Electronic Supplementary Material (ESI) for Polymer Chemistry

Supporting Information

For

High Temperature Synthesis of Vinyl Terminated Polymers Based on Dendronized Acrylates: A Detailed Product Analysis Study

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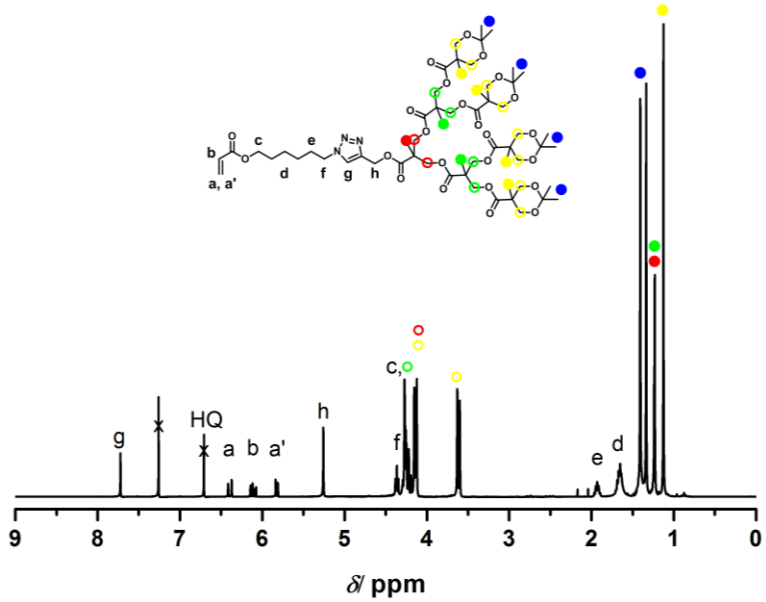


Figure S1. 400 MHz proton spectrum of $(An)_4$-[G3]-triazole-hexyl acrylate (C_6G3) **13a** measured in $CDCl_3$. Hydroquinone (HQ) was added after purification to prevent premature polymerization.

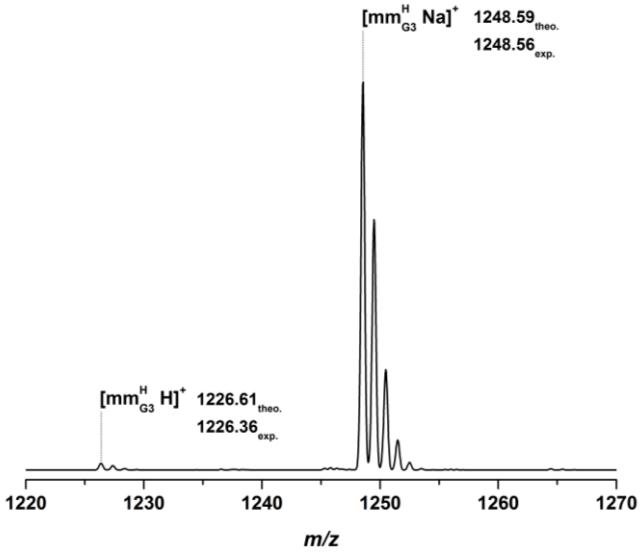


Figure S2. ESI-MS spectrum of $(An)_4$-[G3]-triazole-hexyl acrylate (C_6G3) **13a**.

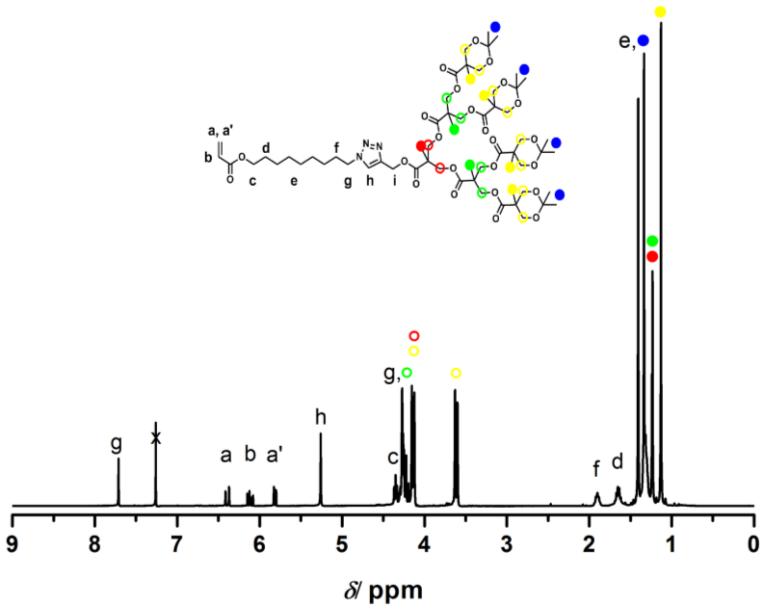


Figure S3. 400 MHz proton spectrum of $(An)_4$-[G3]-triazole-nonanyl acrylate (C_9G3) **13b** measured in $CDCl_3$.

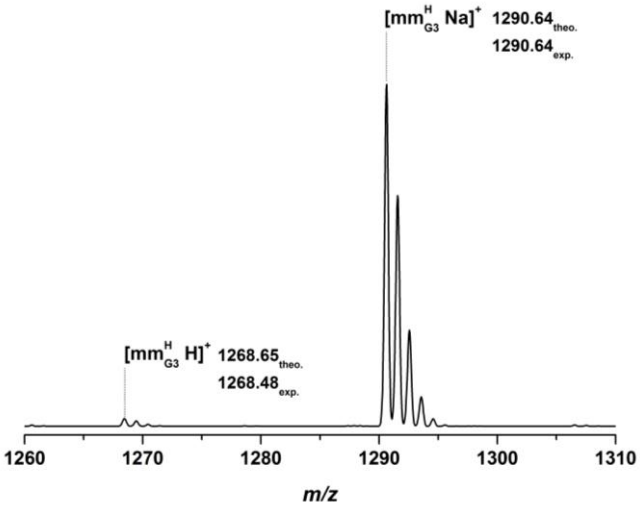
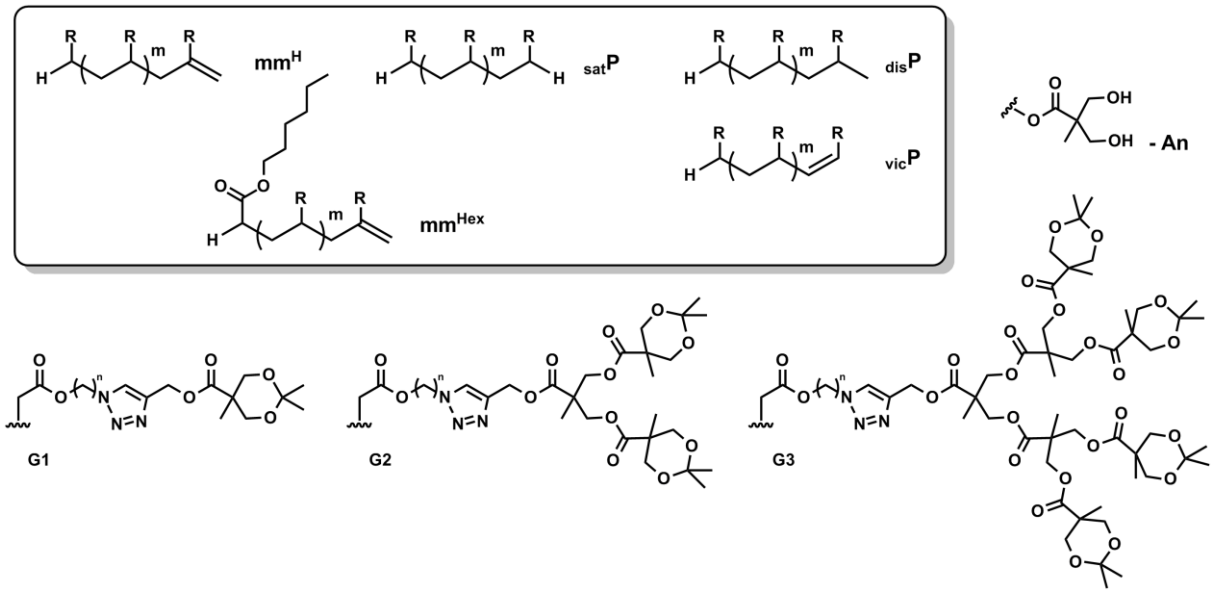


Figure S4. ESI-MS spectrum of $(An)_4$-[G3]-triazole-nonanyl acrylate (C_9G3) **13b**.

ESI-MS spectra of the high temperature acrylate polymerization products as a proof of purity

An overall spectrum as well as a zoom spectrum of one specific repeat unit is shown in the following for each macromonomer. A table with theoretical and experimental *m/z* ratios is additionally provided. G*X* represents the overall repeating units of the monomer C_nGX, whereas –An depicts the amount of deprotection on the grafted macromonomer. Scheme S1 shows all identified species.



Scheme S1. Chemical structures of the identified products in the mass spectrum dendronized macromonomer.

Table S1. Theoretical and experimental *m/z* ratios of the species of the **p(11b) mm** identified via the ESI-MS measurements. The resolution is close to 0.1 amu. (see Figure 3). Listed below are the single charged sodium species $[M+Na]^+$ if not otherwise specified.

Species	G1	- An	$m/z_{theo.}$	$m/z_{exp.}$	$\Delta\ m/z$
mm^{H}	3	1	1336.76	1336.72	0.04
$_{sat}$P	3	0	1364.79	1364.76	0.03
mm^{H}	3	0	1376.79	1376.72	0.07
mm^{H}	3	0	1392.77	1392.72	0.05
mm^{Hex} dc	6	0	1454.85	1454.72	0.13
mm^{Hex}	3	1	1492.88	1492.72	0.16
$_{vic}$P^{Hex}	3	0	1518.89	1518.76	0.13
$_{sat}$P^{Hex}	3	0	1520.91	1520.76	0.15
mm^{Hex}	3	0	1532.91	1532.76	0.15
$_{dis}$P^{Hex}	3	0	1534.93	1534.76	0.17
mm^{H} dc	6	2	1562.40	1562.32	0.08
$_{sat}$P dc	7	1	1576.41	1576.20	0.21
mm^{H} dc	7	1	1582.41	1582.24	0.17
$_{sat}$P dc	7	0	1596.43	1596.28	0.15
mm^{H} dc	7	0	1602.43	1602.28	0.15
$_{sat}$P^{Hex} dc	7	1	1654.47	1654.28	0.19
mm^{Hex} dc	7	1	1660.47	1660.32	0.15
$_{sat}$P^{Hex} dc	7	0	1674.49	1674.28	0.21
mm^{Hex} dc	7	0	1680.49	1680.32	0.17

Table S2. Theoretical and experimental *m/z* ratios of the species of **p(11b) mm** and the hydrogenated analoga identified via the ESI-MS measurements. The resolution is close to 0.1 amu. (see Figure 4). Listed below are the single charged sodium species $[M+Na]^+$ if not otherwise specified.

Species	G1	- An	$m/z_{theo.}$	$m/z_{exp.}$	$m/z_{theo.}$	$m/z_{exp.}$	$\Delta\ m/z$
					hydrogenated		
mm^{H}	3	1	1336.76	1336.72	1338.78	1338.72	0.06
$_{sat}$P dc	6	1	1350.78	1350.72	1350.78	1350.68	0.10
mm^{H} dc	6	1	1356.78	1356.68	1357.79	1357.72	0.07
$_{sat}$P	3	0	1364.79	1364.76	1364.79	1364.76	0.03
$_{sat}$P dc	6	0	1370.79	1370.72	1370.79	1370.72	0.07
mm^{H}	3	0	1376.79	1376.72	1378.81	1378.76	0.05

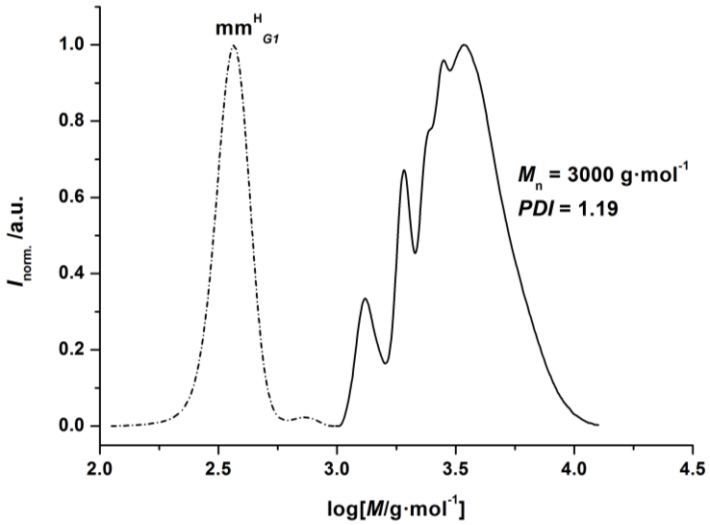


Figure S5. SEC chromatogram of **p(11a) mm**. The trace on the left hand side (dashed) represents the residual monomer, whereas the trace on the right hand side shows the distribution after the polymerization. Both traces have been analysed and normalized separately.

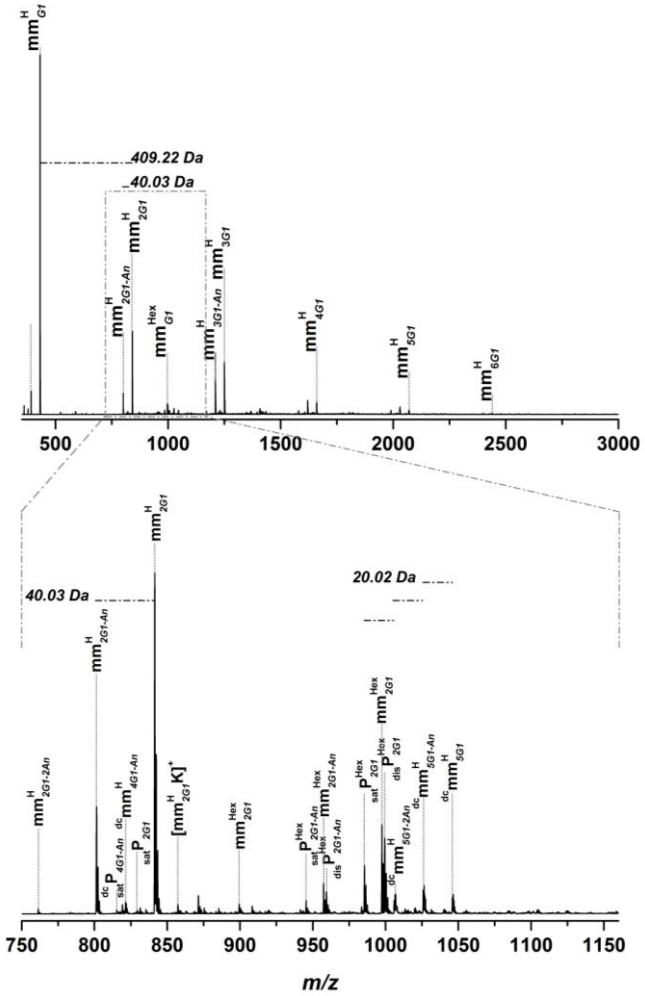
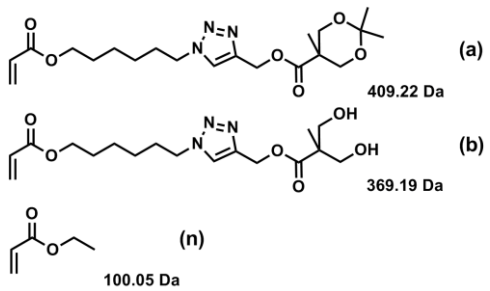


Figure S6. ESI-MS spectrum of **p(11a) mm**. The overall spectrum (above) and the zoom spectrum to a repeat unit (409.22 Da) (below) are depicted. The polymer was synthesized via high temperature acrylate polymerization in solution of hexyl acetate with 5 wt% monomer at 140 °C in an oxygen free atmosphere with $5 \cdot 10^{-3}$ mol L^{-1} AIBN.

Table S3. Theoretical and experimental *m/z* ratios of the species of the **p(11a) mm** identified via the ESI-MS measurements. The resolution is close to 0.1 amu. (see Figure S6).

species	G1	- An	$m/z_{theo.}$	$m/z_{exp.}$	$\Delta\ m/z$
mm^{H}	2	2	761.37	761.36	0.01
mm^{H}	2	1	779.42	779.24	0.18
mm^{H} dc	4	3	781.39	781.40	0.01
$_{sat}$P	2	1	789.40	789.40	0.00
$_{sat}$P dc	4	2	795.40	795.40	0.00
mm^{H}	2	1	801.40	801.40	0.00
mm^{H} dc	4	2	801.40	801.40	0.00
$_{sat}$P dc	4	1	815.42	815.40	0.02
mm^{H}	2	1	817.37	817.40	0.03
mm^{H} dc	4	2	817.37	817.40	0.03
mm^{H}	2	0	819.45	819.20	0.25
mm^{H} dc	4	1	821.42	821.36	0.06
$_{sat}$P	2	0	829.43	829.40	0.03
$_{sat}$P dc	4	0	835.43	835.36	0.07
mm^{H}	2	0	841.43	841.40	0.03
mm^{H} dc	4	0	841.43	841.40	0.03
mm^{H}	2	0	857.41	857.40	0.01
mm^{Hex} dc	4	3	859.44	859.40	0.04
$_{sat}$P^{Hex} dc	4	2	873.46	873.40	0.06
mm^{Hex} dc	4	2	879.46	879.40	0.06
mm^{Hex} dc	4	1	899.47	899.44	0.03
$_{sat}$P^{Hex}	2	2	905.48	905.40	0.08
satP^{Hex} dc	4	0	913.49	913.44	0.05
mm^{Hex}	2	2	917.48	917.40	0.08
mm^{Hex} dc	4	0	919.49	919.40	0.09
$_{dis}$P^{Hex} dc	4	0	920.50	920.40	0.10
$_{sat}$P dc	5	5	939.96	939.44	0.52
$_{sat}$P^{Hex}	1	1	945.52	945.44	0.08
mm^{H} dc	5	5	945.96	945.96	0.00
mm^{Hex}	1	1	957.52	957.44	0.08
$_{dis}$P^{Hex}	1	1	959.98	959.53	0.45
$_{sat}$P dc	5	3	980.00	980.44	0.44
$_{vic}$P^{Hex}	2	0	983.53	983.48	0.05
$_{sat}$P^{Hex}	2	0	985.55	985.48	0.07
mm^{H} dc	5	3	986.00	985.92	0.08

species	G1	- An	m/z theo.	m/z exp.	Δ m/z
mm^{Hex}	2	0	997.55	997.48	0.07
$_{dis}$P^{Hex}	2	0	999.56	999.44	0.12
mm^{H} dc	5	2	1006.01	1005.96	0.05
$_{sat}$P dc	5	1	1020.03	1019.96	0.07
mm^{H} dc	5	1	1026.03	1025.92	0.11
$_{sat}$P dc	5	0	1040.04	1039.96	0.08
mm^{H} dc	5	0	1046.04	1045.96	0.08
mm^{Hex} dc	5	3	1064.05	1064.48	0.43
$_{sat}$P^{Hex} dc	5	2	1078.07	1077.96	0.11
mm^{Hex} dc	3	2	1084.07	1083.96	0.11
$_{vic}$P^{Hex} dc	5	1	1097.08	1097.48	0.40
$_{sat}$P^{Hex} dc	5	1	1098.08	1098.48	0.40
mm^{Hex} dc	5	1	1104.08	1104.00	0.08
$_{sat}$P^{Hex} dc	5	0	1118.10	1118.10	0.00
mm^{Hex} dc	5	0	1124.10	1124.00	0.10



Scheme S2: Chemical structures of the monomers occurring in the copolymerization process of **11a** with ethyl acrylate

Table S4. Theoretical and experimental *m/z* ratios of the species of **p(11a)-*co*-ea mm** identified via the ESI-MS measurements. The resolution is close to 0.1 amu. (see Figure 6). Listed below are the single charged sodium species $[M+Na]^+$ if not otherwise specified.

spezies	G1	-An	EA	$m/z_{theo.}$	$m/z_{exp.}$	Δ m/z
mm^{Hex}	2	2	4	1317.69	1317.60	0.09
$_{sat}$P	3	3	2	1318.66	1318.60	0.06
$_{sat}$P	1	0	9	1320.68	1320.60	0.08
mm^{H}	0	0	13	1323.67	1323.68	0.01
mm^{Hex}	3	2	0	1326.71	1326.60	0.11
$_{sat}$P	2	0	5	1329.69	1329.60	0.09
mm^{H}	3	3	2	1330.66	1330.60	0.06

spezies	G1	-An	EA	$m/z_{theo.}$	$m/z_{exp.}$	Δ m/z
$\mathbf{mm^{H}}$	1	0	9	1332.68	1332.60	0.08
$\mathbf{_{sat}P^{Hex}}$	1	1	8	1336.71	1336.60	0.11
$\mathbf{_{sat}P}$	3	0	1	1338.71	1338.64	0.07
$\mathbf{mm^{H}}$	2	0	5	1341.69	1341.60	0.09
$\mathbf{_{sat}P^{Hex}}$	2	1	4	1345.73	1345.60	0.13
$\mathbf{mm^{Hex}}$	1	1	8	1348.71	1348.60	0.11
$\mathbf{_{sat}P}$	2	2	6	1349.68	1349.60	0.08
$\mathbf{mm^{H}}$	3	0	1	1350.71	1350.60	0.11
$\mathbf{_{sat}P^{Hex}}$	3	1	0	1354.74	1354.64	0.10
$\mathbf{mm^{Hex}}$	2	1	4	1357.73	1357.60	0.13
$\mathbf{_{sat}P}$	3	2	2	1358.70	1358.60	0.10
$\mathbf{mm^{H}}$	2	2	6	1361.68	1361.60	0.08
$\mathbf{mm^{Hex}}$	2	0	1	1366.74	1366.60	0.14
$\mathbf{_{sat}P^{Hex}}$	0	0	12	1367.73	1367.60	0.13
$\mathbf{mm^{H}}$	3	2	2	1370.70	1370.60	0.10
$\mathbf{_{sat}P^{Hex}}$	3	3	1	1374.73	1374.64	0.09
$\mathbf{_{sat}P^{Hex}}$	1	0	8	1376.75	1376.64	0.11
$\mathbf{mm^{Hex}}$	0	0	12	1379.73	1379.68	0.05
$\mathbf{_{sat}P}$	1	1	10	1380.70	1380.60	0.10
$\mathbf{_{sat}P^{Hex}}$	2	0	0	1385.76	1385.64	0.12
$\mathbf{mm^{Hex}}$	3	0	1	1386.73	1386.64	0.09
$\mathbf{mm^{Hex}}$	1	0	8	1388.75	1388.64	0.11
$\mathbf{_{sat}P}$	2	1	6	1389.72	1389.64	0.08
$\mathbf{mm^{H}}$	1	1	10	1392.70	1392.60	0.10
$\mathbf{_{sat}P^{Hex}}$	3	0	0	1394.77	1394.60	0.17
$\mathbf{mm^{Hex}}$	2	0	4	1397.76	1397.64	0.12
$\mathbf{_{sat}P}$	3	1	2	1398.73	1398.64	0.09
$\mathbf{mm^{H}}$	2	1	6	1401.72	1401.60	0.12
$\mathbf{_{sat}P}$	2	2	5	1405.75	1405.64	0.11
$\mathbf{mm^{Hex}}$	3	0	0	1406.77	1406.64	0.13
$\mathbf{mm^{H}}$	3	1	2	1410.73	1410.60	0.13
$\mathbf{_{sat}P}$	0	0	14	1411.72	1411.64	0.08

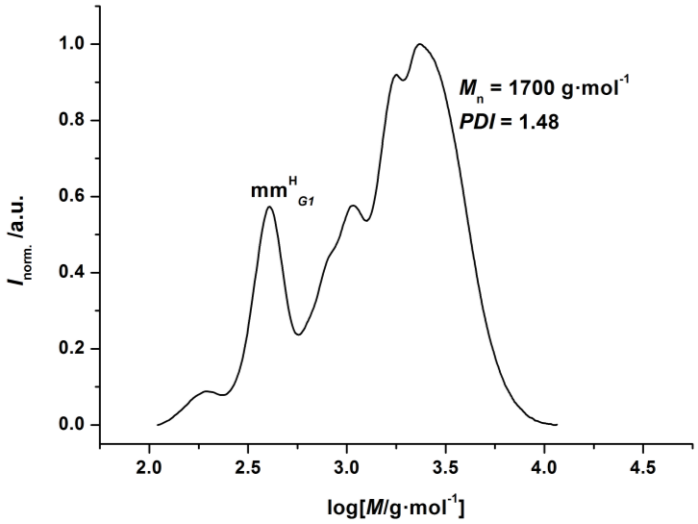


Figure S7. SEC chromatogram of **p(11b)-*co*-ea mm**. The peak on the left hand side represents the residual monomer whereas the shifted trace on the right hand side shows the distribution of the copolymerization product

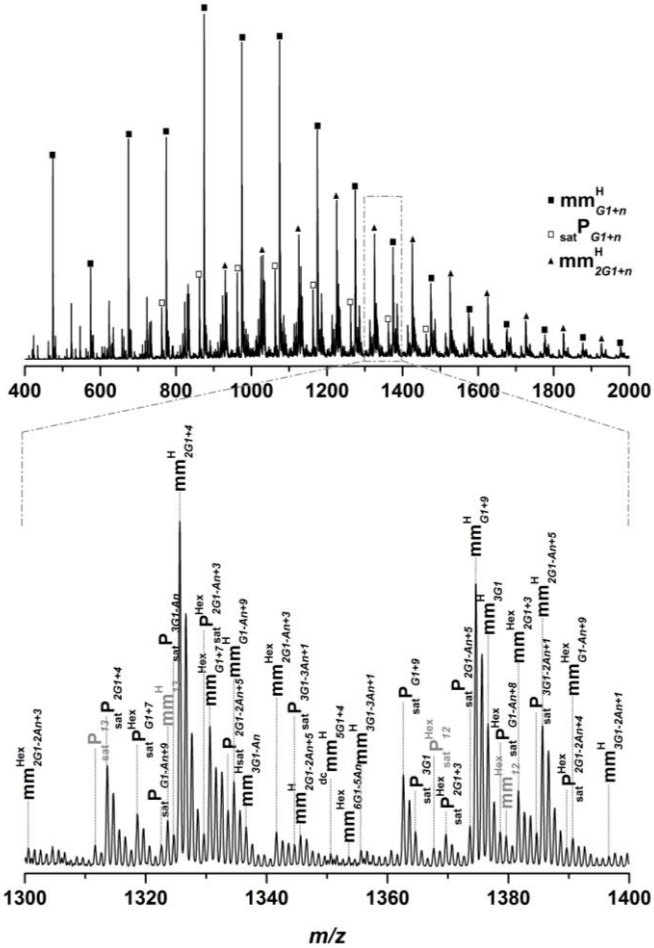


Figure S8. ESI-MS spectrum of **p(11b)-*co*-ea mm**. The overall spectrum (above) and the zoom spectrum to a repeat unit (100.05 Da EA) (below) are depicted. The polymer was synthesized via high temperature acrylate polymerization in solution of hexyl acetate with 2.5 wt% monomer and 2.5 wt% EA at 140 °C in an oxygen free atmosphere with $5 \cdot 10^{-3}$ mol L^{-1} AIBN.

Table S5. Theoretical and experimental *m/z* ratios of the species of **p(11b)-*co*-ea mm** identified via the ESI-MS measurements. The resolution is close to 0.1 amu. (see Figure S8). Listed below are the single charged sodium species $[MNa]^+$ if not otherwise specified.

spezies	G1	G1-An	EA	$m/z_{theo.}$	$m/z_{exp.}$	Δ *m/z*
mm^{Hex}	2	2	4	1317.69	1317.60	0.09
$_{sat}$P	3	3	2	1318.66	1318.60	0.06
$_{sat}$P	1	0	9	1320.68	1320.60	0.08
mm^{H}	0	0	13	1323.67	1323.68	0.01
mm^{Hex}	3	2	0	1326.71	1326.60	0.11
$_{sat}$P	2	0	5	1329.69	1329.60	0.09
mm^{H}	3	3	2	1330.66	1330.60	0.06
mm^{H}	1	0	9	1332.68	1332.60	0.08
$_{sat}$P^{Hex}	1	1	8	1336.71	1336.60	0.11
$_{sat}$P	3	0	1	1338.71	1338.64	0.07
mm^{H}	2	0	5	1341.69	1341.60	0.09
$_{sat}$P^{Hex}	2	1	4	1345.73	1345.60	0.13
mm^{Hex}	1	1	8	1348.71	1348.60	0.11
$_{sat}$P	2	2	6	1349.68	1349.60	0.08
mm^{H}	3	0	1	1350.71	1350.60	0.11
$_{sat}$P^{Hex}	3	1	0	1354.74	1354.64	0.10
mm^{Hex}	2	1	4	1357.73	1357.60	0.13
$_{sat}$P	3	2	2	1358.70	1358.60	0.10
mm^{H}	2	2	6	1361.68	1361.60	0.08
mm^{Hex}	2	0	1	1366.74	1366.60	0.14
$_{sat}$P^{Hex}	0	0	12	1367.73	1367.60	0.13
mm^{H}	3	2	2	1370.70	1370.60	0.10
$_{sat}$P^{Hex}	3	3	1	1374.73	1374.64	0.09
$_{sat}$P^{Hex}	1	0	8	1376.75	1376.64	0.11
mm^{Hex}	0	0	12	1379.73	1379.68	0.05
$_{sat}$P	1	1	10	1380.70	1380.60	0.10
$_{sat}$P^{Hex}	2	0	0	1385.76	1385.64	0.12
mm^{Hex}	3	0	1	1386.73	1386.64	0.09
mm^{Hex}	1	0	8	1388.75	1388.64	0.11
$_{sat}$P	2	1	6	1389.72	1389.64	0.08
mm^{H}	1	1	10	1392.70	1392.60	0.10
$_{sat}$P^{Hex}	3	0	0	1394.77	1394.60	0.17
mm^{Hex}	2	0	4	1397.76	1397.64	0.12
$_{sat}$P	3	1	2	1398.73	1398.64	0.09
mm^{H}	2	1	6	1401.72	1401.60	0.12

spezies	G1	G1-An	EA	$m/z_{theo.}$	$m/z_{exp.}$	Δ m/z
$_{sat}$**P**	2	2	5	1405.75	1405.64	0.11
mm^{Hex}	3	0	0	1406.77	1406.64	0.13
mm^{H}	3	1	2	1410.73	1410.60	0.13
$_{sat}$**P**	0	0	14	1411.72	1411.64	0.08

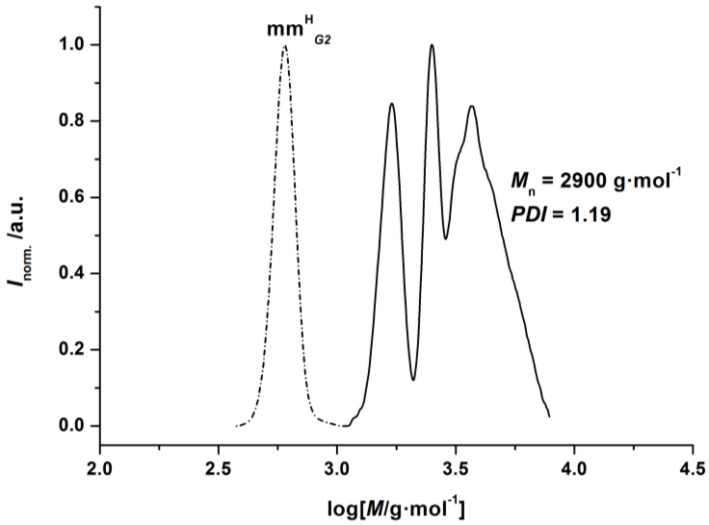


Figure S9. SEC chromatogram of **p(12a) mm**. The trace on the left hand side (dashed) represents the residual monomer whereas the trace on the right hand side shows the distribution after the polymerization. Both traces have been analysed and normalized separately.

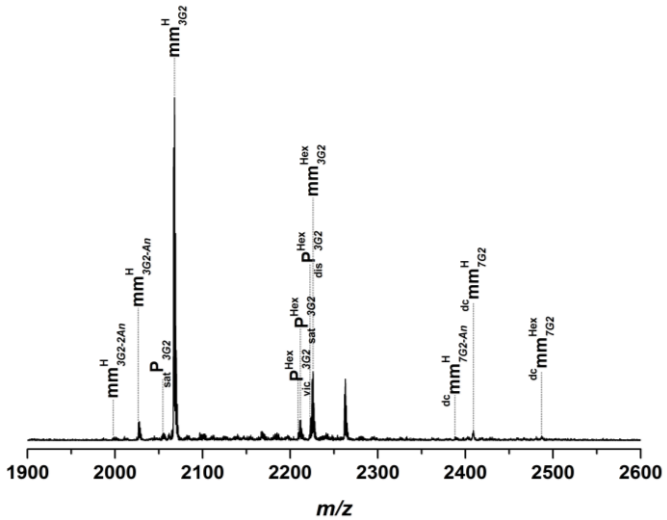


Figure S10. ESI-MS spectrum of **p(12a) mm**. The zoom spectrum to a repeat unit (681.35 Da) is depicted. The polymer was synthesized via high temperature acrylate polymerization in solution of hexyl acetate with 5 wt% monomer at 140 °C in an oxygen free atmosphere with $5 \cdot 10^{-3}$ mol L^{-1} AIBN.

Table S6. Theoretical and experimental *m/z* ratios of the species of **p(12a) mm** identified via the ESI-MS measurements. The resolution is close to 0.1 amu. (see Figure S10). Listed below are the single charged sodium species $[M+Na]^+$ if not otherwise specified.

species	G3	- An	$m/z_{theo.}$	$m/z_{exp.}$	$\Delta\ m/z$
$\mathbf{mm^H}$	3	2	1986.97	1986.82	0.15
$\mathbf{mm^H}$	3	1	2027.00	2026.82	0.18
$\mathbf{_{sat}P}$	3	0	2055.03	2055.00	0.03
$\mathbf{mm^H}$	3	0	2067.03	2066.91	0.12
$\mathbf{mm^H\ [K]^+}$	3	0	2083.01	2083.00	0.01
$\mathbf{_{vic}P^{Hex}}$	3	0	2209.13	2209.09	0.04
$\mathbf{_{sat}P^{Hex}}$	3	0	2211.15	2210.91	0.24
$\mathbf{mm^{Hex}}$	3	0	2223.15	2223.00	0.15
$\mathbf{_{dis}P^{Hex}}$	3	0	2225.16	2225.09	0.07
unassigned				2261.91	
$\mathbf{_{sat}P\ dc}$	7	1	2383.16	2382.91	0.25
$\mathbf{mm^H\ dc}$	7	1	2389.16	2389.09	0.07
$\mathbf{_{sat}P\ dc}$	7	0	2403.19	2403.18	0.01
$\mathbf{mm^H\ dc}$	7	0	2409.19	2409.09	0.10
$\mathbf{_{sat}P^{Hex}\ dc}$	7	0	2481.30	2481.00	0.30
$\mathbf{mm^{Hex}\ dc}$	7	0	2487.30	2487.09	0.21

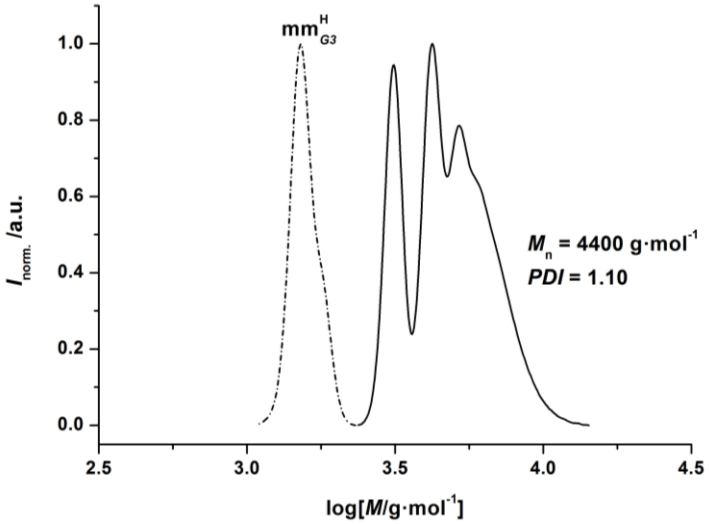


Figure S11. SEC chromatogram of **p(13a) mm**. The trace on the left hand side (dashed) represents the residual monomer whereas the trace on the right hand side shows the distribution after the polymerization. Both traces have been analysed and normalized separately.

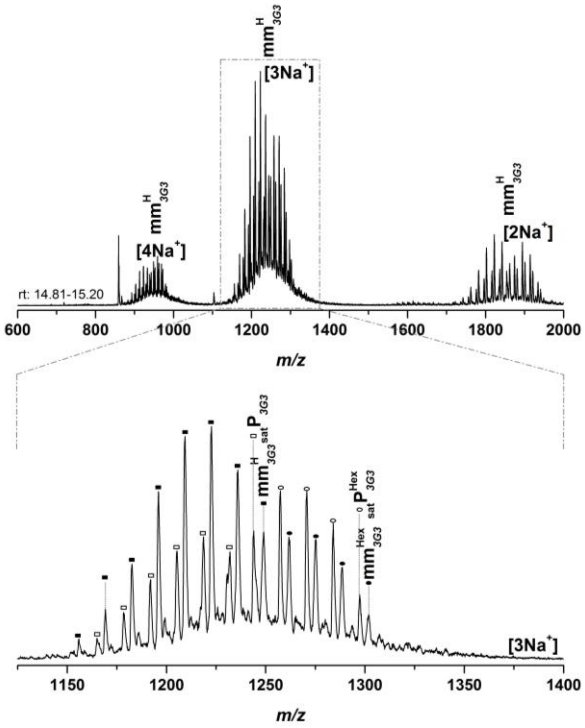


Figure S12. SEC-ESI-MS spectrum of **p(13a) mm**. The spectrum at a specific retention time (14.81-15.20 min) is shown above, whereas the spectrum below represents the zoom to the detected triple charged species. The polymer was synthesized via high temperature acrylate polymerization in solution of hexyl acetate with 5 wt% monomer at 140 °C in an oxygen free atmosphere with $5 \cdot 10^{-3}$ mol L^{-1} AIBN.

Table S7. Theoretical and experimental *m/z* ratios of the species of **p(13a) mm** identified via the SEC-ESI-MS measurements. The resolution is close to 0.1 amu. (see Figure S12). Listed below are the triple charged sodium species $[M+3Na]^{3+}$ if not otherwise specified.

species	G3	- An	*m/z* theo.	*m/z* exp.	Δ *m/z*
$\mathbf{mm^H}$	3	7	1155.87	1155.83	0.04
$\mathbf{^{sat}P}$	3	6	1165.22	1165.00	0.22
$\mathbf{mm^H}$	3	6	1169.22	1169.25	0.03
$\mathbf{_{sat}P}$	3	5	1178.58	1178.33	0.25
$\mathbf{mm^H}$	3	5	1182.58	1182.67	0.09
$\mathbf{_{sat}P}$	3	4	1191.93	1191.92	0.01
$\mathbf{mm^H}$	3	4	1195.93	1195.92	0.01
$\mathbf{_{sat}P}$	3	3	1205.29	1205.25	0.04
$\mathbf{mm^H}$	3	3	1209.29	1209.33	0.04
$\mathbf{_{sat}P}$	3	2	1218.64	1218.58	0.06
$\mathbf{mm^H}$	3	2	1222.64	1222.67	0.03
$\mathbf{_{sat}P^{Hex}}$	3	5	1230.65	1230.58	0.07
$\mathbf{_{sat}P}$	3	1	1231.99	1232.00	0.01
$\mathbf{mm^H}$	3	1	1235.99	1235.92	0.07

species	G3	- An	m/z theo.	m/z exp.	Δ m/z
$_{sat}\mathbf{P}^{Hex}$	3	4	1244.00	1243.92	0.08
$\mathbf{mm}^{Hex}$	3	4	1248.00	-	
$\mathbf{mm}^{H}$	3	0	1249.35	1248.92	0.43
$_{sat}\mathbf{P}^{Hex}$	3	3	1257.36	1257.33	0.03
$\mathbf{mm}^{Hex}$	3	3	1261.36	1261.67	0.31
$_{sat}\mathbf{P}^{Hex}$	3	2	1270.71	1270.67	0.04
$\mathbf{mm}^{Hex}$	3	2	1274.71	1275.00	0.29
$_{sat}\mathbf{P}^{Hex}$	3	1	1284.07	1284.00	0.07
$\mathbf{mm}^{Hex}$	3	1	1288.07	1288.33	0.26
$_{sat}\mathbf{P}^{Hex}$	3	0	1297.42	1297.33	0.09
$\mathbf{mm}^{Hex}$	3	0	1301.42	1301.83	0.41

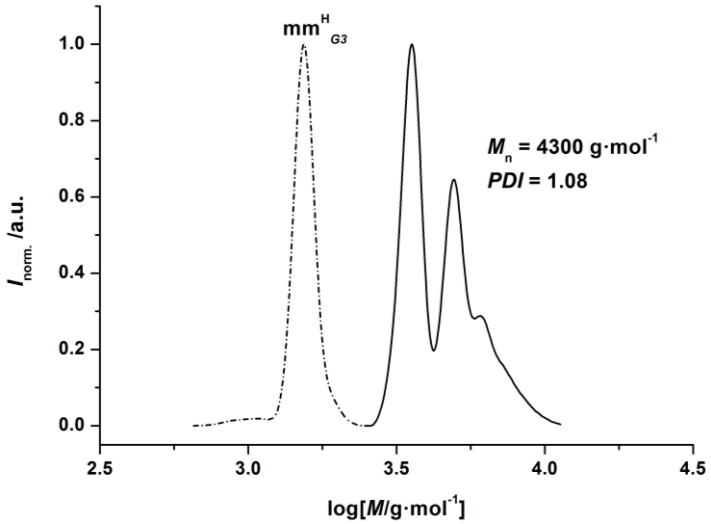


Figure S13. SEC chromatogram of **p(13b) mm**. The trace on the left hand side (dashed) represents the residual monomer whereas the trace on the right hand side shows the distribution after the polymerization. Both traces have been analysed and normalized separately to focus on the formation of species with higher molecular weight.

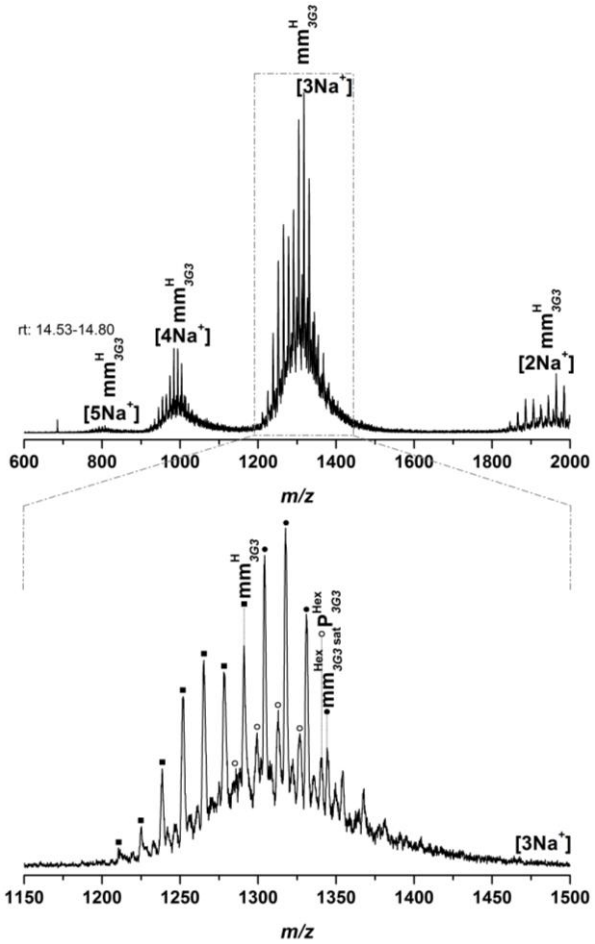


Figure S14. SEC-ESI-MS spectrum of **p(13b) mm**. The spectrum at a specific retention time (14.53-14.80 min) is shown above, whereas the spectrum below represents the zoom to the detected triple charged species. The polymer was synthesized via high temperature acrylate polymerization in solution of hexyl acetate with 5 wt% monomer at 140 °C in an oxygen free atmosphere with $5 \cdot 10^{-3}$ mol L^{-1} AIBN.

Table S8. Theoretical and experimental *m/z* ratios of the species of **p(13b) mm** identified via the ESI-MS measurements (see Figure S14).. The resolution is close to 0.1 amu. Listed below are the triple charged sodium species $[M+3Na]^{3+}$ if not otherwise specified. For the calculation the molar mass was used due to less resolution at higher charges.

species	G3	- An	$m/z_{\text{theo.}}$	$m/z_{\text{exp.}}$	Δ *m/z*
mm$^{\mathbf{H}}$	3	6	1211.30	1211.58	0.28
mm$^{\mathbf{H}}$	3	5	1224.66	1225.00	0.34
mm$^{\mathbf{H}}$	3	4	1238.01	1238.58	0.57[a]
mm$^{\mathbf{H}}$	3	3	1251.37	1252.00	0.63[a]
mm$^{\mathbf{H}}$	3	2	1264.72	1265.25	0.53[a]
$_{\text{sat}}$**P**$^{\mathbf{Hex}}$	3	5	1272.73	1272.00	0.73[a]
mm$^{\mathbf{H}}$	3	1	1278.07	1278.42	0.35
$_{\text{sat}}$**P**$^{\mathbf{Hex}}$	3	4	1286.08	1285.75	0.33
mm$^{\mathbf{H}}$	3	0	1291.43	1291.00	0.43
$_{\text{sat}}$**P**$^{\mathbf{Hex}}$	3	3	1299.44	1299.33	0.11
mm$^{\mathbf{Hex}}$	3	3	1303.44	1304.17	0.73[a]
$_{\text{sat}}$**P**$^{\mathbf{Hex}}$	3	2	1312.79	1313.00	0.21
mm$^{\mathbf{Hex}}$	3	2	1316.79	1317.58	0.79[a]
$_{\text{sat}}$**P**$^{\mathbf{Hex}}$	3	1	1326.15	1326.58	0.43
mm$^{\mathbf{Hex}}$	3	1	1330.15	1330.92	0.77[a]
$_{\text{sat}}$**P**$^{\mathbf{Hex}}$	3	0	1339.50	1340.33	0.83[a]
mm$^{\mathbf{Hex}}$	3	0	1343.50	1344.58	1.08[a]

[a] assignments outside experimental accuracy