Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Stereospecific polymerization of conjugated dienes using neodymium alkylborohydride complexes

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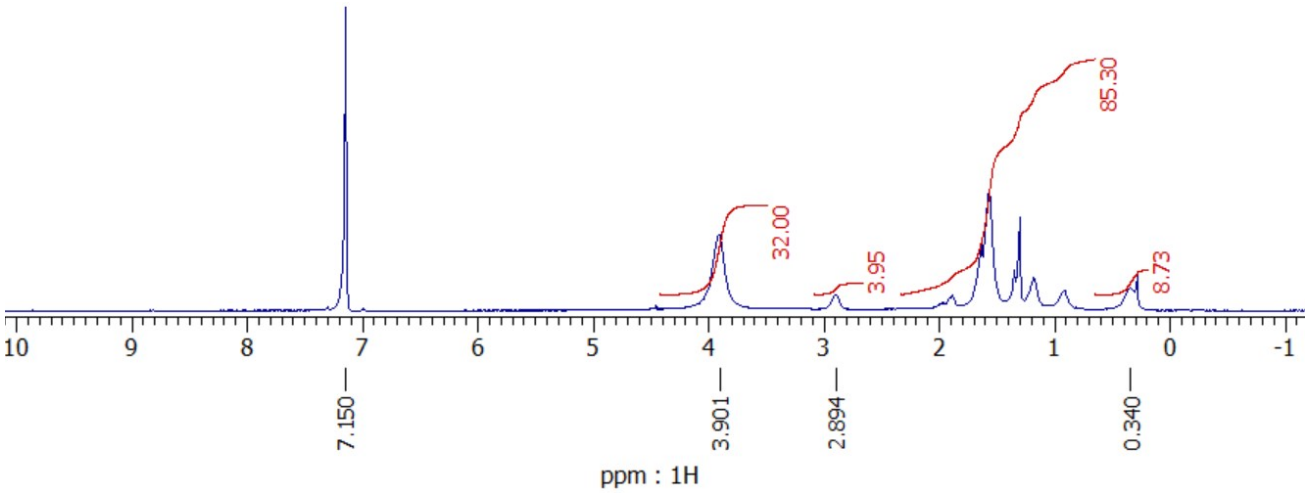

Figure S1. ^{1}H NMR spectrum of complex **3** (500 MHz, in C_6D_6).

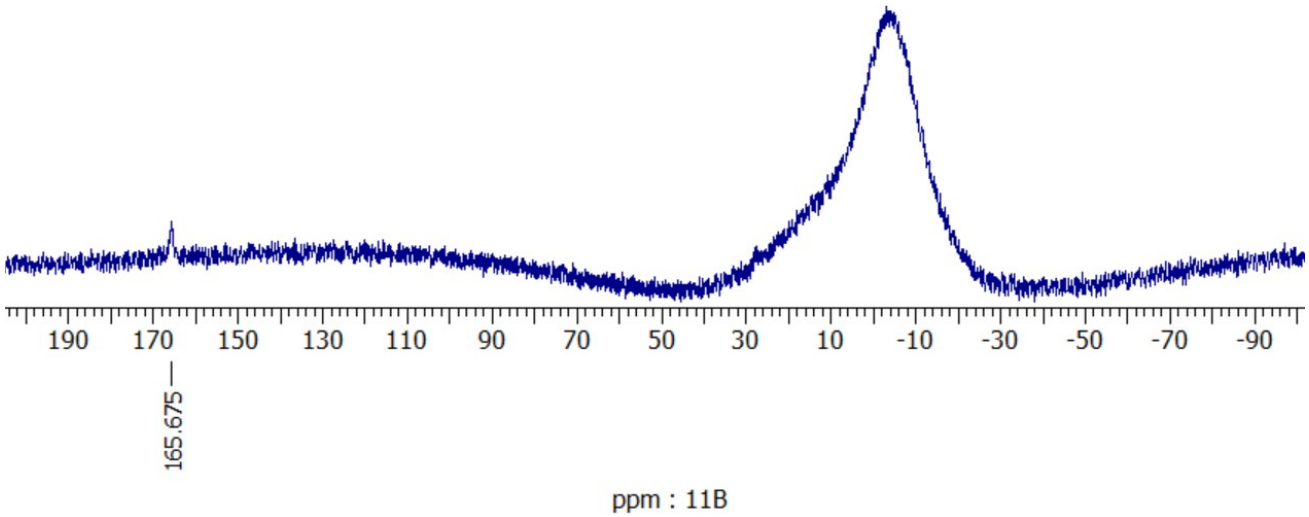

Figure S2. ^{11}B NMR spectrum of complex **3** (160 MHz, in C_6D_6).

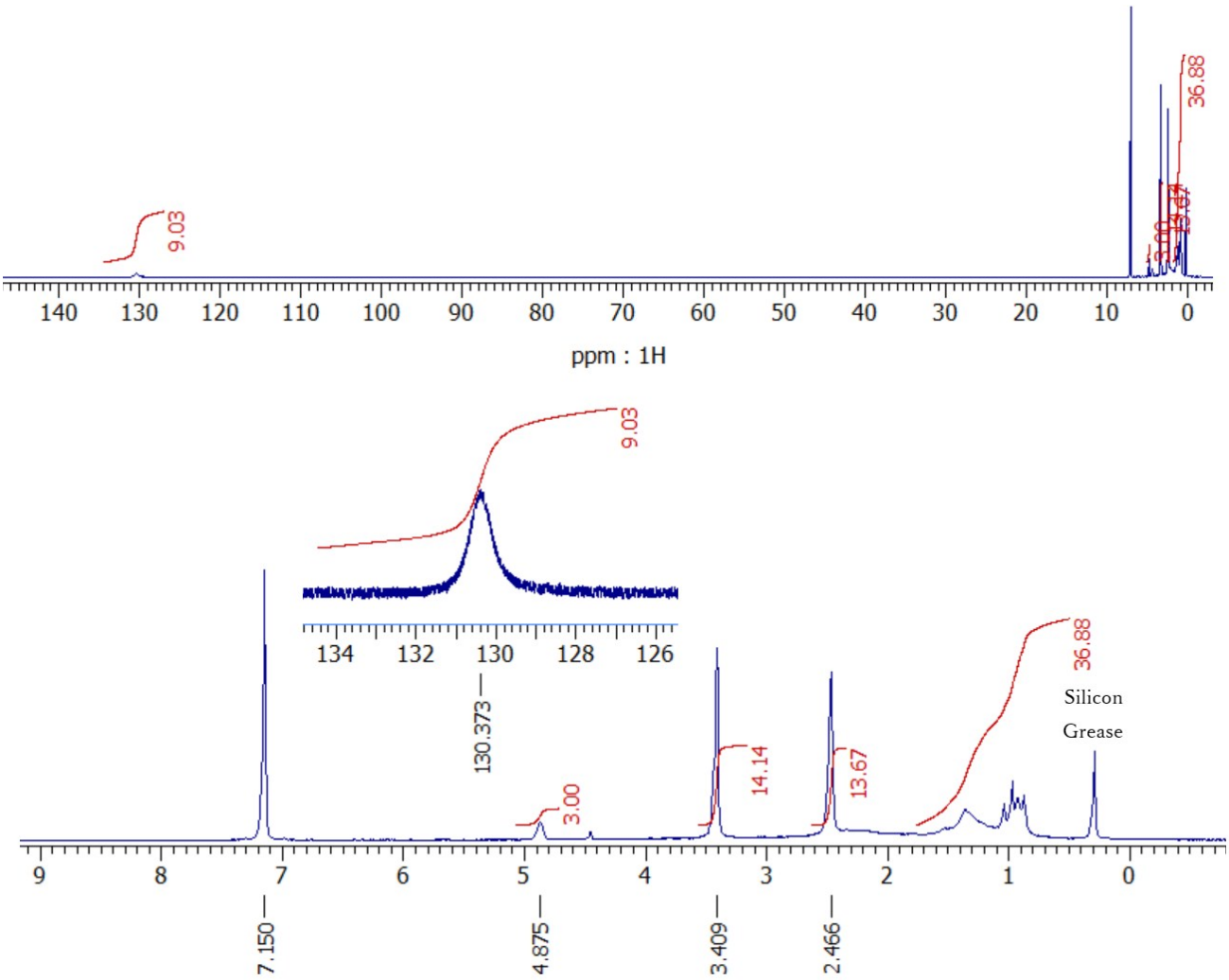

Figure S3. ^{1}H NMR spectrum of complex **4** (500 MHz, in C_6D_6).

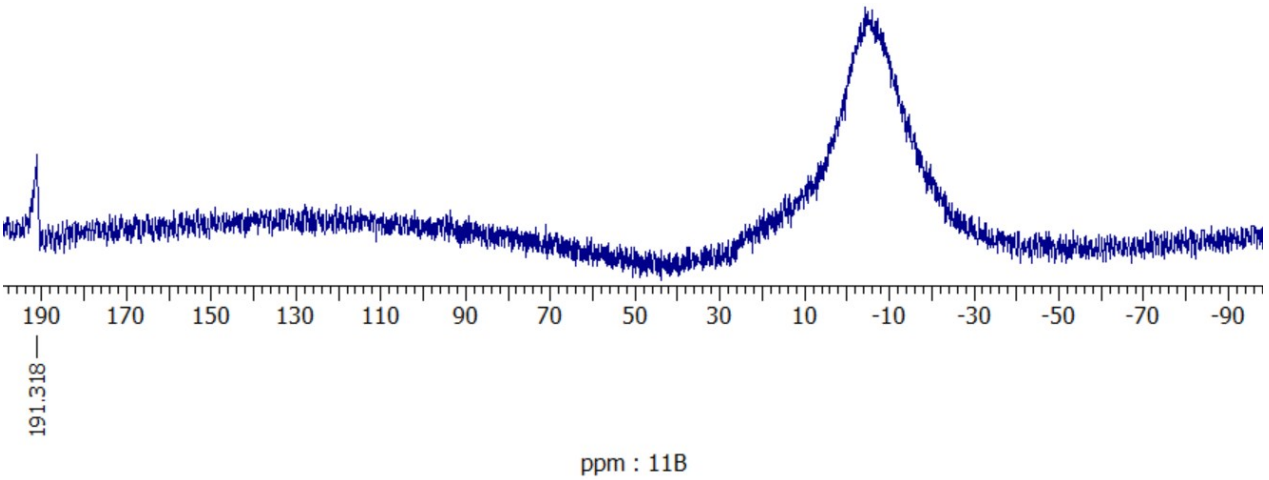

Figure S4. ^{11}B NMR spectrum of complex **4** (160 MHz, in C_6D_6).

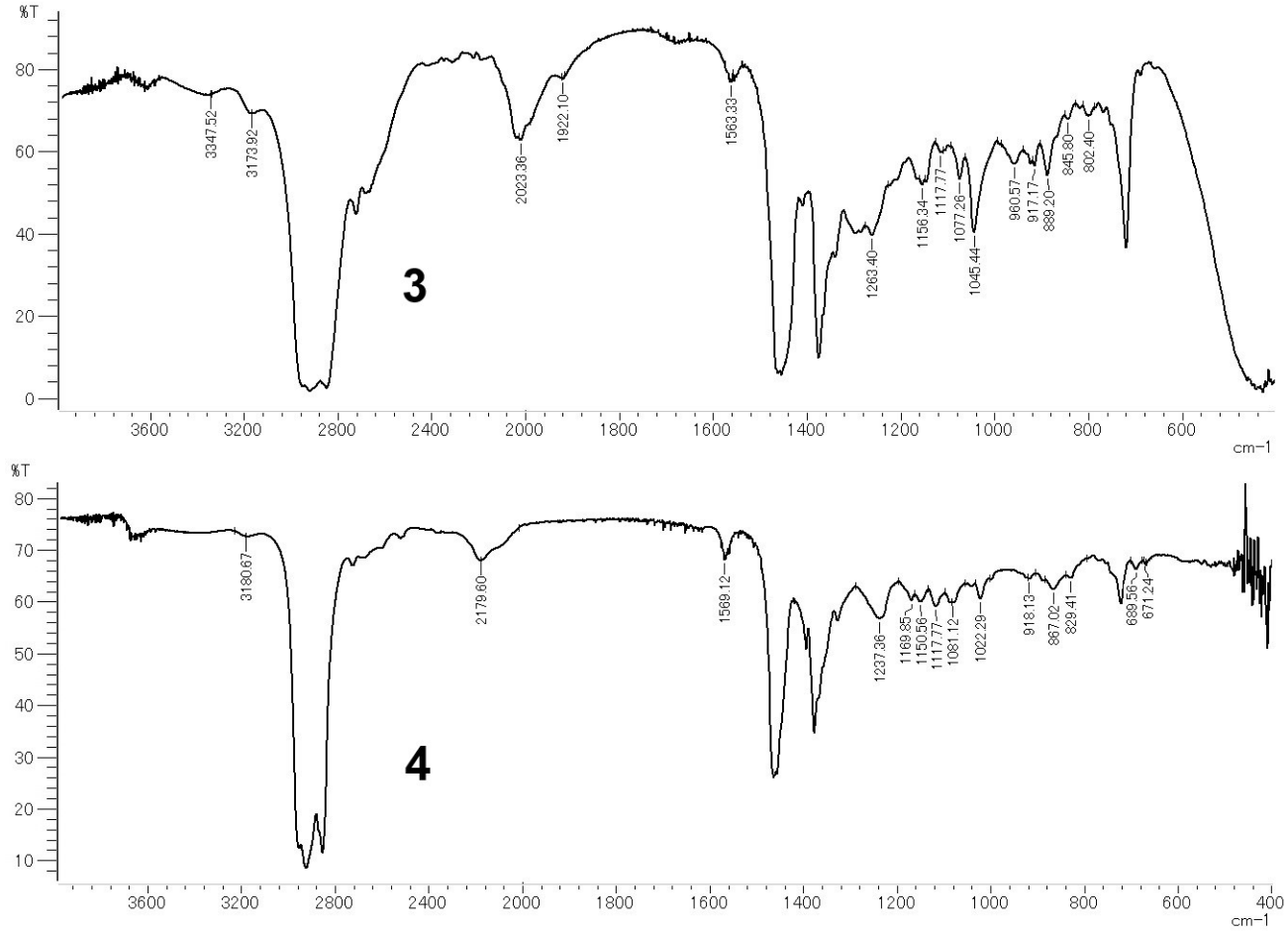

Figure S5. IR spectra of complexes **3** and **4** (Nujol).

Table S1. Crystal refinement data for complexes **3** and **4**.

Compound	**3**	**4**
Wavelength (Å)	0.71069 Å	0.71069 Å
Temperature (K)	123	123
Empirical formula	$C_{40}H_{80}B_4NdO_2$ $C_{24}H_{48}NaO_6$	$C_{30}H_{72}B_3NdO_3$
Formula weight	1236.13	657.54
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	$P2_1/c$
a (Å)	11.2257(11)	11.2474(14)
b (Å)	11.2958(11)	16.788(2)
c (Å)	14.3024(14)	20.353(2)
α (deg)	77.2071(13)	90
β (deg)	80.0236(14)	101.486(2)
γ (deg)	79.6023(13)	90
Volume ($Å^3$)	1722.7(3)	3766.1(7)
Z	1	4
D_{calc} (g/cm^3)	1.192	1.160
μ (mm^{-1})	0.808	1.403
F(000)	667.0	1404.0
Crystal size (mm)	0.2 x 0.2 x 0.2	0.1 x 0.1 x 0.05
θ_{max} (deg)	27.405	27.381
Index ranges	$-12 \le h \le 14$	$-14 \le h \le 14$
	$-14 \le k \le 14$	$-21 \le k \le 20$
	$-10 \le l \le 18$	$-26 \le l \le 9$
No. of reflections observed	7558	8506
No. of parameters refined	527	402
T_{min}, T_{max}	0.6789, 0.7455	0.6599, 0.7455
R_1	0.0373	0.0484
wR_2	0.0963	0.0998
GoF on F^2	1.049	0.994

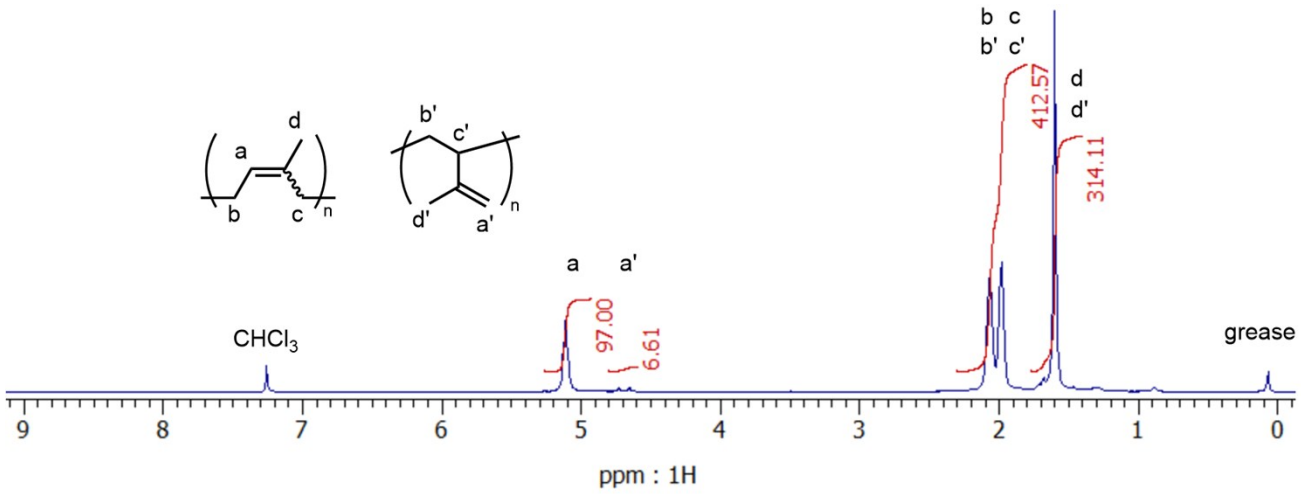

Figure S6. ^{1}H NMR of polyisoprene obtained in Table 2, run 2 (500 MHz, in $CDCl_3$).

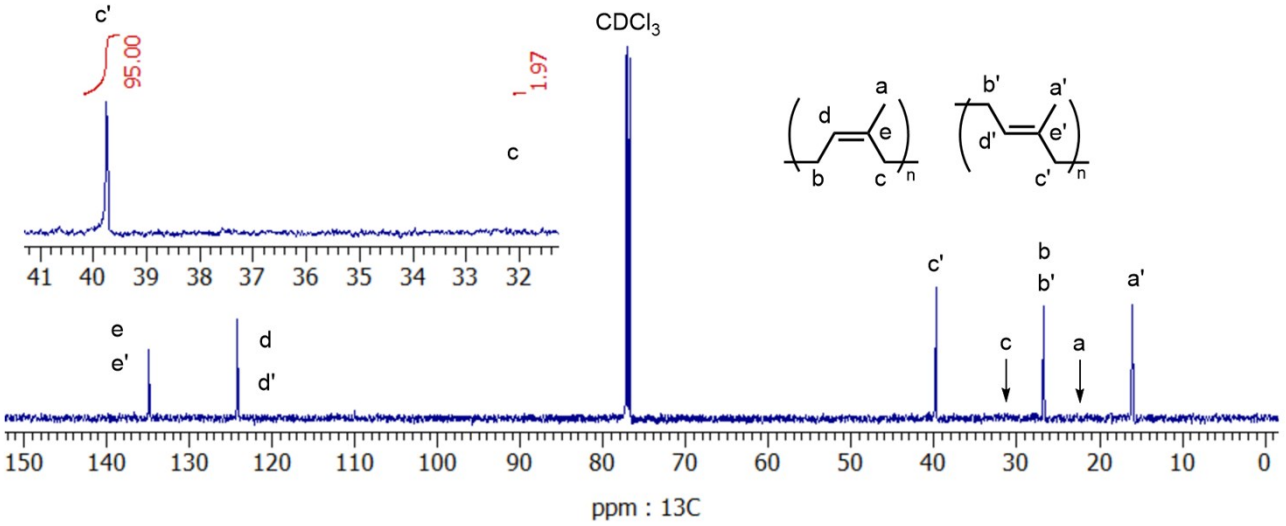

Figure S7. ^{13}C NMR of polyisoprene obtained in Table 2, run 2 (125 MHz, in $CDCl_3$).

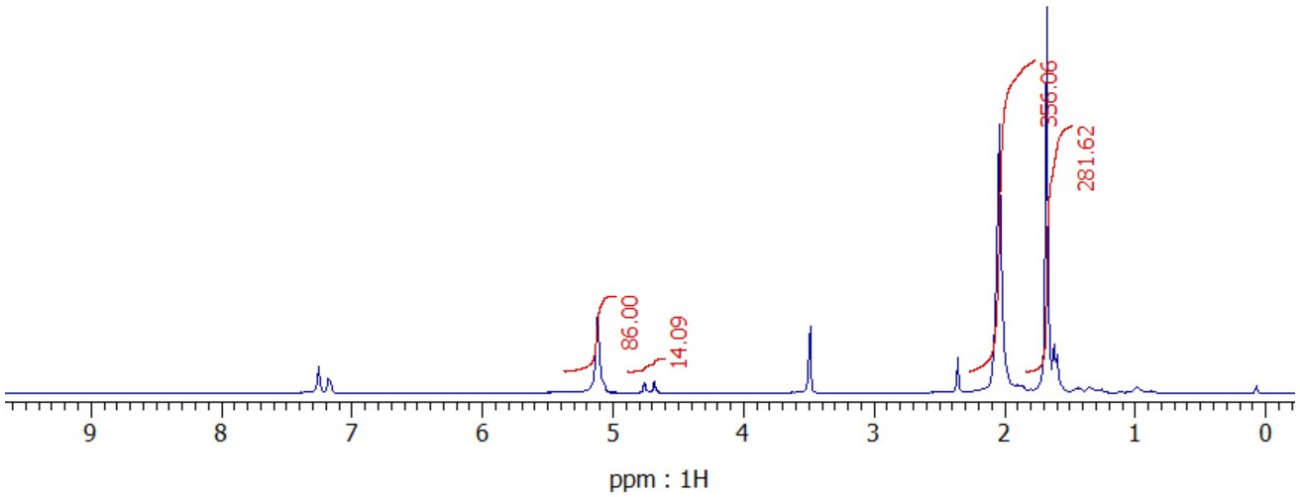

Figure S8. ^{1}H NMR of polyisoprene obtained in Table 2, run 3 (500 MHz, in $CDCl_3$).

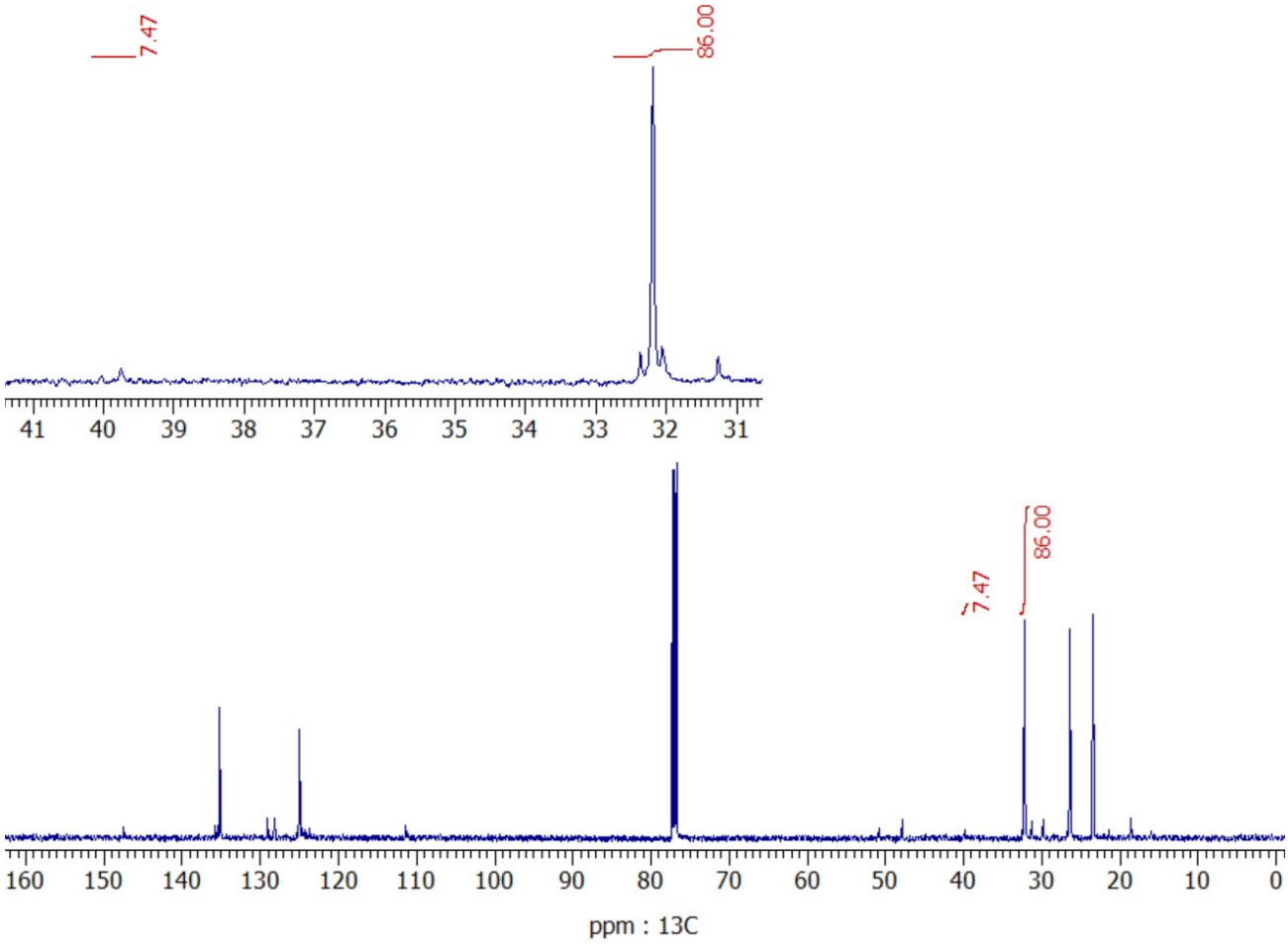

Figure S9. ^{13}C NMR of polyisoprene obtained in Table 2, run 3 (125 MHz, in $CDCl_3$).

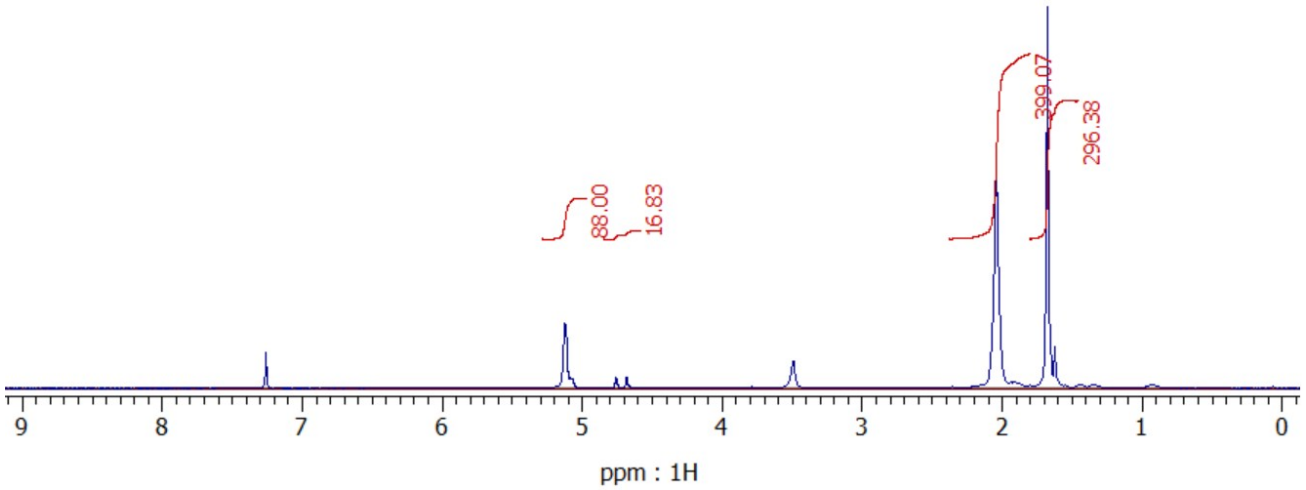

Figure S10. ^{1}H NMR of polyisoprene obtained in Table 2, run 4 (500 MHz, in $CDCl_3$).

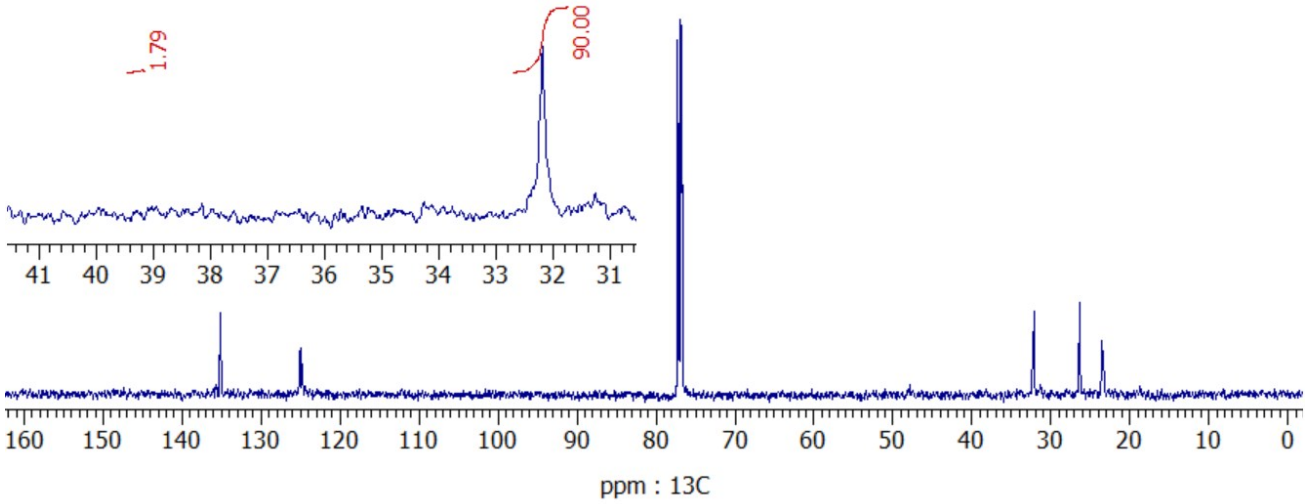

Figure S11. ^{13}C NMR of polyisoprene obtained in Table 2, run 4 (125 MHz, in $CDCl_3$).

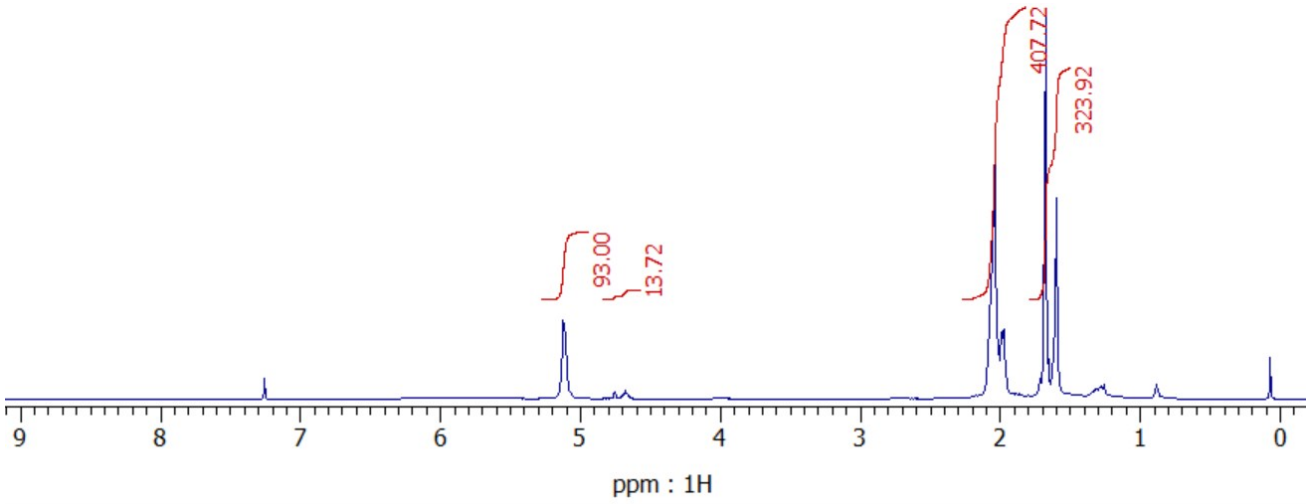

Figure S12. ^{1}H NMR of polyisoprene obtained in Table 2, run 5 (500 MHz, in $CDCl_3$).

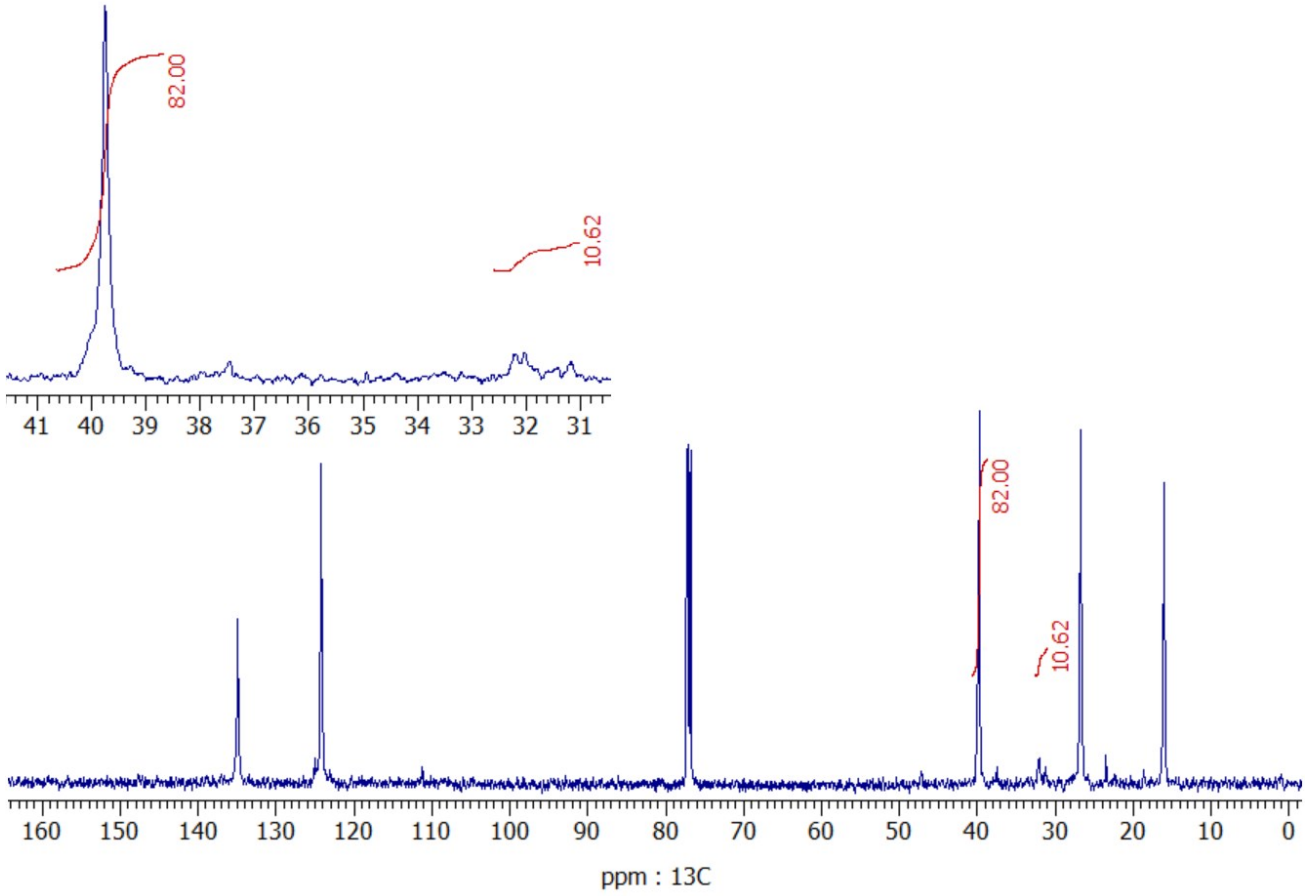

Figure S13. ^{13}C NMR of polyisoprene obtained in Table 2, run 5 (125 MHz, in $CDCl_3$).

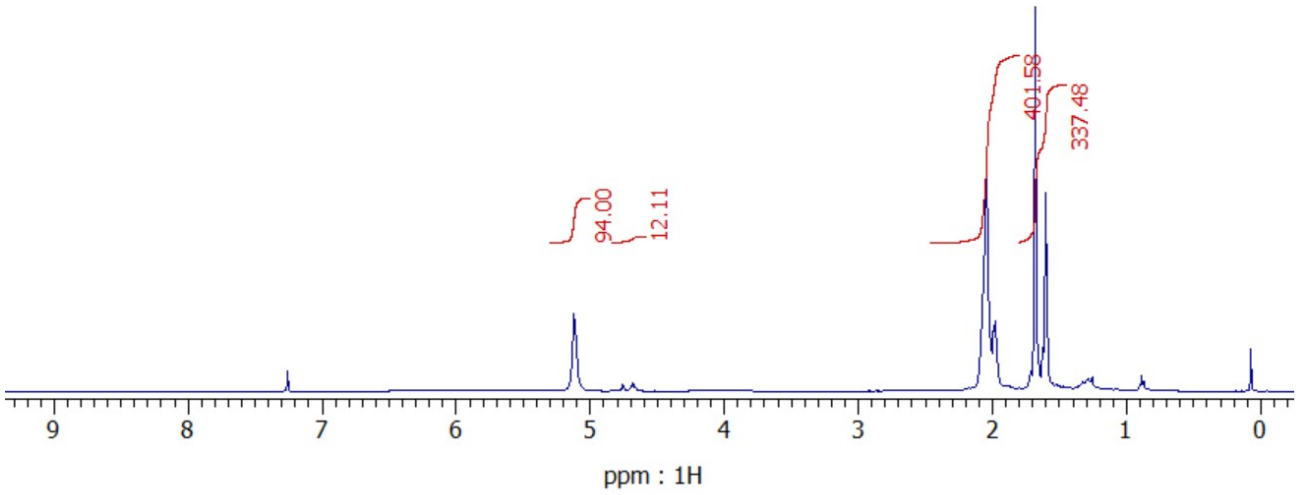

Figure S14. ^{1}H NMR of polyisoprene obtained in Table 2, run 6 (500 MHz, in $CDCl_3$).

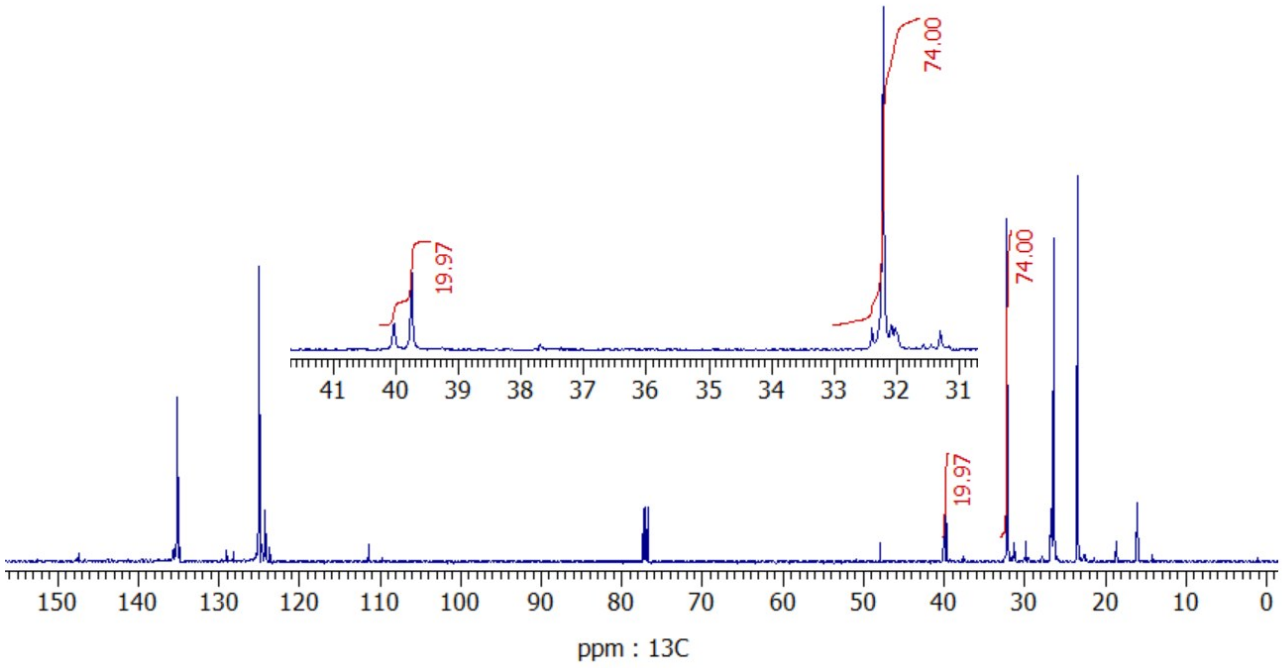

Figure S15. ^{13}C NMR of polyisoprene obtained in Table 2, run 6 (125 MHz, in $CDCl_3$).

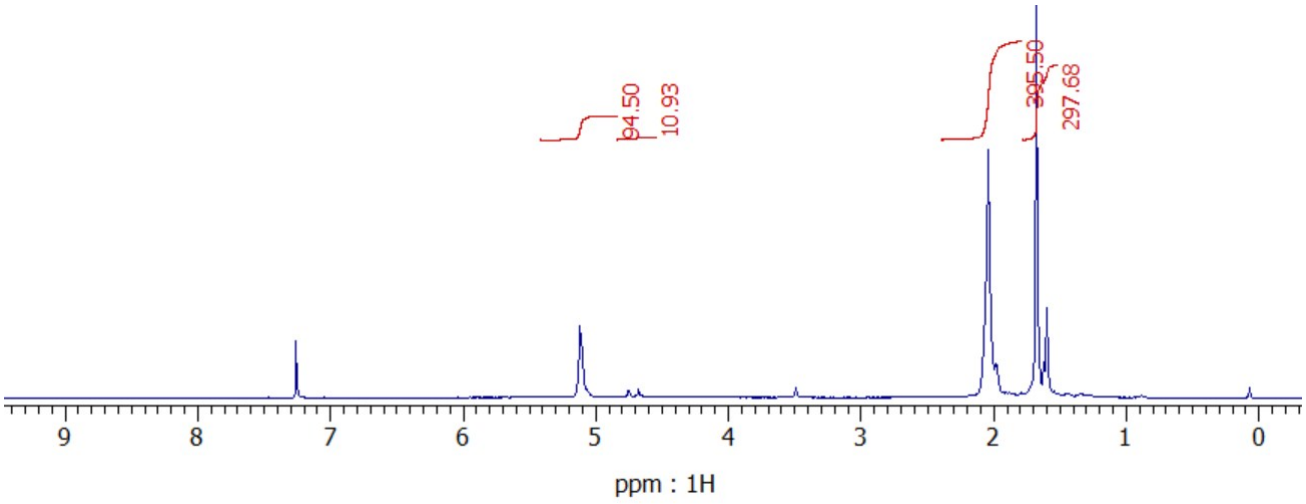

Figure S16. ^{1}H NMR of polyisoprene obtained in Table 2, run 7 (500 MHz, in $CDCl_3$).

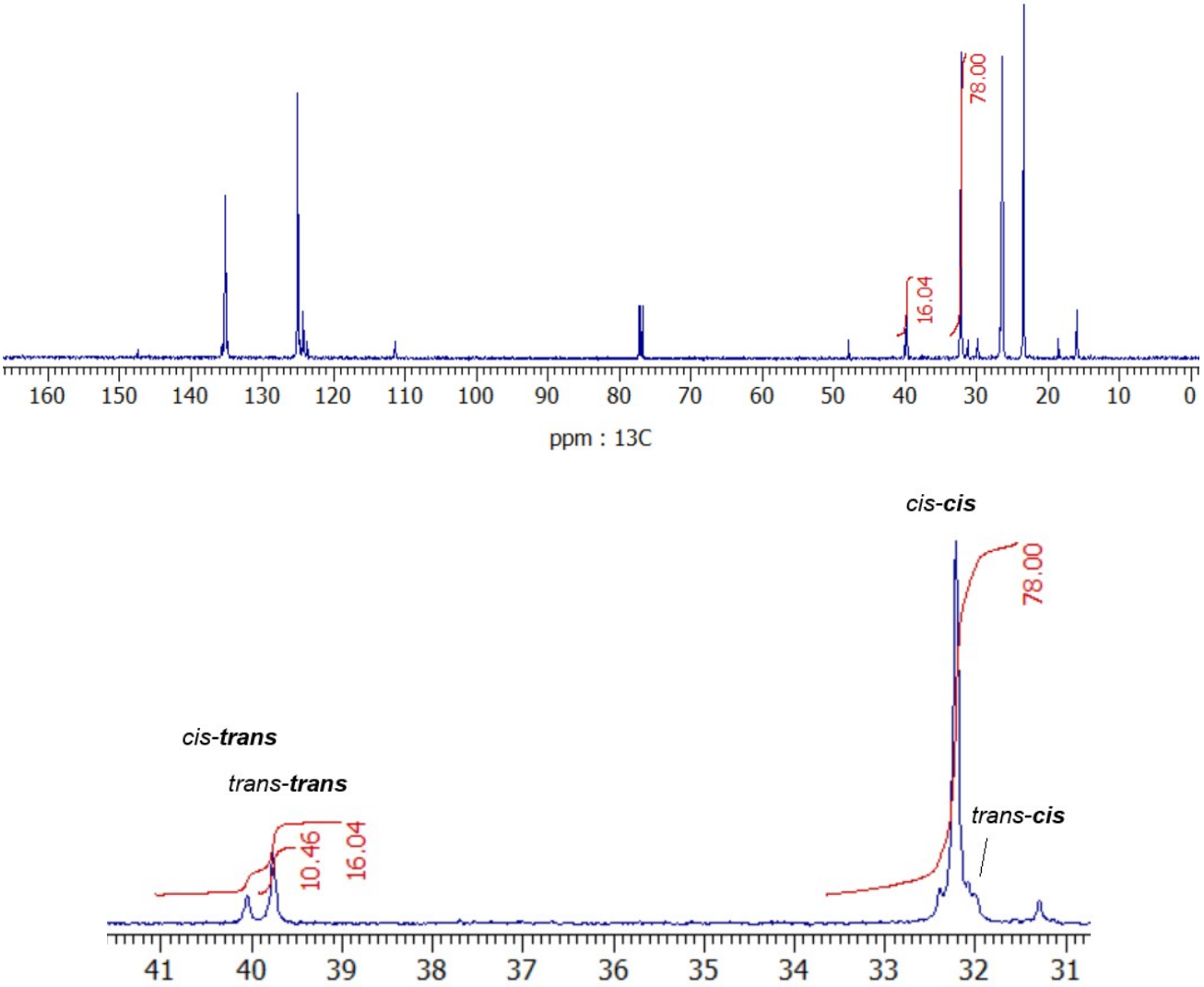

Figure S17. ^{13}C NMR of polyisoprene obtained in Table 2, run 7 (125 MHz, in $CDCl_3$).

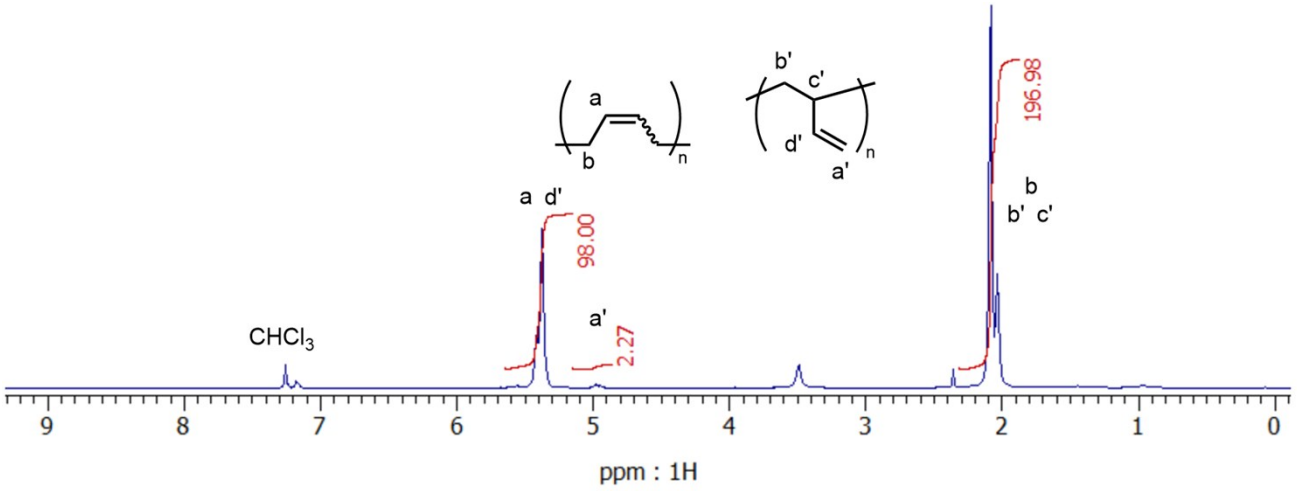

Figure S18. ^{1}H NMR of polybutadiene obtained in Table 2, run 10 (500 MHz, in $CDCl_3$).

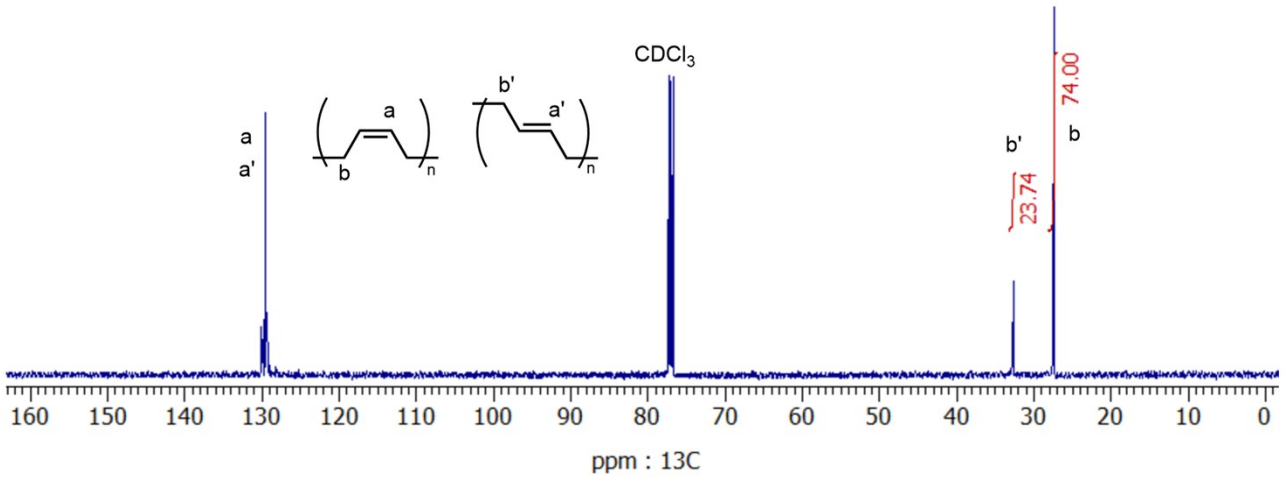

Figure S19. ^{13}C NMR of polybutadiene obtained in Table 2, run 10 (125 MHz, in $CDCl_3$).

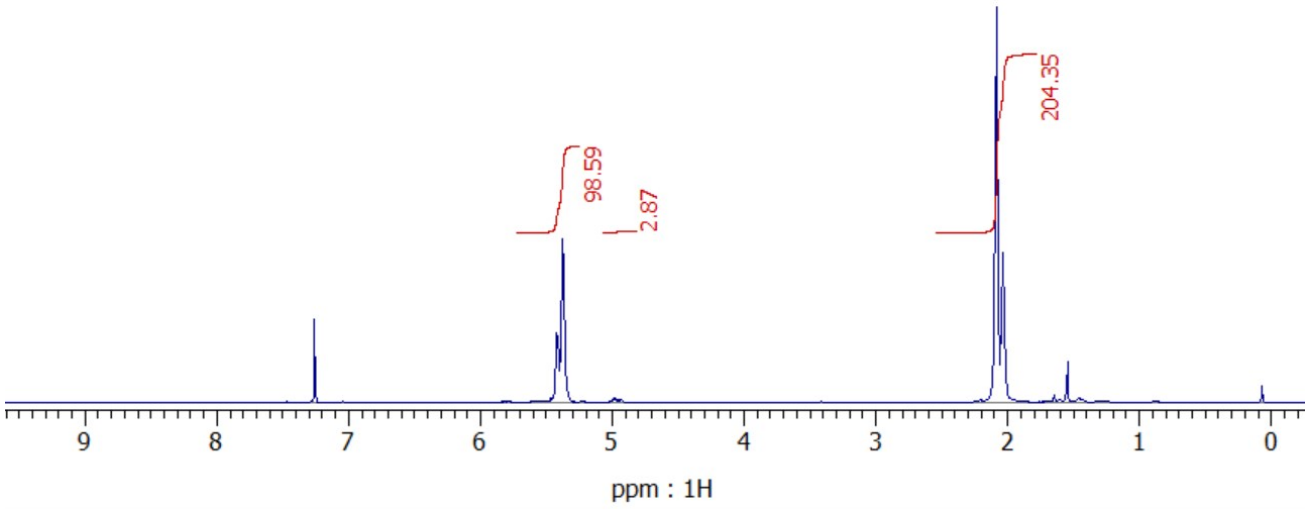

Figure S20. ^{1}H NMR of polyisoprene obtained in Table 2, run 11 (500 MHz, in $CDCl_3$).

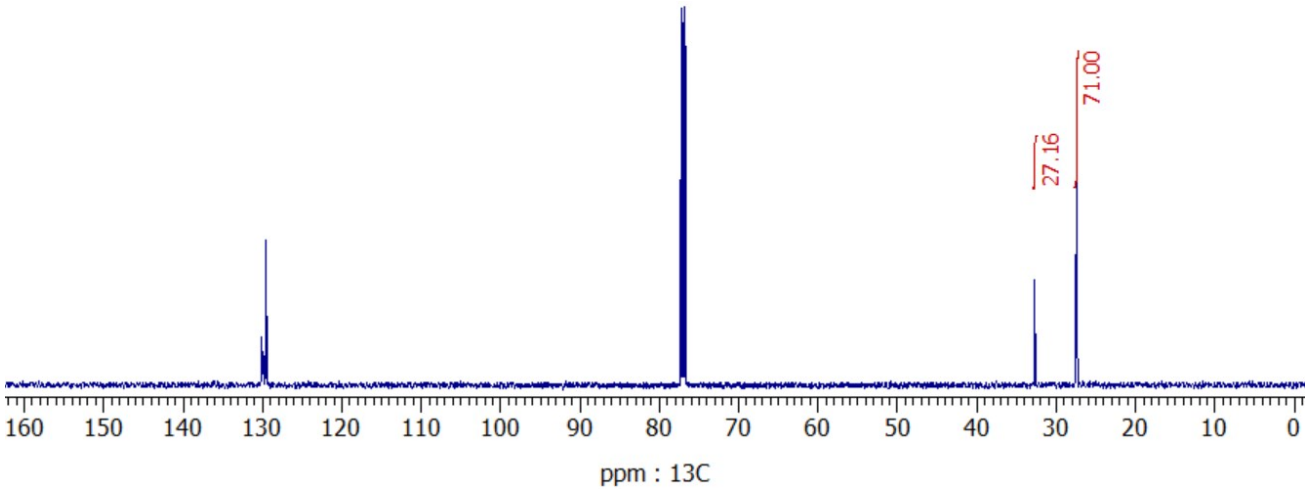

Figure S21. ^{13}C NMR of polyisoprene obtained in Table 2, run 11 (125 MHz, in $CDCl_3$).

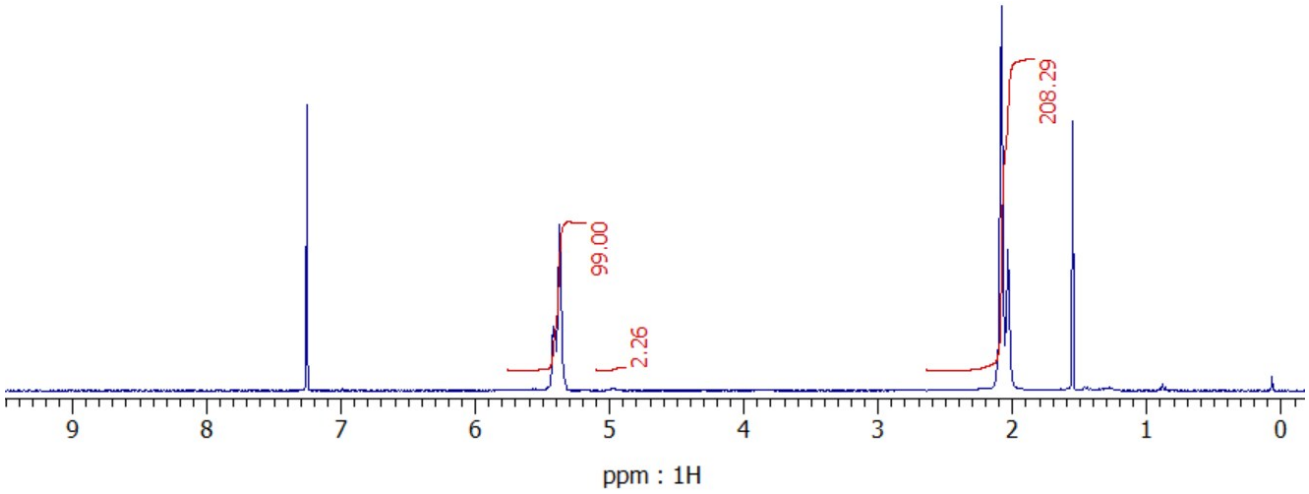

Figure S22. ^{1}H NMR of polybutadiene obtained in Table 2, run 12 (500 MHz, in $CDCl_3$).

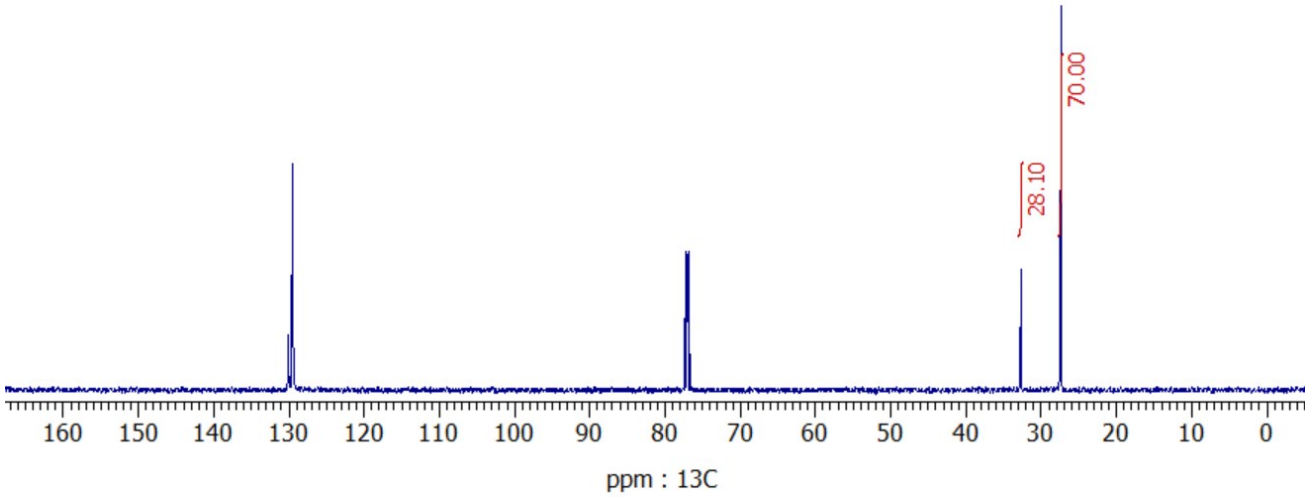

Figure S23. ^{13}C NMR of polybutadiene obtained in Table 2, run 12 (125 MHz, in $CDCl_3$).

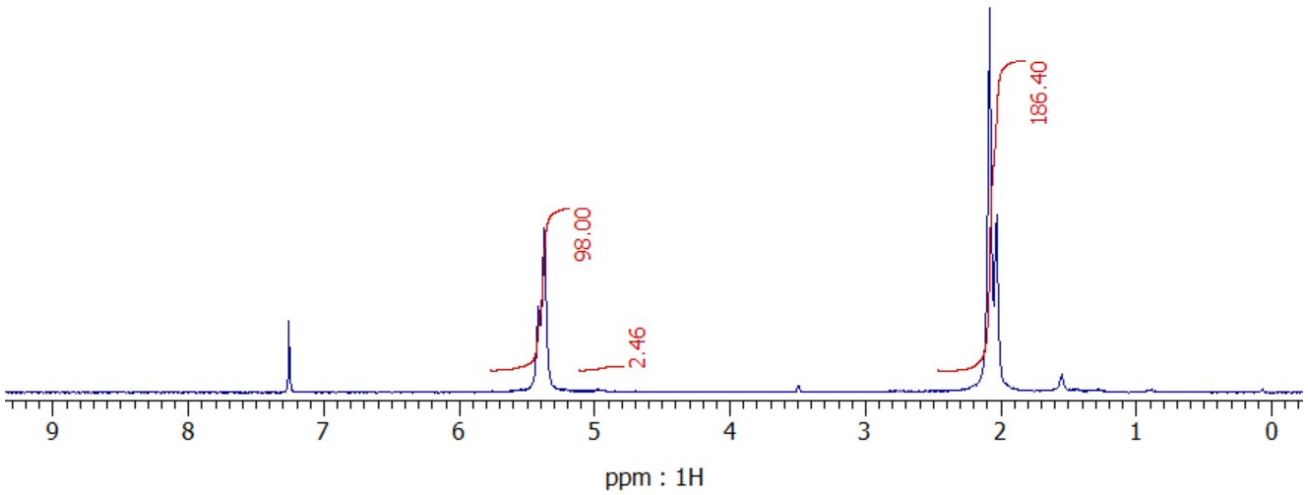

Figure S24. ^{1}H NMR of polybutadiene obtained in Table 2, run 13 (500 MHz, in $CDCl_3$).

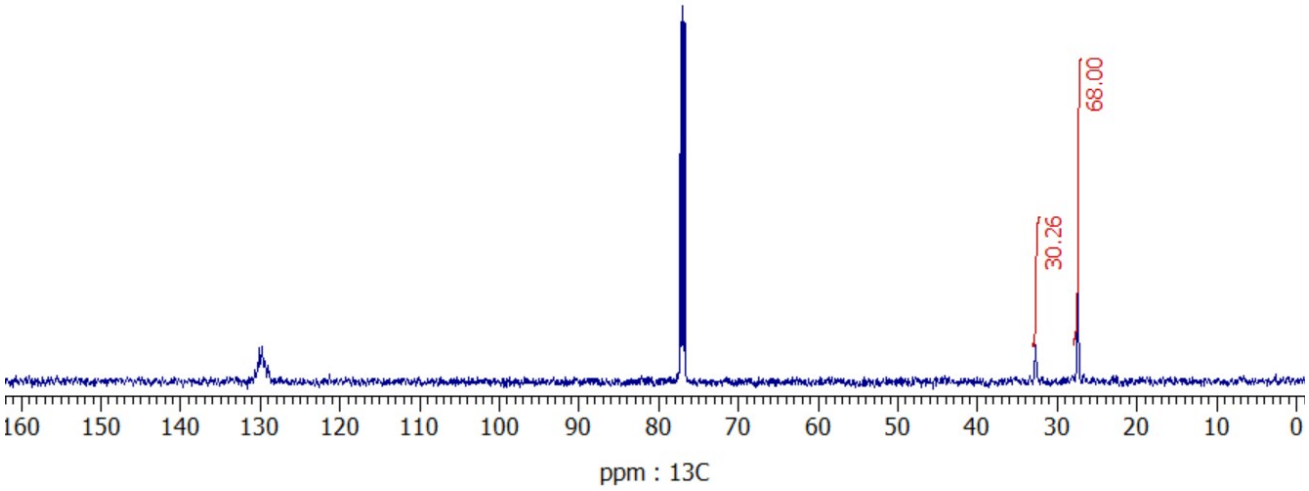

Figure S25. ^{13}C NMR of polybutadiene obtained in Table 2, run 13 (125 MHz, in $CDCl_3$).

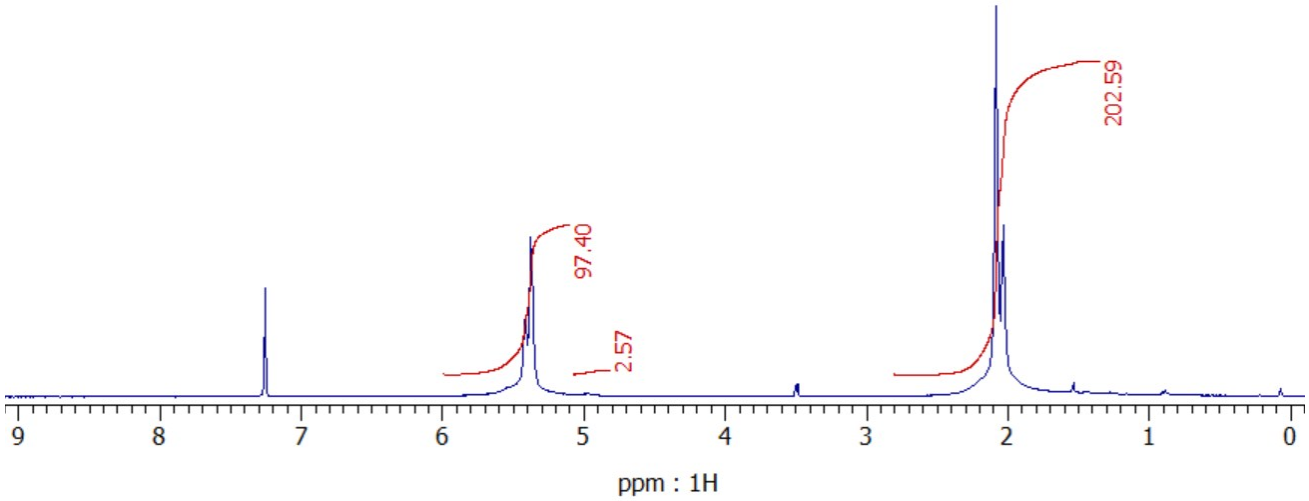

Figure S26. ^{1}H NMR of polybutadiene obtained in Table 2, run 14 (500 MHz, in $CDCl_3$).

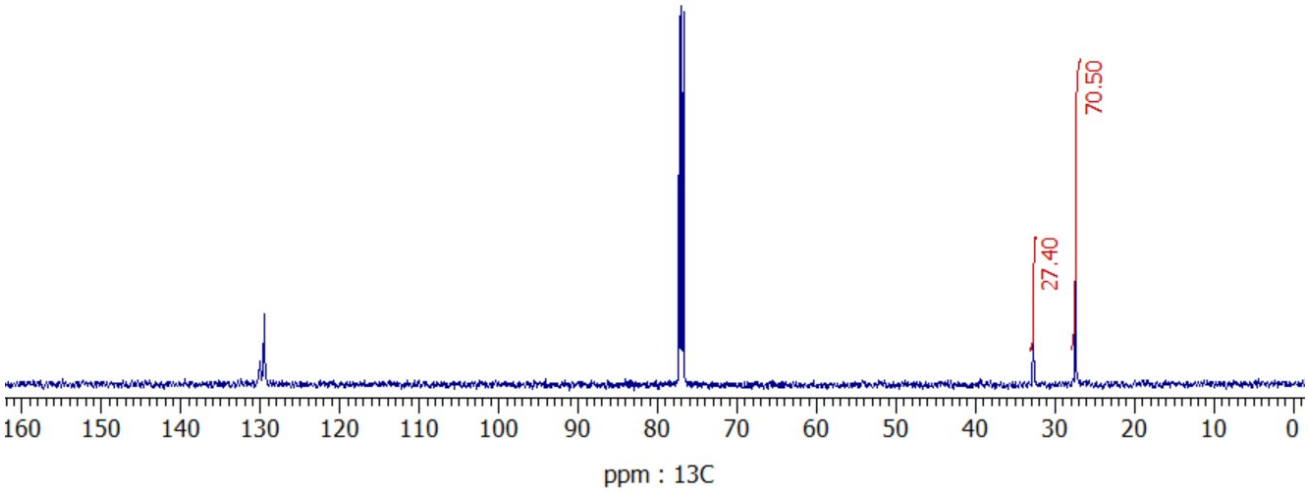

Figure S27. ^{13}C NMR of polybutadiene obtained in Table 2, run 14 (125 MHz, in $CDCl_3$).

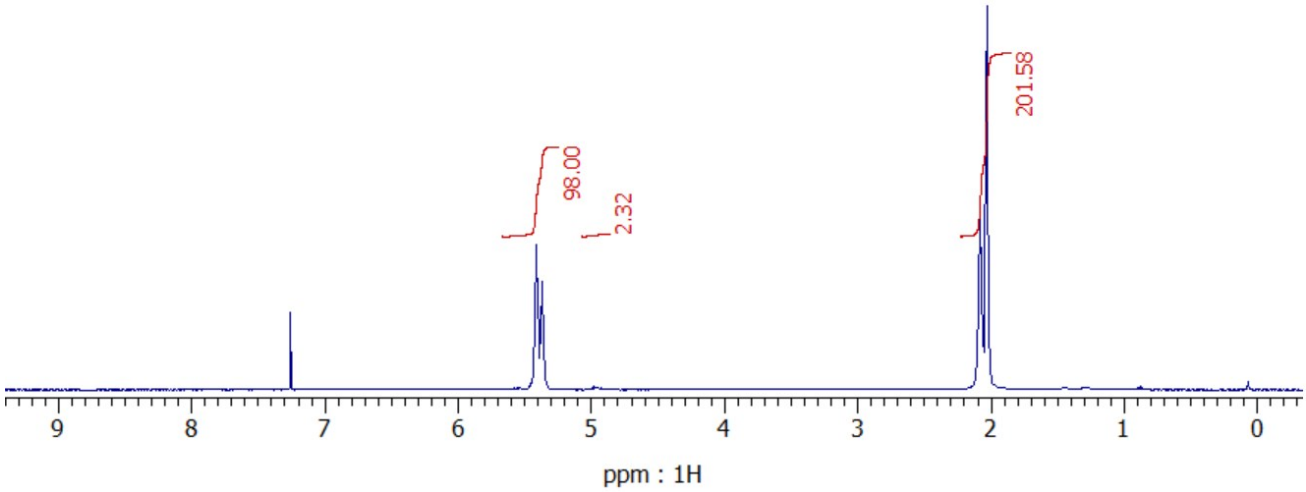

Figure S28. ^{1}H NMR of polybutadiene obtained in Table 2, run 15 (500 MHz, in $CDCl_3$).

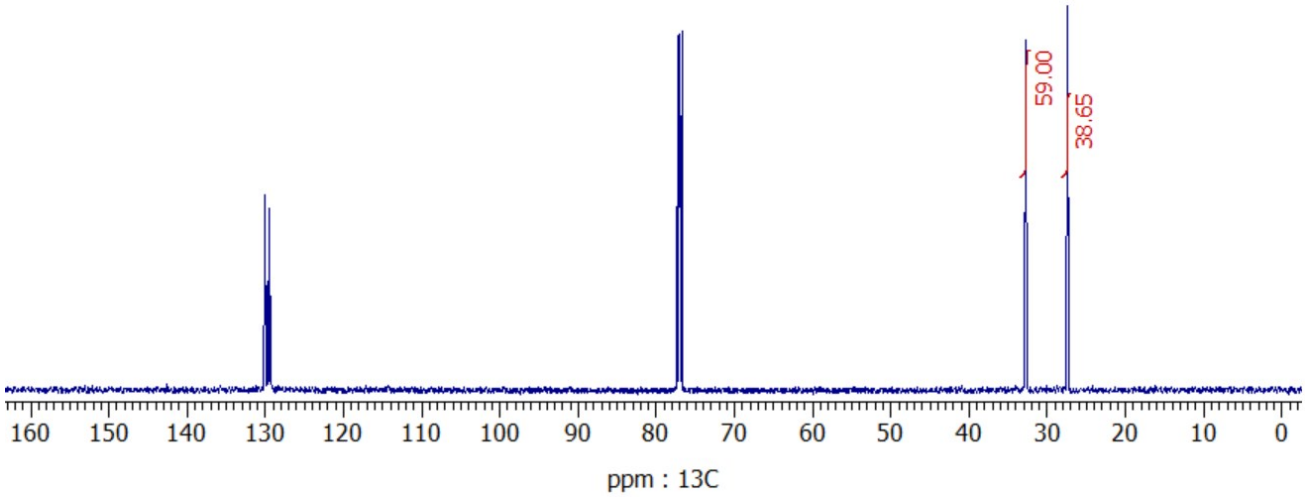

Figure S29. ^{13}C NMR of polybutadiene obtained in Table 2, run 15 (125 MHz, in $CDCl_3$).

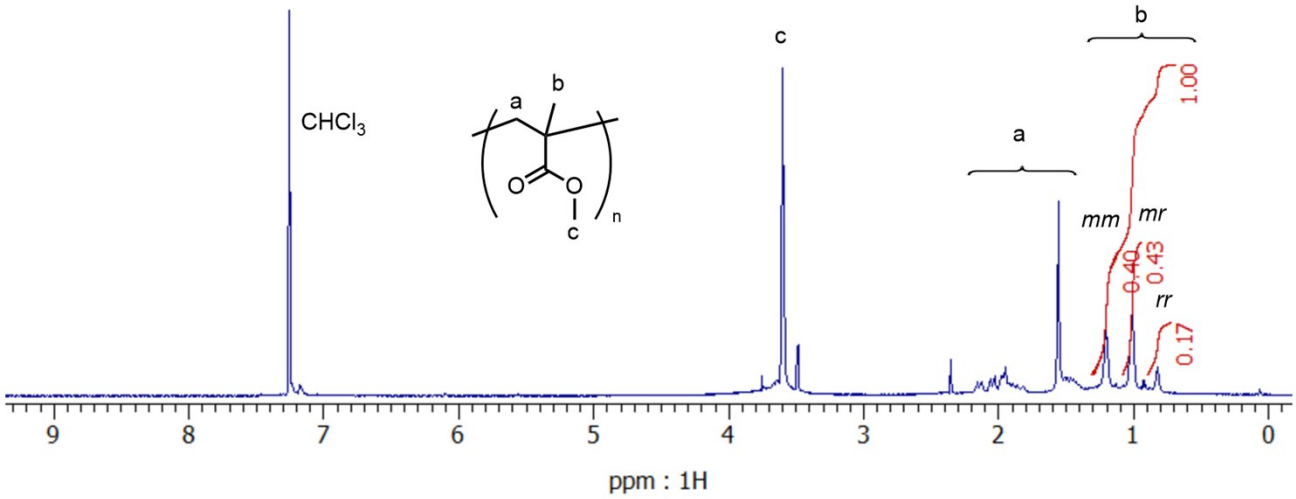

Figure S30. ^{1}H NMR of PMMA obtained in Table 3, run 1 (500 MHz, in $CDCl_3$).

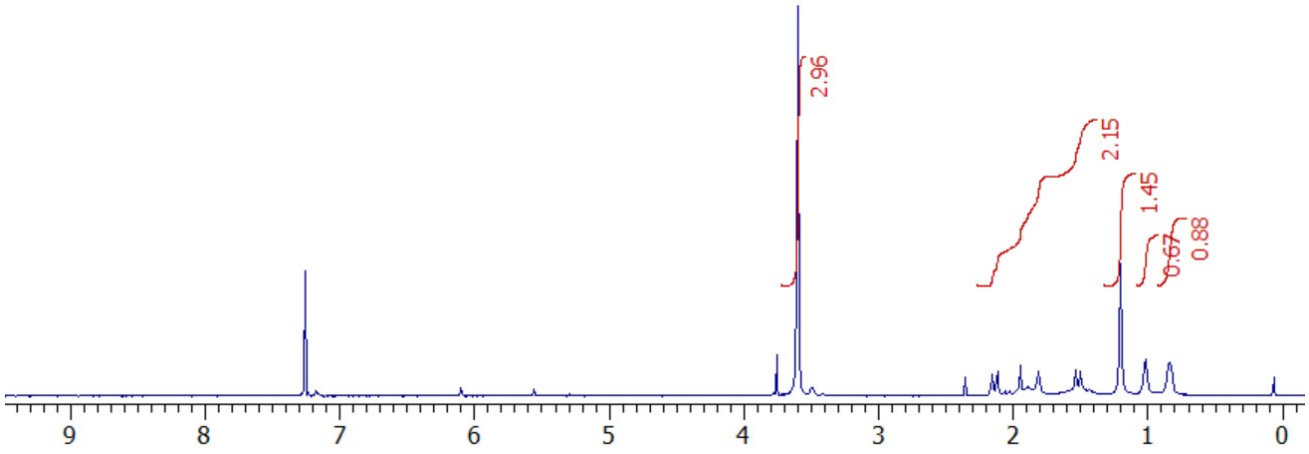

Figure S31. ^{1}H NMR of PMMA obtained in Table 3, run 2 (500 MHz, in $CDCl_3$).

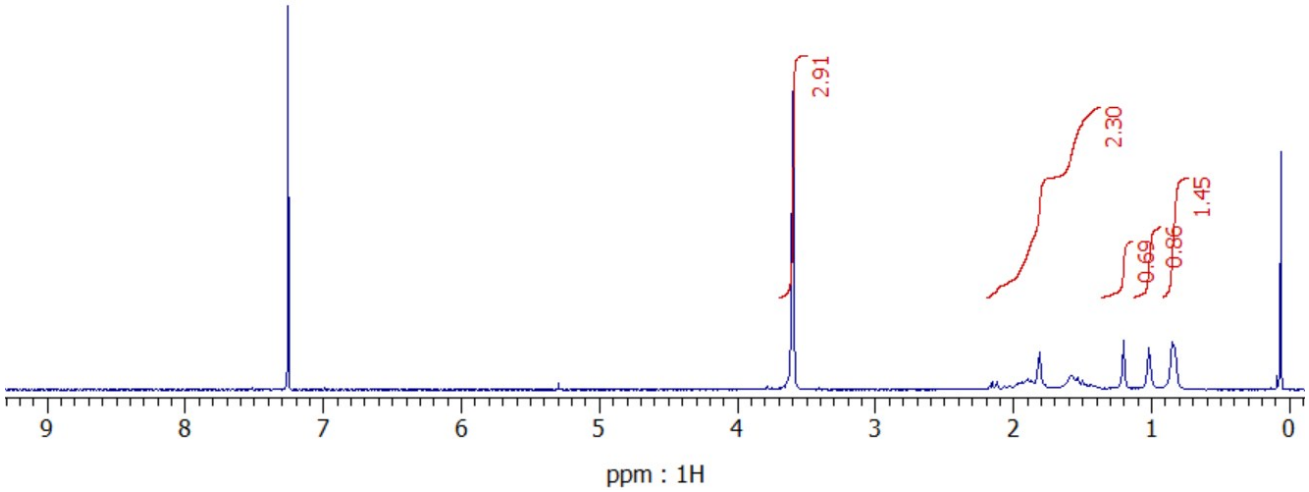

Figure S32. ^{1}H NMR of PMMA obtained in Table 3, run 3 (500 MHz, in $CDCl_3$).

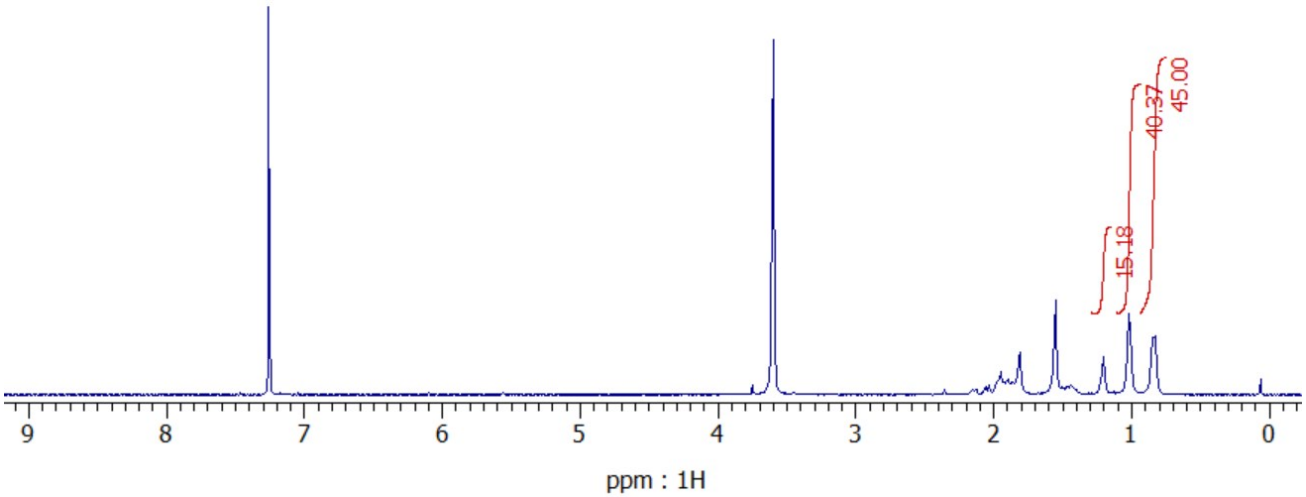

Figure S33. ^{1}H NMR of PMMA obtained in Table 3, run 6 (500 MHz, in $CDCl_3$).