

Supplementary Information

π -Carbazolyl supported bis(alkyl) complexes of Sc, Y and La for α -olefin polymerization and hydrogenation

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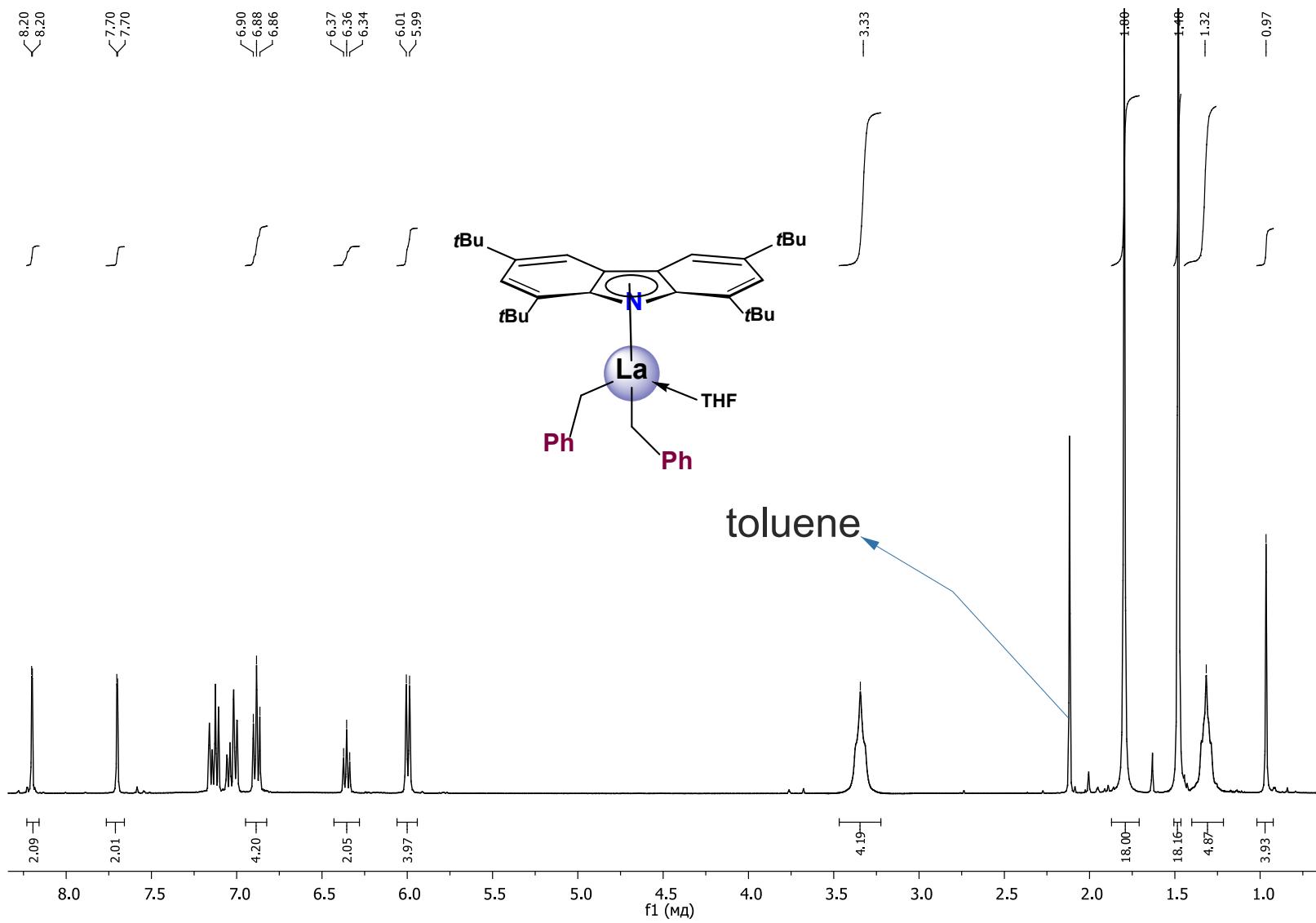


Figure S1. ^1H NMR spectrum of $[t\text{Bu}_4\text{Carb}]\text{La}(\text{CH}_2\text{C}_6\text{H}_5)_2(\text{THF})$ (**1-La**) (400 MHz, C_6D_6 , 293 K).

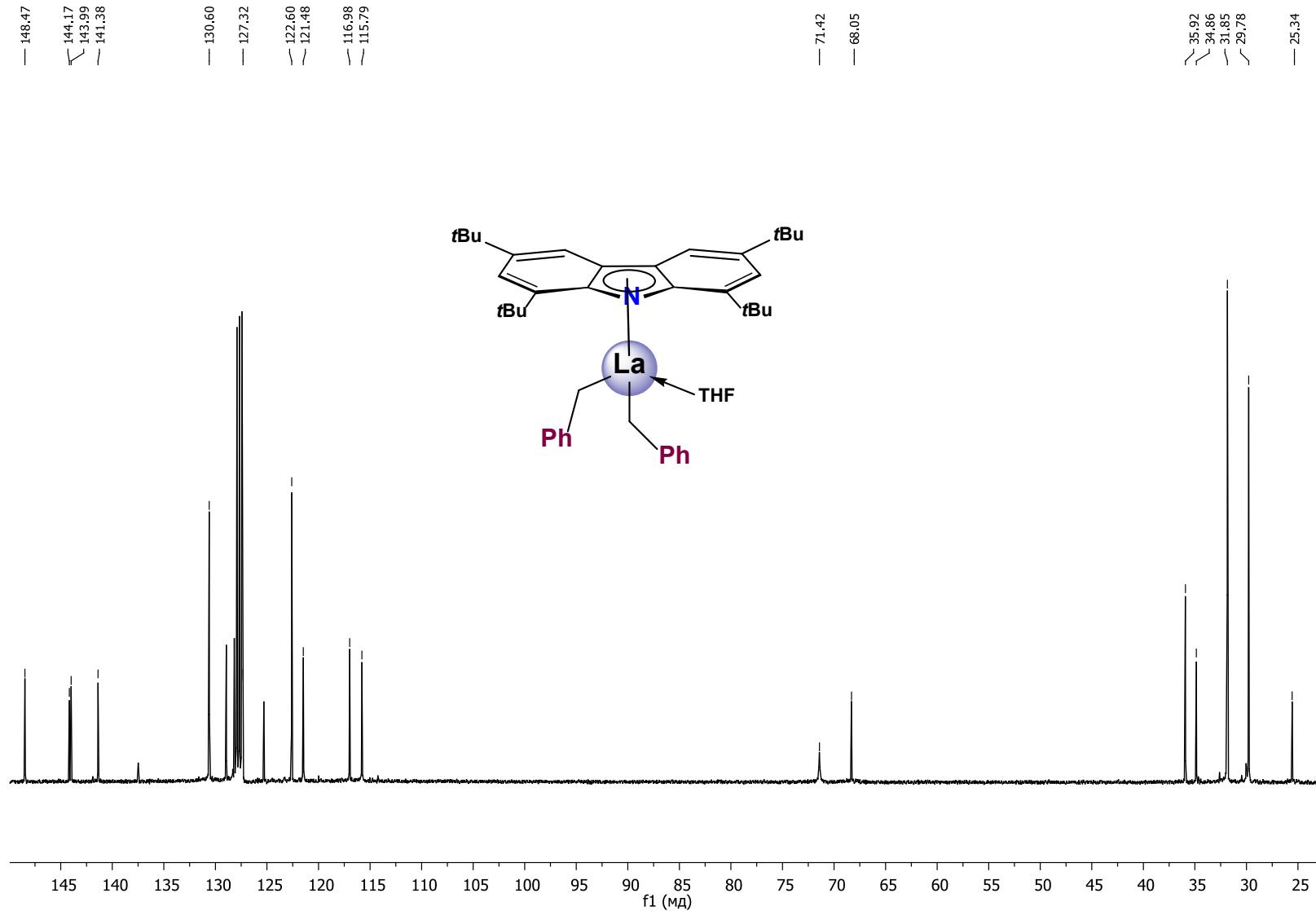


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[t\text{Bu}_4\text{Carb}]\text{La}(\text{CH}_2\text{C}_6\text{H}_5)_2(\text{THF})$ (**1-La**) (100 MHz, C_6D_6 , 293 K).

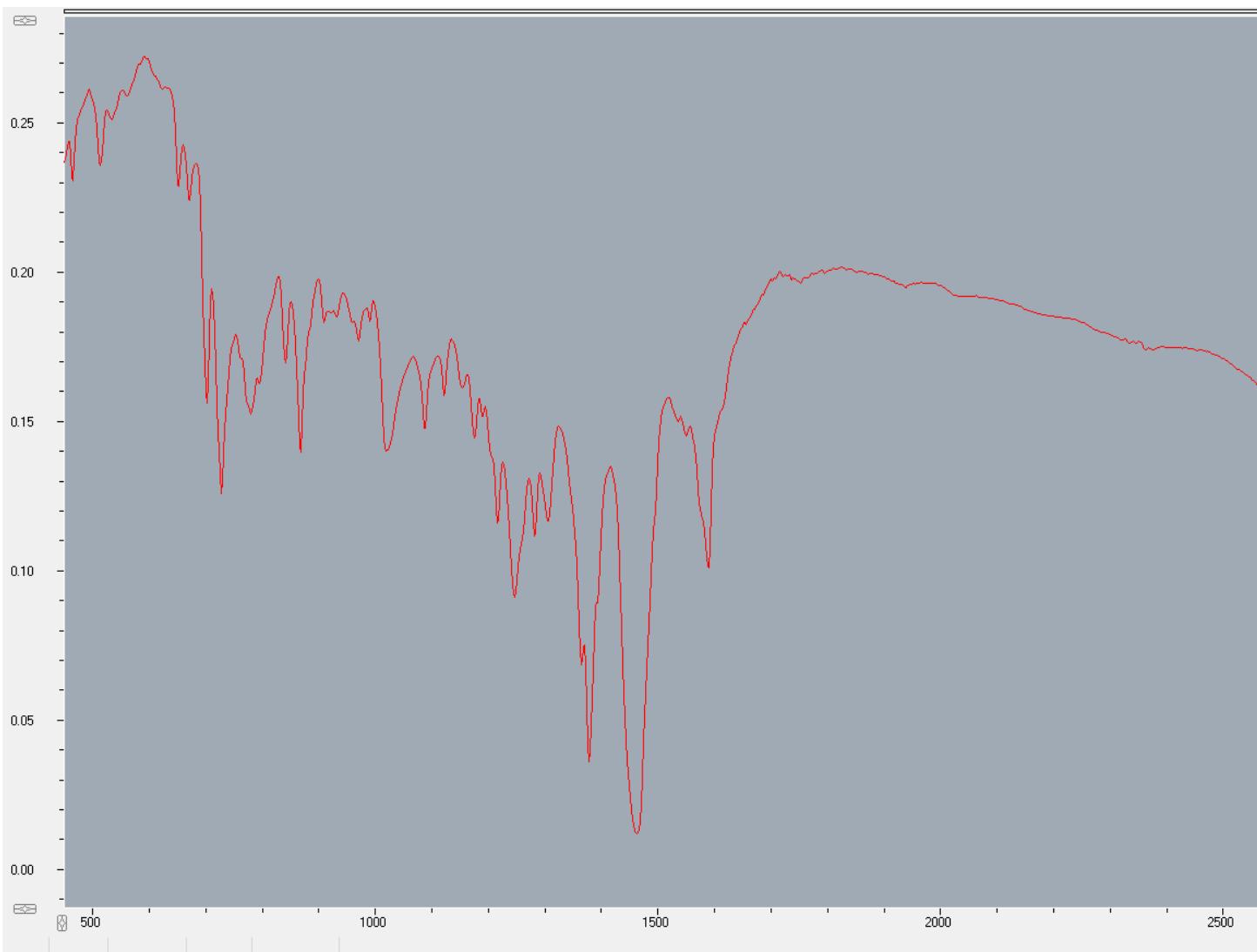


Figure S3. IR spectrum of complex $[t\text{Bu}_4\text{Carb}]\text{La}(\text{CH}_2\text{C}_6\text{H}_5)_2(\text{THF})$ (**1-La**) (KBr, Nujol mull).

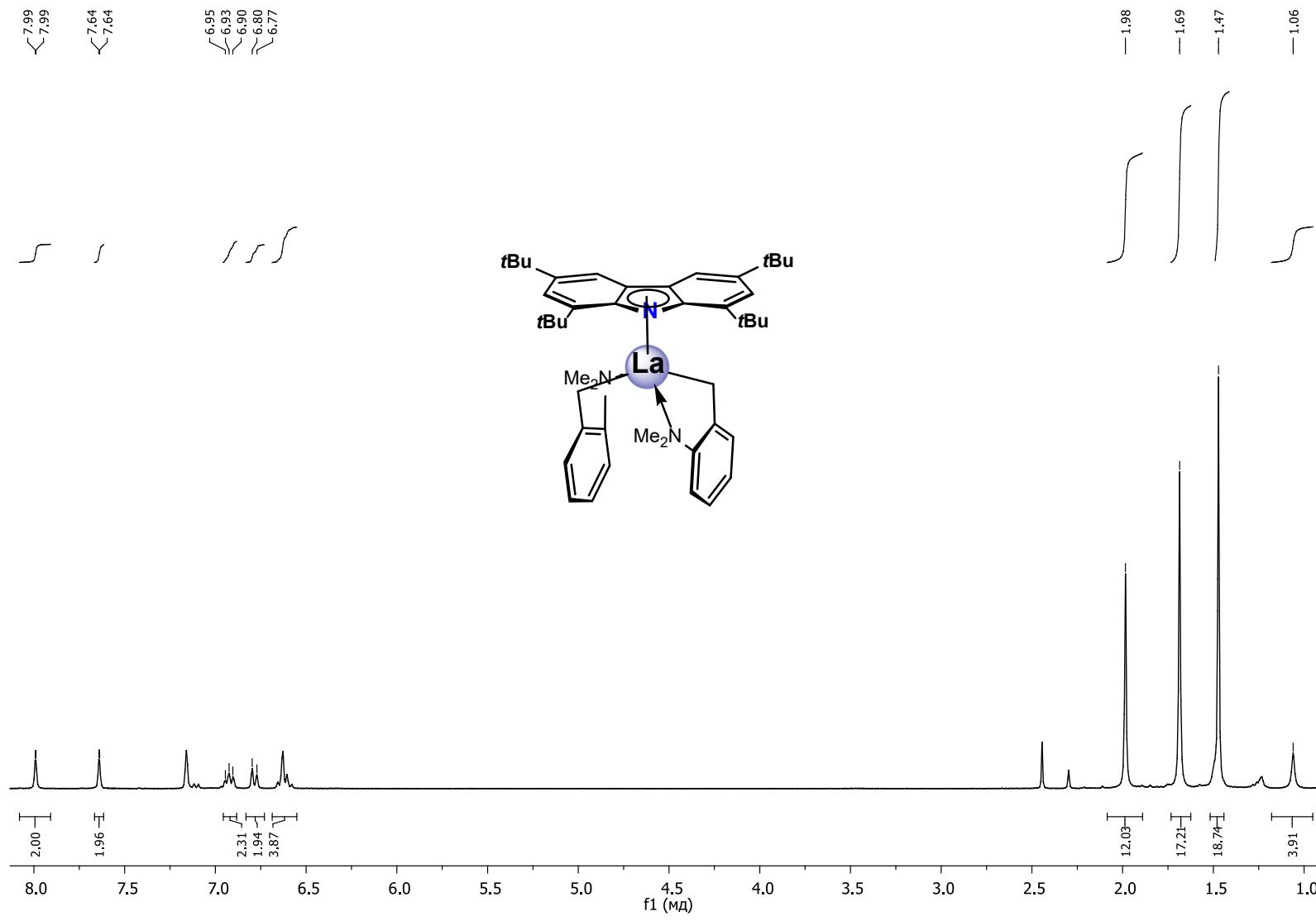


Figure S4. ^1H NMR spectrum of $[t\text{Bu}_4\text{Carb}]\text{La}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-La**) (300 MHz, C₆D₆, 293 K).

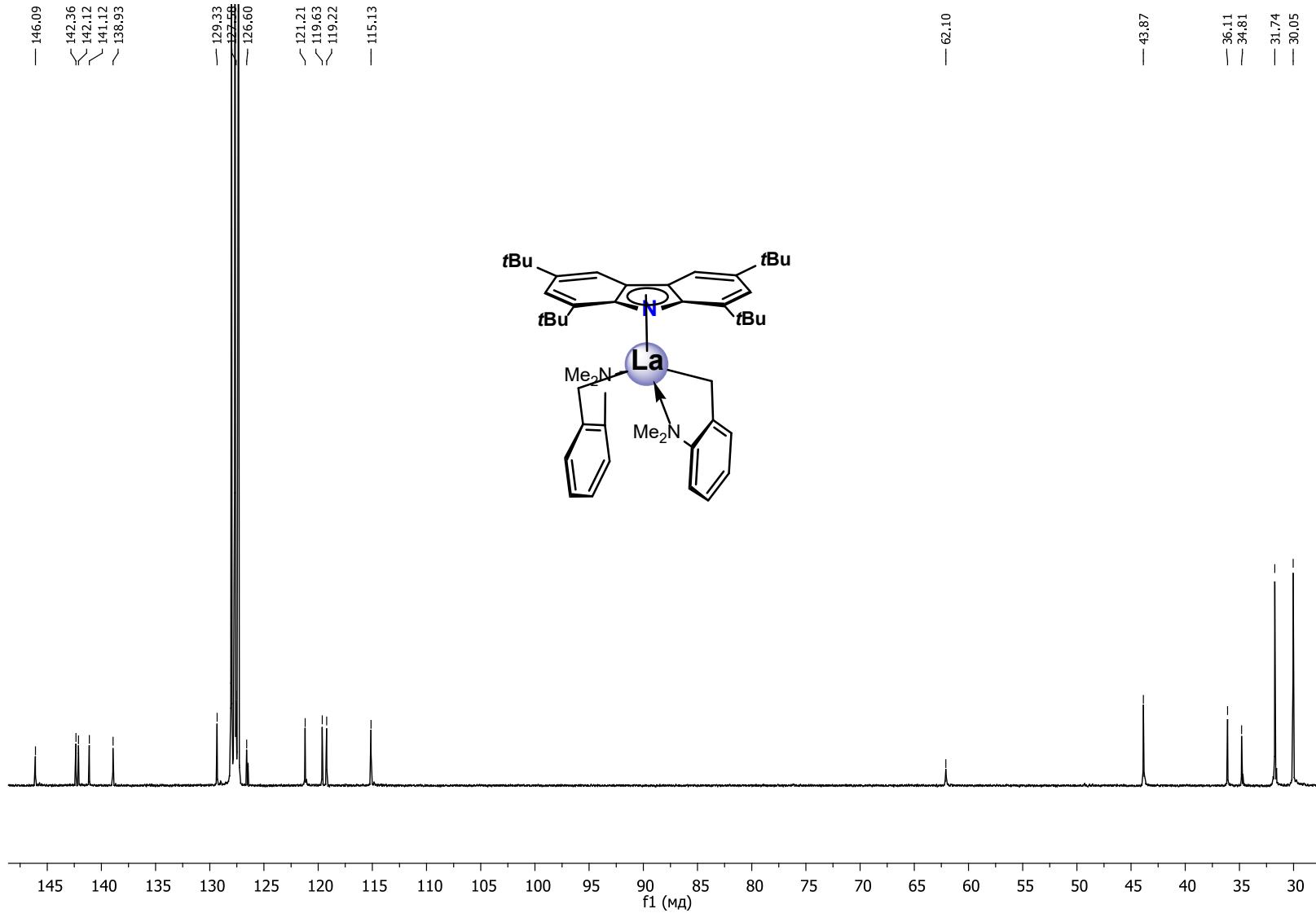


Figure S5. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of $[\text{tBu}_4\text{Carb}]\text{La}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-La**) (75 MHz, C₆D₆, 293 K).

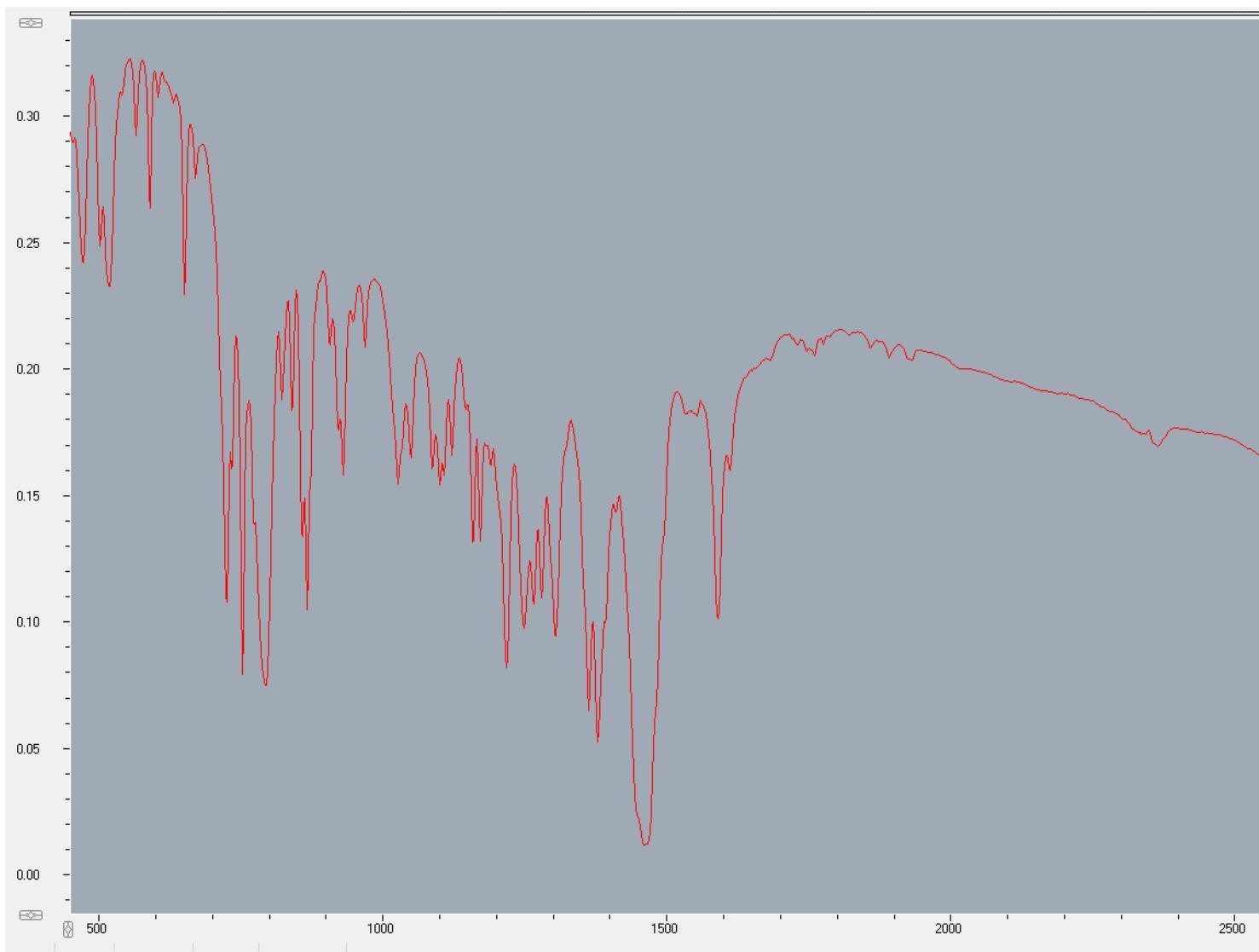


Figure S6. IR spectrum of complex $[t\text{Bu}_4\text{Carb}]\text{La}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-La**) (KBr, Nujol mull).

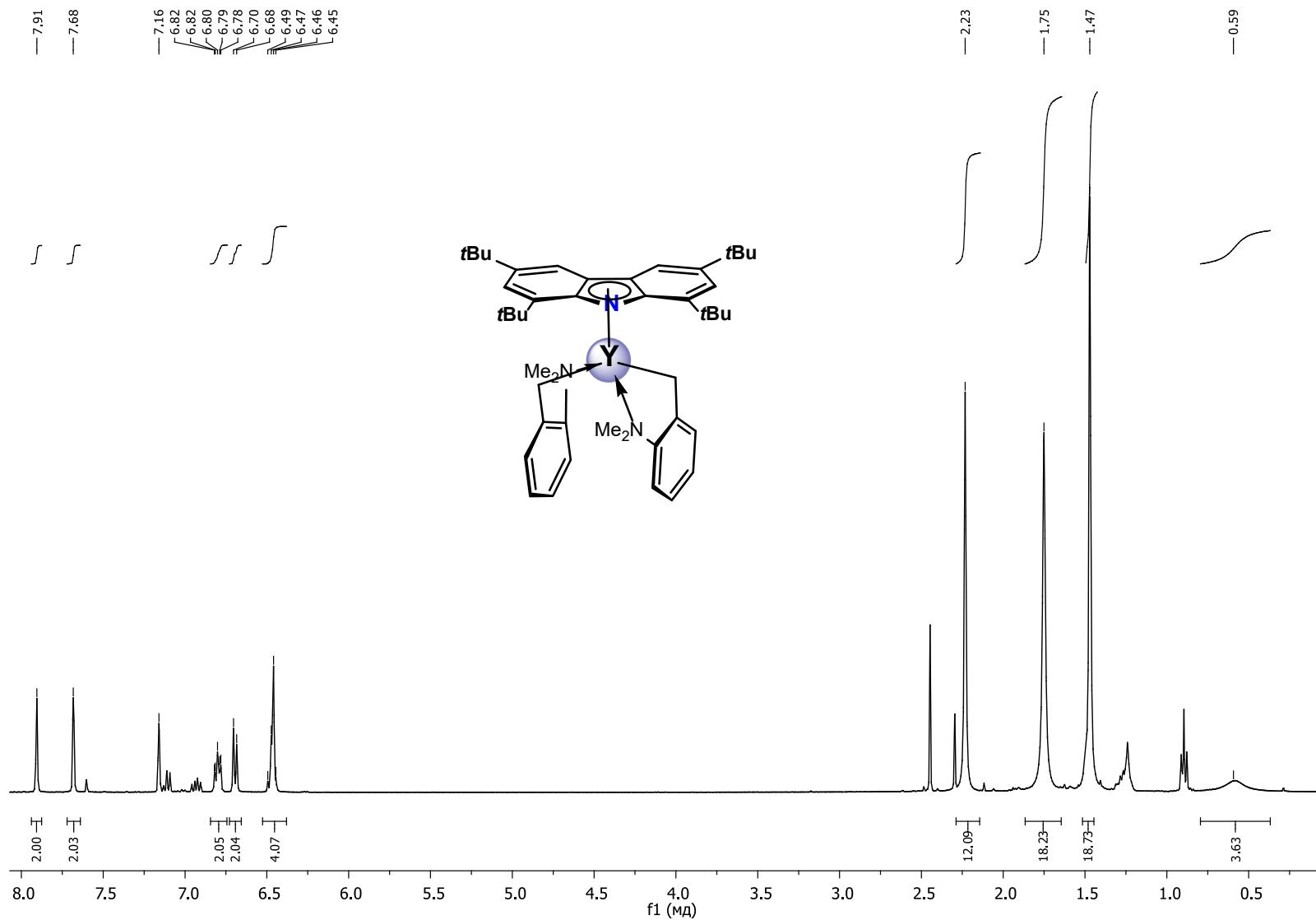


Figure S7. ^1H NMR spectrum of $[t\text{Bu}_4\text{Carb}]Y(\text{o-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-Y**) (400 MHz, C_6D_6 , 293 K).

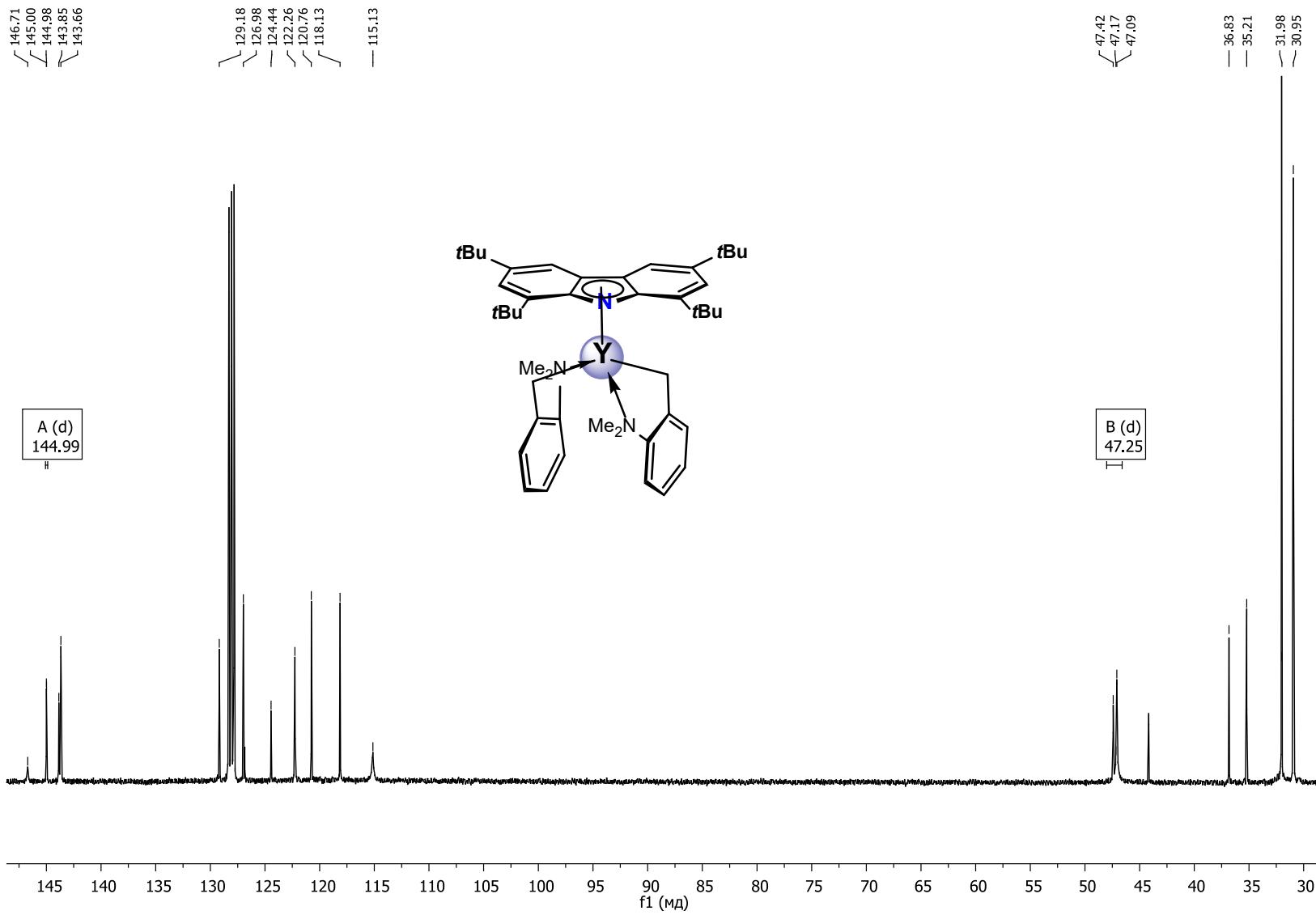


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{tBu}_4\text{Carb}] \text{Y}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-Y**) (100 MHz, C_6D_6 , 293 K).

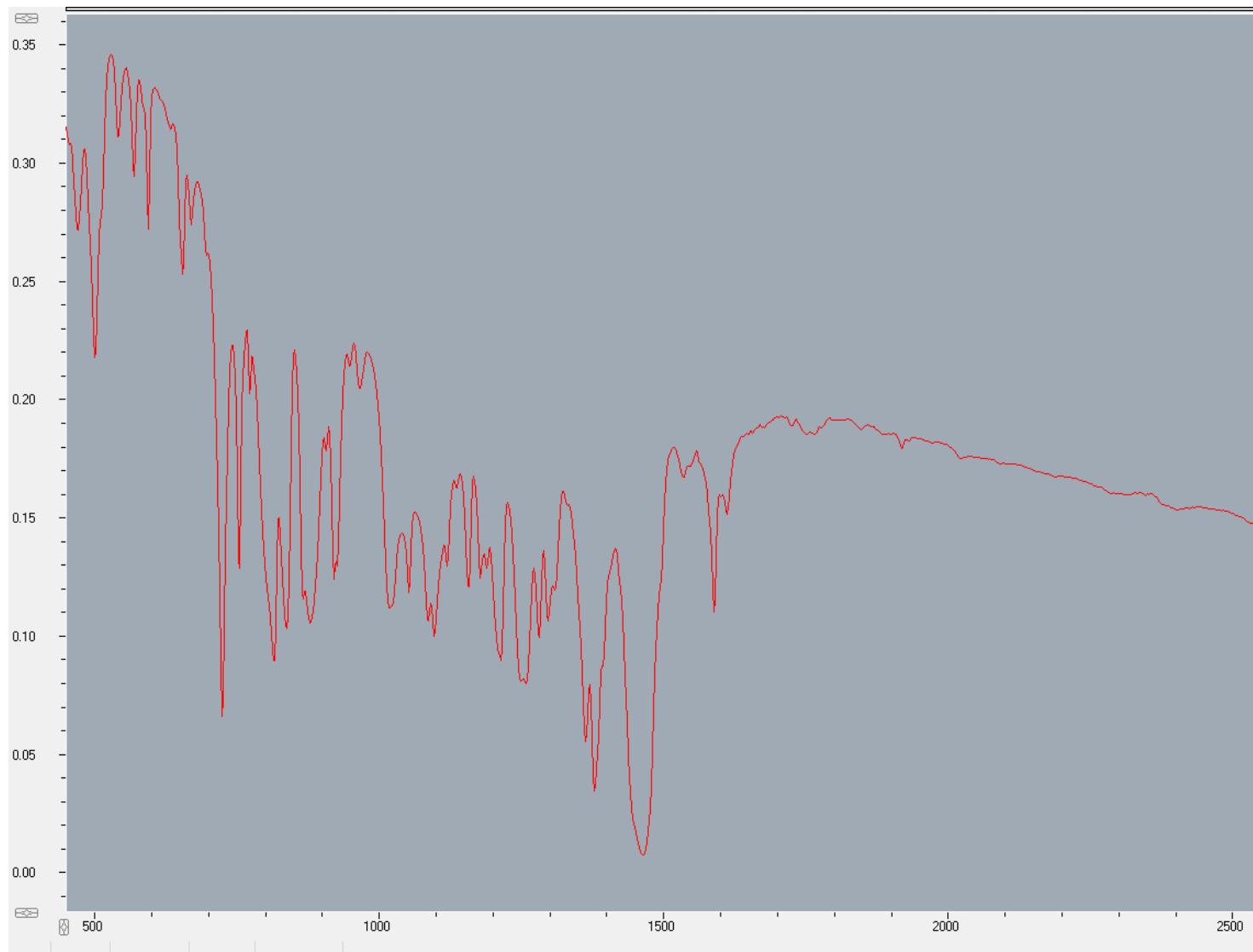


Figure S9. IR spectrum of complex $[t\text{Bu}_4\text{Carb}]\text{Y}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-Y**) (KBr, Nujol mull).

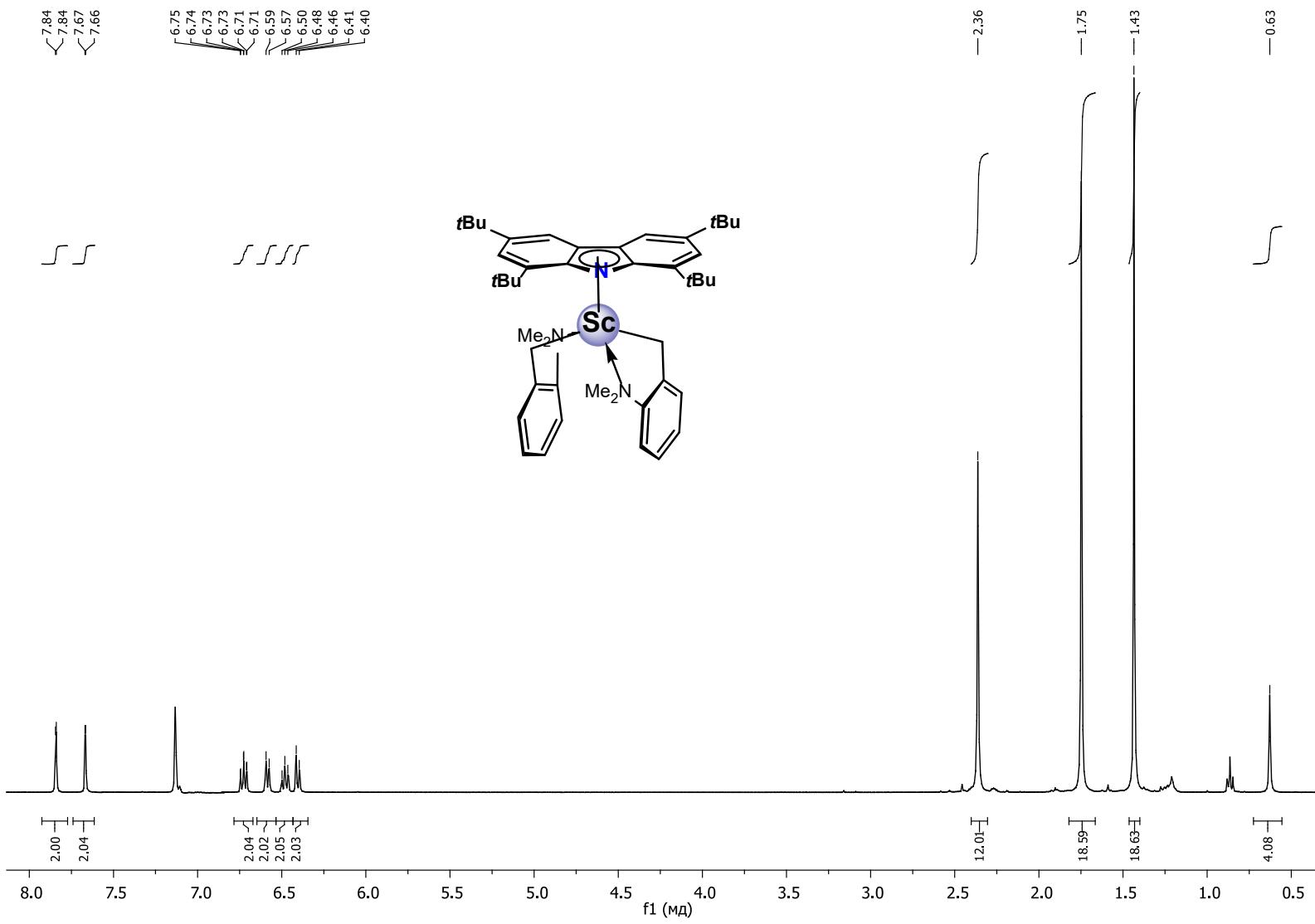


Figure S10. ^1H NMR spectrum of $[t\text{Bu}_4\text{Carb}]\text{Sc}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-Sc**) (400 MHz, C_6D_6 , 293 K).

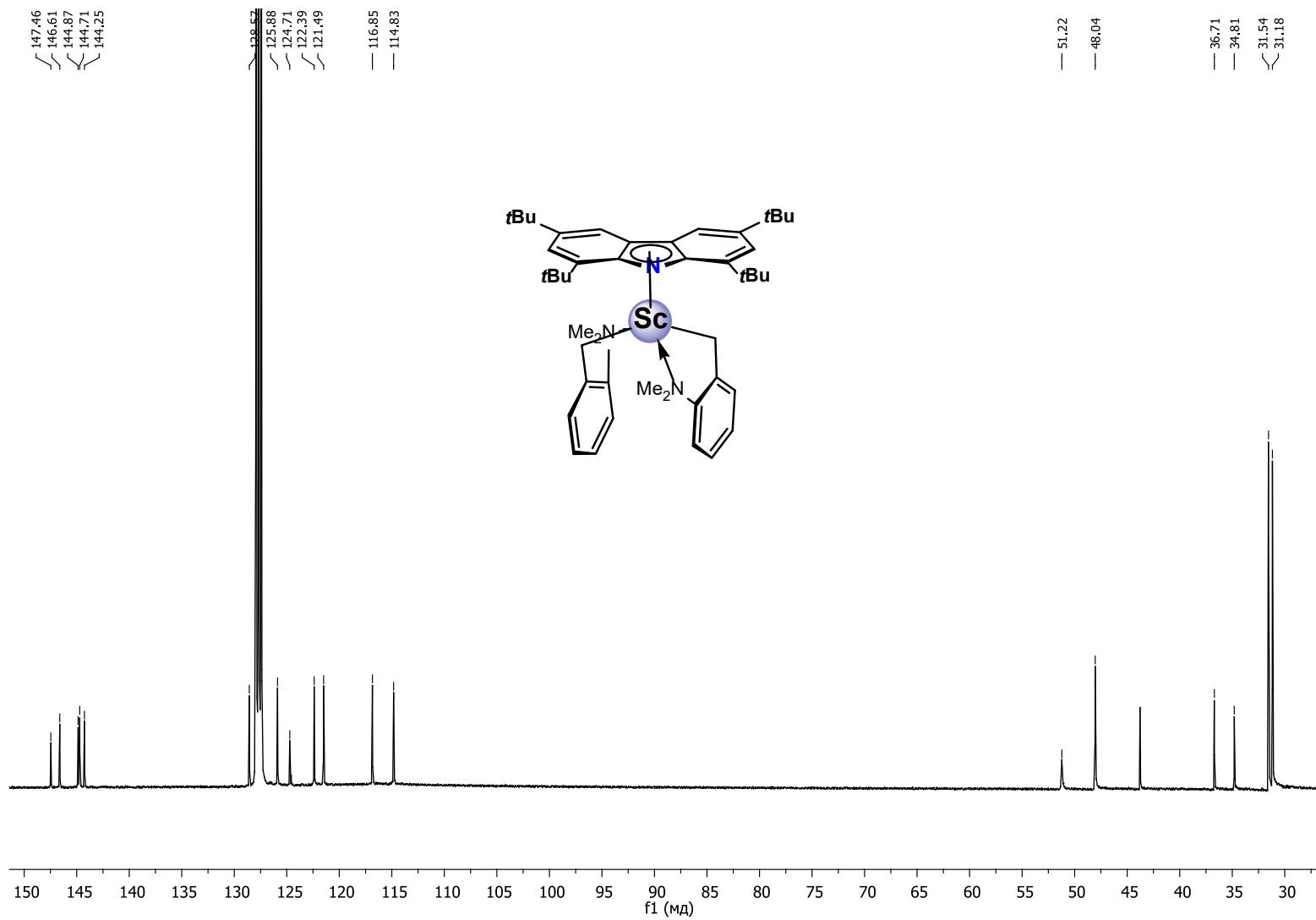


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{tBu}_4\text{Carb}]\text{Sc}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-Sc**) (100 MHz, C_6D_6 , 293 K).

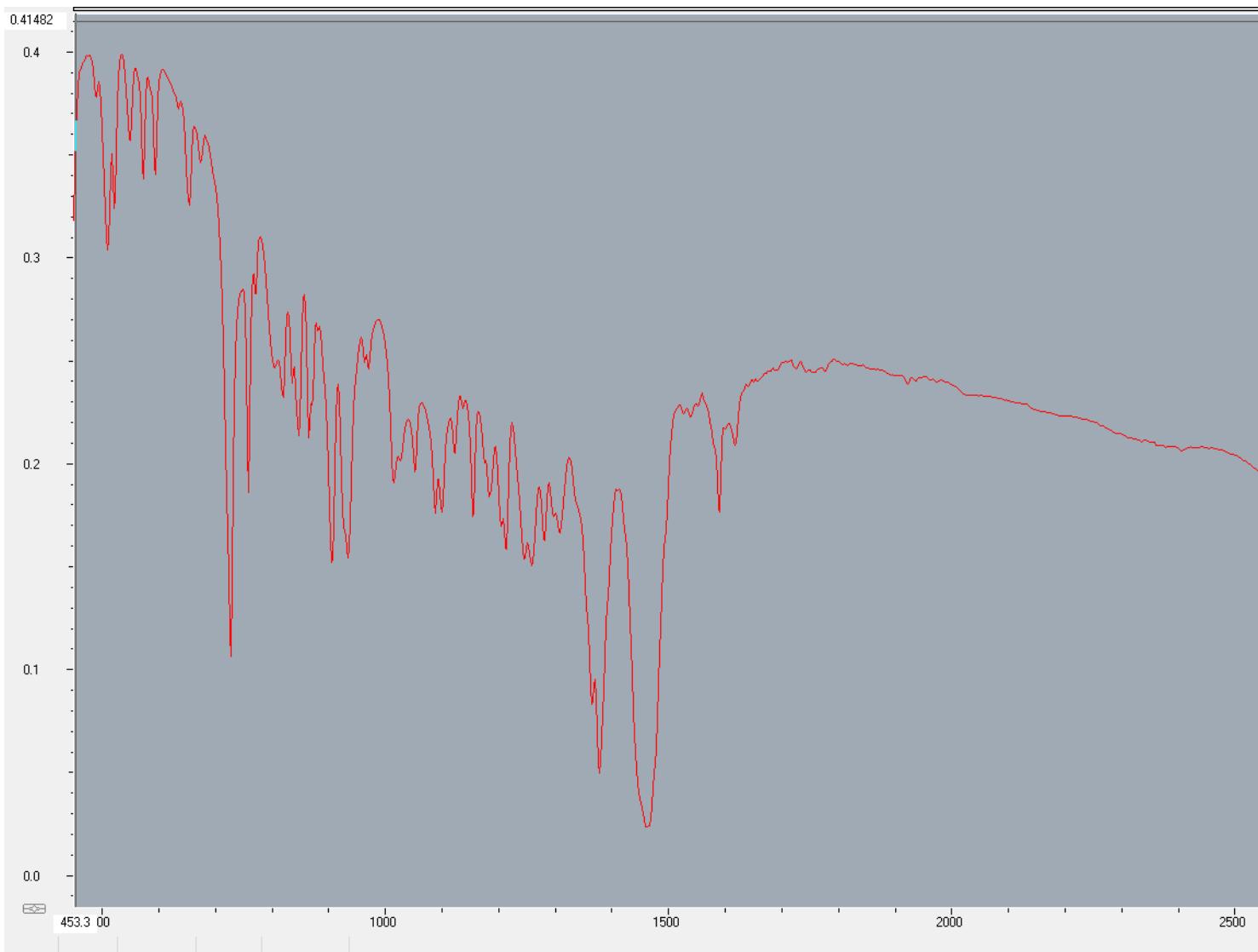


Figure S12. IR spectrum of complex $[t\text{Bu}_4\text{Carb}]\text{Sc}(o\text{-NMe}_2\text{C}_6\text{H}_5\text{CH}_2)_2$ (**2-Sc**) (KBr, Nujol mull).

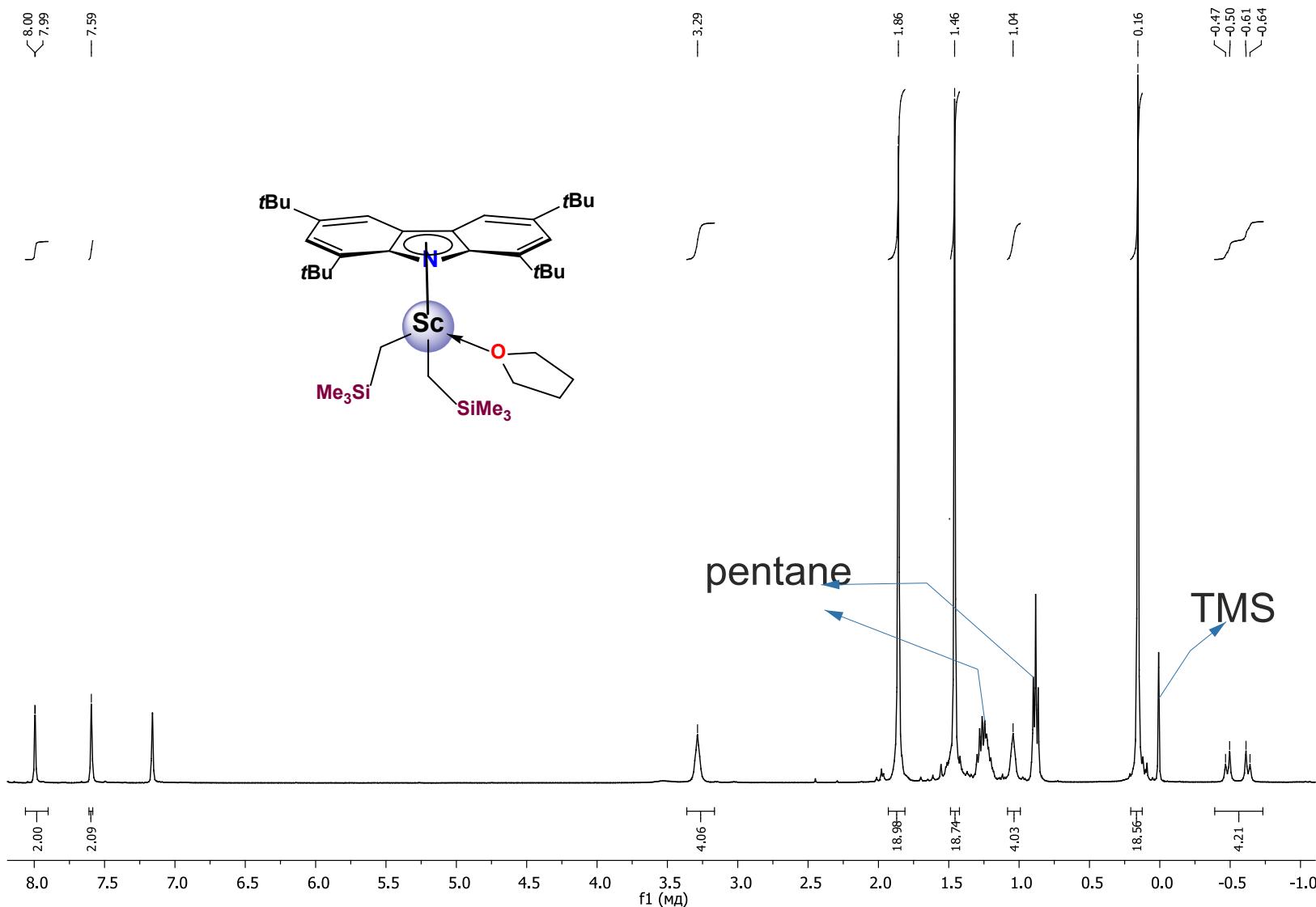


Figure S13. ^1H NMR spectrum of $[t\text{Bu}_4\text{Carb}]\text{Sc}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**3-Sc**) (400 MHz, C_6D_6 , 293 K).

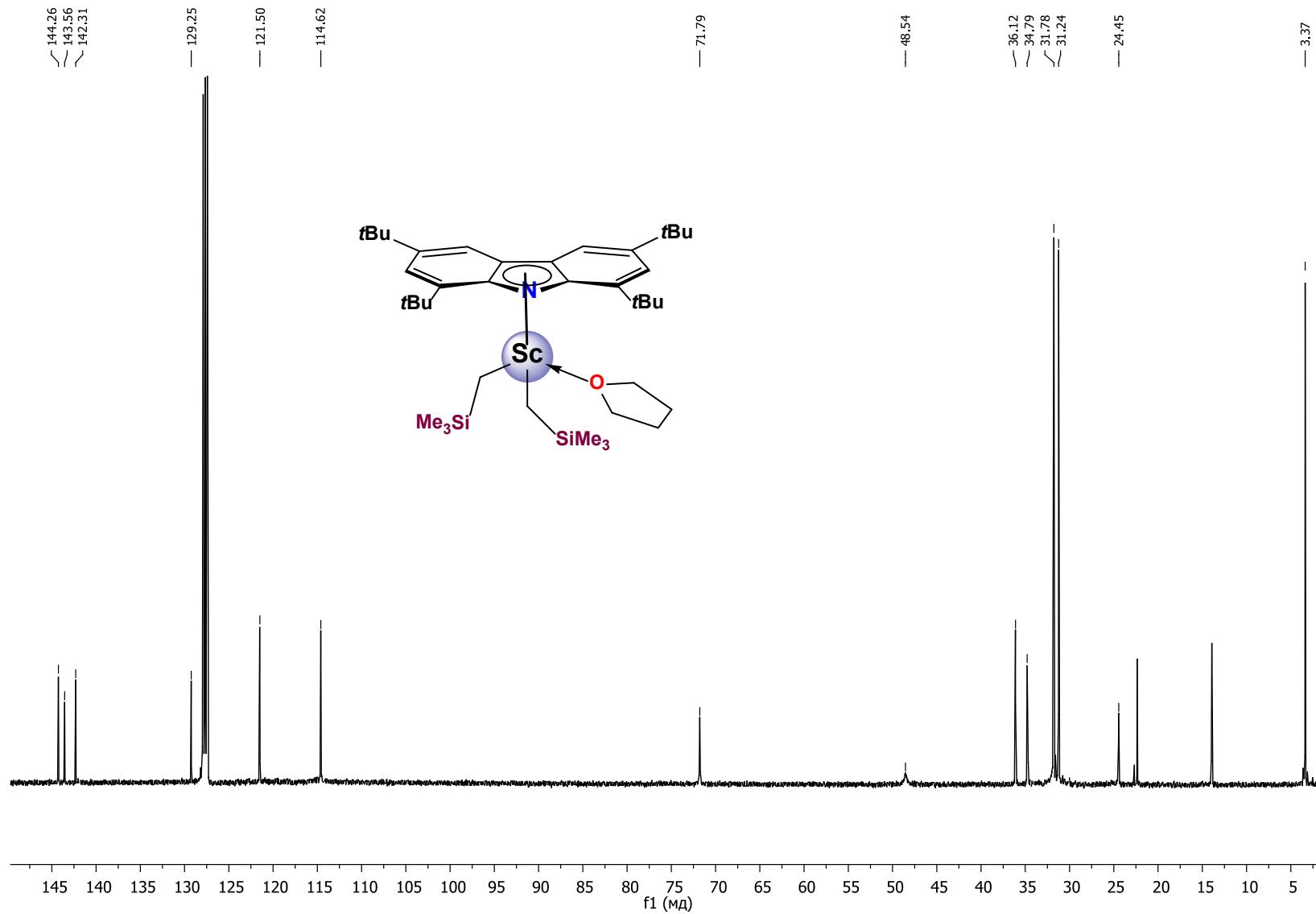


Figure S14. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of $[\text{tBu}_4\text{Carb}]\text{Sc}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**3-Sc**) (100 MHz, C_6D_6 , 293 K).

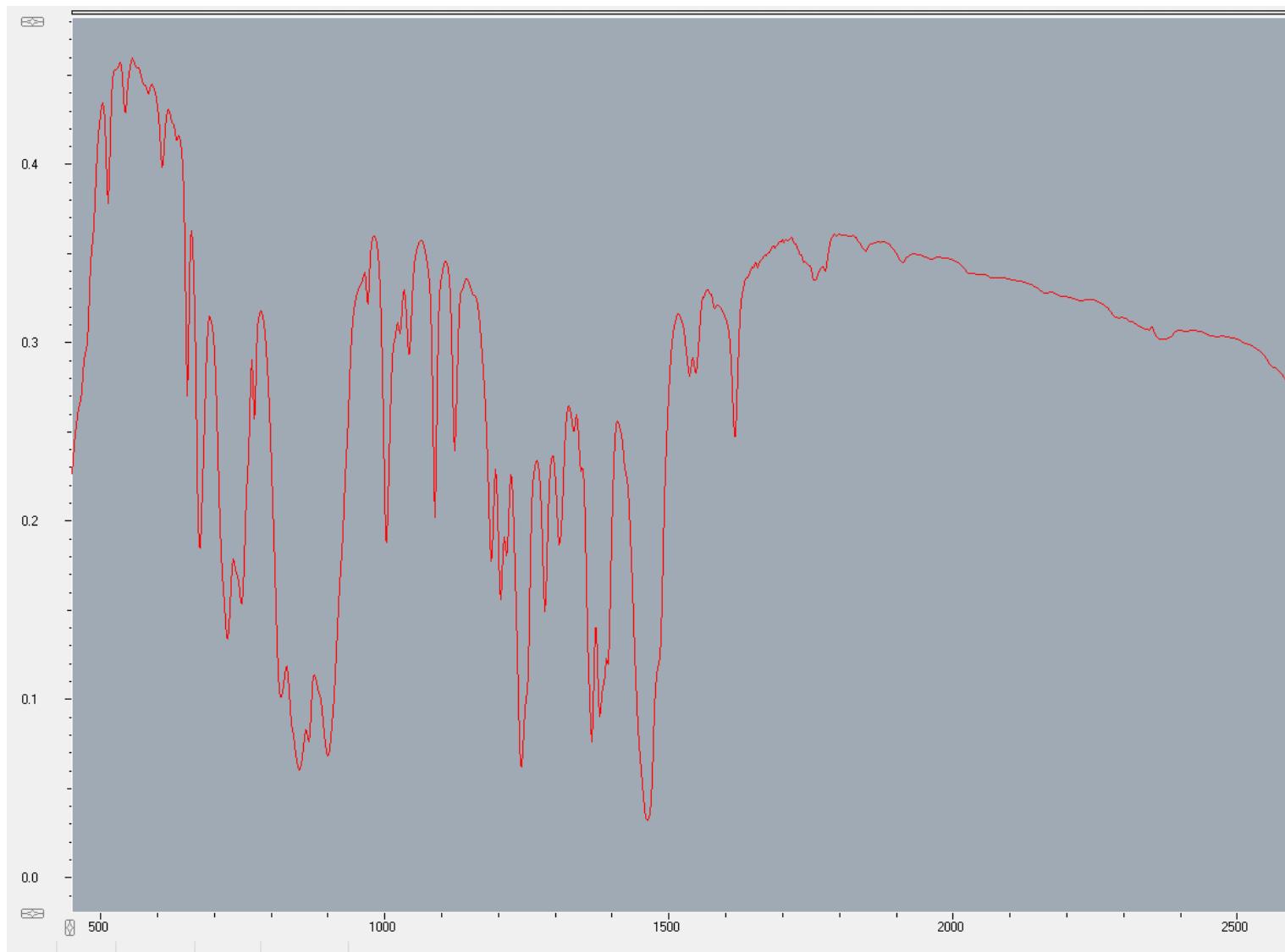


Figure S15. IR spectrum of complex $[t\text{Bu}_4\text{Carb}]\text{Sc}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**3-Sc**) (KBr, Nujol mull).

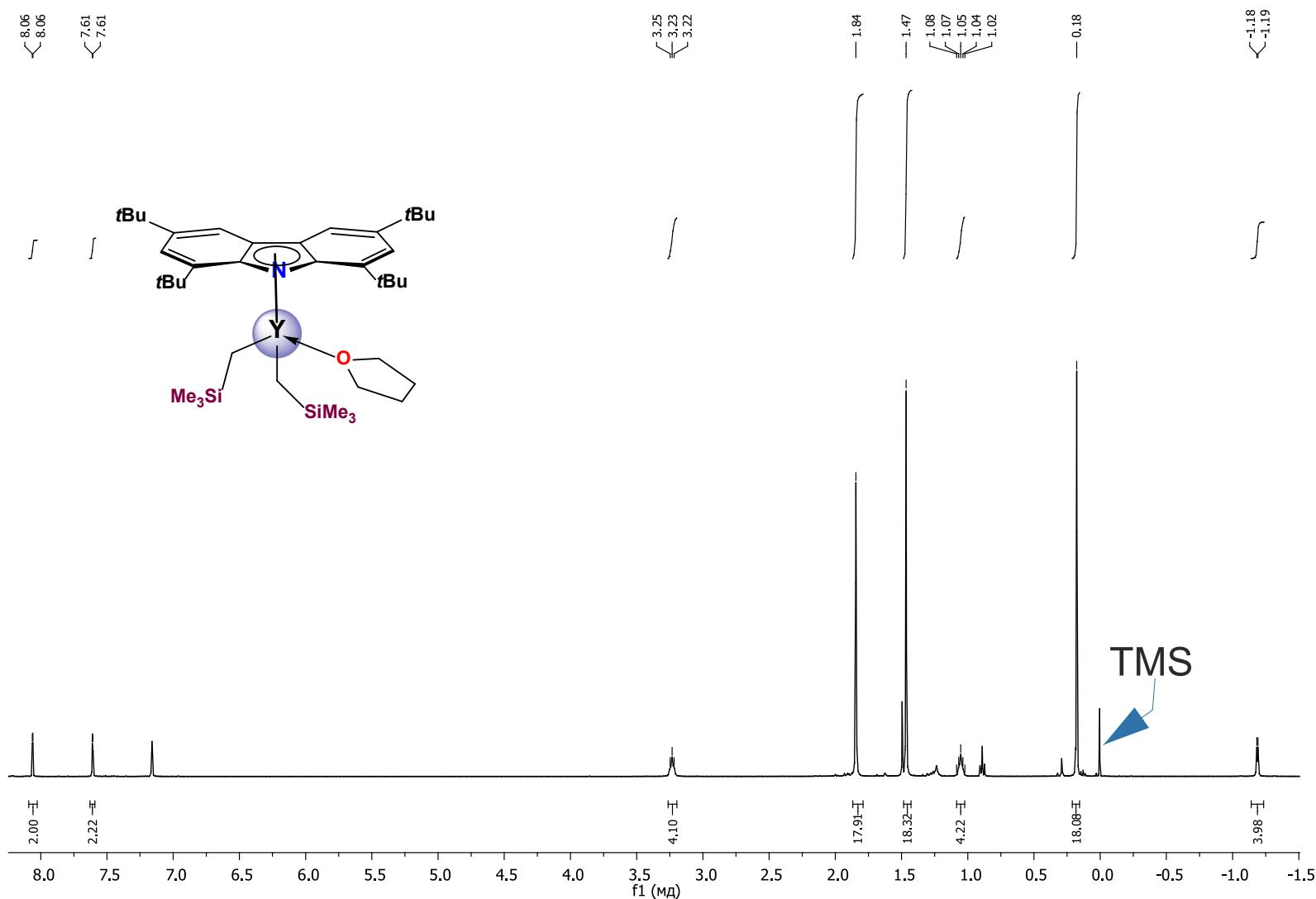


Figure S16. ^1H NMR spectrum of $[t\text{Bu}_4\text{Carb}]Y(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**3-Y**) (400 MHz, C_6D_6 , 293 K).

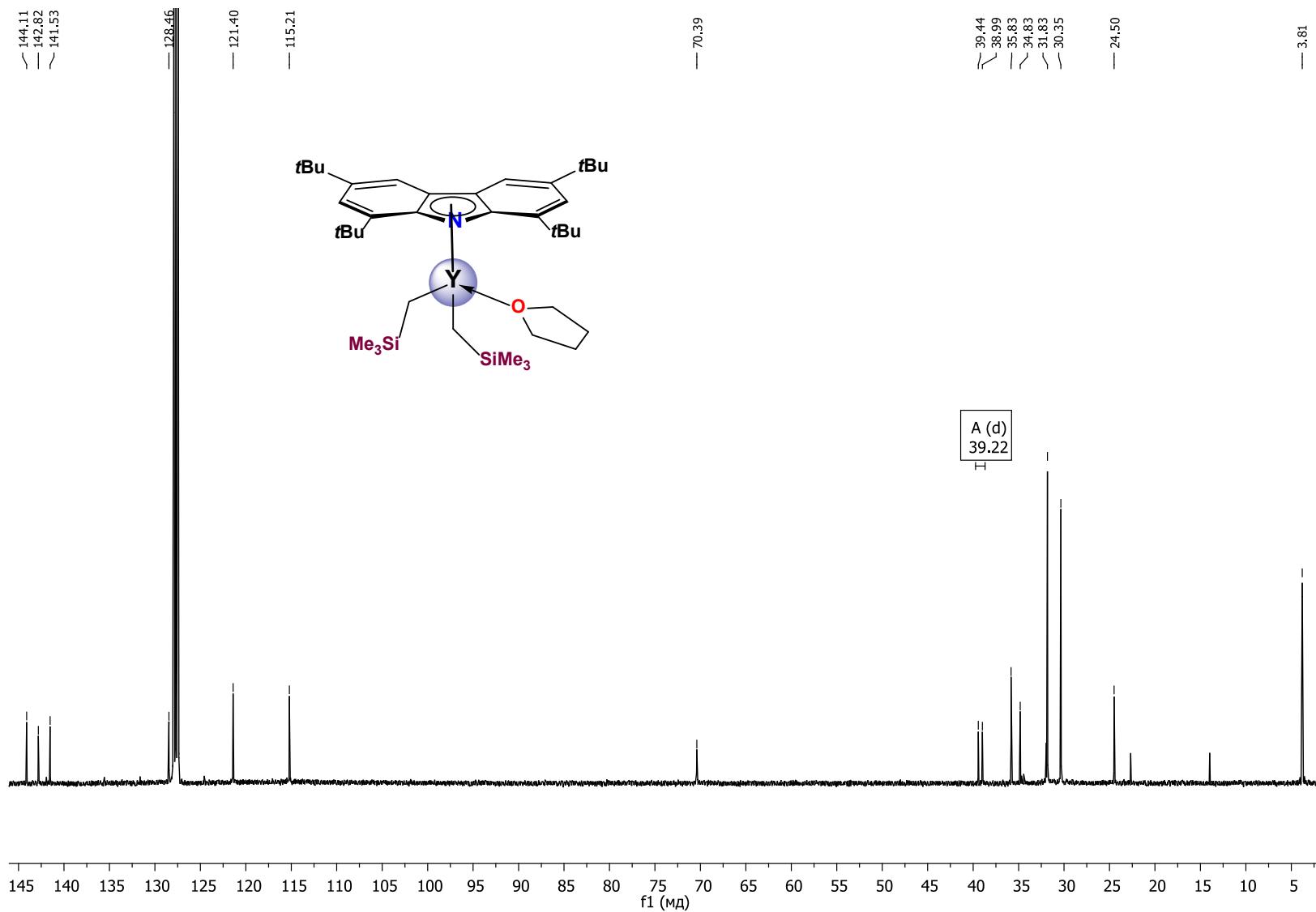


Figure S17. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of $[\text{tBu}_4\text{Carb}]Y(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**3-Y**) (100 MHz, C_6D_6 , 298 K).

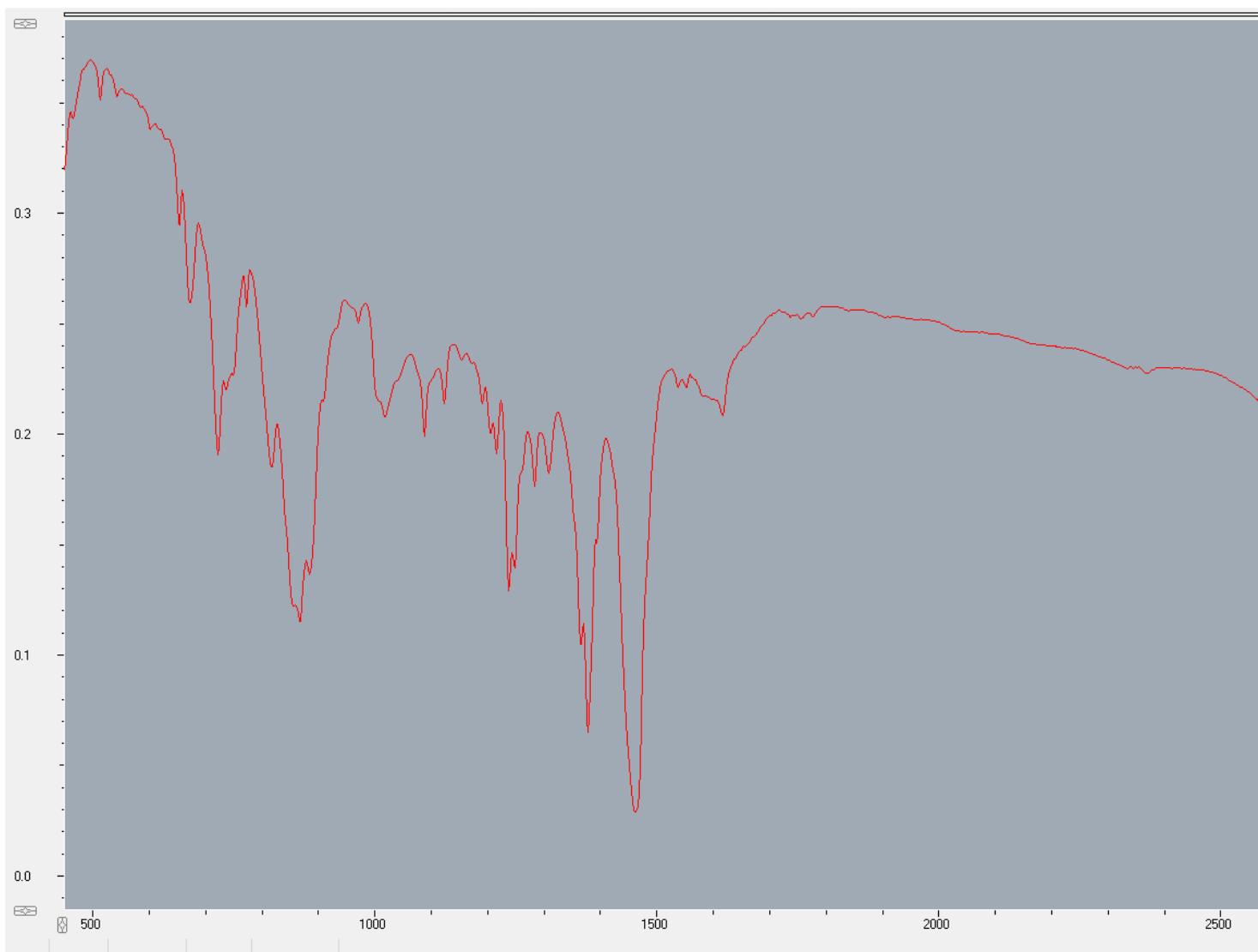


Figure S18. IR spectrum of complex $[t\text{Bu}_4\text{Carb}]\text{Y}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**3-Y**) (KBr, Nujol mull).

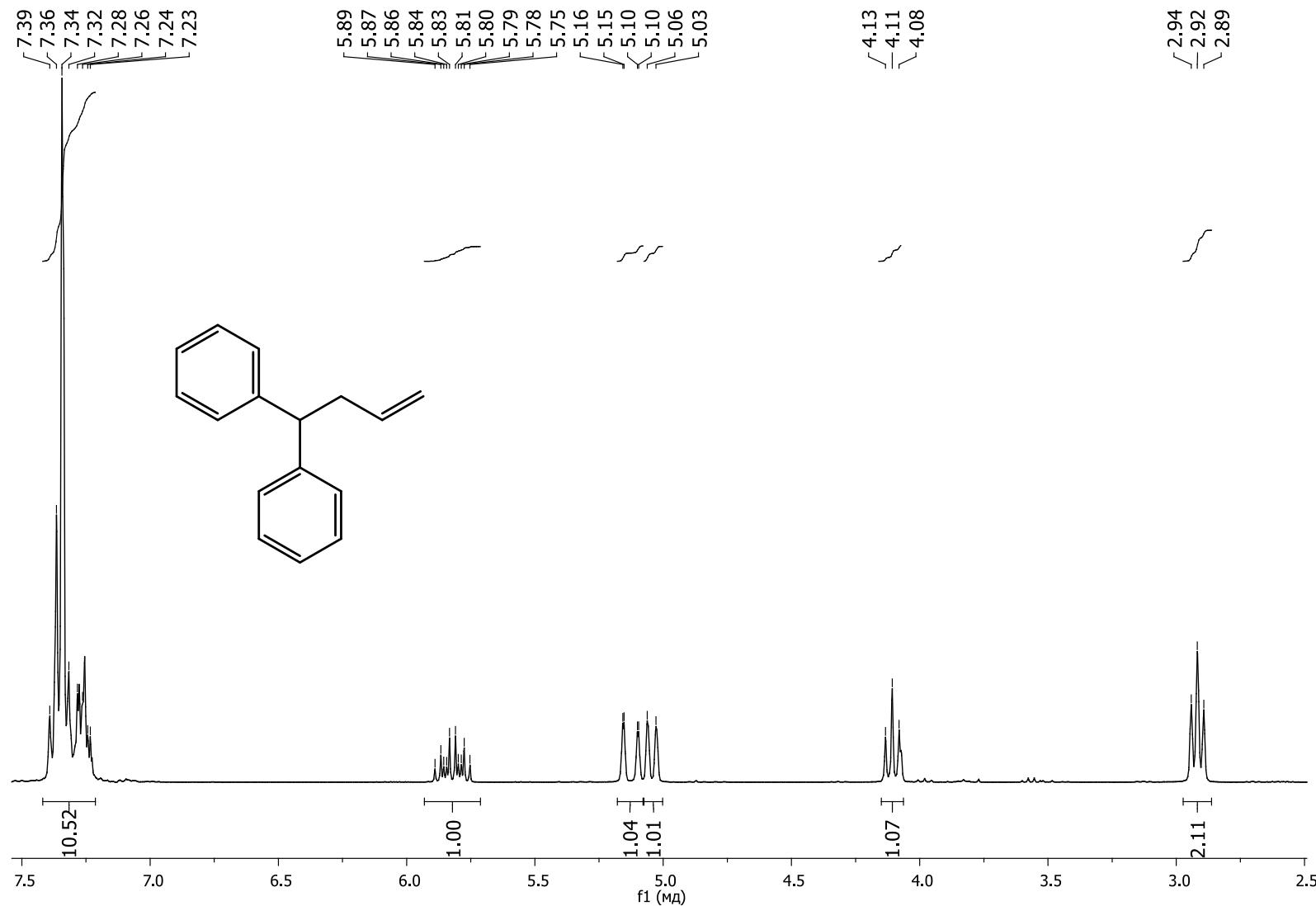


Figure S19. ^1H NMR spectrum of 4,4-diphenyl-but-1-ene (300 MHz, CDCl_3 , 300 K).



Figure S20. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4,4-diphenyl-but-1-ene (75 MHz, CDCl_3 , 300 K).

0858_Polyolefine
Polyhexene. 70(1)

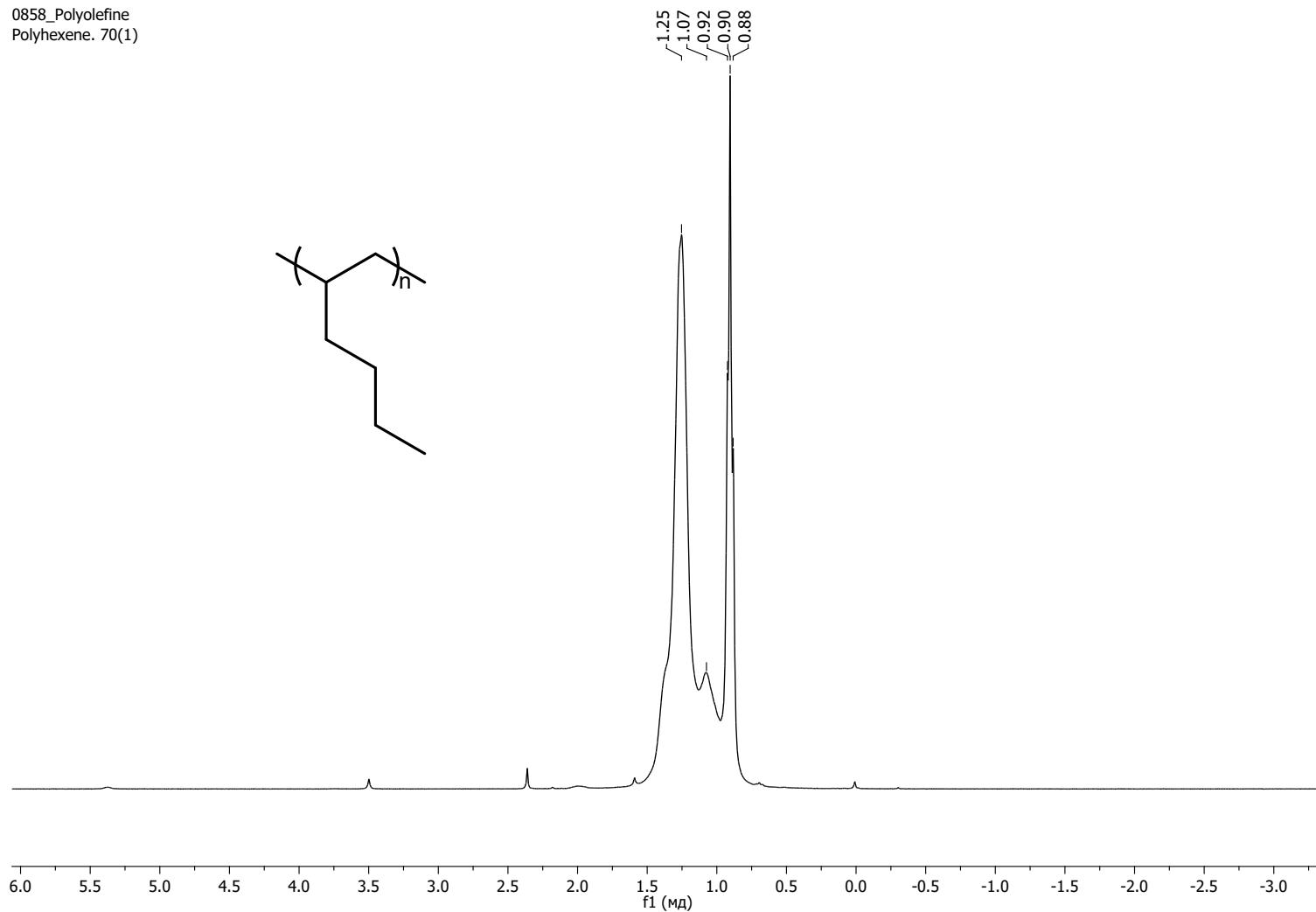


Figure S21. ^1H NMR spectrum of poly(1-hexene) (300 MHz, CDCl_3 , 300 K).

0858_Polyolefine
Polyhexene. 70(1)

~40.68
~40.29

34.63
34.54
34.33
34.23
33.94
33.73
32.33
30.69
30.41
28.71
28.35
28.28

~23.27

14.17

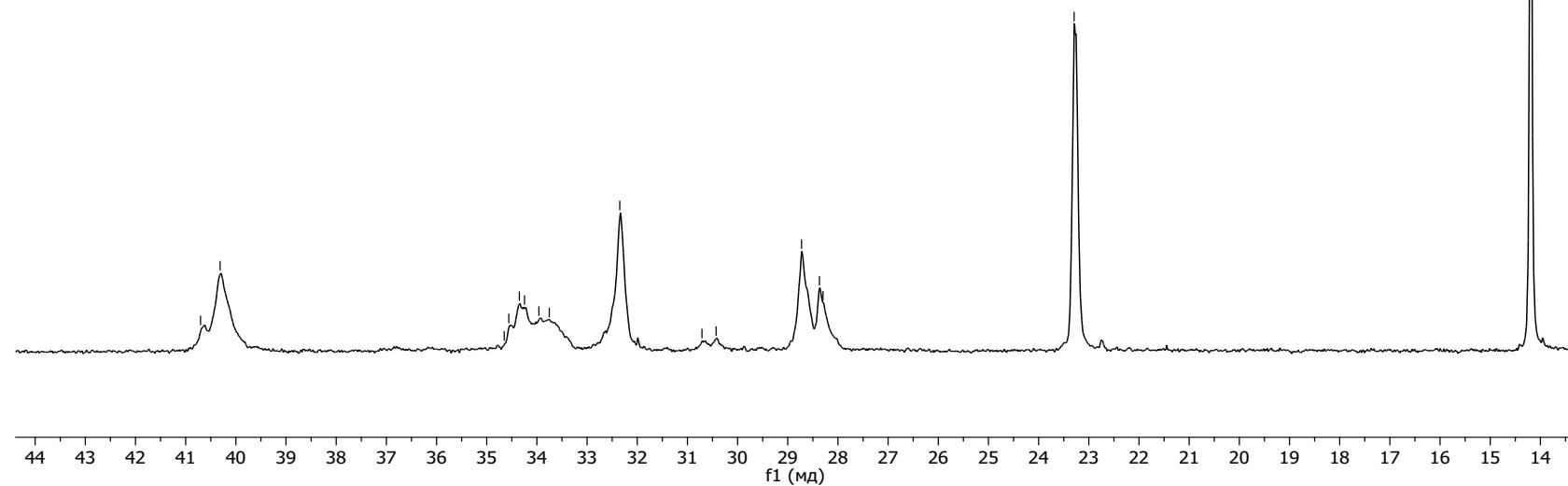
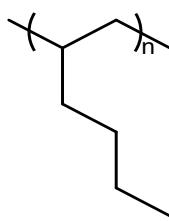


Figure S22. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(1-hexene) (75 MHz, CDCl_3 , 300 K).

0858_Polyolefine
Polyheptene. 69(1)

~1.31
~1.26
~1.24
~1.21
-1.06
~0.90
~0.88
~0.86

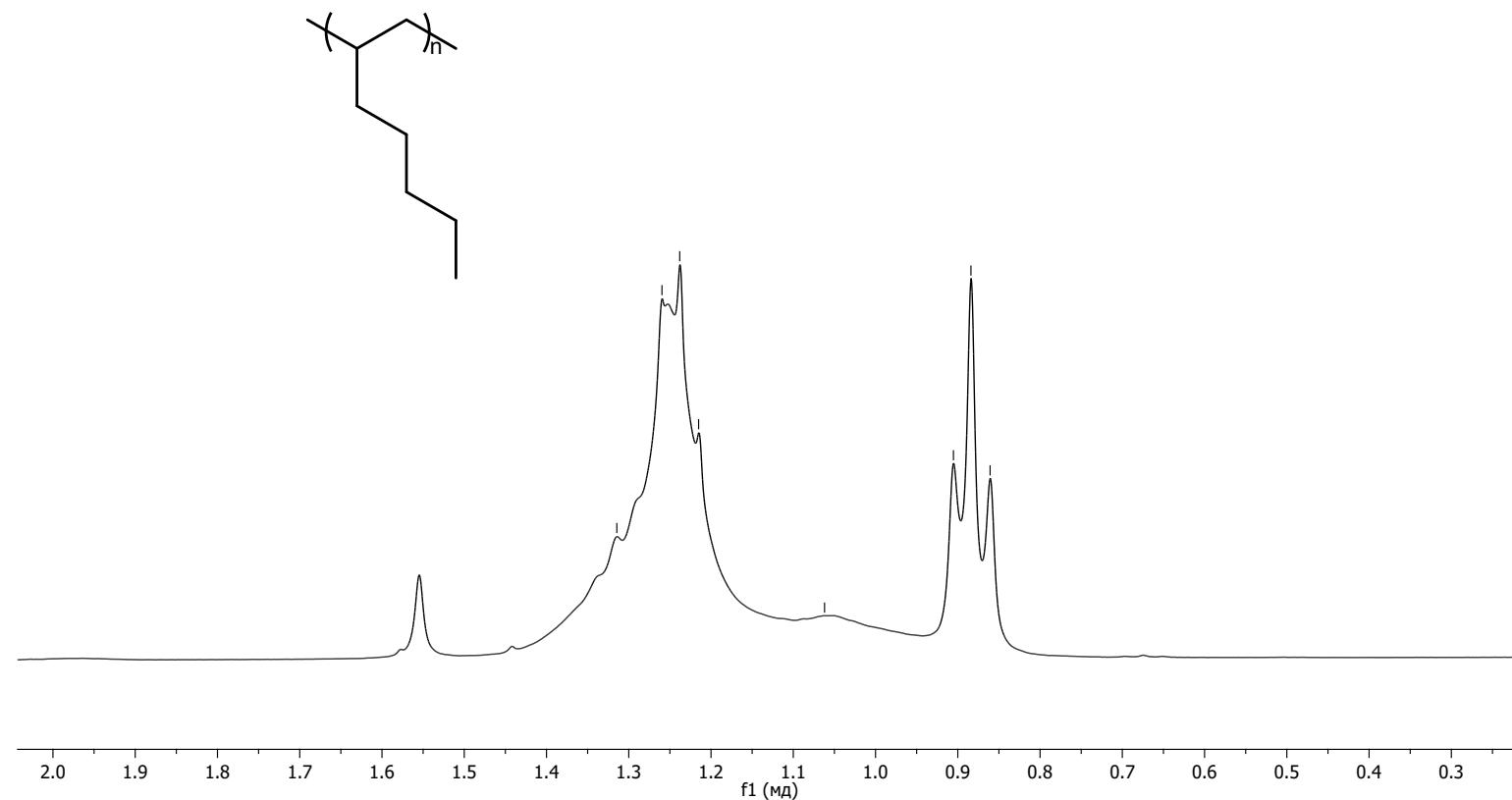


Figure S23. ^1H NMR spectrum of poly(1-heptene) (300 MHz, CDCl_3 , 300 K).

0858_Polyolefine
Polyheptene. 69(1)

40.71
40.30
40.17

34.80
34.56
34.32
34.04
33.71
32.51

26.10
25.72
25.55

22.74

-14.12

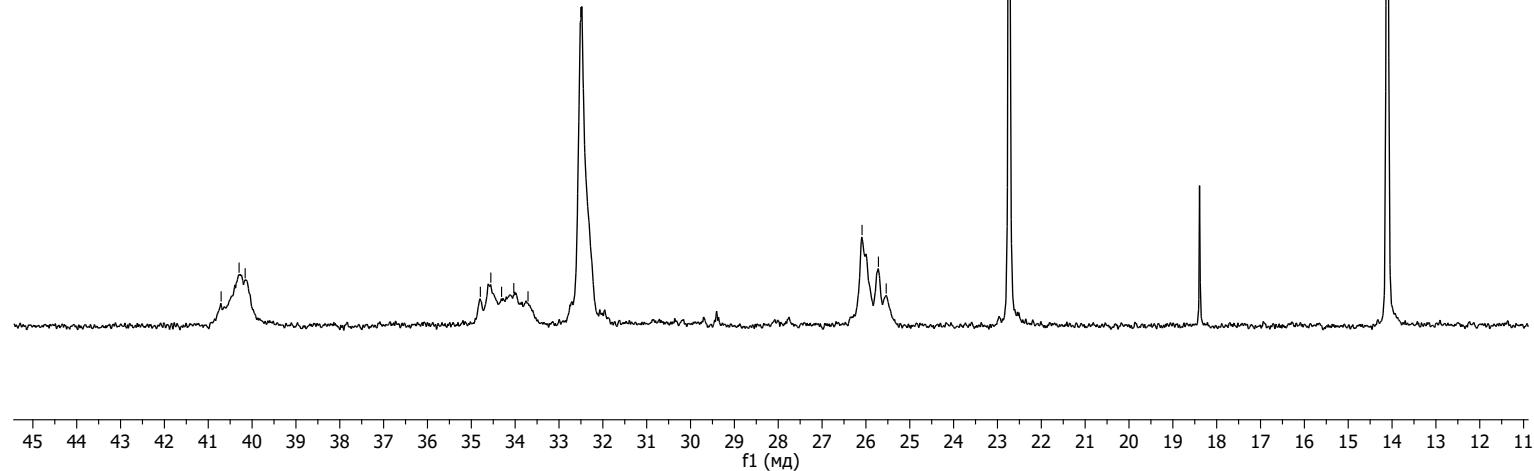
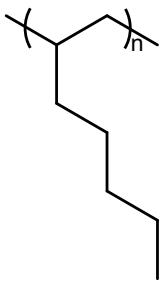


Figure S24. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(1-heptene) (75 MHz, CDCl_3 , 300 K).

0781_Polyolefine
Polyoctene

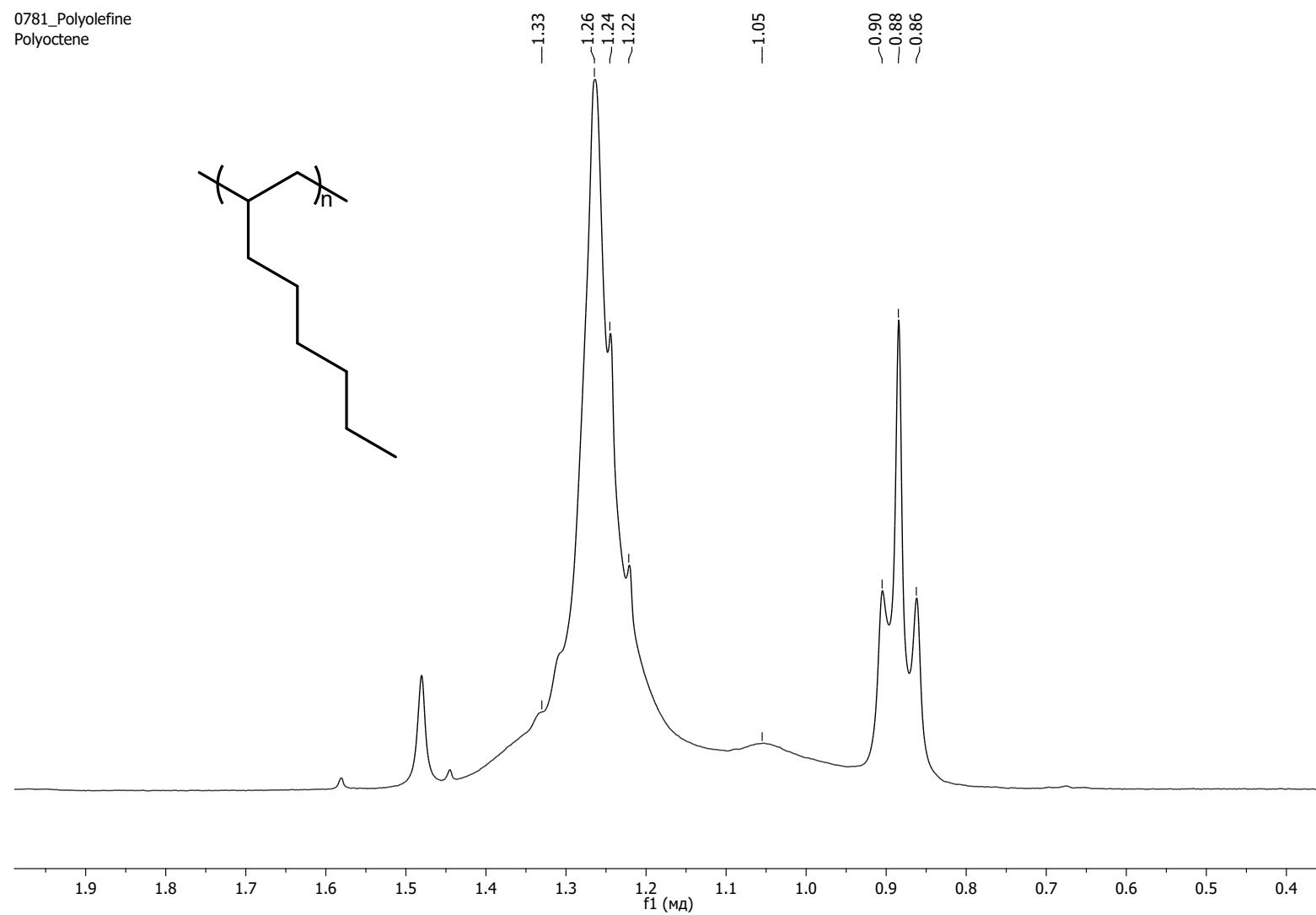


Figure S25. ^1H NMR spectrum of poly(1-octene) (300 MHz, CDCl_3 , 300 K).

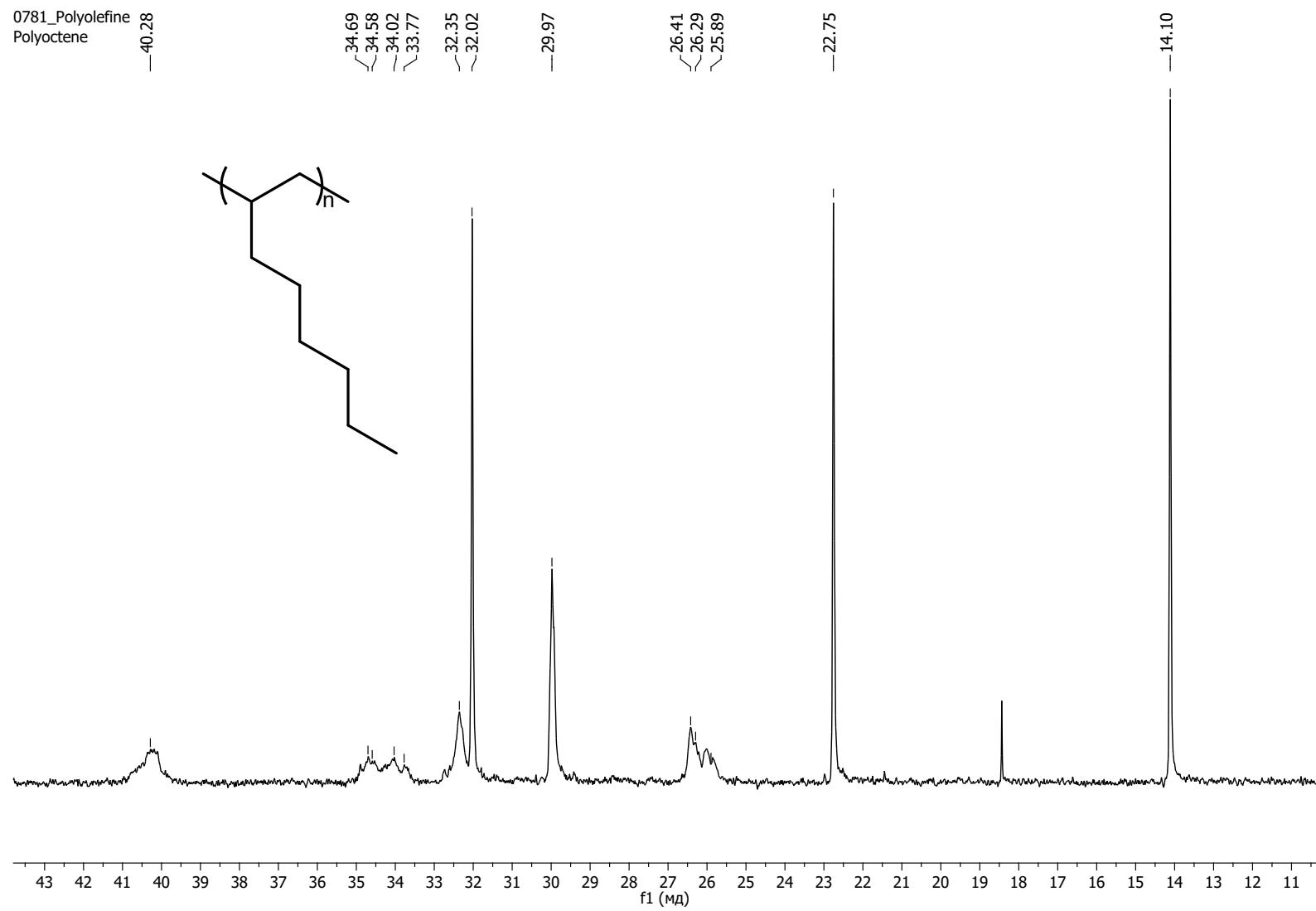


Figure S26. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(1-octene) (75 MHz, CDCl_3 , 300 K).

0781_Polyolefine
polynonene

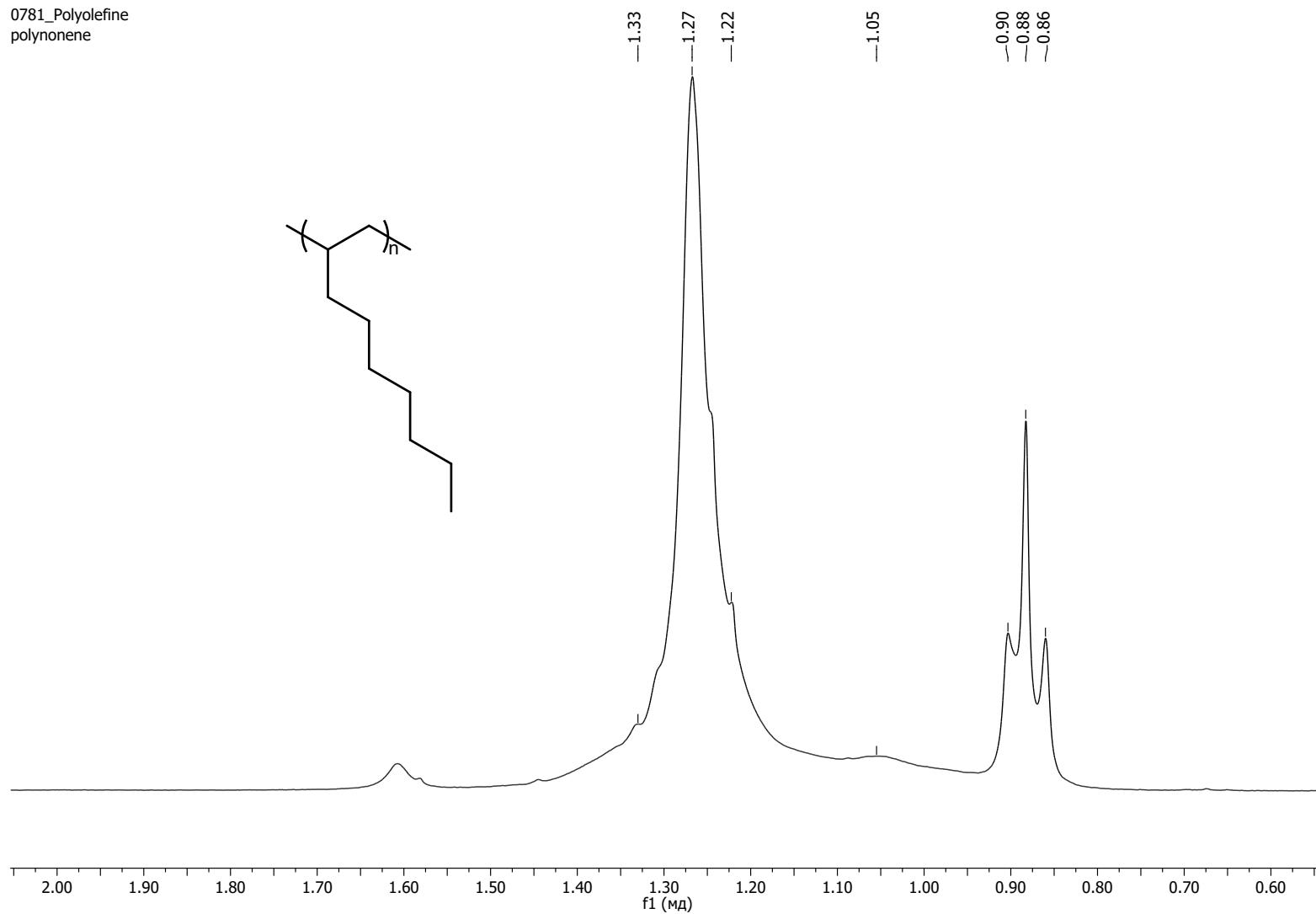


Figure S27. ^1H NMR spectrum of poly(1-nonene) (300 MHz, CDCl_3 , 300 K).

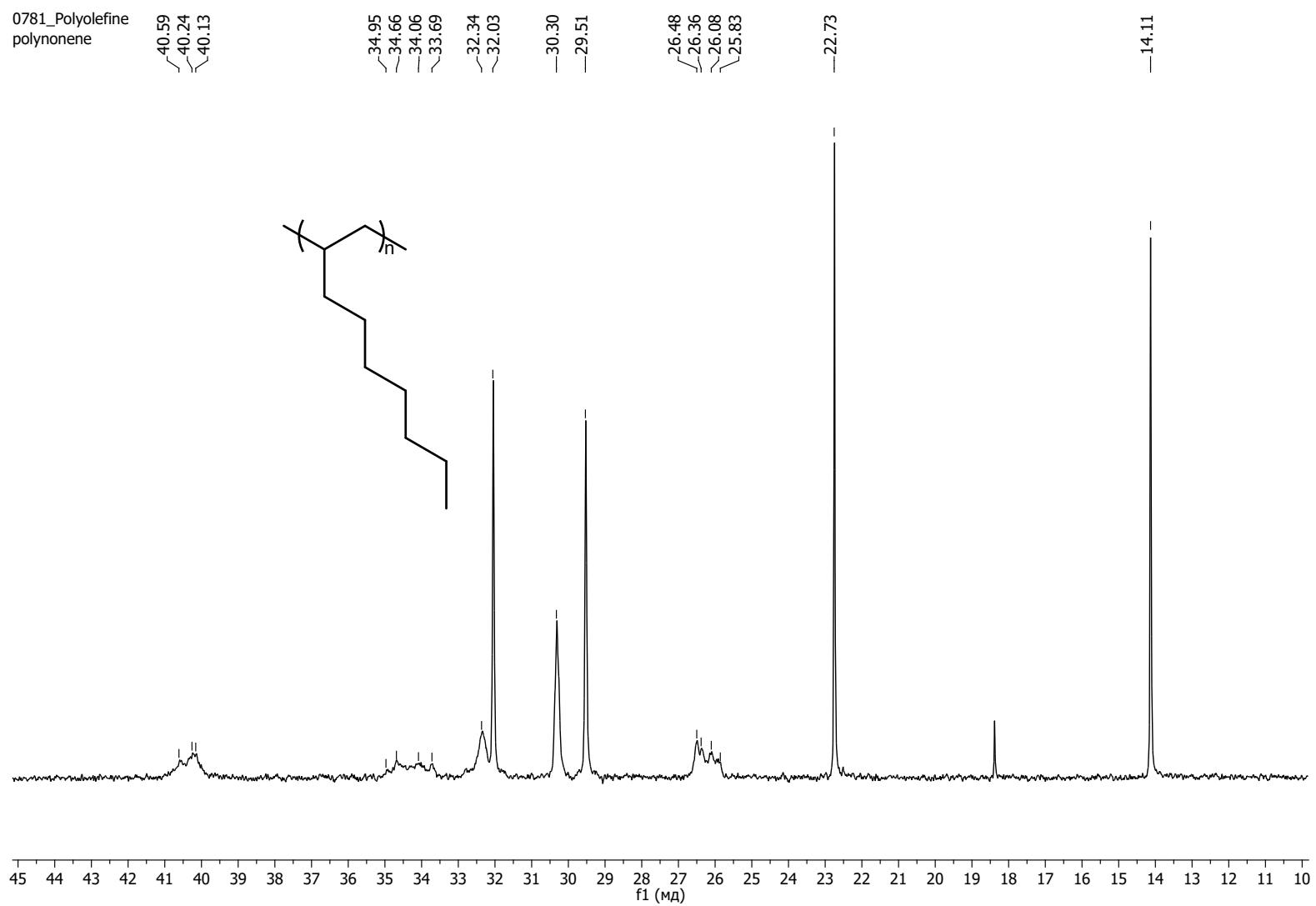


Figure S28. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(1-nonene) (75 MHz, CDCl_3 , 300 K).

0858_Polyolefine
Polydecene. 69(2)

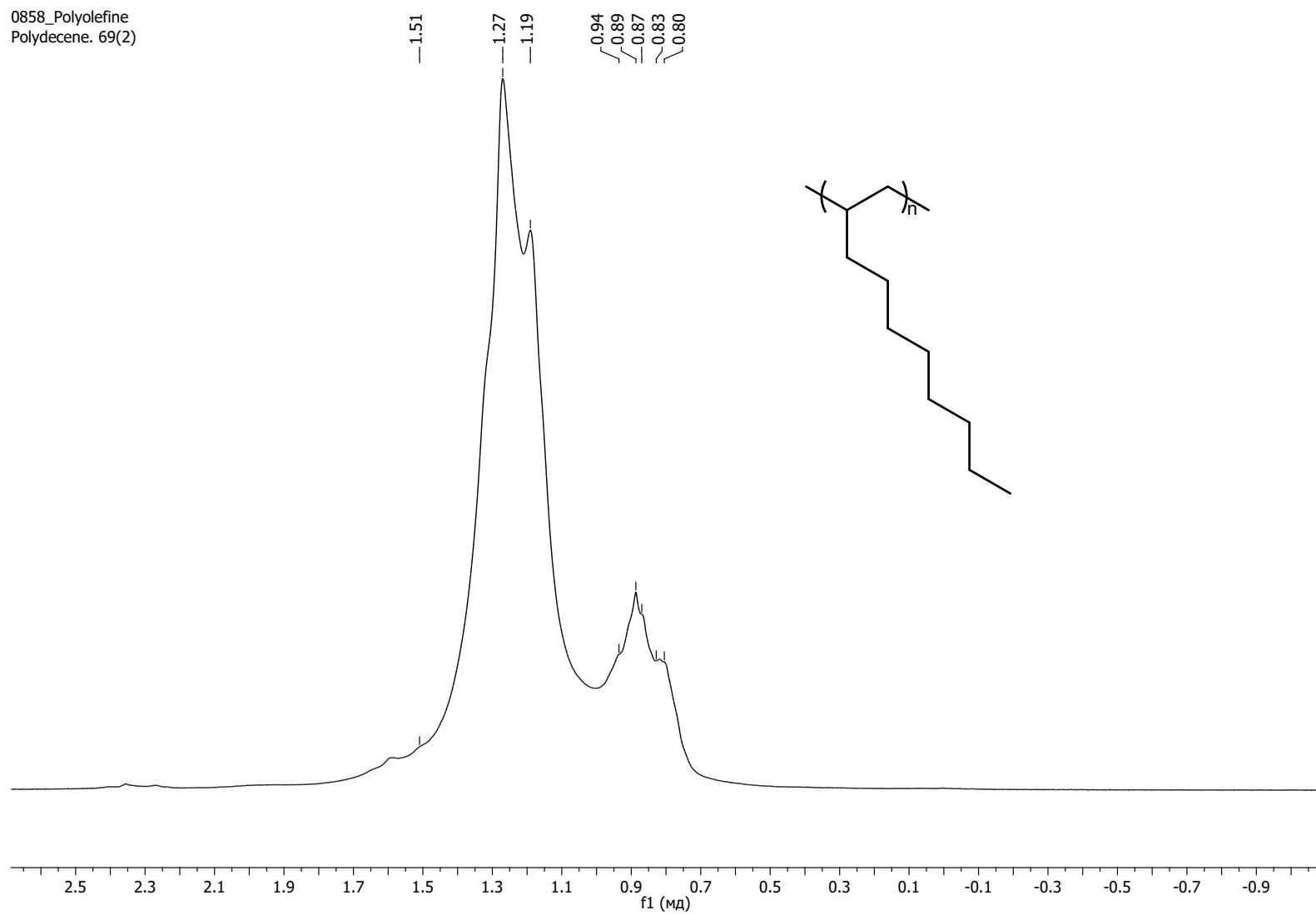


Figure S29. ^1H NMR spectrum of poly(1-decene) (300 MHz, CDCl_3 , 300 K).

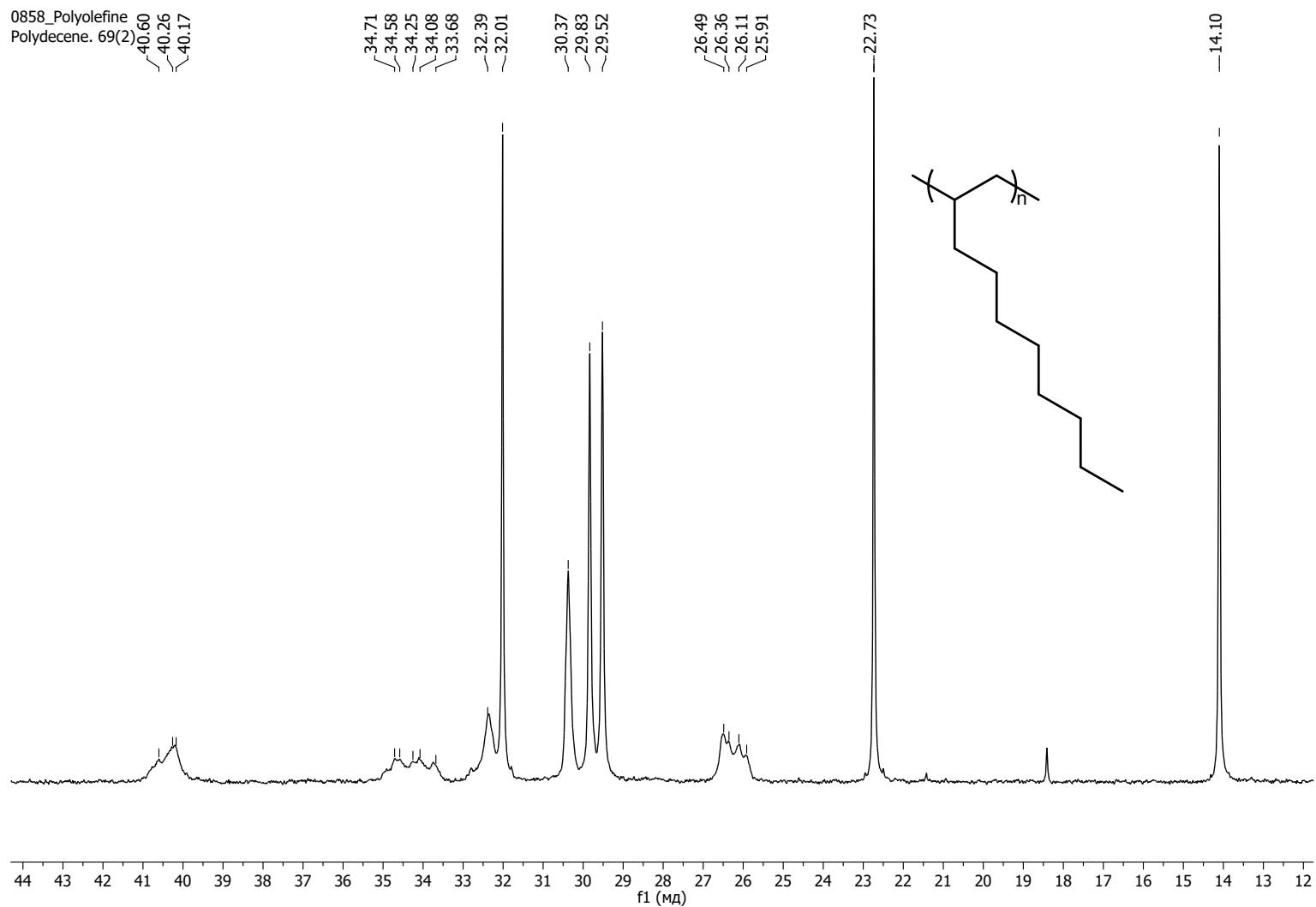


Figure S30. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(1-decene) (75 MHz, CDCl_3 , 300 K).

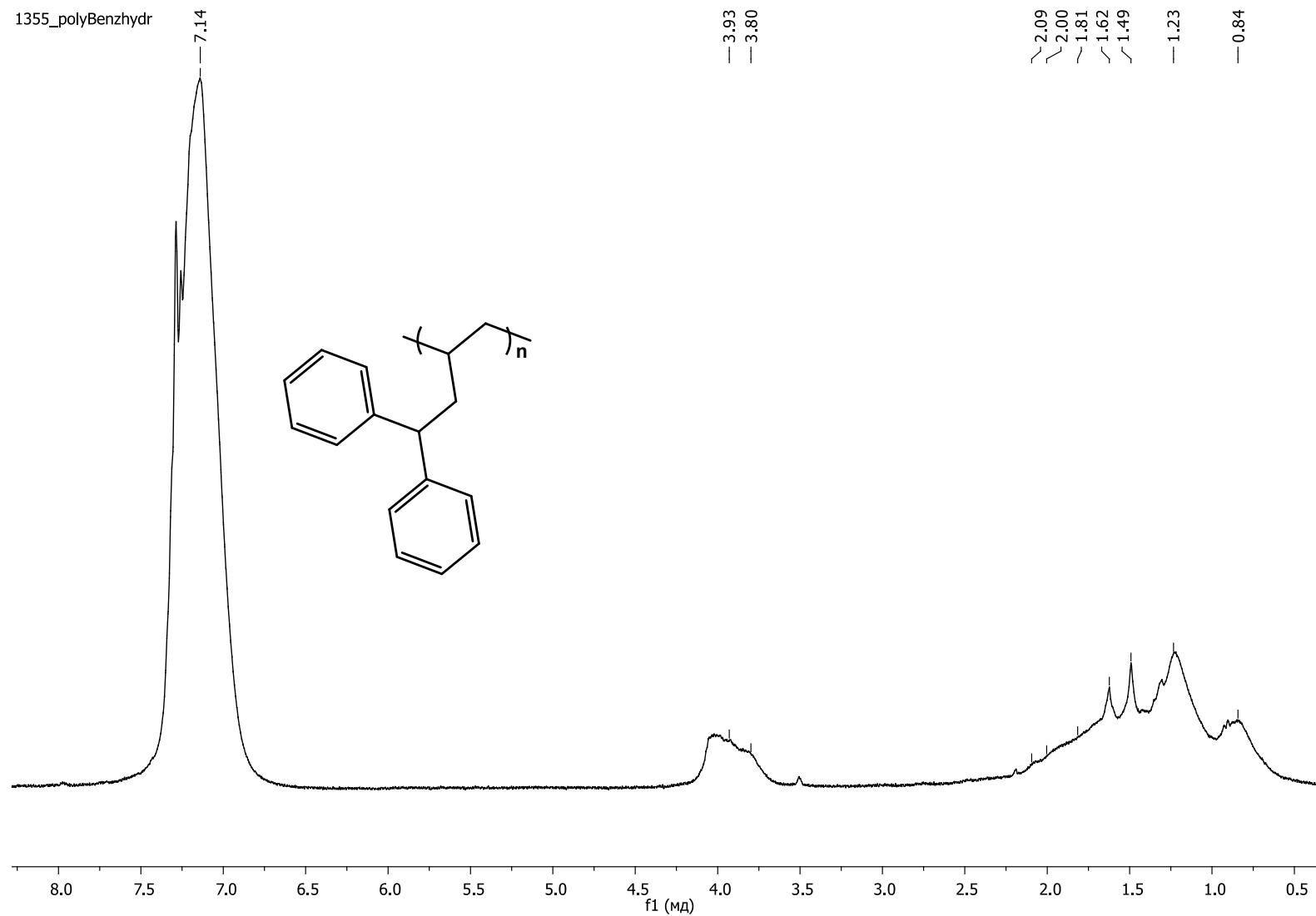


Figure S31. ¹H NMR spectrum of poly(4,4-diphenyl-but-1-ene) (300 MHz, CDCl₃, 300 K).

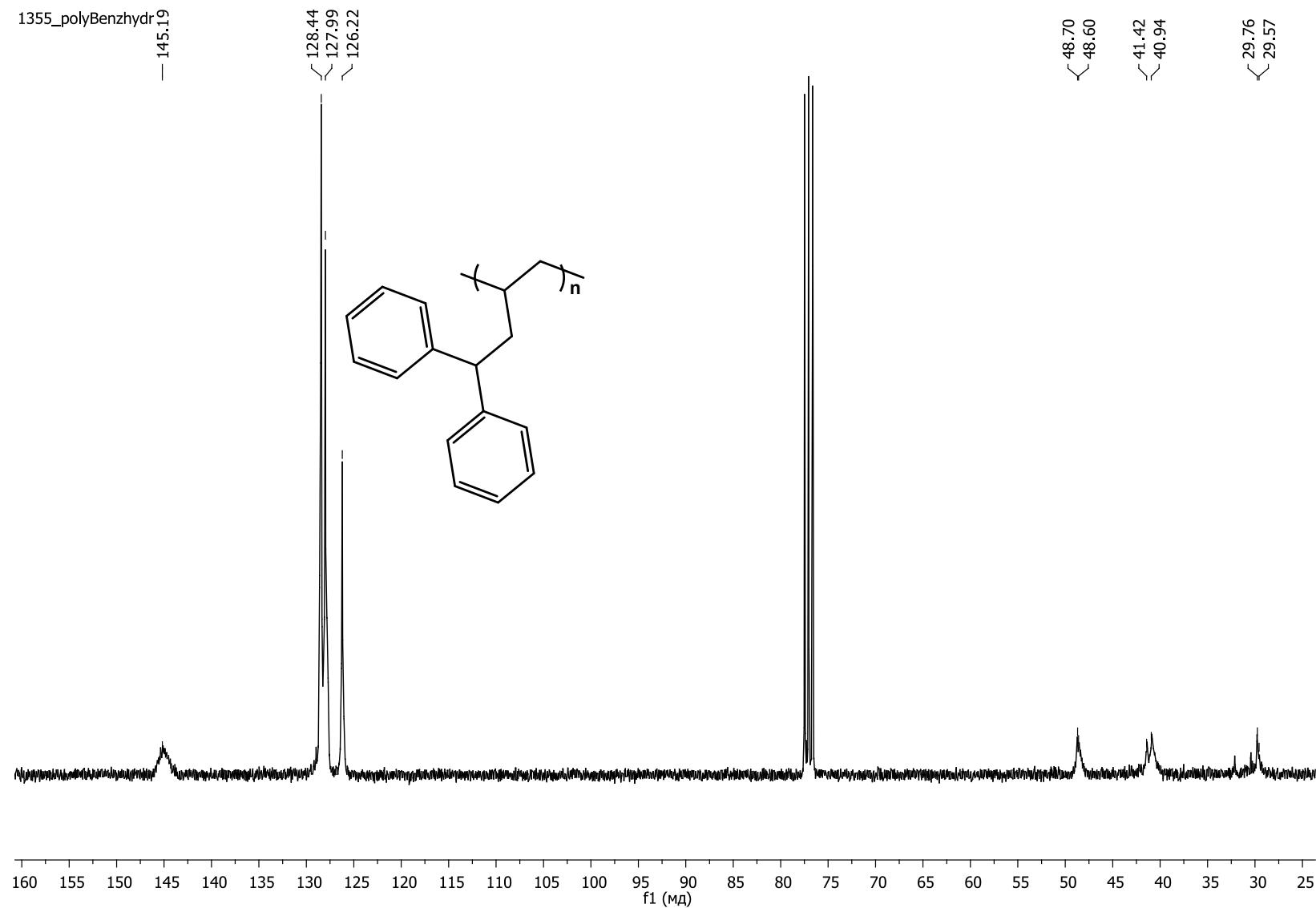


Figure S32. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(4,4-diphenyl-but-1-ene) (75 MHz, CDCl_3 , 300 K).

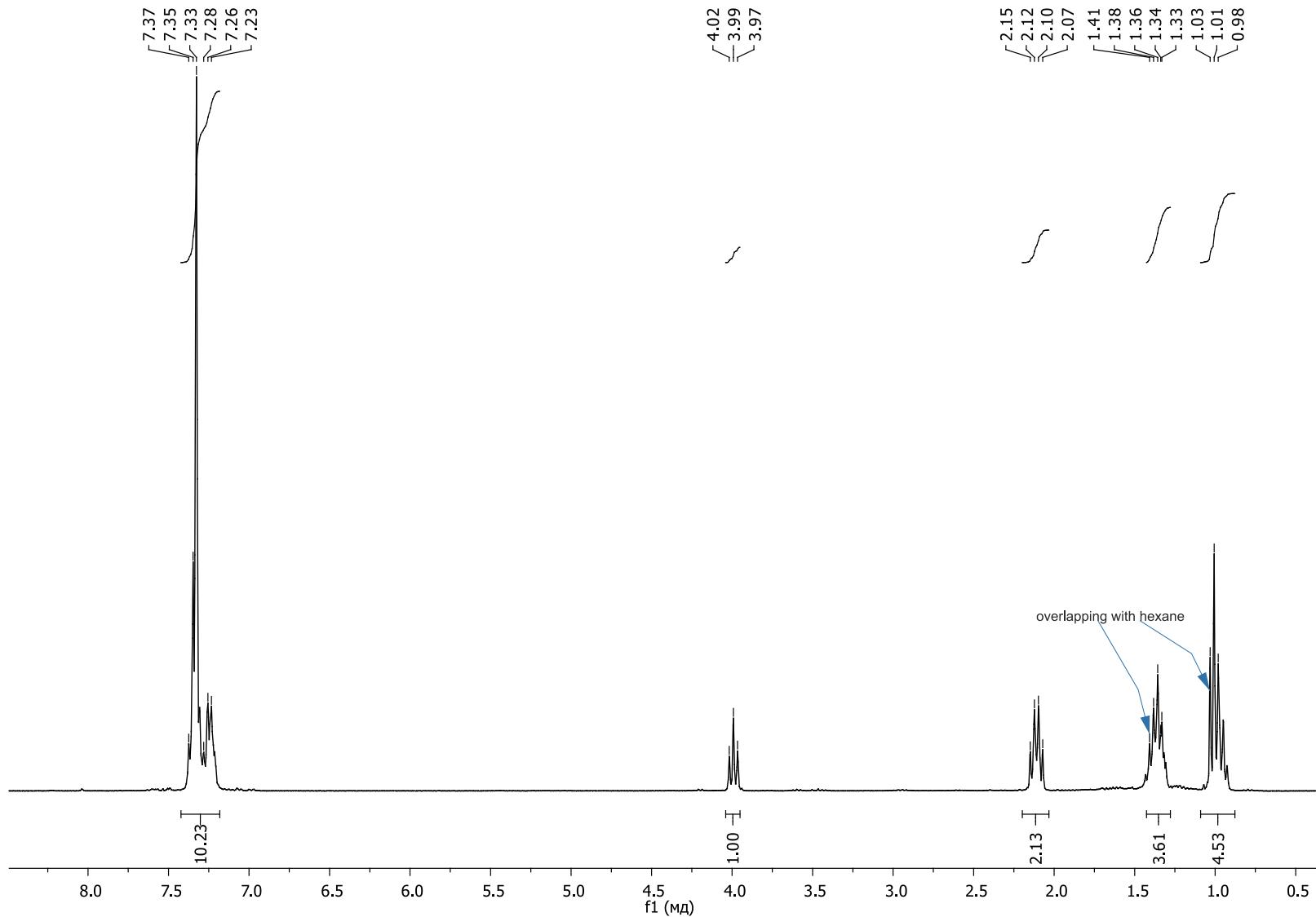


Figure S33. ^1H NMR spectrum of 1,1-diphenylbutane (300 MHz, CDCl_3 , 300 K).

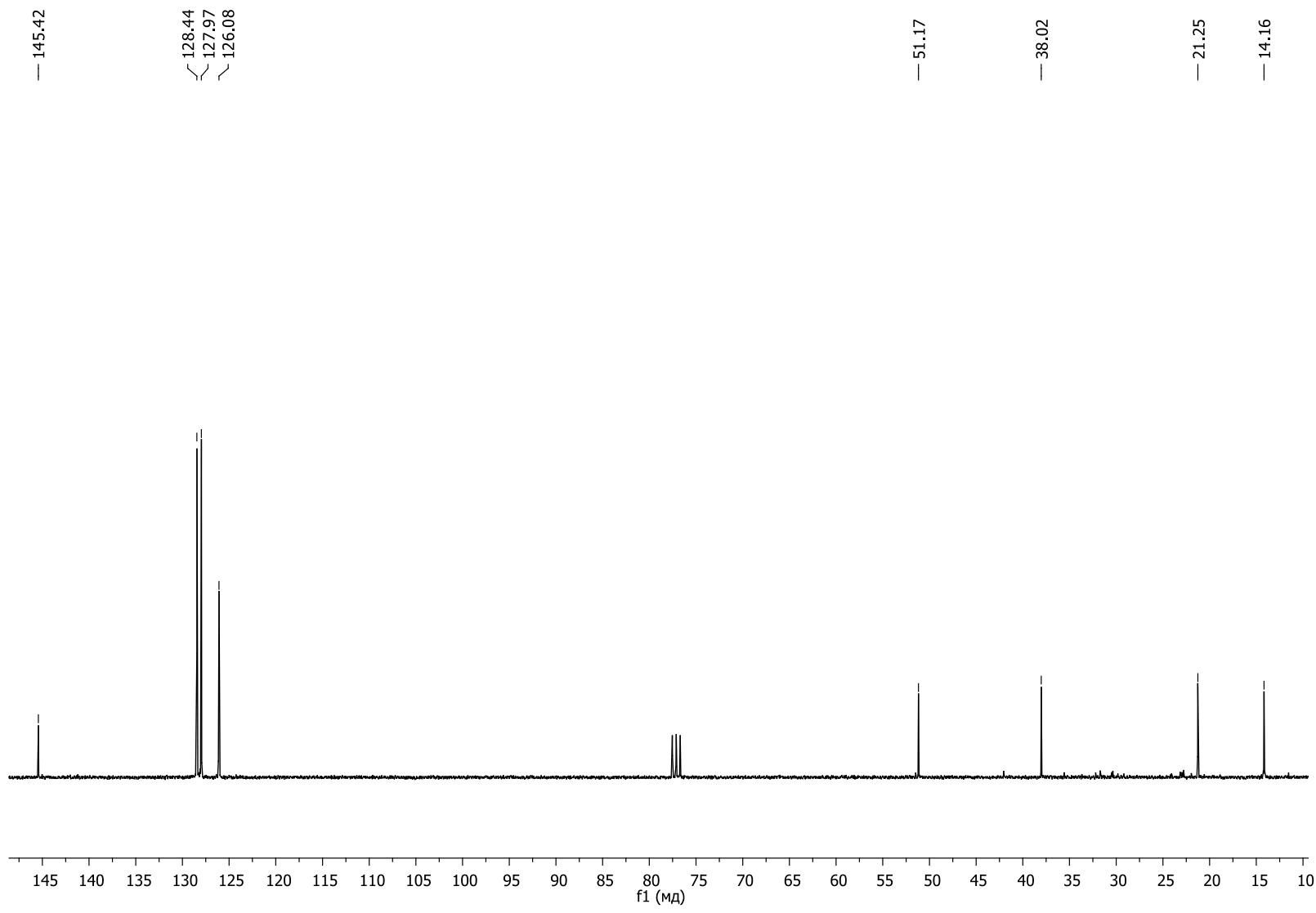


Figure S34. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of 1,1-diphenylbutane (75 MHz, CDCl_3 , 300 K).

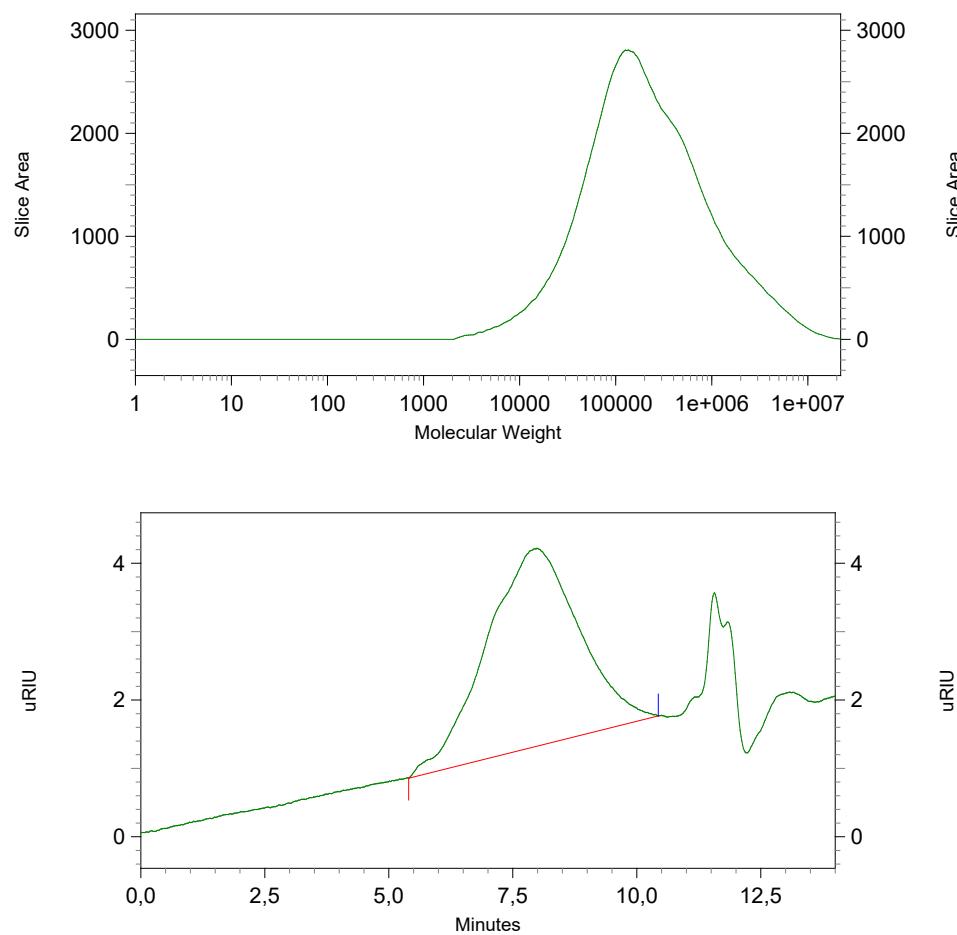


Figure S35. GPC of poly(1-hexene) (Table 2, Entry 5).

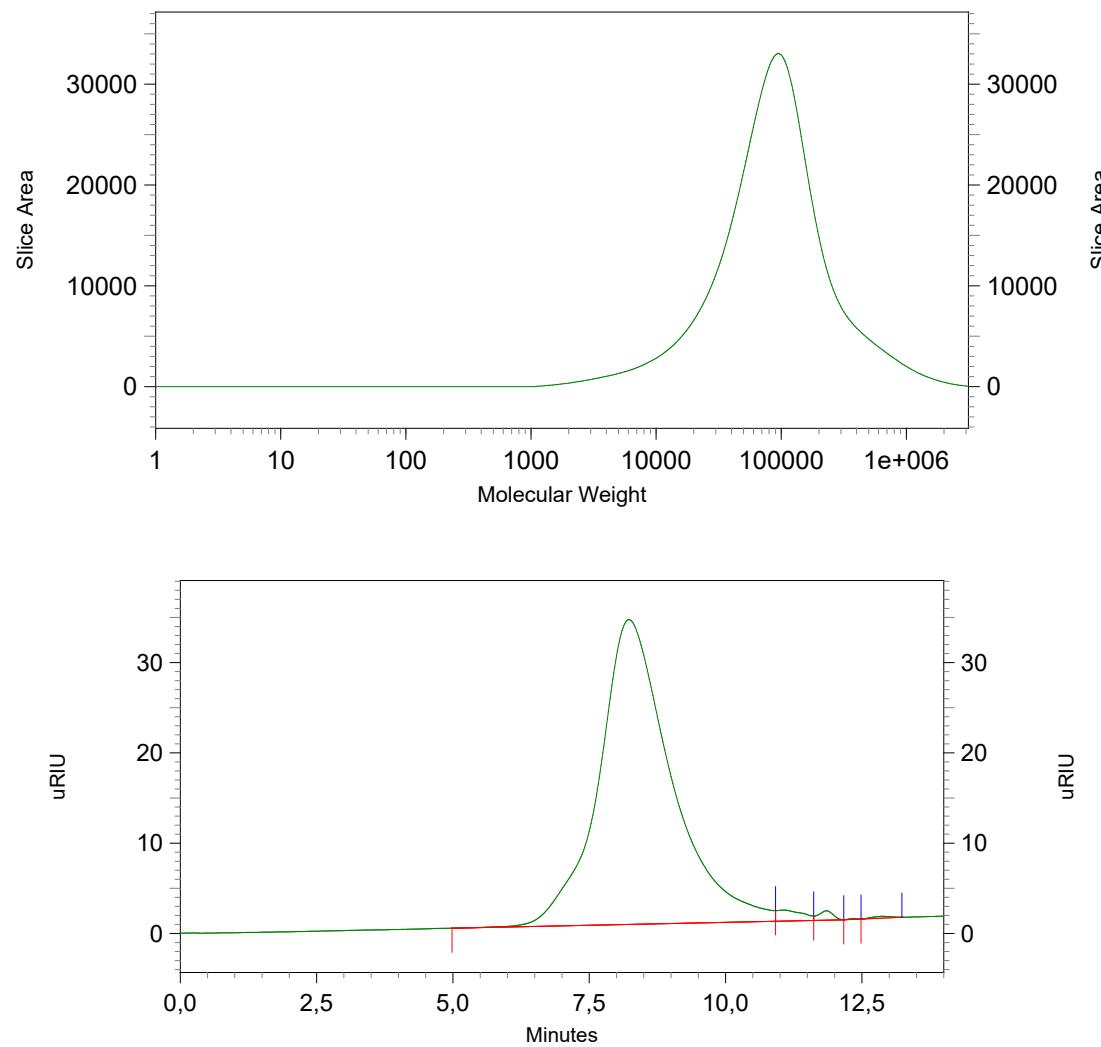


Figure S36. GPC of poly(1-hexene) (Table 2, Entry 6).

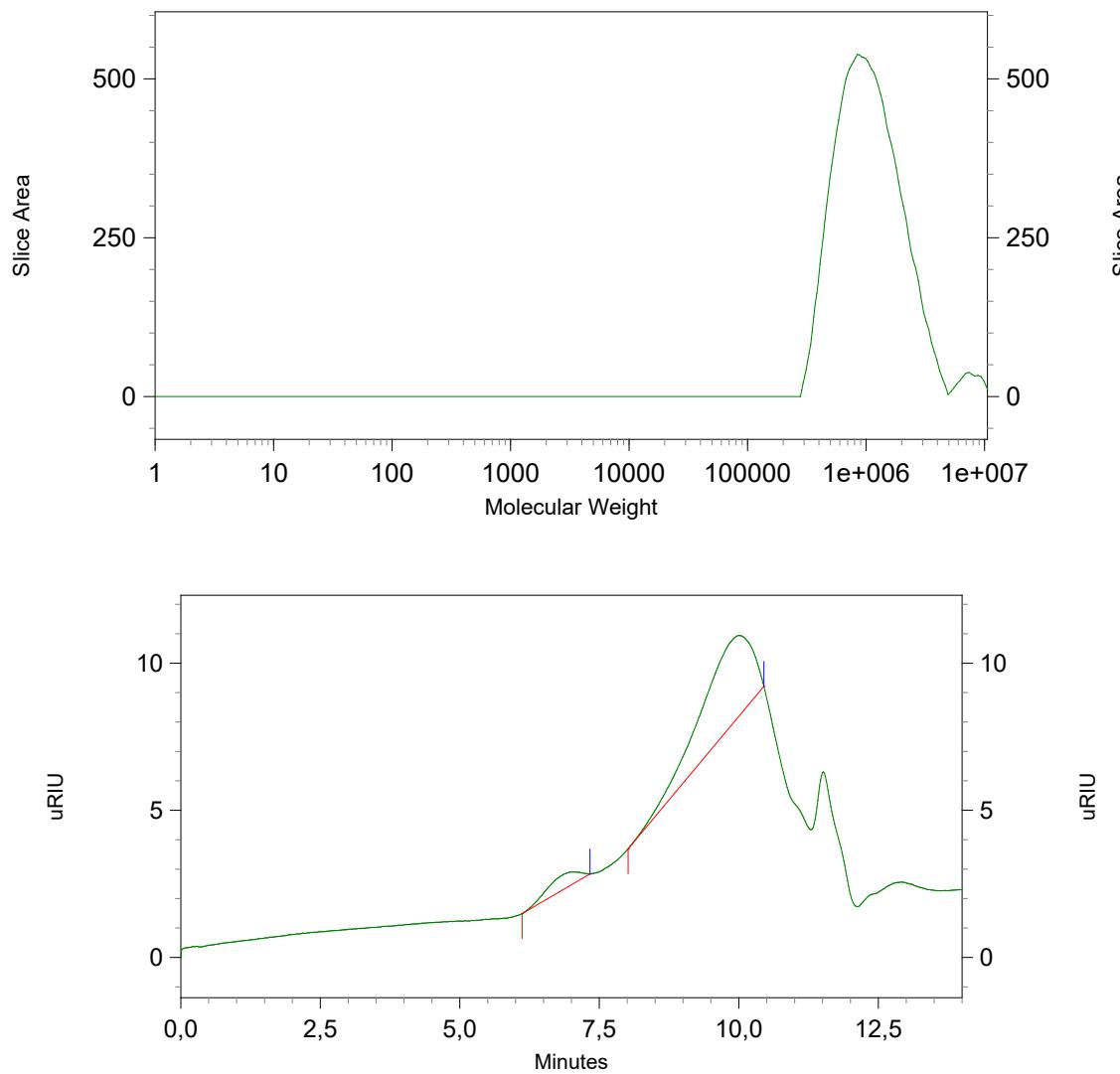


Figure S37. GPC of poly(1-hexene) (Table 2, Entry 7).

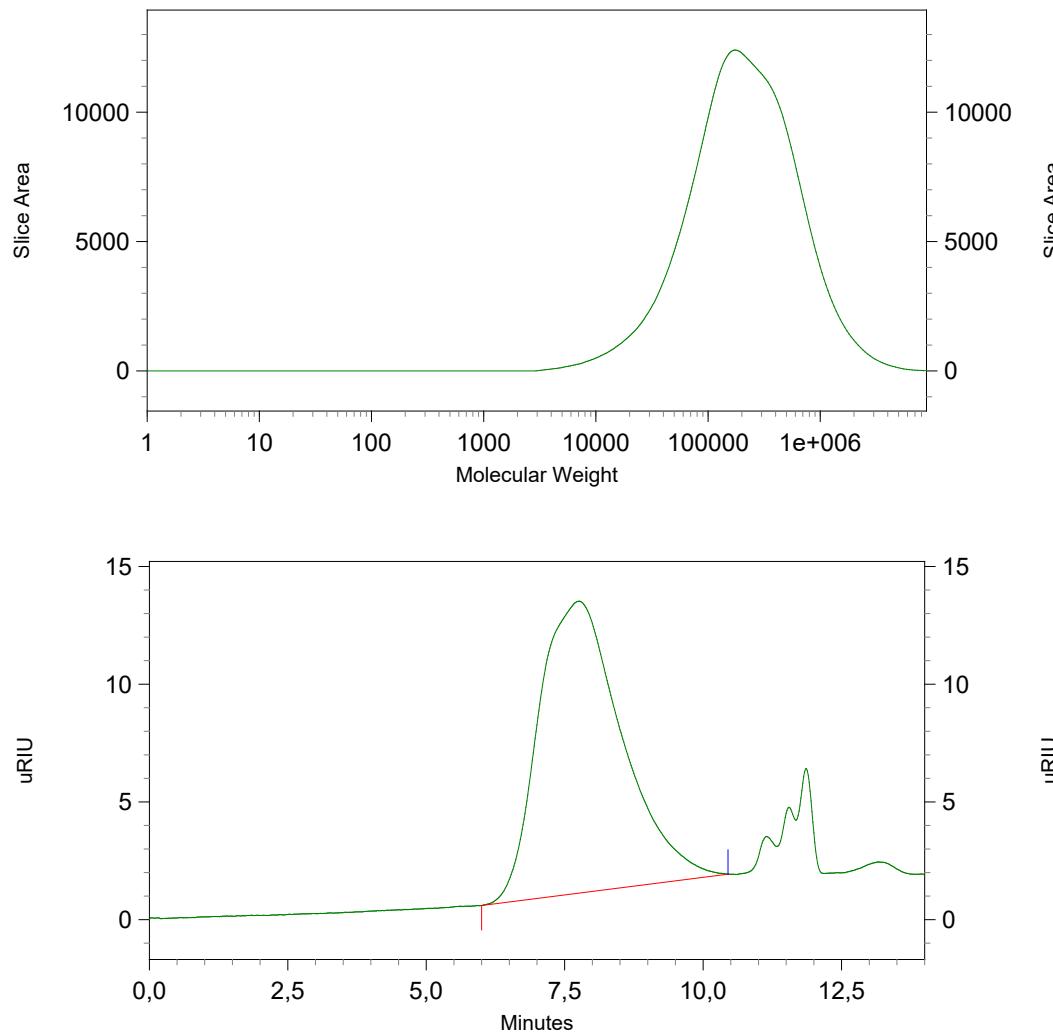


Figure S38. GPC of poly(1-hexene) (Table 2, Entry 8).

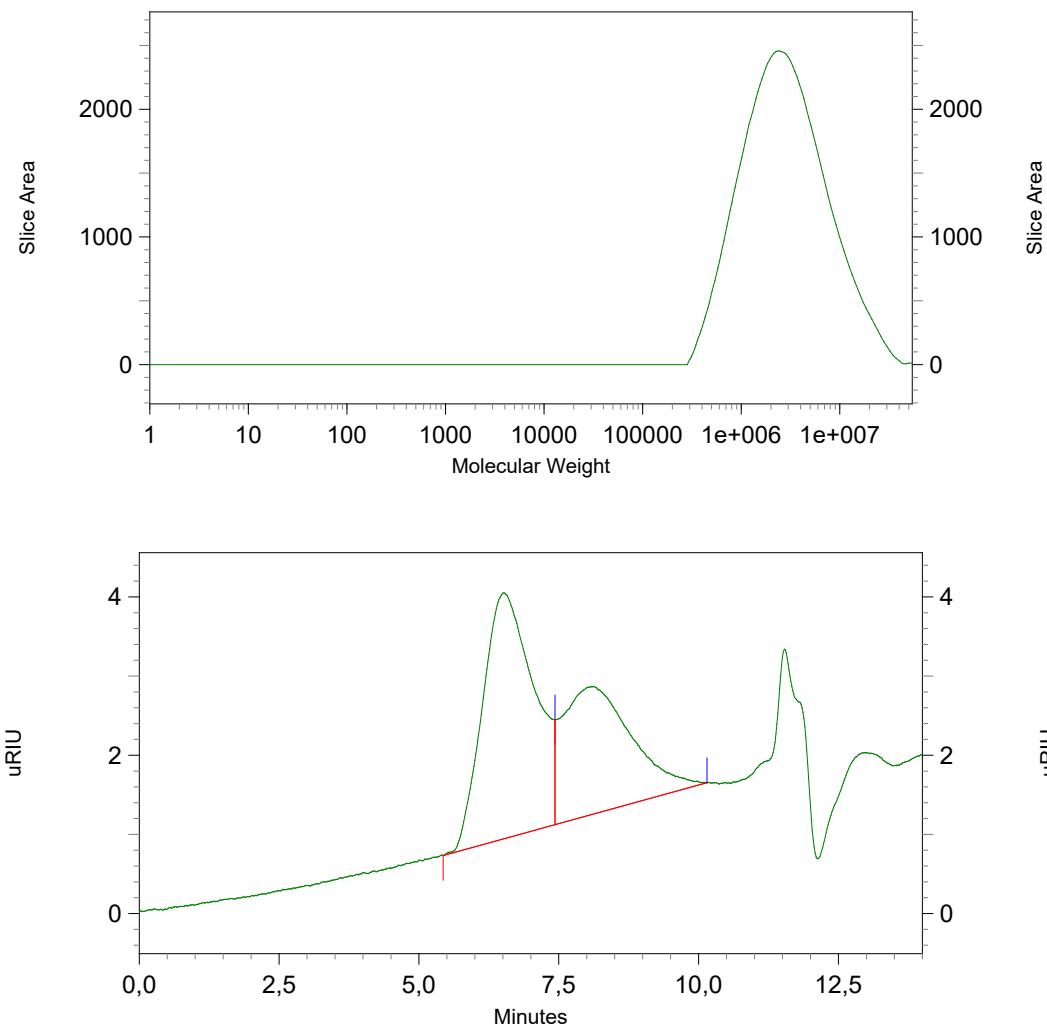


Figure S39. GPC of poly(1-hexene) (Table 2, Entry 9).

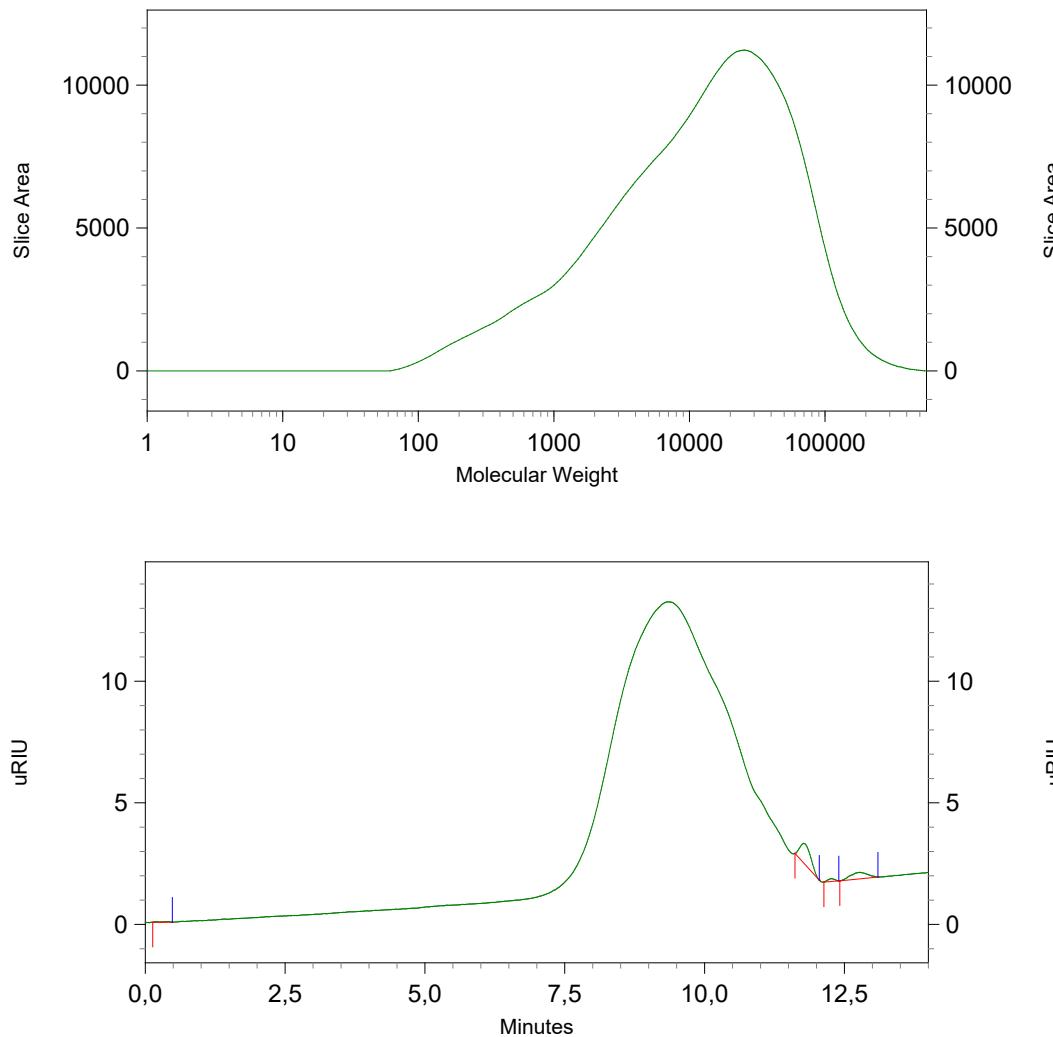


Figure S40. GPC of poly(1-hexene) (Table 2, Entry 10).

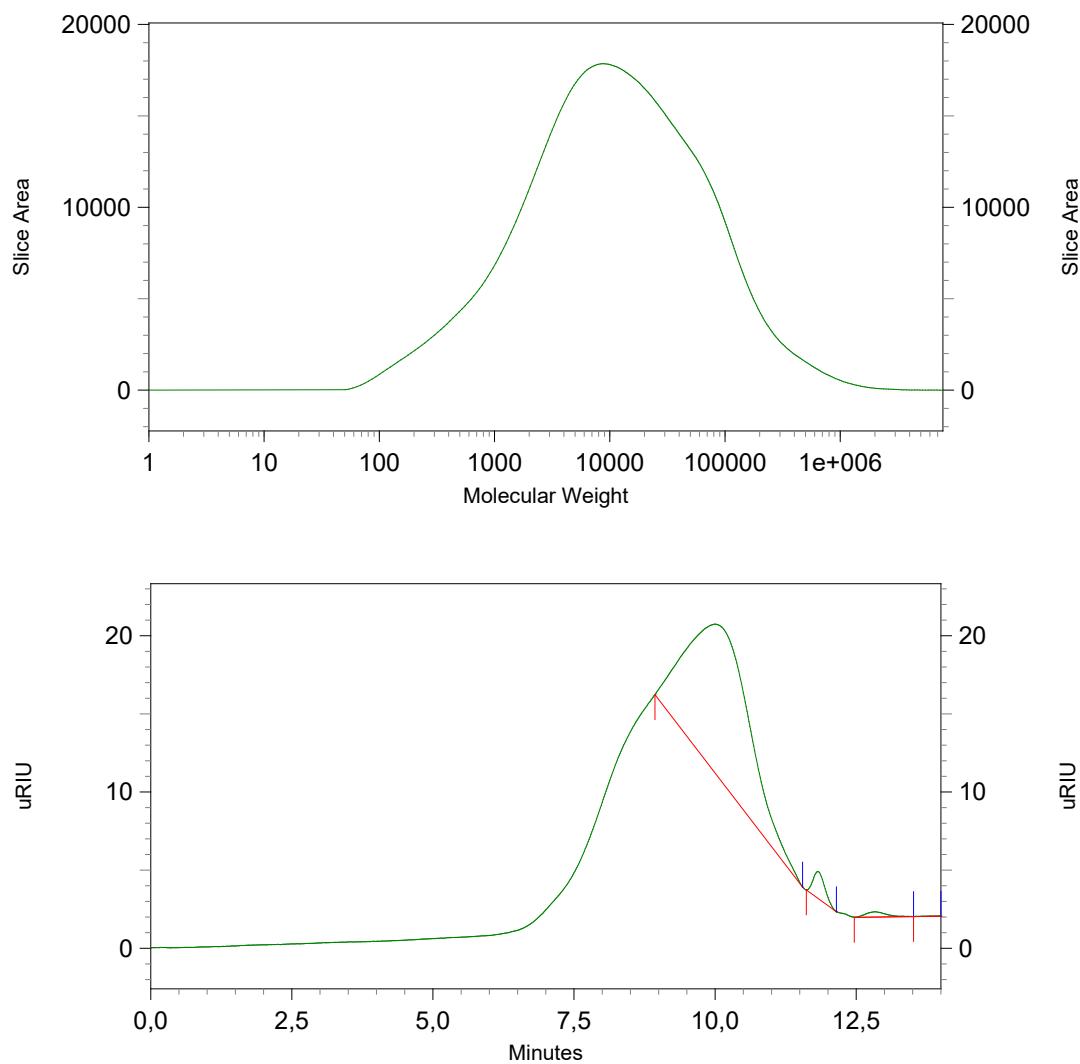


Figure S41. GPC of poly(1-hexene) (Table 2, Entry 11).

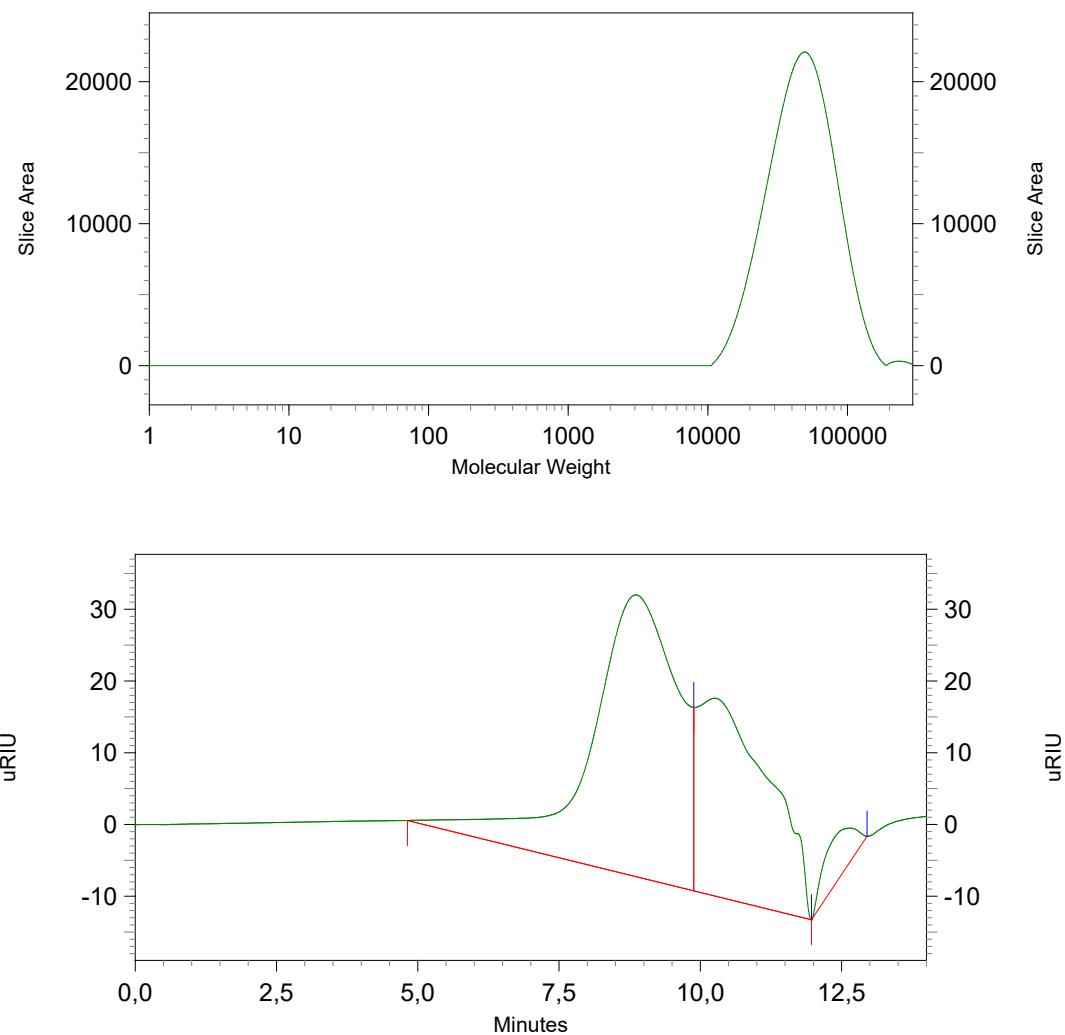


Figure S42. GPC of poly(1-heptene) (Table 2, Entry 12).

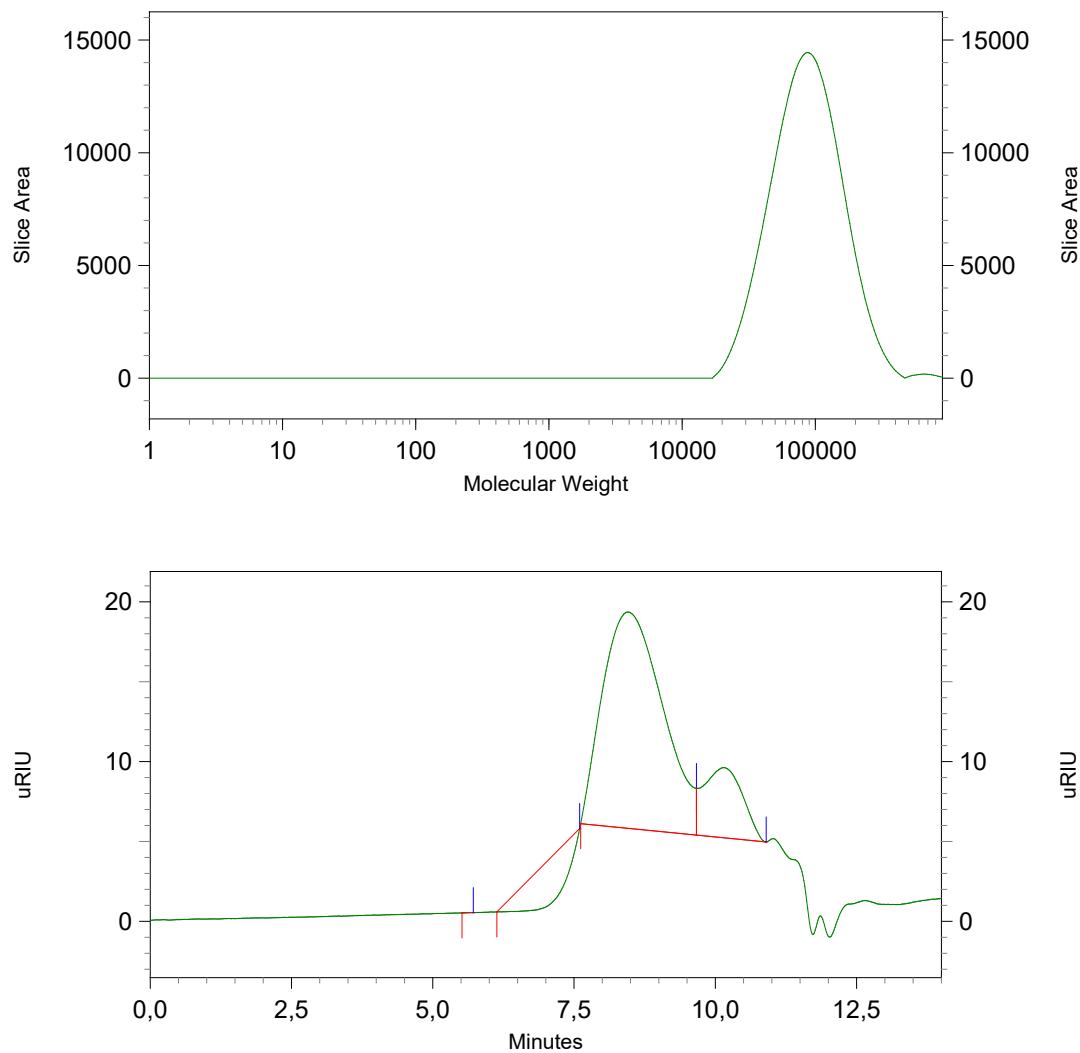


Figure S43. GPC of poly(1-octene) (Table 2, Entry 13).

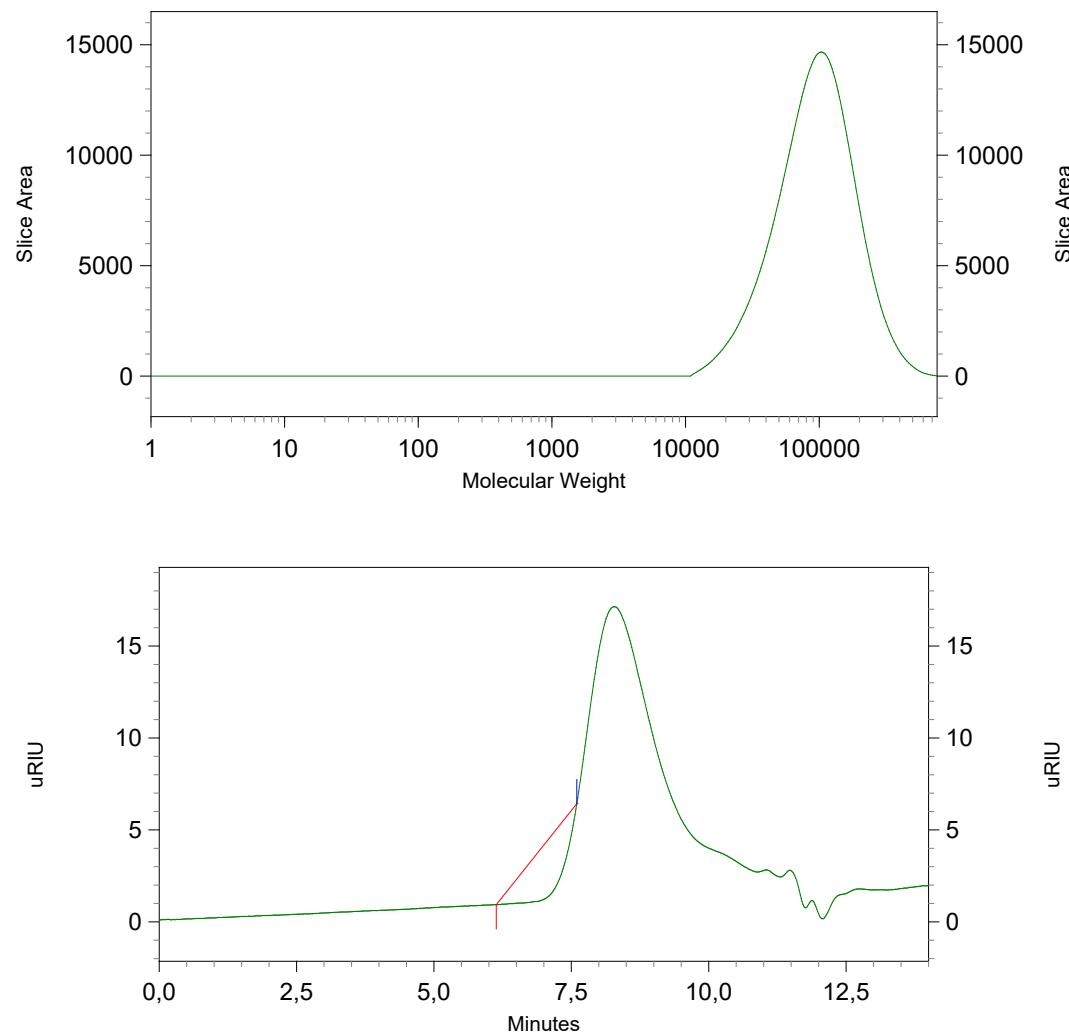


Figure S44. GPC of poly(1-nonene) (Table 2, Entry 14).

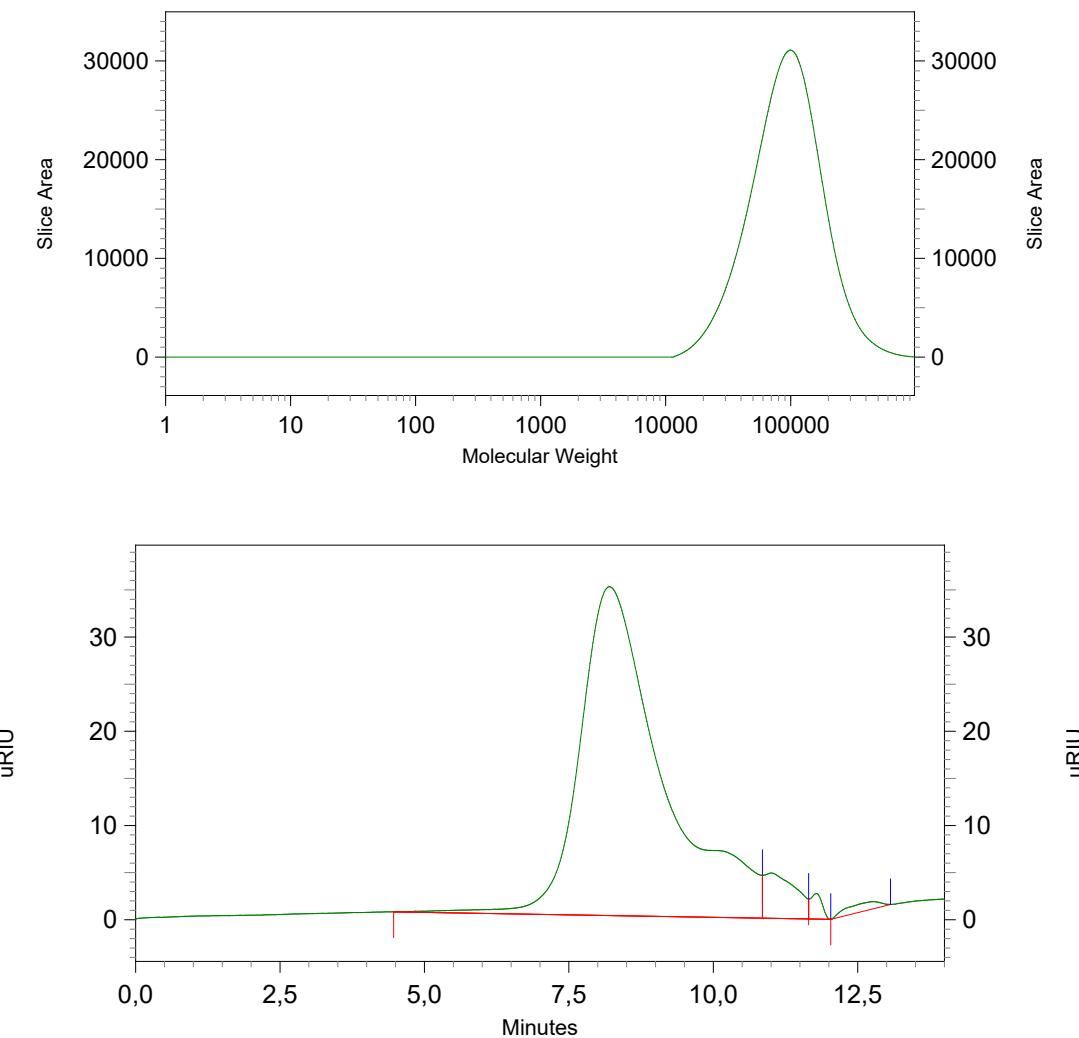


Figure S45. GPC of poly(1-decene) (Table 2, Entry 15).

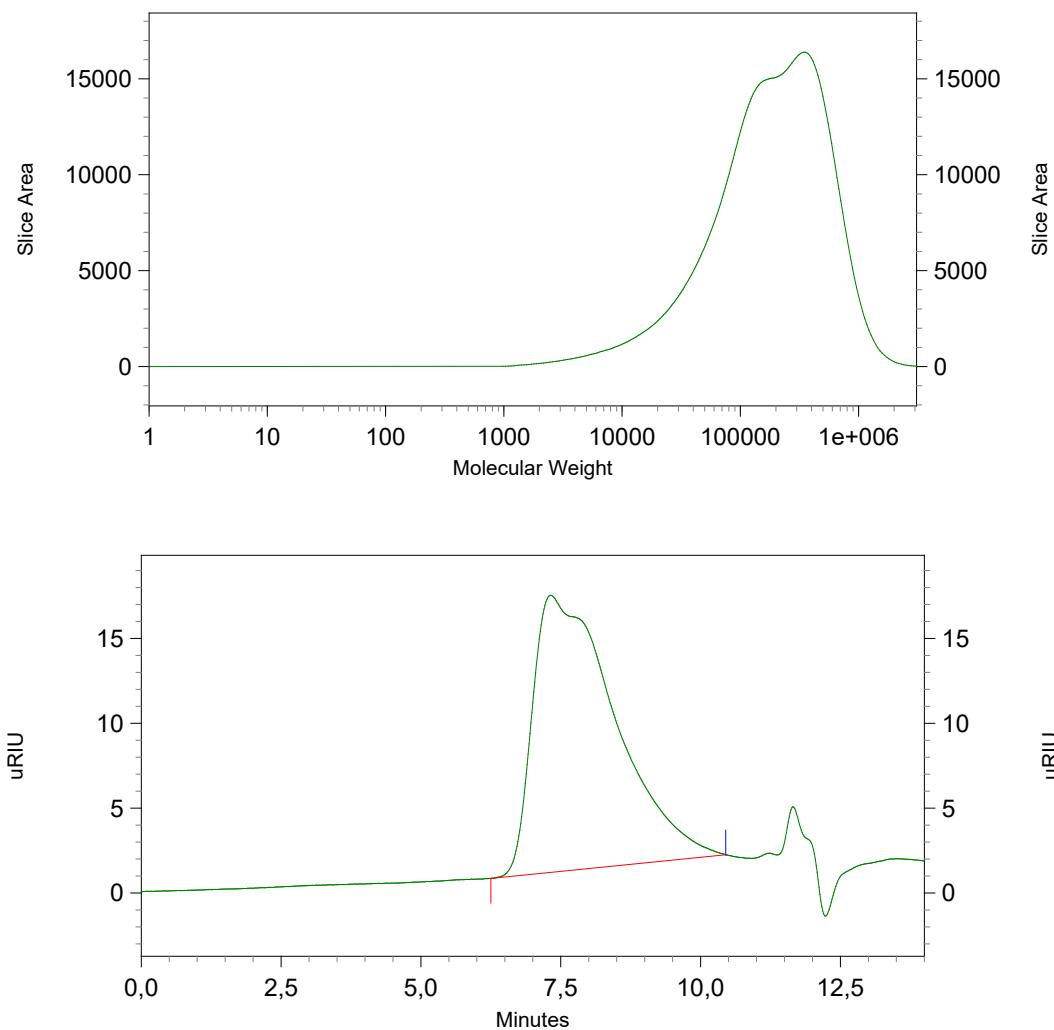


Figure S46. GPC of poly(1-decene) (Table 2, Entry 16).

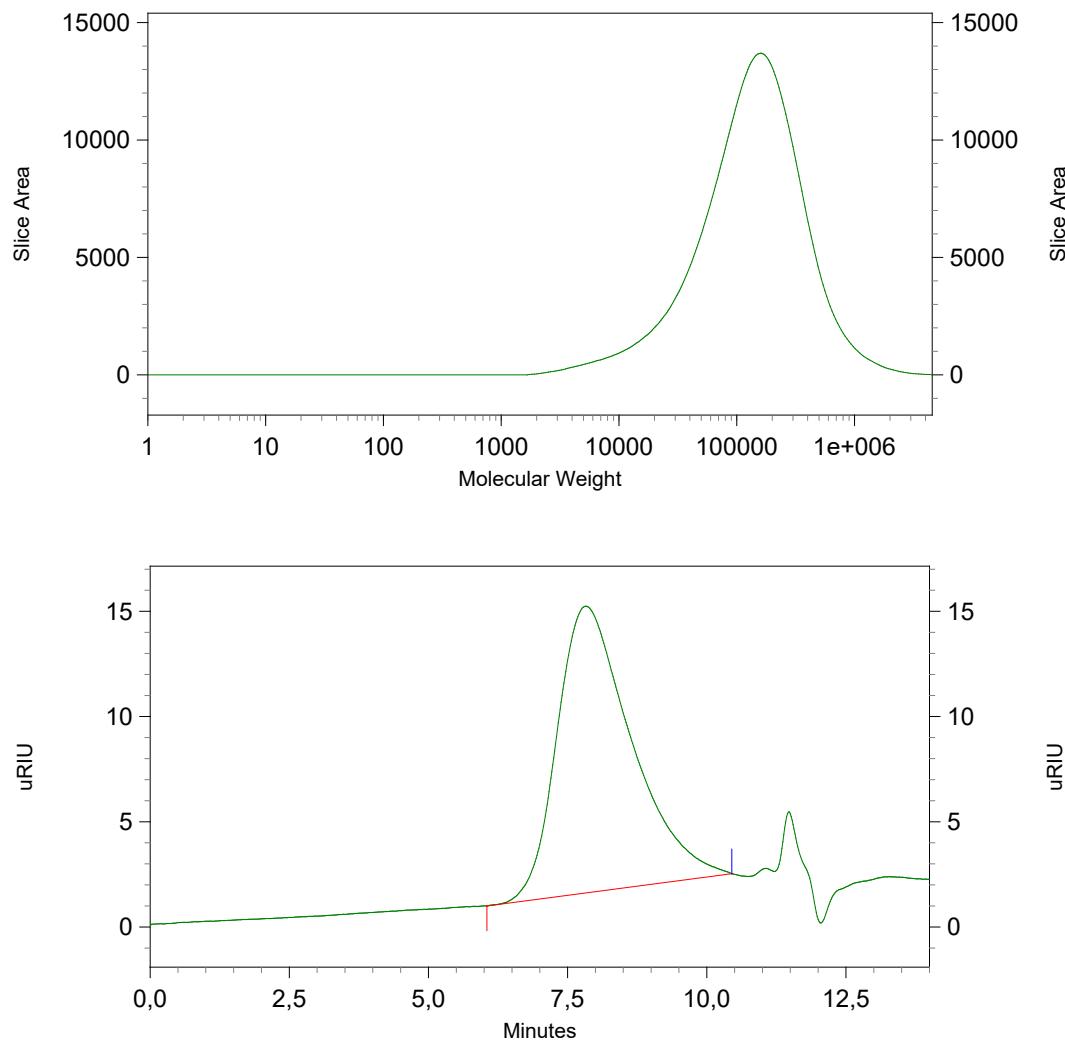


Figure S47. GPC of poly(1-decene) (Table 2, Entry 17).

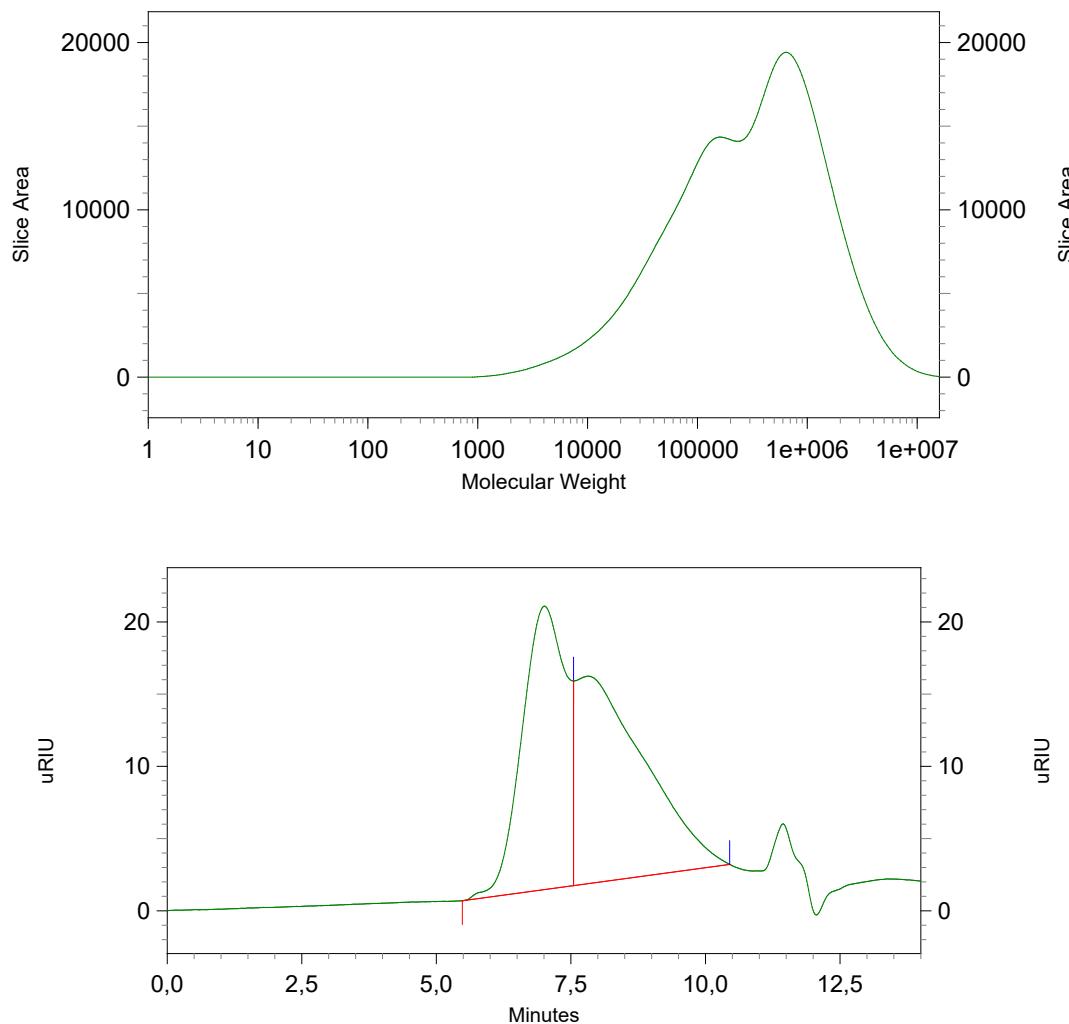


Figure S48. GPC of poly(1-decene) (Table 2, Entry 18).

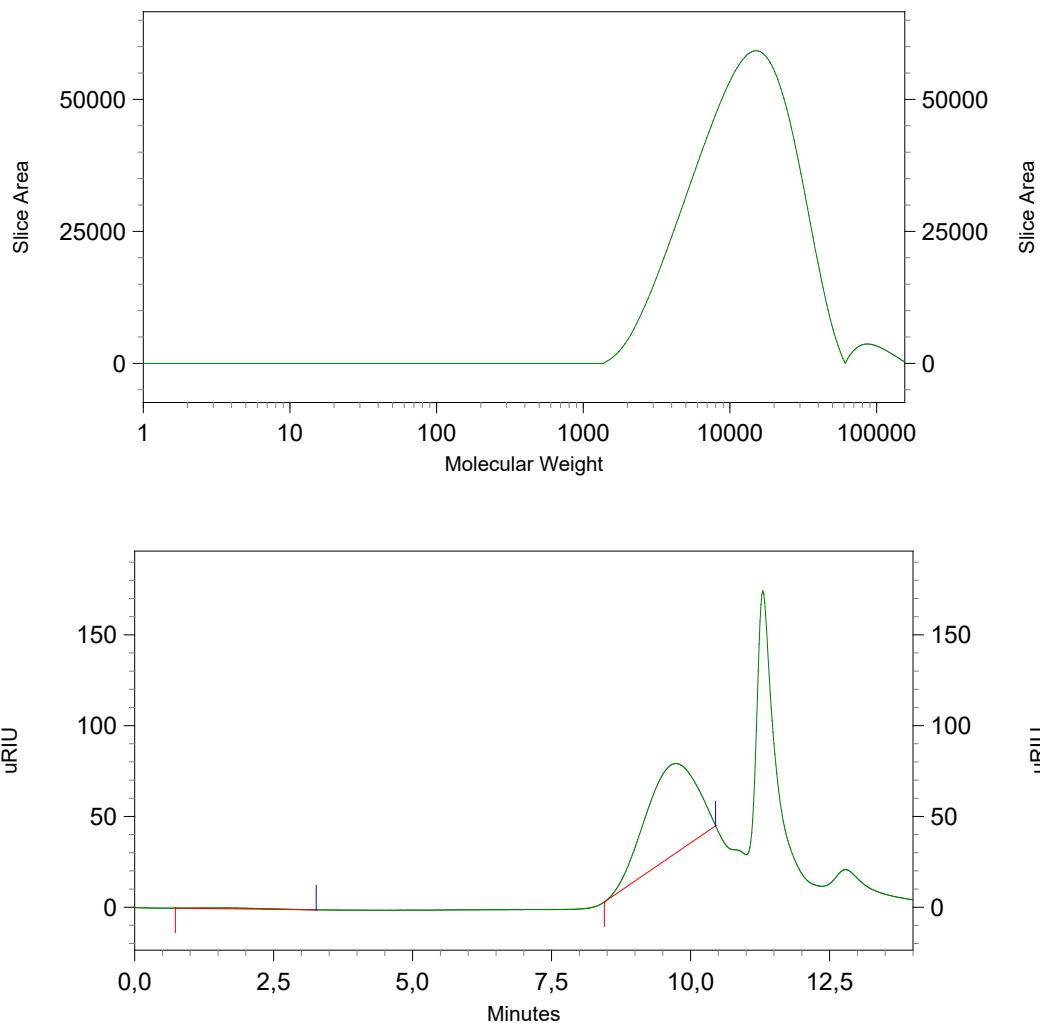


Figure S49. GPC of poly(4,4-diphenyl-but-1-ene) (Table 2, Entry 19).

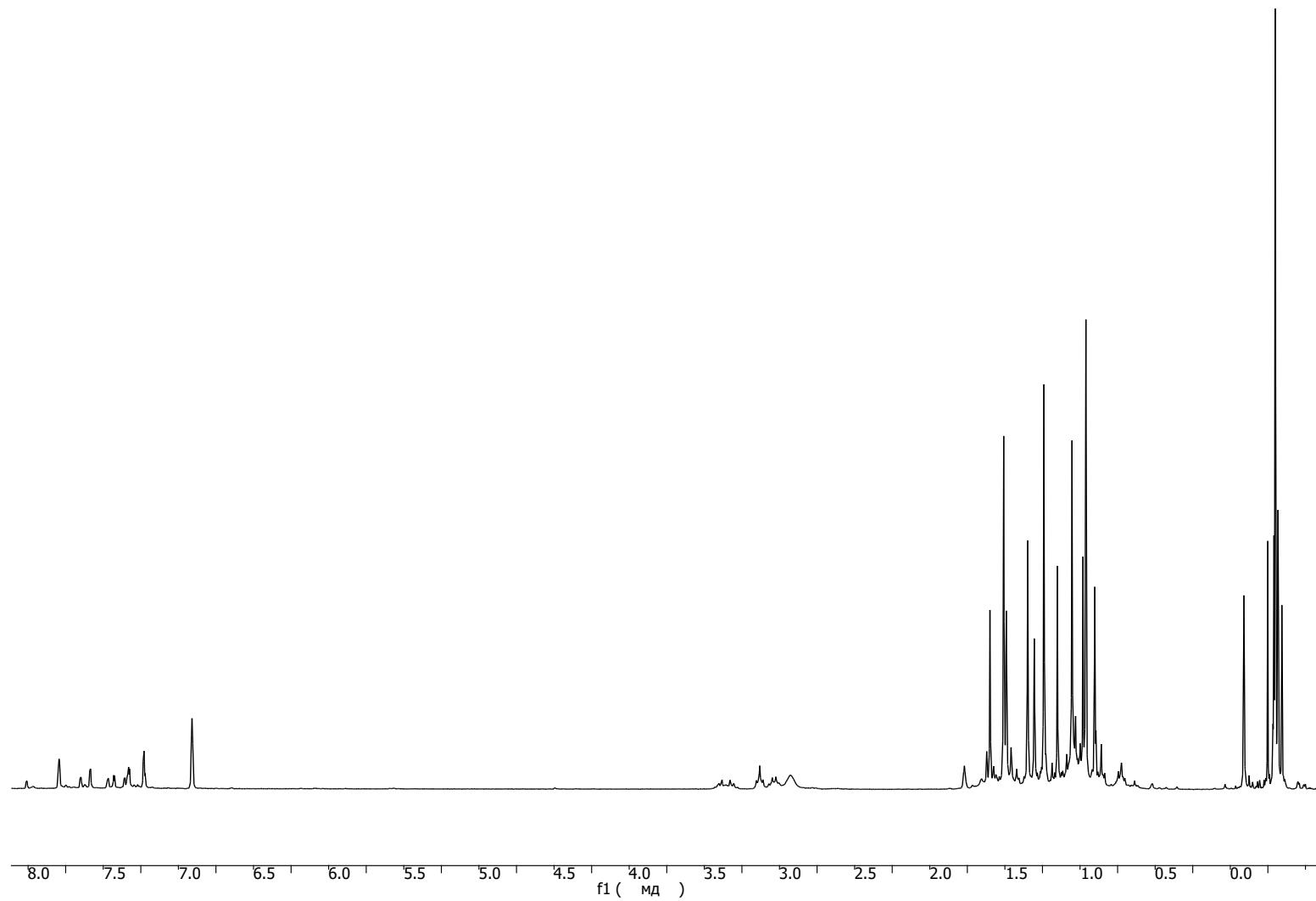


Figure S50. ¹H NMR spectrum of the reaction of **3-Sc** with B(C₆F₅)₃ (300 MHz, C₆D₆, 300 K).

3426_tBu4CarbSc(+)

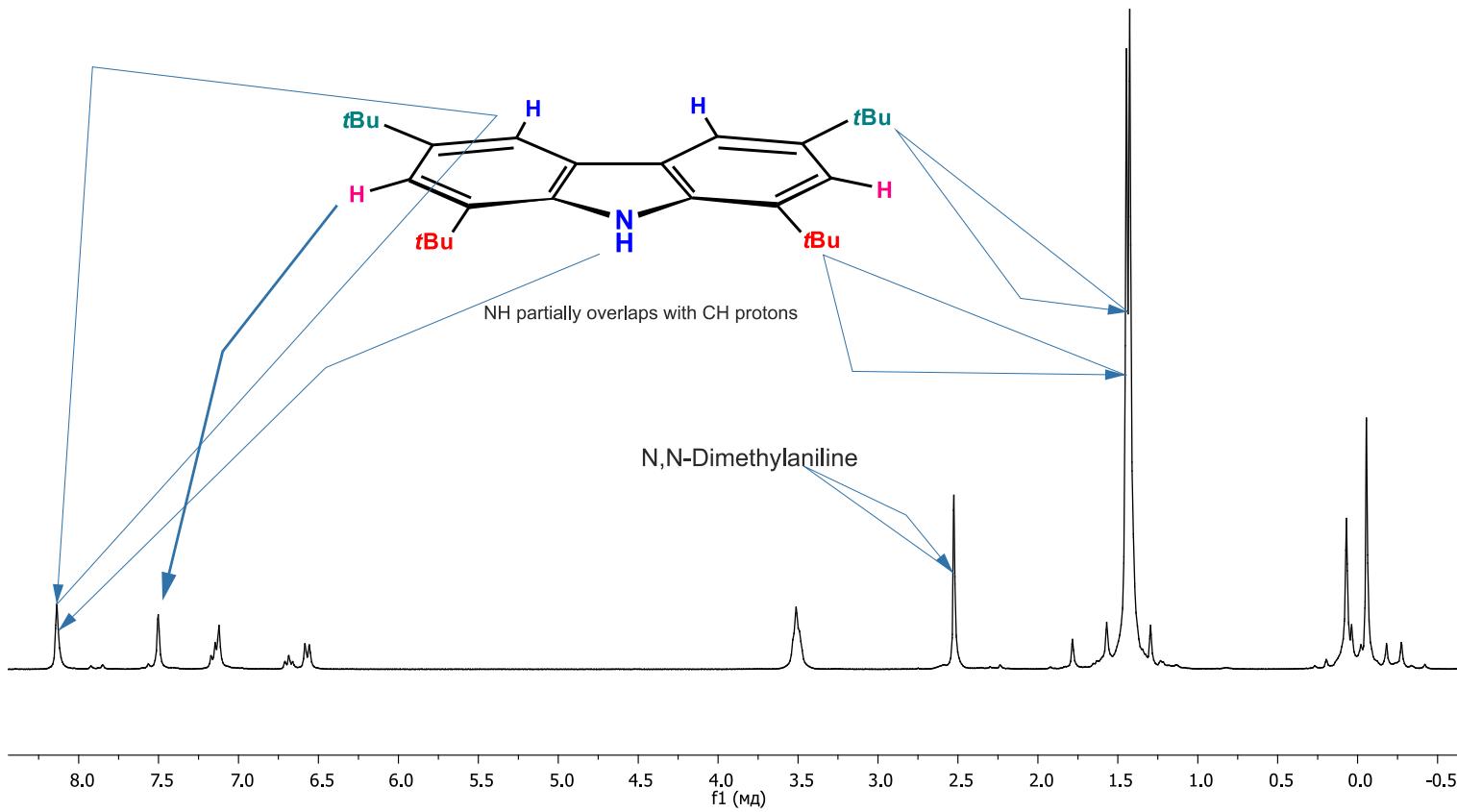


Figure S51. ¹H NMR spectrum of the reaction of **3-Sc** with [PhNHMe₂][B(C₆F₅)₄] (300 MHz, C₆D₆, 300 K).

3426_tBu4CarbSc(+)
tBu4CarbScR2 + TB

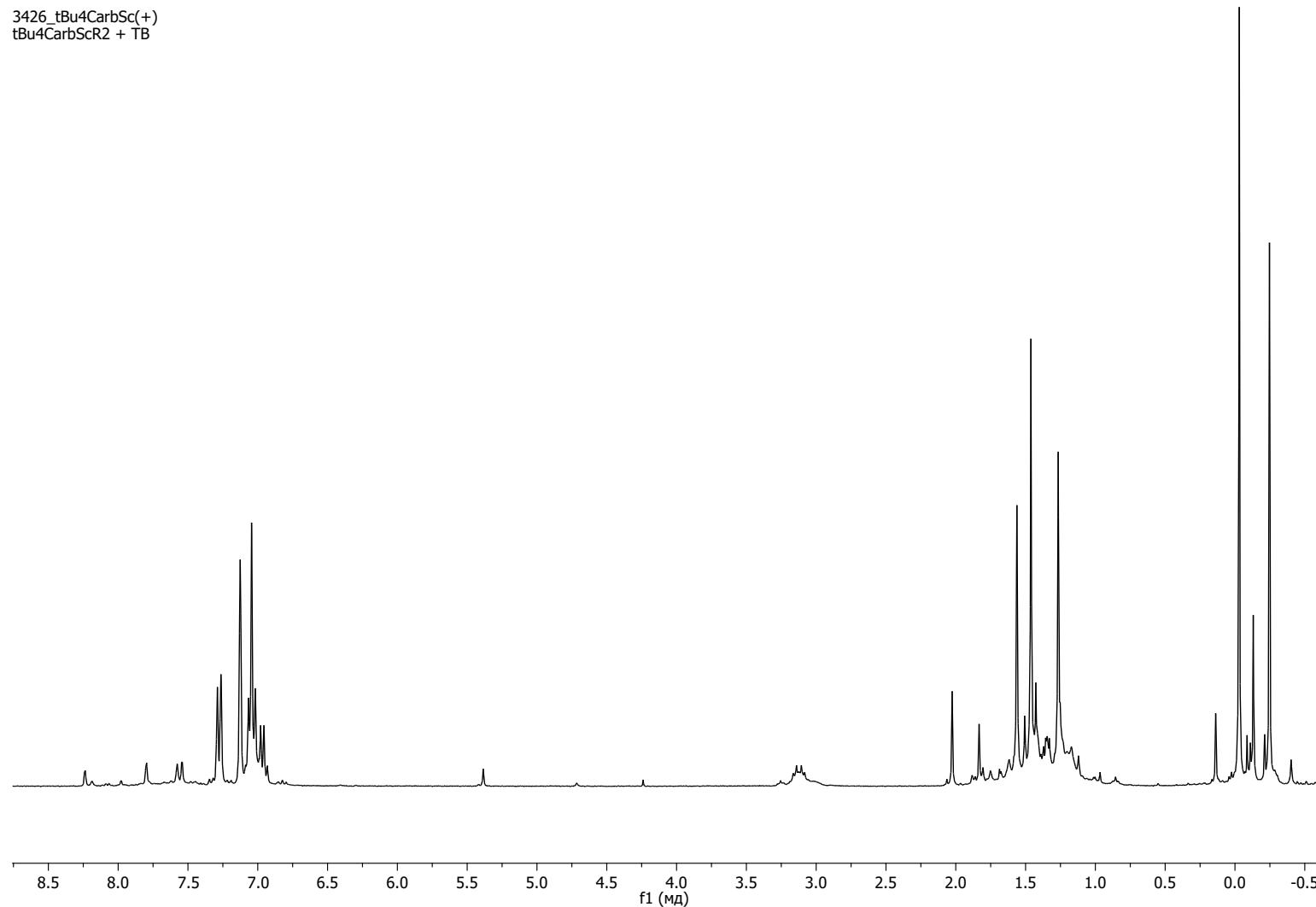


Figure S52. ¹H NMR spectrum of the reaction of **3-Sc** with [Ph₃C][B(C₆F₅)₄] (300 MHz, C₆D₆, 300 K).

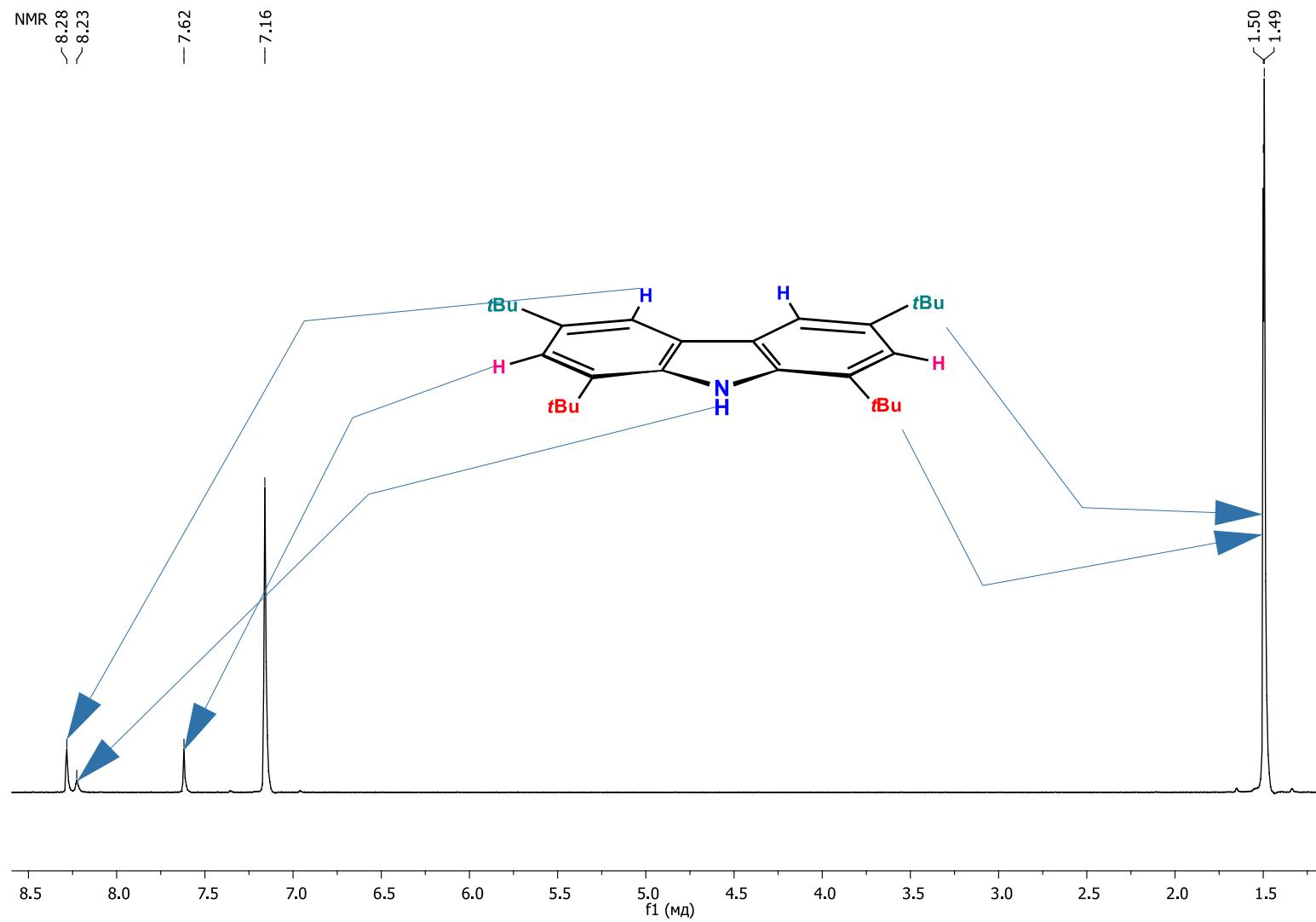


Figure S53. ^1H NMR spectrum of the tBu_4CarbH (400 MHz, C_6D_6 , 298 K).

Table S1. Crystal Data and Structure Refinement Details for Complexes **1-La**, **2-Y**, **2-Sc**, **3-Sc**

	1-La	2-Y	2-Sc	3-Sc
Empirical formula	C ₄₆ H ₆₂ LaNO	C ₄₆ H ₆₄ N ₃ Y, C ₇ H ₈	C ₄₆ H ₆₄ N ₃ Sc, ½C ₆ H ₁₄	C ₄₀ H ₇₀ NOScSi ₂ , C ₅ H ₁₂
Formula weight	783.87	840.04	747.04	754.25
T, K	100	120	120	100
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> - <i>I</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> , Å	10.4113(3)	21.112(13)	41.78(2)	10.9924(5)
<i>b</i> , Å	10.6661(3)	12.629(8)	12.672(6)	15.8617(7)
<i>c</i> , Å	19.7627(6)	18.607(11)	18.072(8)	27.3052(12)
<i>α</i> , deg	88.4910(10)	90	90	90
<i>β</i> , deg	82.5190(10)	107.171(10)	112.604(12)	93.099(2)
<i>γ</i> , deg	68.7340(10)	90	90	90
<i>V</i> , Å ³	2027.24(10)	4740(5)	8833(7)	4753.9(4)
<i>Z</i>	2	4	8	4
<i>d</i> _{calc} , g/cm ³	1.284	1.177	1.124	1.054

μ , mm ⁻¹	1.087	1.267	0.202	0.236
F_{000}	820	1800	3256	1664
Crystal size, mm	0.25×0.11×0.04	0.10×0.10×0.01	0.35×0.15×0.03	0.17×0.09×0.05
θ range for data collection, deg	2.05-27.89	1.90-26.02	1.69-25.03	2.26-25.12
HKL indices	-13≤h≤13, -14≤k≤14, -25≤l≤25	-26≤h≤26, -15≤k≤15, -22≤l≤22	-49≤h≤49, -15≤k≤15, -21≤l≤21	-13≤h≤13, -18≤k≤18, -32≤l≤32
Reflns collected	20152	60951	59336	53000
Independent reflns ($I > 2\sigma(I)$)	8292	4041	3097	5769
R_{int}	0.0246	0.4026	0.5174	0.1048
Compl. to θ , %	99.1	99.9	99.9	99.6
Data / restraints / params	9575 / 0 / 470	9335 / 699 / 572	7787 / 585 / 524	8443 / 182 / 550
$S(F^2)$	1.060	0.991	1.002	1.042
Final R indices ($F^2 > 2\sigma(F^2)$)	$R_1 = 0.0312$, $wR_2 = 0.0703$	$R_1 = 0.0806$, $wR_2 = 0.1258$	$R_1 = 0.1175$, $wR_2 = 0.2627$	$R_1 = 0.0579$, $wR_2 = 0.1146$
R indices (all data)	$R_1 = 0.0406$,	$R_1 = 0.2129$,	$R_1 = 0.2802$,	$R_1 = 0.1027$,

	$wR_2 = 0.0733$	$wR_2 = 0.1616$	$wR_2 = 0.3567$	$wR_2 = 0.1318$
Largest diff peak and hole, e/Å ³	1.13 / -1.01	0.55 / -0.56	1.07 / -0.74	0.41 / -0.40