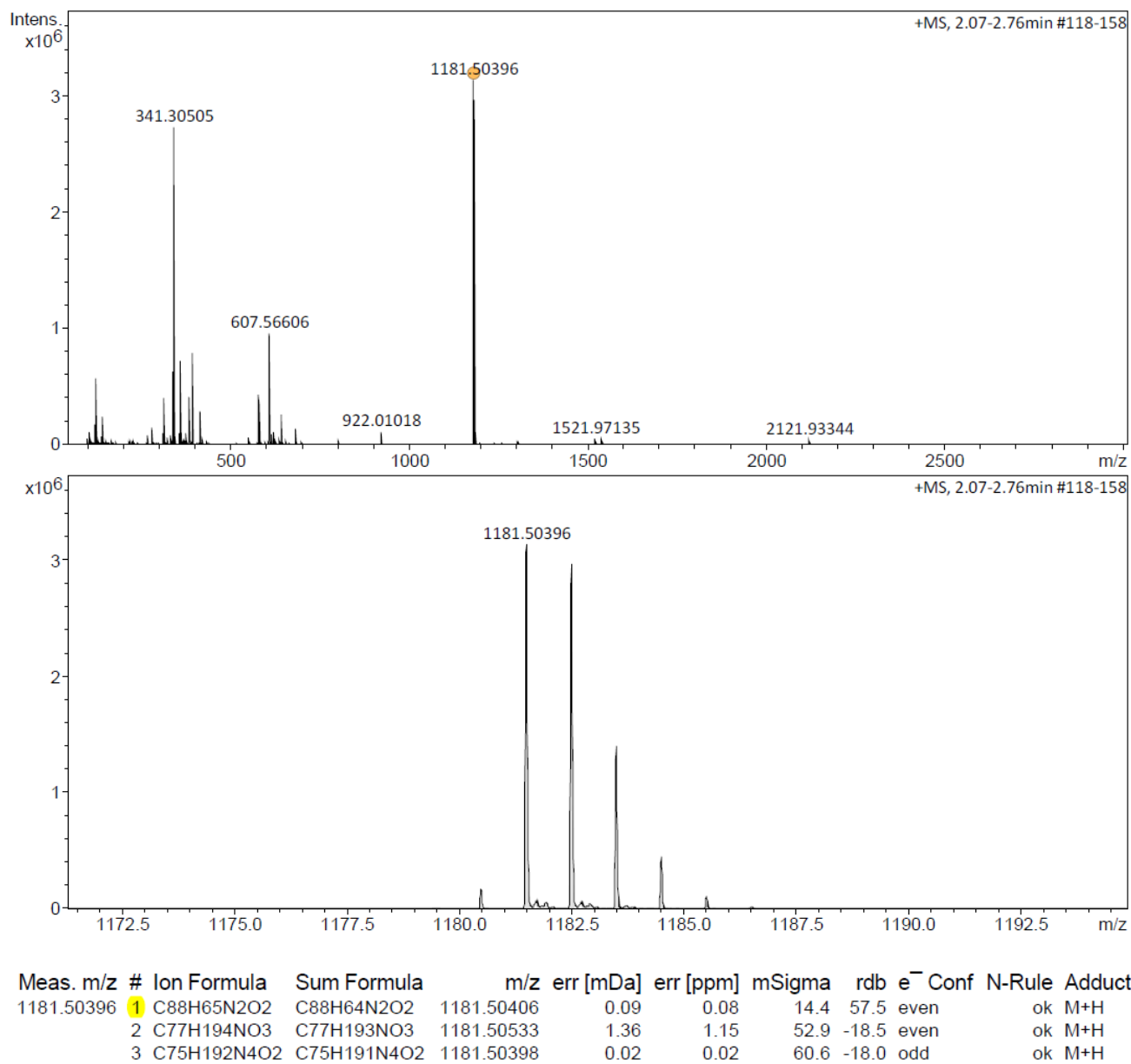


Fig S 6. Mass spectrum of diimine **2a**.

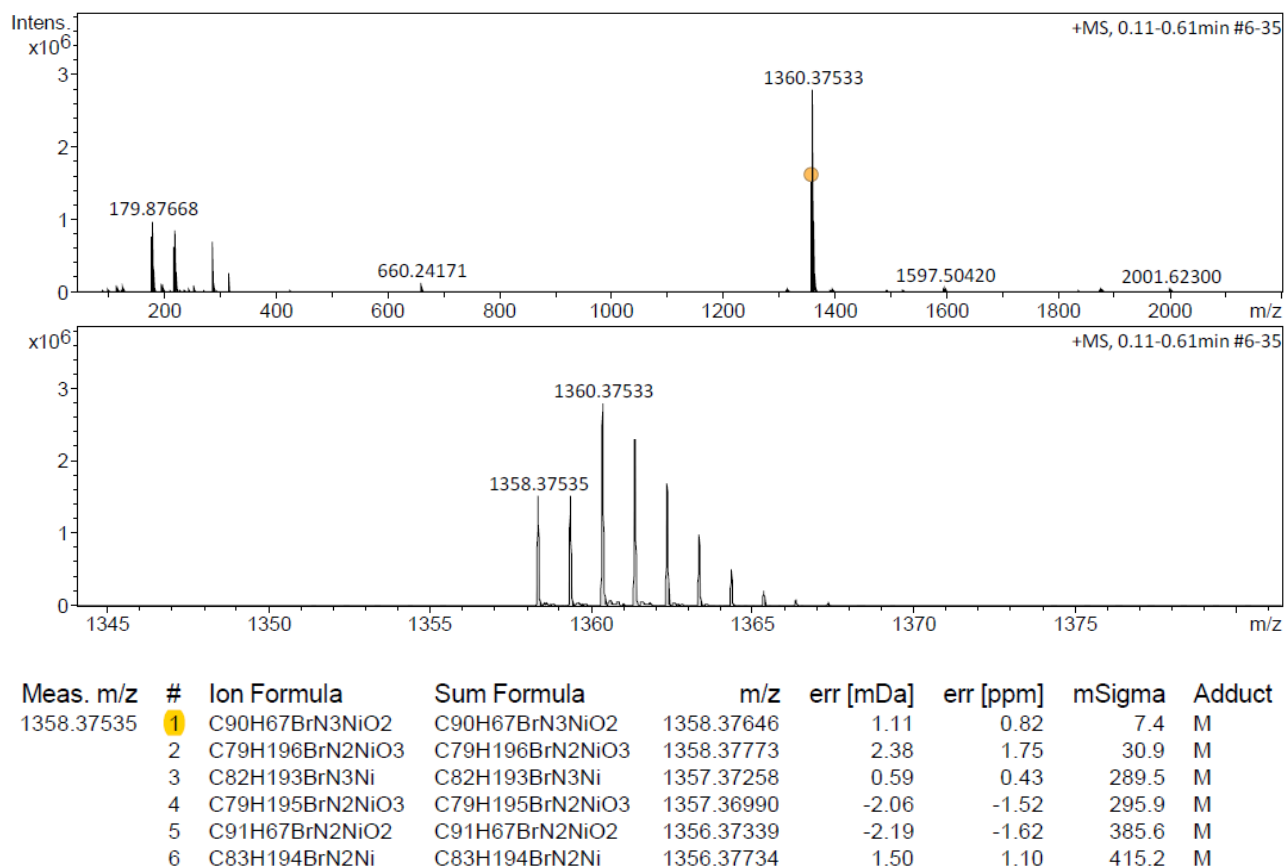
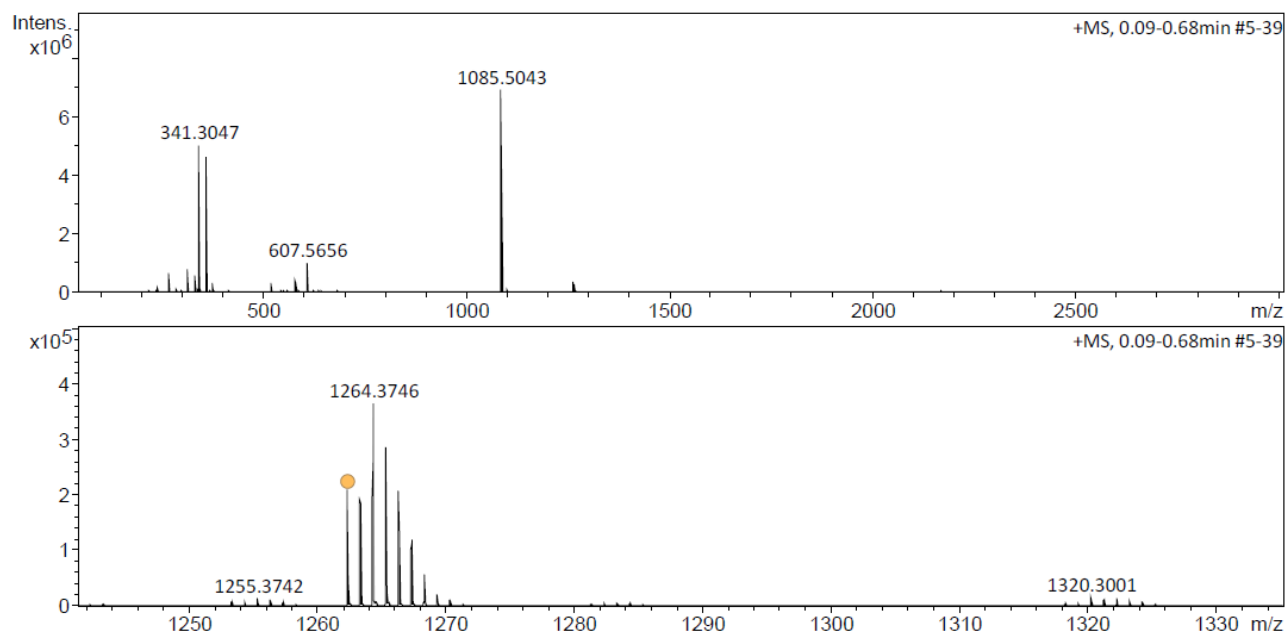


Fig S 7. Mass spectrum of nickel complex **3a**.



Meas. m/z #	Ion Formula	Sum Formula	m/z err [mDa]	err [ppm]	mSigma	rdB	e ⁻	Conf	N-Rule	Adduct
1262.375152	1 C82H67BrN3NiO2	C82H67BrN3NiO2	1262.376460	1.3	1.0	9.9	50.5	even	ok	M
2	C80H65BrN6NiO	C80H65BrN6NiO	1262.375117	-0.0	-0.0	10.2	51.0	odd	ok	M
3	C78H63BrN9Ni	C78H63BrN9Ni	1262.373774	-1.4	-1.1	12.1	51.5	even	ok	M
4	C79H69BrN2NiO5	C79H69BrN2NiO5	1262.373780	-1.4	-1.1	15.1	46.0	odd	ok	M
1	C82H67BrN3NiO2	C82H66BrN3NiO2	1262.376460	1.3	1.0	9.9	50.5	even	ok	M+H
2	C80H65BrN6NiO	C80H64BrN6NiO	1262.375117	-0.0	-0.0	10.2	51.0	odd	ok	M+H
3	C78H63BrN9Ni	C78H62BrN9Ni	1262.373774	-1.4	-1.1	12.1	51.5	even	ok	M+H
4	C79H69BrN2NiO5	C79H68BrN2NiO5	1262.373780	-1.4	-1.1	15.1	46.0	odd	ok	M+H

Fig S 8. Mass spectrum of nickel complex **3b**.

Infrared spectra

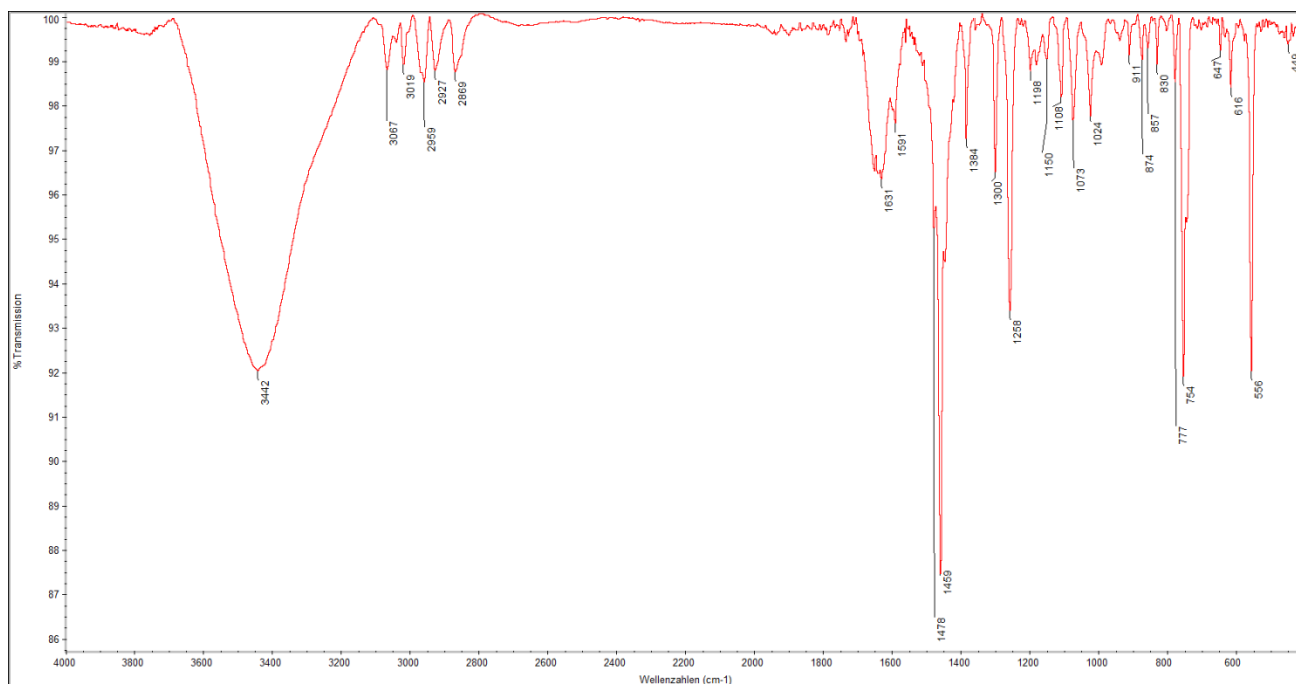


Fig S 9. Infrared spectrum of diimine **2a**.

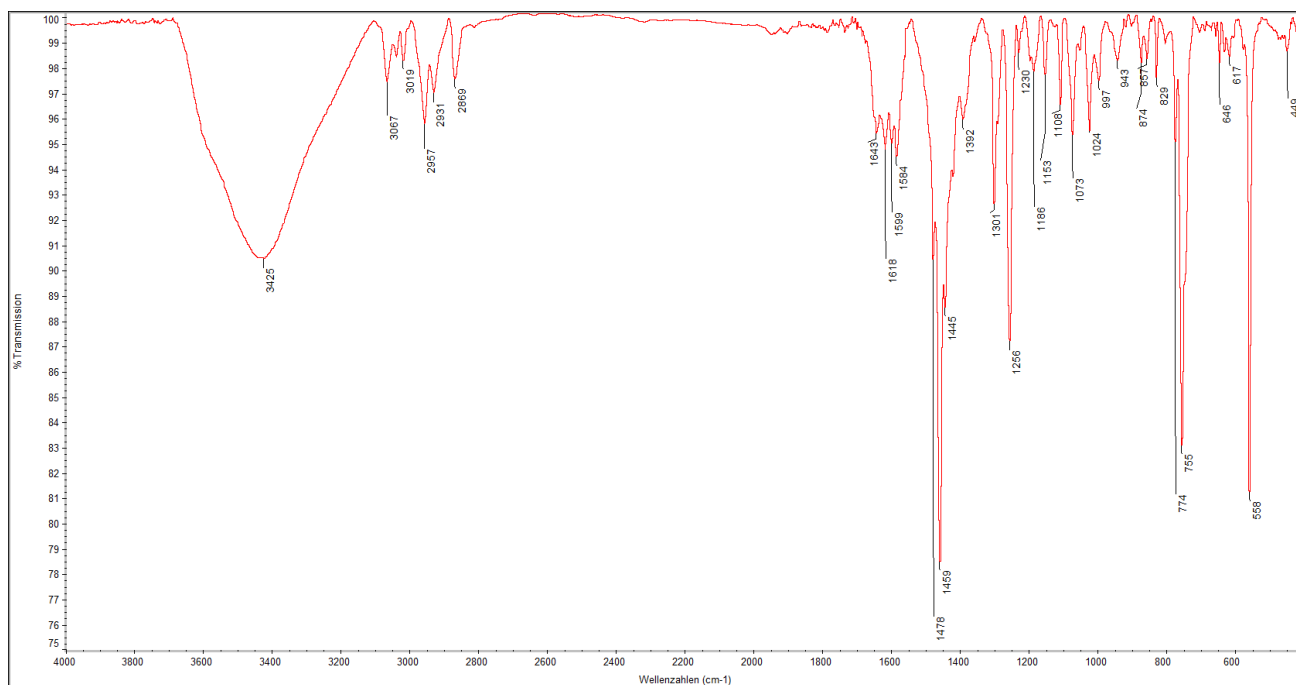


Fig S 10. Infrared spectrum of nickel complex **3a**.

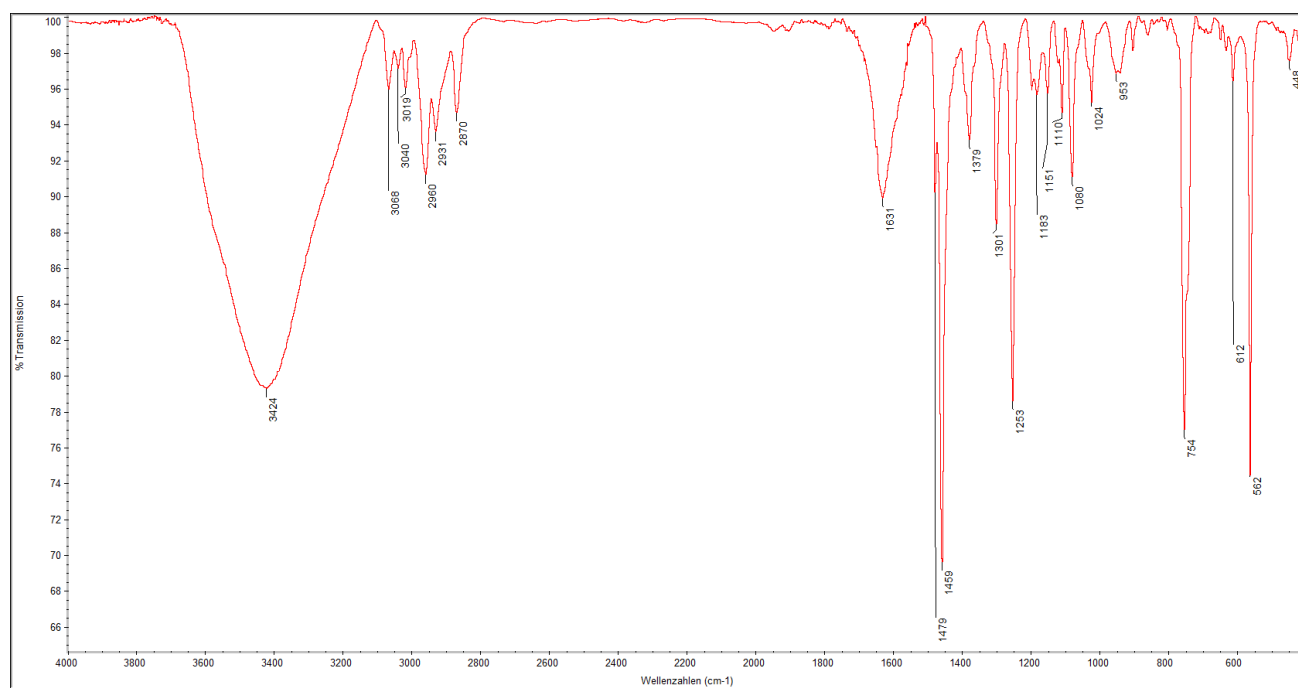


Fig S 11. Infrared spectrum of nickel complex **3b**.

Ethene polymerization and polymer characterization

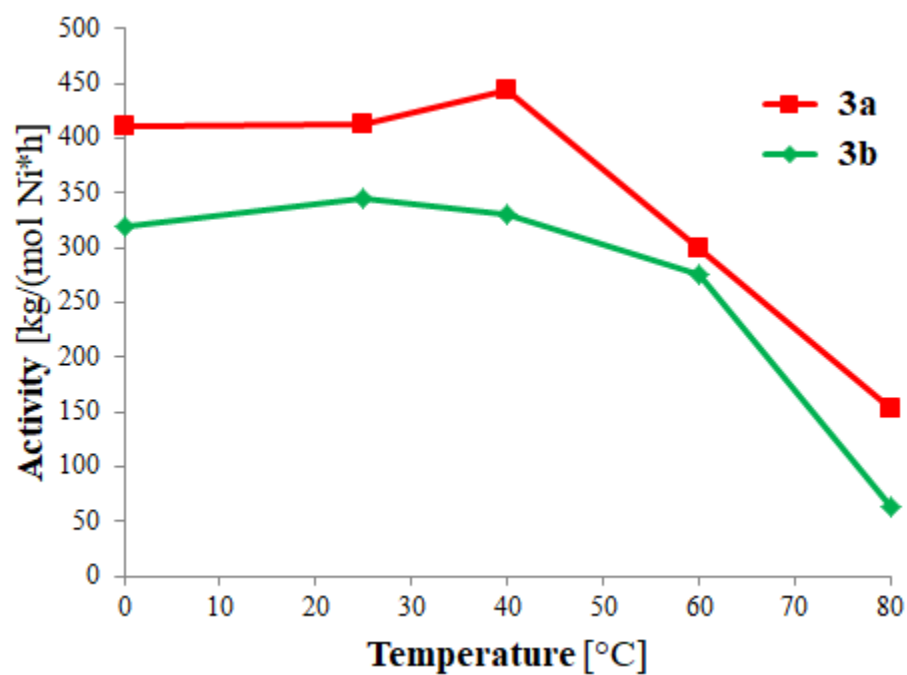


Fig S 12. Activity of catalyst in ethene polymerization at 1 atm.

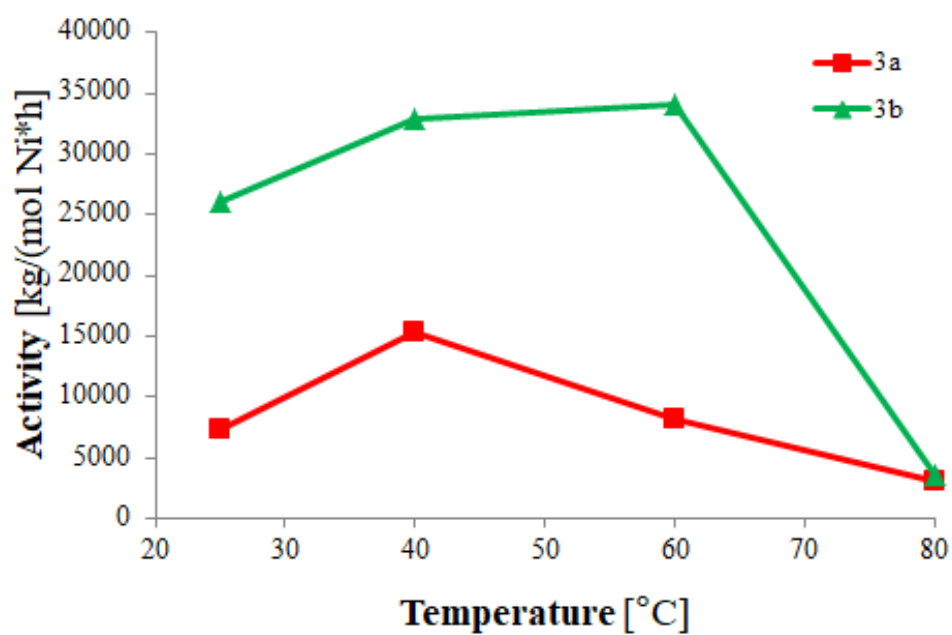


Fig S 13. Activity of catalysts in ethene polymerization at 7 atm.

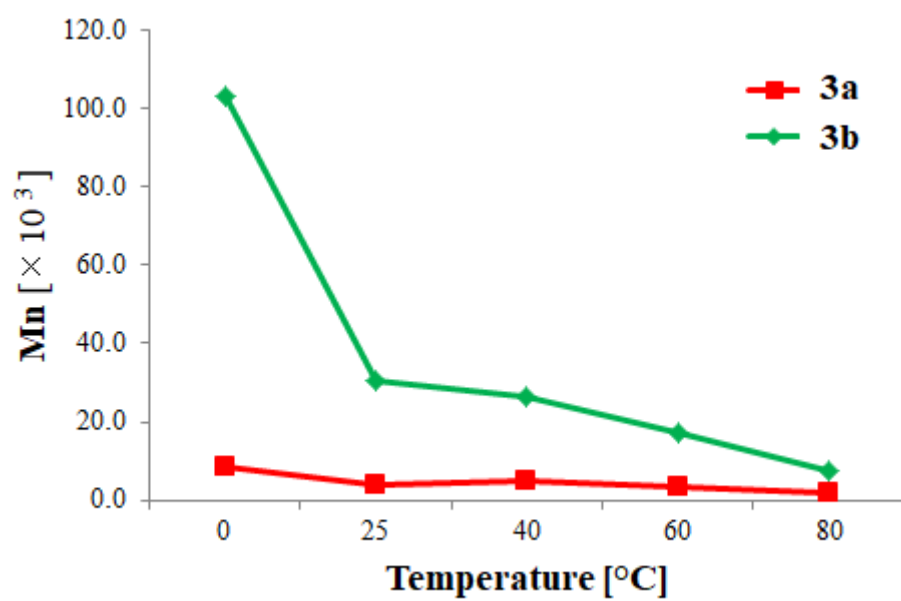


Fig S 14. M_n of synthesized PE at 1 atm.

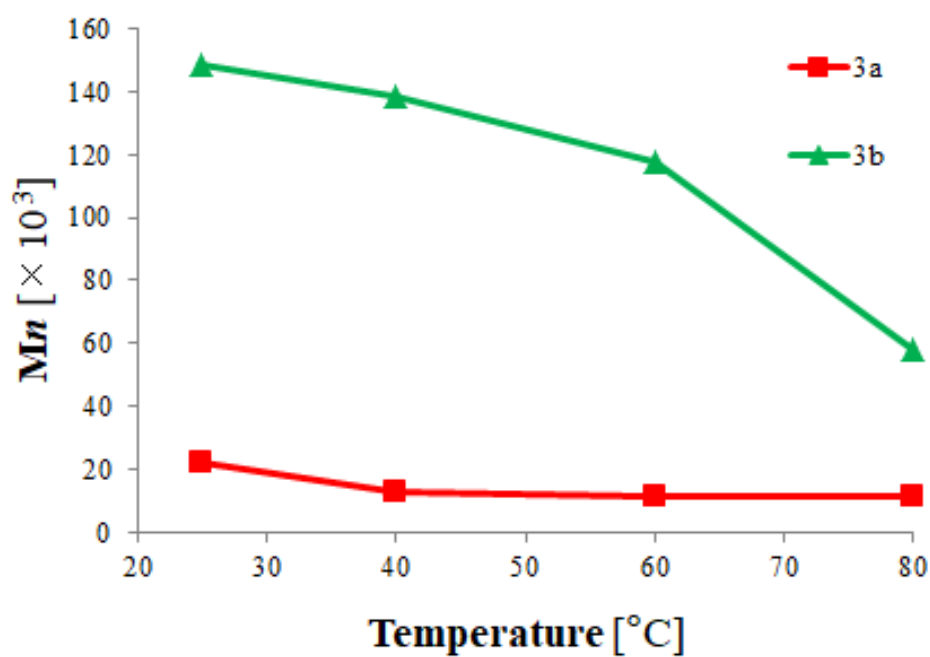


Fig S 15. M_n of synthesized PE at 7 atm.

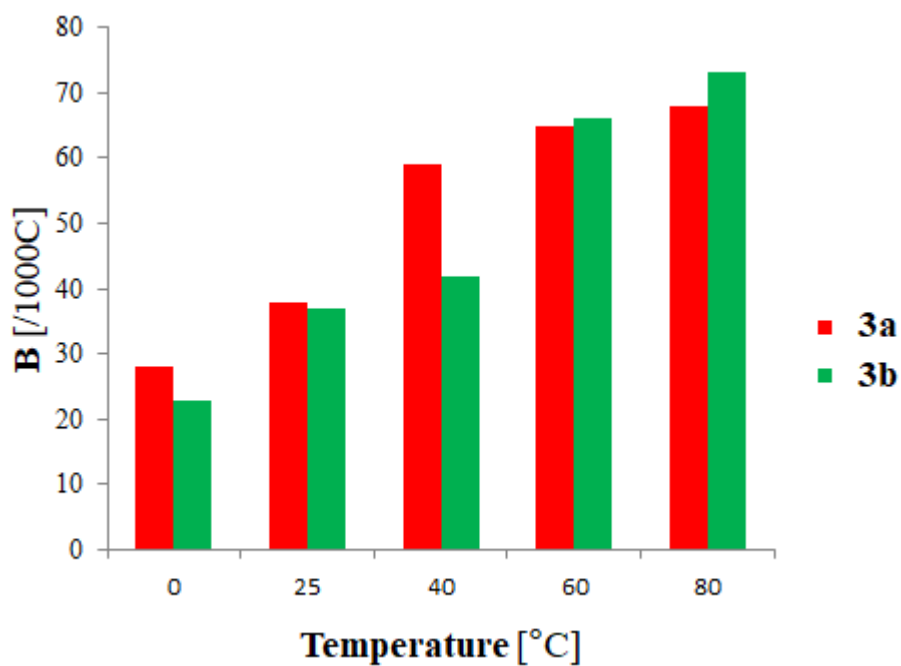


Fig S 16. Temperature-dependent branching number of synthesized PE at 1 atm, determined by ^1H NMR spectroscopy [2].

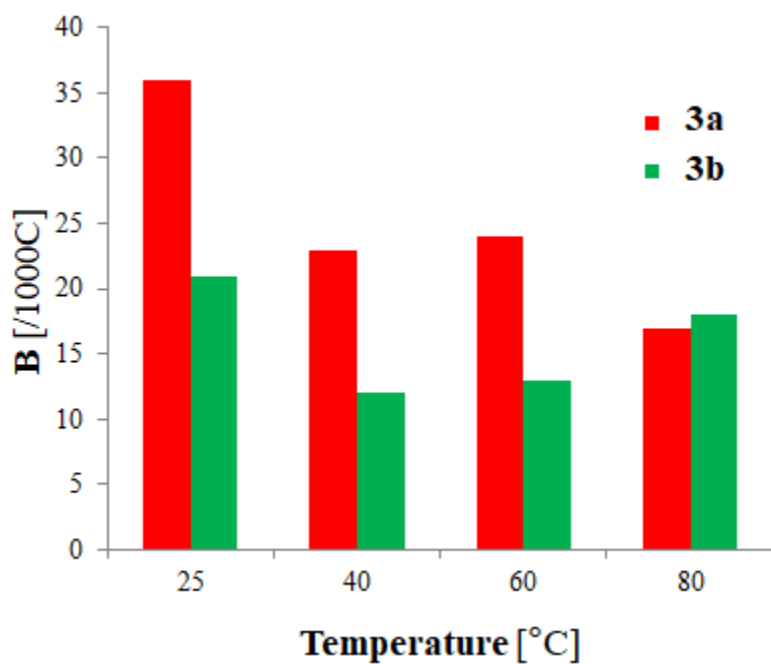


Fig S 17. Temperature-dependent branching number of synthesized PE at 7 atm, determined by ^1H NMR spectroscopy [2].

[2] O. Daugulis *et al.*, *Organometallics* **2002**, *21*, 5935-5943.

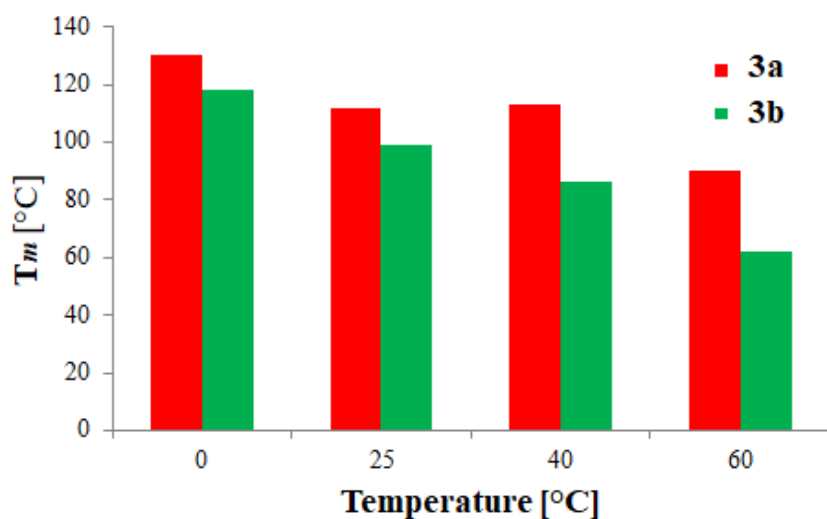


Fig S 18. Temperature-dependent melting point of synthesized PE at 1 atm.

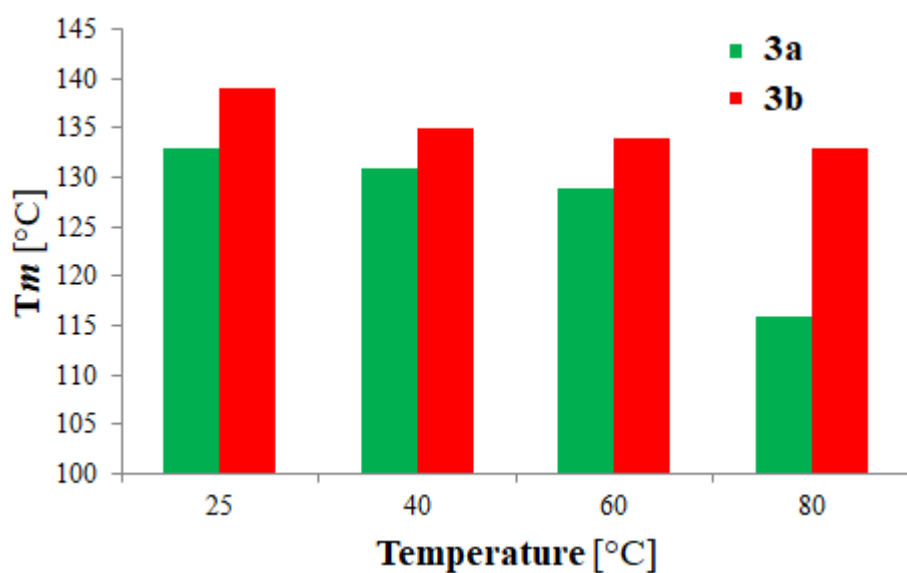


Fig S 19. Temperature-dependent melting point of synthesized PE at 7 atm.

Table S1. Microstructure of synthesized PE ^[a]

Entry	P [atm]	Cat.	T [°C]	Branch [%]			
				Methyl	Ethyl	Pr	Long
1	1	3a	0	100	0	0	0
2	1	3a	25	49	25	16	10
3	1	3a	40	47	25	18	10
4	1	3a	60	35	39	12	14
5	1	3a	80	29	34	20	17
6	1	3b	0	100	0	0	0
7	1	3b	25	52	19	17	12
8	1	3b	40	50	29	13	8
9	1	3b	60	45	29	16	10
10	1	3b	80	37	30	17	16
11	7	3a	25	100	0	0	0
12	7	3a	40	100	0	0	0
13	7	3a	60	100	0	0	0
14	7	3a	80	100	0	0	0
15	7	3b	25	– ^[b]	– ^[b]	– ^[b]	– ^[b]
16	7	3b	40	100	0	0	0
17	7	3b	60	100	0	0	0
18	7	3b	80	100	0	0	0

[a] Determined by ¹³C NMR spectrometry in 1,1,2,2-tetrachloroethane-*d*₂ at 100 °C. [b] Not determined due to the insufficient solubility of sample in solvent.

¹³C NMR spectra were measured with following parameter: Inverse gated decoupling, temperature 100 °C, pulse width 90 °, acquisition time 2.4 s, acquisition delay time 6.0 s.

¹³C NMR spectra were assigned according to reported literature [3].

[3] G. B. Galland *et al.*, *Macromolecules* **1999**, 32, 1620-1625

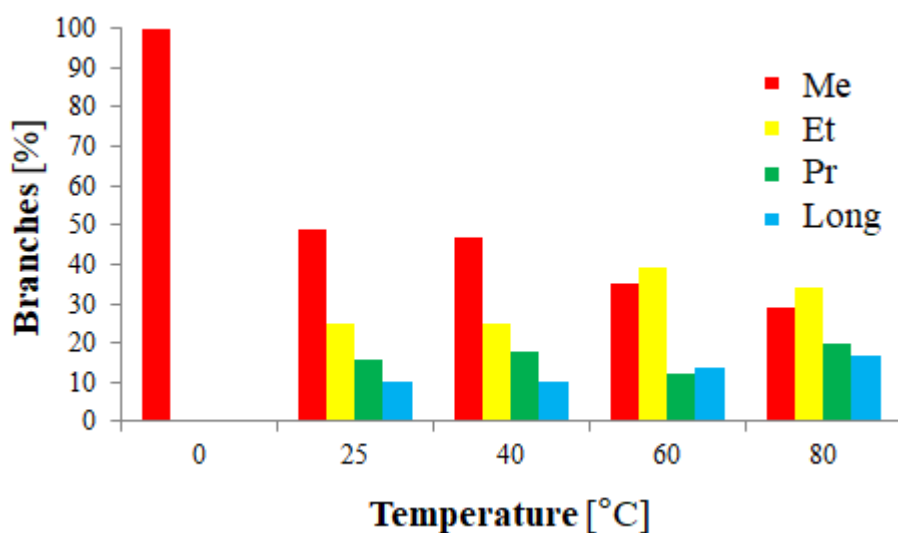


Fig S 20. Microstructure: Temperature-dependent branches of synthesized PE by **3a** at 1 atm, determined by ^{13}C NMR spectroscopy [3].

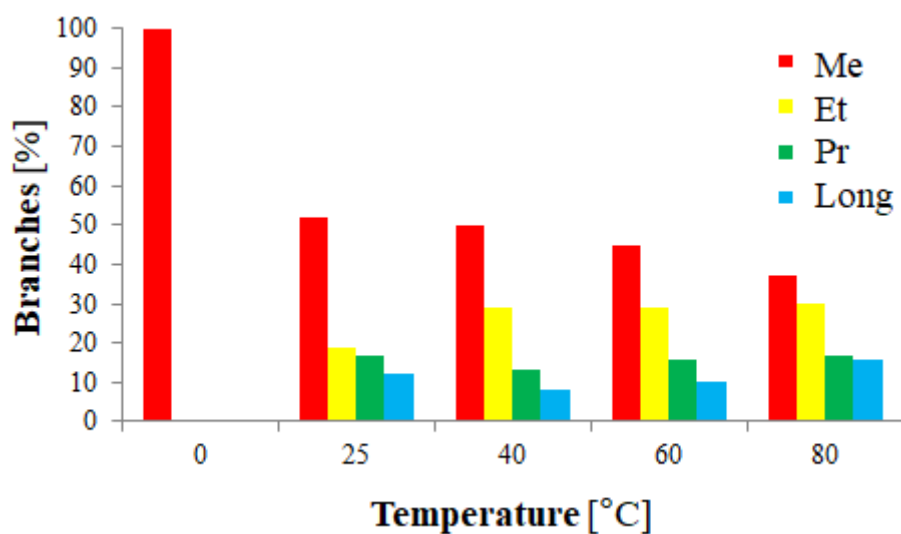


Fig S 21. Microstructure: Temperature-dependent branches of synthesized PE by **3b** at 1 atm, determined by ^{13}C NMR spectroscopy [3].

Polymerization at atmospheric pressure

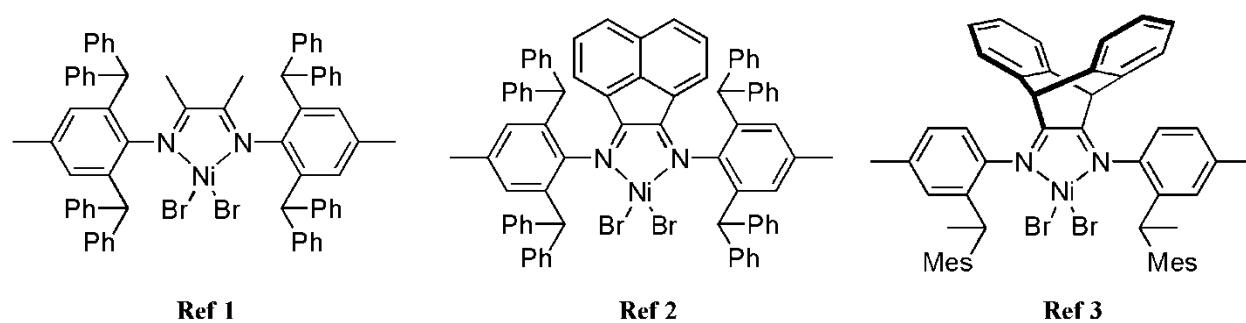


Fig S 22. Reported catalysts.

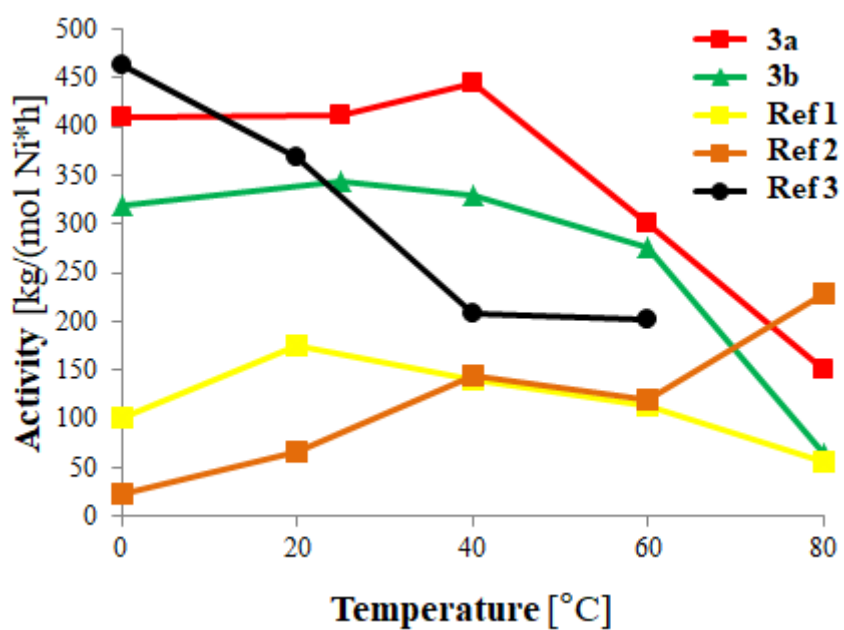


Fig S 23. Comparison of activity on ethene polymerization at 1 atm.

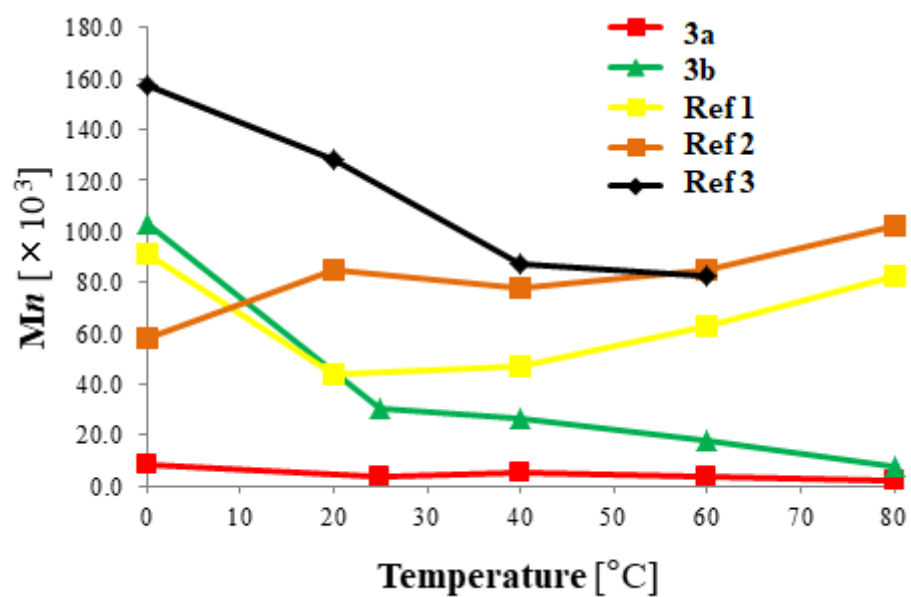


Fig S 24. M_n of PE synthesized at 1 atm pressure ethene.

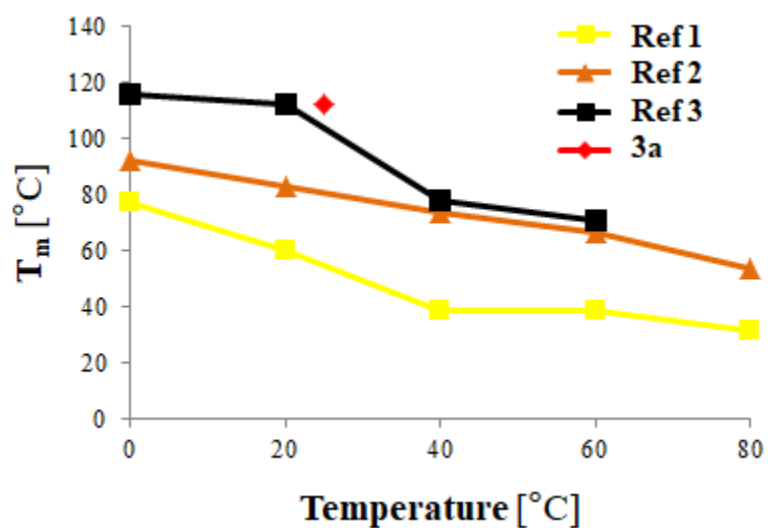


Fig S 25. Melting point of PE synthesized at 1 atm pressure ethene.

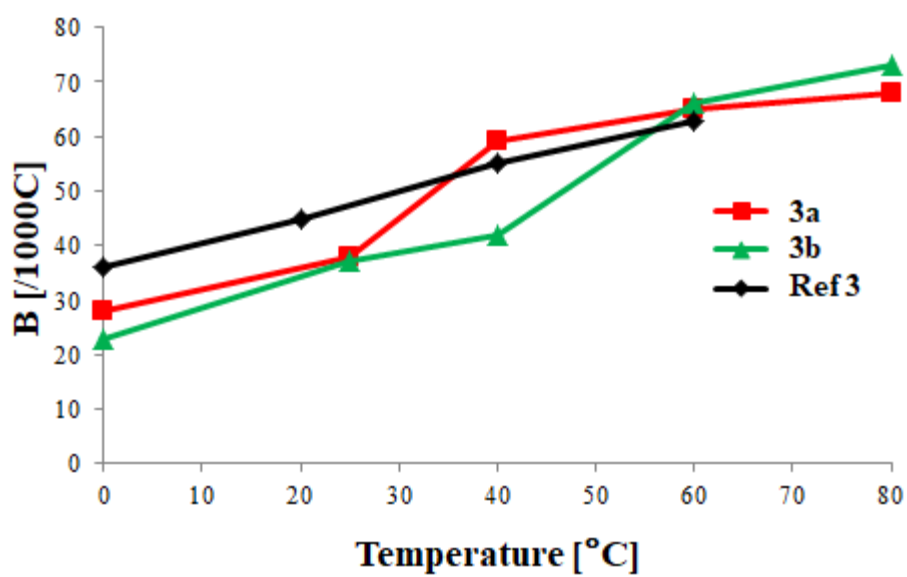


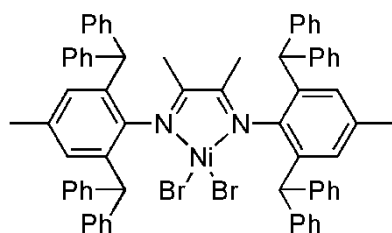
Fig S 26. Branching density of PE synthesized at 1 atm pressure ethene, determined by ^1H NMR spectroscopy [2].

Polymerization at high pressure of ethene

Table S2. Comparison with reported polymerization data at high pressure

Entry	P	Cat.	Activator	T	Time	Yield ^[d]	Activity ^[d]	M _n ^[e]	PDI	T _m ^[f]	B ^[g]	
	atm	μmol	eq.	°C	min	g	kg(mol Ni) ⁻¹ h ⁻¹	×10 ³		°C	/1000C	
1 ^[a]	7	3a	0.2	500	25	30	1.60	7400	22.1	3.2	139	36
2 ^[a]	7	3a	0.2	500	40	30	1.72	15300	12.5	3.4	135	23
3 ^[a]	7	3a	0.2	500	60	30	1.65	8200	11.7	3.2	134	24
4 ^[a]	7	3a	0.2	500	80	30	1.38	3100	11.2	4.0	133	17
5 ^[a]	7	3b	0.05	1000	25	30	0.32	26000	148.6	3.0	133	21
6 ^[a]	7	3b	0.05	1000	40	30	0.82	32800	138.4	3.2	131	12
7 ^[a]	7	3b	0.05	1000	60	30	0.85	34000	117.4	2.6	119	12
8 ^[a]	7	3b	0.05	1000	80	30	0.31	3600	57.9	2.5	116	18
9 ^[a]	7	Ref 1	1	500	25	30	0.18	360	n.d.	n.d.	n.d.	n.d.
10 ^[a]	7	Ref 1	1	500	40	30	0.27	540	n.d.	n.d.	n.d.	n.d.
11 ^[a]	7	4b	1	500	25	30	1.78	3560	n.d.	n.d.	n.d.	n.d.
12 ^[a]	7	4b	1	500	40	30	2.17	4340	n.d.	n.d.	n.d.	n.d.
13 ^[b]	9	4b	2.4	500 ^[c]	20	30	5.52	4600	149	2.2	57	53
14 ^[b]	9	4b	2.4	500 ^[c]	40	30	3.77	3142	80	2.8	50	71
15 ^[b]	9	4b	2.4	500 ^[c]	60	30	1.60	1333	45	2.7	n.d.	88
16 ^[b]	9	4b	2.4	500 ^[c]	80	30	1.00	833	37	3.1	n.d.	96
17 ^[b]	9	4a	2.4	500 ^[c]	20	10	4.22	3520	64	2.8	n.d.	55
18 ^[b]	9	4a	2.4	500 ^[c]	40	10	3.14	2620	48	3.3	n.d.	70
19 ^[b]	9	4a	2.4	500 ^[c]	60	10	2.15	1790	33	3.1	n.d.	83
20 ^[b]	9	4a	2.4	500 ^[c]	80	10	0.75	630	21	2.8	n.d.	101

[a] The reactions were conducted by us. Reaction conditions : precatalyst, Et₂AlCl, toluene (50 mL), 30 min. [b] Data from reported literatures. [c] Used MAO instead of Et₂AlCl. [d] Average value of two experiments. [e] Determined by GPC in trichlorobenzene at 150 °C with PE standard. [f] Melting temperature was determined by differential scanning calorimetry (DSC, second heating). [g] Numbers of branches per 1000 carbons, as determined by ¹H NMR spectrometry. [Ref 1] J. L. Rhinehart *et al.*, *J. Am. Chem. Soc.* **2013**, 135, 16316-16319. [4a, 4b] R. Wang *et al.*, *ChemCatChem* **2016**, 8, 434-440.



Ref 1

Fig S 27. Reported catalysts.

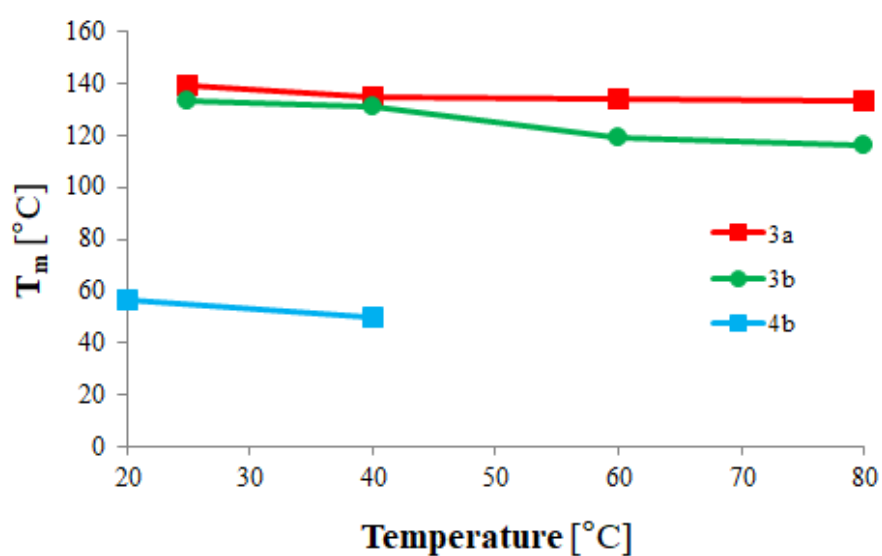


Fig S 28. Melting point of PE synthesized at high ethene pressure (7 atm for **3a** conducted by us; 9 atm for **4b** from reported literature).

Copolymerization comparison with literature data

Table S3. Comparison with reported polymerization data at 1 atm

Entry	Cat.	Activator	T	Time	Yield ^[e]	Activity ^[e]	M _n ^[f]	PDI	T _m ^[g]	B ^[h]	
	μmol	eq.	°C	min	g	kg(mol Ni) ⁻¹ h ⁻¹	×10 ³		°C	/1000C	
1 ^[a]	3a	10	100	0	30	2.05	410	8.4	4.7	130	28
2 ^[a]	3a	10	100	25	30	2.06	412	3.8	3.3	112	38
3 ^[a]	3a	10	100	40	30	2.22	444	4.8	3.1	113	59
4 ^[a]	3a	10	100	60	30	1.50	300	3.3	2.8	- ^[i]	65
5 ^[a]	3a	10	100	80	30	0.76	152	1.7	2.6	- ^[i]	68
6 ^[a]	3b	10	100	0	30	1.60	320	103.0	3.2	118	23
7 ^[a]	3b	10	100	25	30	1.72	344	30.5	3.3	n.d.	37
8 ^[a]	3b	10	100	40	30	1.65	330	26.2	2.9	n.d.	42
9 ^[a]	3b	10	100	60	30	1.38	276	17.4	2.8	- ^[i]	66
10 ^[a]	3b	10	100	80	30	0.32	64	7.7	2.8	- ^[i]	73
11 ^[b]	Ref 1	1.57	100 ^[c]	0	45	0.12	102	91	1.2	77	n.d.
12 ^[b]	Ref 1	1.57	100 ^[c]	20	15	0.07	176	44	1.1	60	n.d.
13 ^[b]	Ref 1	1.57	100 ^[c]	40	15	0.06	140	47	1.1	39	n.d.
14 ^[b]	Ref 1	1.57	100 ^[c]	60	15	0.05	115	63	1.1	39	n.d.
15 ^[b]	Ref 1	1.57	100 ^[c]	80	15	0.02	56	82	1.2	32	n.d.
16 ^[b]	Ref 2	5	100 ^[c]	0	15	0.03	23	58	1.1	92	n.d.
17 ^[b]	Ref 2	5	100 ^[c]	20	15	0.08	66	85	1.1	83	n.d.
18 ^[b]	Ref 2	5	100 ^[c]	40	15	0.18	145	78	1.2	74	n.d.
19 ^[b]	Ref 2	5	100 ^[d]	60	15	0.15	121	85	1.1	67	n.d.
20 ^[b]	Ref 2	5	100 ^[d]	80	15	0.29	230	102	1.3	54	n.d.
21 ^[b]	Ref 3	10	300 ^[d]	0	30	2.32	464	157	1.6	116	36
22 ^[b]	Ref 3	10	300 ^[d]	20	30	1.84	368	128	1.3	112	45
23 ^[b]	Ref 3	10	300 ^[d]	40	30	1.04	208	87	1.2	78	55
24 ^[b]	Ref 3	10	300 ^[d]	60	30	1.01	202	82	1.4	71	63

[a] The reactions were conducted by us. Reaction conditions : precatalyst, Et₂AlCl, toluene (50 mL), 30 min. [b] Data from reported literatures. [c] PMAO-IP [d] MAO [e] Average value of two experiments. [f] Determined by GPC in trichlorobenzene at 150 °C with PE standard. [g] Melting temperature was determined by differential scanning calorimetry (DSC, second heating). [h] Numbers of branches per 1000 carbons, as determined by ¹H NMR spectrometry. [i] Amorphous polymer. [Ref 1] J. L. Rhinehart *et al.*, *J. Am. Chem. Soc.* **2013**, 135, 16316-16319. [Ref 2] J. L. Rhinehart *et al.*, *ACS Catal.* **2014**, 4, 2501-2504. [Ref 3] B. K. Long *et al.*, *Angew. Chem. Int. Ed.* **2016**, 55, 7106-7110.

NMR spectra

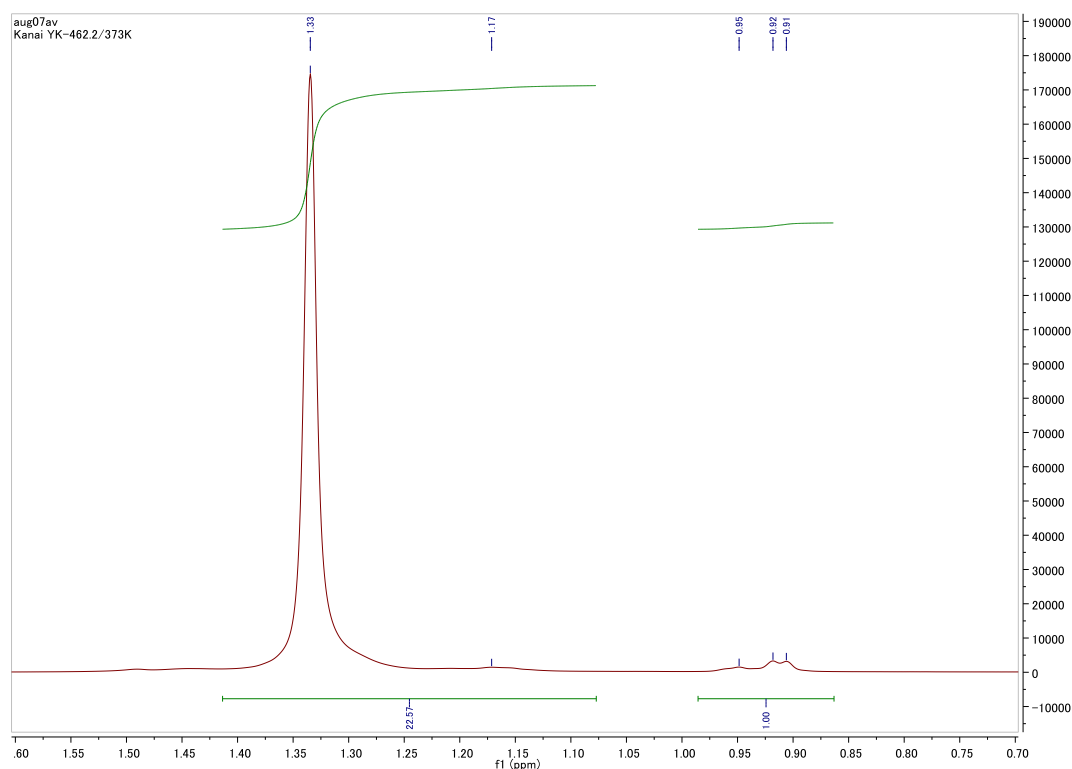


Fig S 29. ^1H NMR spectrum of PE (Table 1, #1).

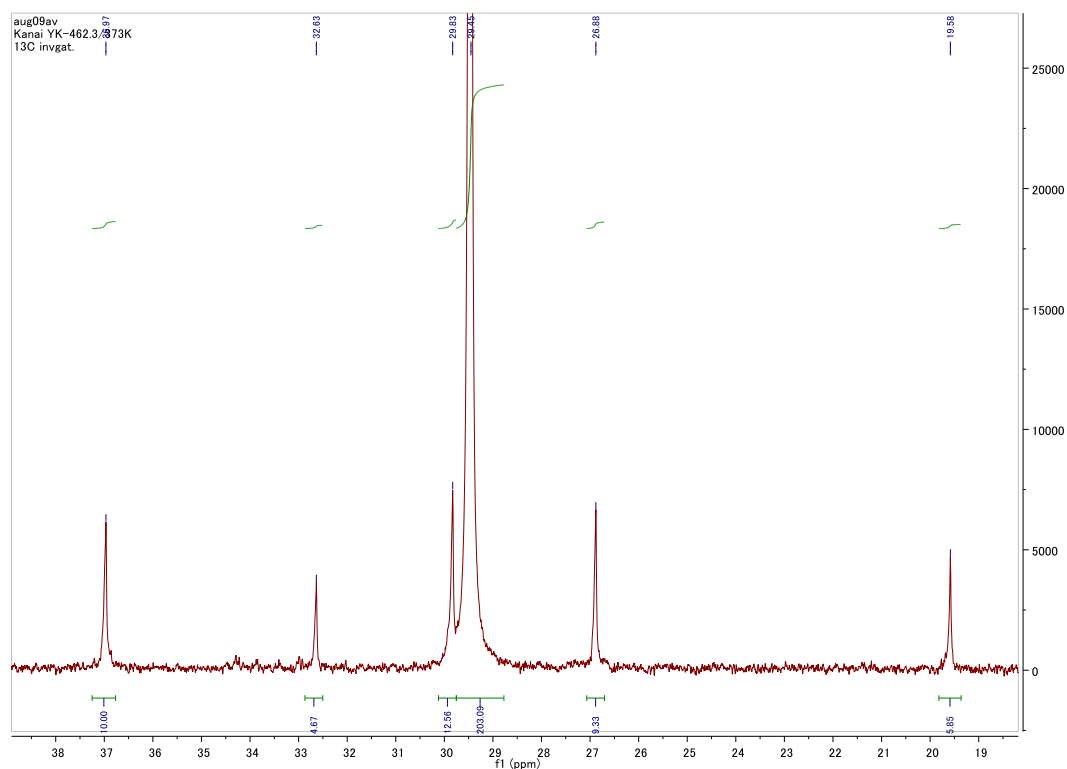


Fig S 30. ^{13}C NMR spectrum of PE (Table 1, #1).

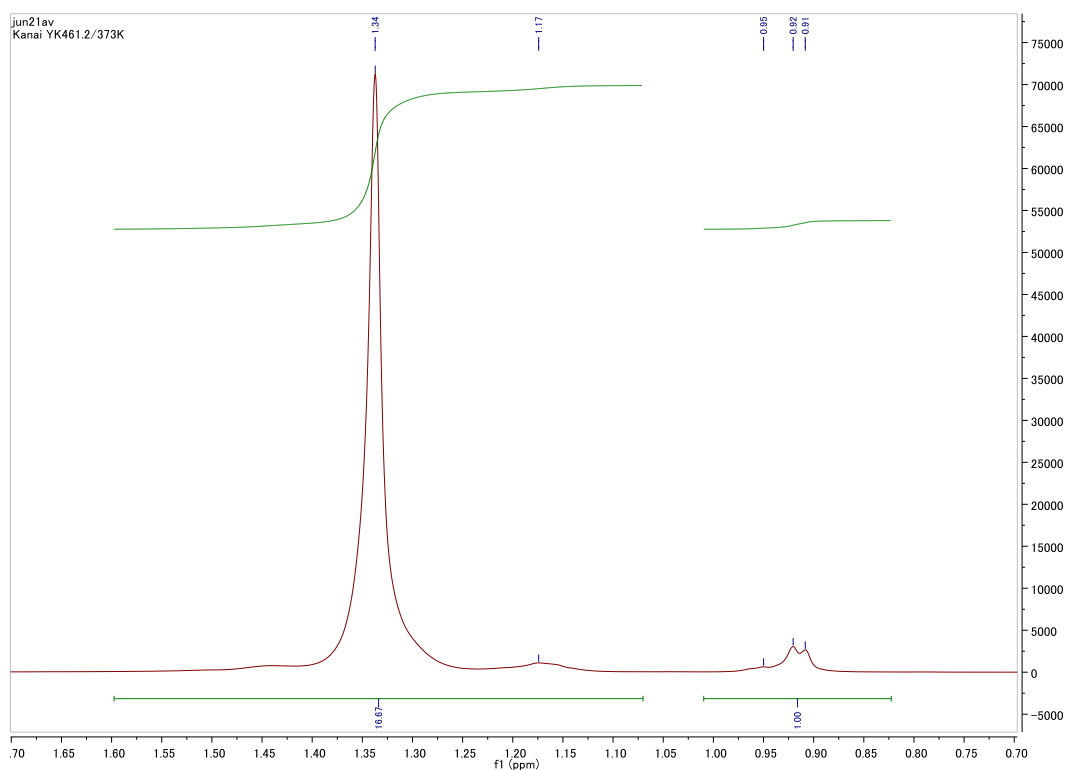


Fig S 31. ^1H NMR spectrum of PE (Table 1, #2).

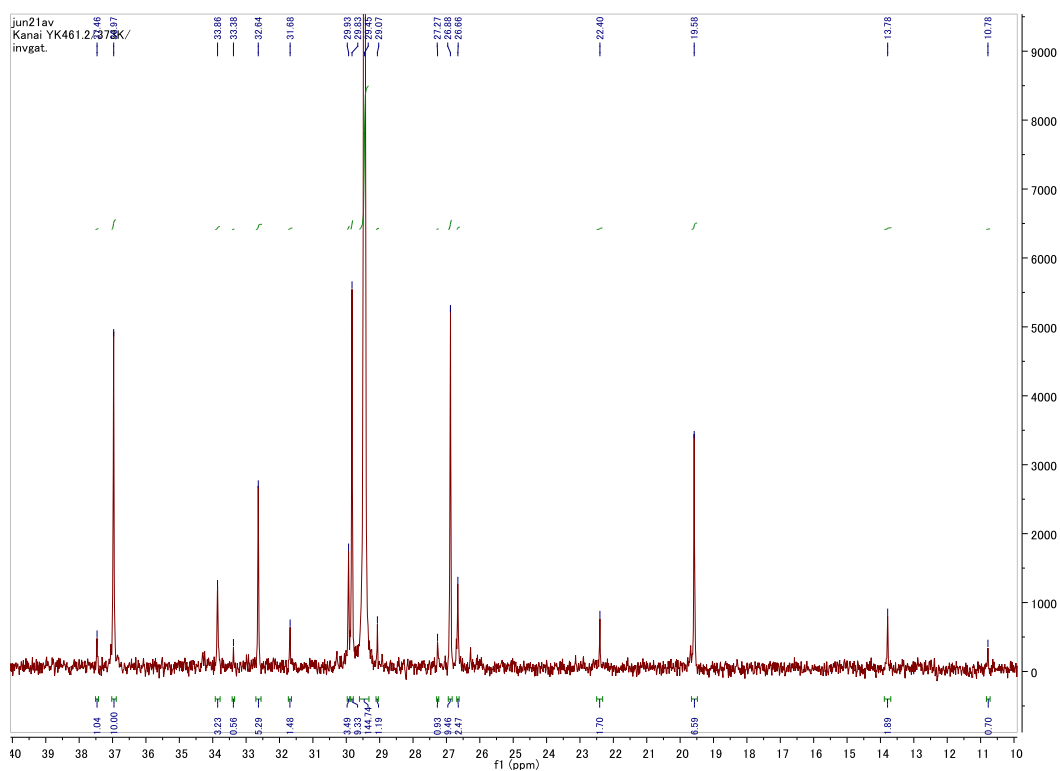


Fig S 32. ^{13}C NMR spectrum of PE (Table 1, #2).

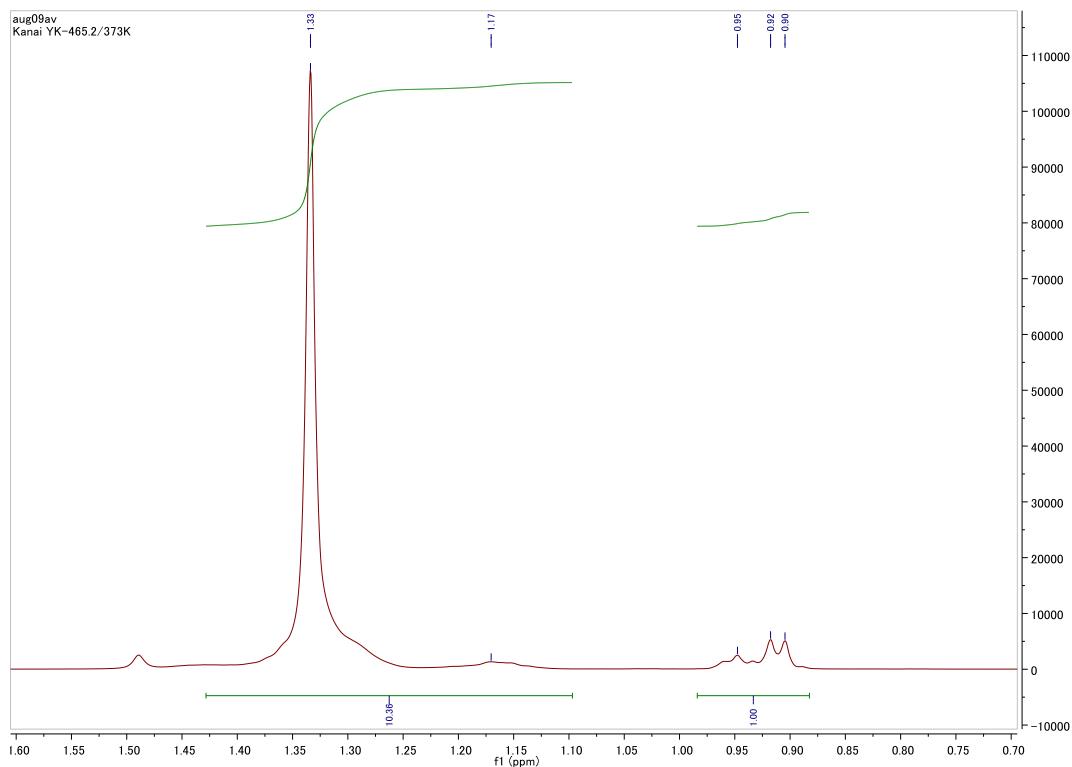


Fig S 33. ^1H NMR spectrum of PE (Table 1, #3).

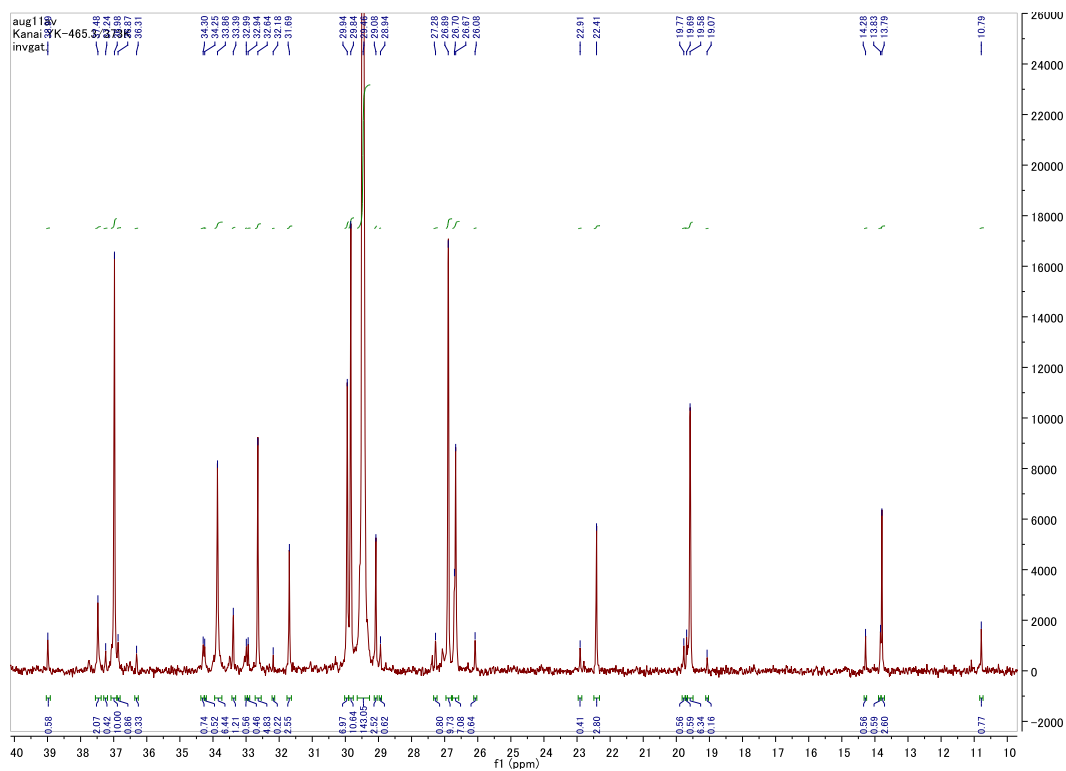


Fig S 34. ^{13}C NMR spectrum of PE (Table 1, #3).

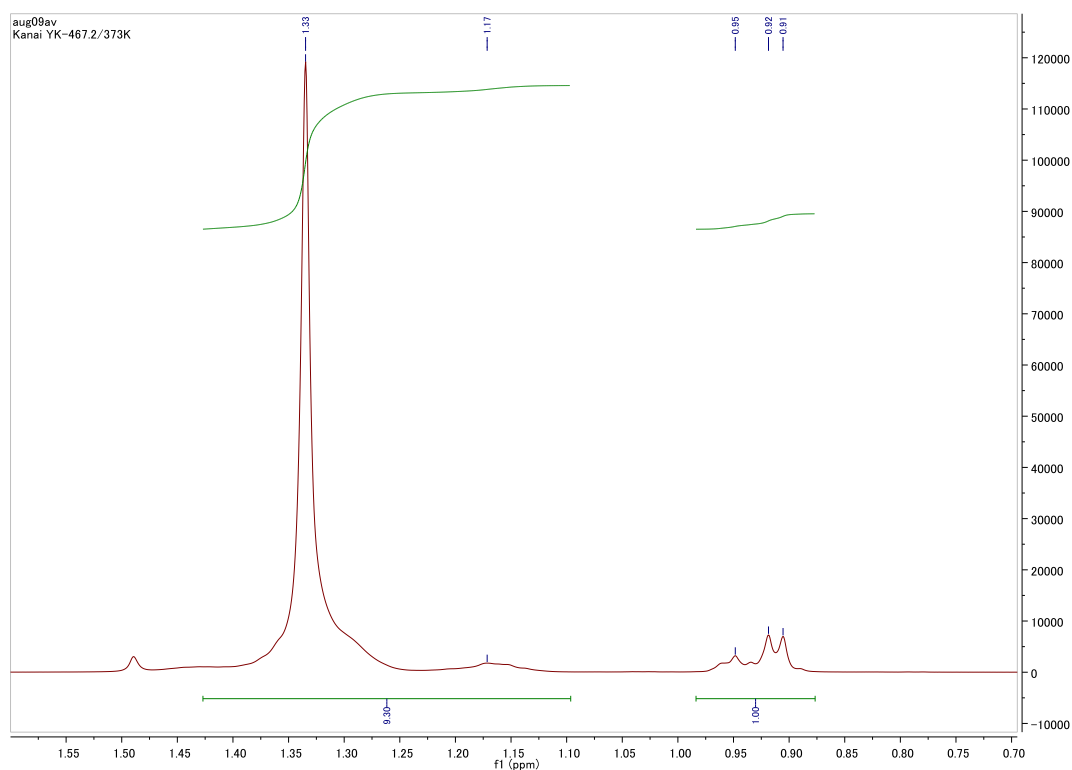


Fig S 35. ^1H NMR spectrum of PE (Table 1, #4).

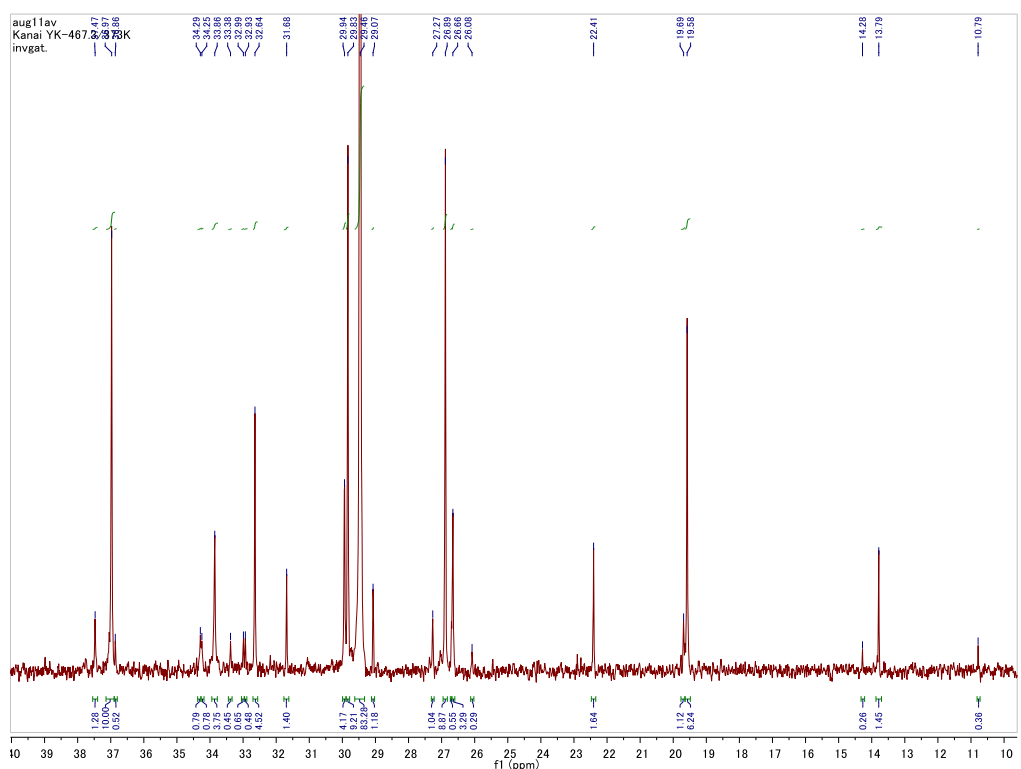
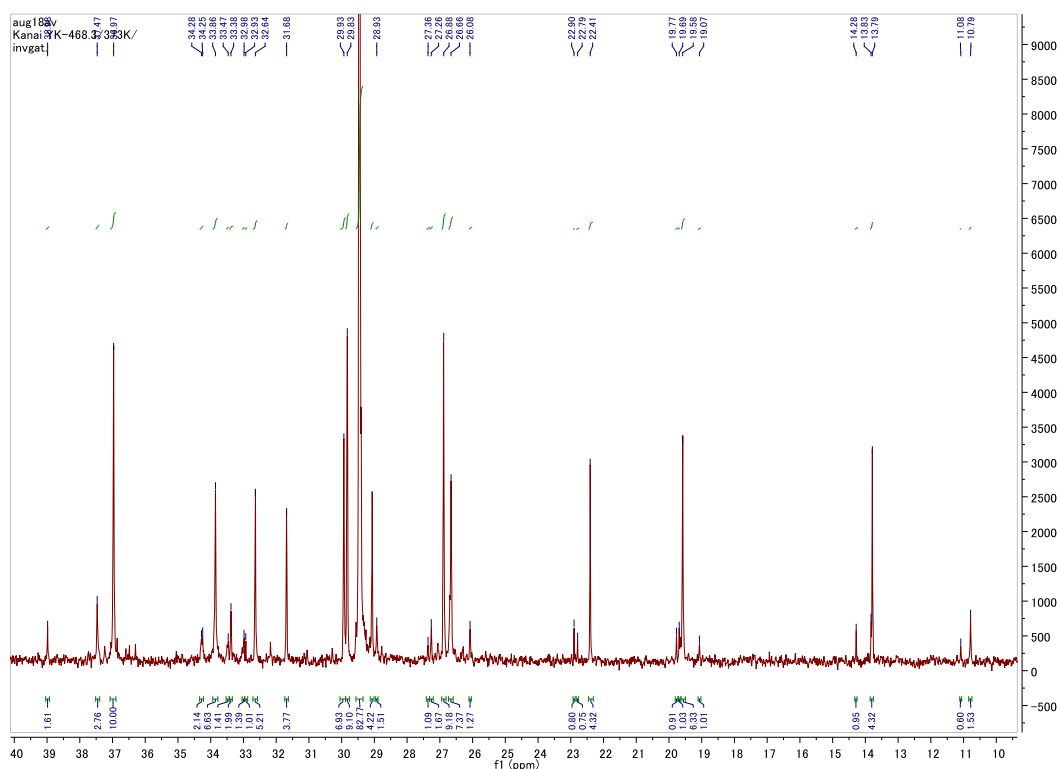
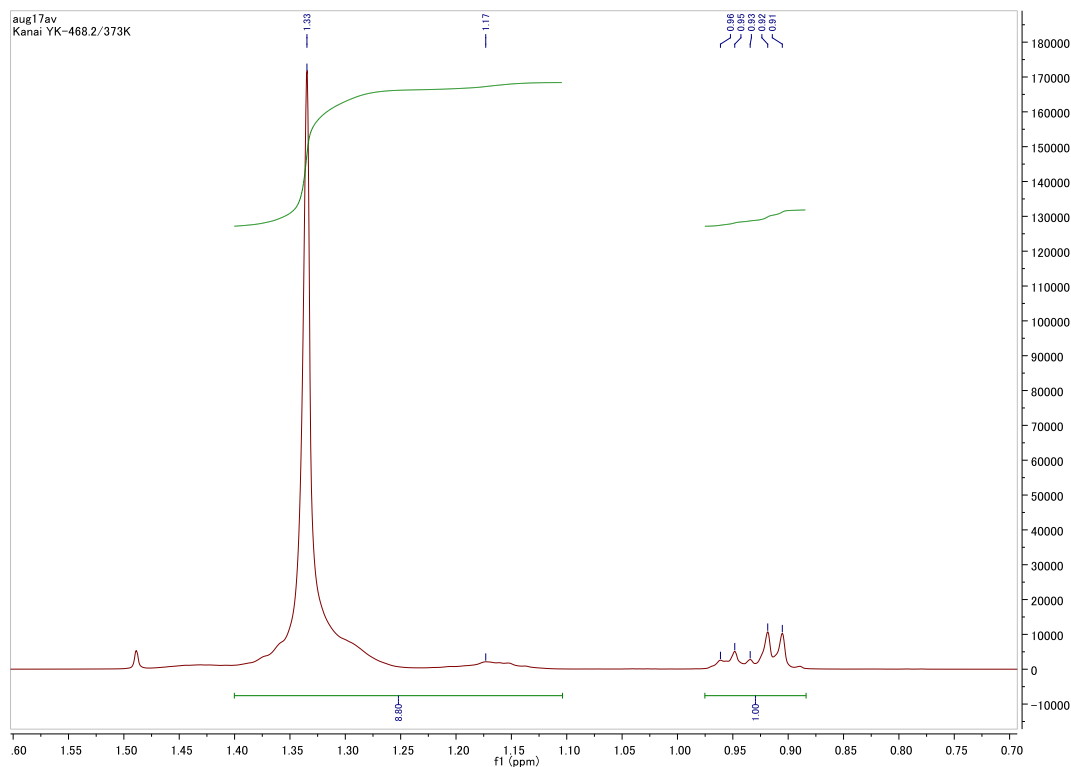


Fig S 36. ^{13}C NMR spectrum of PE (Table 1, #4).



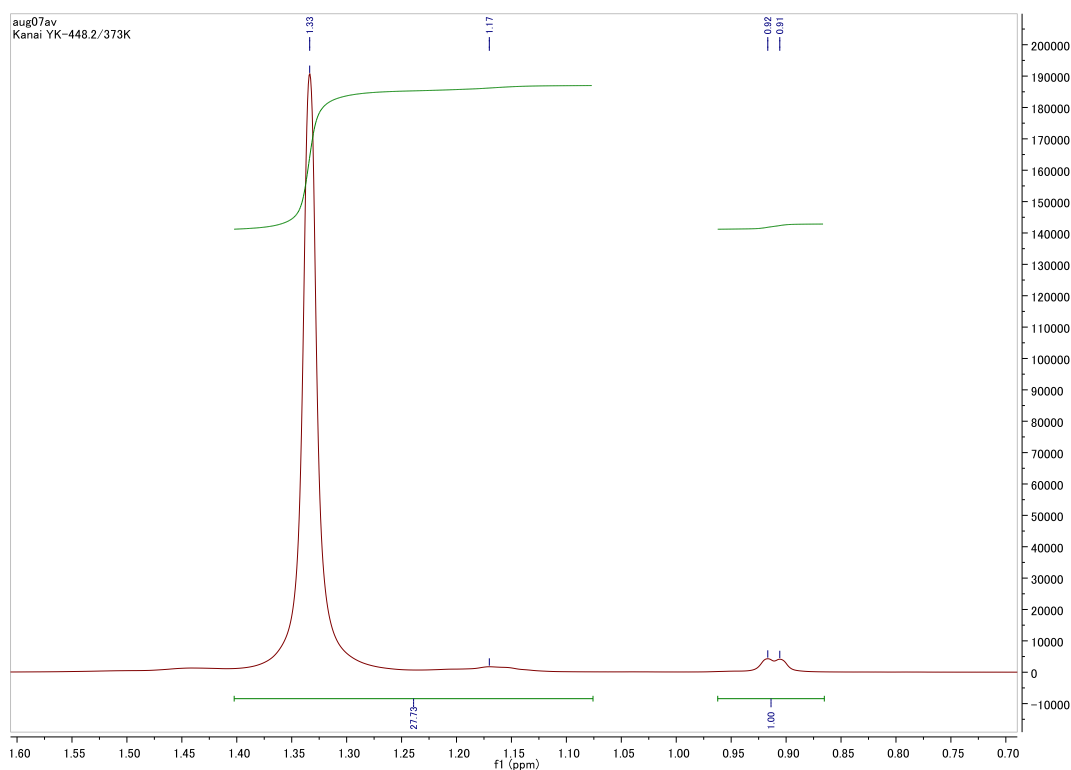


Fig S 39. ^1H NMR spectrum of PE (Table 1, #6).

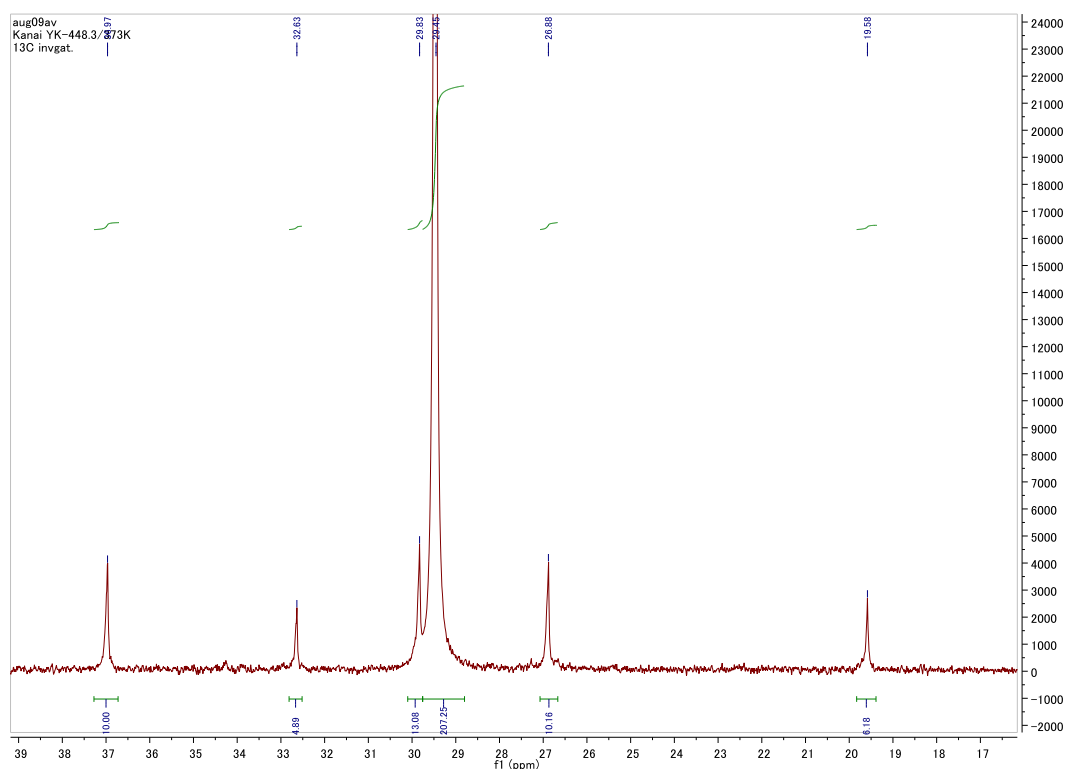


Fig S 40. ^{13}C NMR spectrum of PE (Table 1, #6).

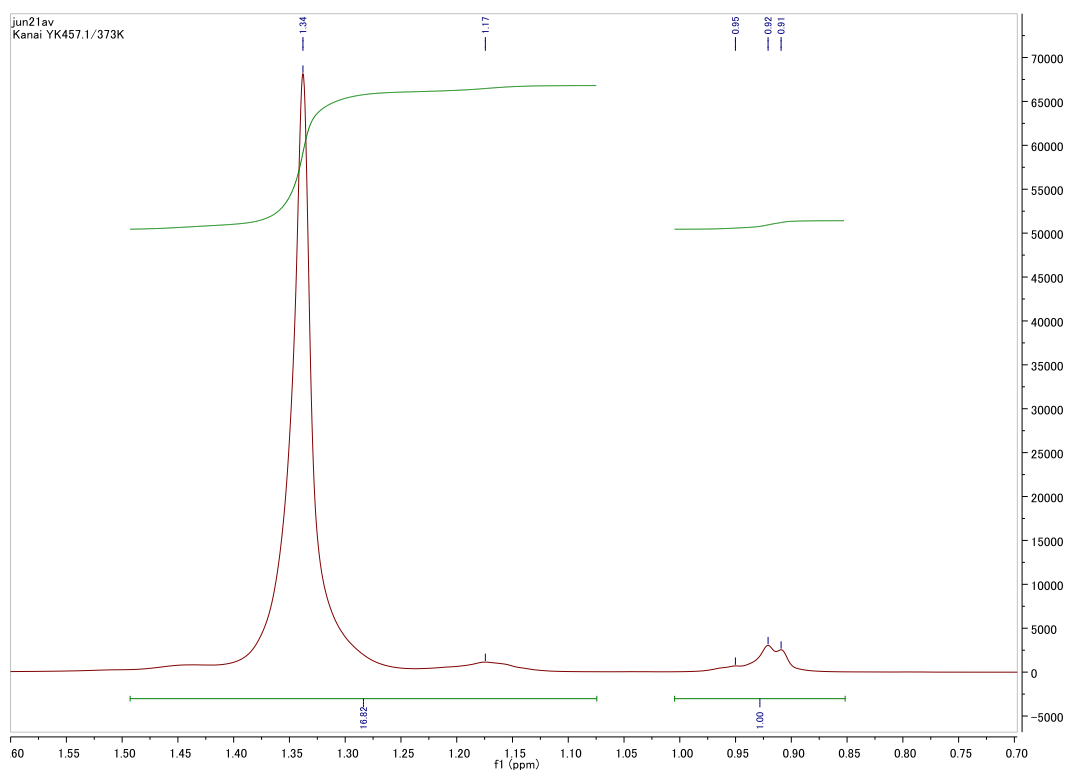


Fig S 41. ^1H NMR spectrum of PE (Table 1, #7).

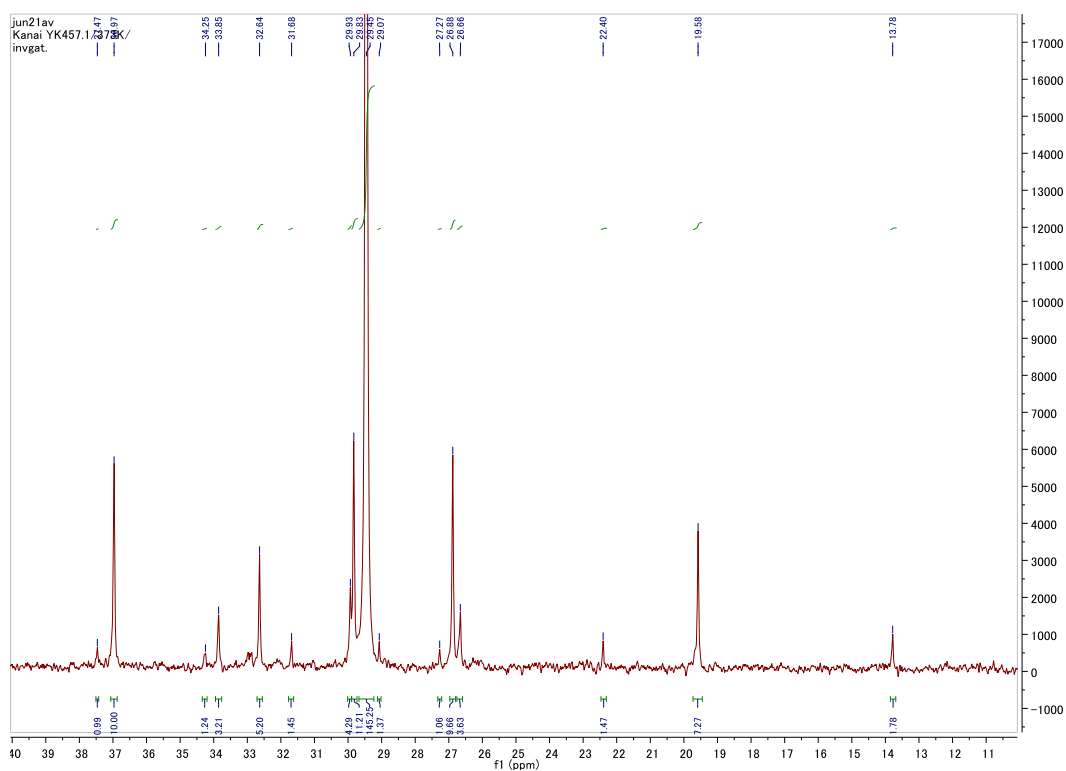


Fig S 42. ^{13}C NMR spectrum of PE (Table 1, #7).

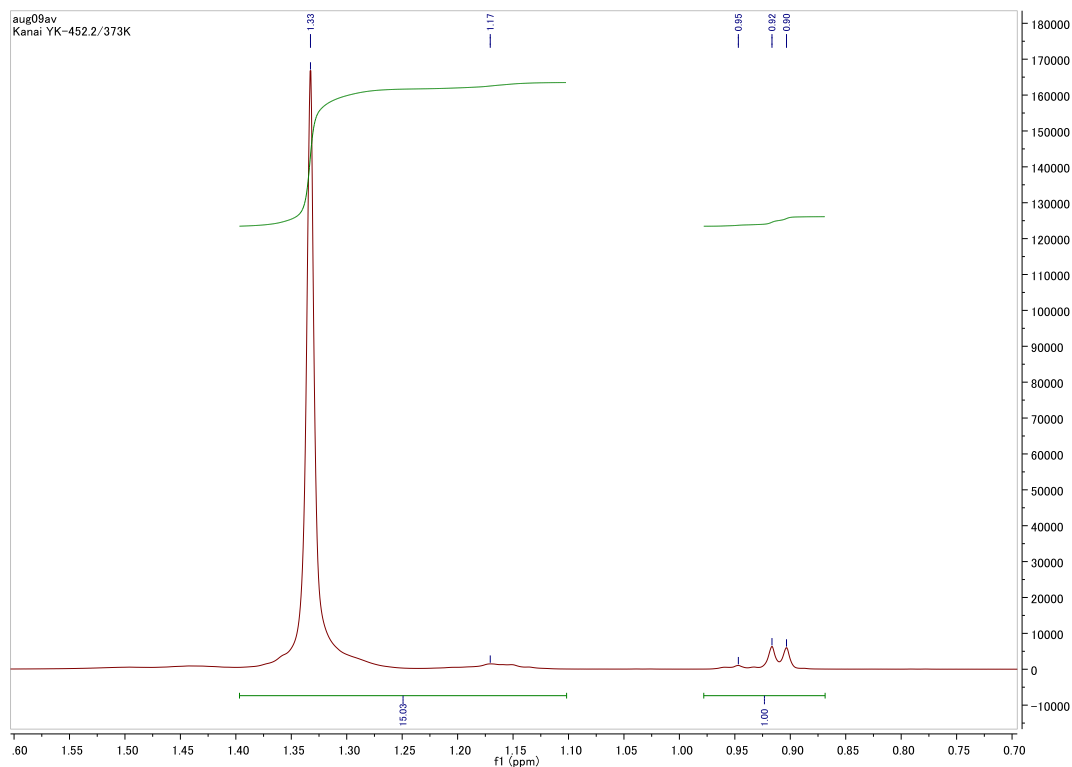


Fig S 43. ^1H NMR spectrum of PE (Table 1, #8).

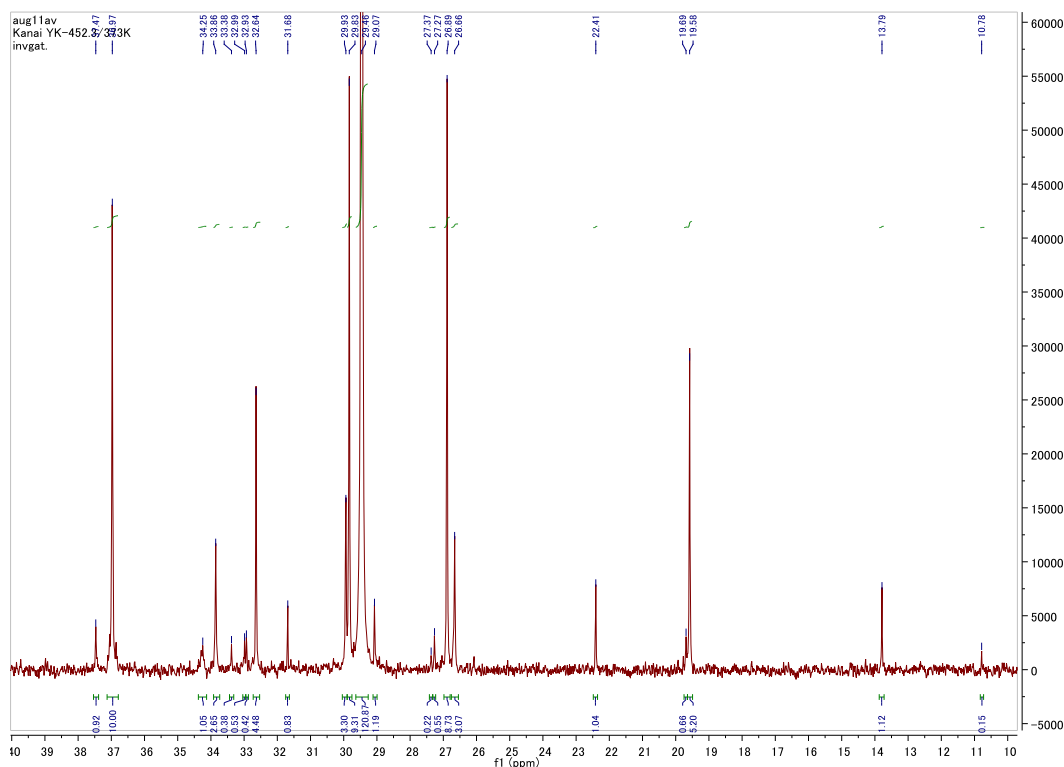


Fig S 44. ^{13}C NMR spectrum of PE (Table 1, #8).

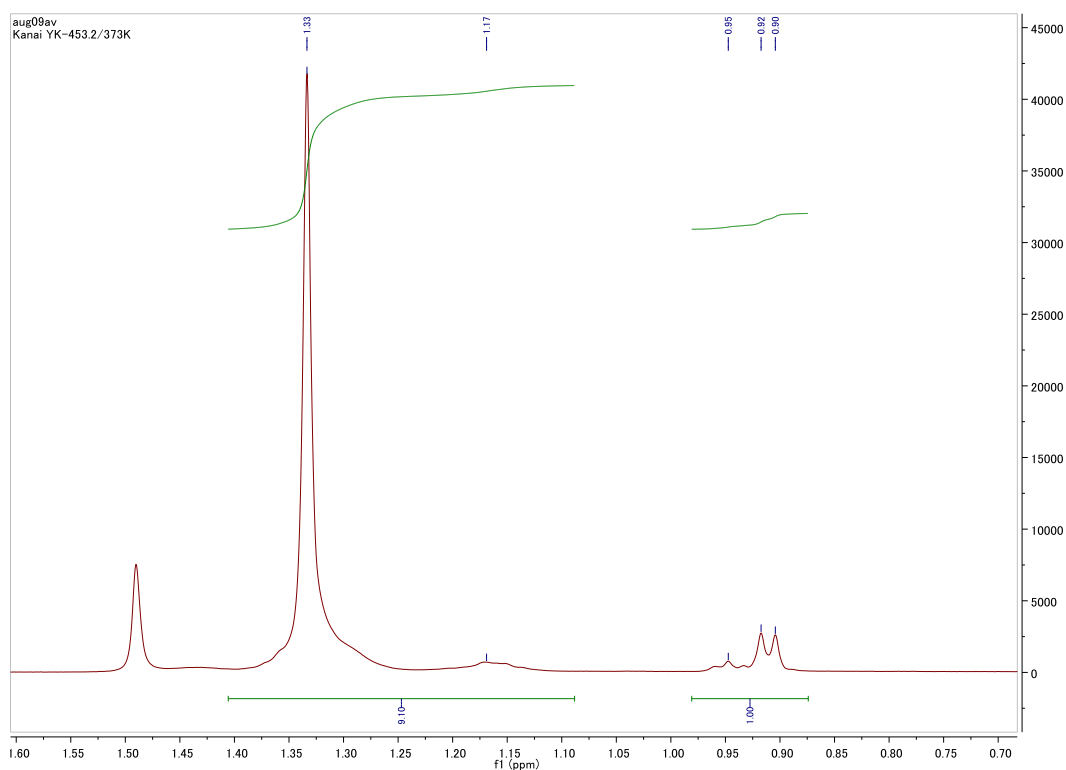


Fig S 45. ^1H NMR spectrum of PE (Table 1, #9).

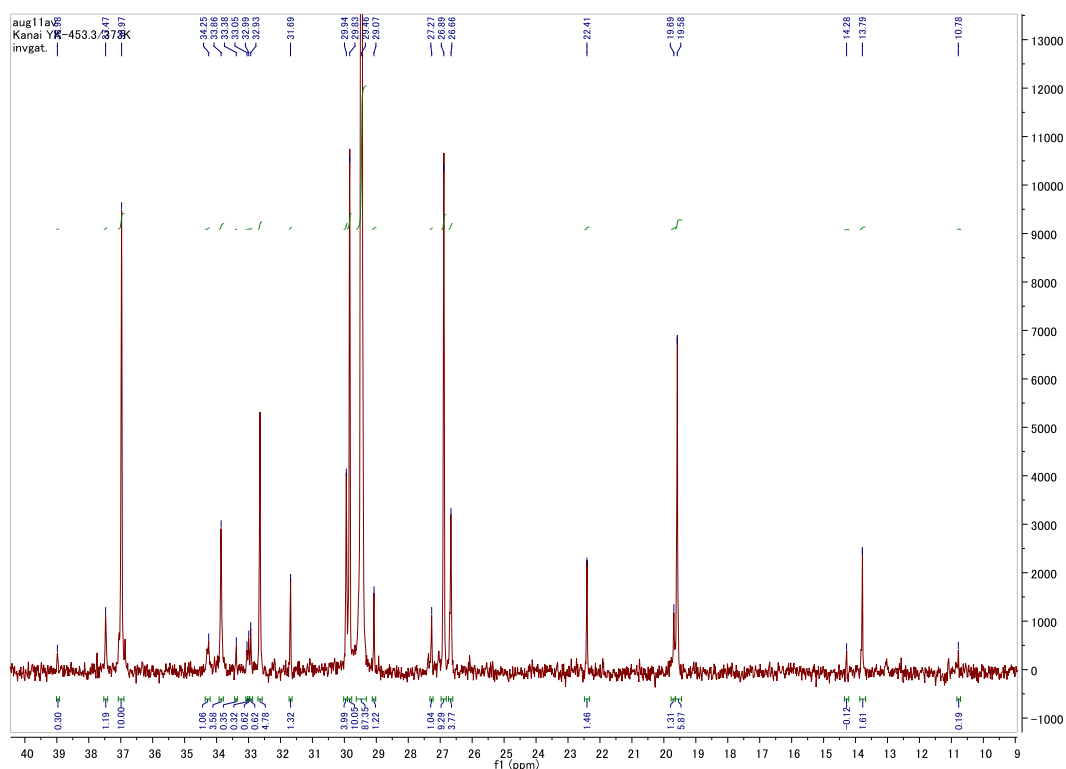


Fig S 46. ^{13}C NMR spectrum of PE (Table 1, #9).

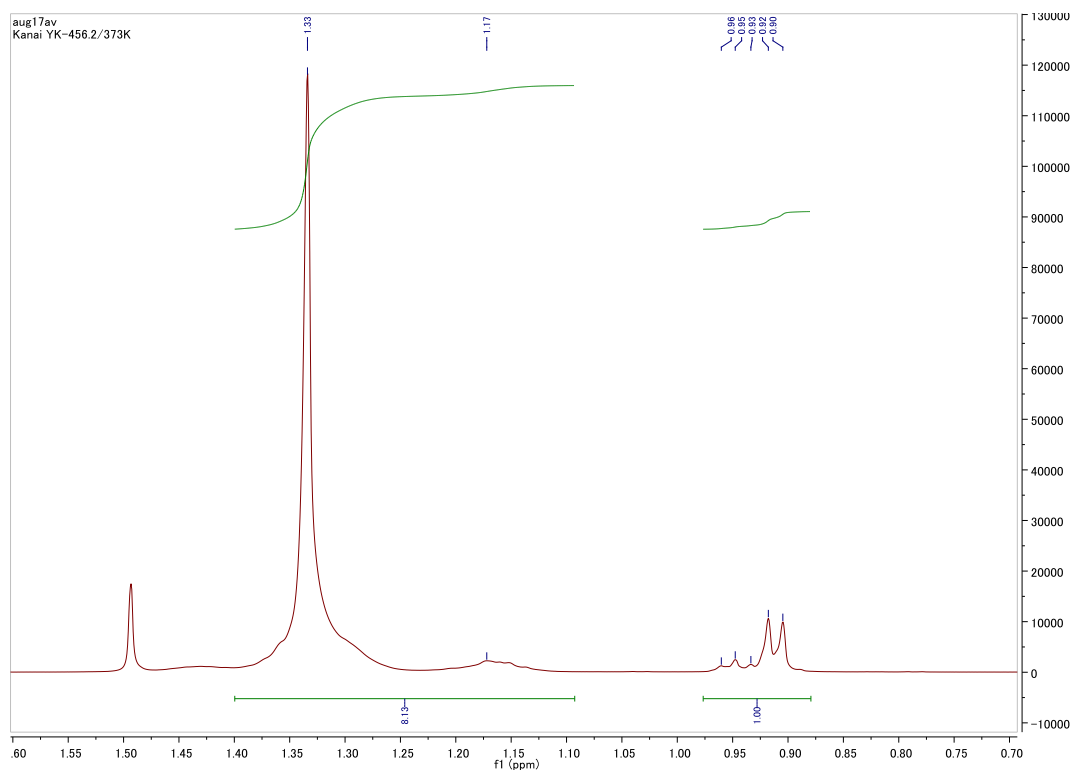


Fig S 47. ^1H NMR spectrum of PE (Table 1, #10).

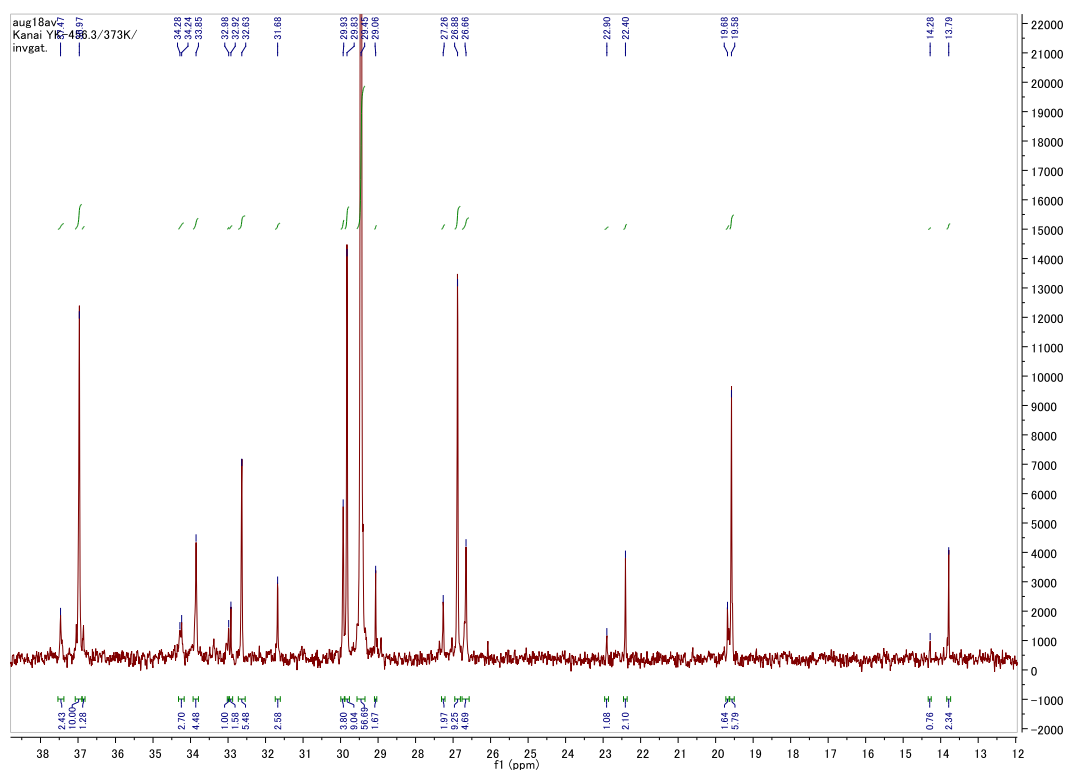


Fig S 48. ^{13}C NMR spectrum of PE (Table 1, #10).

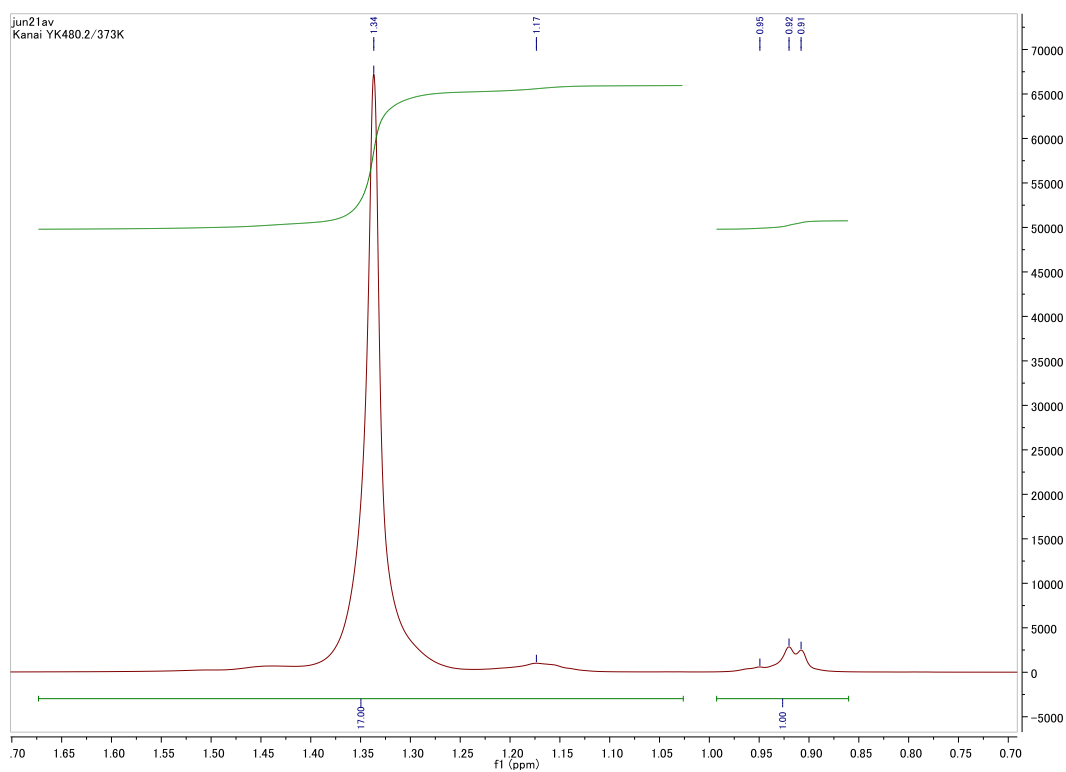


Fig S 49. ^1H NMR spectrum of PE (Table 1, #11).

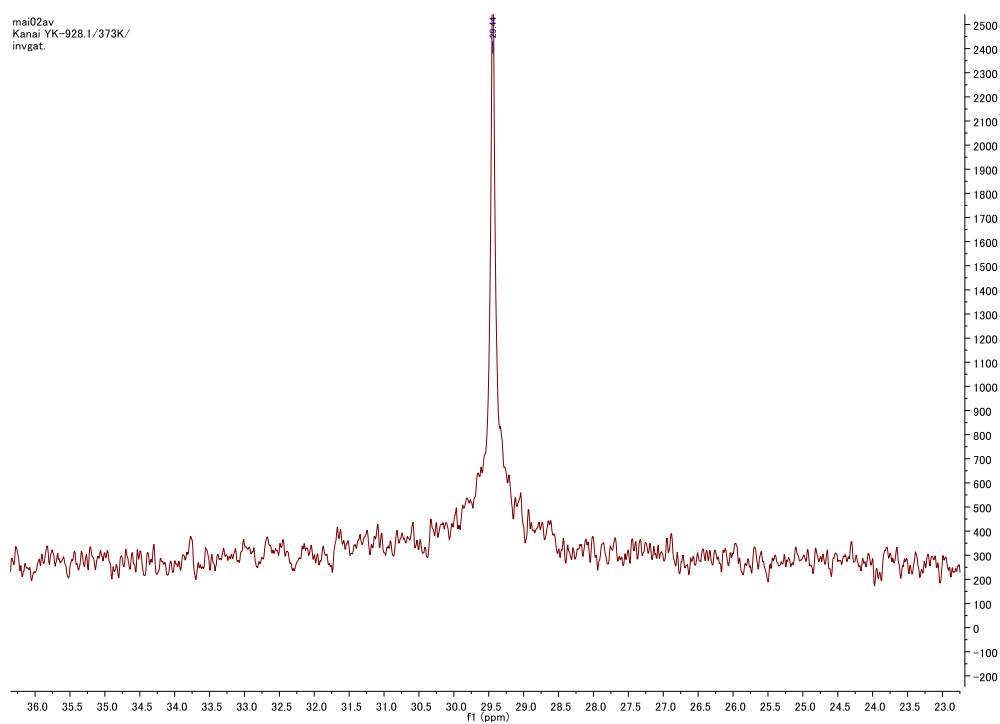


Fig S 50. ^{13}C NMR spectrum of PE (Table 1, #11).

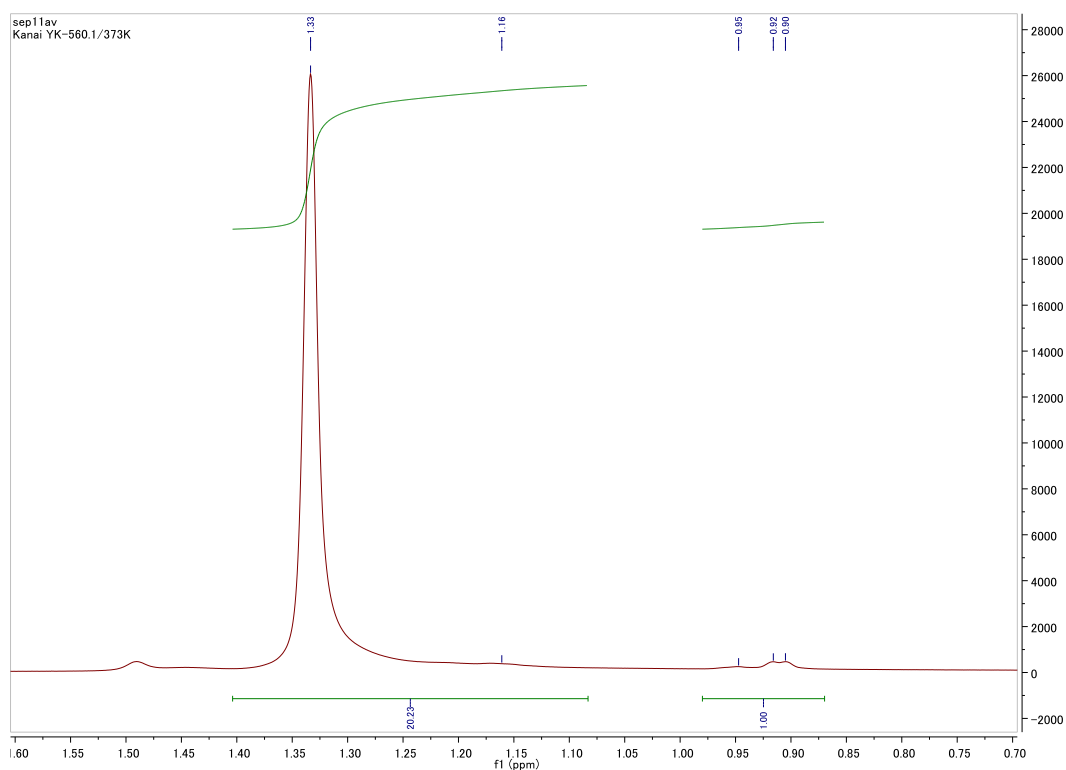


Fig S 51. ^1H NMR spectrum of PE (Table 1, #12).

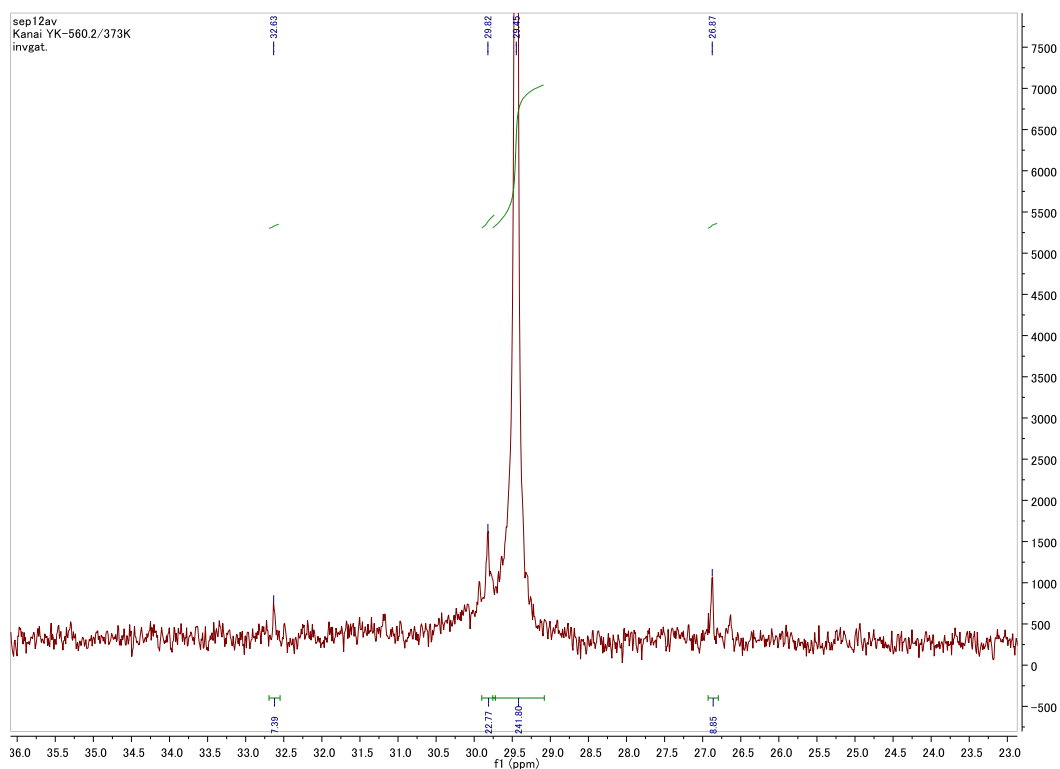


Fig S 52. ^{13}C NMR spectrum of PE (Table 1, #12).

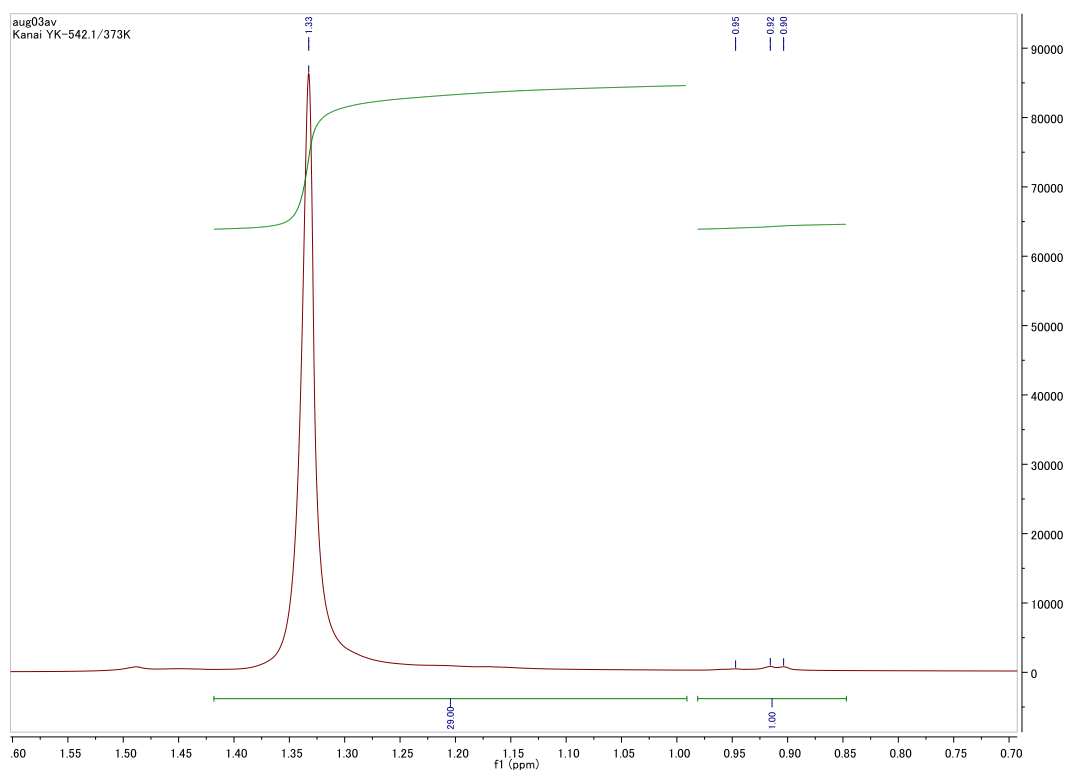


Fig S 53. ^1H NMR spectrum of PE (Table 1, #13).

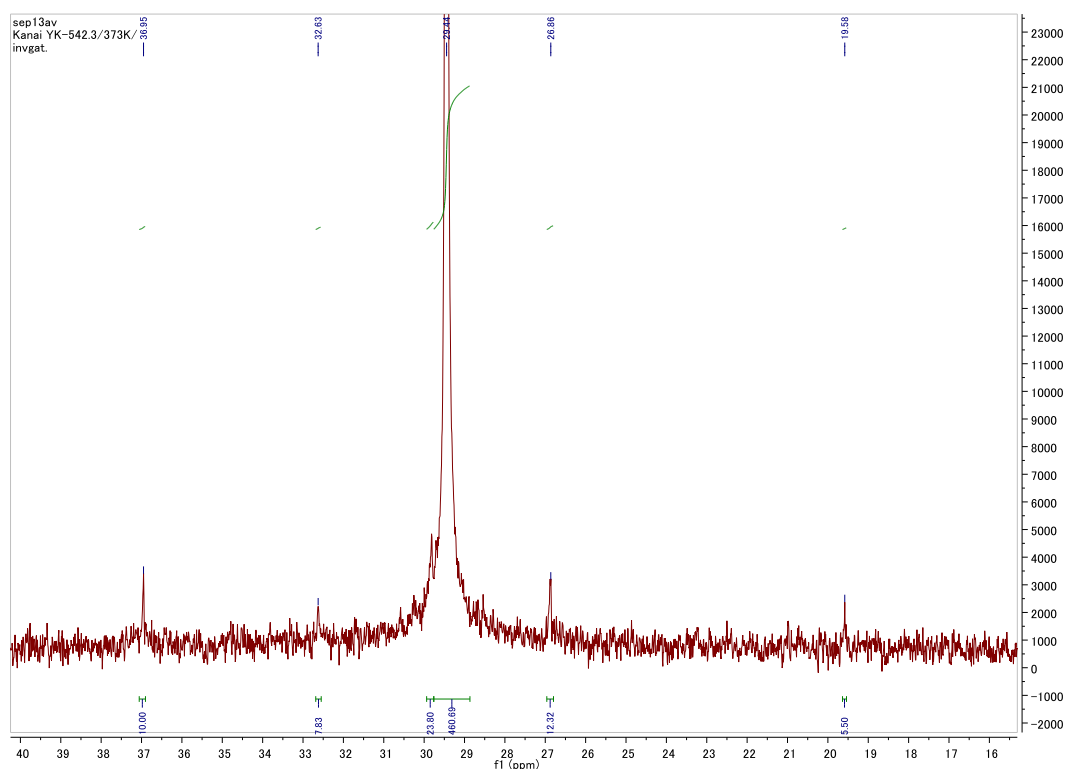


Fig S 54. ^{13}C NMR spectrum of PE (Table 1, #13).

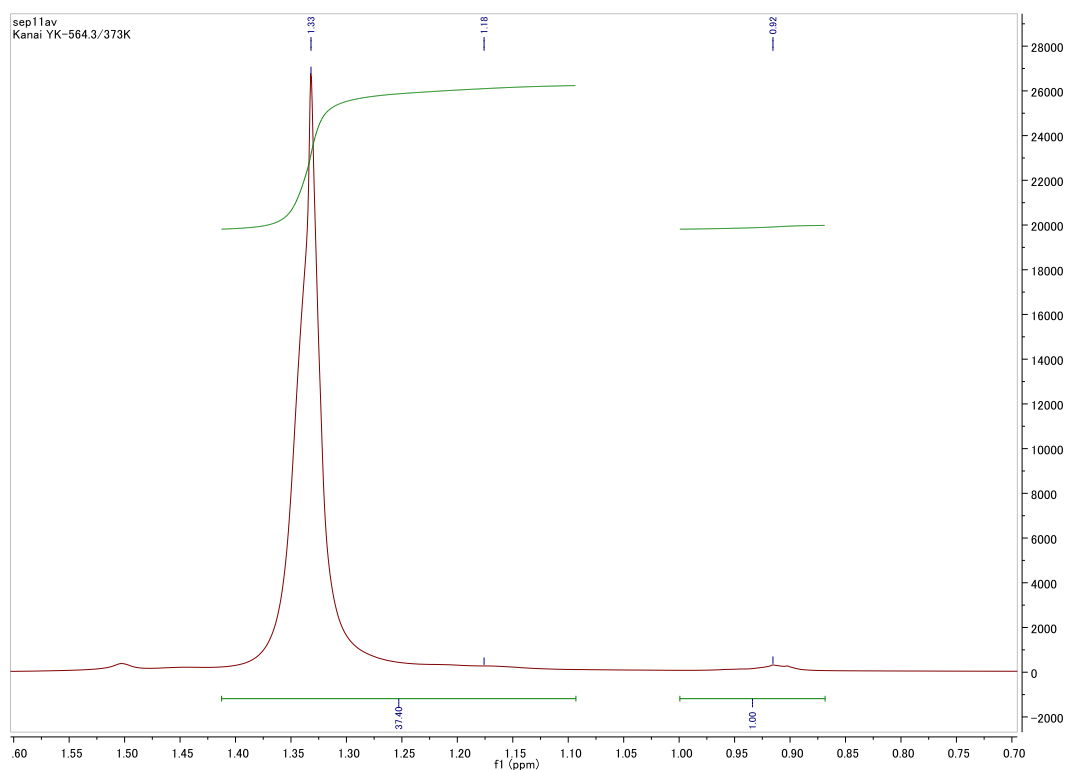


Fig S 55. ^1H NMR spectrum of PE (Table 1, #14).

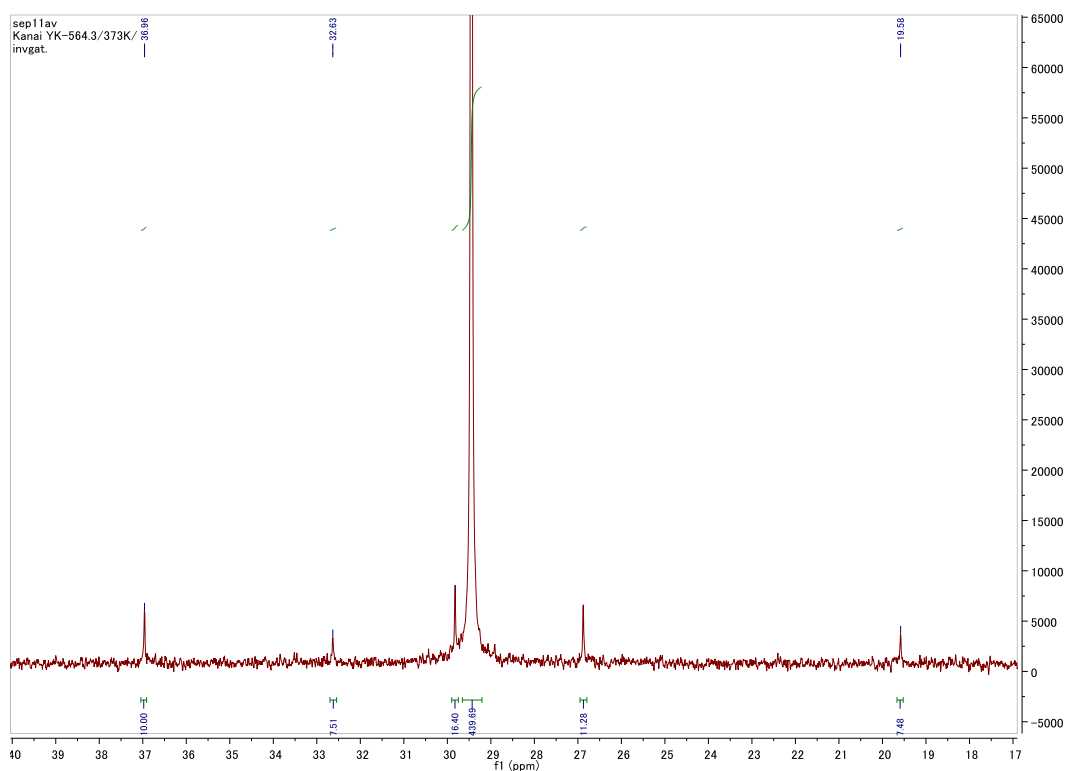


Fig S 56. ^{13}C NMR spectrum of PE (Table 1, #14).

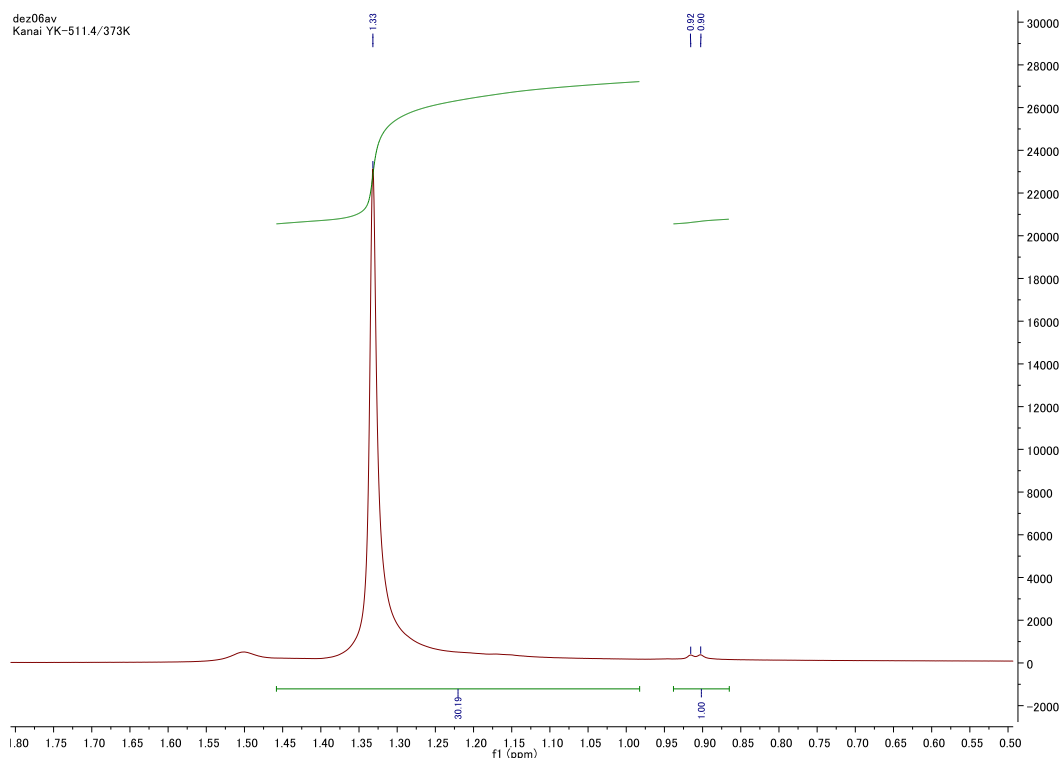


Fig S 57. ^1H NMR spectrum of PE (Table 1, #15).

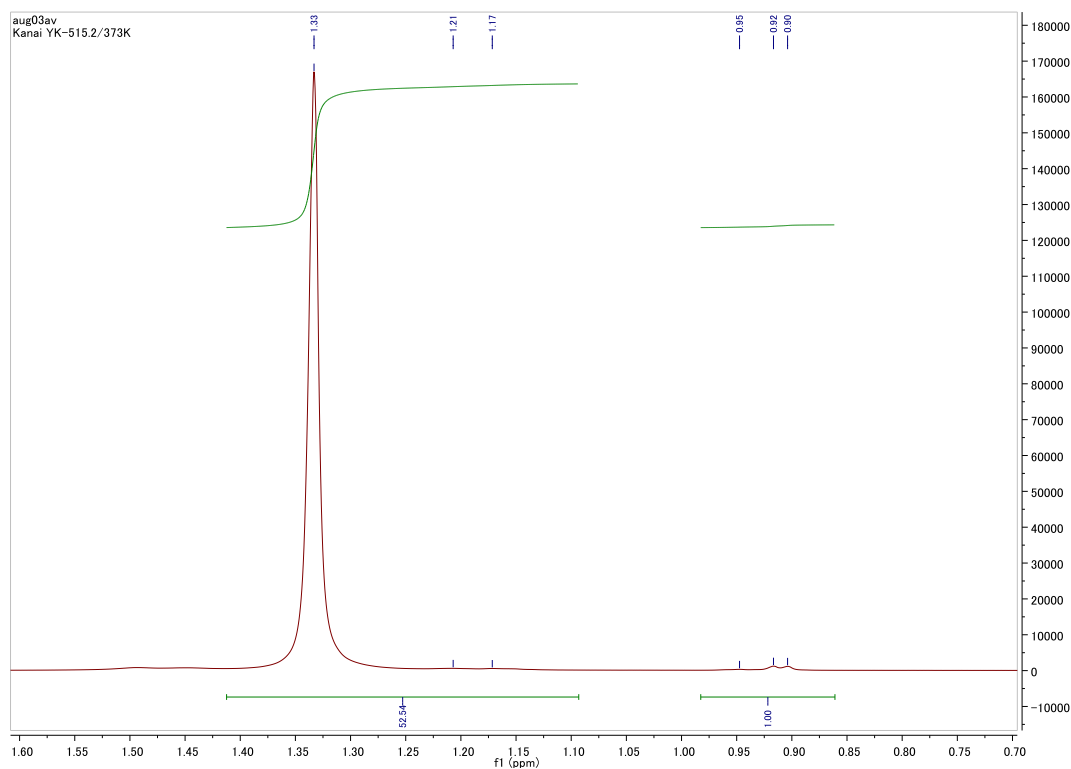


Fig S 58. ^1H NMR spectrum of PE (Table 1, #16).

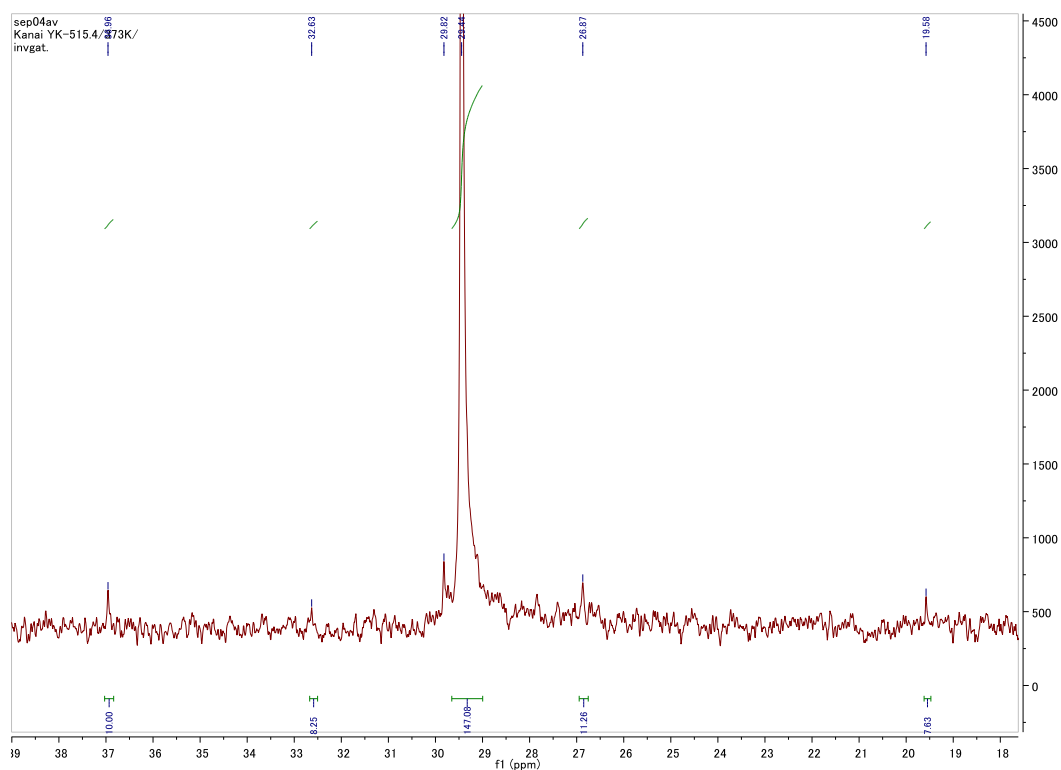


Fig S 59. ^{13}C NMR spectrum of PE (Table 1, #16).

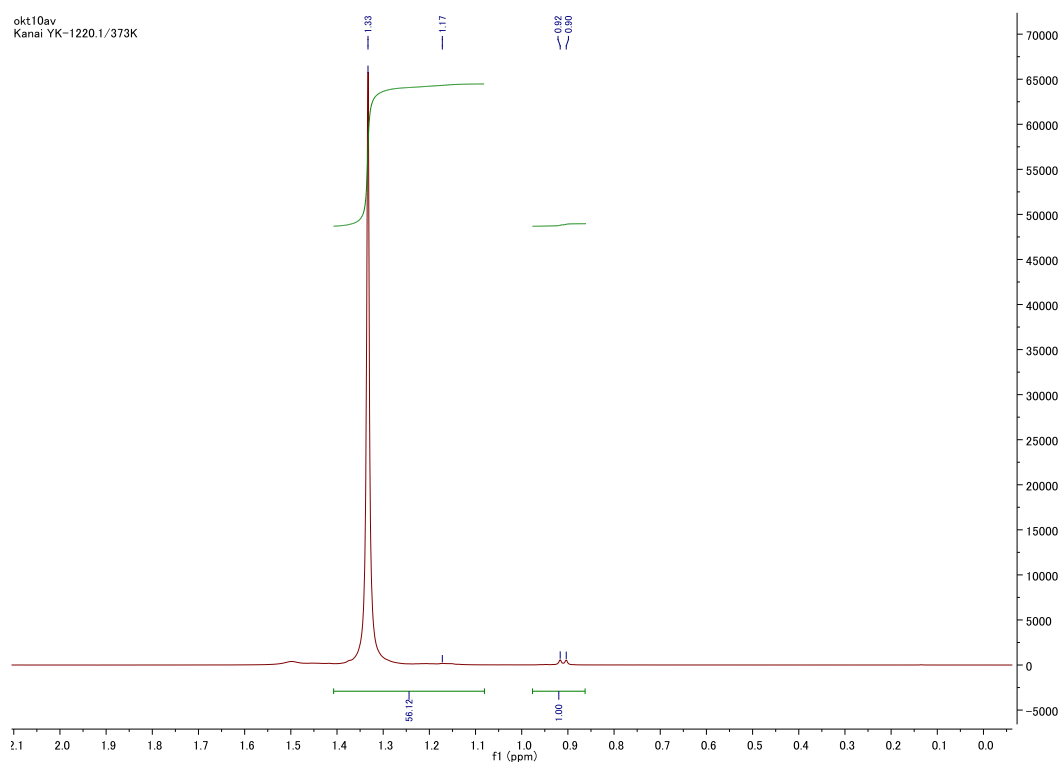


Fig S 60. ^1H NMR spectrum of PE (Table 1, #17).

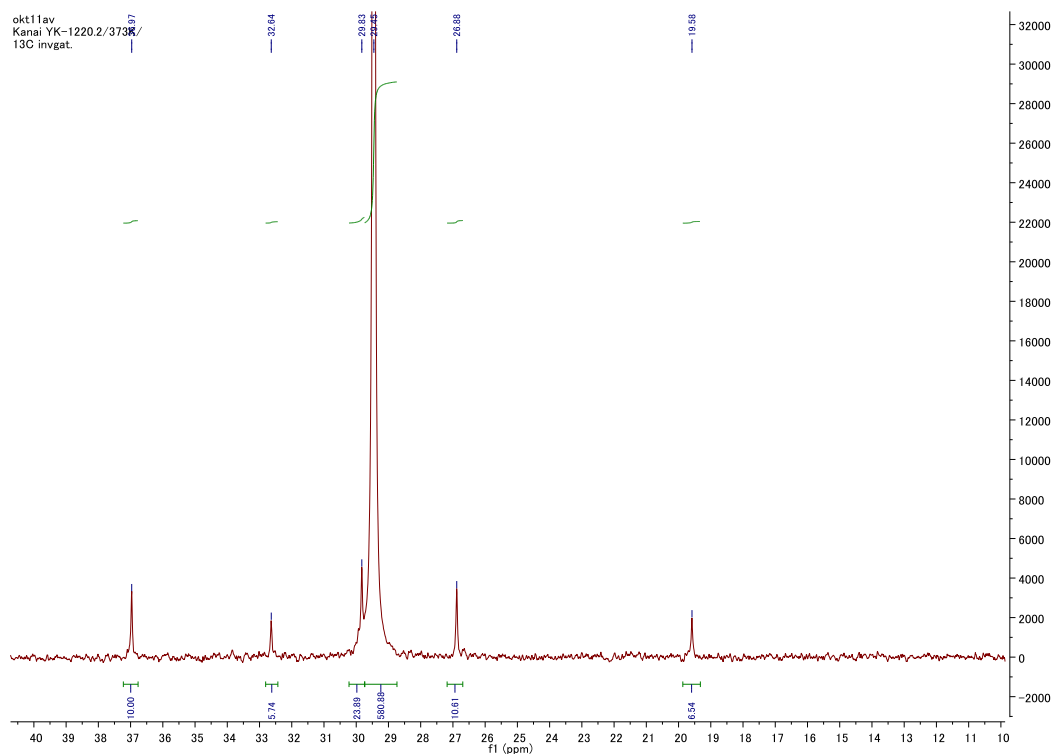


Fig S 61. ^{13}C NMR spectrum of PE (Table 1, #17).

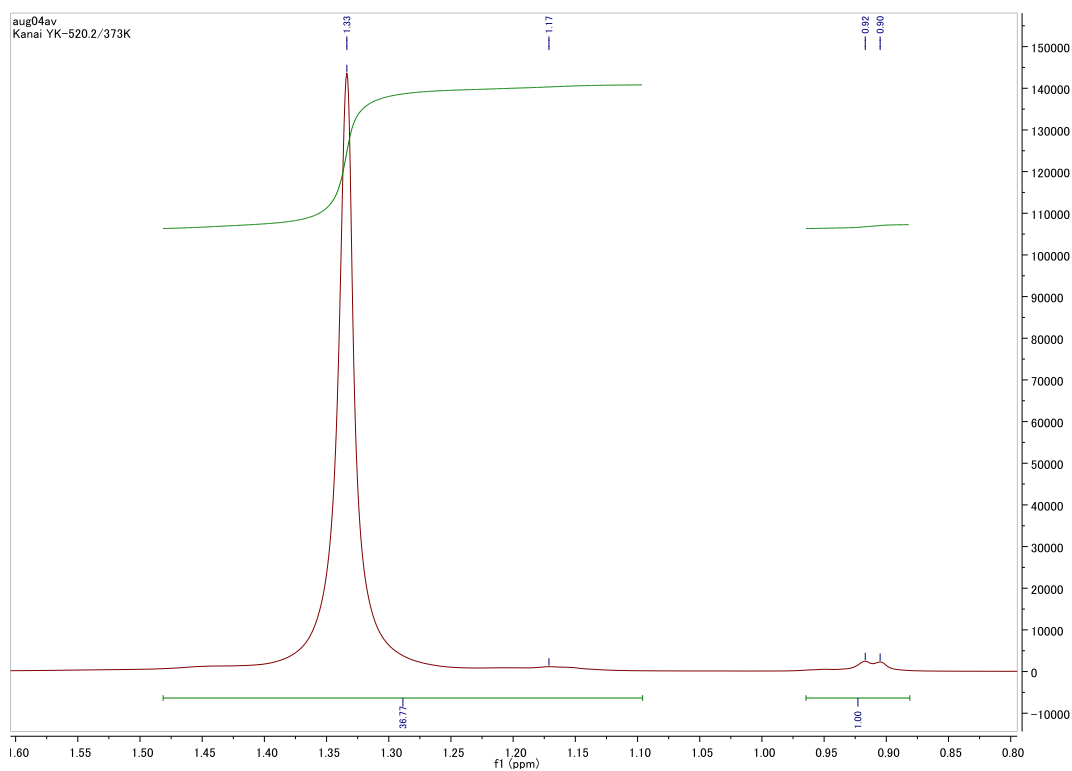
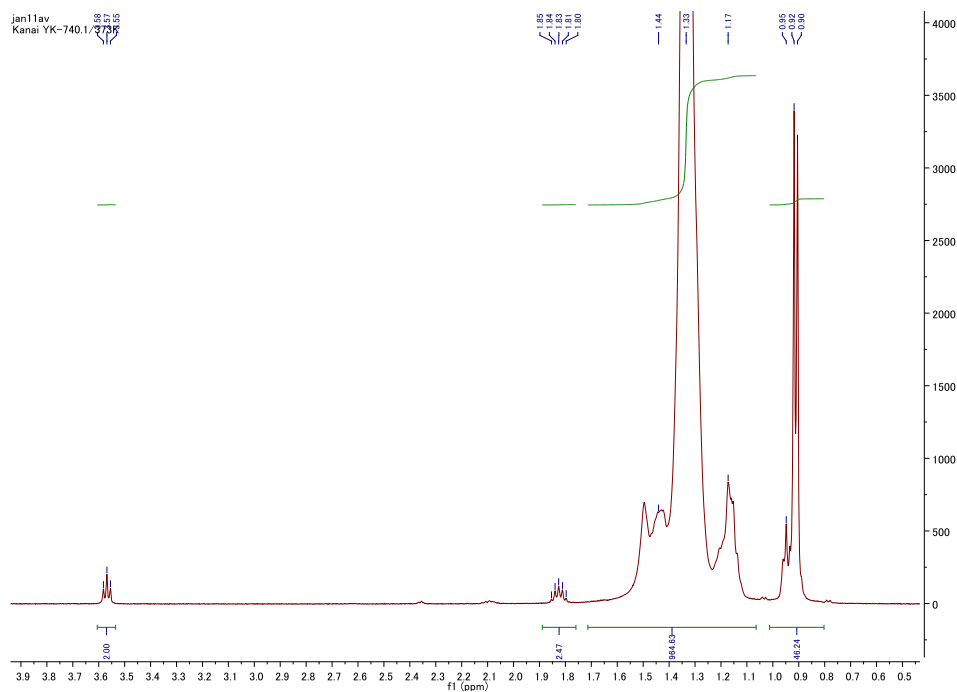
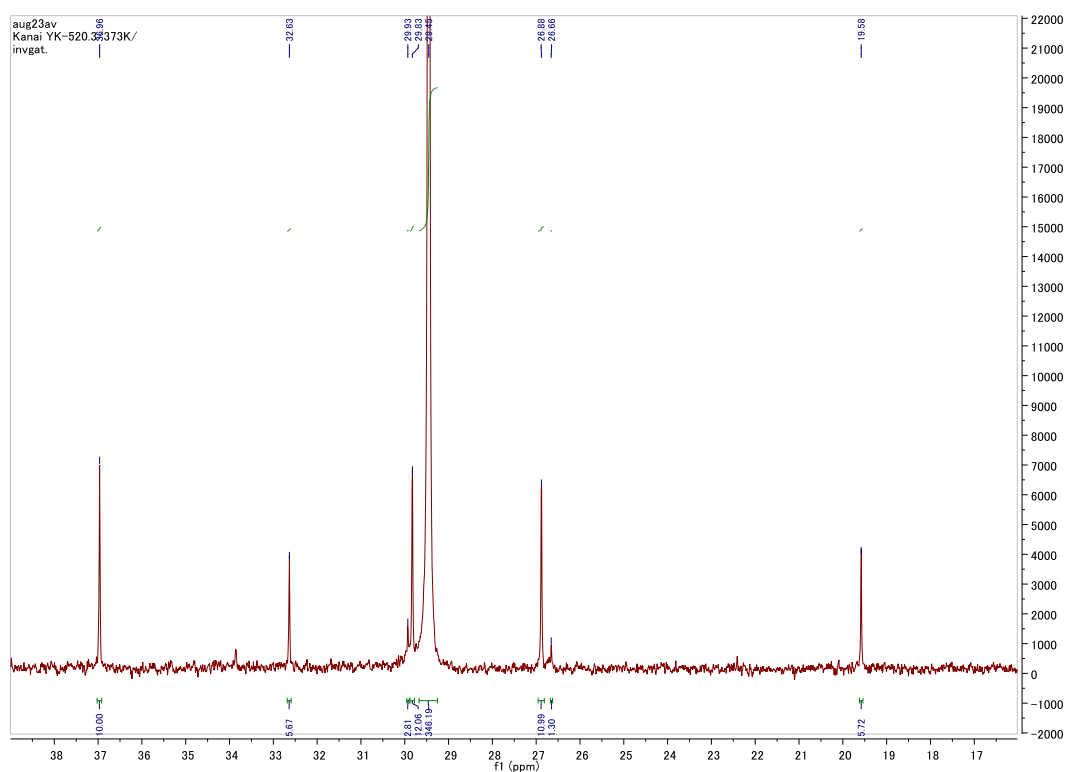


Fig S 62. ^1H NMR spectrum of PE (Table 1, #18).



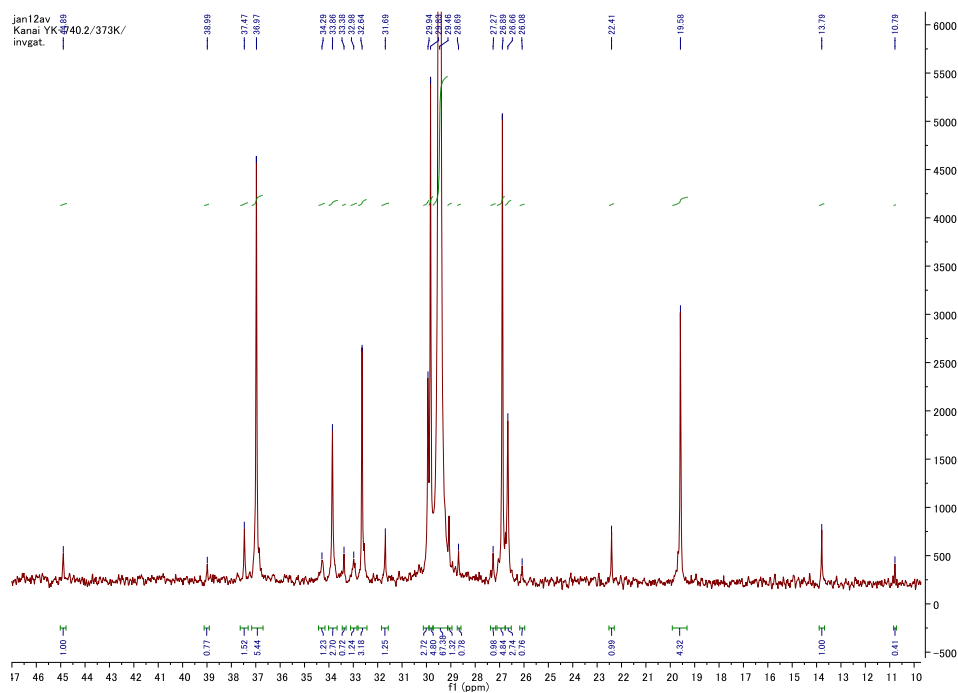


Fig S 65. ^{13}C NMR spectrum of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #8, 0.02 M).

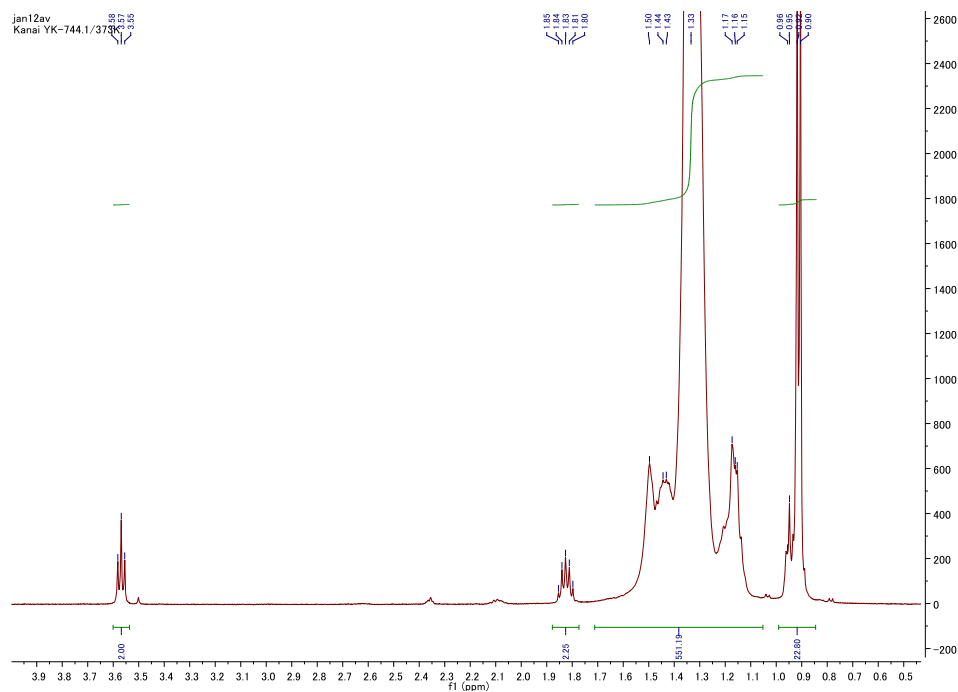


Fig S 66. ^1H NMR spectrum of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #9, 0.04 M).

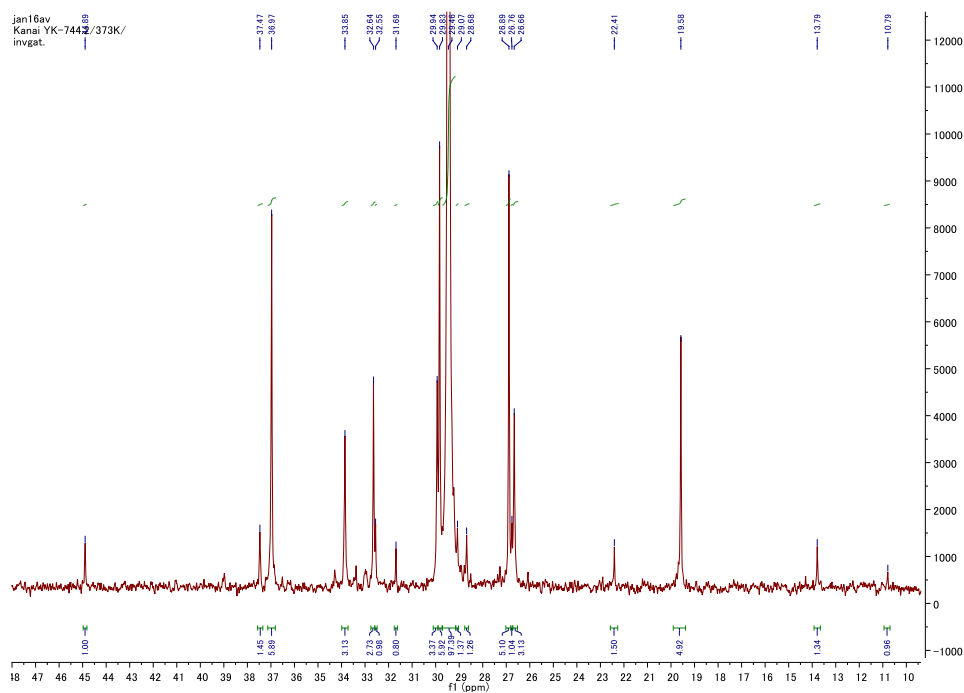


Fig S 67. ^{13}C NMR spectrum of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #9, 0.04 M).

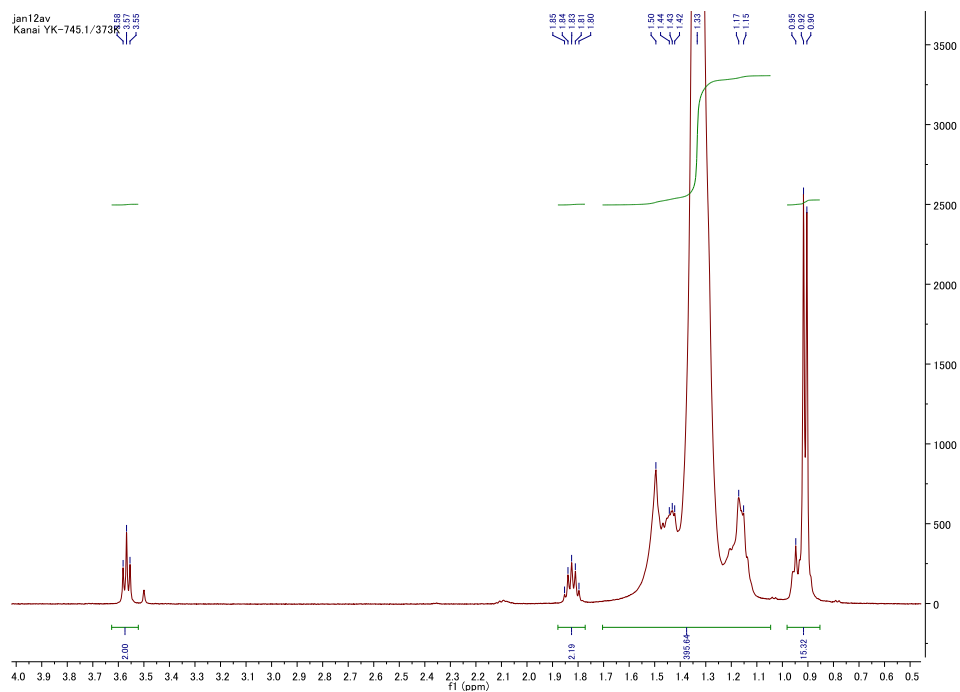


Fig S 68. ^1H NMR spectrum of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #10, 0.06 M).

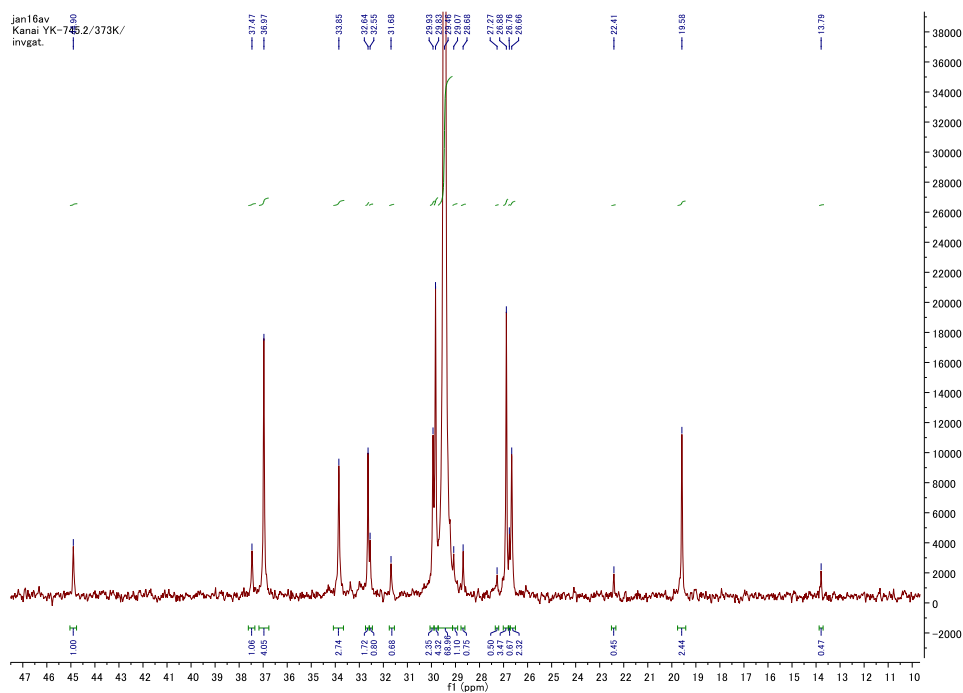


Fig S 69. ^{13}C NMR spectrum of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #10, 0.06 M).

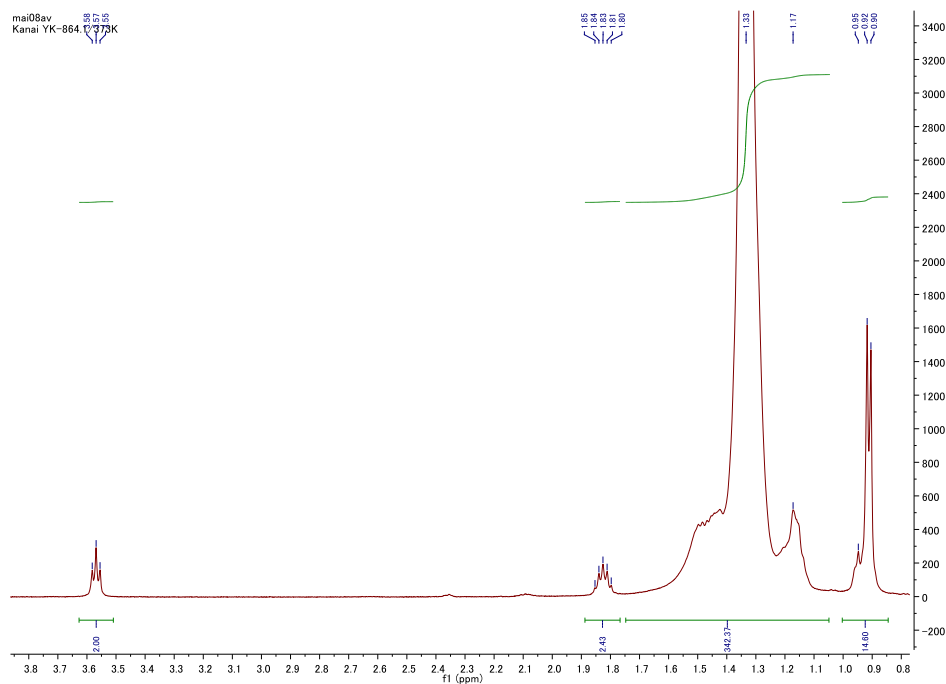


Fig S 70. ^1H NMR spectrum of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, # 11, 0.06 M).

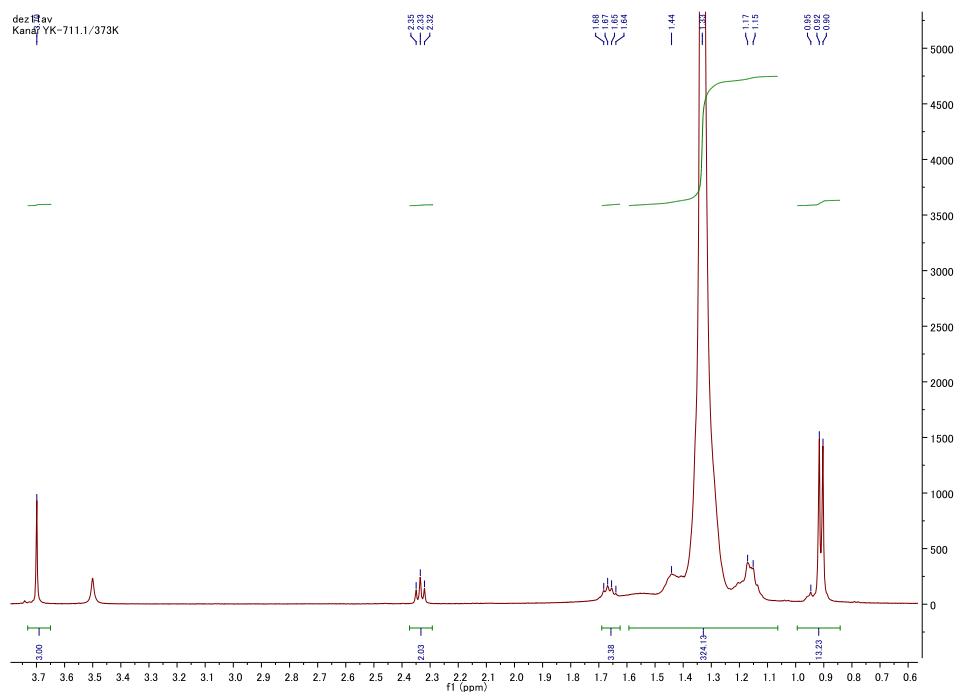


Fig S 71. ^1H NMR spectrum of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, #1, 0.05 M).

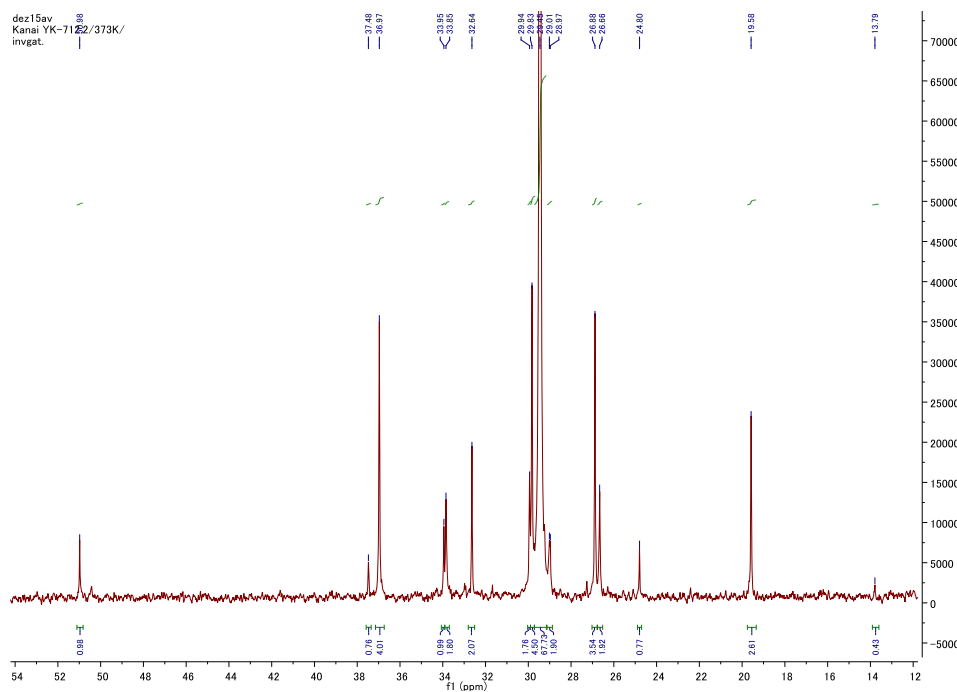


Fig S 72. ^{13}C NMR spectrum of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, #1, 0.05 M).

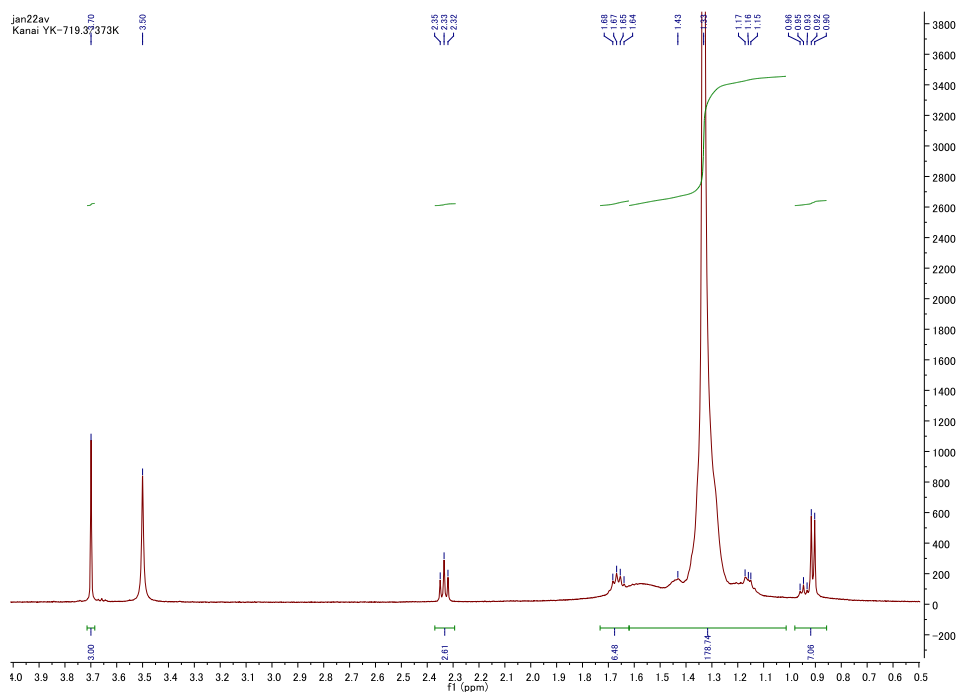


Fig S 73. ^1H NMR spectrum of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, # 2, 0.10 M).

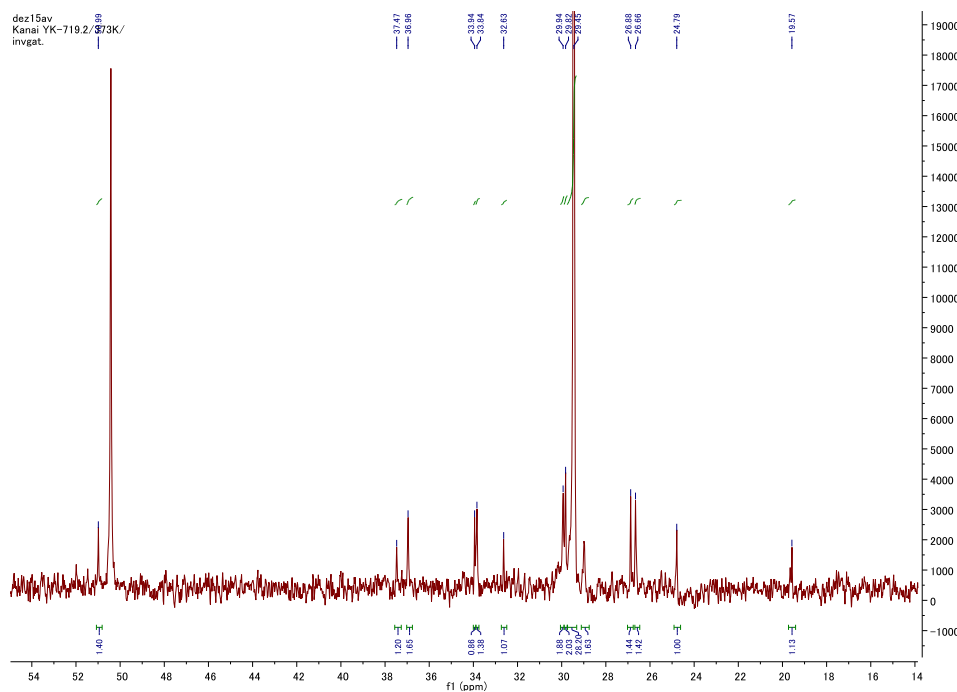


Fig S 74. ^{13}C NMR spectrum of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, #2, 0.10 M).

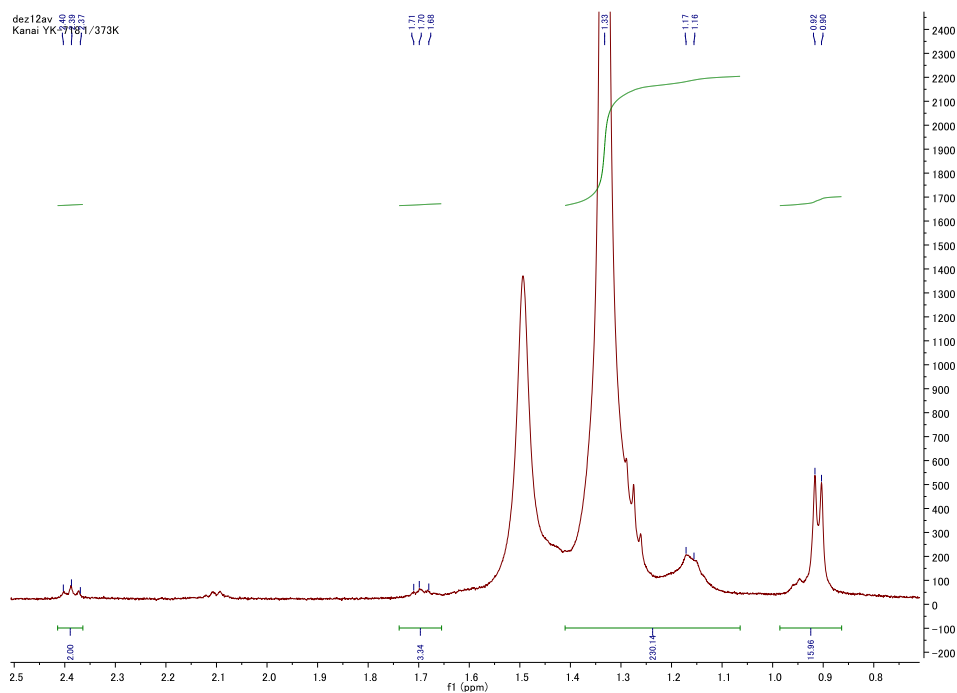


Fig S 75. ^1H NMR spectrum of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #4, 0.02 M).

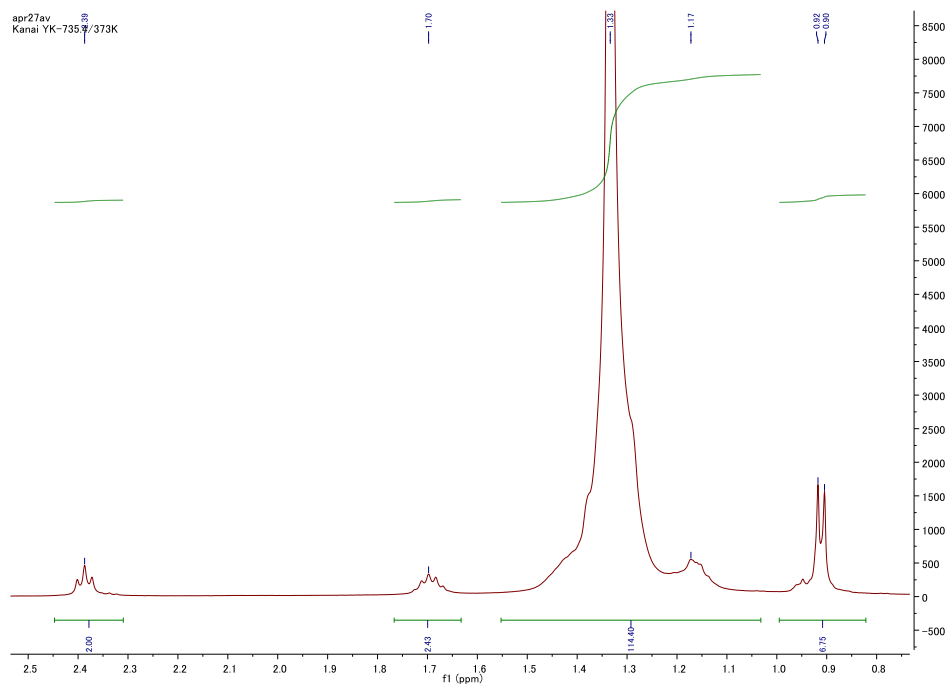


Fig S 76. ^1H NMR spectrum of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #5, 0.06 M).

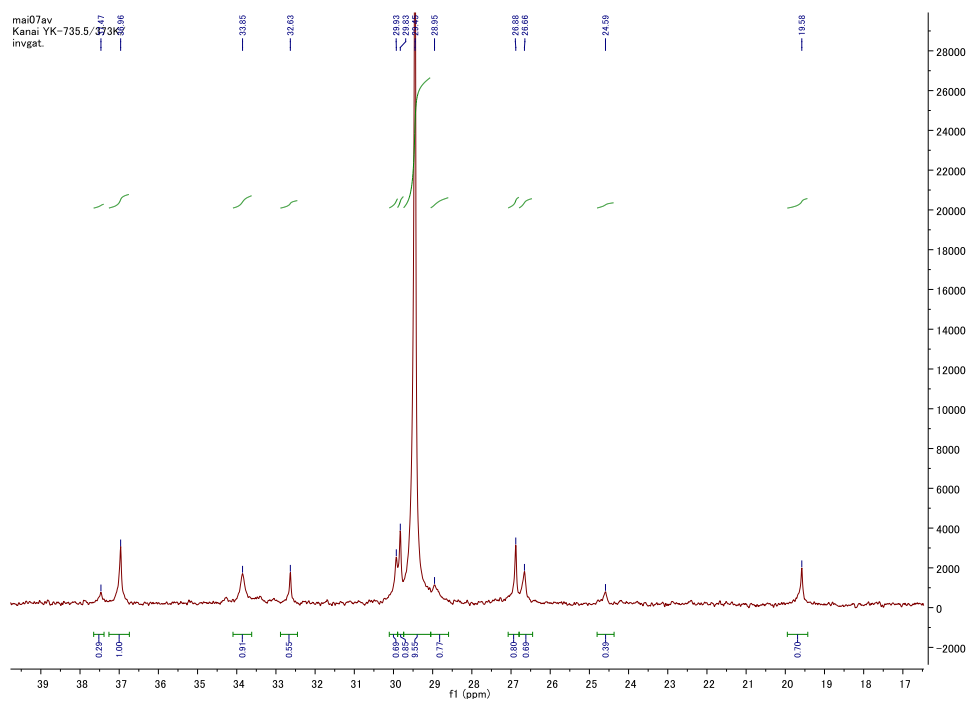


Fig S 77. ^{13}C NMR spectrum of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #5, 0.06 M).

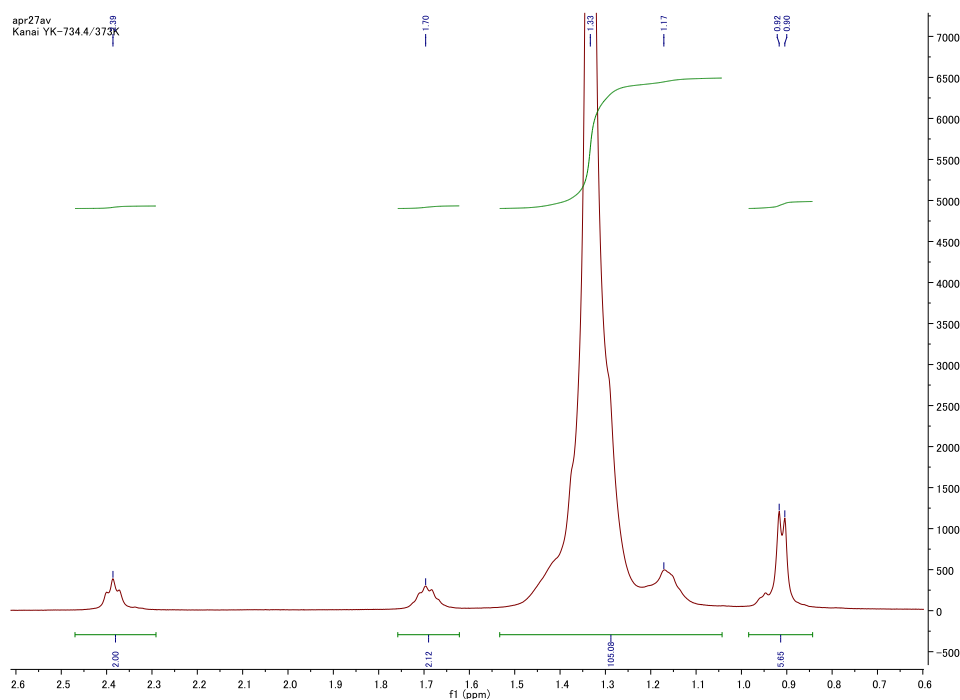


Fig S 78. ^1H NMR spectrum of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #6, 0.1 M).

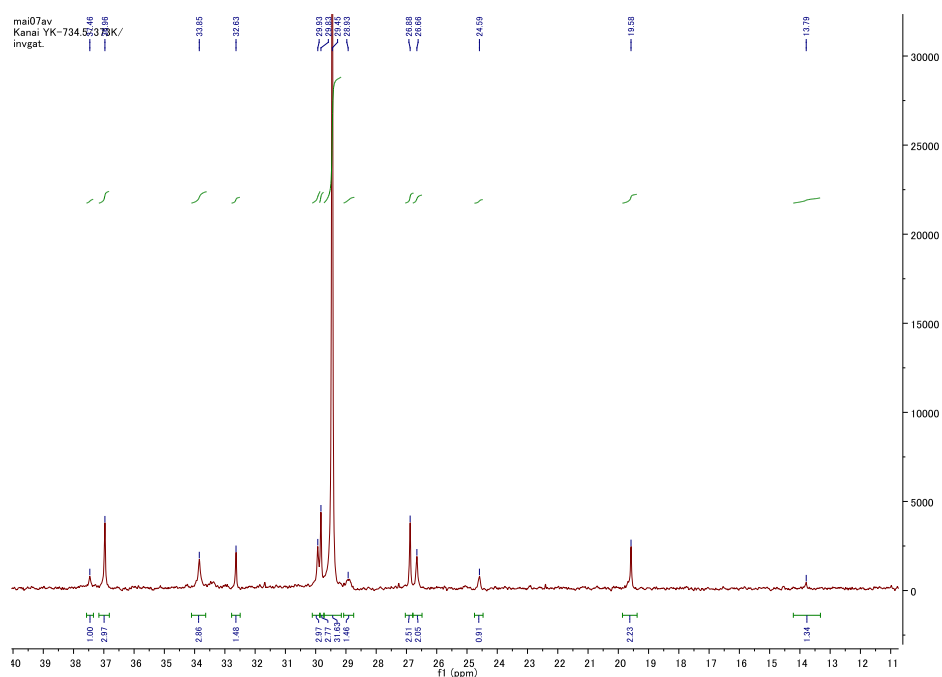


Fig S 79. ^{13}C NMR spectrum of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #6, 0.10 M).

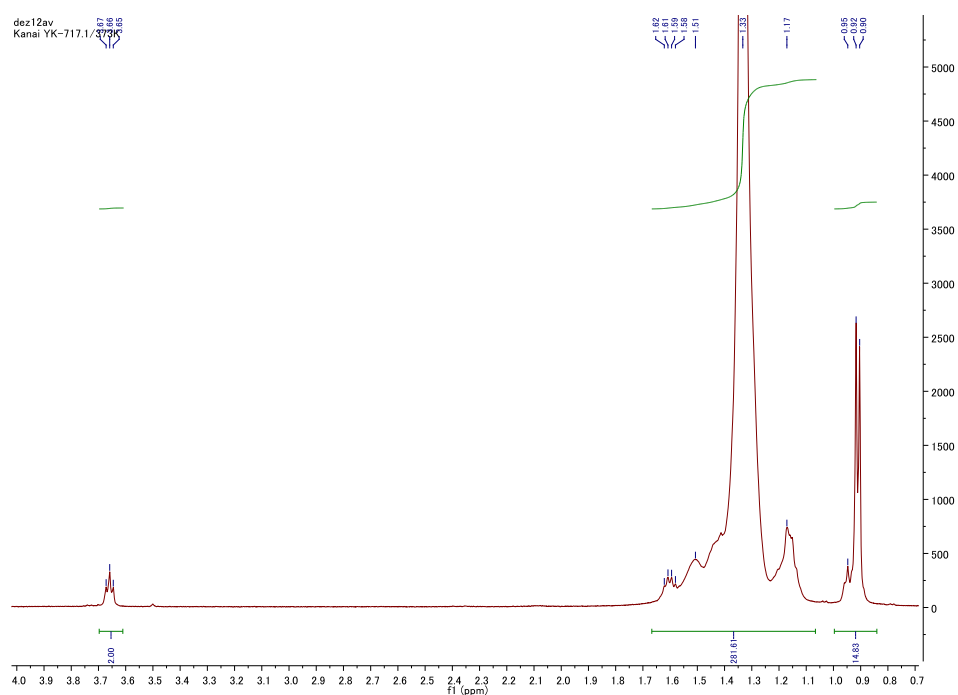


Fig S 80. ^1H NMR spectrum of ethene/5-hexen-1-ol copolymer synthesized at 1 atm (Table 2, #12, 0.06 M).

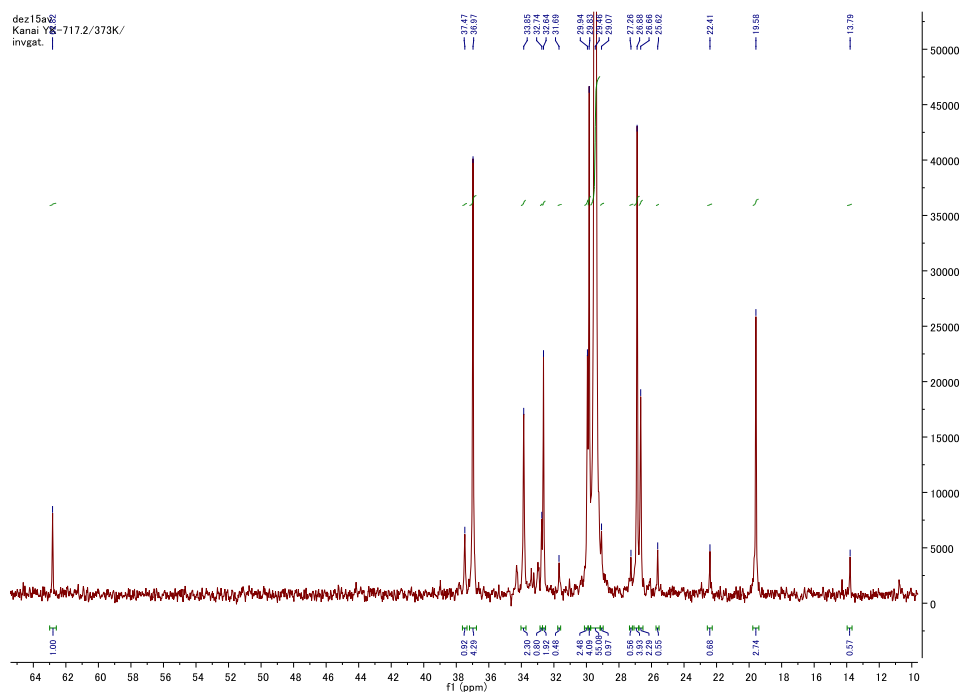


Fig S 81. ^{13}C NMR spectrum of ethene/5-hexen-1-ol copolymer synthesized at 1 atm (Table 2, #12, 0.06 M).

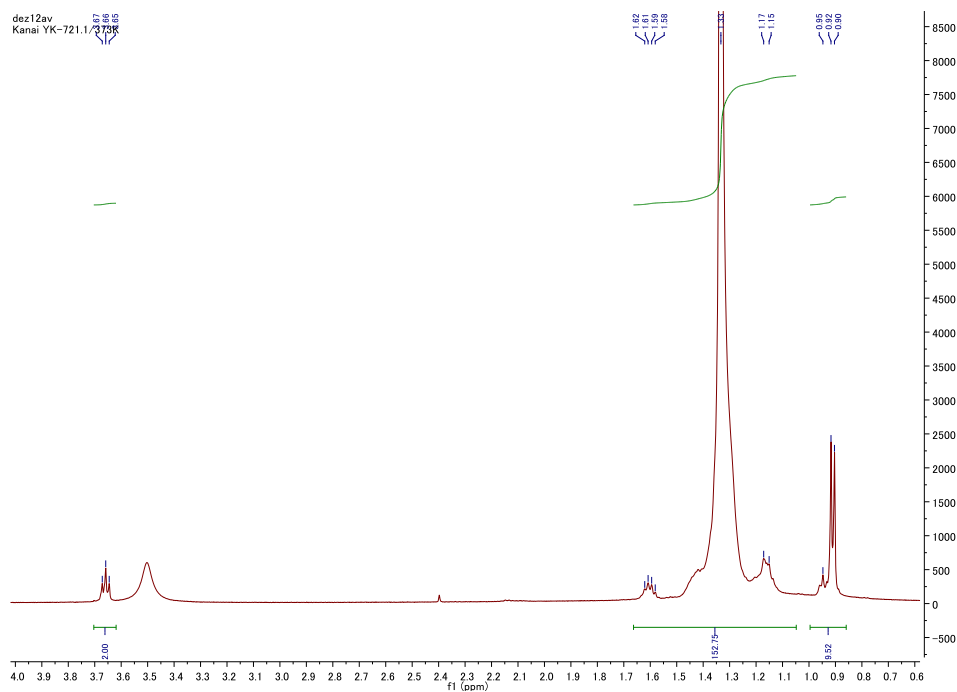


Fig S 82. ^1H NMR spectrum of ethene/5-hexen-1-ol copolymer synthesized at 1 atm (Table 2, #13, 0.08 M).

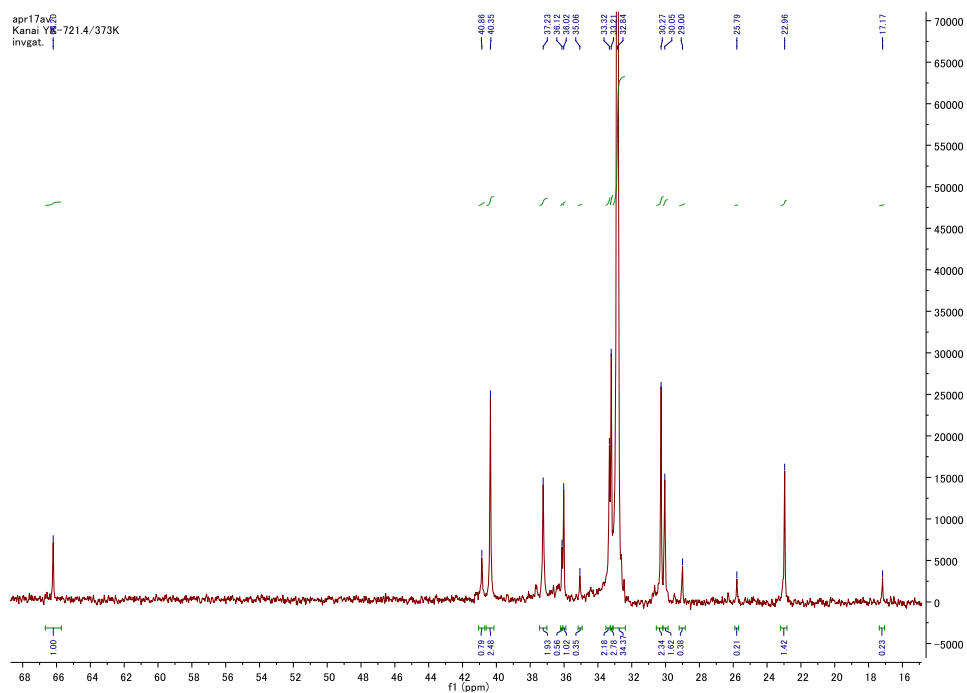


Fig S 83. ^{13}C NMR spectrum of ethene/5-hexen-1-ol copolymer synthesized at 1 atm (Table 2, #13, 0.08 M).

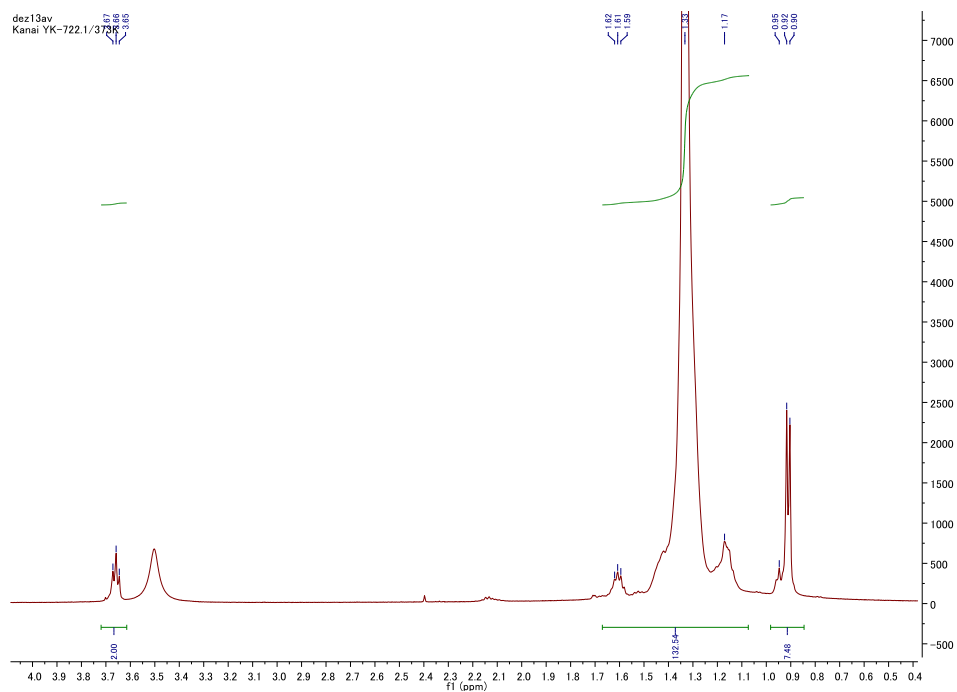


Fig S 84. ^1H NMR spectrum of ethene/5-hexen-1-ol copolymer synthesized at 1 atm (Table 2, #14, 0.10 M).

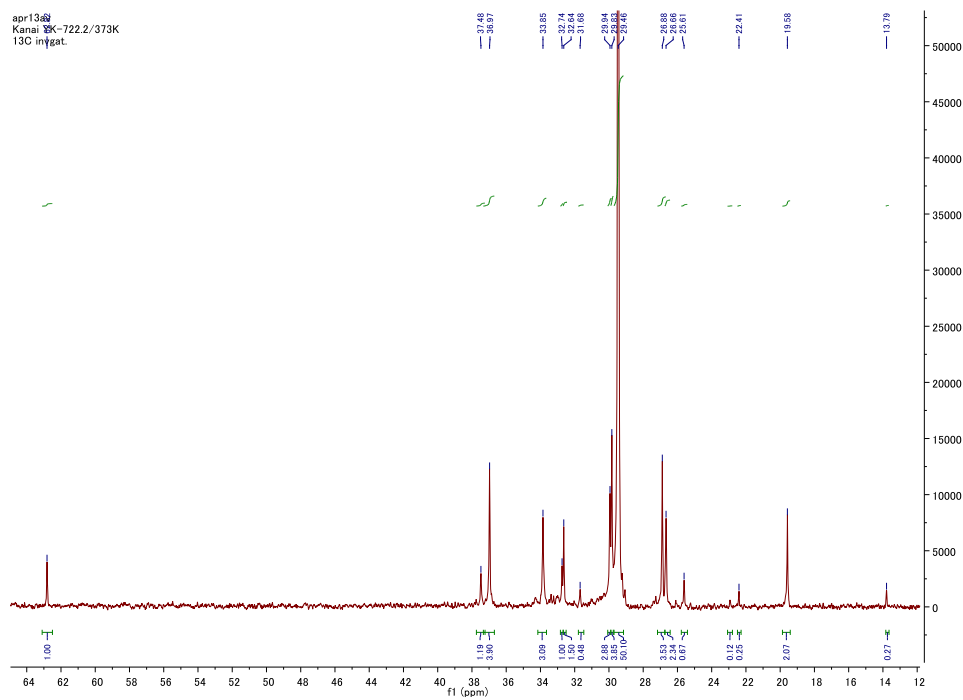
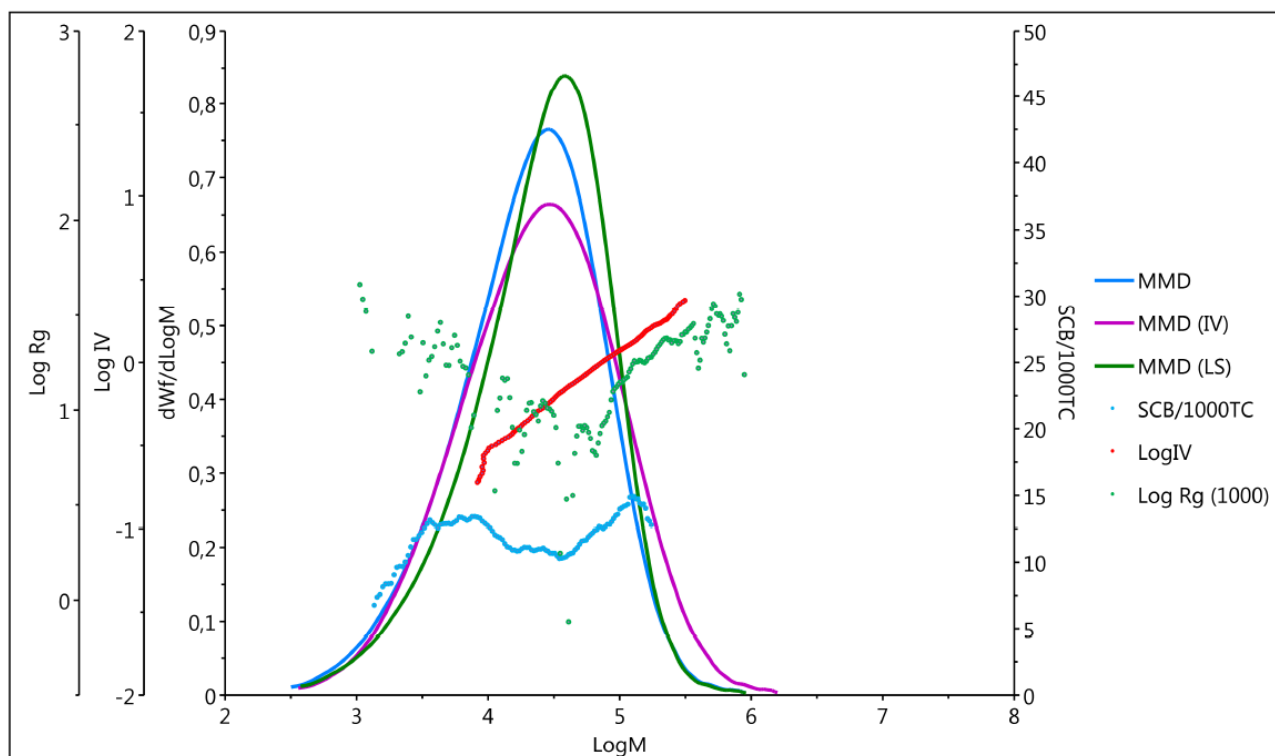


Fig S 85. ^{13}C NMR spectrum of ethene/5-hexen-1-ol copolymer synthesized at 1 atm (Table 2, #14, 0.10 M).

Gel permeation chromatography



Results (Conventional)

Mw	39886	g/mol
Mn	8399	g/mol
Mw / Mn	4,7	
Mz	119233	g/mol
Mp	28659	g/mol
Mv	33692	g/mol
IVmwd	0,78	dL/g
Bulk CH3 / 1000C	15,1	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,91	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	56507	g/mol
Mn UC	9392	g/mol
Mz UC	223934	g/mol
IV Bulk	0,63	dL/g

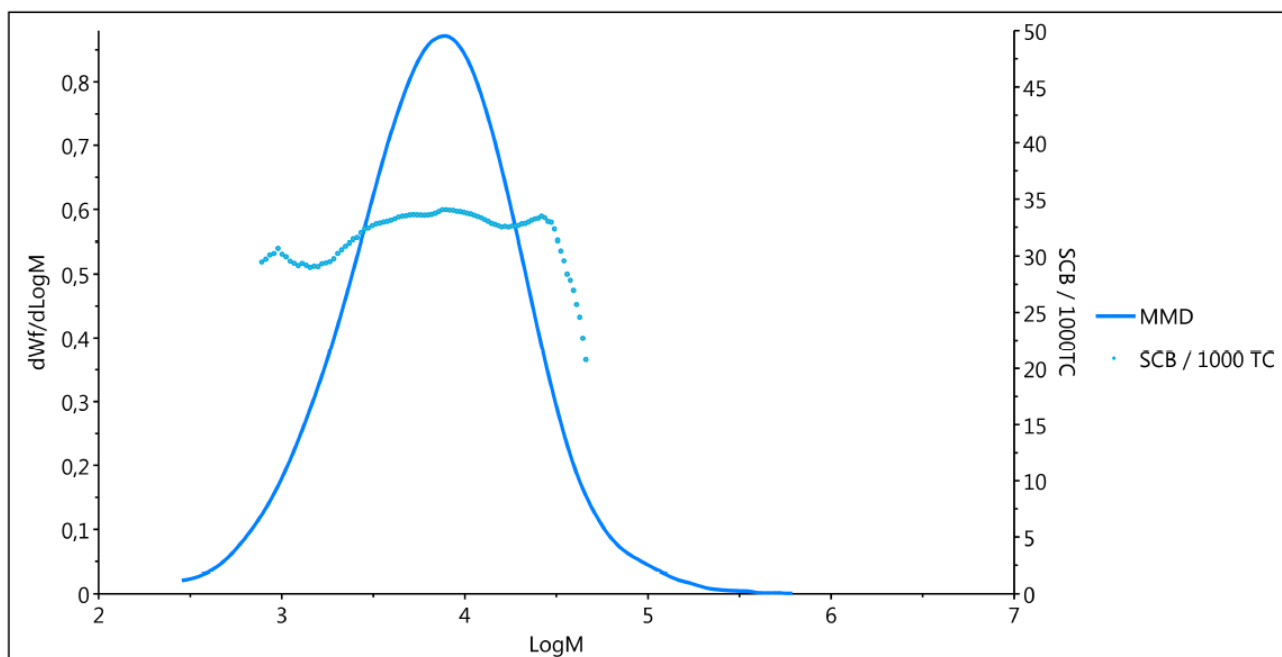
Performance

Mass recovery	0,00	%
Flow Marker	44,57	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	44250	g/mol
Mn Abs	10300	g/mol
Mz Abs	110661	g/mol
Mw / Mn Abs	4	
Rg Slice	8,2	nm

Fig S 86. GPC of PE (Table 1, #1).



Results

Mw 12628 g/mol
Mn 3847 g/mol
Mw / Mn 3,28
Mz 48734 g/mol
Mp 7685 g/mol
Mv 10635 g/mol
IVmwd 0,3376 dL/g
Bulk CH3 / 1000C 38,815

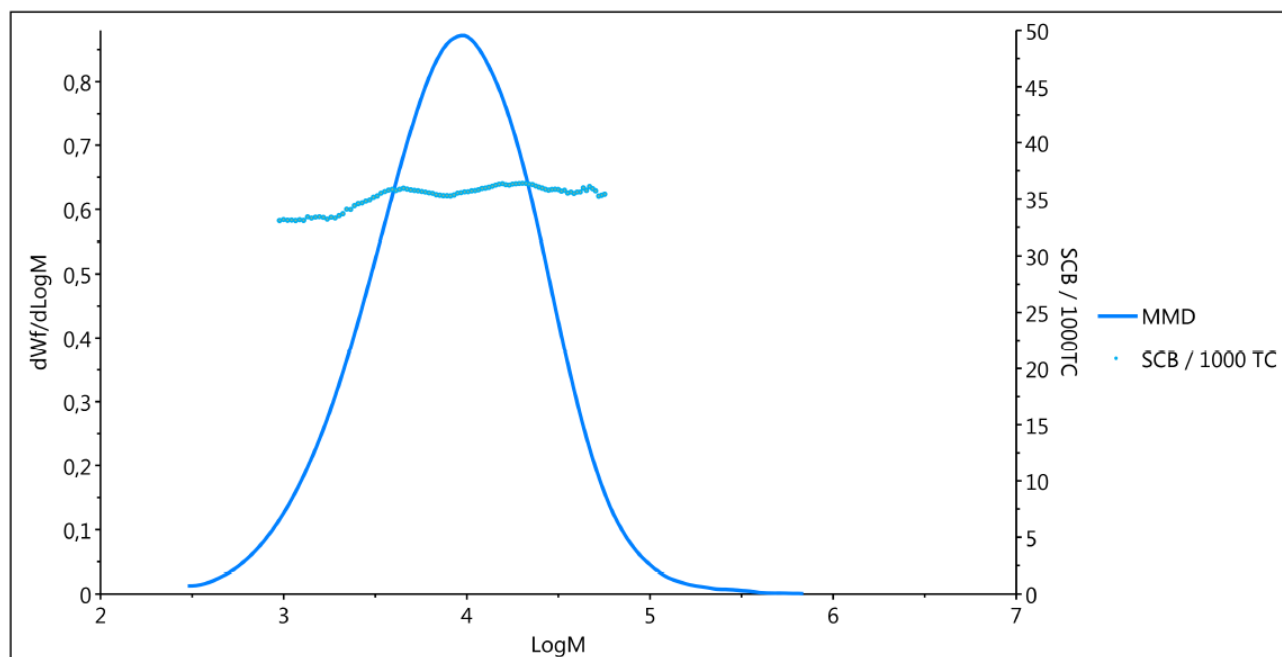
Performance

Flow Marker 44,57 mL
Mass recovery 100 %

Calibrations

Calib Flow Marker 44,68 mL
Calib Mass constant 0,47 mL·V/mg

Fig S 87. GPC of PE (Table 1, #2).



Results

Mw 14883 g/mol
Mn 4795 g/mol
Mw / Mn 3,10
Mz 49548 g/mol
Mp 9396 g/mol
Mv 12765 g/mol
IVmwd 0,3854 dL/g
Bulk CH3 / 1000C 41,703

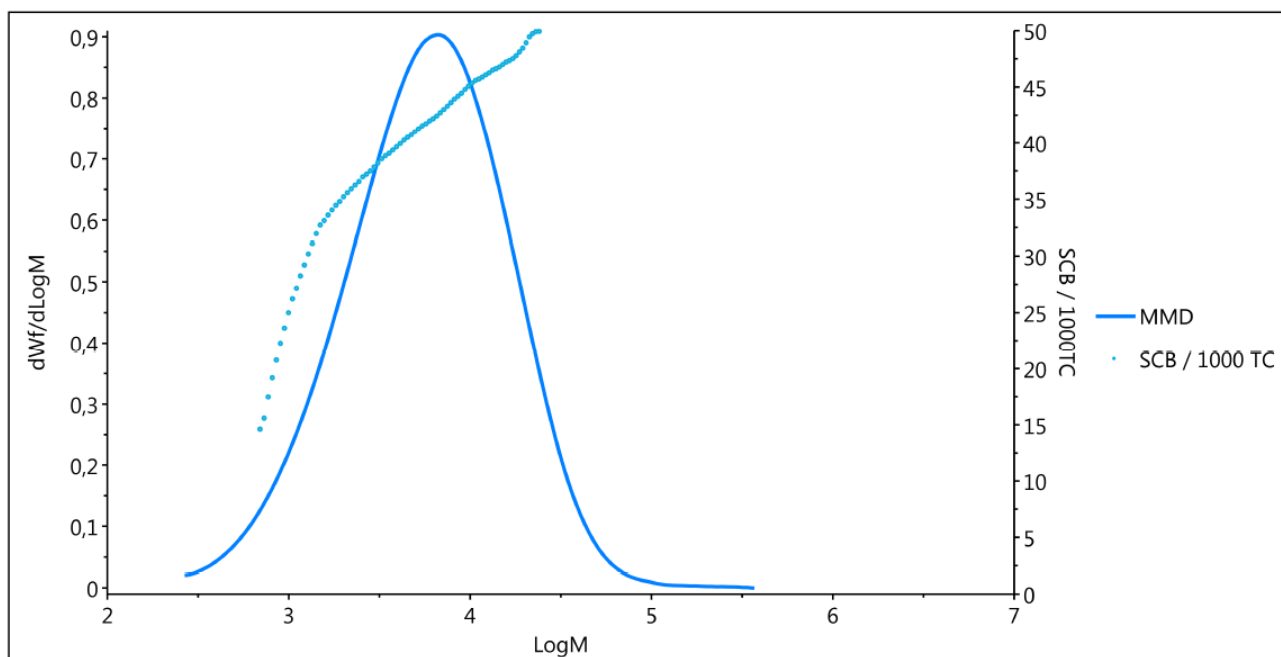
Performance

Flow Marker 44,75 mL
Mass recovery 99 %

Calibrations

Calib Flow Marker 44,68 mL
Calib Mass constant 0,47 mL·V/mg

Fig S 88. GPC of PE (Table 1, #3).



Results

Mw	9280	g/mol
Mn	3341	g/mol
Mw / Mn	2,78	
Mz	24646	g/mol
Mp	6610	g/mol
Mv	8141	g/mol
IVmwd	0,2781	dL/g
Bulk CH3 / 1000C	48,922	

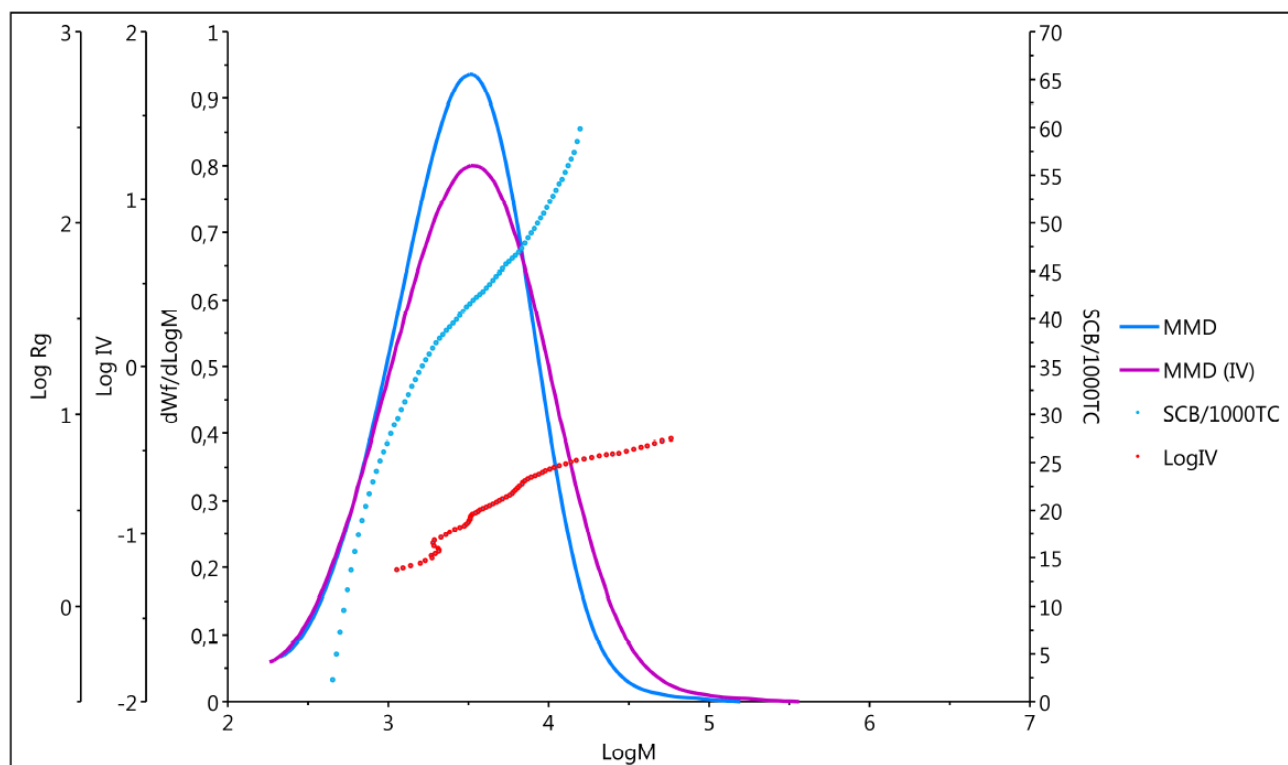
Performance

Flow Marker	44,56	mL
Mass recovery	99	%
Plate Count	5833	

Calibrations

Calib Flow Marker	44,68	mL
Calib Mass constant	0,44	mL·V/mg

Fig S 89. GPC of PE (Table 1, #4).



Results (Conventional)

Mw	4394	g/mol
Mn	1701	g/mol
Mw / Mn	2,6	
Mz	11697	g/mol
Mp	3245	g/mol
Mv	3865	g/mol
IVmwd	0,16	dL/g
Bulk CH3 / 1000C	55,0	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	1,09	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,45	mL·V/mg
dn/dc	-0,1040	ml / g

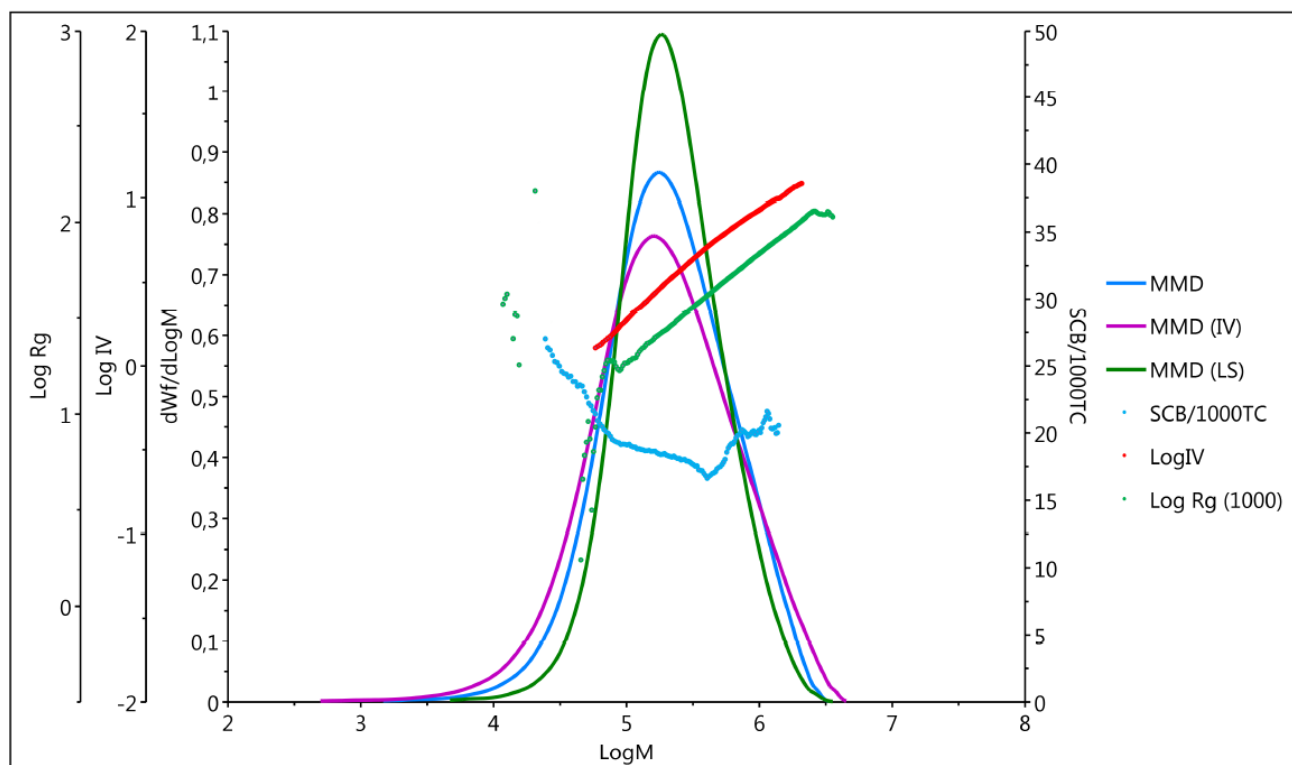
Results (Visco)

Mw UC	5990	g/mol
Mn UC	1697	g/mol
Mz UC	24617	g/mol
IV Bulk	0,14	dL/g

Performance

Mass recovery	98,84	%
Flow Marker	44,48	mL
Calib Flow Marker	44,68	mL

Fig S 90. GPC of PE (Table 1, #5).



Results (Conventional)

Mw	337692	g/mol
Mn	103929	g/mol
Mw / Mn	3,2	
Mz	770556	g/mol
Mp	175753	g/mol
Mv	295083	g/mol
IVmwd	3,76	dL/g
Bulk CH3 / 1000C	20,2	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,88	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	364635	g/mol
Mn UC	73232	g/mol
Mz UC	1014997	g/mol
IV Bulk	3,81	dL/g

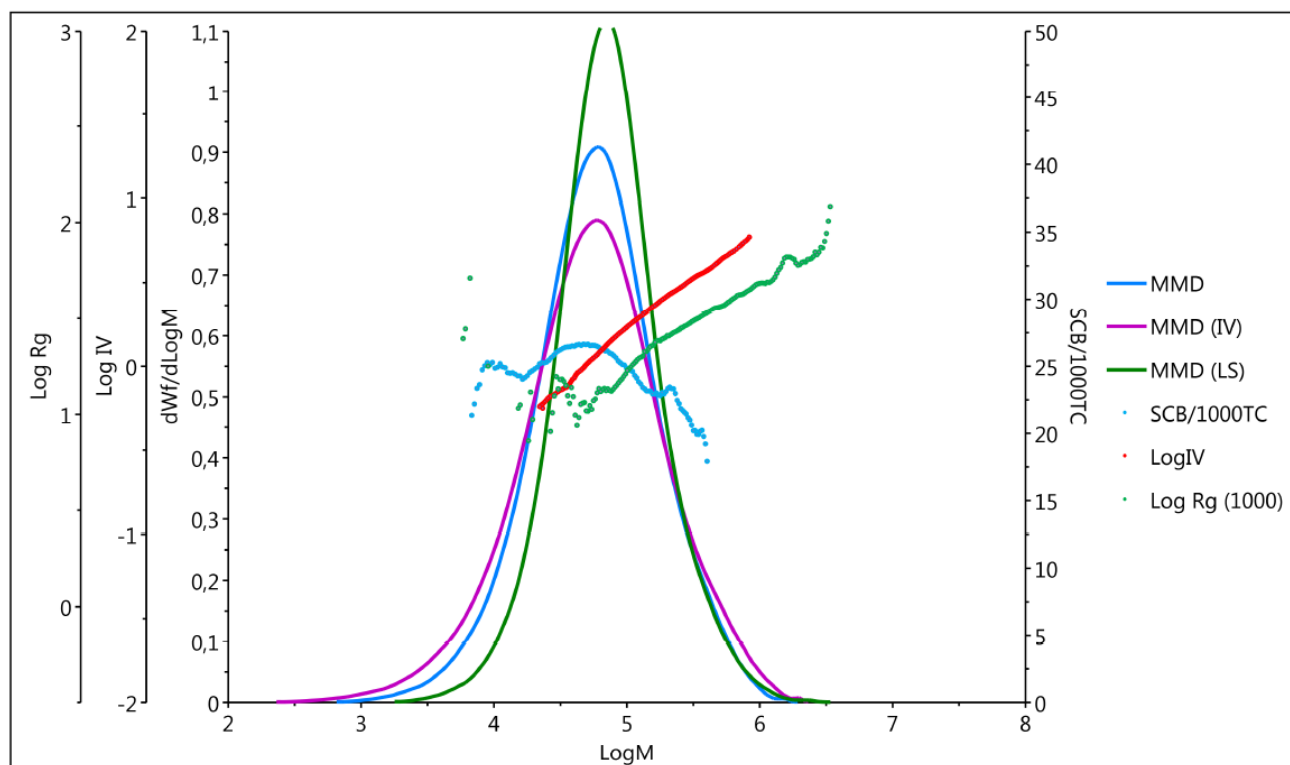
Performance

	0,00	
Mass recovery	99,31	%
Flow Marker	44,73	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	312504	g/mol
Mn Abs	141760	g/mol
Mz Abs	650112	g/mol
Mw / Mn Abs	2	
Rg Slice	37,8	nm

Fig S 91. GPC of PE (Table 1, #6).



Results (Conventional)

Mw	101574	g/mol
Mn	30487	g/mol
Mw / Mn	3,3	
Mz	275000	g/mol
Mp	60790	g/mol
Mv	87416	g/mol
IVmwd	1,55	dL/g
Bulk CH3 / 1000C	23,1	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,68	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	112627	g/mol
Mn UC	21819	g/mol
Mz UC	372661	g/mol
IV Bulk	1,59	dL/g

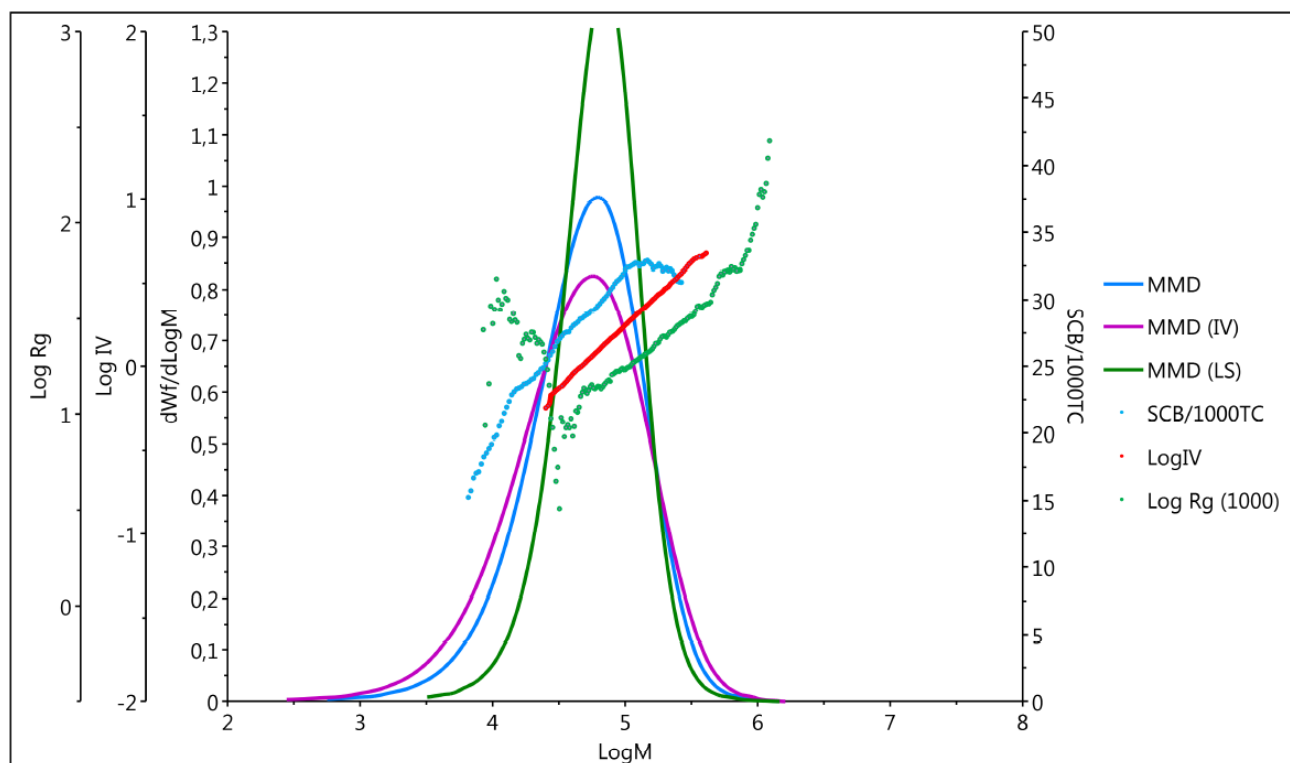
Performance

	0,00	
Mass recovery	98,18	%
Flow Marker	44,55	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	114468	g/mol
Mn Abs	47358	g/mol
Mz Abs	347161	g/mol
Mw / Mn Abs	2	
Rg Slice	19,8	nm

Fig S 92. GPC of PE (Table 1, #7).



Results (Conventional)

Mw	74861	g/mol
Mn	26186	g/mol
Mw / Mn	2,9	
Mz	151829	g/mol
Mp	62155	g/mol
Mv	67202	g/mol
IVmwd	1,28	dL/g
Bulk CH3 / 1000C	29,2	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,70	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,47	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	76169	g/mol
Mn UC	18760	g/mol
Mz UC	182489	g/mol
IV Bulk	1,43	dL/g

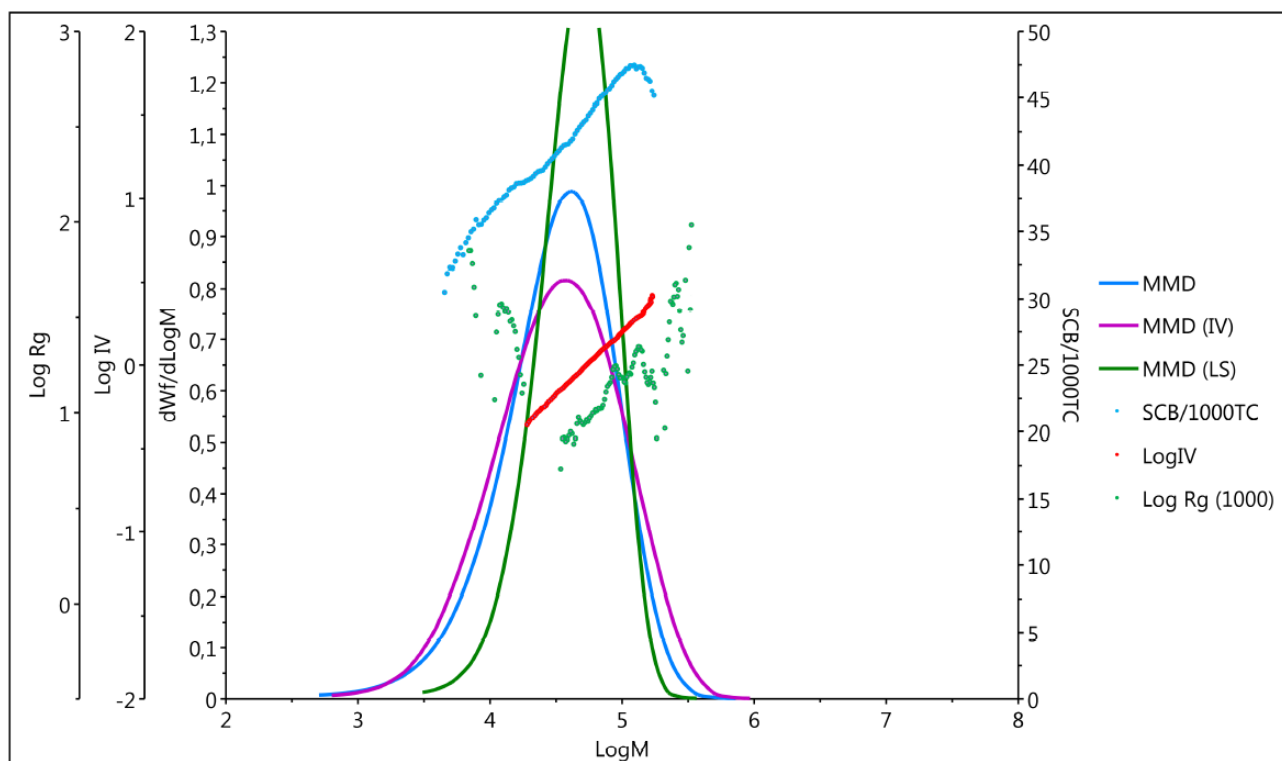
Performance

	0,00	
Mass recovery	99,00	%
Flow Marker	44,49	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	78569	g/mol
Mn Abs	47045	g/mol
Mz Abs	104203	g/mol
Mw / Mn Abs	2	
Rg Slice	17,0	nm

Fig S 93. GPC of PE (Table 1, #8).



Results (Conventional)

Mw	48543	g/mol
Mn	17443	g/mol
Mw / Mn	2,8	
Mz	92439	g/mol
Mp	41188	g/mol
Mv	43834	g/mol
IVmwd	0,94	dL/g
Bulk CH3 / 1000C	42,3	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,73	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,47	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	55132	g/mol
Mn UC	16805	g/mol
Mz UC	126187	g/mol
IV Bulk	0,94	dL/g

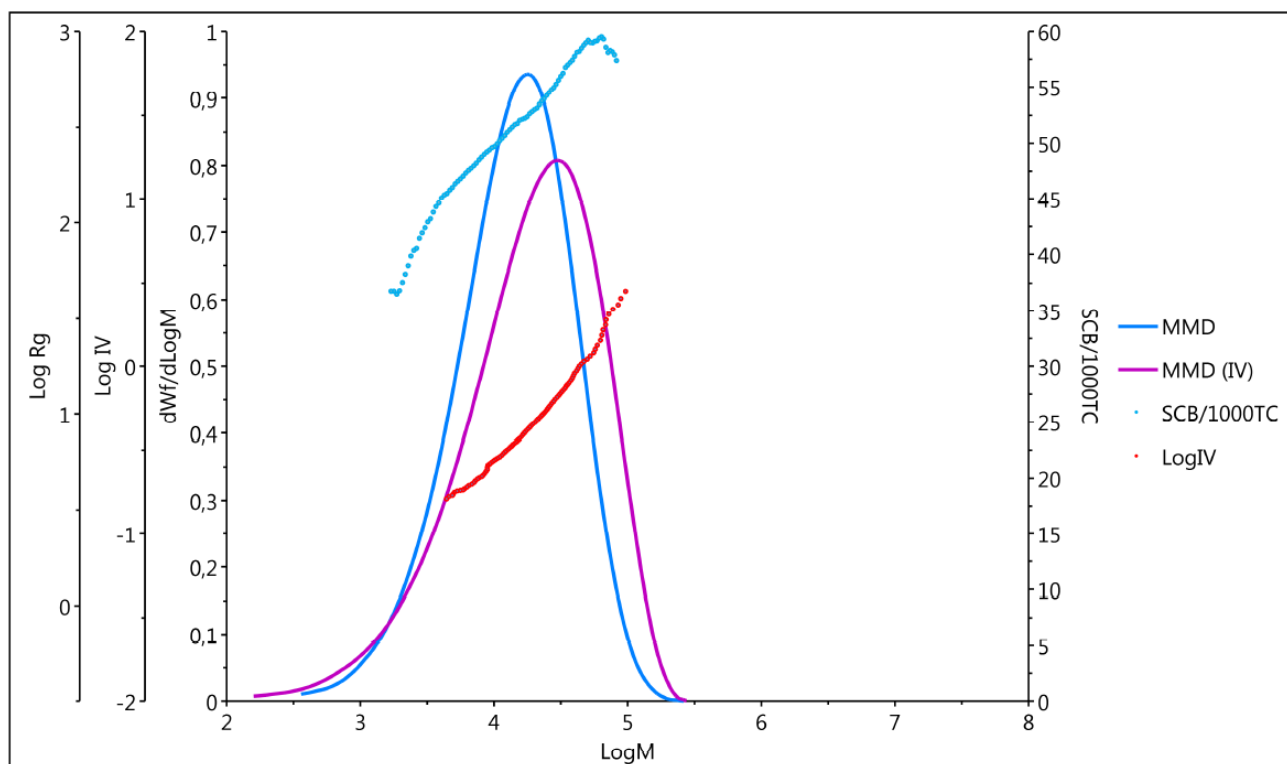
Performance

Mass recovery	0,00	%
Flow Marker	44,49	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	52973	g/mol
Mn Abs	33469	g/mol
Mz Abs	73396	g/mol
Mw / Mn Abs	2	
Rg Slice	10,5	nm

Fig S 94. GPC of PE (Table 1, #9).



Results (Conventional)

Mw	21270	g/mol
Mn	7688	g/mol
Mw / Mn	2,8	
Mz	41715	g/mol
Mp	17821	g/mol
Mv	19079	g/mol
IVmwd	0,52	dL/g
Bulk CH3 / 1000C	55,2	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	1,01	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,33	mL·V/mg
dn/dc	-0,1040	ml / g

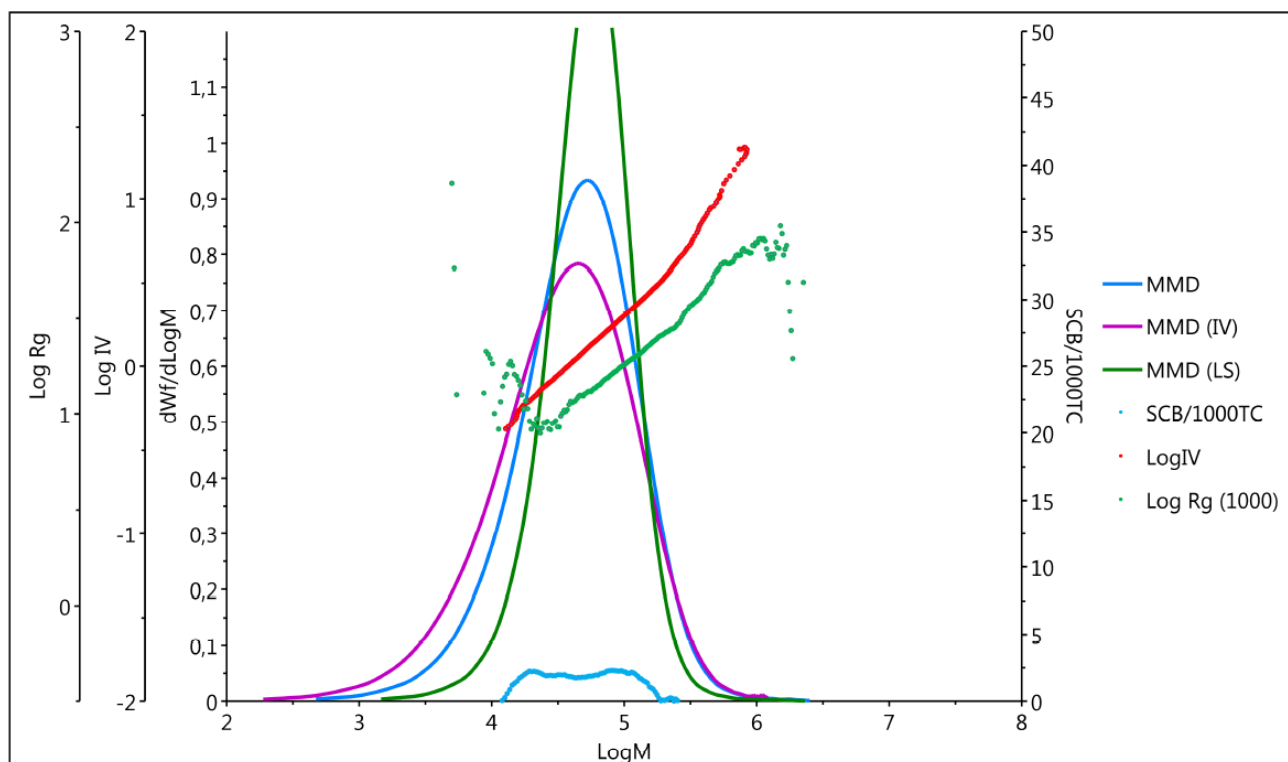
Results (Visco)

Mw UC	31704	g/mol
Mn UC	7157	g/mol
Mz UC	64604	g/mol
IV Bulk	0,40	dL/g

Performance

Mass recovery	0,00	%
Flow Marker	44,47	mL
Calib Flow Marker	44,68	mL

Fig S 95. GPC of PE (Table 1, #10).



Results (Conventional)

Mw	71436	g/mol
Mn	22058	g/mol
Mw / Mn	3,2	
Mz	199226	g/mol
Mp	52701	g/mol
Mv	62525	g/mol
IVmwd	1,22	dL/g
Bulk CH3 / 1000C	2,8	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,99	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,48	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	65022	g/mol
Mn UC	13181	g/mol
Mz UC	180642	g/mol
IV Bulk	1,52	dL/g

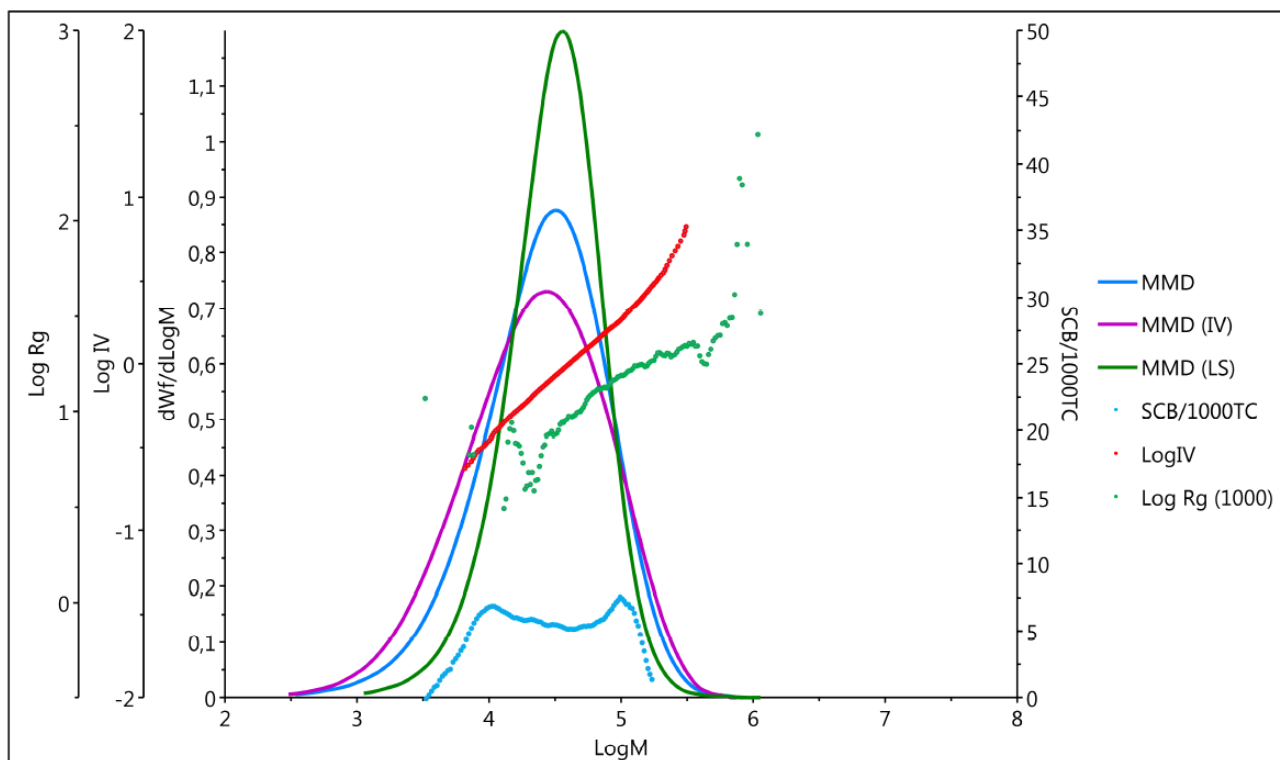
Performance

	0,00	
Mass recovery	99,69	%
Flow Marker	44,53	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	69240	g/mol
Mn Abs	37954	g/mol
Mz Abs	117346	g/mol
Mw / Mn Abs	2	
Rg Slice	16,8	nm

Fig S 96. GPC of PE (Table 1, #11).



Results (Conventional)

Mw	42836	g/mol
Mn	12485	g/mol
Mw / Mn	3,4	
Mz	97054	g/mol
Mp	32122	g/mol
Mv	37657	g/mol
IVmwd	0,84	dL/g
Bulk CH3 / 1000C	7,3	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,99	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,47	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	42427	g/mol
Mn UC	9658	g/mol
Mz UC	108606	g/mol
IV Bulk	0,97	dL/g

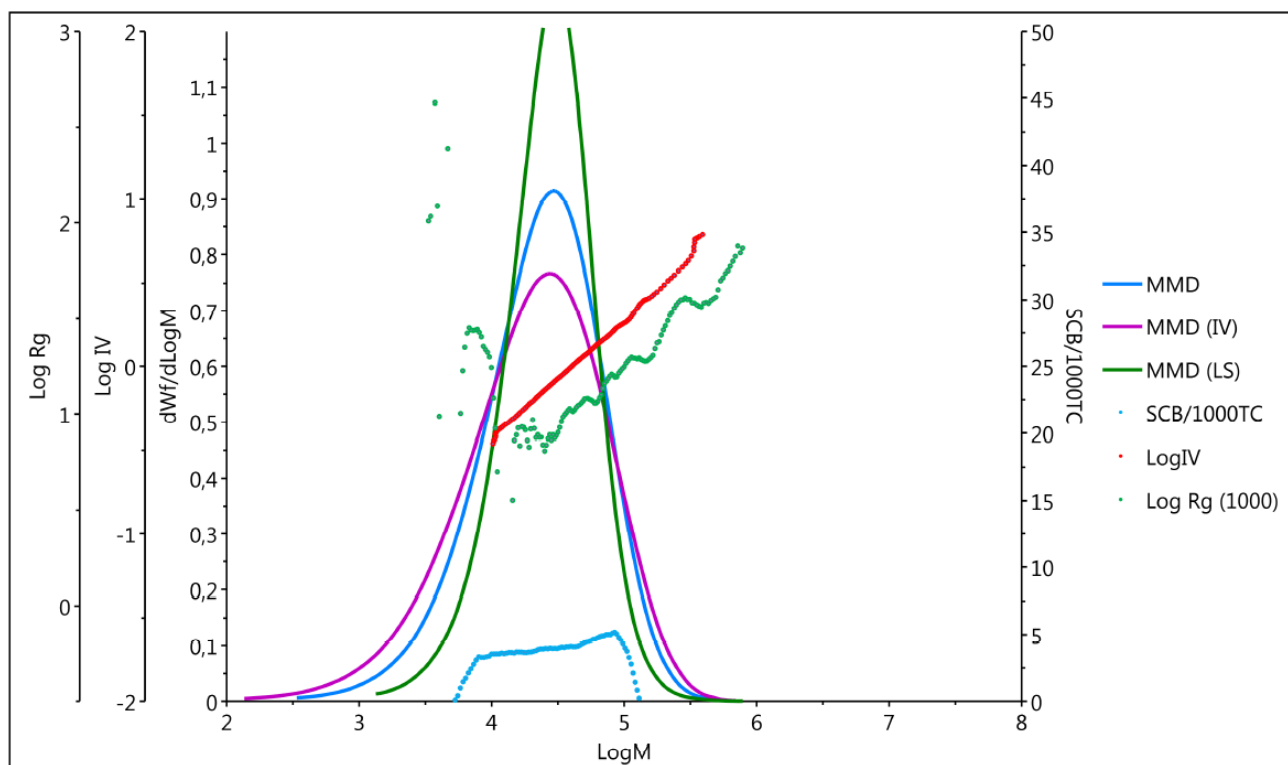
Performance

	0,00	
Mass recovery	98,94	%
Flow Marker	44,53	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	42177	g/mol
Mn Abs	20560	g/mol
Mz Abs	76365	g/mol
Mw / Mn Abs	2	
Rg Slice	11,8	nm

Fig S 97. GPC of PE (Table 1, #12).



Results (Conventional)

Mw	37192	g/mol
Mn	11664	g/mol
Mw / Mn	3,2	
Mz	80710	g/mol
Mp	29381	g/mol
Mv	32955	g/mol
IVmwd	0,77	dL/g
Bulk CH3 / 1000C	4,8	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	1,04	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	38236	g/mol
Mn UC	7615	g/mol
Mz UC	98085	g/mol
IV Bulk	0,87	dL/g

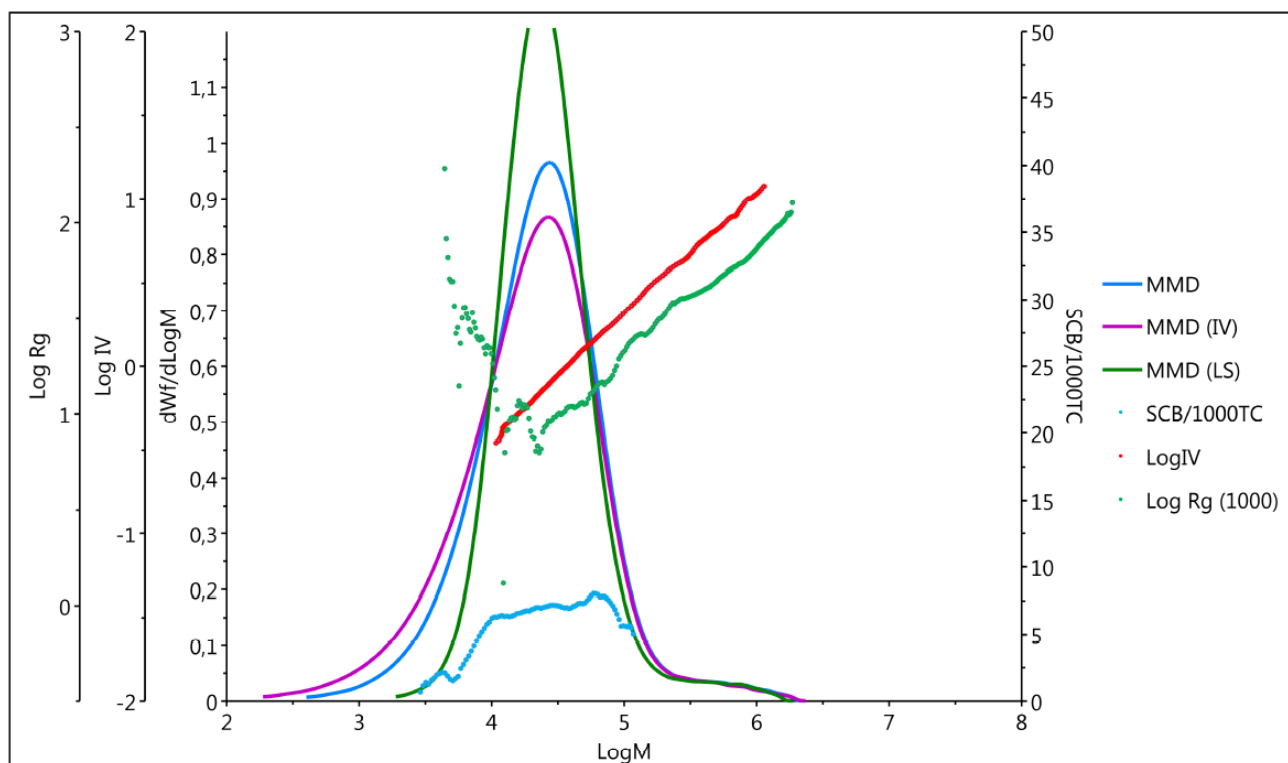
Performance

	0,00	
Mass recovery	99,11	%
Flow Marker	44,52	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	35885	g/mol
Mn Abs	18466	g/mol
Mz Abs	67637	g/mol
Mw / Mn Abs	2	
Rg Slice	11,2	nm

Fig S 98. GPC of PE (Table 1, #13).



Results (Conventional)

Mw	48149	g/mol
Mn	11982	g/mol
Mw / Mn	4,0	
Mz	336177	g/mol
Mp	27265	g/mol
Mv	37995	g/mol
IVmwd	0,85	dL/g
Bulk CH3 / 1000C	8,4	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,97	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	46154	g/mol
Mn UC	7855	g/mol
Mz UC	343802	g/mol
IV Bulk	1,00	dL/g

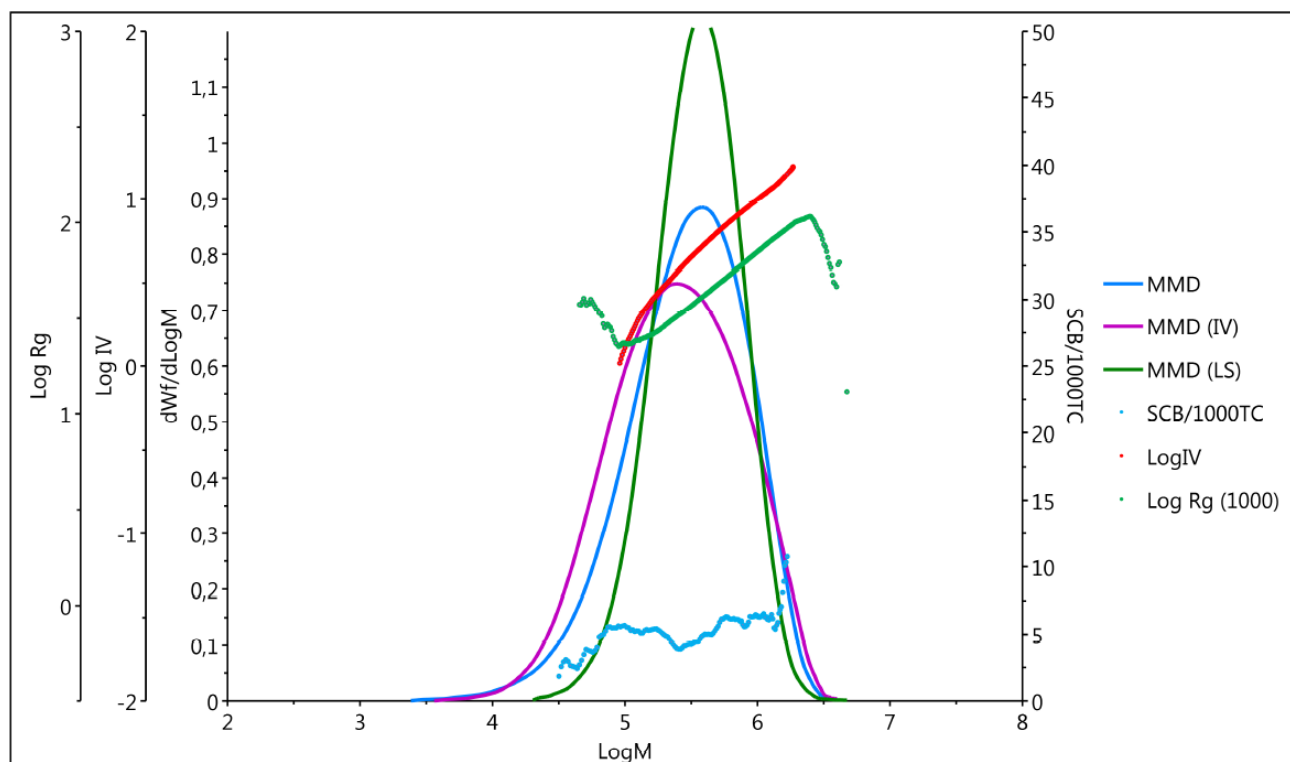
Performance

	0,00	
Mass recovery	98,57	%
Flow Marker	44,53	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	45034	g/mol
Mn Abs	19623	g/mol
Mz Abs	283096	g/mol
Mw / Mn Abs	2	
Rg Slice	10,7	nm

Fig S 99. GPC of PE (Table 1, #14).



Results (Conventional)

Mw	450732	g/mol
Mn	148616	g/mol
Mw / Mn	3,0	
Mz	851327	g/mol
Mp	382191	g/mol
Mv	404604	g/mol
IVmwd	4,72	dL/g
Bulk CH3 / 1000C	5,2	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,71	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,49	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	422792	g/mol
Mn UC	127940	g/mol
Mz UC	925726	g/mol
IV Bulk	5,35	dL/g

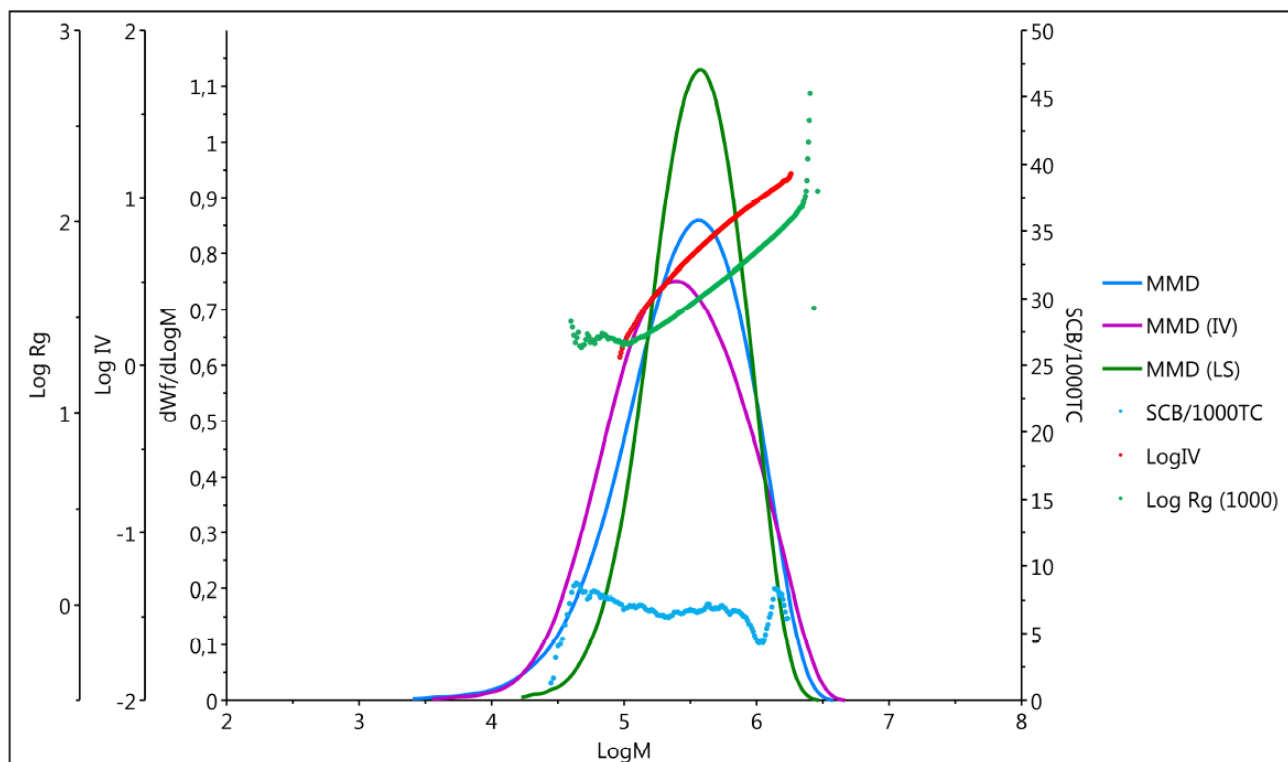
Performance

	0,00	
Mass recovery	99,94	%
Flow Marker	44,55	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	448992	g/mol
Mn Abs	261890	g/mol
Mz Abs	687172	g/mol
Mw / Mn Abs	2	
Rg Slice	48,6	nm

Fig S 100. GPC of PE (Table 1, #15).



Results (Conventional)

Mw	446733	g/mol
Mn	138416	g/mol
Mw / Mn	3,2	
Mz	860268	g/mol
Mp	364977	g/mol
Mv	399128	g/mol
IVmwd	4,68	dL/g
Bulk CH3 / 1000C	5,8	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,69	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,49	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	433204	g/mol
Mn UC	127410	g/mol
Mz UC	985337	g/mol
IV Bulk	5,12	dL/g

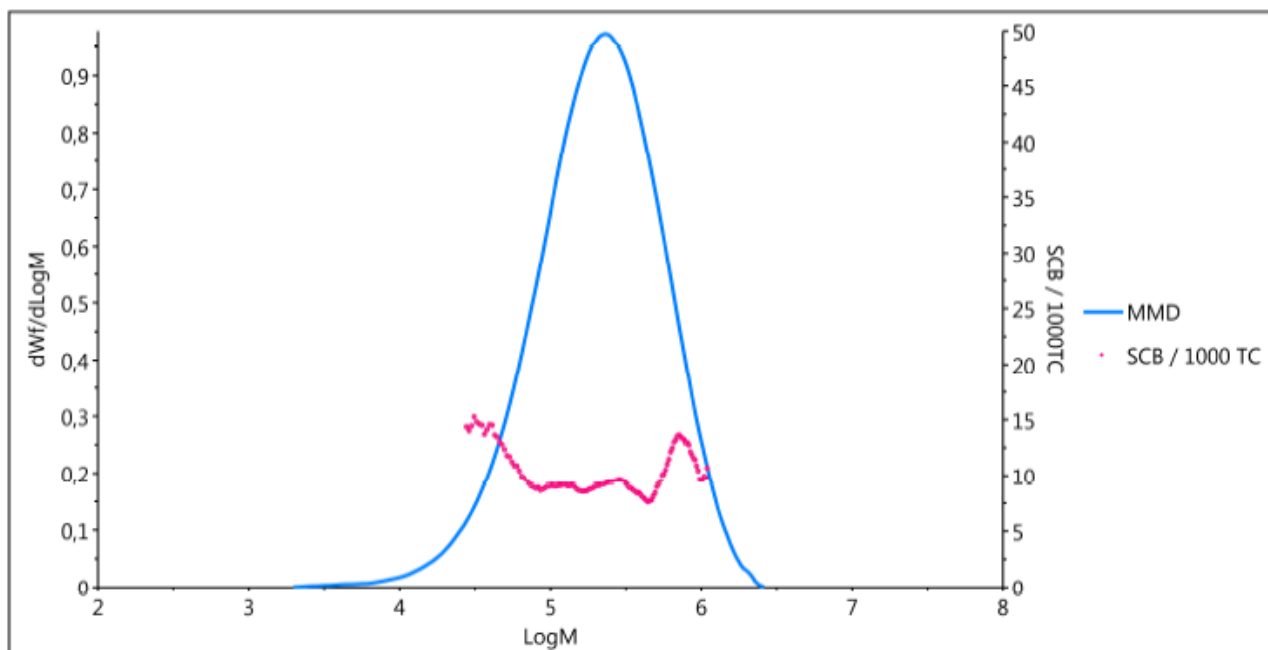
Performance

	0,00	
Mass recovery	99,38	%
Flow Marker	44,54	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	444173	g/mol
Mn Abs	240149	g/mol
Mz Abs	701184	g/mol
Mw / Mn Abs	2	
Rg Slice	49,9	nm

Fig S 101. GPC of PE (Table 1, #16).



Results

Mw 307238 g/mol
Mn 117453 g/mol
Mw / Mn 2,62
Mz 585972 g/mol
Mp 230518 g/mol
Mv 277134 g/mol
IVmwd 3,5888 dL/g
Bulk CH3 / 1000C 10,200

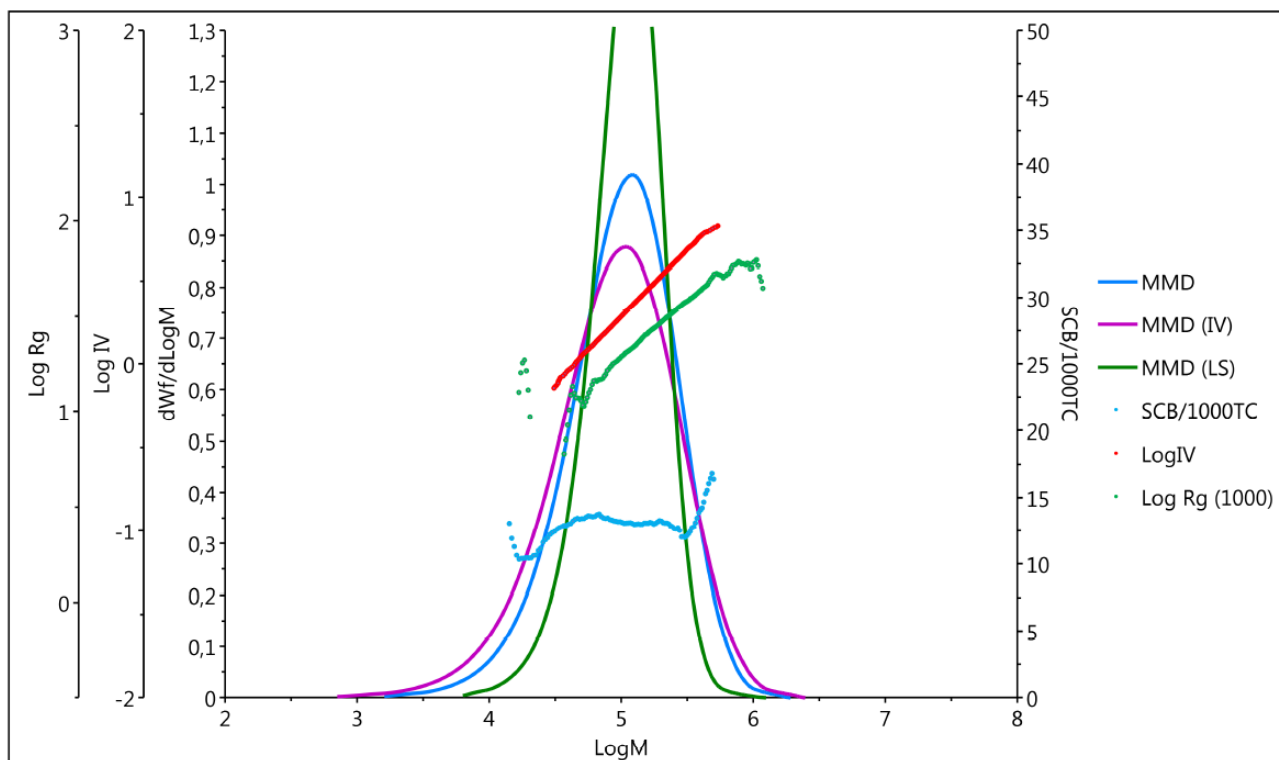
Performance

Flow Marker 44,84 mL
Mass recovery 99 %

Calibrations

Calib Flow Marker 44,82 mL
Calib Mass constant 0,46 mL·V/mg
Q-Factor -0,3649

Fig S 102. GPC of PE (Table 1, #17).



Results (Conventional)

Mw	145934	g/mol
Mn	57909	g/mol
Mw / Mn	2,5	
Mz	277185	g/mol
Mp	121101	g/mol
Mv	132174	g/mol
IVmwd	2,10	dL/g
Bulk CH3 / 1000C	13,5	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,81	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,44	mL·V/mg
dn/dc	-0,1040	ml / g

Results (Visco)

Mw UC	146190	g/mol
Mn UC	42038	g/mol
Mz UC	336690	g/mol
IV Bulk	2,30	dL/g

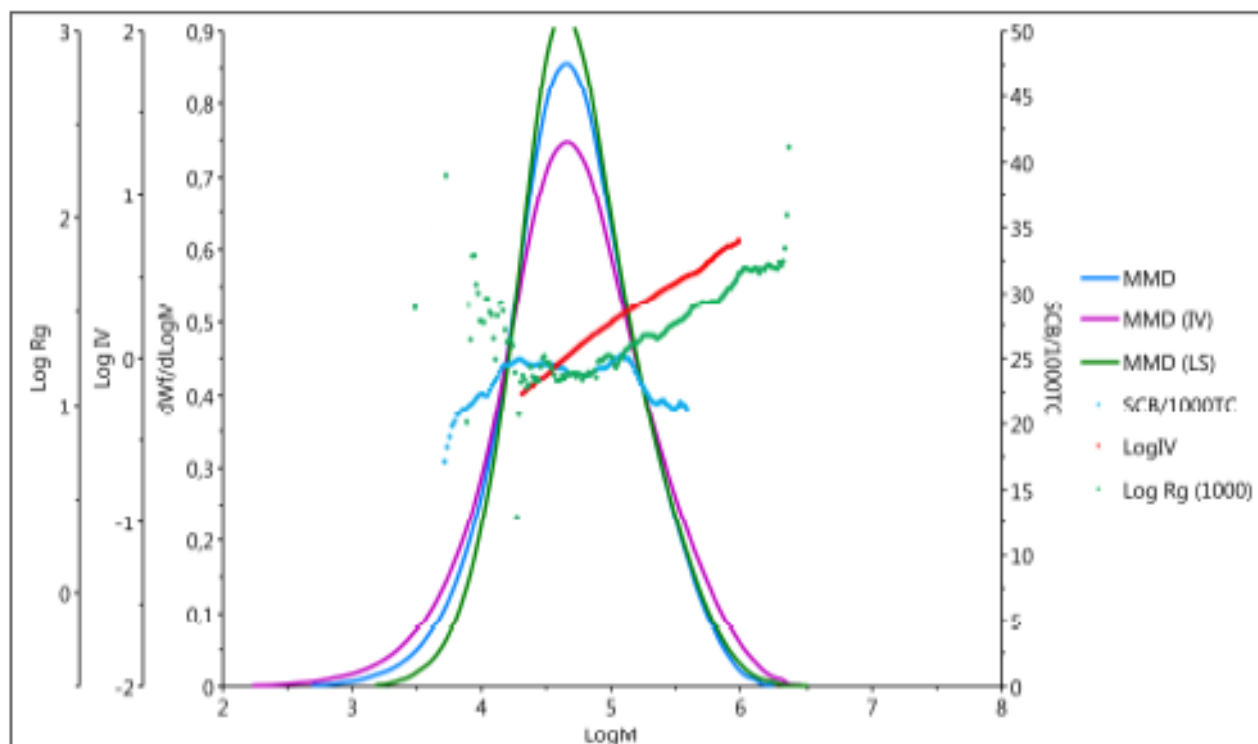
Performance

	0,00	
Mass recovery	99,67	%
Flow Marker	44,52	mL
Calib Flow Marker	44,68	mL

Results (LS)

Mw Abs	129152	g/mol
Mn Abs	84460	g/mol
Mz Abs	178408	g/mol
Mw / Mn Abs	2	
Rg Slice	25,4	nm

Fig S 103. GPC of PE (Table 1, #18).



Results (Conventional)

Mw	92473	g/mol
Mn	24645	g/mol
Mw / Mn	3.8	
Mz	271064	g/mol
Mp	45338	g/mol
Mv	78289	g/mol
IV/mvd	1,44	dL/g
Bulk CH3 / 1000C	24,9	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,97	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g
Q-Factor	-0,3649	

Results (Visco)

Mw UC	113139	g/mol
Mn UC	18410	g/mol
Mz UC	438332	g/mol
IV Bulk	1,36	dL/g

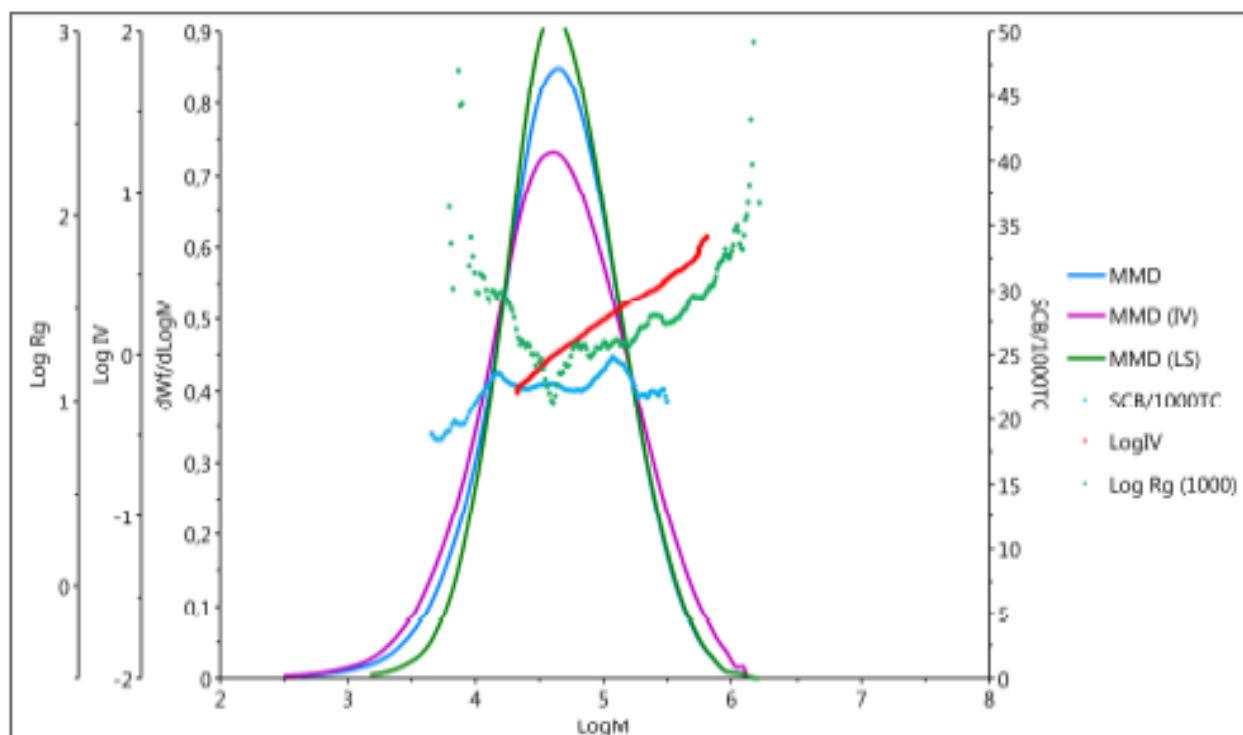
Performance

Mass recovery	98,83	%
Flow Marker	44,85	mL
Calib Flow Marker	44,82	mL

Results (LS)

Mw Abs	98929	g/mol
Mn Abs	32465	g/mol
Mz Abs	306256	g/mol
Mw / Mn Abs	3	
Rg Slice	23,6	nm

Fig S 104. GPC of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #8, 0.02 M).



Results (Conventional)

Mw	77553	g/mol
Mn	21077	g/mol
Mw / Mn	3.7	
Mz	207578	g/mol
Mp	44245	g/mol
Mv	66691	g/mol
IV/mvd	1,28	dL/g
Bulk CH3 / 1000C	24,2	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0.99	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g
Q-Factor	-0,3649	

Results (Visco)

Mw UC	90262	g/mol
Mn UC	18022	g/mol
Mz UC	285147	g/mol
IV Bulk	1,24	dL/g

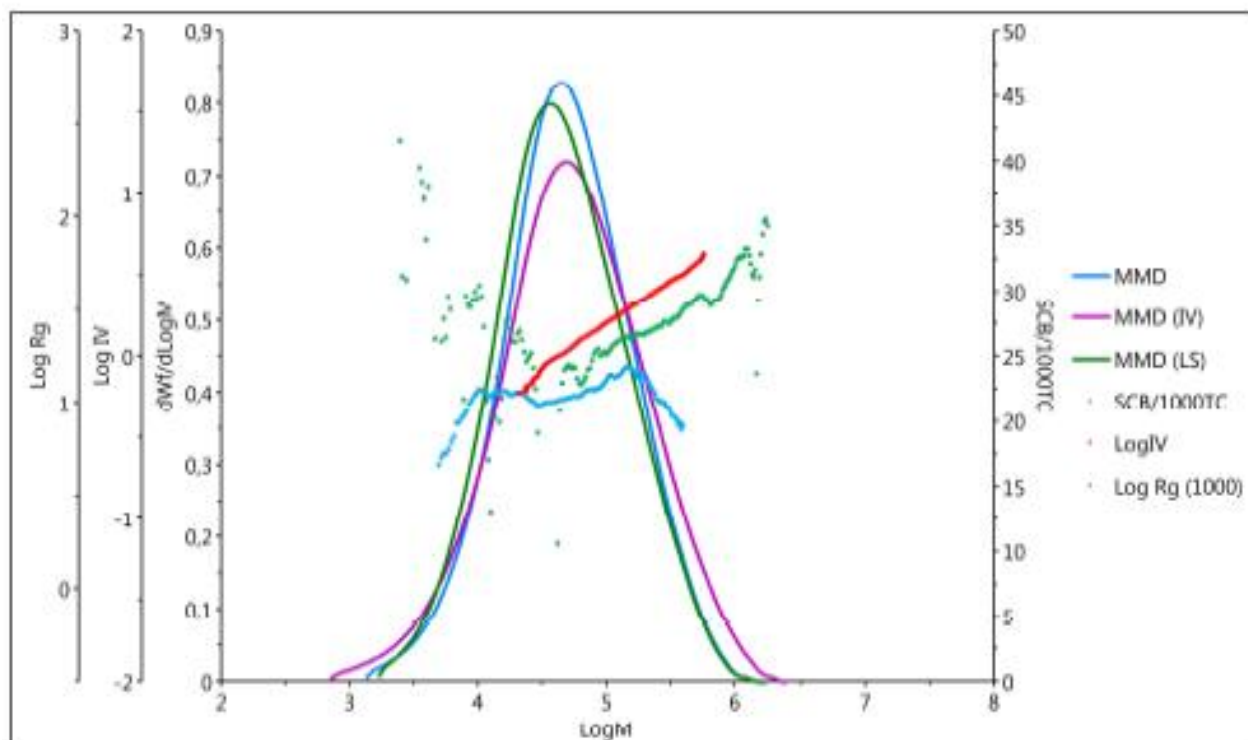
Performance

Mass recovery	0,00	%
Flow Marker	44,86	mL
Calib Flow Marker	44,82	mL

Results (LS)

Mw Abs	83676	g/mol
Mn Abs	28972	g/mol
Mz Abs	236110	g/mol
Mw / Mn Abs	3	
Rg Slice	21,0	nm

Fig S 105. GPC of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #9, 0.04 M).



Results (Conventional)

Mw	89688	g/mol
Mn	25518	g/mol
Mw / Mn	3.5	
Mz	241561	g/mol
Mp	44924	g/mol
Mv	76741	g/mol
IV _{bulk}	1.41	dL/g
Bulk CH ₃ / 1000C	22.6	

Analysis Conditions

Flow Rate	1.00	ml / min
Columns Temp	150	°C
Concentration	1.00	mg / ml
Injection Volume	200	μL
Calib Mass constant	0.42	mL·V/mg
dn/dc	-0.1040	ml / g
Q-Factor	-0.3649	

Results (Visco)

Mw UC	117298	g/mol
Mn UC	21664	g/mol
Mz UC	393860	g/mol
IV Bulk	1.26	dL/g

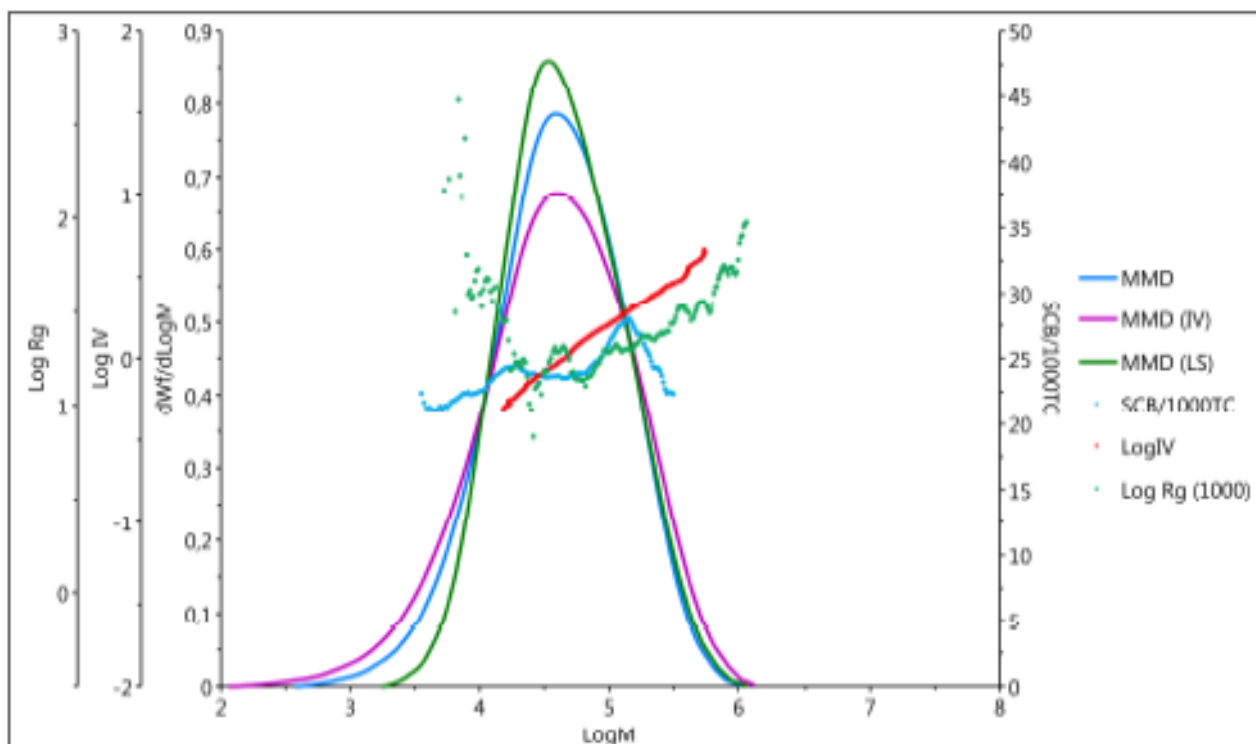
Performance

Mass recovery	96.01	%
Flow Marker	44.92	mL
Calib Flow Marker	44.82	mL

Results (LS)

Mw Abs	86717	g/mol
Mn Abs	23490	g/mol
Mz Abs	252024	g/mol
Mw / Mn Abs	4	
Rg Slice	22.8	nm

Fig S 106. GPC of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #10, 0.06 M).



Results (Conventional)

Mw	71978	g/mol
Mn	18803	g/mol
Mw / Mn	3.8	
Mz	181751	g/mol
Mp	39067	g/mol
Mv	61876	g/mol
IV/mvd	1,21	dL/g
Bulk CH3 / 1000C	20,2	

Analysis Conditions

Flow Rate	1,00	ml / min
Columns Temp	150	°C
Concentration	0,96	mg / ml
Injection Volume	200	uL
Calib Mass constant	0,46	mL·V/mg
dn/dc	-0,1040	ml / g
Q-Factor	-0,3649	

Results (Visco)

Mw UC	82700	g/mol
Mn UC	13094	g/mol
Mz UC	249822	g/mol
IV Bulk	1,24	dL/g

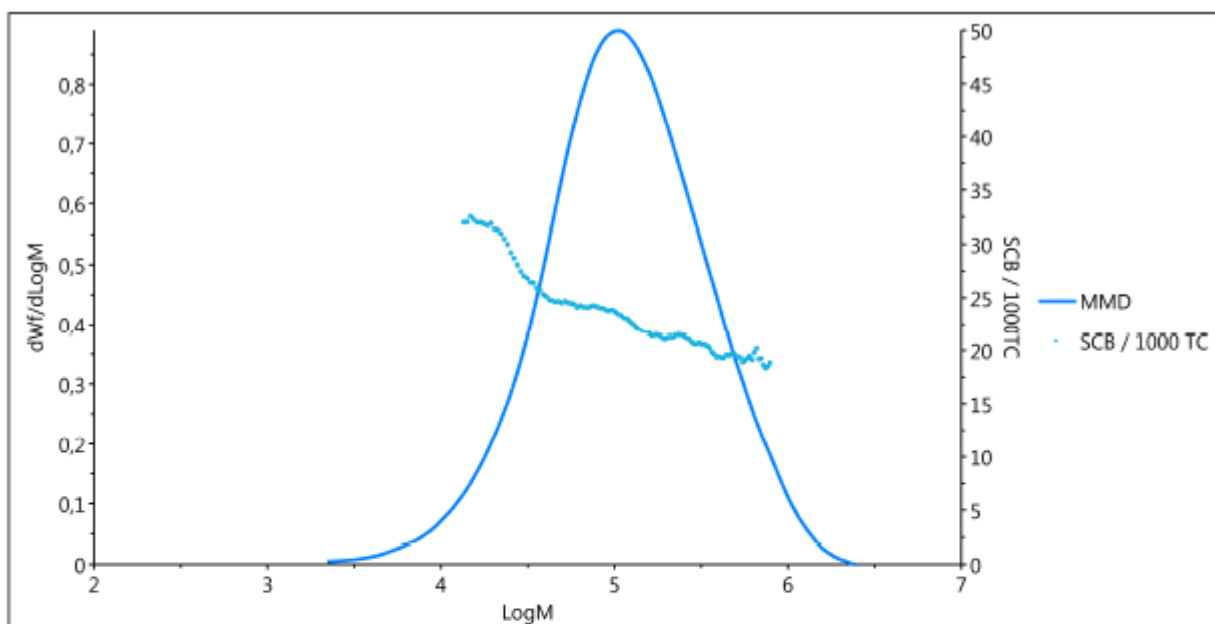
Performance

Mass recovery	96,23	%
Flow Marker	44,85	mL
Calib Flow Marker	44,82	mL

Results (LS)

Mw Abs	78358	g/mol
Mn Abs	26962	g/mol
Mz Abs	208209	g/mol
Mw / Mn Abs	3	
Rg Slice	19,7	nm

Fig S 107. GPC of ethene/11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #11, 0.06 M).



Results

Mw 189307 g/mol
Mn 61863 g/mol
Mw / Mn 3,06
Mz 451178 g/mol
Mp 104798 g/mol
Mv 163024 g/mol
IVmwd 0,6144 dL/g
Bulk CH3 / 1000C 23,861

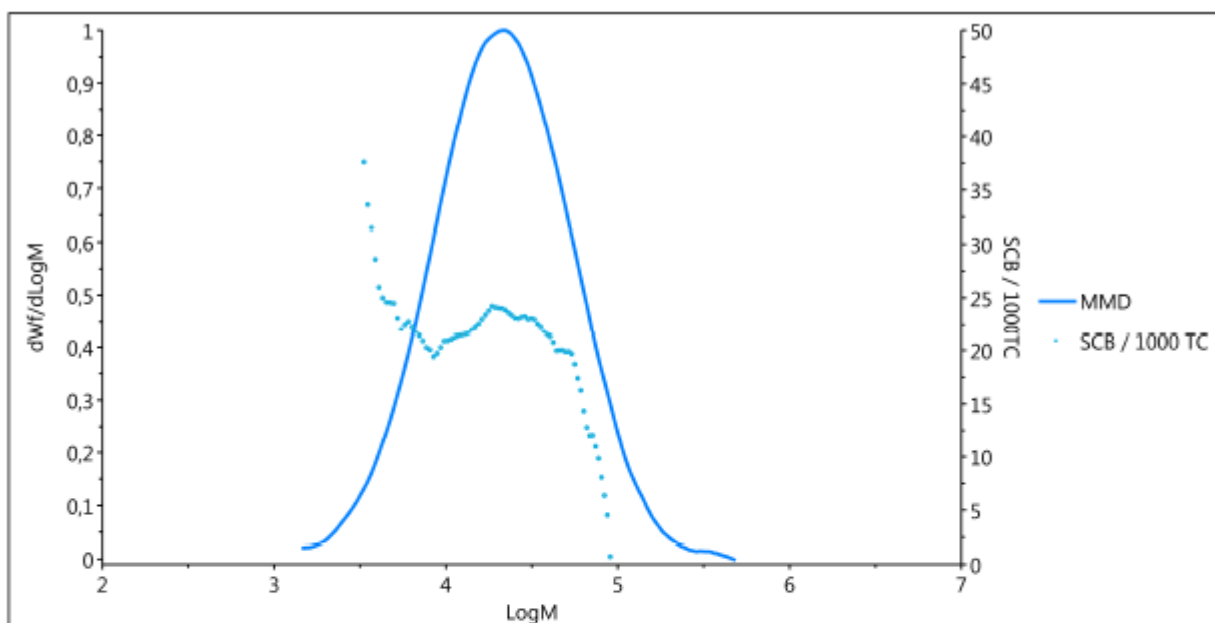
Performance

Flow Marker 44,82 mL
Mass recovery 97 %

Calibrations

Calib Flow Marker 44,82 mL
Calib Mass constant 0,32 mL·V/mg

Fig S 108 GPC of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, #1, 0.05 M).



Results

Mw	31679	g/mol
Mn	14149	g/mol
Mw / Mn	2,24	
Mz	68374	g/mol
Mp	21497	g/mol
Mv	28108	g/mol
IVmwd	0,1705	dL/g
Bulk CH3 / 1000C	18,509	

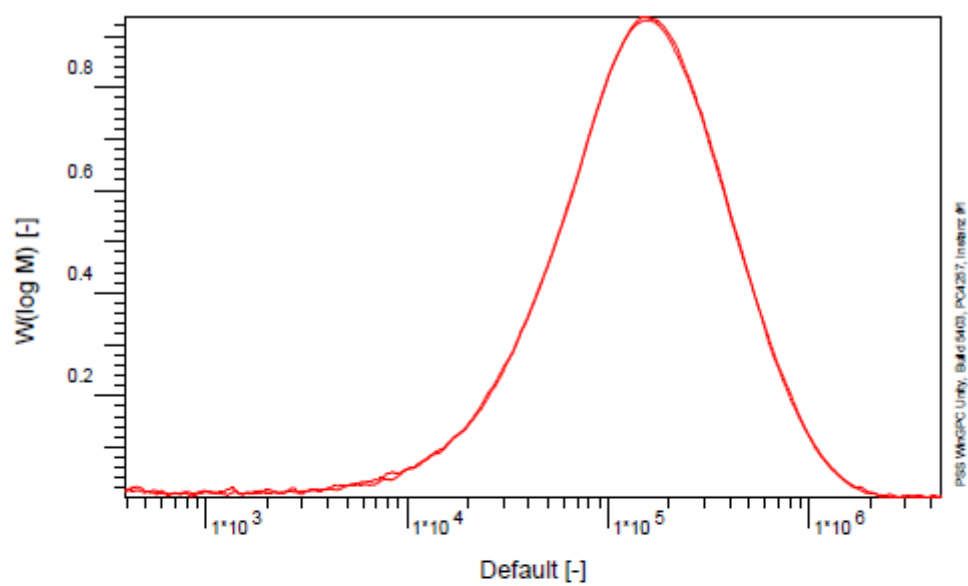
Performance

Flow Marker	44,82	mL
Mass recovery	42	%

Calibrations

Calib Flow Marker	44,82	mL
Calib Mass constant	0,21	mL·V/mg

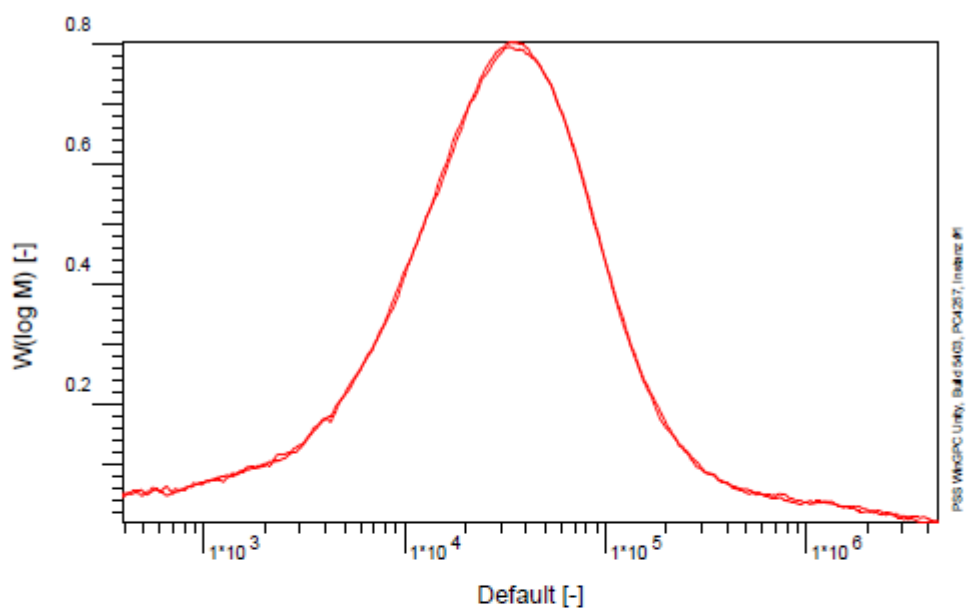
Fig S 109. GPC of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, #2, 0.1 M).



Kurve 1 : 730
Kurve 2 : 730

	IR-Detektor	IR-Detektor	
$\overline{M}_n$:	3.9819e4	3.5807e4	g/mol
$\overline{M}_w$:	2.2092e5	2.2093e5	g/mol
$\overline{M}_z$:	5.0474e5	5.3242e5	g/mol
$\overline{M}_v$:	0.000000	0.000000	g/mol
$\overline{D}$:	5.5780e0	6.2047e0	
[η] :	0.000000	0.000000	ml/g
Vp :	1.9067e1	1.9020e1	ml
Mp :	1.5486e5	1.6191e5	g/mol
FI :	1.790e-1	1.577e-1	ml ^{1/2} V
< 392	0.00	0.00	
w% :	100.00	100.00	
> 4537190	0.00	0.00	

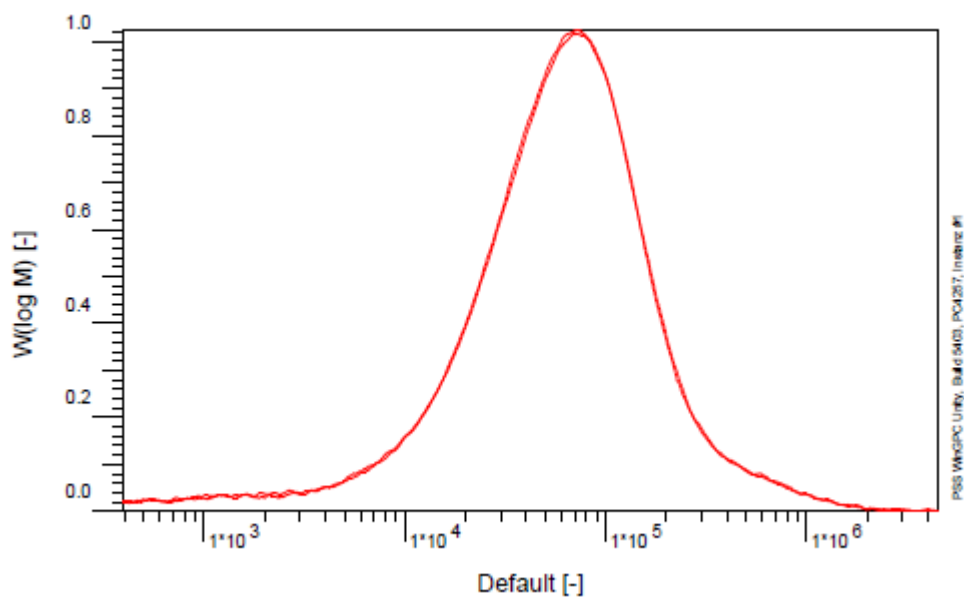
Fig S 110. GPC of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #4, 0.02 M).



Kurve 1 : 735
Kurve 2 : 735

	<u>IR-Detektor</u>	<u>IR-Detektor</u>	
<u>Mn</u> :	9.0936e3	9.0764e3	g/mol
<u>Mw</u> :	8.1120e4	8.5697e4	g/mol
<u>Mz</u> :	7.5099e5	8.4355e5	g/mol
<u>Mv</u> :	0.000000	0.000000	g/mol
<u>D</u> :	8.9206e0	9.4417e0	
[<u>n</u>] :	0.000000	0.000000	ml/g
<u>Vp</u> :	2.0664e1	2.0700e1	ml
<u>Mp</u> :	3.4089e4	3.2961e4	g/mol
<u>FI</u> :	1.491e-1	1.327e-1	ml ² /V
< 392	0.00	0.00	
w% :	100.00	100.00	
> 4537190	0.00	0.00	

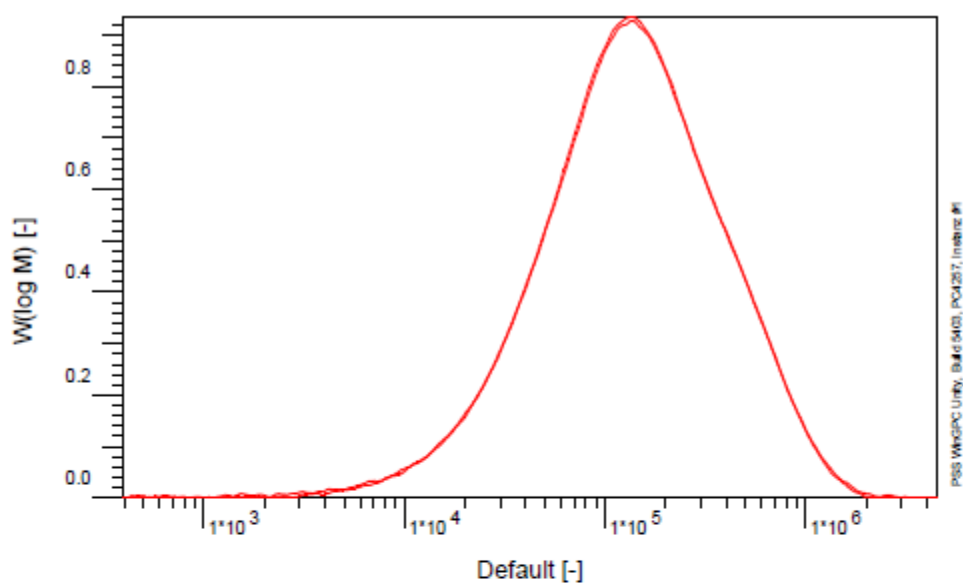
Fig S 111. GPC of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #5, 0.06 M).



Kurve 1 : 734
Kurve 2 : 734

	IR-Detektor	IR-Detektor	
<u>Mn</u> :	1.9427e4	1.8681e4	g/mol
<u>Mw</u> :	1.0261e5	1.0400e5	g/mol
<u>Mz</u> :	3.8218e5	4.0756e5	g/mol
<u>Mv</u> :	0.000000	0.000000	g/mol
<u>D</u> :	5.2819e0	5.5670e0	
[<u>n</u>] :	0.000000	0.000000	ml/g
<u>Vp</u> :	1.9858e1	1.9861e1	ml
<u>Mp</u> :	7.2663e4	7.2445e4	g/mol
<u>FI</u> :	1.762e-1	1.640e-1	ml*V
< 392	0.00	0.00	
w% :	100.00	100.00	
> 4537190	0.00	0.00	

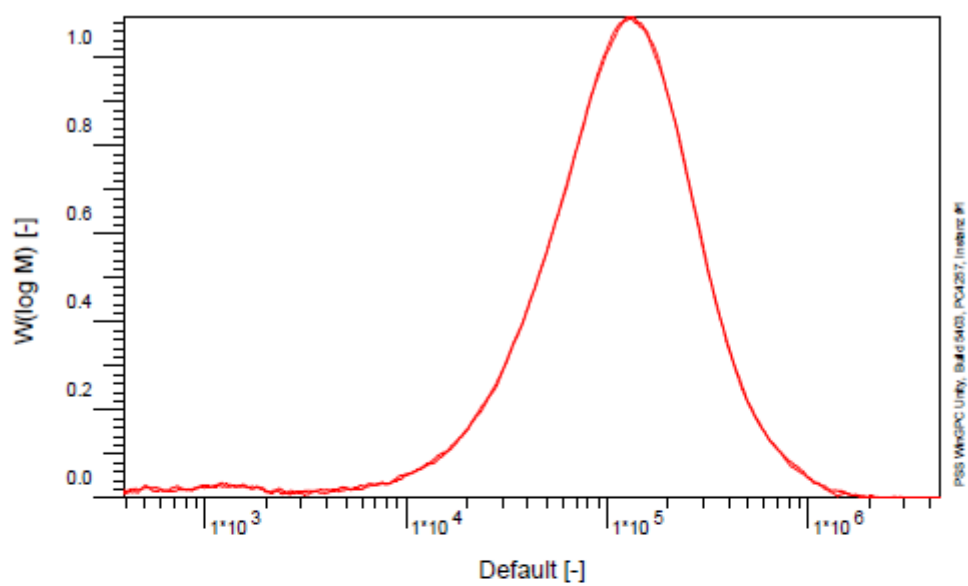
Fig S 112. GPC of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #6, 0.1 M).



Kurve 1 : 717
 Kurve 2 : 717

	IR-Detektor	IR-Detektor	
$\overline{M}_n$:	7.1616e4	5.7640e4	g/mol
$\overline{M}_w$:	2.1191e5	2.1523e5	g/mol
$\overline{M}_z$:	4.5525e5	4.9003e5	g/mol
$\overline{M}_v$:	0.000000	0.000000	g/mol
$\overline{D}$:	2.9590e0	3.7340e0	
$[\eta]$:	0.000000	0.000000	ml/g
V_p :	1.9197e1	1.9183e1	ml
M_p :	1.3666e5	1.3842e5	g/mol
FI :	2.651e-1	2.334e-1	ml ¹ /V
< 392	0.00	0.00	
w% :	100.00	100.00	
> 4537190	0.00	0.00	

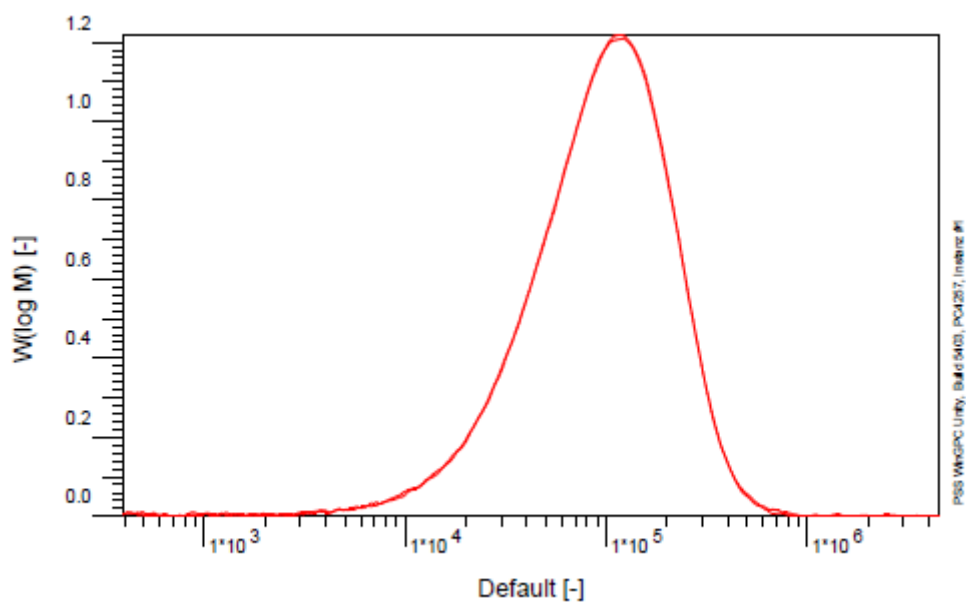
Fig S 113. GPC of ethene/5-Hexene-1-ol copolymer synthesized at 1 atm (Table 3, Entry 7, 0.06 M).



Kurve 1 : 721
 Kurve 2 : 721

	IR-Detektor	IR-Detektor	
$\overline{Mn}$:	2.7769e4	3.0128e4	g/mol
$\overline{Mw}$:	1.6242e5	1.6105e5	g/mol
$\overline{Mz}$:	3.4762e5	3.2749e5	g/mol
$\overline{Mv}$:	0.000000	0.000000	g/mol
D :	5.8489e0	5.3456e0	
[η] :	0.000000	0.000000	ml/g
Vp :	1.9237e1	1.9240e1	ml
Mp :	1.3144e5	1.3102e5	g/mol
FI :	1.384e-1	1.193e-1	ml ¹ /V
< 392	0.00	0.00	
w% :	100.00	100.00	
> 4537190	0.00	0.00	

Fig S 114. GPC of ethene/5-Hexene-1-ol copolymer synthesized at 1 atm (Table 2, # 8, 0.08 M).



Kurve 1 : 722
 Kurve 2 : 722

	<u>IR-Detektor</u>	<u>IR-Detektor</u>	
<u>Mn</u> :	4.7019e4	4.5108e4	g/mol
<u>Mw</u> :	1.1889e5	1.2151e5	g/mol
<u>Mz</u> :	1.8528e5	2.3133e5	g/mol
<u>Mv</u> :	0.000000	0.000000	g/mol
<u>D</u> :	2.5288e0	2.6939e0	
[<u>n</u>] :	0.000000	0.000000	ml/g
<u>Vp</u> :	1.9344e1	1.9331e1	ml
<u>Mp</u> :	1.1863e5	1.2016e5	g/mol
<u>FI</u> :	1.819e-1	1.591e-1	ml*V
< 392	0.00	0.00	
w% :	100.00	100.00	
> 4537190	0.00	0.00	

Fig S 115. GPC of ethene/5-Hexene-1-ol copolymer synthesized at 1 atm (Table 2, #8, 0.1 M).

Differential scanning calorimetry

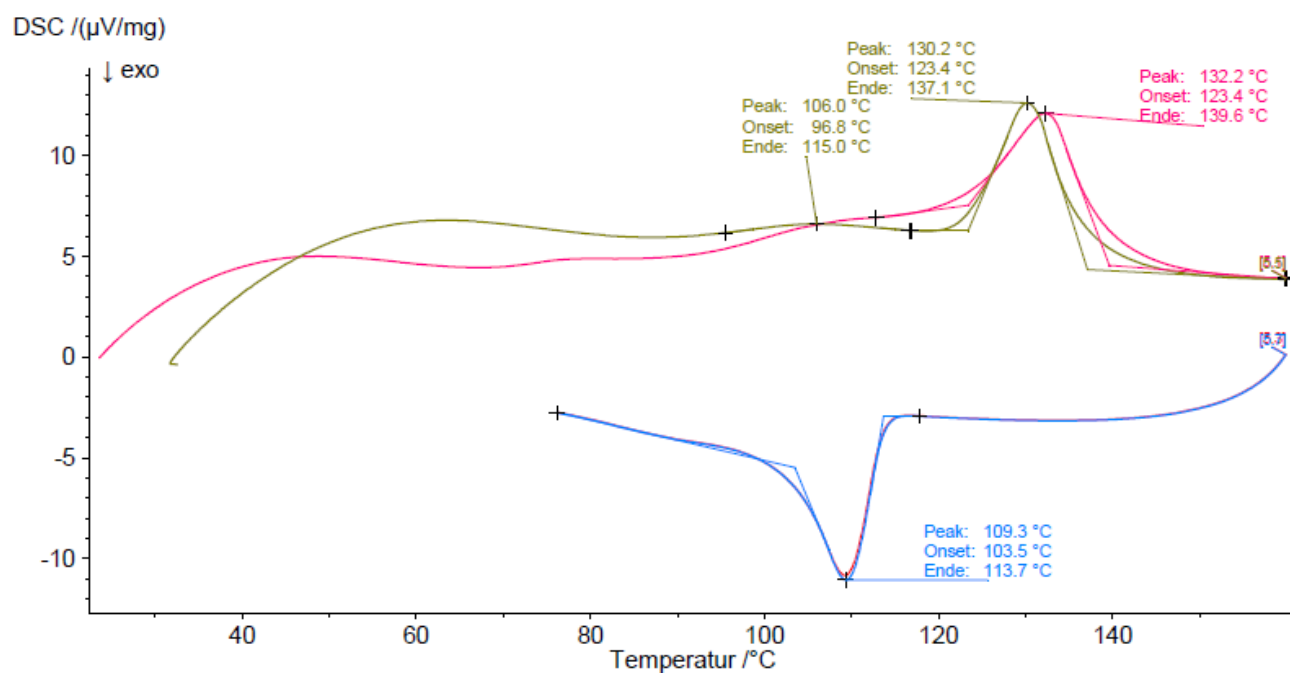


Fig S 116. DSC of PE (Table 1, #1).

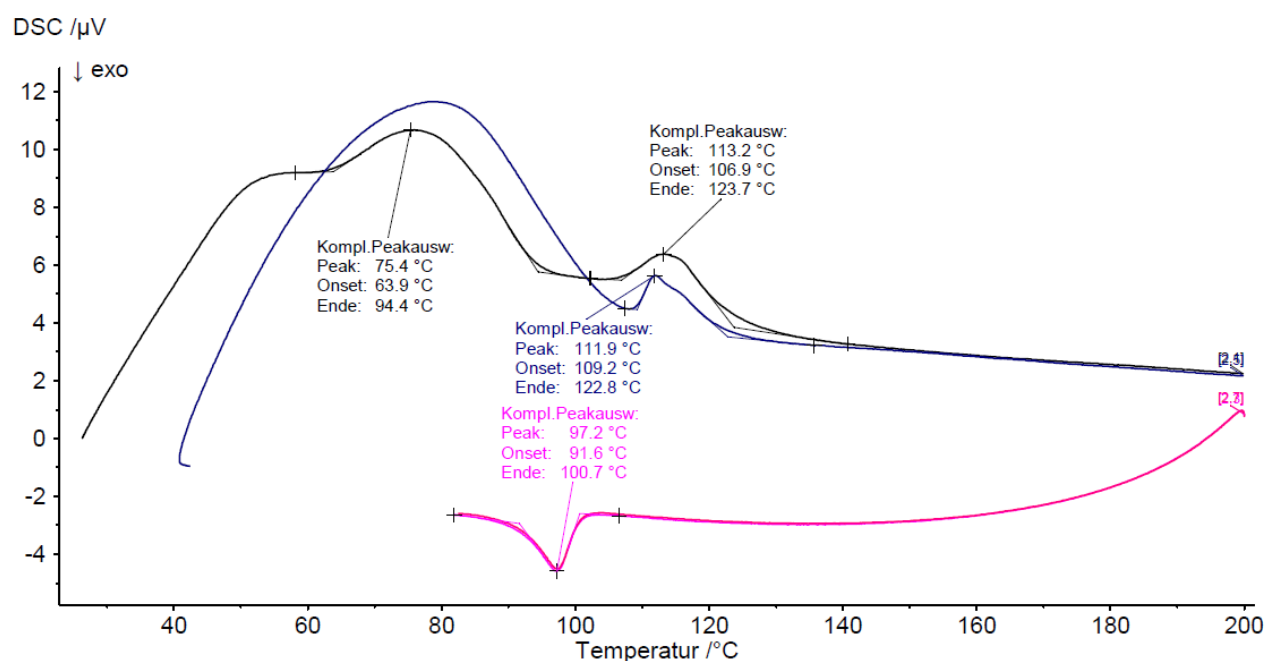


Fig S 117. DSC of PE (Table 1, #2).

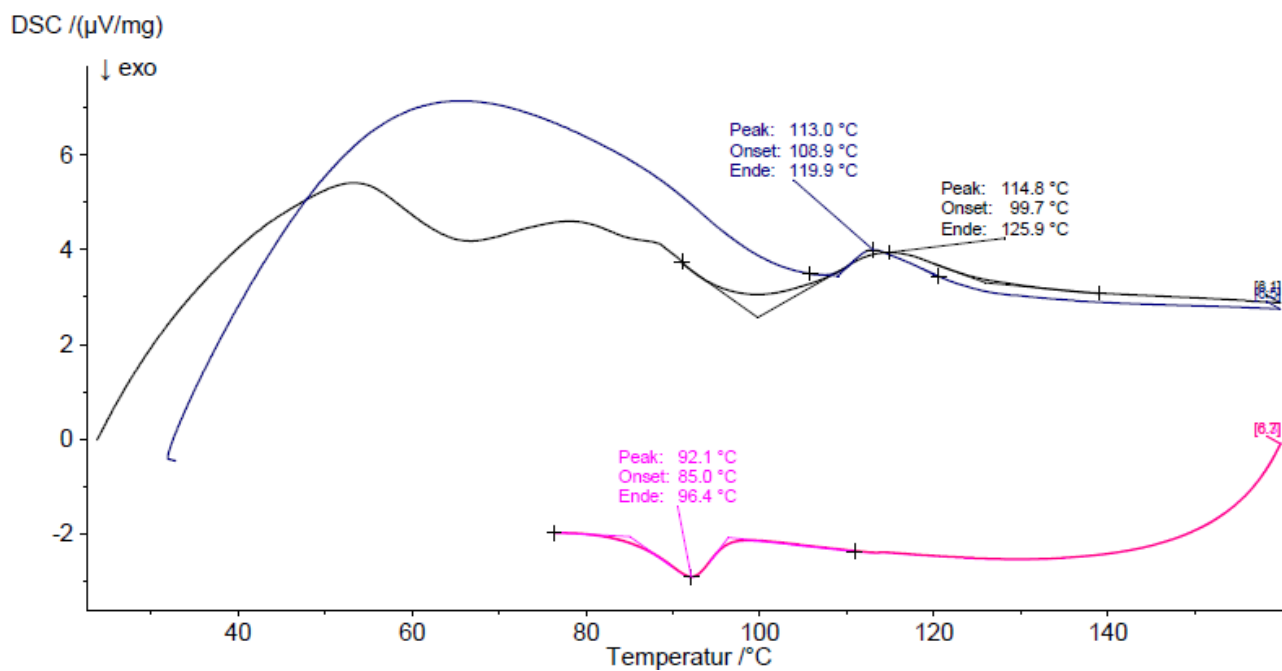


Fig S 118. DSC of PE (Table 1, #3).

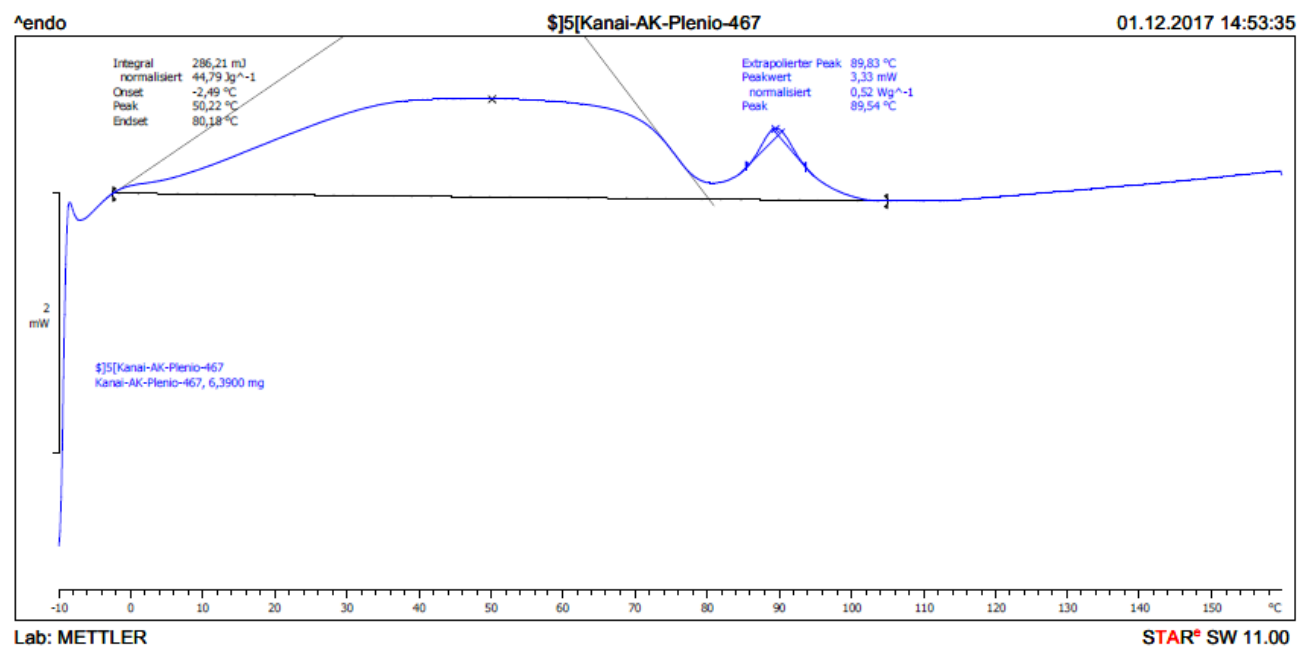


Fig S 119 DSC of PE (Table 1, #4).

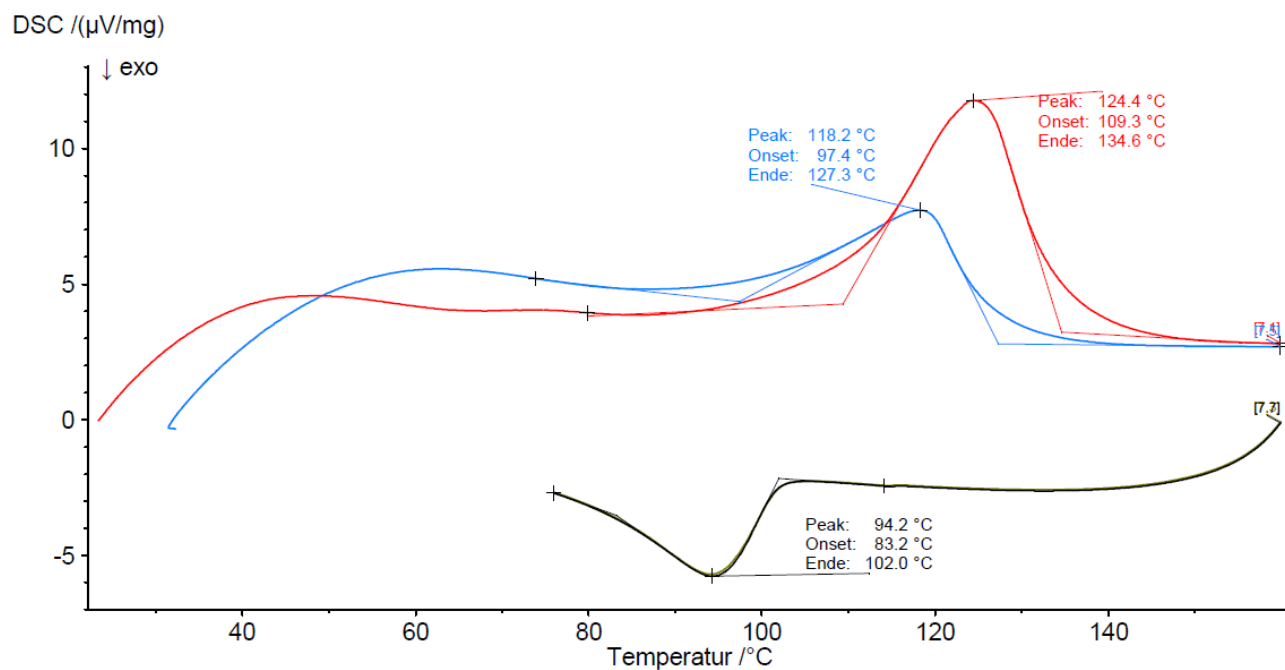


Fig S 120. DSC of PE (Table 1, #6).

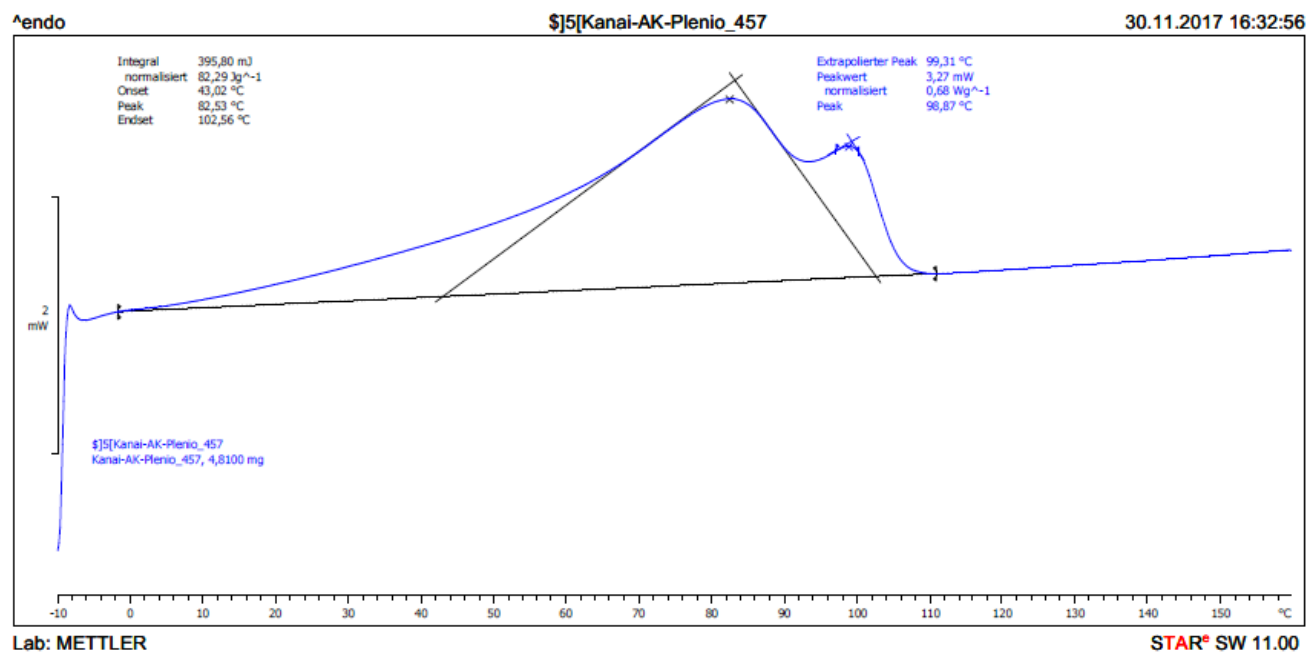


Fig S 121. DSC of PE (Table 1, #7).

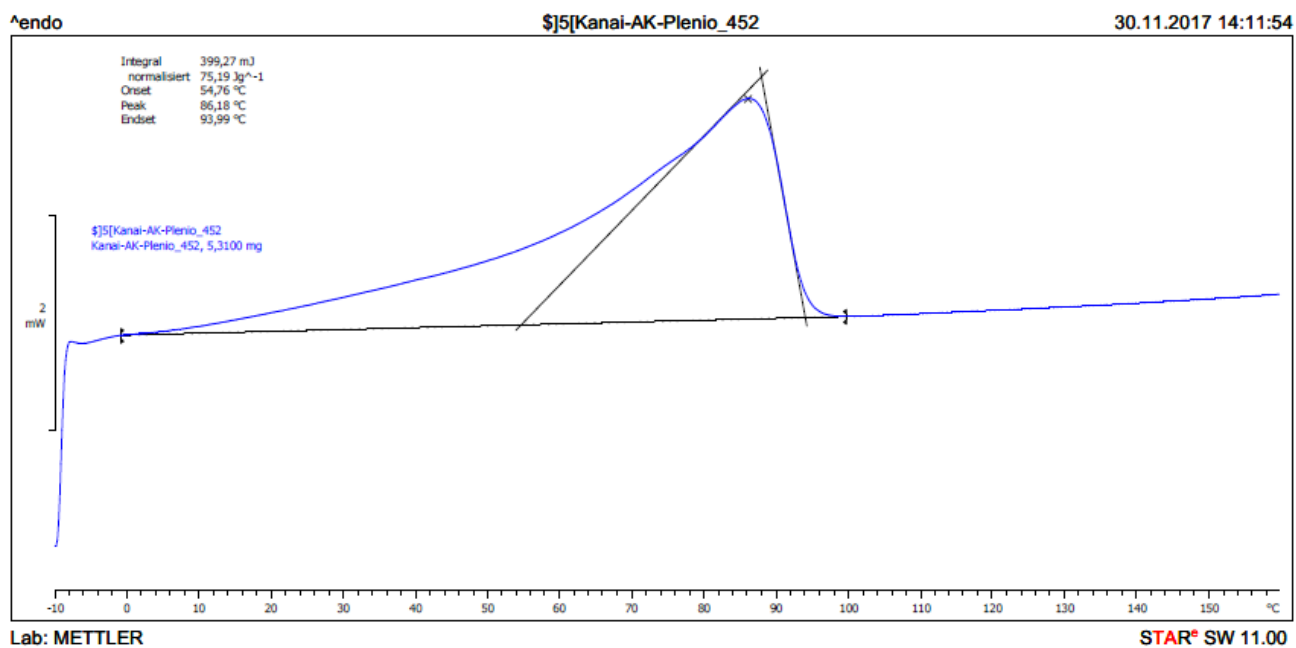


Fig S 122. DSC of PE (Table 1, #8).

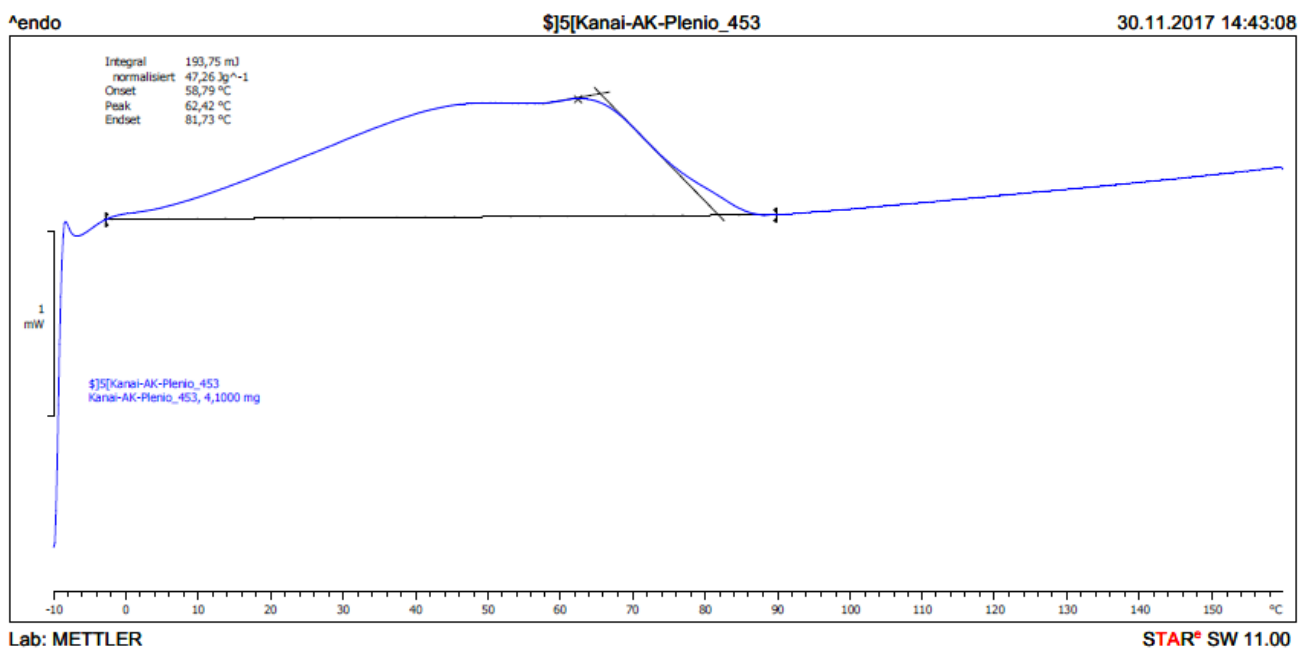


Fig S 123. DSC of PE (Table 1, #9).

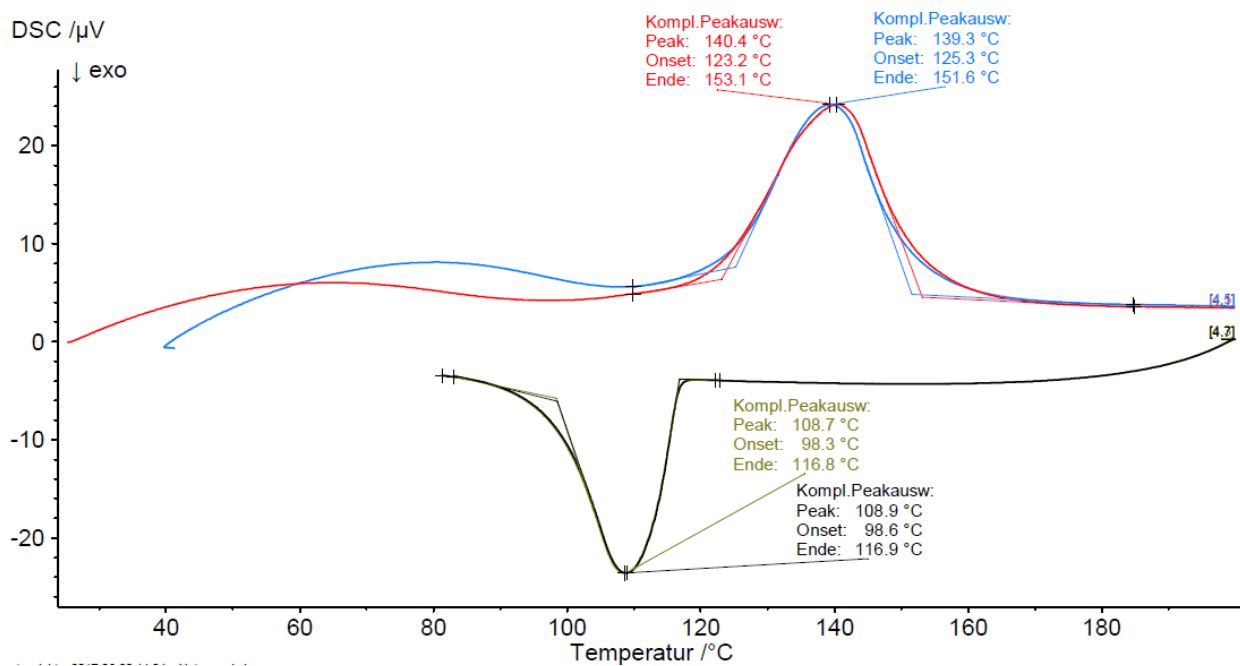


Fig S 124. DSC of PE (Table 1, #11).

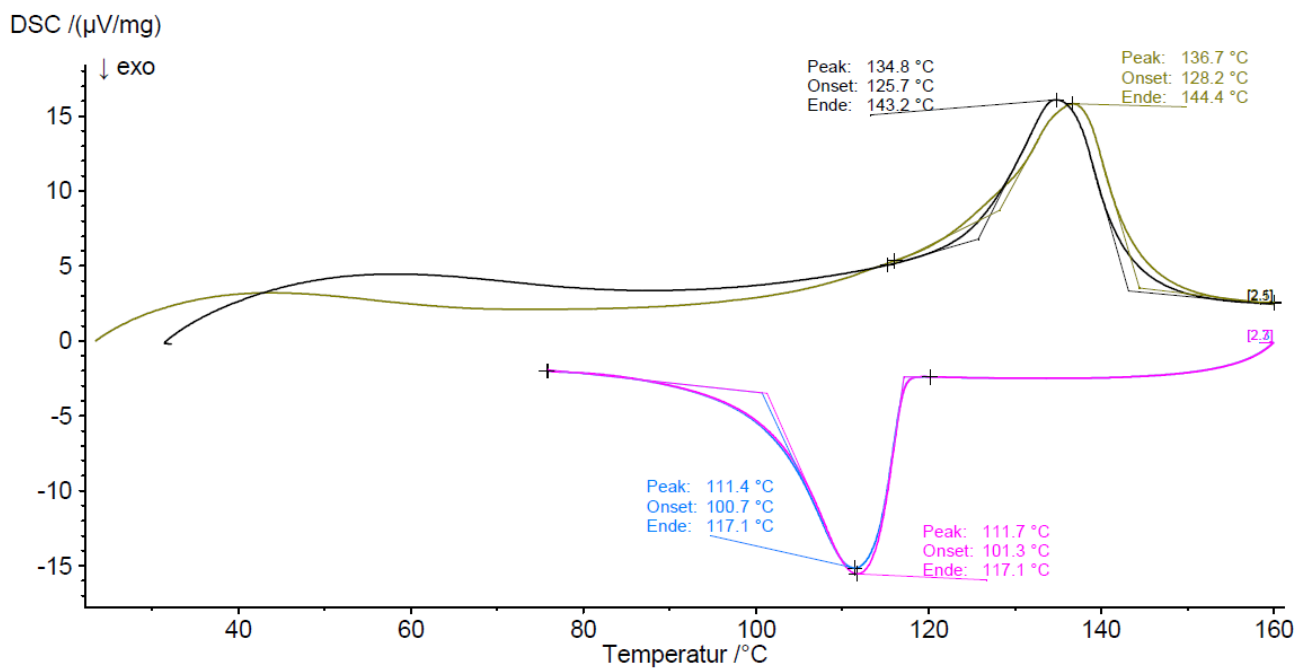


Fig S 125. DSC of PE (Table 1, #12).

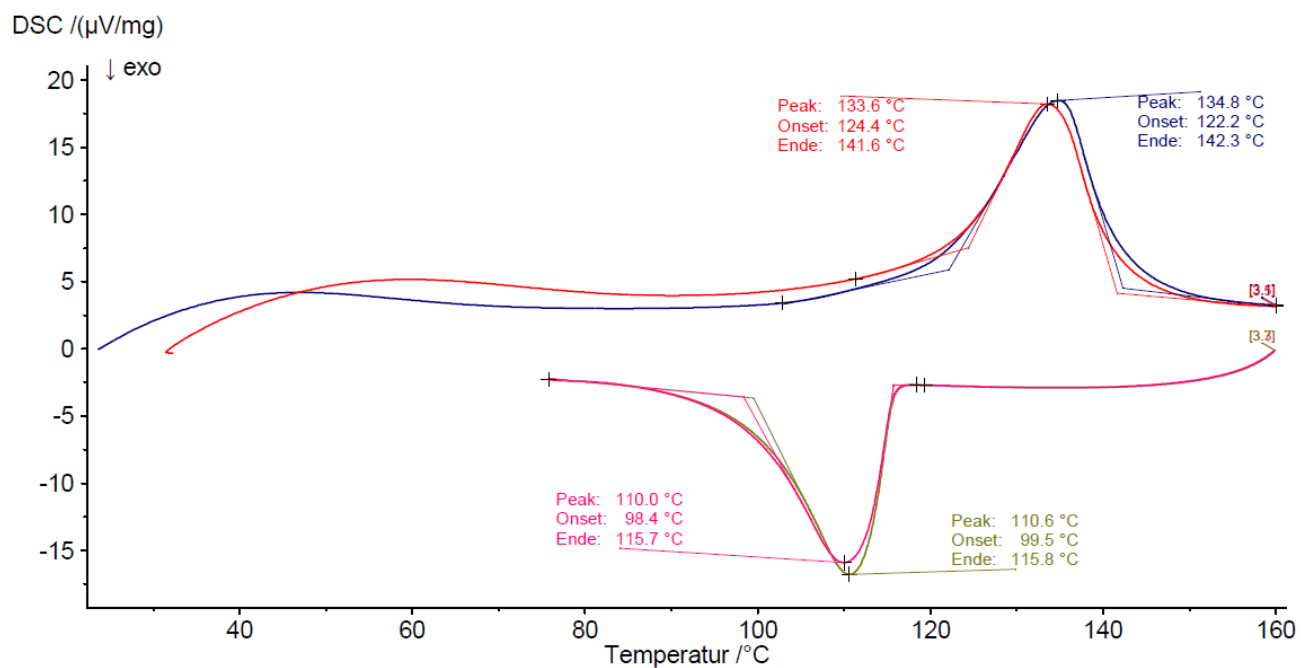


Fig S 126. DSC of PE (Table 1, #13).

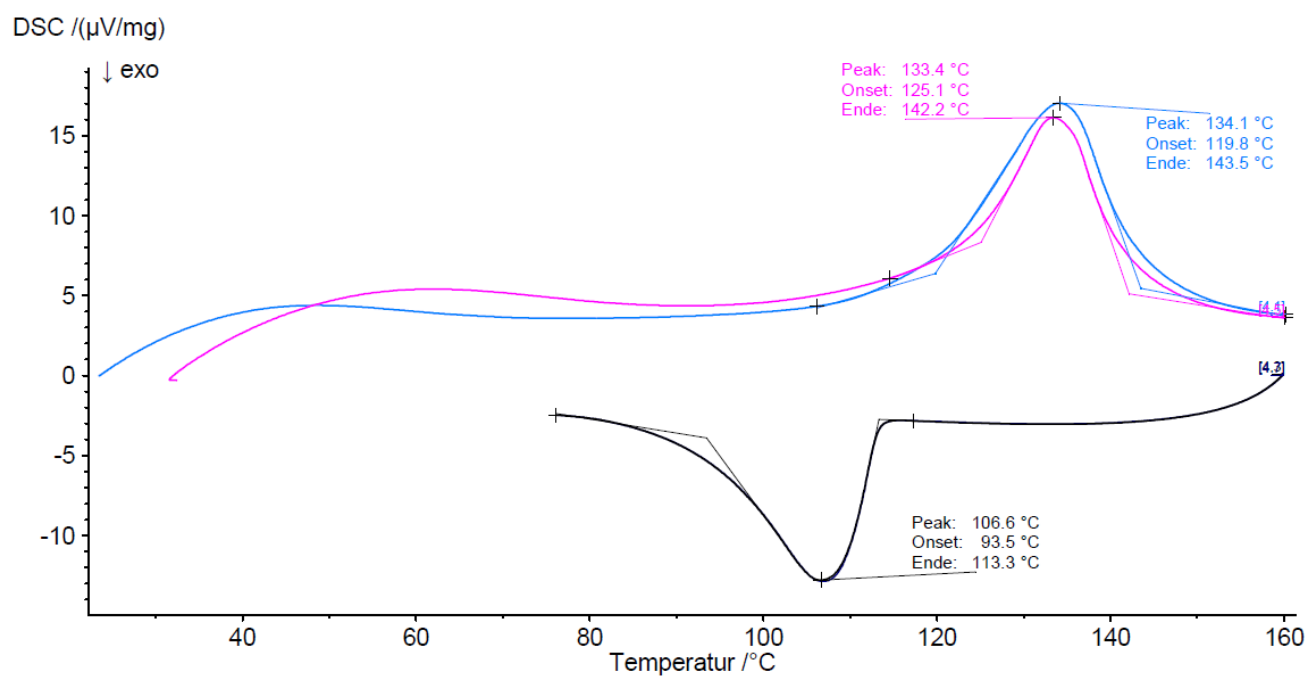


Fig S 127. DSC of PE (Table 1, #14).

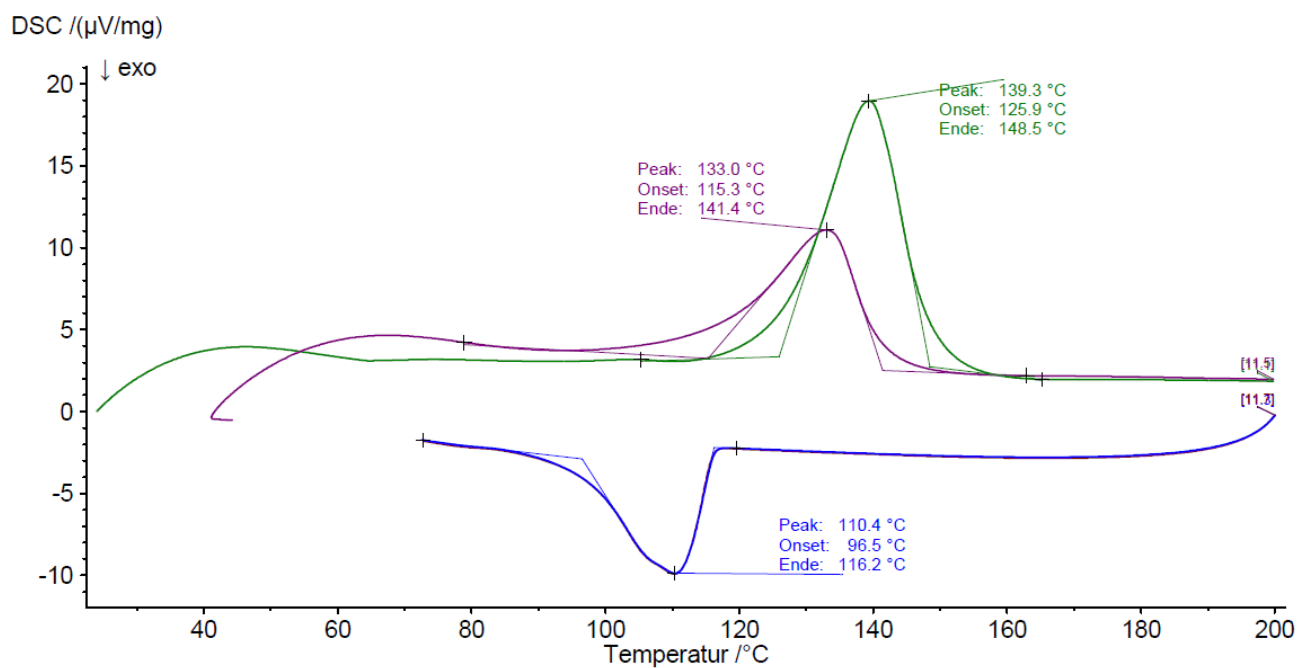


Fig S 128. DSC of PE (Table 1, #15).

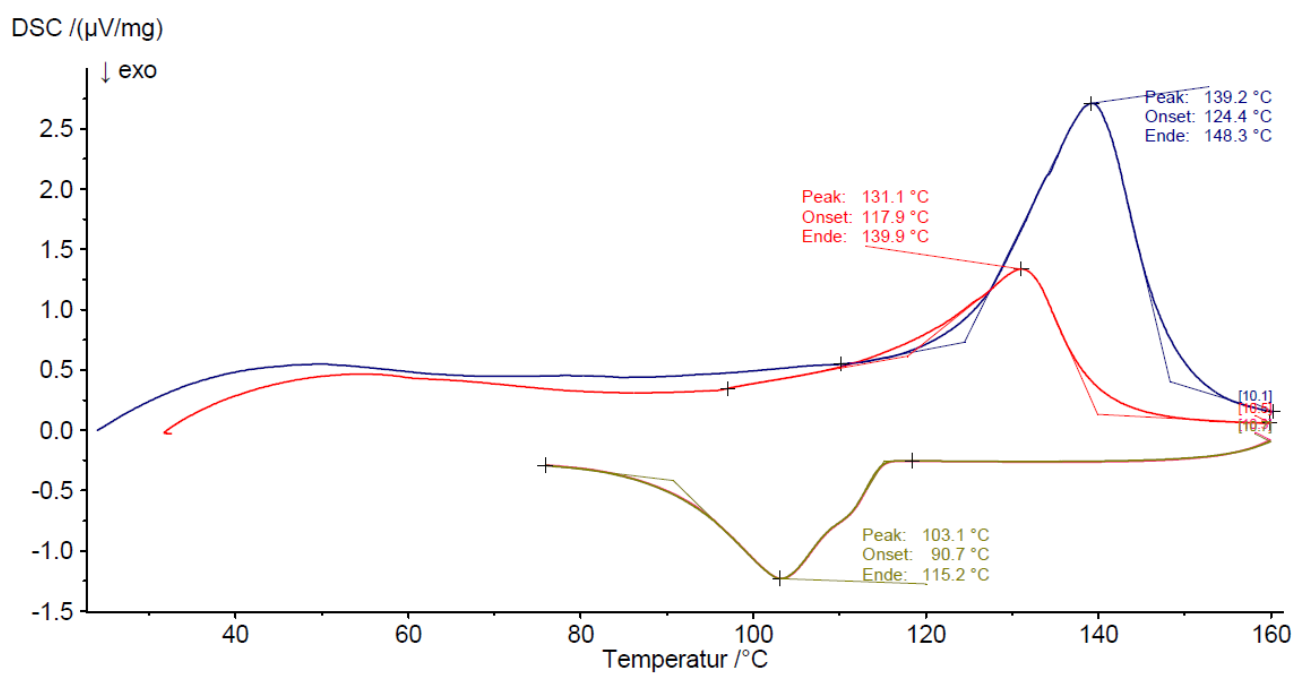


Fig S 129. DSC of PE (Table 1, #16).

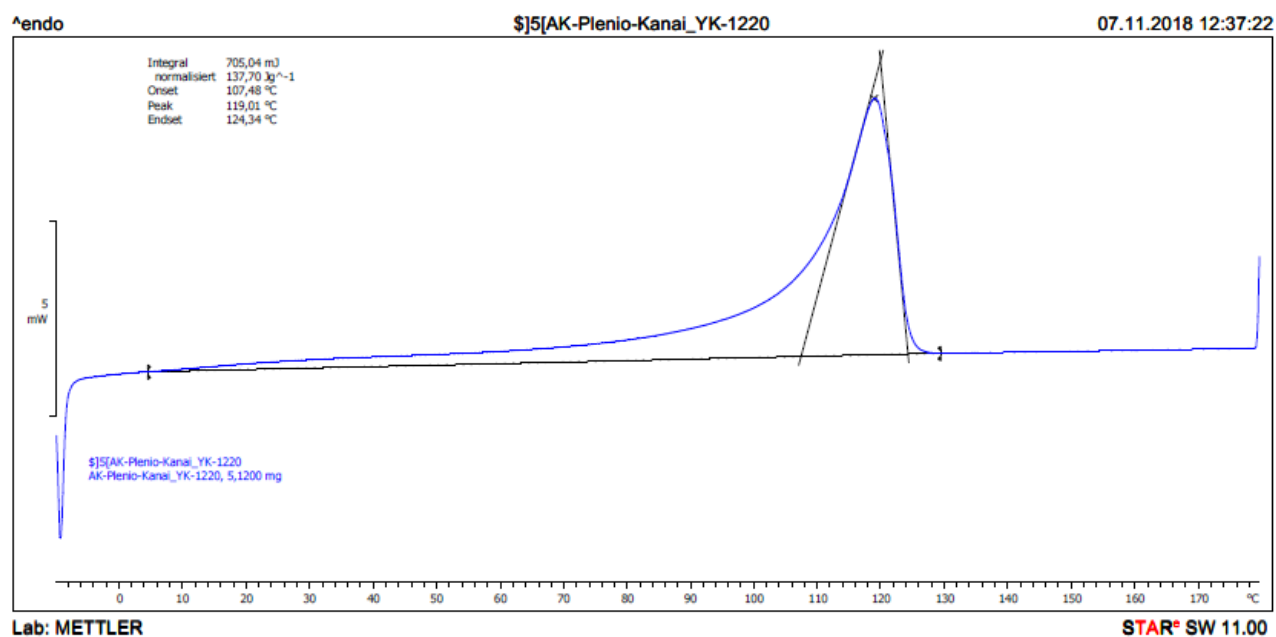


Fig S 130. DSC of PE (Table 1, #17).

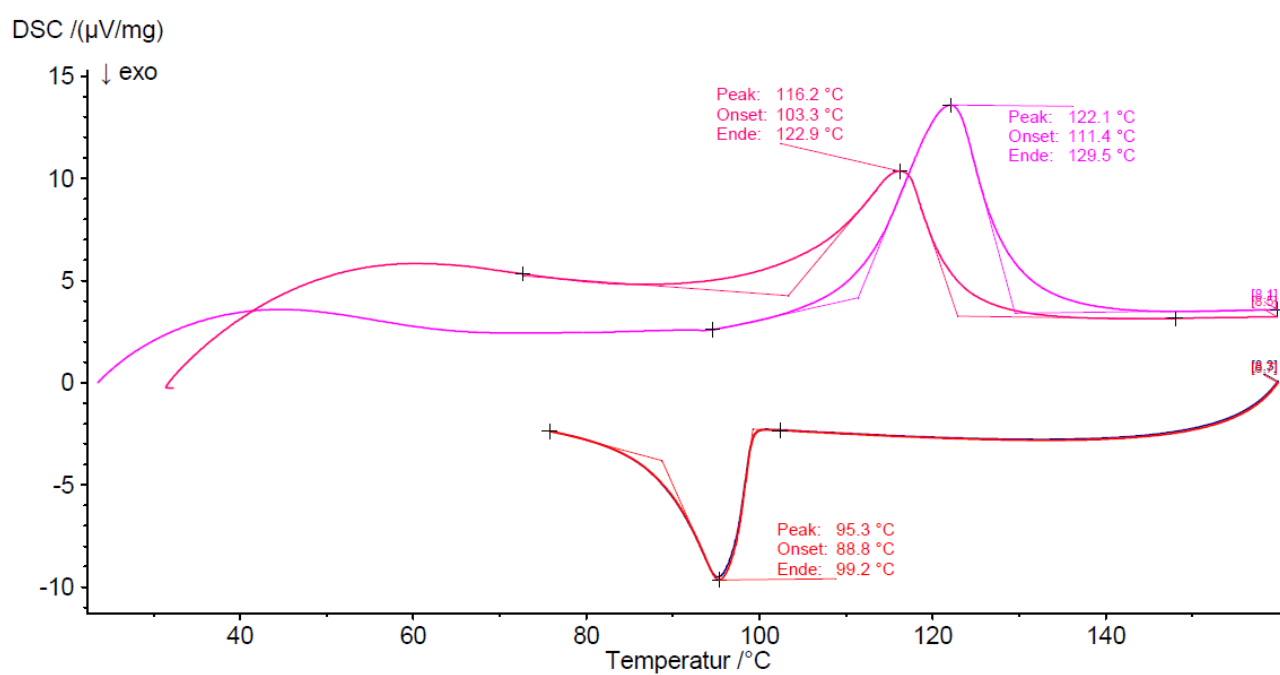


Fig S 131. DSC of PE (Table 1, #18).

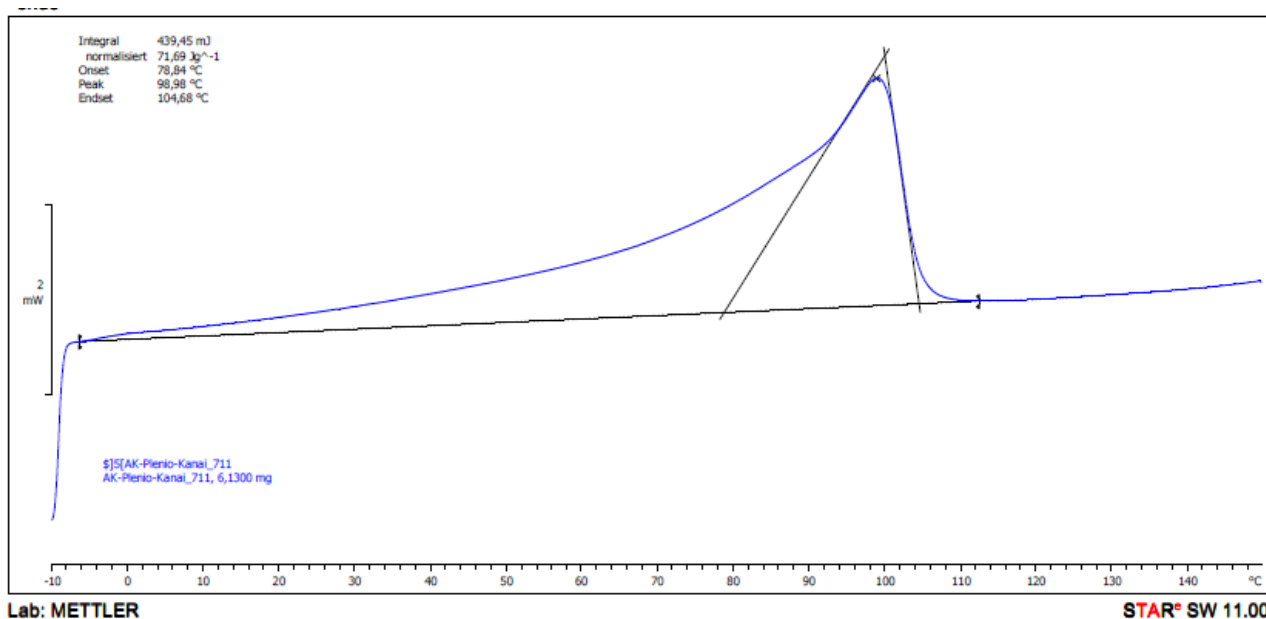


Fig S 132. DSC of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, #1, 0.05 M).

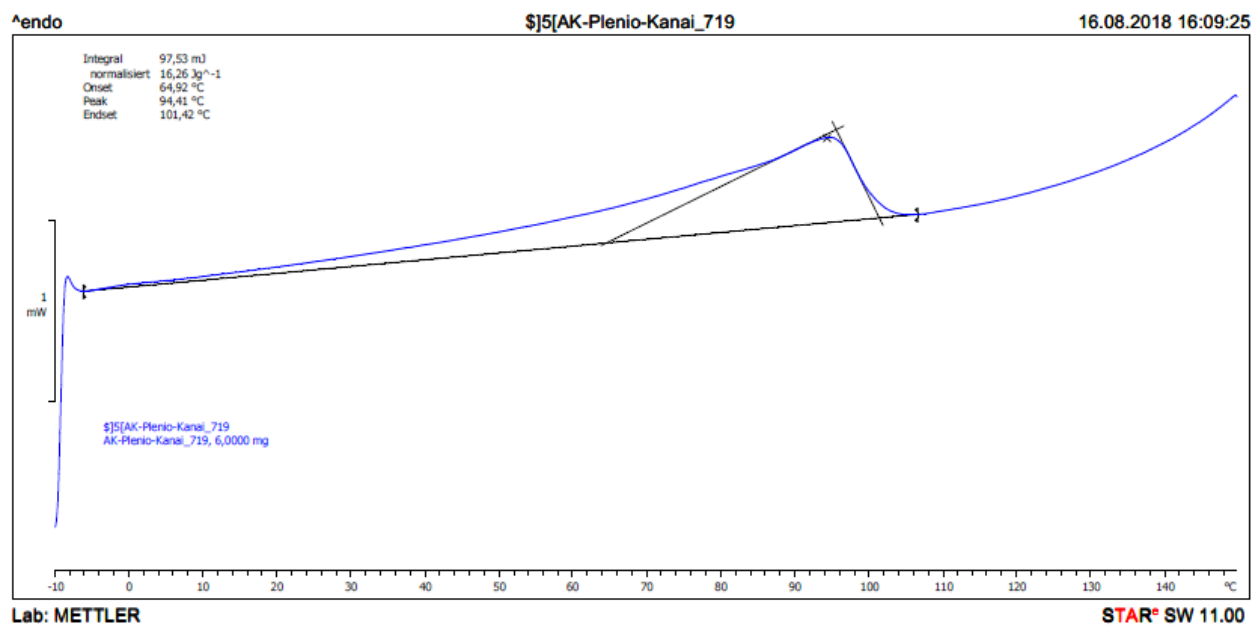


Fig S 133. DSC of ethene/methyl 10-undecenoate copolymer synthesized at 1 atm (Table 2, #1, 0.1 M).

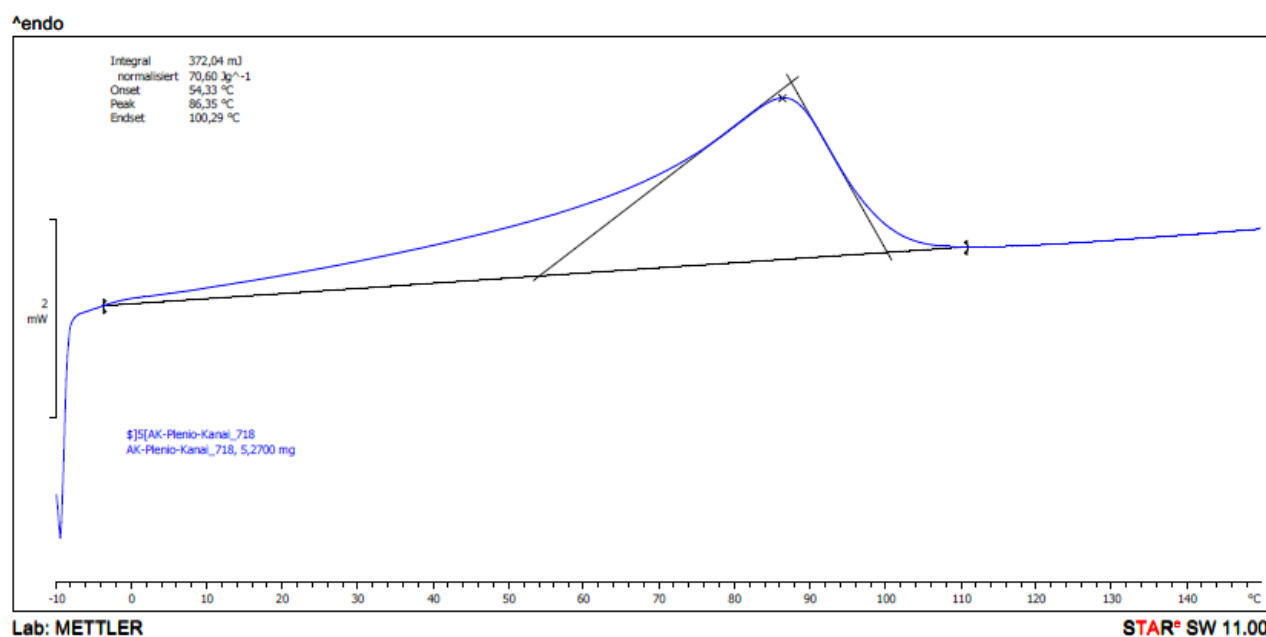


Fig S 134. DSC of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #4, 0.02 M).

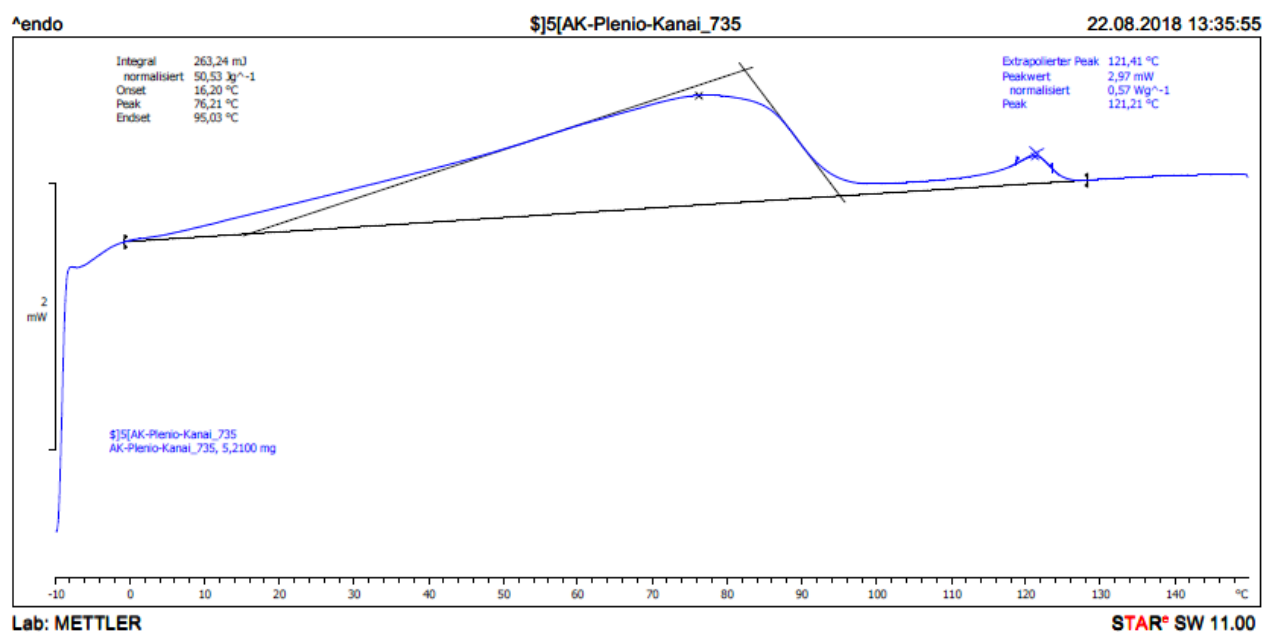


Fig S 135. DSC of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #5, 0.06 M).

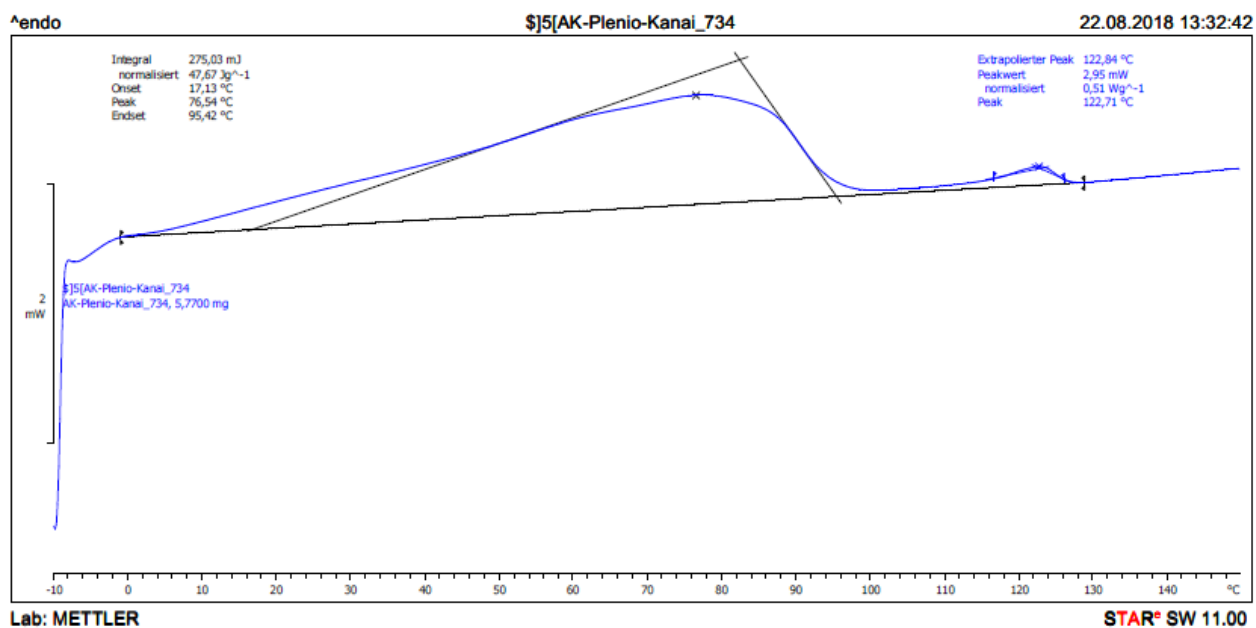


Fig S 136. DSC of ethene/10-undecenoic acid copolymer synthesized at 1 atm (Table 2, #6, 0.1 M).

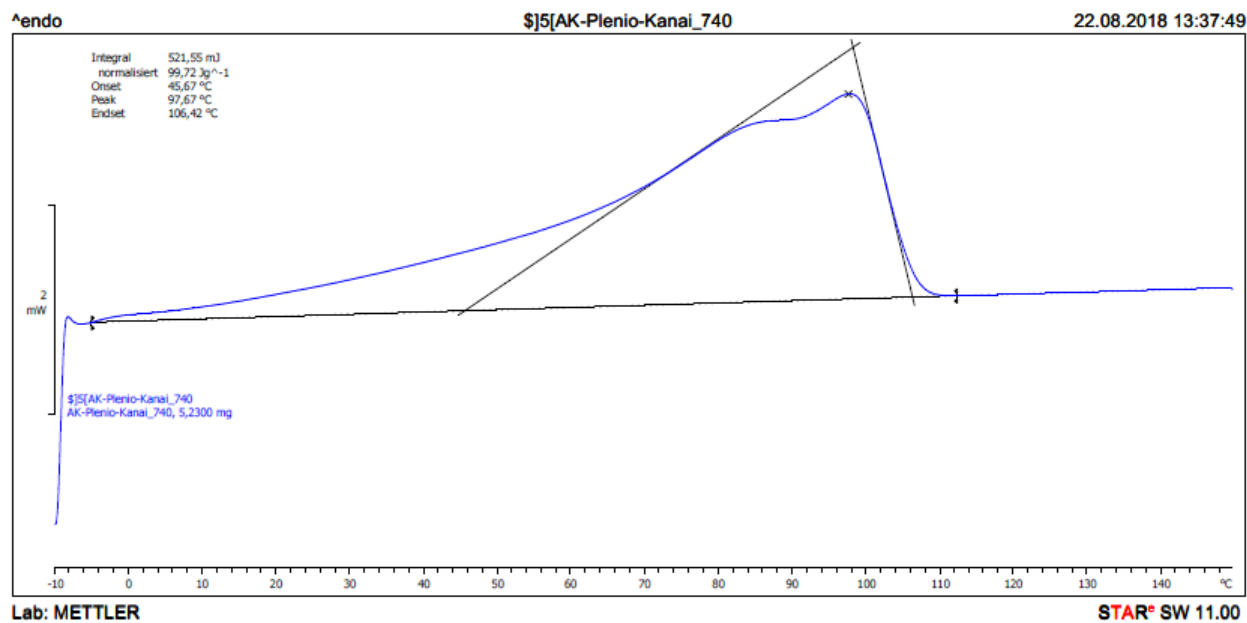


Fig S 137. DSC of ethene/methyl 11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #8, 0.02 M).

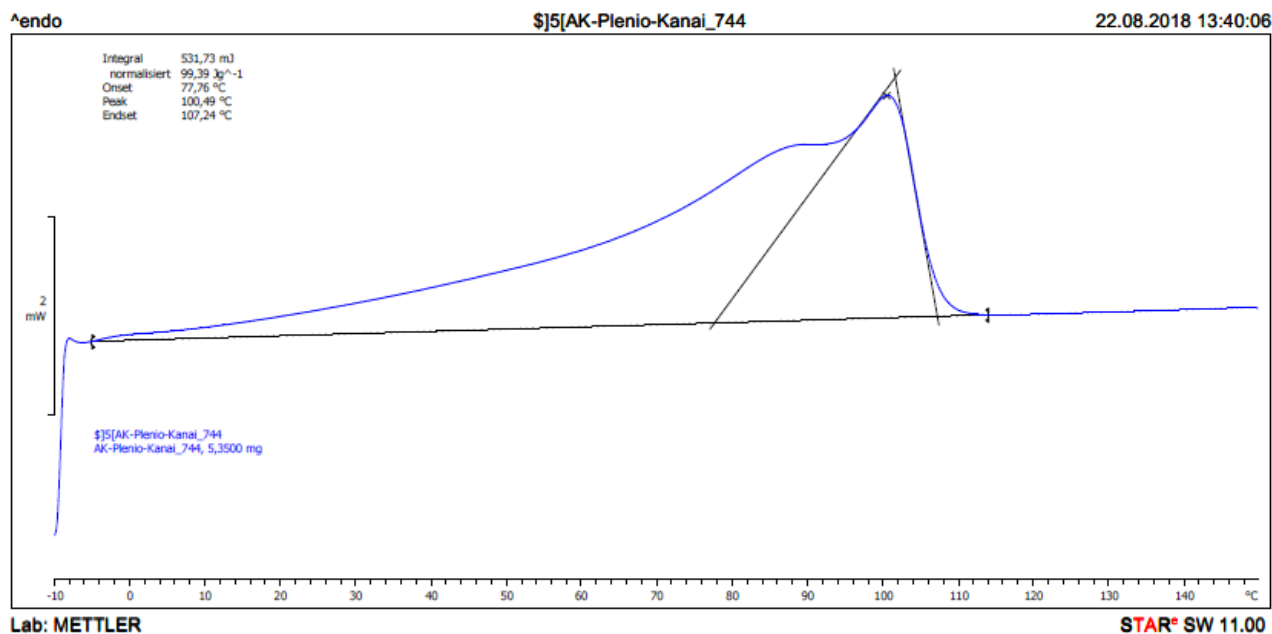


Fig S 138. DSC of ethene/methyl 11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #9, 0.04 M).

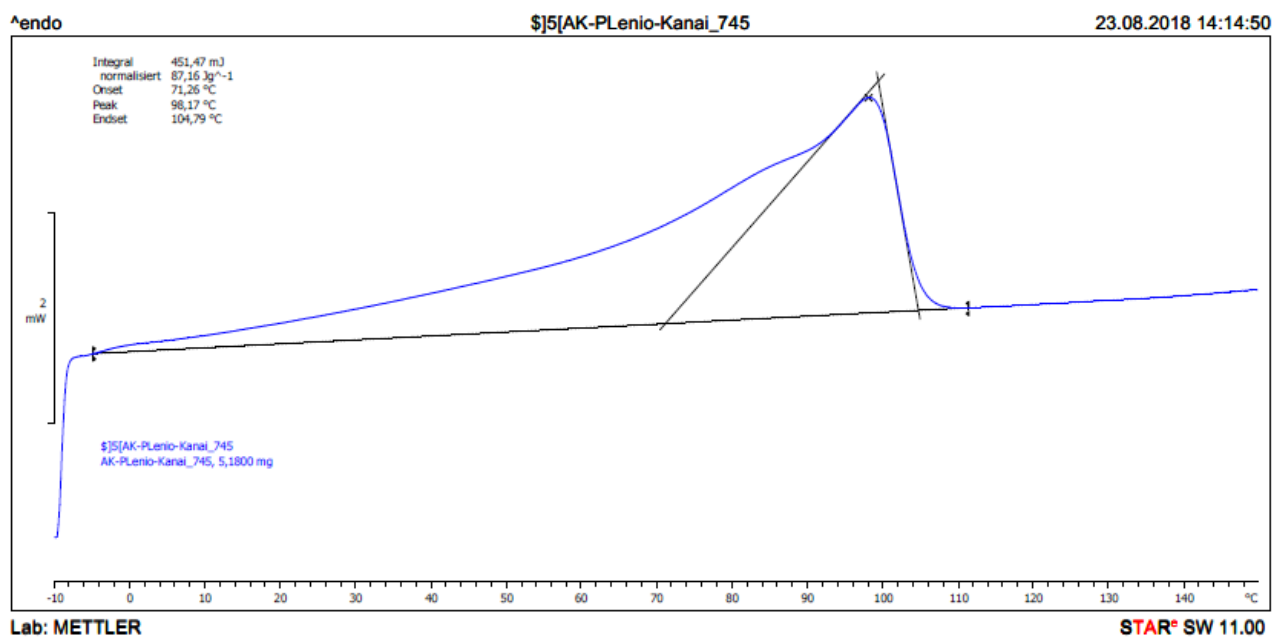


Fig S 139. DSC of ethene/methyl 11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #10, 0.06 M).

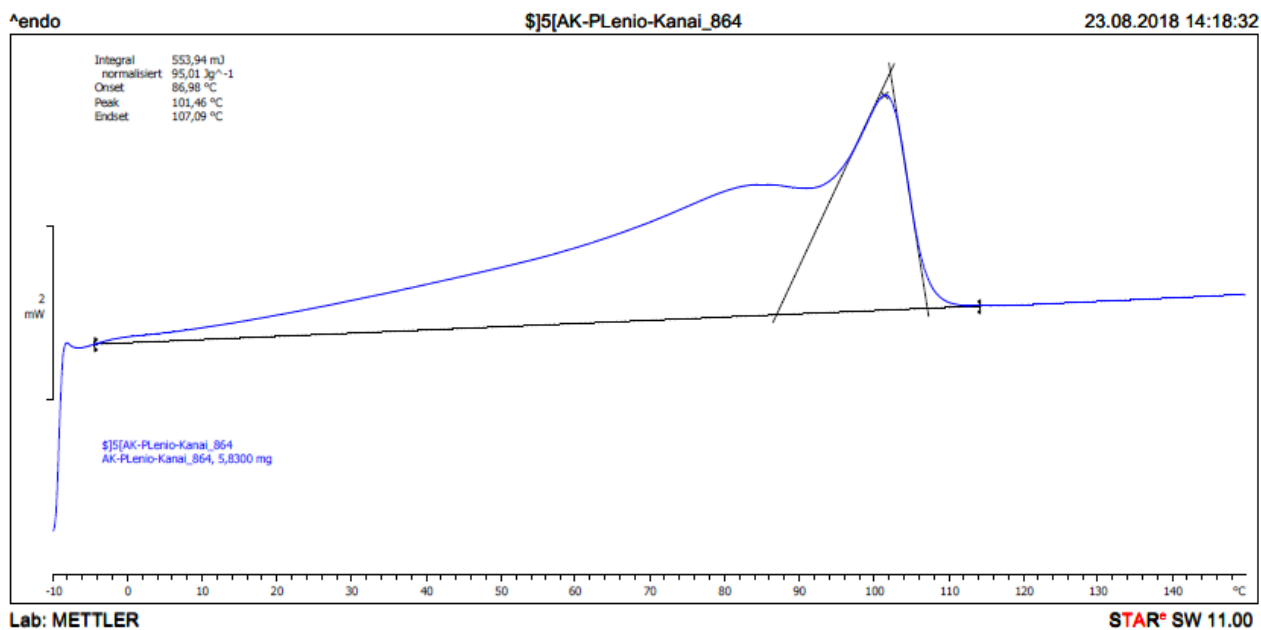


Fig S 140. DSC of ethene/methyl 11-chloro-1-undecene copolymer synthesized at 1 atm (Table 2, #11, 0.06 M).

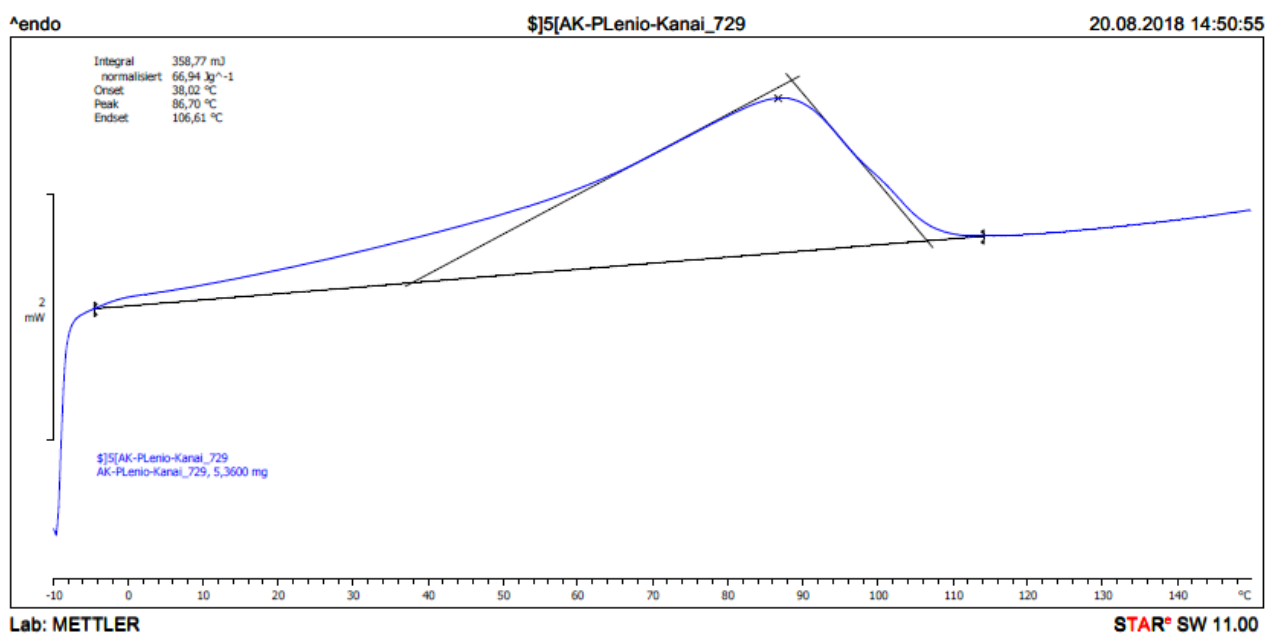


Fig S 141. DSC of ethene/5-Hexene-1-ol copolymer synthesized at 1 atm (Table 2, #12, 0.06 M).

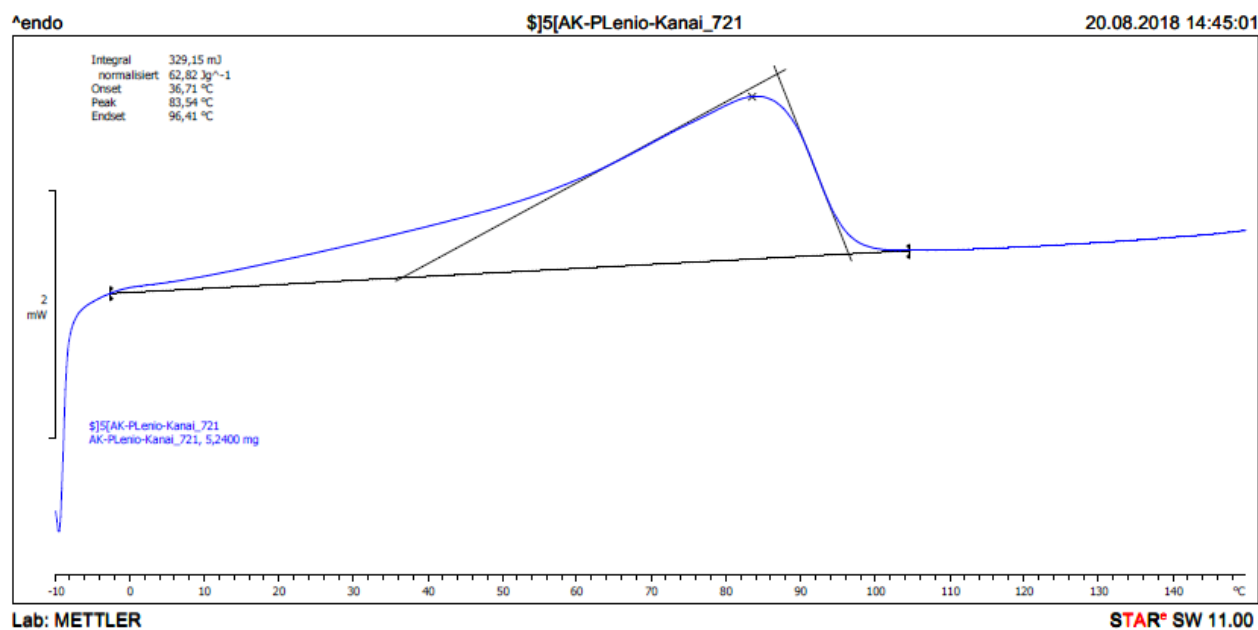


Fig S 142. DSC of ethene/5-Hexene-1-ol copolymer synthesized at 1 atm (Table 2, #13, 0.08 M).

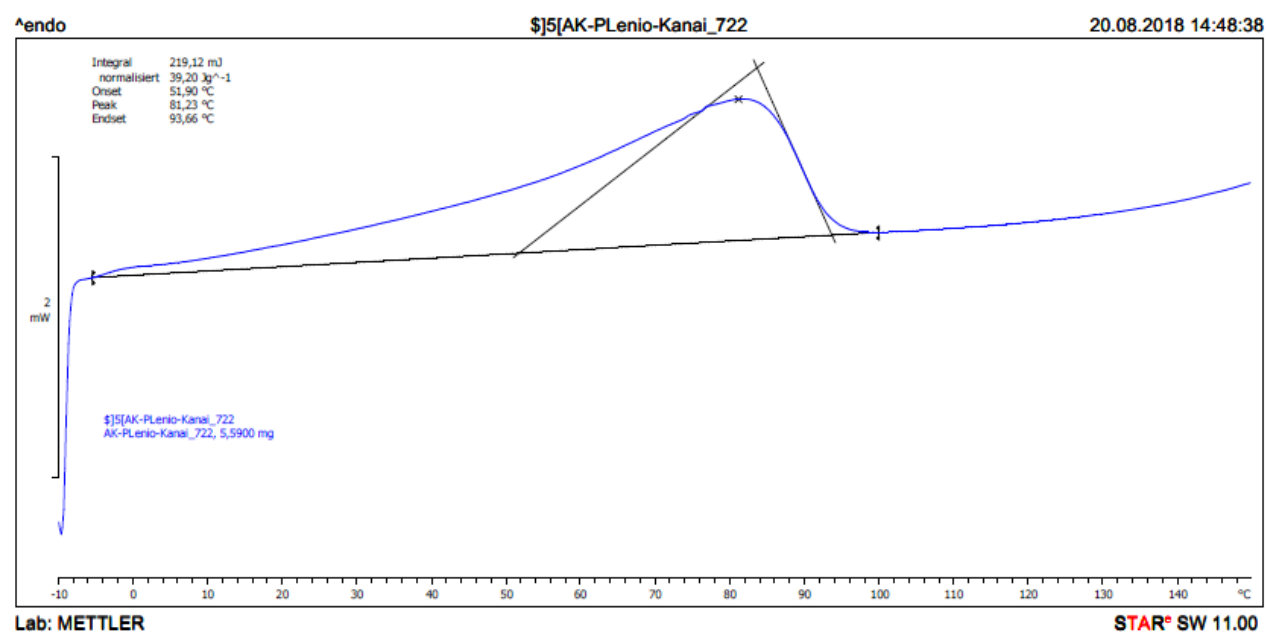


Fig S 143. DSC of ethene/5-Hexene-1-ol copolymer synthesized at 1 atm (Table 2, #14, 0.1 M).

X-ray crystal structure of nickel complex [(2a)NiBr(H₂O)₃Br]

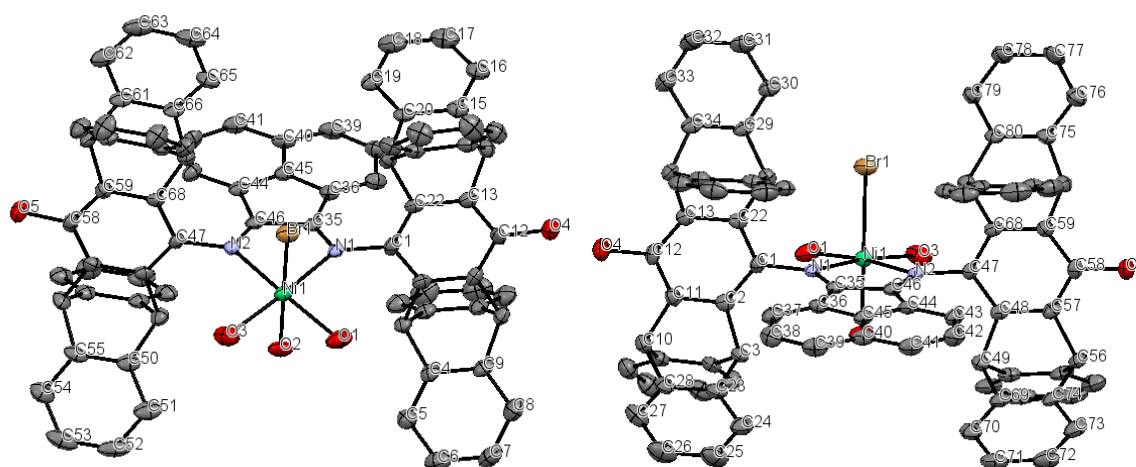


Fig S 144. X-ray crystal structure of nickel complex [(2a)NiBr(H₂O)₃Br]

Table S4. Crystal data and structure refinement for YK1.

Identification code	YK1	
Empirical formula	C106 H109 Br2 N2 Ni O8	
Formula weight	1757.48	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.983(1) Å α = 88.540(6)°. b = 17.146(1) Å β = 74.140(6)°. c = 19.897(1) Å γ = 75.369(7)°.	
Volume	4435.1(5) Å ³	
Z	2	
Density (calculated)	1.316 Mg/m ³	
Absorption coefficient	1.180 mm ⁻¹	
F(000)	1842	
Crystal size	0.280 x 0.140 x 0.080 mm ³	
Theta range for data collection	2.458 to 25.348°.	
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 20, -23 ≤ l ≤ 23	
Reflections collected	32250	
Independent reflections	16184 [R(int) = 0.0558]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.912 and 0.734
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16184 / 67 / 1117
Goodness-of-fit on F^2	1.001
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0602$, $wR_2 = 0.1387$
R indices (all data)	$R_1 = 0.1111$, $wR_2 = 0.1664$
Extinction coefficient	n/a
Largest diff. peak and hole	0.638 and -0.533 e.Å ⁻³

SambVca-buried volume

V Free	V Buried	V Total	V Exact
785.8	650.5	1436.3	1436.8

%V_Free	%V_Bur	% Tot/Ex
54.7	45.3	100.0

Quadrant	V_f	V_b	V_t	%V_f	%V_b
SW	186.8	172.3	359.1	52.0	48.0
NW	205.6	153.4	359.0	57.3	42.7
NE	205.4	153.7	359.0	57.2	42.8
SE	188.0	171.0	359.0	52.4	47.6

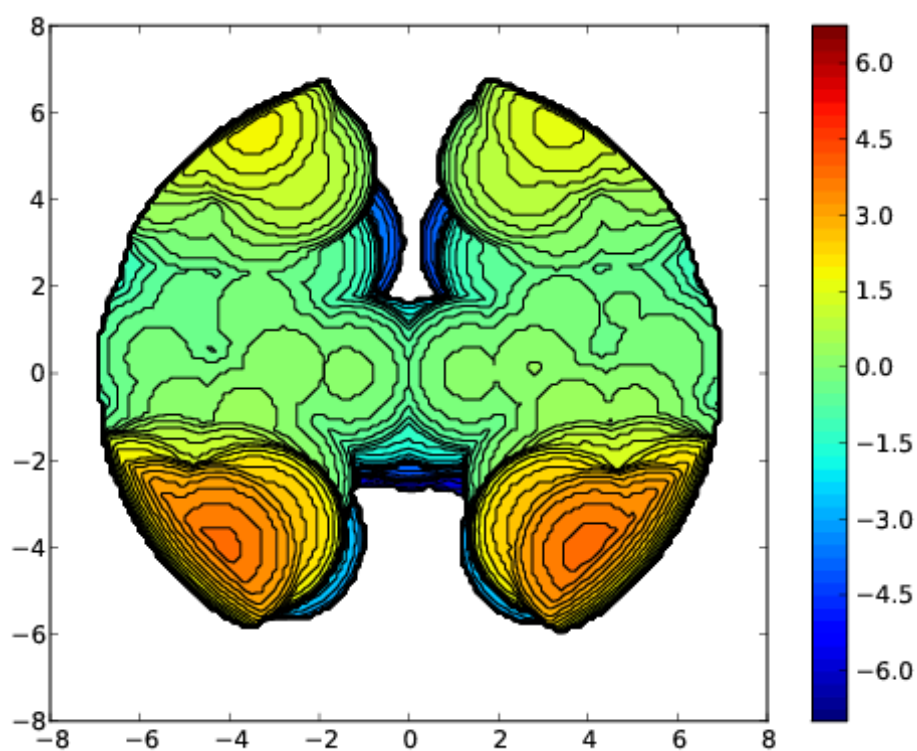


Figure S145. Buried-volume plot :

https://www.molnac.unisa.it/OMtools/sambvca2.0/process/sambvca_result_page.php?uploadDir=job_dir_1014587097&which_axis=6&addH=false

File content

130

O 6.97191 0.48939 -2.09195
O -6.93999 0.46342 -2.32423
N 1.36868 -0.00000 -1.62209
N -1.36868 -0.00000 -1.63304
C 2.81966 0.13765 -1.68474
C 3.64682 -0.97555 -1.50339
C 3.20079 -2.42442 -1.33665
H 2.20822 -2.52457 -1.27431
C 3.92968 -2.97944 -0.12967
C 3.34945 -3.61861 0.95262
H 2.40409 -3.69230 1.01951
C 4.17574 -4.15260 1.94549
H 3.79283 -4.60382 2.68764
C 5.54893 -4.02469 1.85167
H 6.10297 -4.39577 2.53061
C 6.13144 -3.35972 0.77482
H 7.07449 -3.26512 0.72116
C 5.31844 -2.83961 -0.21873
C 5.76789 -2.17167 -1.50086
H 6.75980 -2.06812 -1.55994
C 5.02704 -0.84565 -1.61065
C 5.60633 0.37160 -1.92879
C 4.78158 1.46702 -2.14796
C 5.22986 2.79976 -2.73817
H 6.22005 2.85652 -2.87125
C 4.45402 2.93458 -4.02884
C 4.97840 3.07796 -5.29468
H 5.91856 3.12798 -5.42468
C 4.10864 3.15051 -6.38381
H 4.46528 3.23613 -7.26146
C 2.74571 3.09905 -6.21041
H 2.16899 3.16539 -6.96242
C 2.20861 2.95255 -4.93798
H 1.26703 2.91100 -4.81972
C 3.05164 2.86402 -3.84304
C 2.65507 2.65138 -2.38318

H 1.66565 2.59719 -2.24884
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C 3.80558 -3.15034 -2.55465
C 3.11296 -3.87645 -3.50801
H 2.16664 -3.95093 -3.46461
C 3.82632 -4.49569 -4.52926
H 3.35927 -4.99154 -5.19167
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H 5.67945 -4.83964 -5.29317
C 5.89786 -3.64824 -3.64717
H 6.84213 -3.56194 -3.69705
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C 3.30319 3.80221 -1.61158
C 2.65424 4.74617 -0.84990
H 1.71835 4.68441 -0.69791
C 3.39280 5.79688 -0.30426
H 2.94936 6.45818 0.21209
C 4.73750 5.88943 -0.49465
H 5.22011 6.61213 -0.11088
C 5.41124 4.92930 -1.25418
H 6.35033 4.98750 -1.38198
C 4.68765 3.89104 -1.81892
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C 2.44143 -0.82037 -6.13248
H 3.27861 -0.93695 -6.56693
C 1.28049 -0.90911 -6.87383
H 1.33435 -1.09141 -7.80353
C 0.01458 -0.73092 -6.27307
C -1.25193 -0.80344 -6.90129
H -1.30592 -0.95827 -7.83736
C -2.39587 -0.65284 -6.17313
H -3.22904 -0.69245 -6.62547
C -2.39606 -0.44209 -4.77566
H -3.21054 -0.36040 -4.29260
C -1.16987 -0.35490 -4.13697

C 0.01479 -0.49919 -4.88660
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C -2.80805 0.13725 -1.69290
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C -3.96899 -2.97217 -0.23055
C -3.43967 -3.55700 0.92188
H -2.49920 -3.62519 1.04036
C -4.30503 -4.03305 1.88272
H -3.95690 -4.44340 2.66518
C -5.67320 -3.91899 1.71968
H -6.25176 -4.26177 2.38970
C -6.21177 -3.31533 0.59791
H -7.15323 -3.22255 0.50152
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C -5.74700 -2.19927 -1.69658
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C -5.00870 -0.85127 -1.74383
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H -4.21477 3.54045 -7.20946
C -2.54451 3.21427 -6.10767
H -1.93262 3.25991 -6.83508
C -2.08439 2.99854 -4.82024
H -1.15272 2.90051 -4.65960
C -2.97528 2.92352 -3.77227
C -2.63024 2.67024 -2.30192
H -1.64786 2.61014 -2.12806
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C -3.70225 -3.13058 -2.66305
C -2.96153 -3.78915 -3.61151

H -2.02176 -3.87041 -3.50768
C -3.59234 -4.33920 -4.72515
H -3.08192 -4.79590 -5.38352
C -4.95971 -4.21817 -4.87010
H -5.38648 -4.59062 -5.63142
C -5.71713 -3.55888 -3.91139
H -6.65910 -3.48539 -4.01503
C -5.09453 -3.00700 -2.80094
C -4.70540 3.87614 -1.75166
C -5.47394 4.83600 -1.15666
H -6.40909 4.87264 -1.31610
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H -5.38447 6.43688 0.11328
C -3.49416 5.69699 -0.08147
H -3.07993 6.33340 0.48987
C -2.71979 4.70354 -0.68324
H -1.78459 4.66081 -0.52237
C -3.32836 3.78499 -1.51200