

## Supporting information

# One-shot activating reagent of neodymium carboxylate for highly *cis*-1,4 specific butadiene polymerization

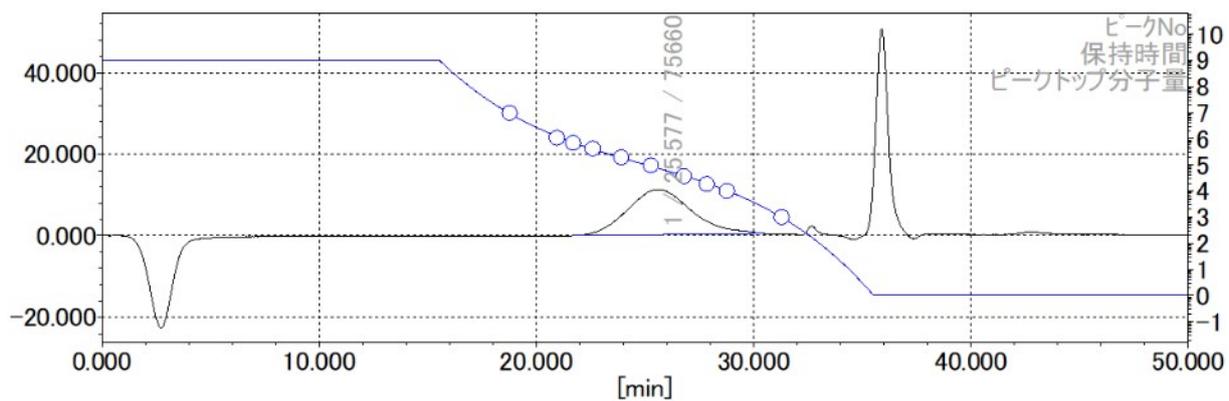
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Graduate School of Advanced Science and Engineering, Hiroshima University, 1-4-1 Kagamiyama, Higashi-Hiroshima 739-8527, Japan.

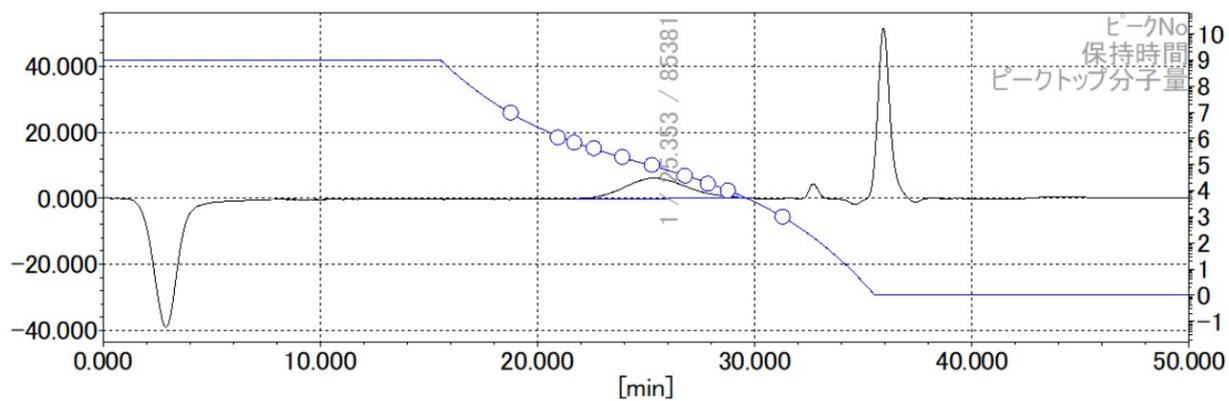
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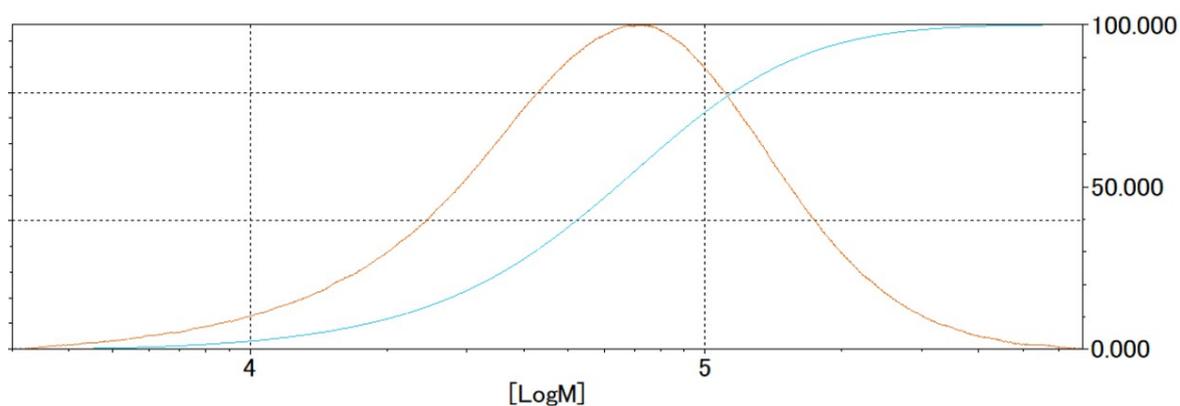
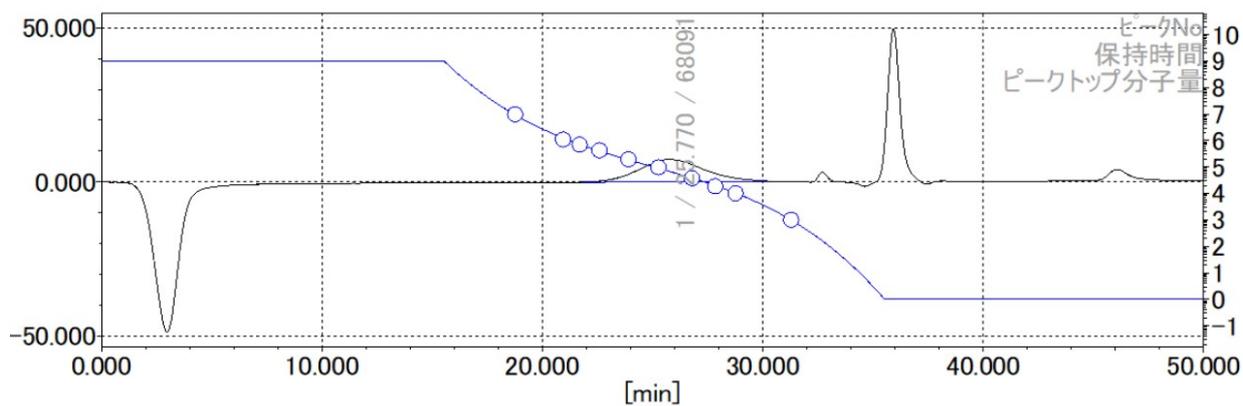
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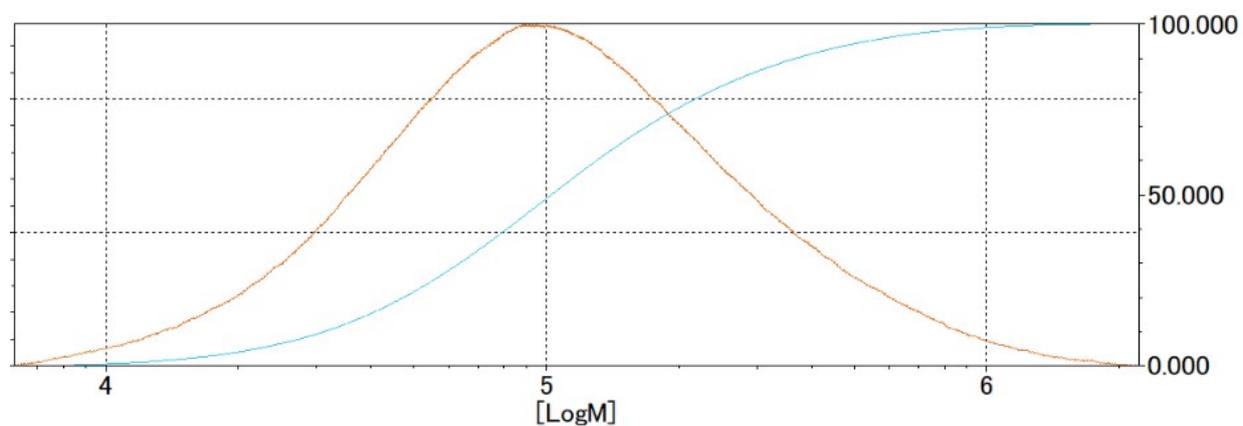
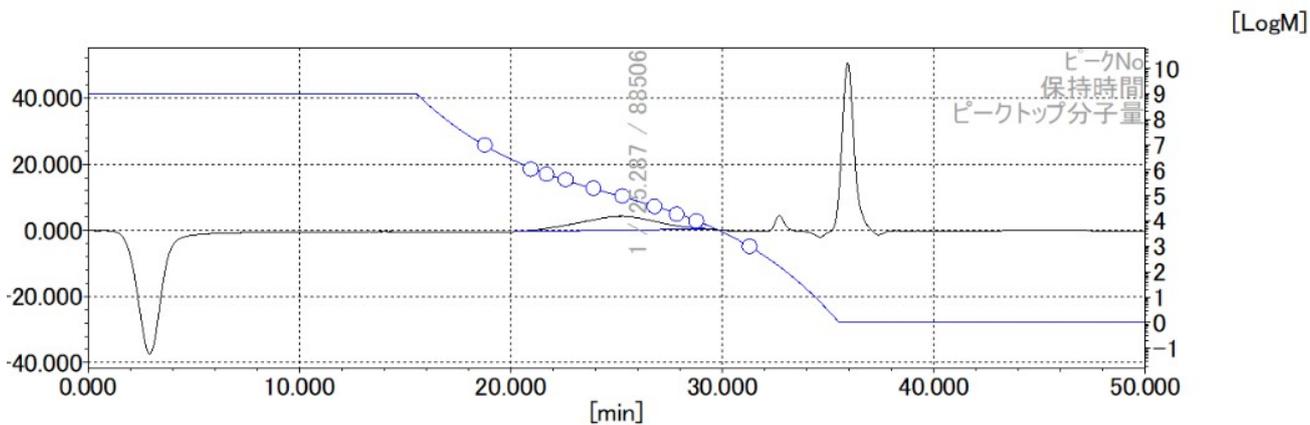
**Figure S1.** GPC traces of synthesized polybutadienes obtained in run 1.



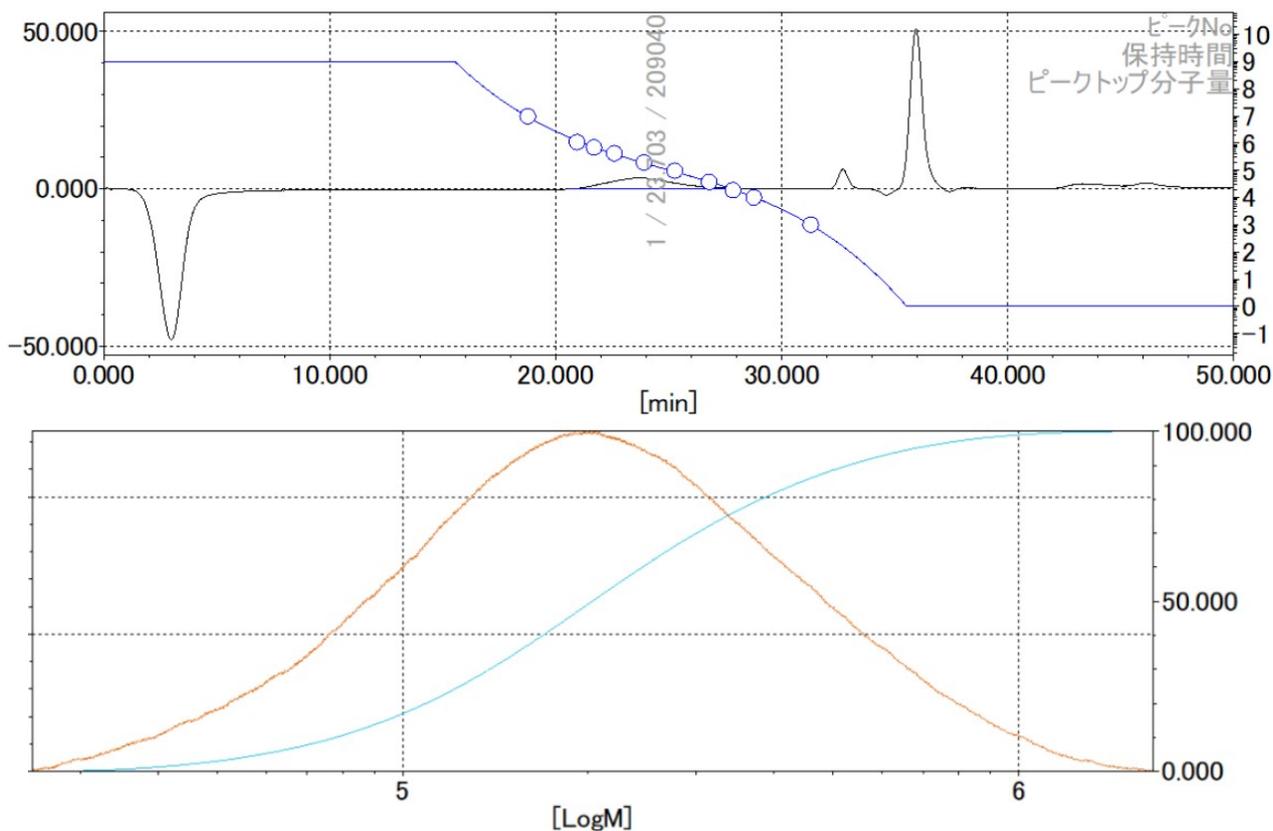
**Figure S2.** GPC traces of synthesized polybutadienes obtained in run 2.



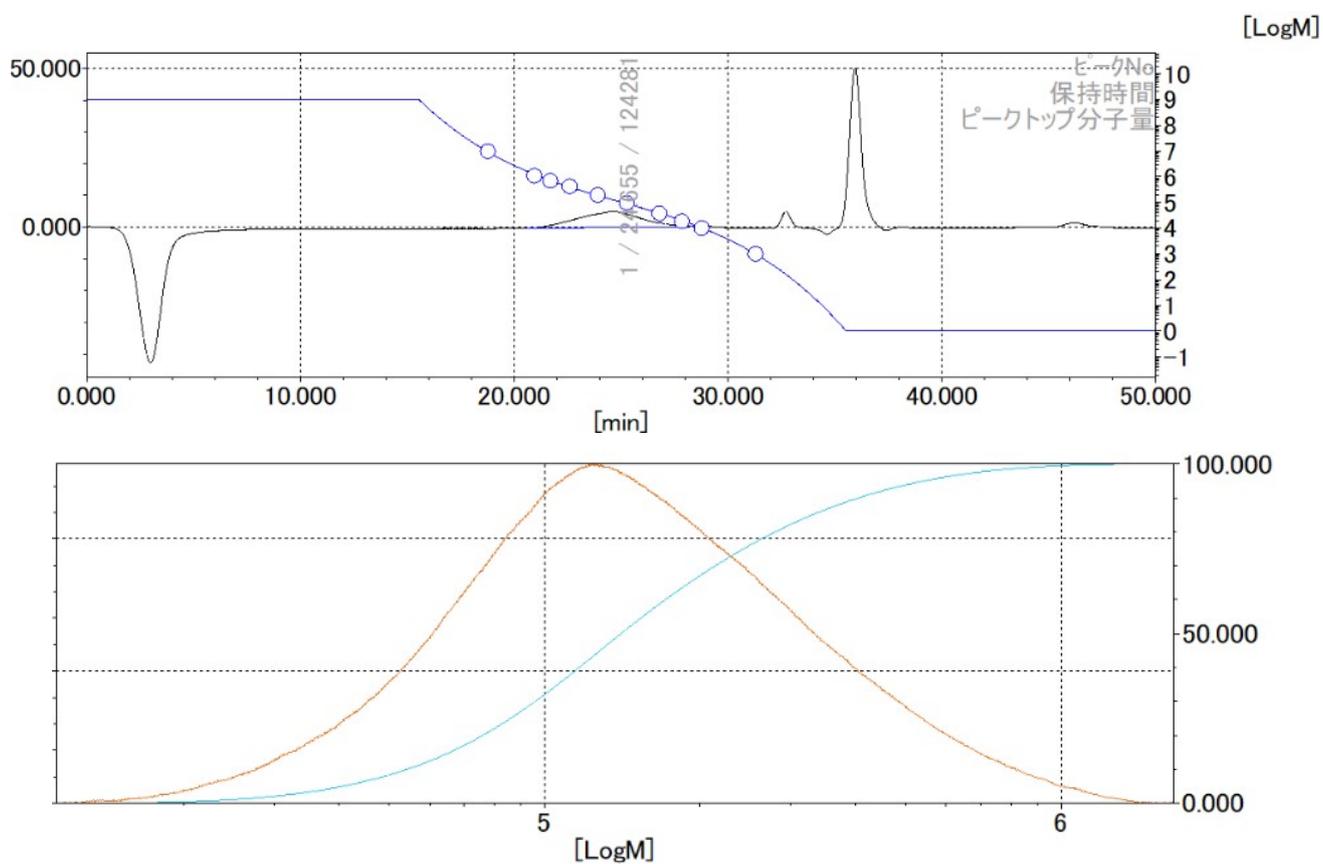
**Figure S3.** GPC traces of synthesized polybutadienes obtained in run 3.



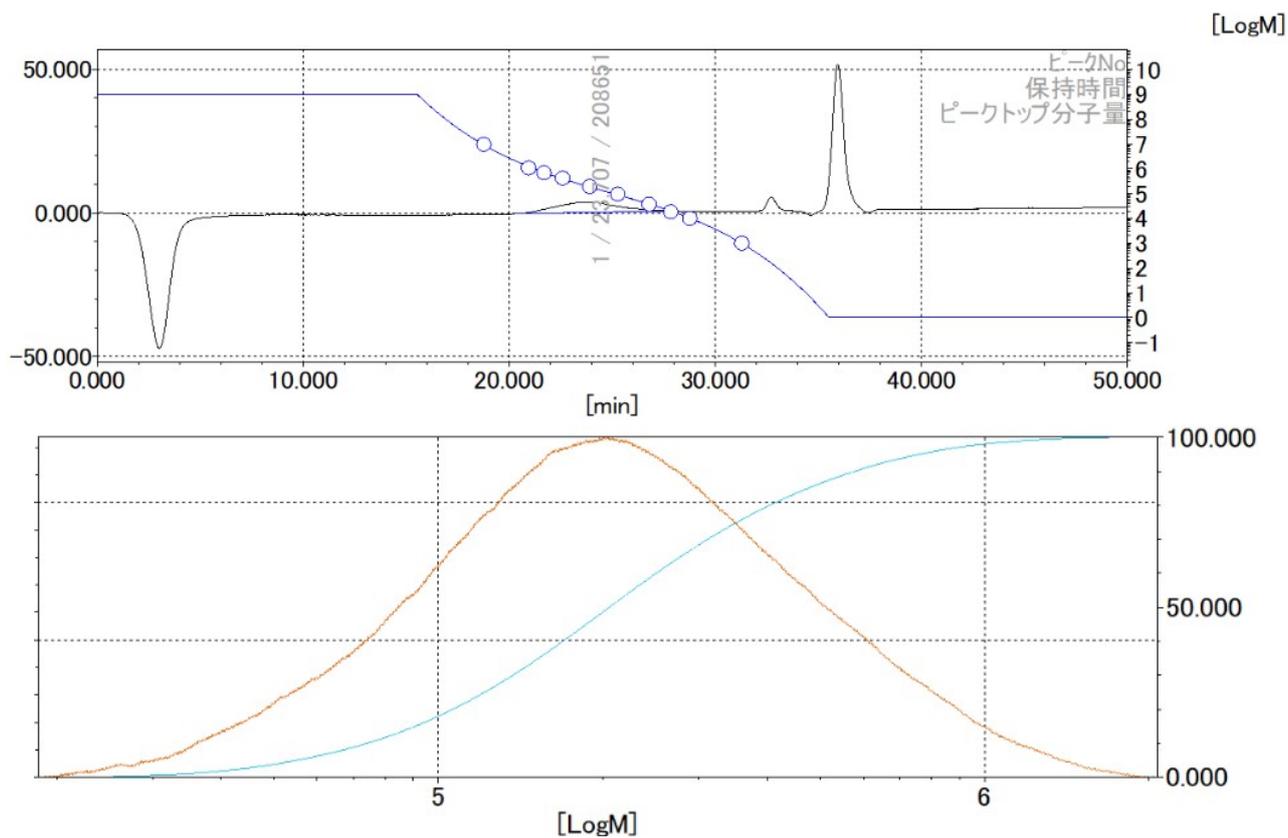
**Figure S4.** GPC traces of synthesized polybutadienes obtained in run 4.



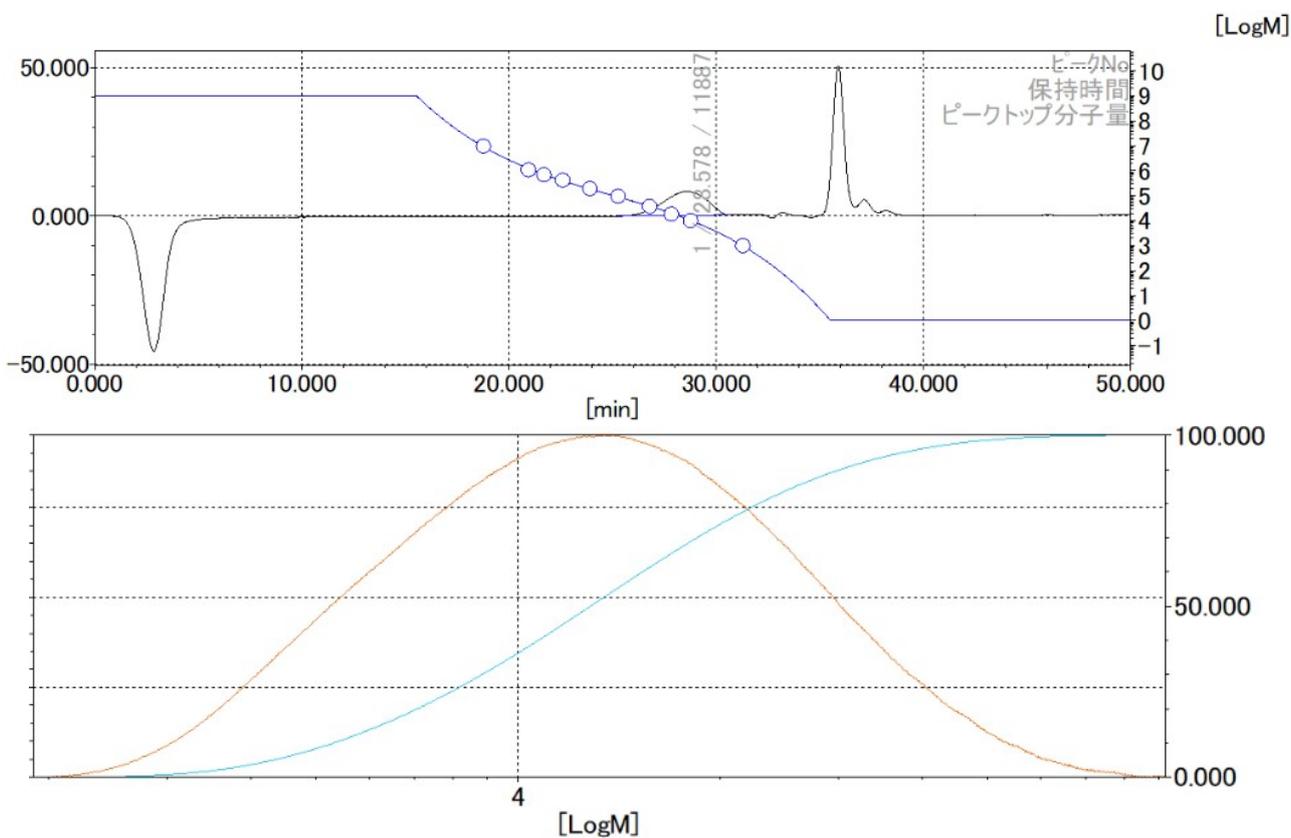
**Figure S5.** GPC traces of synthesized polybutadienes obtained in run 5.



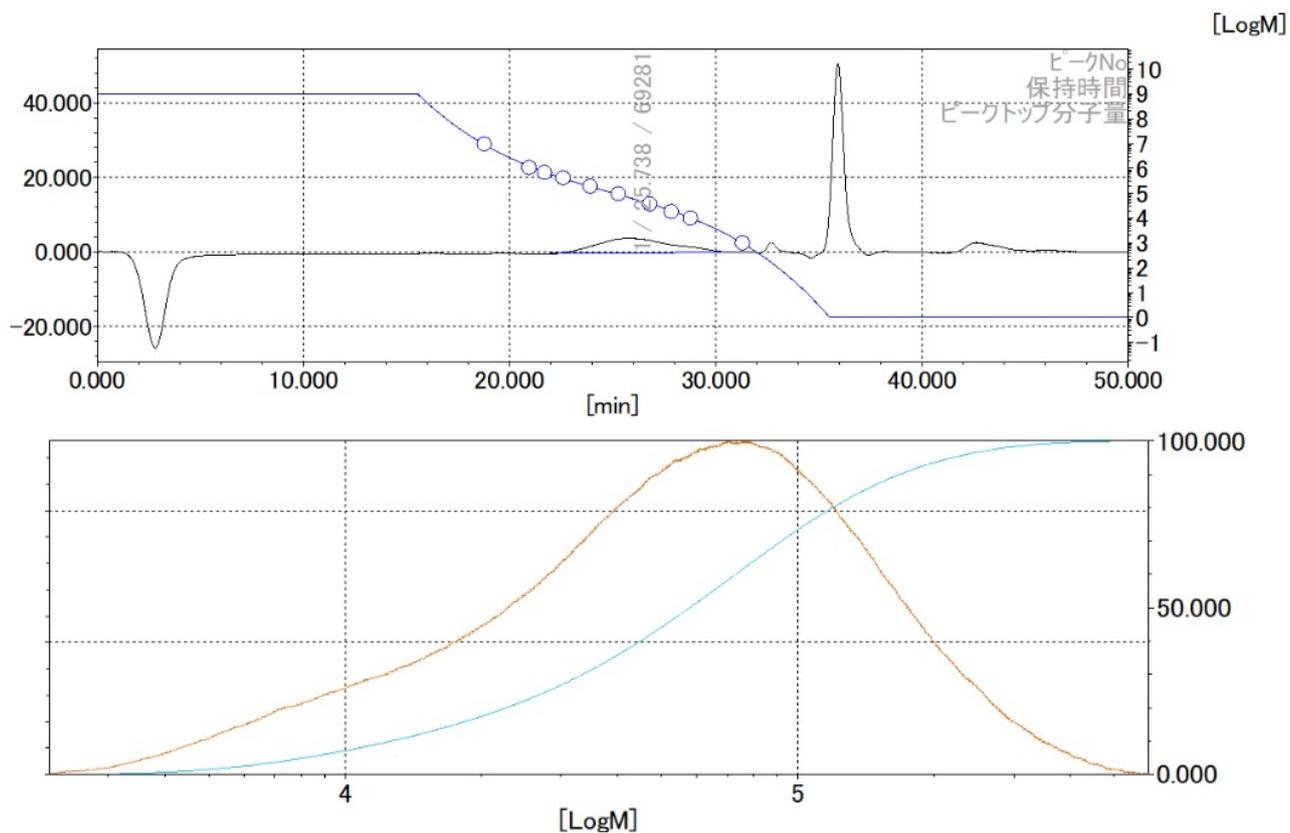
**Figure S6.** GPC traces of synthesized polybutadienes obtained in run 6.



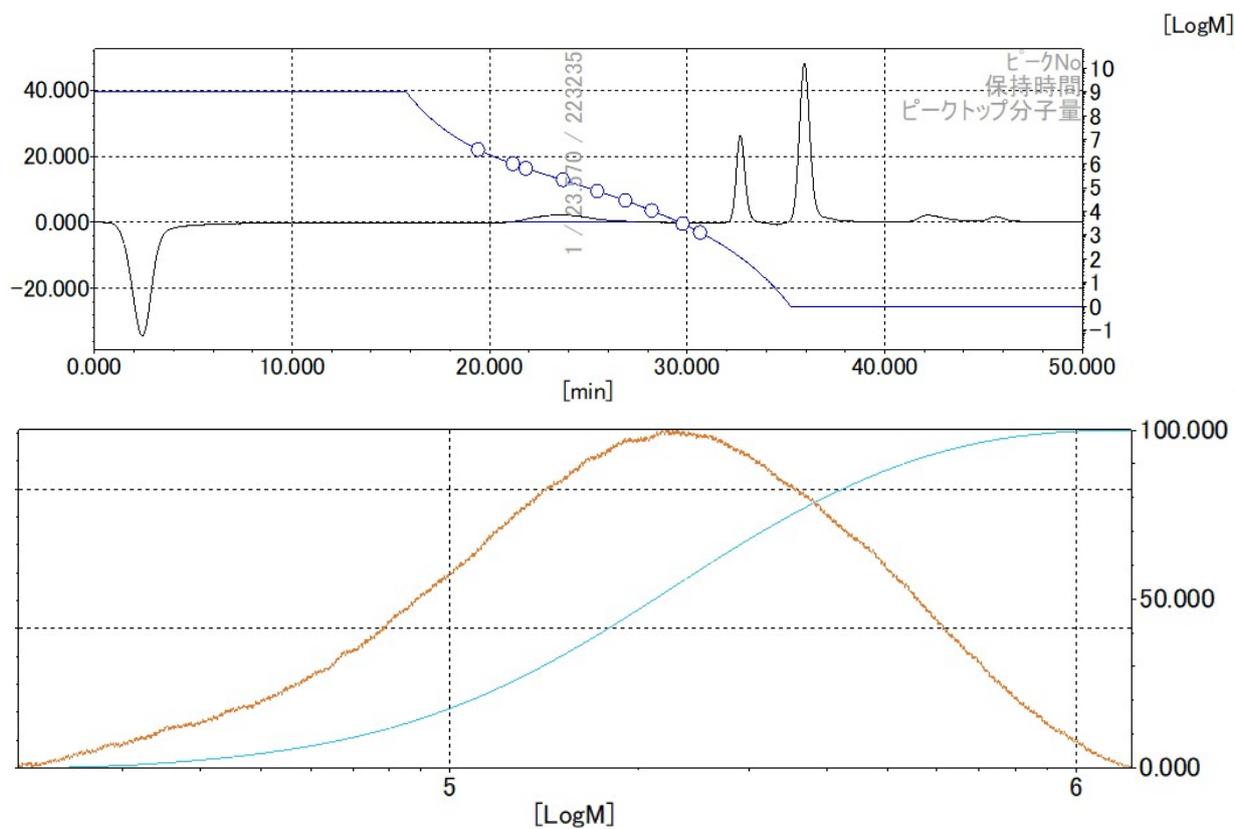
**Figure S7.** GPC traces of synthesized polybutadienes obtained in run 7.



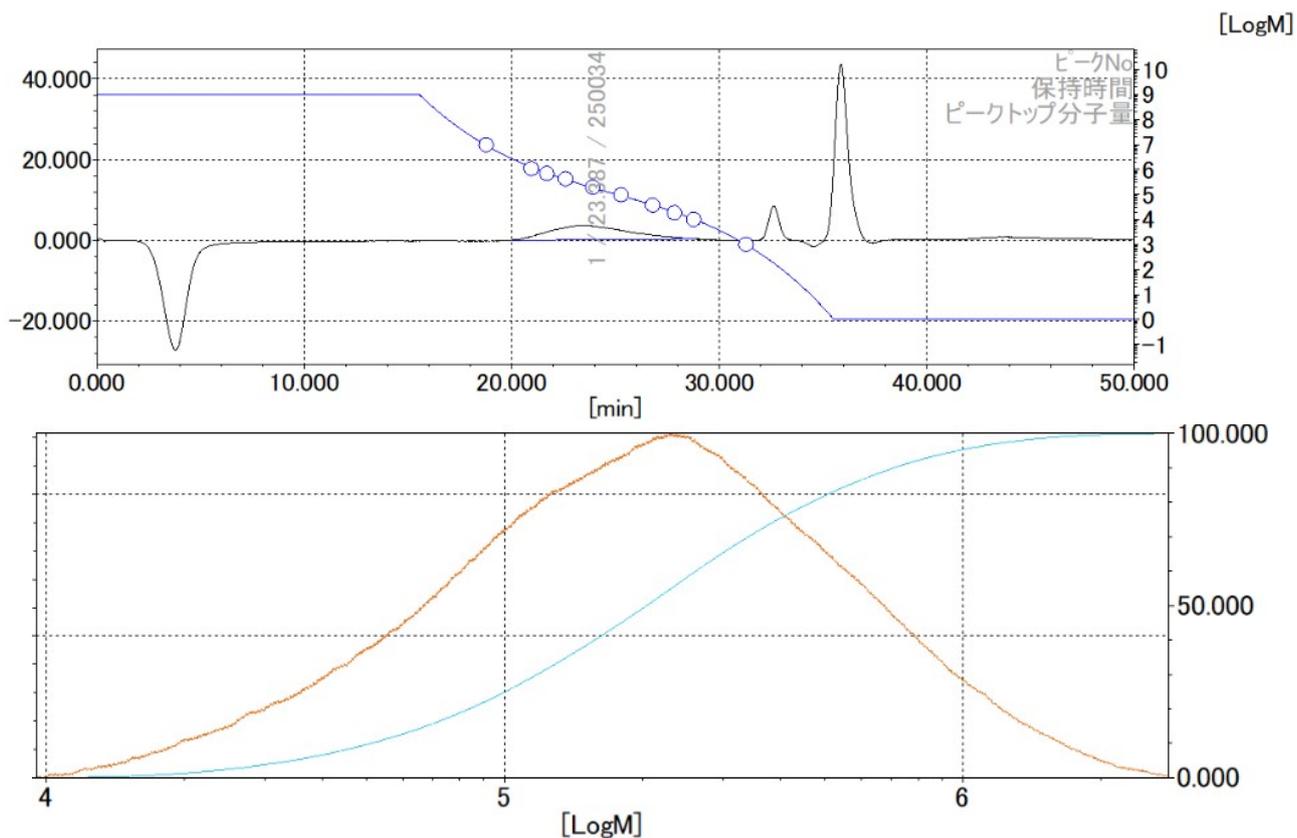
**Figure S8.** GPC traces of synthesized polybutadienes obtained in run 8.



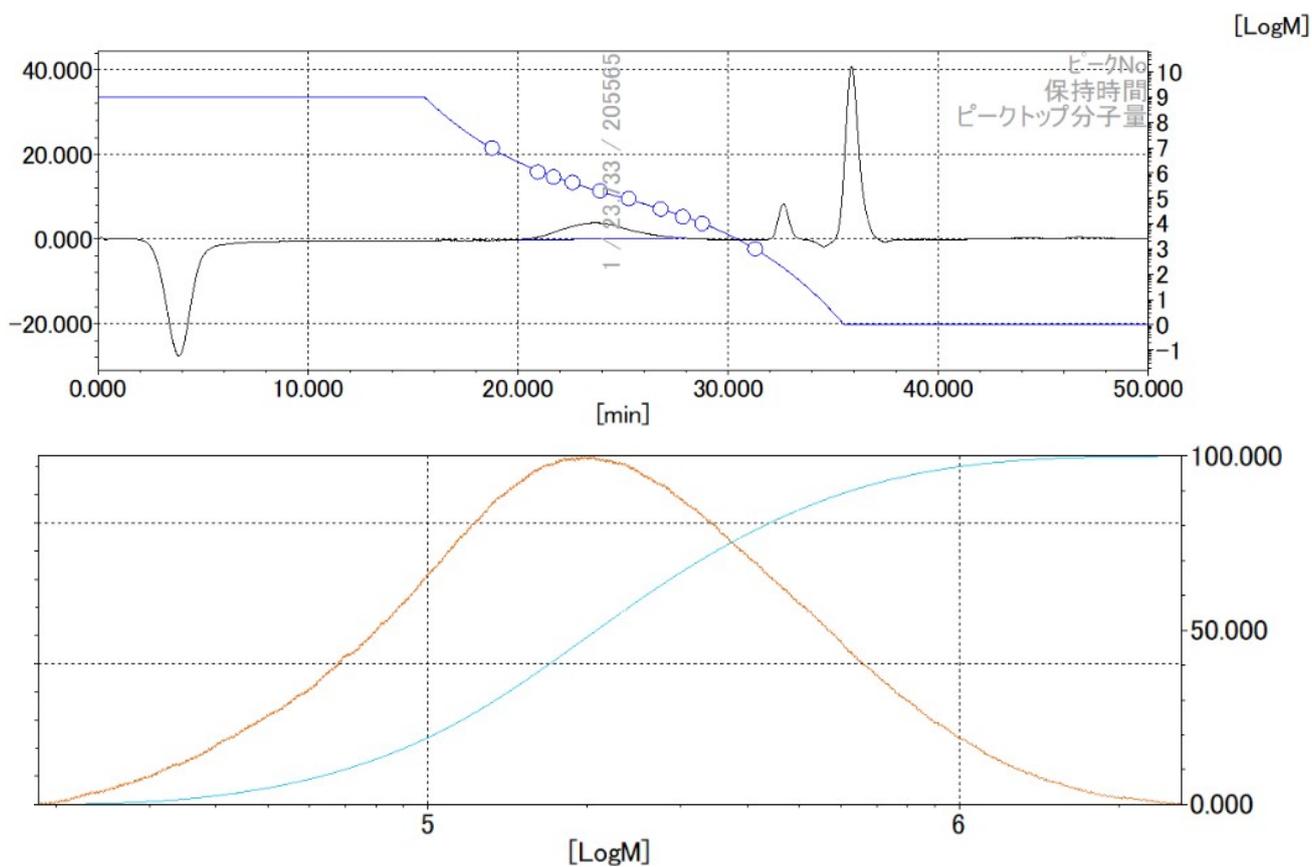
**Figure S9.** GPC traces of synthesized polybutadienes obtained in run 9.



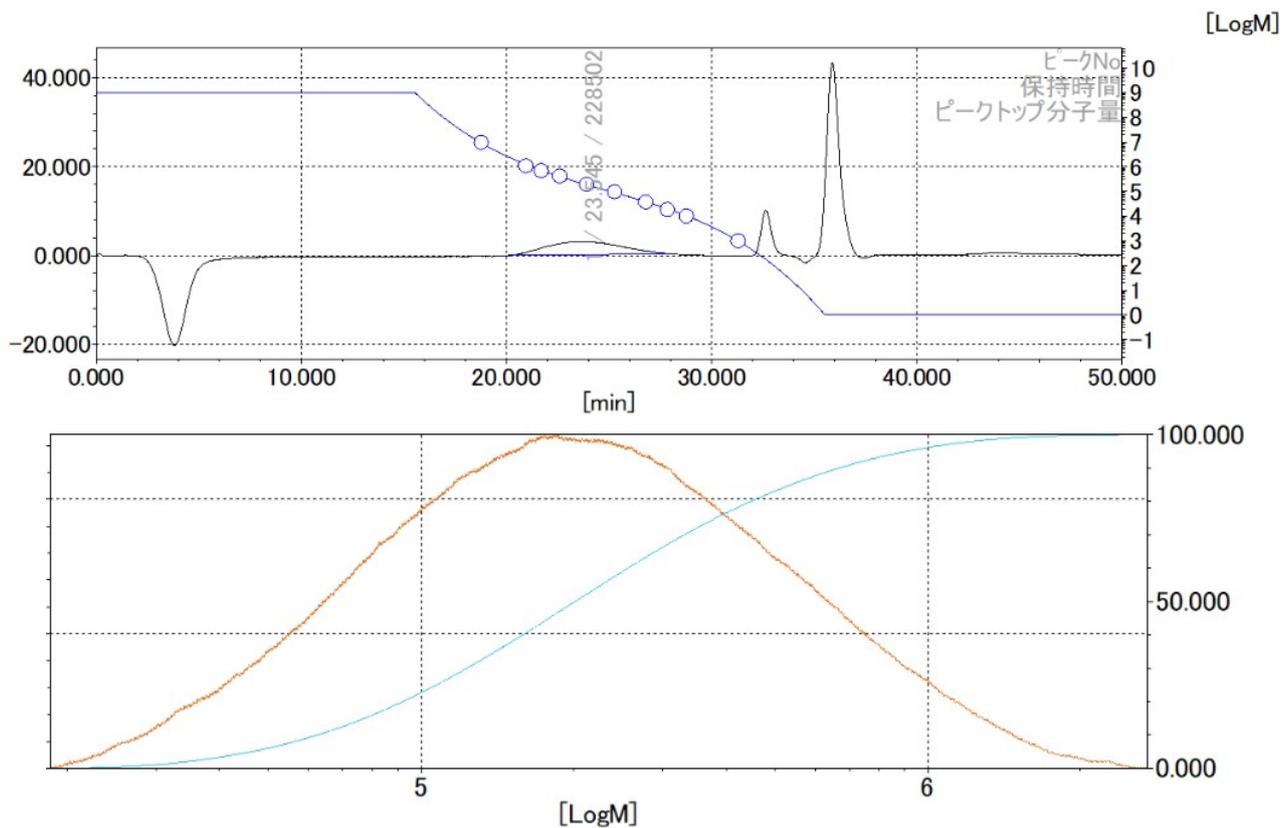
**Figure S10.** GPC traces of synthesized polybutadienes obtained in run 10.



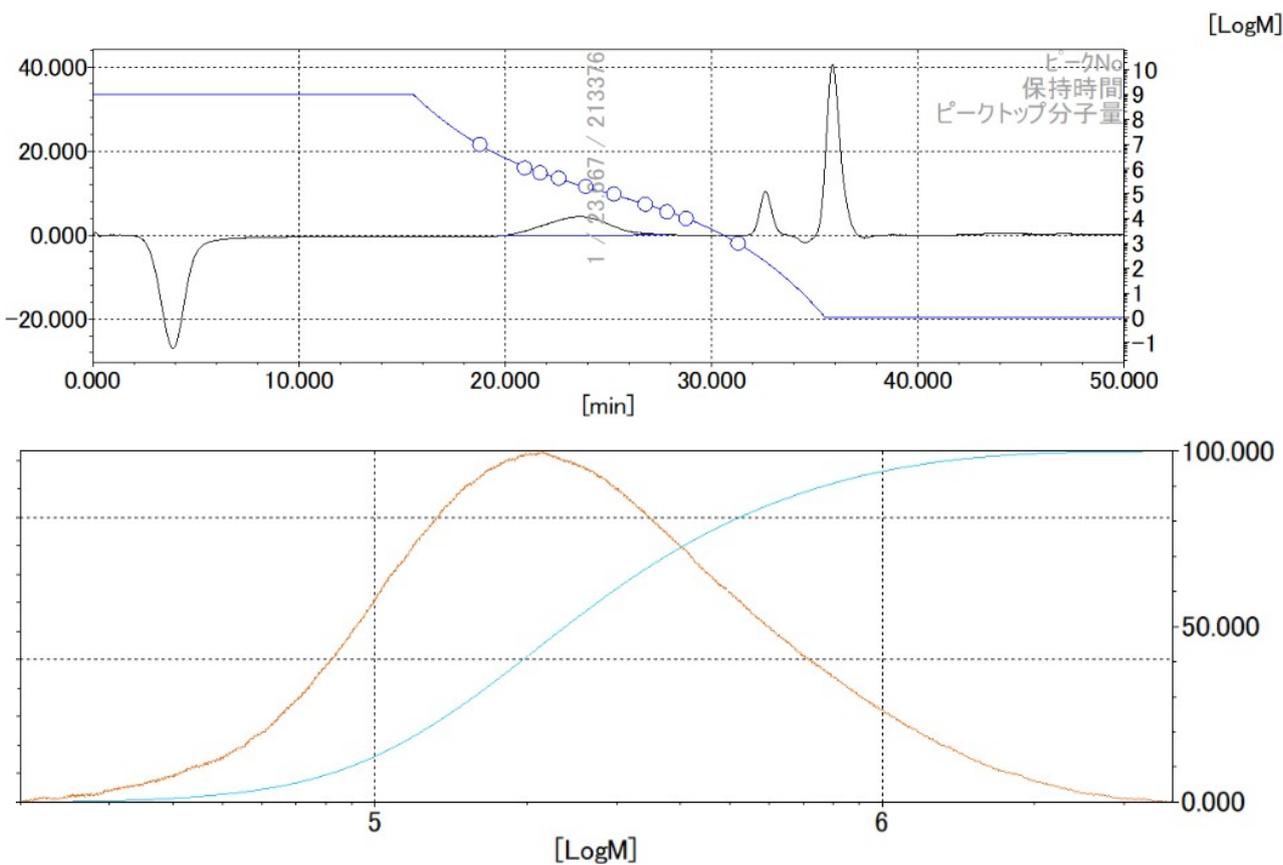
**Figure S11.** GPC traces of synthesized polybutadienes obtained in run 11.



**Figure S12.** GPC traces of synthesized polybutadienes obtained in run 12.



**Figure S13.** GPC traces of synthesized polybutadienes obtained in run 13.



**Figure S14.** GPC traces of synthesized polybutadienes obtained in run 14.

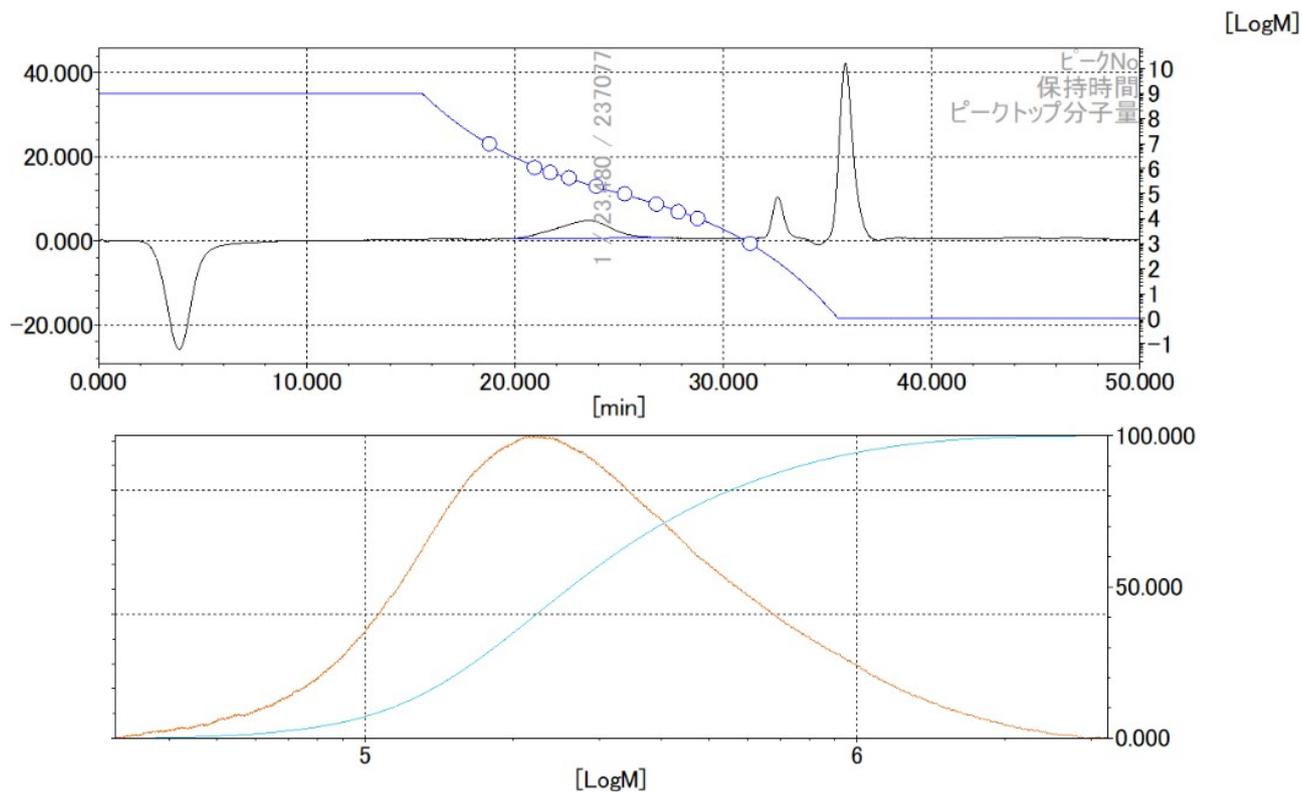


Figure S15. GPC traces of synthesized polybutadienes obtained in run 15.

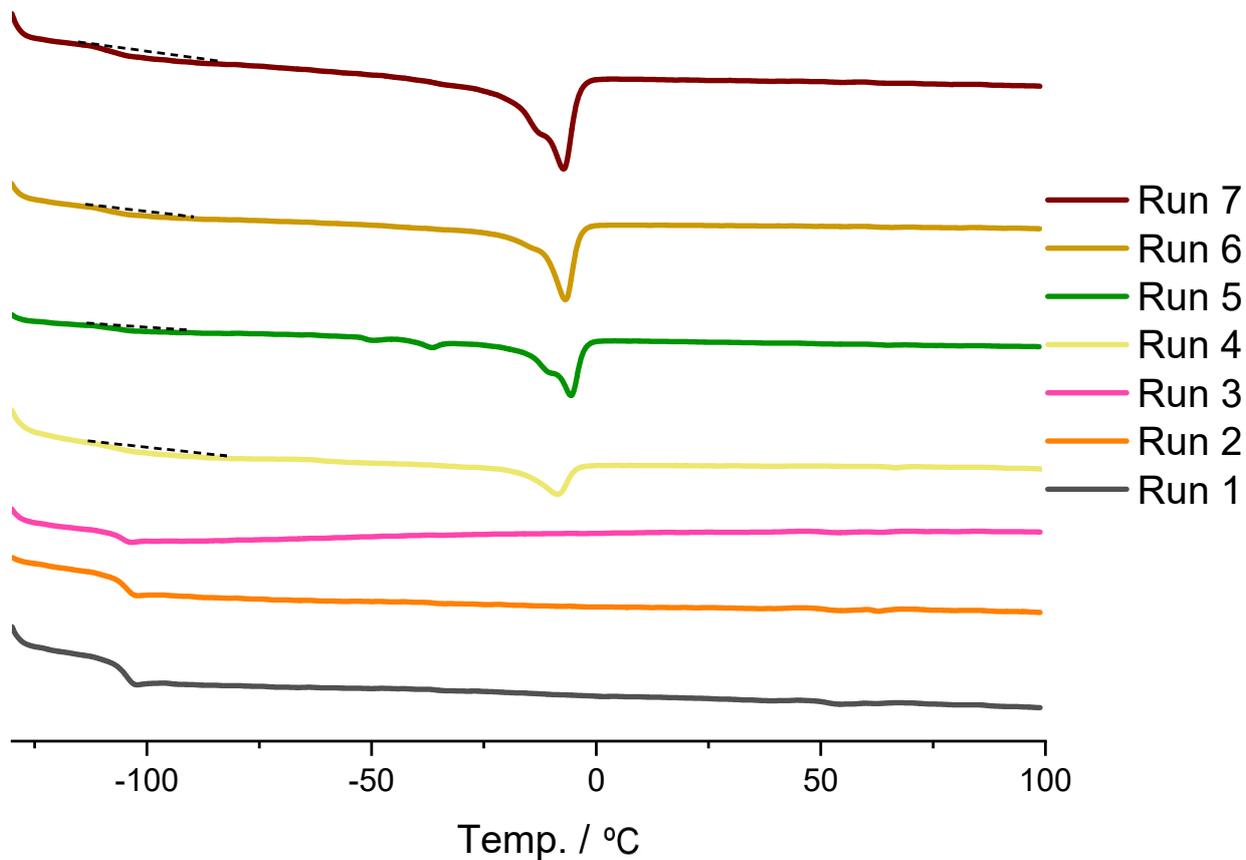
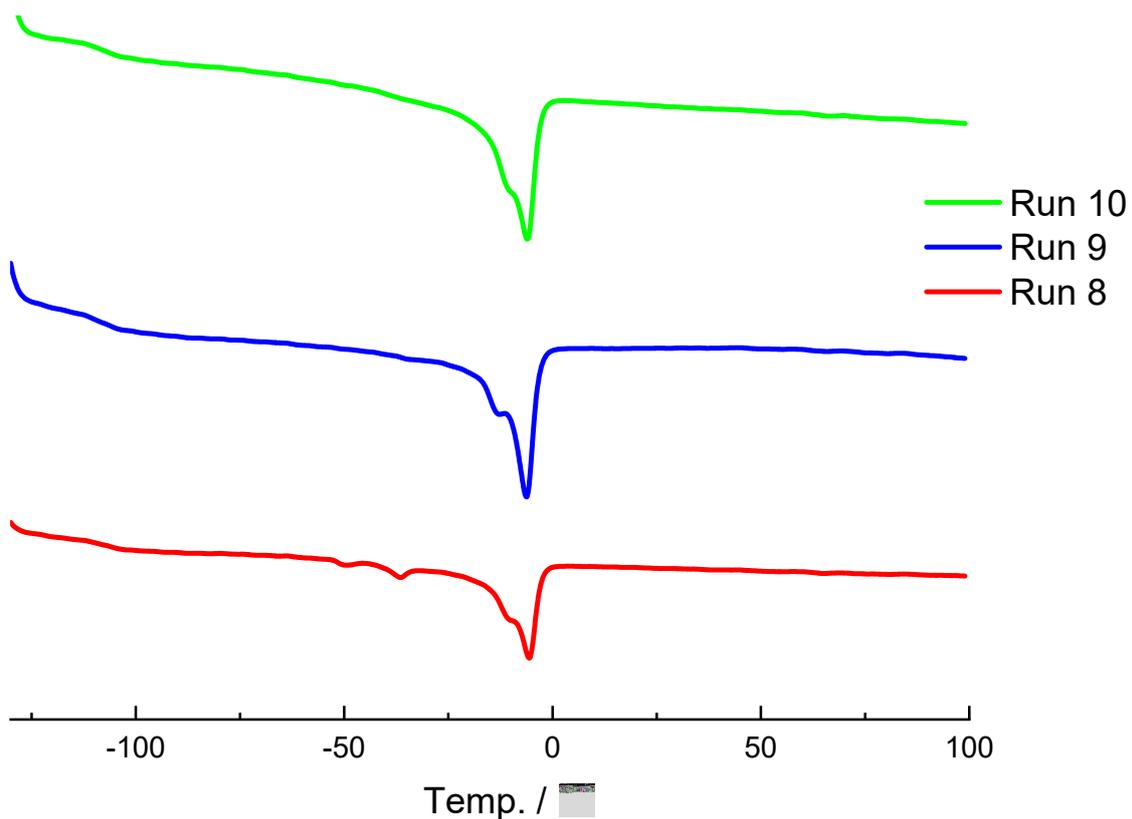
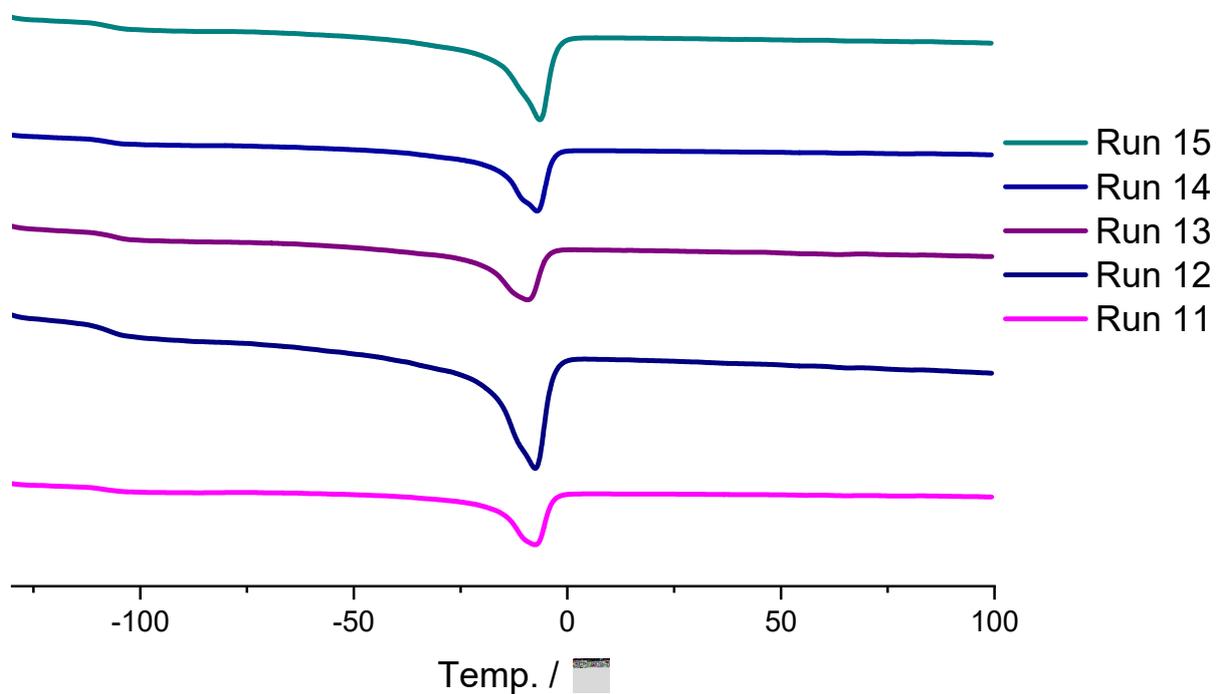


Figure S16. DSC traces of the polybutadienes obtained in Table 1.

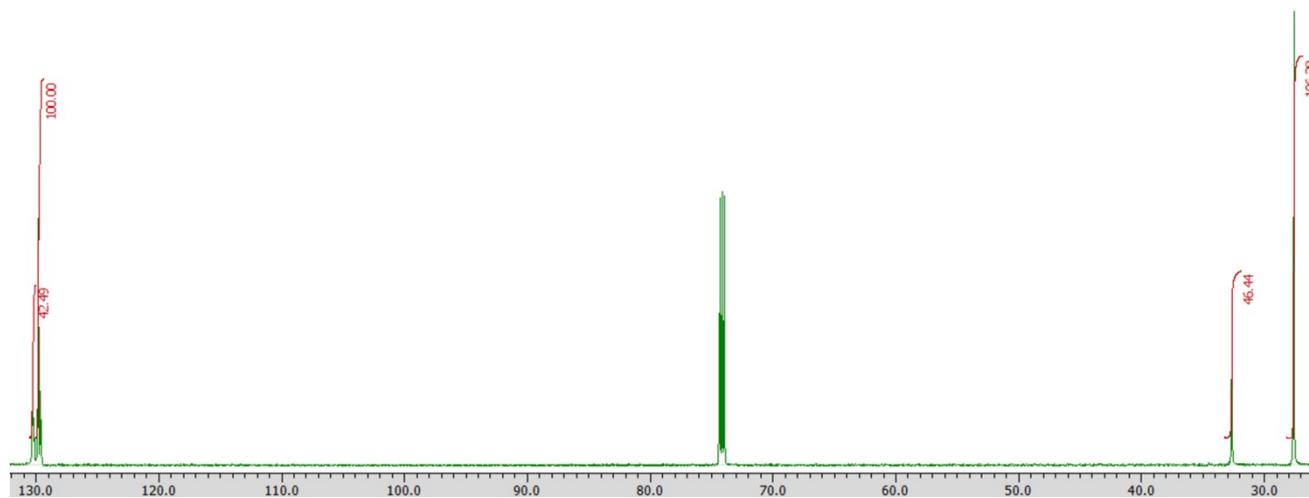


**Figure S17.** DSC traces of the polybutadienes obtained in Table 2.



**Figure S18.** DSC traces of the polybutadienes obtained in Table 3.

Run 1



Run 5

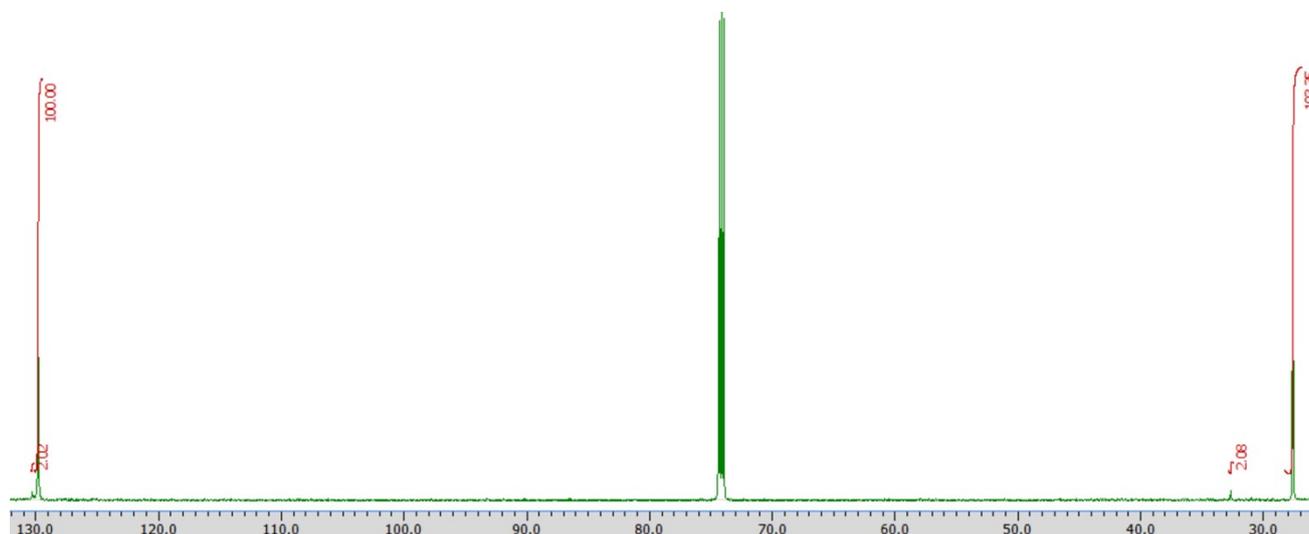
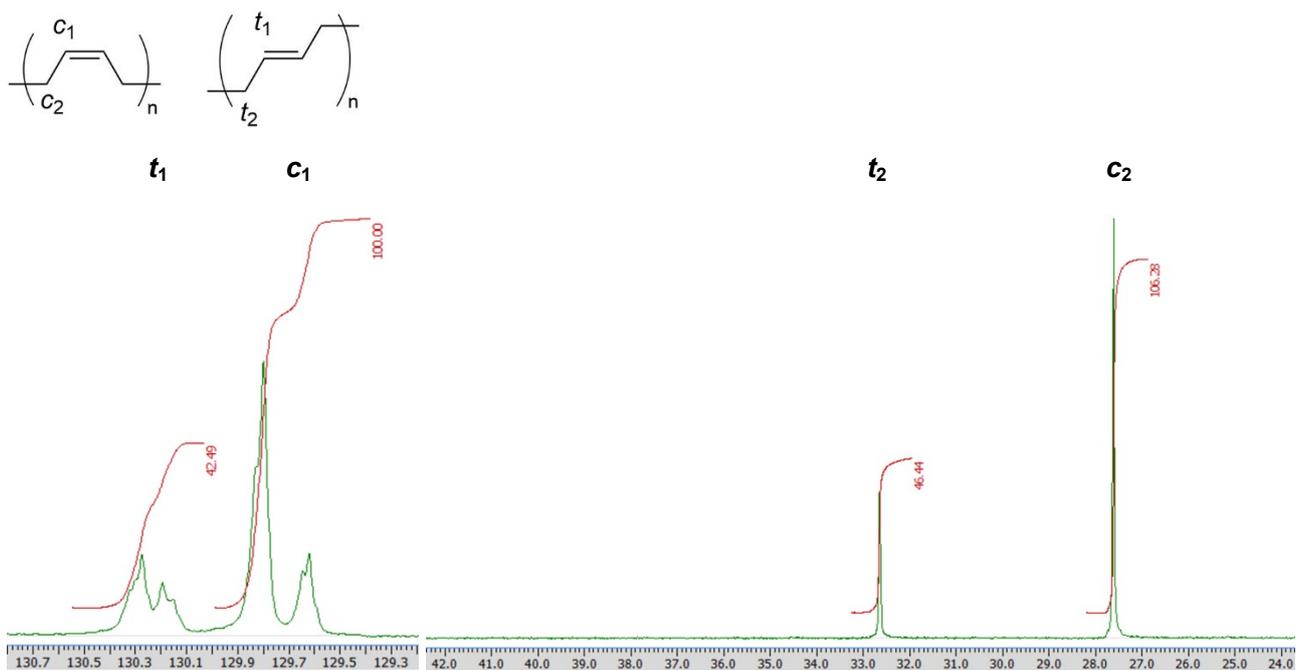
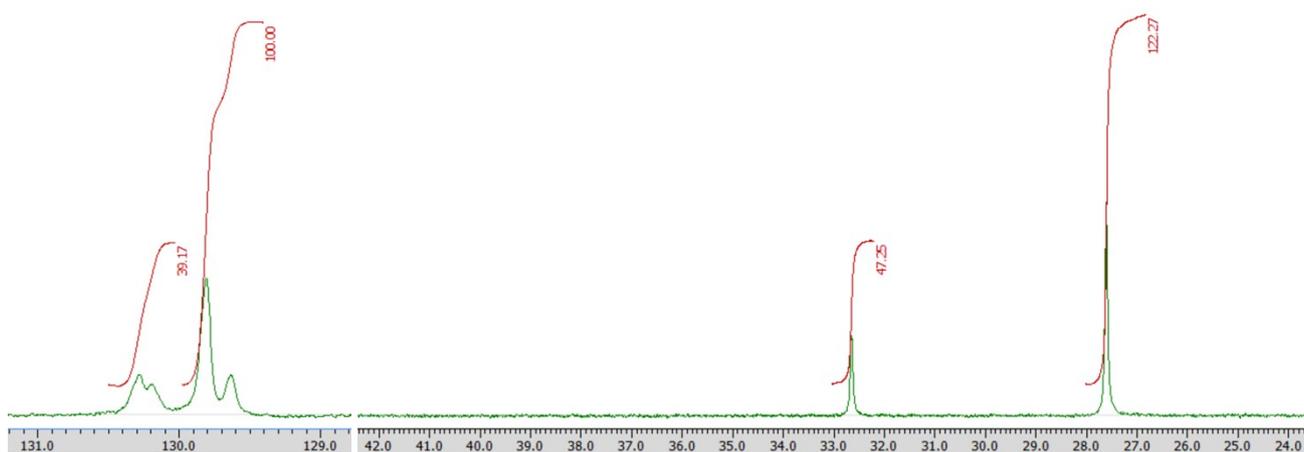


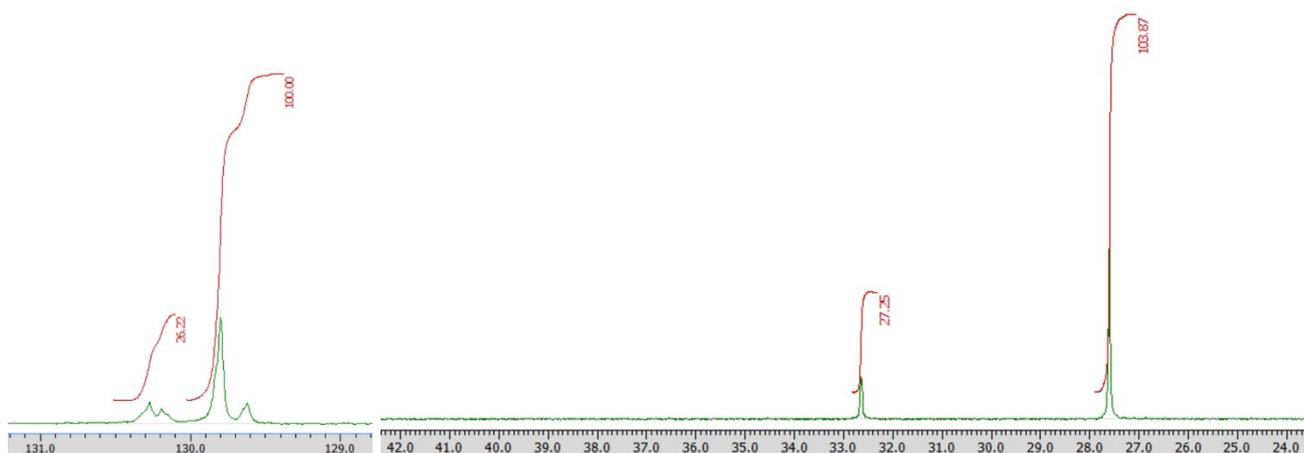
Figure S19. Full <sup>13</sup>C NMR spectra comparison of polybutadiene (in C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub>, 150 MHz, 130 °C).



**Figure S20. An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 1 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).**

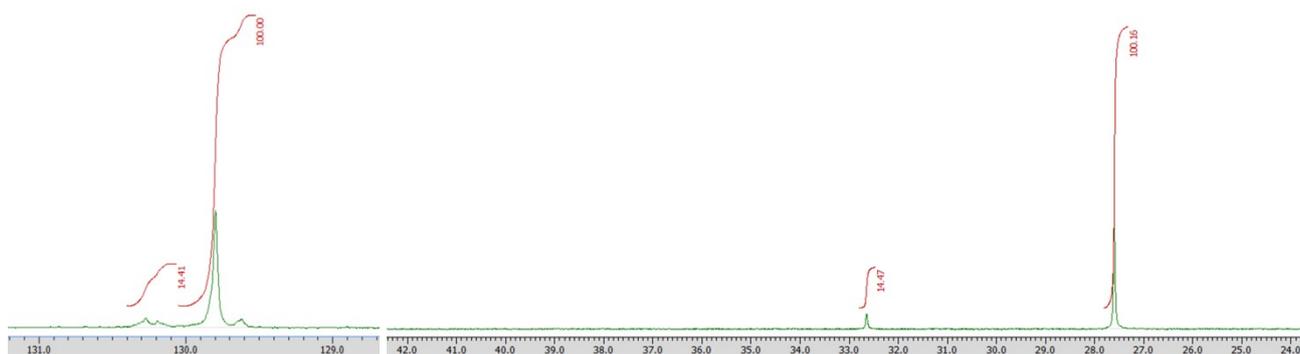


**Figure S21. An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 2 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).**

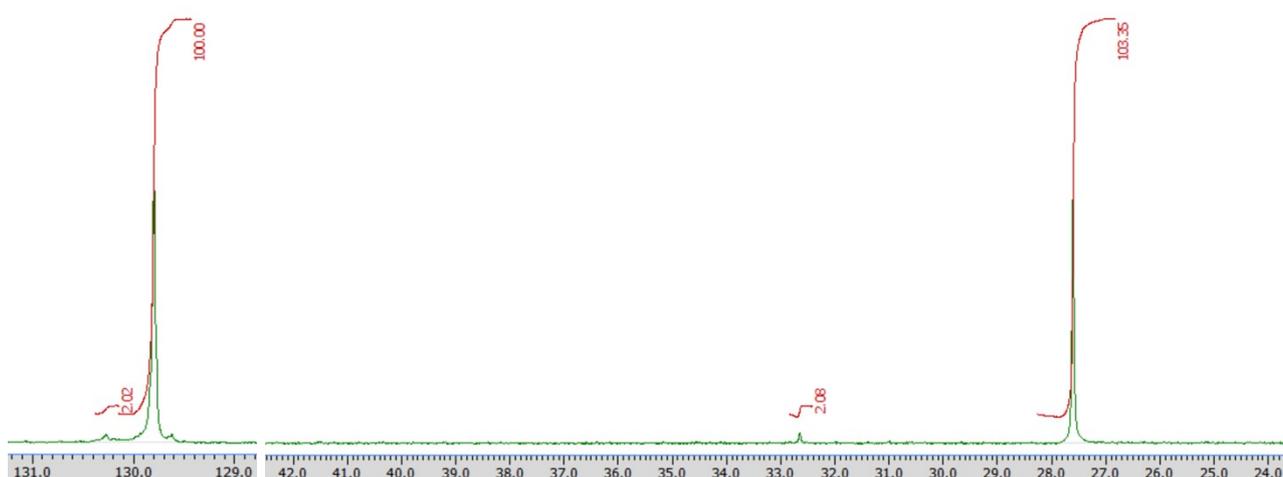


**Figure S22. An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 3 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).**

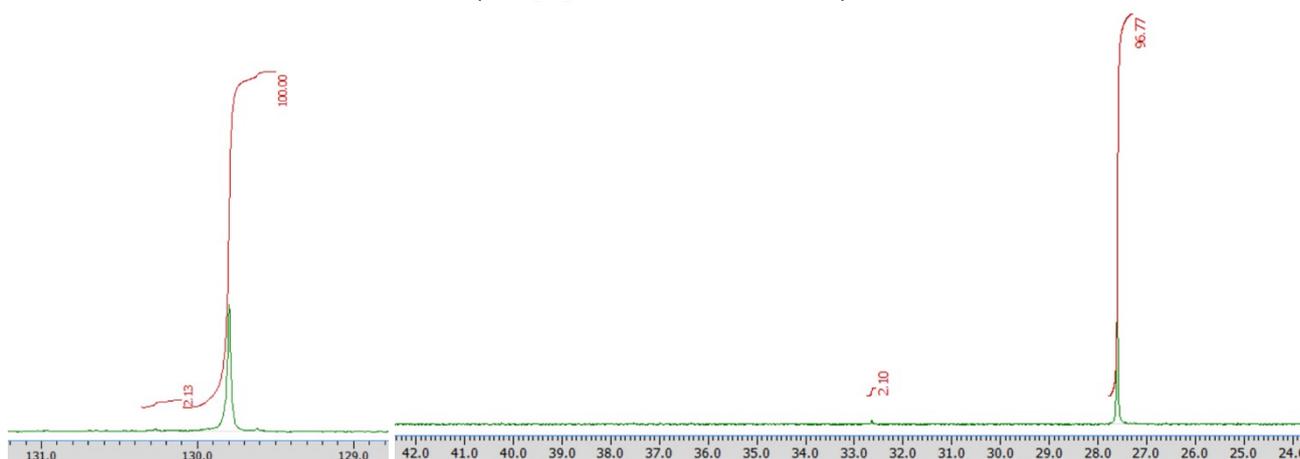
(in  $C_2D_2Cl_4$ , 150 MHz, 130 °C).



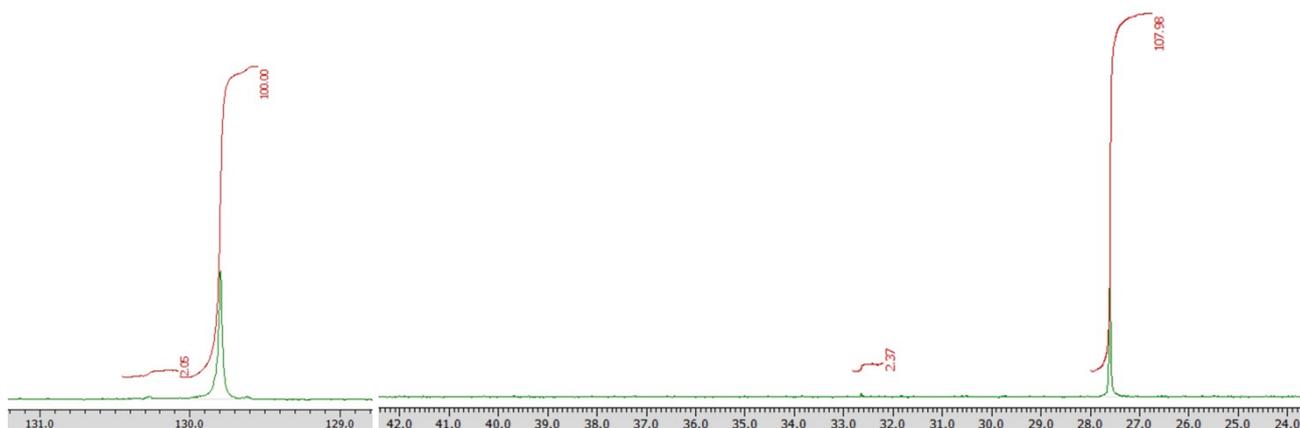
**Figure S23.** An enlarged view of  $^{13}C$  NMR spectrum of polybutadiene obtained in run 4 (in  $C_2D_2Cl_4$ , 150 MHz, 130 °C).



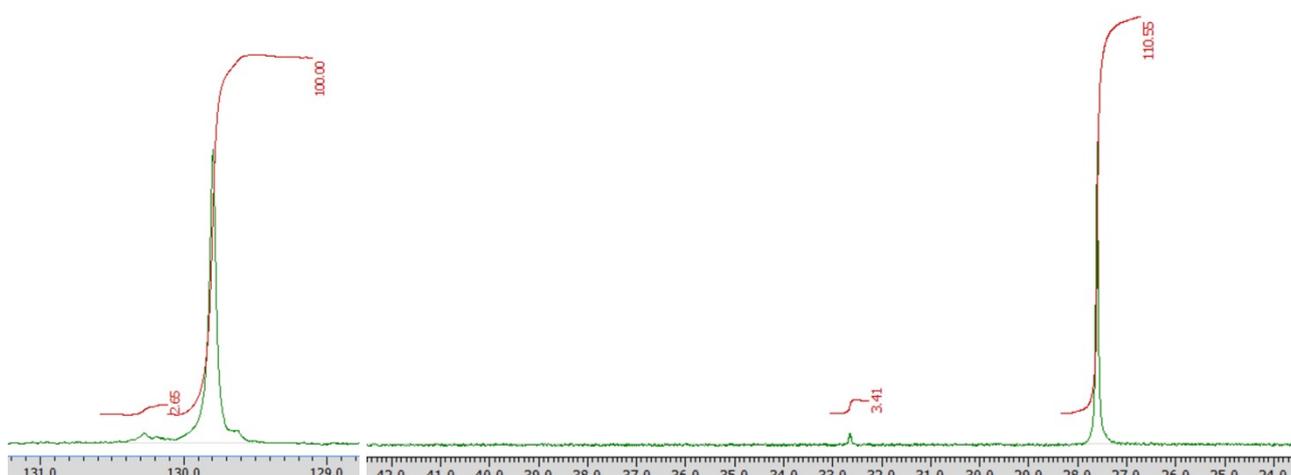
**Figure S24.** An enlarged view of  $^{13}C$  NMR spectrum of polybutadiene obtained in run 5 (in  $C_2D_2Cl_4$ , 150 MHz, 130 °C).



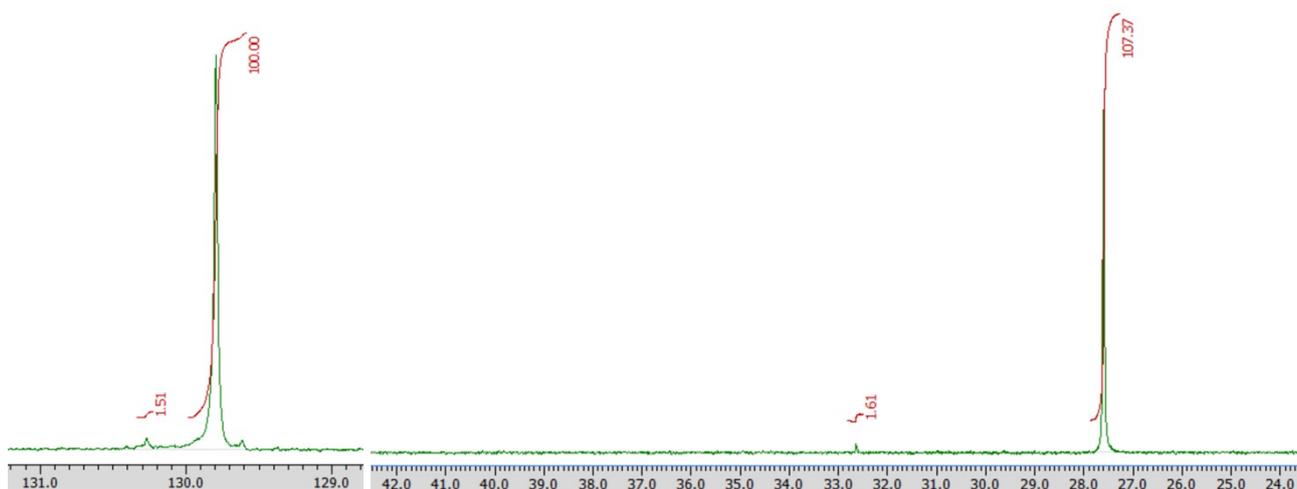
**Figure S25.** An enlarged view of  $^{13}C$  NMR spectrum of polybutadiene obtained in run 6 (in  $C_2D_2Cl_4$ , 150 MHz, 130 °C).



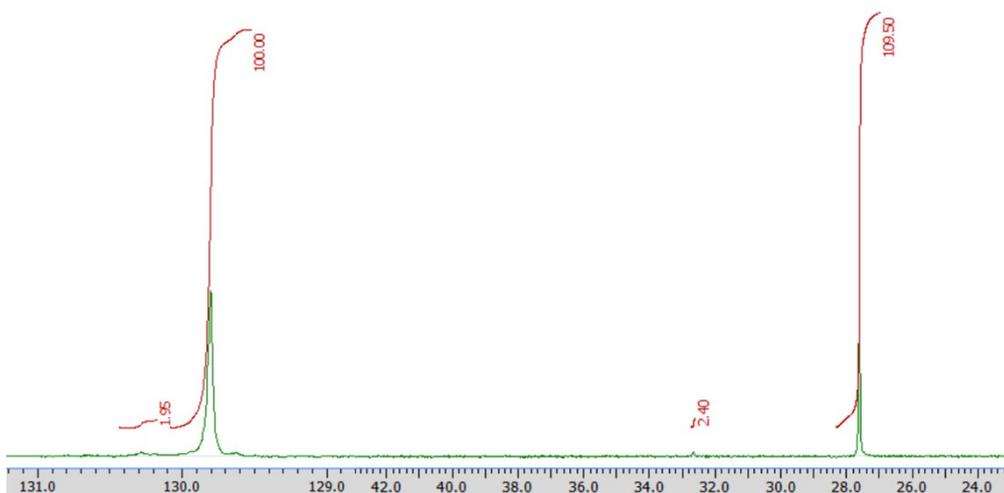
**Figure S26.** An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 7 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).



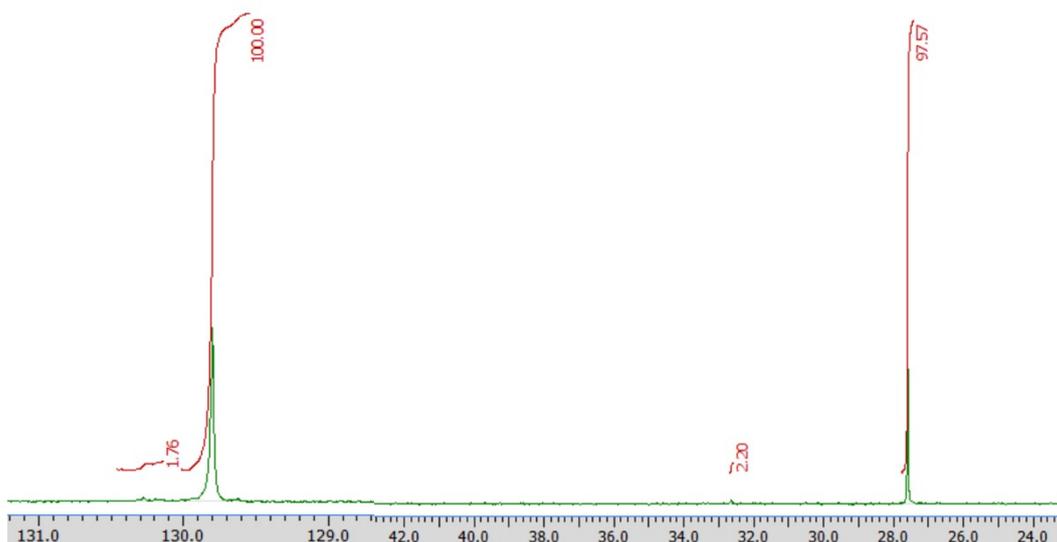
**Figure S27.** An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 9 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).



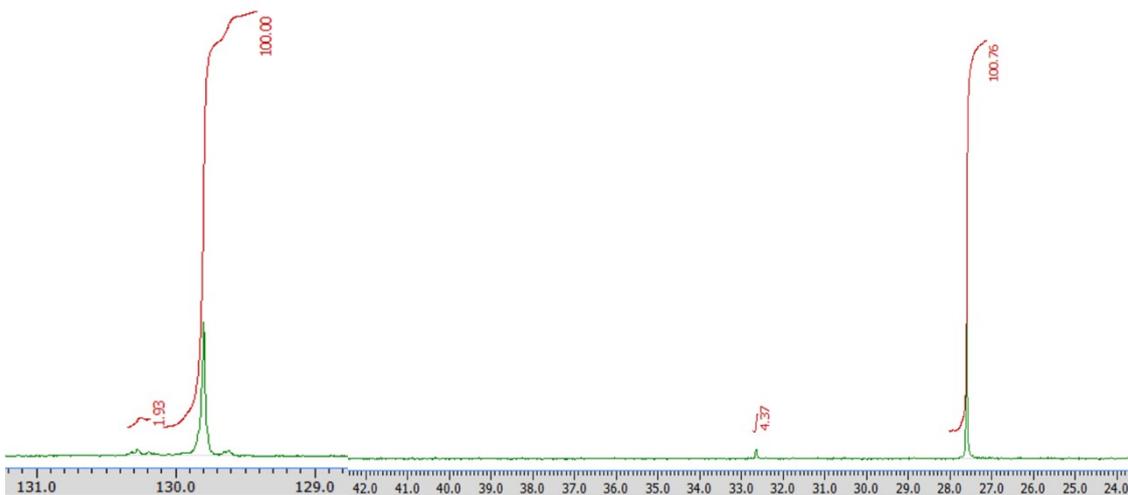
**Figure S28.** An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 10 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).



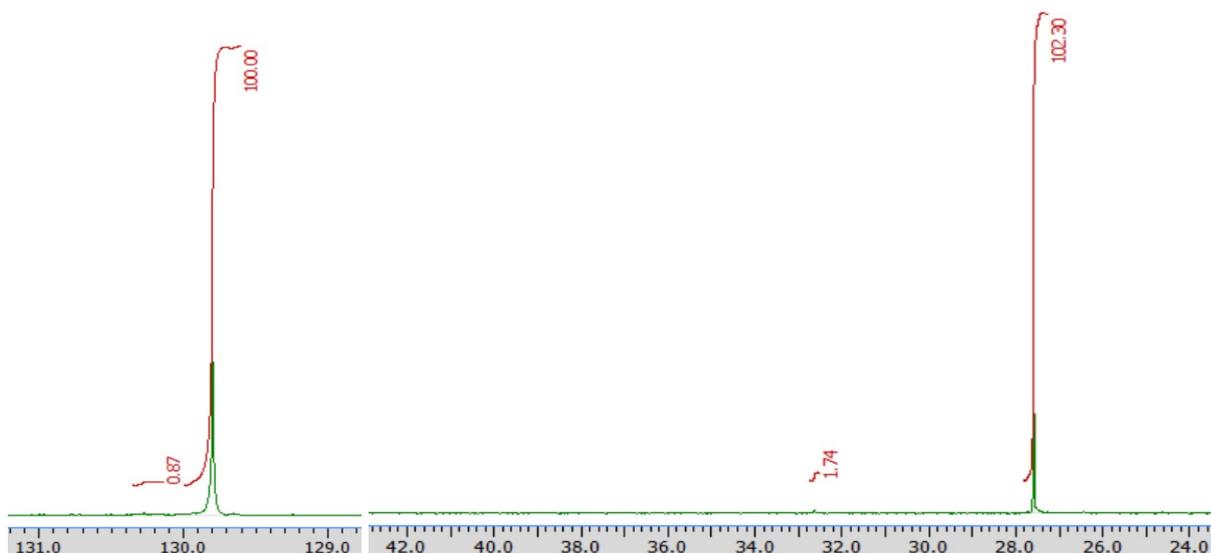
**Figure S29.** An enlarged view of <sup>13</sup>C NMR spectrum of polybutadiene obtained in run 11 (in C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub>, 150 MHz, 130 °C).



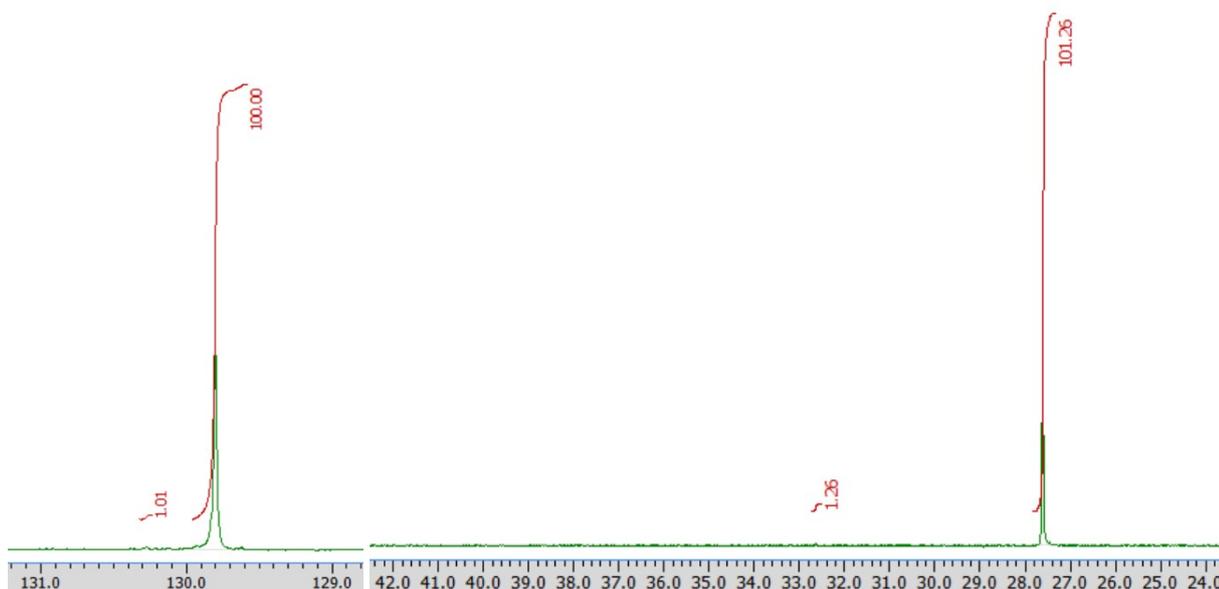
**Figure S30.** An enlarged view of <sup>13</sup>C NMR spectrum of polybutadiene obtained in run 12 (in C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub>, 150 MHz, 130 °C).



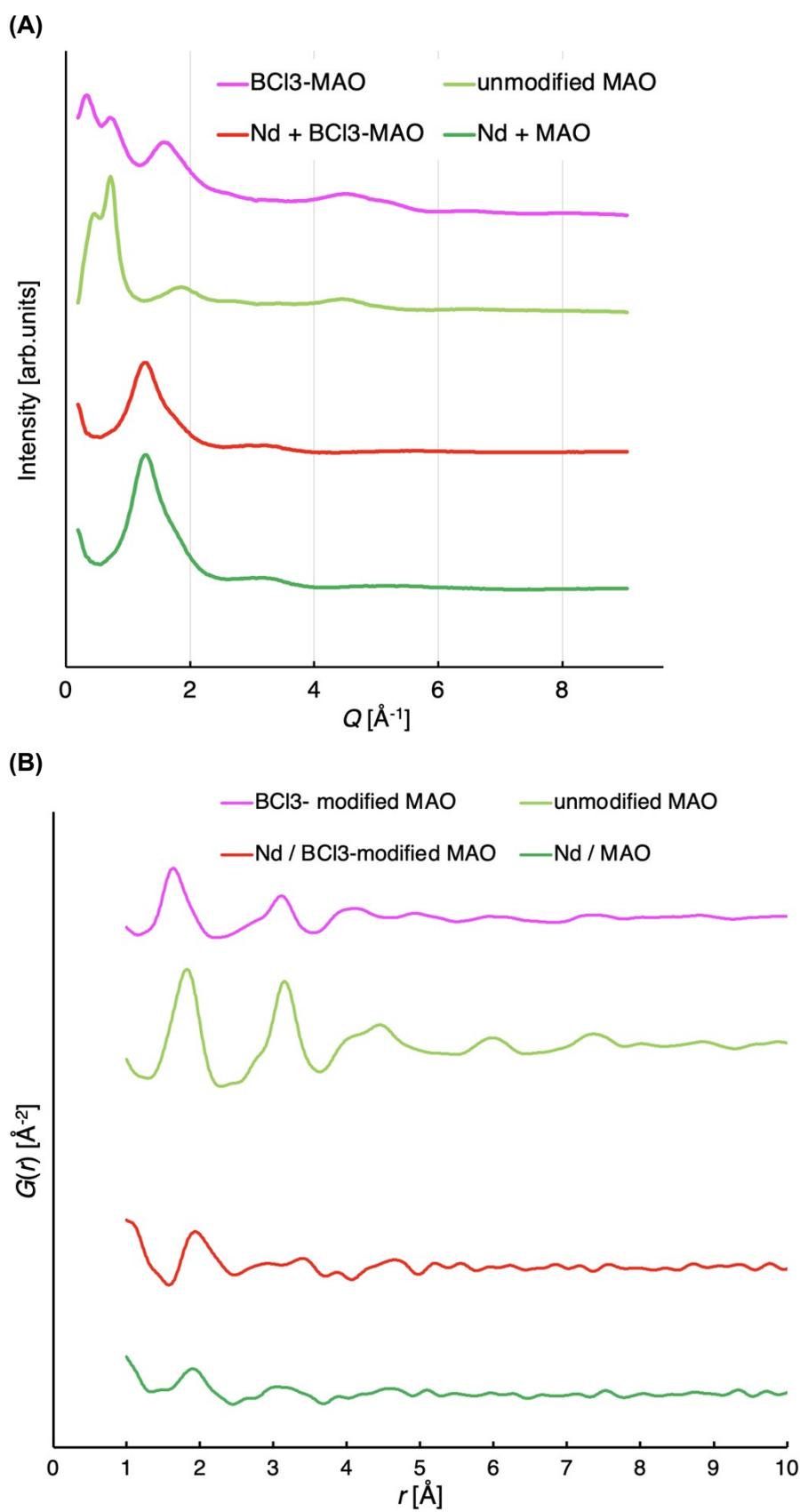
**Figure S31.** An enlarged view of <sup>13</sup>C NMR spectrum of polybutadiene obtained in run 13 (in C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub>, 150 MHz, 130 °C).



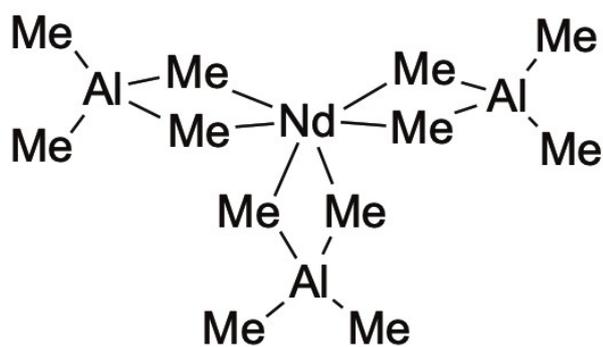
**Figure S32.** An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 14 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).



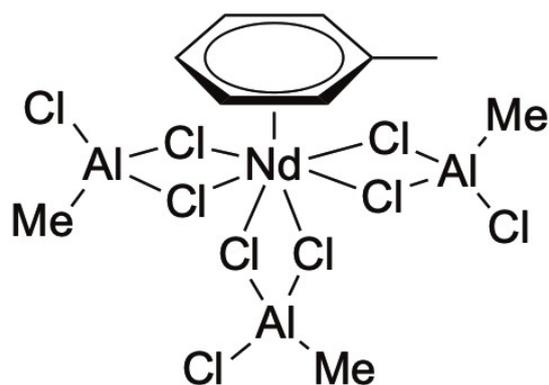
**Figure S33.** An enlarged view of  $^{13}\text{C}$  NMR spectrum of polybutadiene obtained in run 15 (in  $\text{C}_2\text{D}_2\text{Cl}_4$ , 150 MHz, 130 °C).



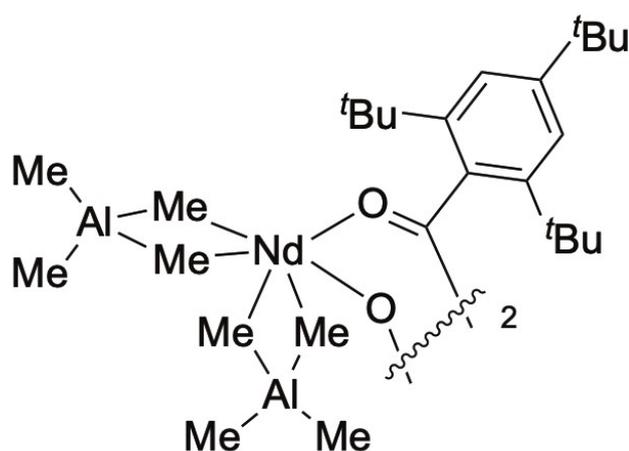
**Figure S34.** A) X-ray scattering patterns and B) Full PDF curves of MAO and Nd/MAO mixtures. Scattering intensities of the quartz capillary was subtracted prior to the analyses.



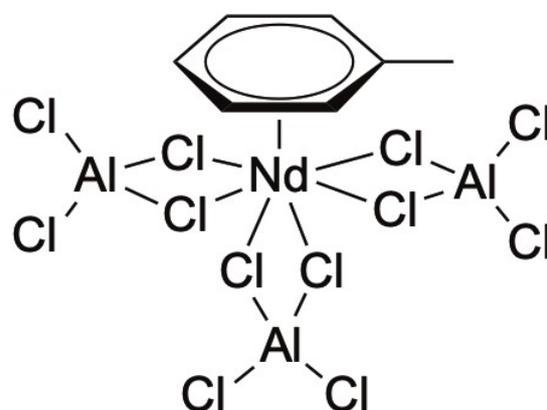
ref. 34 Nd-Al (Å): 3.150, 3.153, 3.156;  
Nd-C (Å): 2.578, 2.563, 2.605, 2.609, 2.601, 2.595.



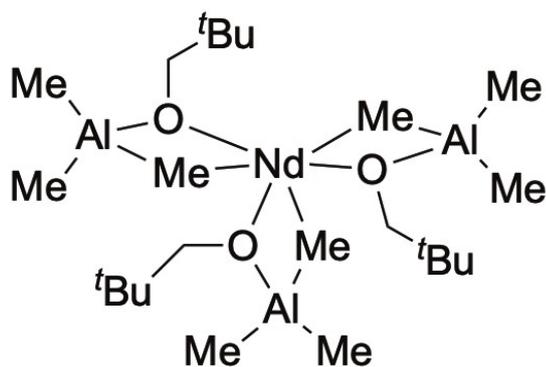
ref. 36 Nd-Al (Å): 3.749, 3.836, 3.839;  
Nd-Cl (Å): 2.864, 2.883, 2.784, 2.848, 2.885, 2.848.



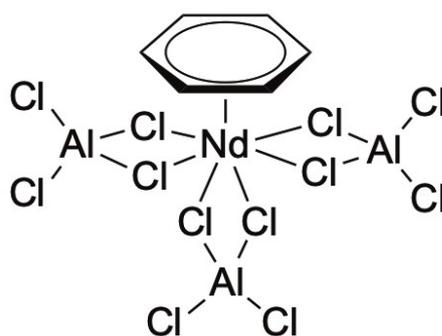
ref. 19 Nd-Al (Å): 3.178, 3.189;  
Nd-C (Å): 2.615, 2.620, 2.614, 2.626;  
Nd-O (Å): 2.282, 2.365.



ref. 37 Nd-Al (Å): 3.715, 3.793, 3.804;  
Nd-Cl (Å): 2.864, 2.902, 2.857, 2.845, 2.876, 2.798.



ref. 35 Nd-Al (Å): 3.276;  
Nd-C (Å): 2.698; Nd-O (Å): 2.294.



ref. 38 Nd-Al (Å): 3.680, 3.771, 3.782;  
Nd-Cl (Å): 2.883, 2.842, 2.796, 2.845, 2.861, 2.889.

**Figure S35.** Representative interatomic distances for reported neodymium aluminate complexes.