

Bis(alkyl) Sc and Y complexes supported by bi- and tridentate amidinate ligands. Synthesis, structure and catalytic activity in polymerization of isoprene and 1-heptene.

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Contents:

Table 1S. Crystallographic data and structure refinement details for 1-4	3
Figure S1. ¹ H NMR spectrum (400 MHz, C ₆ D ₆ , 20 °C) of {(2,6-Me ₂ C ₆ H ₃)NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Y(CH ₂ SiMe ₃) ₂ (THF) (1).	5
Figure S2. ¹³ C{ ¹ H} NMR spectrum (100.62 MHz, C ₆ D ₆ , 20 °C) of {(2,6-Me ₂ C ₆ H ₃)NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Y(CH ₂ SiMe ₃) ₂ (THF) (1).	6
Figure S3. IR spectrum of {(2,6-Me ₂ C ₆ H ₃)NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Y(CH ₂ SiMe ₃) ₂ (THF) (1).	7
Figure S4. ¹ H NMR spectrum (400 MHz, C ₆ D ₆ , 20 °C) of {(2,6-Me ₂ C ₆ H ₃)NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (THF) (2).	8
Figure S5. ¹³ C{ ¹ H} NMR spectrum (100.62 MHz, C ₆ D ₆ , 20 °C) of {(2,6-Me ₂ C ₆ H ₃)NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (THF) (2).	9
Figure S6. IR spectrum of {(2,6-Me ₂ C ₆ H ₃)NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (THF) (2).	10
Figure S7. ¹ H NMR spectrum (400 MHz, C ₆ D ₆ , 20 °C) of {2-[Ph ₂ P(O)]C ₆ H ₄ NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (3).....	11
Figure S8. ¹³ C{ ¹ H} NMR spectrum (100.62 MHz, C ₆ D ₆ , 20 °C) of {2-[Ph ₂ P(O)]C ₆ H ₄ NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (3).....	12
Figure S9. ³¹ P{ ¹ H} NMR spectrum (161.99 MHz, C ₆ D ₆ , 20 °C) of {2-[Ph ₂ P(O)]C ₆ H ₄ NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (3).....	13
Figure S10. IR spectrum of {2-[Ph ₂ P(O)]C ₆ H ₄ NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (3).	14
Figure S11. ¹ H NMR spectrum (400 MHz, C ₆ D ₆ , 20 °C) of {2-[Ph ₂ P(NPh)]C ₆ H ₄ NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (4).....	15
Figure S12. ¹³ C{ ¹ H} NMR spectrum (100.62 MHz, C ₆ D ₆ , 20 °C) of {2-[Ph ₂ P(NPh)]C ₆ H ₄ NC(tBu)N(2,6-Me ₂ C ₆ H ₃)}Sc(CH ₂ SiMe ₃) ₂ (4).....	16

Figure S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, C_6D_6 , 20 °C) of $\{2\text{-}[\text{Ph}_2\text{P}(\text{NPh})]\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2$ (4).....	17
Figure S14. IR spectrum of $\{2\text{-}[\text{Ph}_2\text{P}(\text{NPh})]\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2$ (4).	18
Figure S 15. GPC of PIP sample (Table 1, entry 1).	20
Figure S 16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 1).	21
Figure S 17. GPC of PIP sample (Table 1, entry 2).	23
Figure S 18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 2).	24
Figure S 19. GPC of PIP sample (Table 1, entry 5).	26
Figure S 20. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 5).	27
Figure S 21. GPC of PIP sample (Table 1, entry 7).	29
Figure S 22. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 7).	30
Figure S 23. GPC of PIP sample (Table 1, entry 8).	32
Figure S 24. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 8).	33
Figure S 25. GPC of PIP sample (Table 1, entry 10).	35
Figure S 26. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 10).	36
Figure S 27. GPC of PIP sample (Table 1, entry 11).	38
Figure S 28. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 11).	39
Figure S 29. GPC of PIP sample (Table 1, entry 15).	41
Figure S 30. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 15).	42
Figure S 31. GPC of PIP sample (Table 1, entry 16).	44
Figure S 32. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 16).	45
Figure S 33. GPC of PIP sample (Table 1, entry 17).	47
Figure S 34. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 17).	48
Figure S 35. GPC of polyheptene sample (Table 2, entry 2).	50
Figure S 36. GPC of polyheptene sample (Table 2, entry 3).	52
Figure S 37. GPC of polyheptene sample (Table 2, entry 4).	54
Figure S 38. GPC of polyheptene sample (Table 2, entry 6).	56
Figure S 39. GPC of polyheptene sample (Table 2, entry 8).	58

Table 1S. Crystallographic data and structure refinement details for **1-4**.

Compound	1	2	3	4
Empirical formula	C ₃₃ H ₅₇ N ₂ OSi ₂ Y	C ₃₃ H ₅₇ N ₂ OScSi ₂	C ₃₉ H ₅₄ N ₂ OPScSi ₂	C ₄₅ H ₅₉ N ₃ PScSi ₂ , ½C ₇ H ₈
Formula weight	642.89	598.94	698.95	820.13
<i>T</i> [K]	100(2)	150(2)	100(2)	200(2)
Wavelength [Å]	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> [Å]	11.1445(5)	11.1928(5)	11.4383(5)	12.6969(4)
<i>b</i> [Å]	11.4646(5)	11.3356(5)	19.1282(8)	24.2752(9)
<i>c</i> [Å]	15.5390(7)	15.4964(4)	18.8454(8)	15.3631(7)
α [°]	94.646(2)	94.893(3)	90	90
β [°]	99.027(2)	98.012(3)	103.7300(10)	94.631(4)
γ [°]	111.260(2)	111.928(5)	90	90
<i>V</i> [Å ³]	1806.72(14)	1785.79(13)	4005.4(3)	4719.8(3)
<i>Z</i>	2	2	4	4
ρ_{calcd} [g cm ⁻³]	1.182	1.114	1.159	1.154
Absorption coefficient [mm ⁻¹]	1.705	0.299	0.314	0.275
<i>F</i> ₀₀₀	688	652	1496	1756
Crystal dimensions [mm]	0.36 0.24 0.09	0.51×0.39×0.19	0.11×0.09×0.09	0.53×0.27×0.10
θ range for data collection [°]	2.00-27.09	3.04-27.10	2.12-26.07	2.33-25.96
<i>hkl</i> indices	-14≤ <i>h</i> ≤14, -14≤ <i>k</i> ≤14, -19≤ <i>l</i> ≤19	-14≤ <i>h</i> ≤14, -14≤ <i>k</i> ≤14, -19≤ <i>l</i> ≤19	-14≤ <i>h</i> ≤14, -23≤ <i>k</i> ≤23, -23≤ <i>l</i> ≤23	-15≤ <i>h</i> ≤15, -29≤ <i>k</i> ≤29, -18≤ <i>l</i> ≤18
Reflections collected	19408	28484	42934	66482
Independent	6387	6304	6579	6120

reflections				
$R_{\text{int}} [I > 2\sigma(I)]$	0.0412	0.0295	0.0365	0.0942
Completeness to θ [%]	99.6	98.6	99.5	99.9
Data / restraints / parameters	7928 / 1084 / 627	7773/14/416	7879/0/426	9226/48/531
$S(F^2)$	1.039	1.042	1.073	1.071
Final R indices [$F^2 > 2\sigma(F^2)$]	$R_1 = 0.0384,$ $wR_2 = 0.0879$	$R_1 = 0.0421,$ $wR_2 = 0.1065$	$R_1 = 0.0386,$ $wR_2 = 0.0827$	$R_1 = 0.0672,$ $wR_2 = 0.1364$
Final R indices (all data)	$R_1 = 0.0554,$ $wR_2 = 0.0940$	$R_1 = 0.0564,$ $wR_2 = 0.1161$	$R_1 = 0.0509,$ $wR_2 = 0.0882$	$R_1 = 0.1124,$ $wR_2 = 0.1572$
Largest diff. peak and hole [$\text{e}\text{\AA}^{-3}$]	0.62 / -0.68	0.37 / -0.35	0.30 / -0.34	0.44 / -0.37

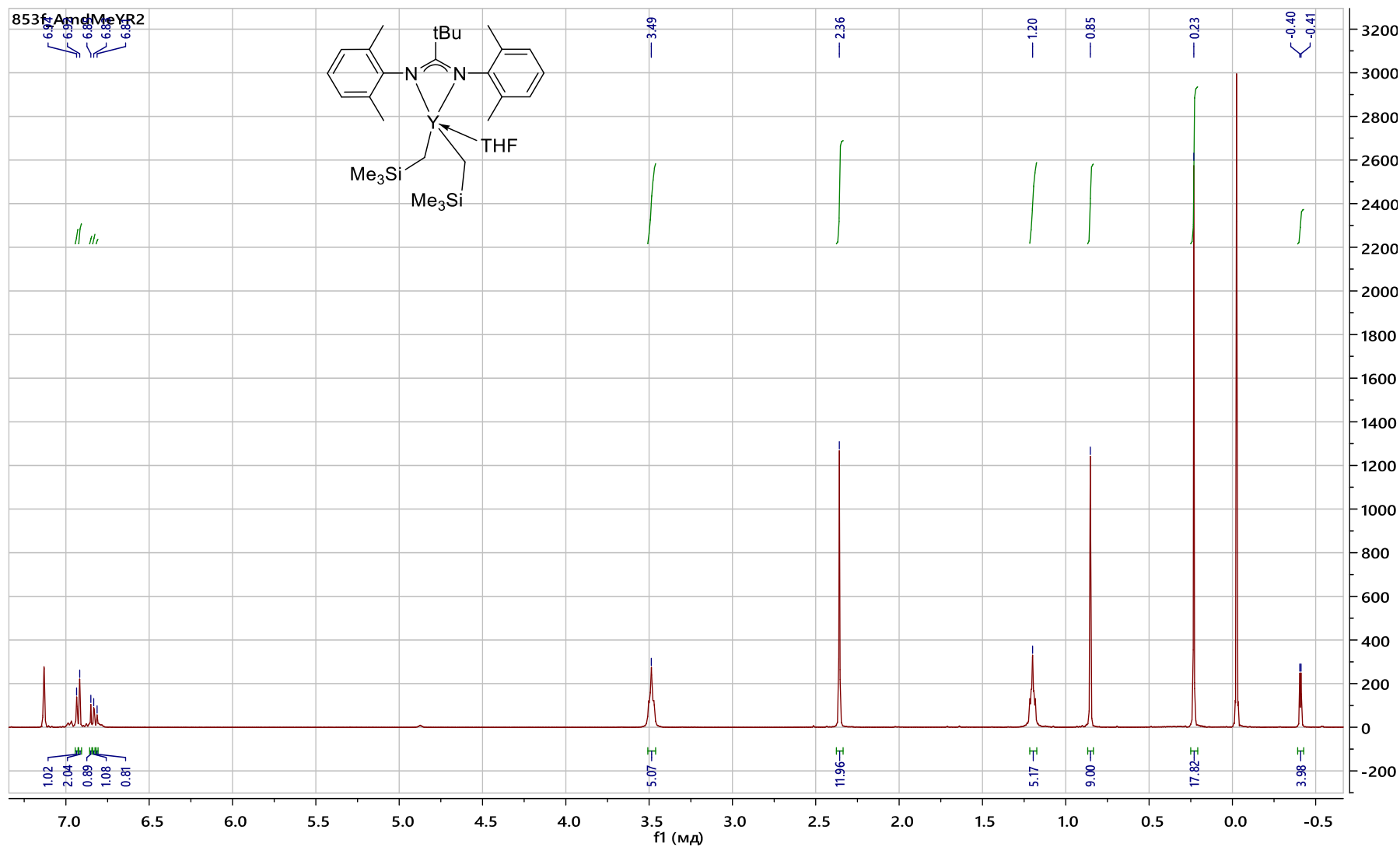


Figure S1. ^1H NMR spectrum (400 MHz, C_6D_6 , 20 $^\circ\text{C}$) of $\{(2,6\text{-Me}_2\text{C}_6\text{H}_3)\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Y}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**1**).

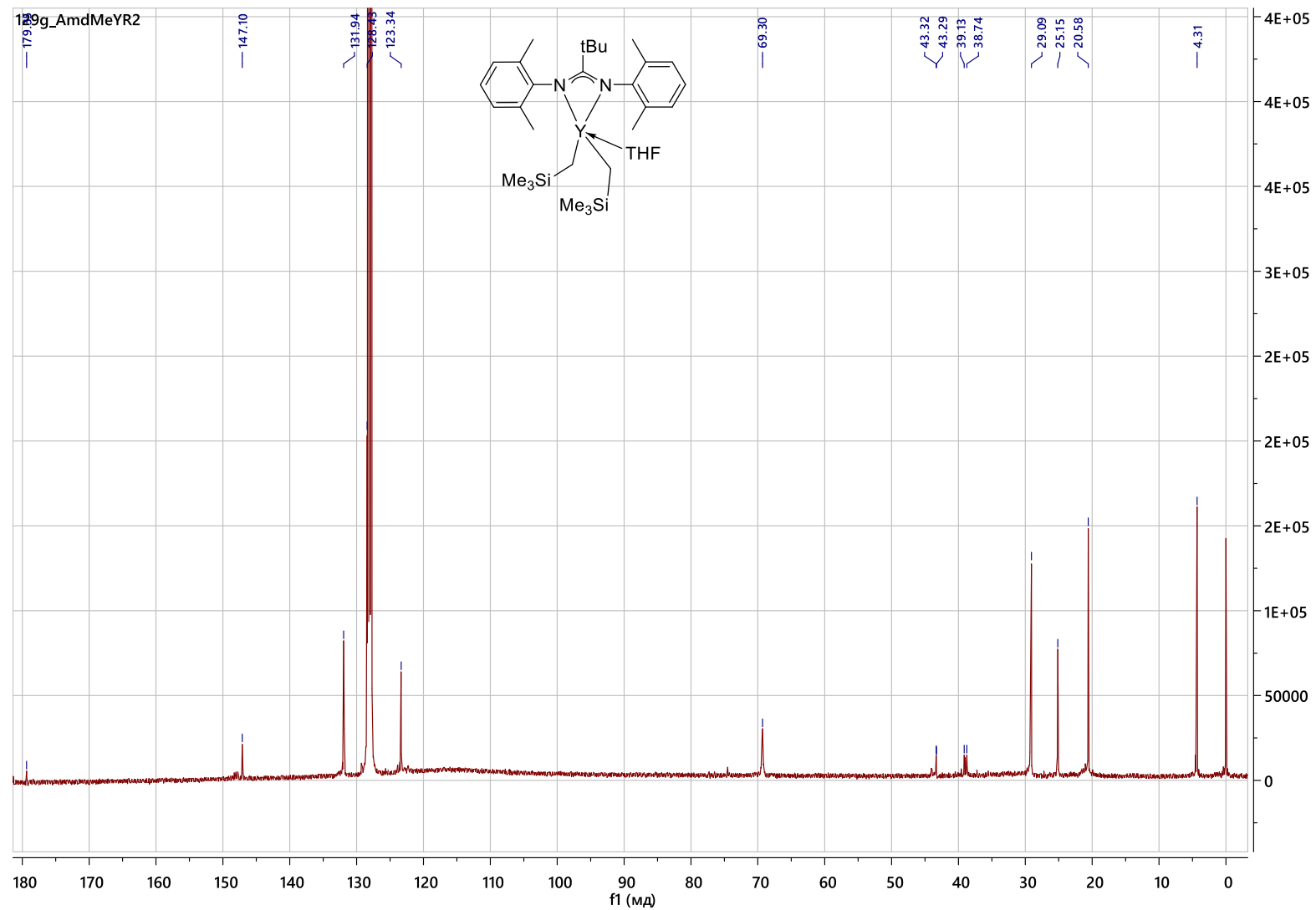


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.62 MHz, C_6D_6 , 20 °C) of $\{(2,6\text{-Me}_2\text{C}_6\text{H}_3)\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Y}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**1**).

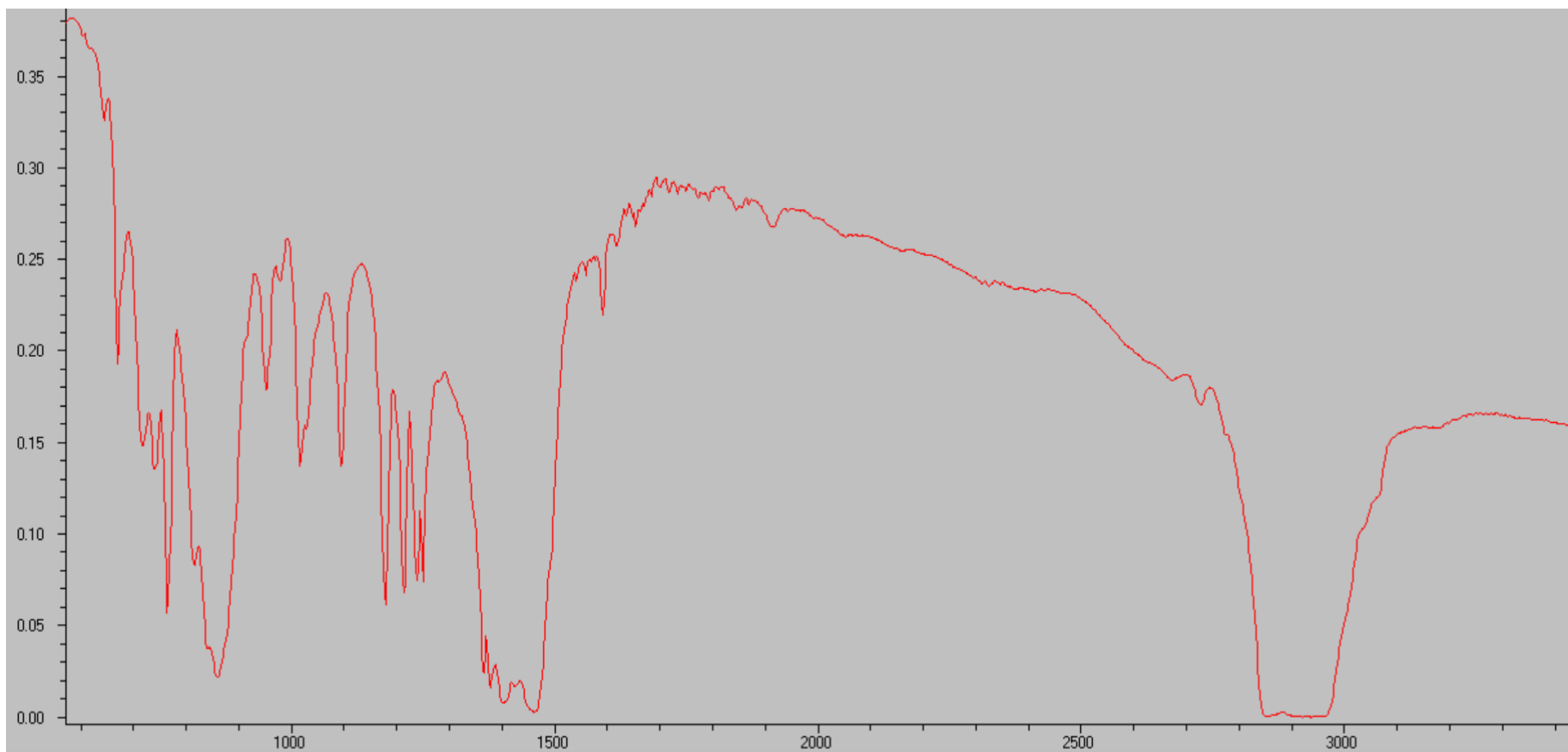


Figure S3. IR spectrum of $\{(2,6\text{-Me}_2\text{C}_6\text{H}_3)\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Y}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**1**).

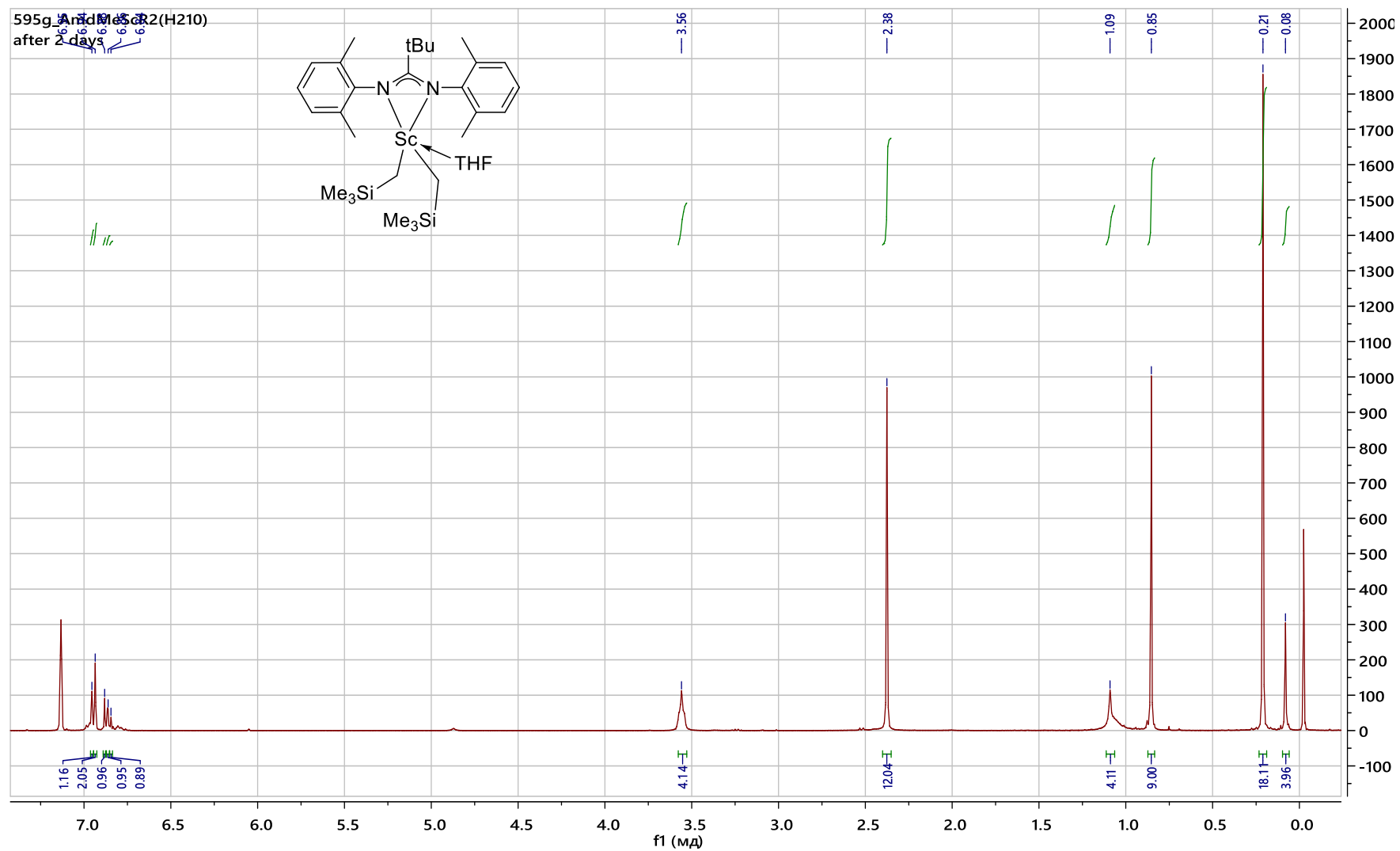


Figure S4. ^1H NMR spectrum (400 MHz, C_6D_6 , 20 °C) of $\{(2,6\text{-Me}_2\text{C}_6\text{H}_3)\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**2**).

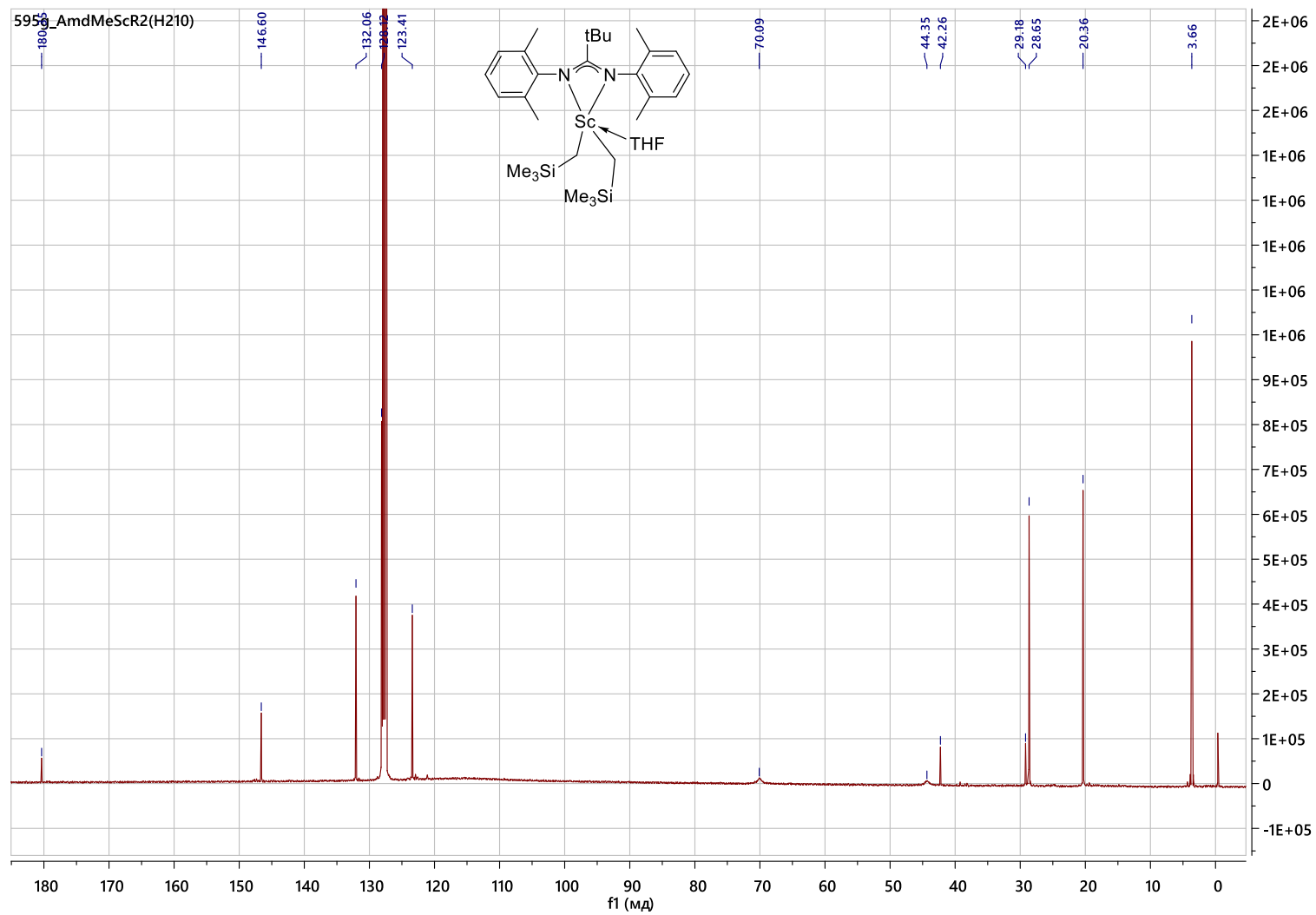


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.62 MHz, C_6D_6 , 20 °C) of $\{(2,6\text{-Me}_2\text{C}_6\text{H}_3)\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**2**).

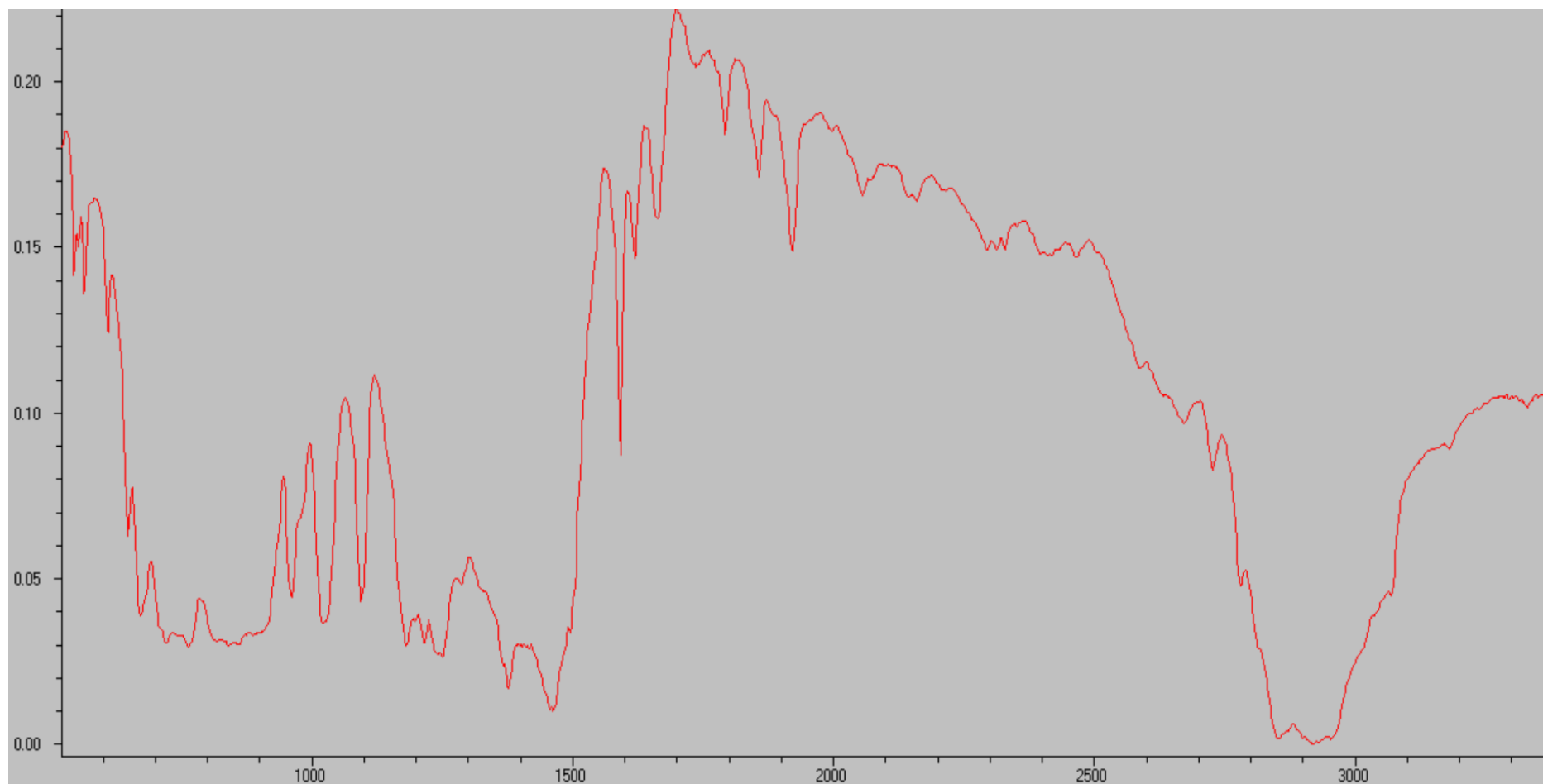


Figure S6. IR spectrum of $\{(2,6\text{-Me}_2\text{C}_6\text{H}_3)\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (**2**).

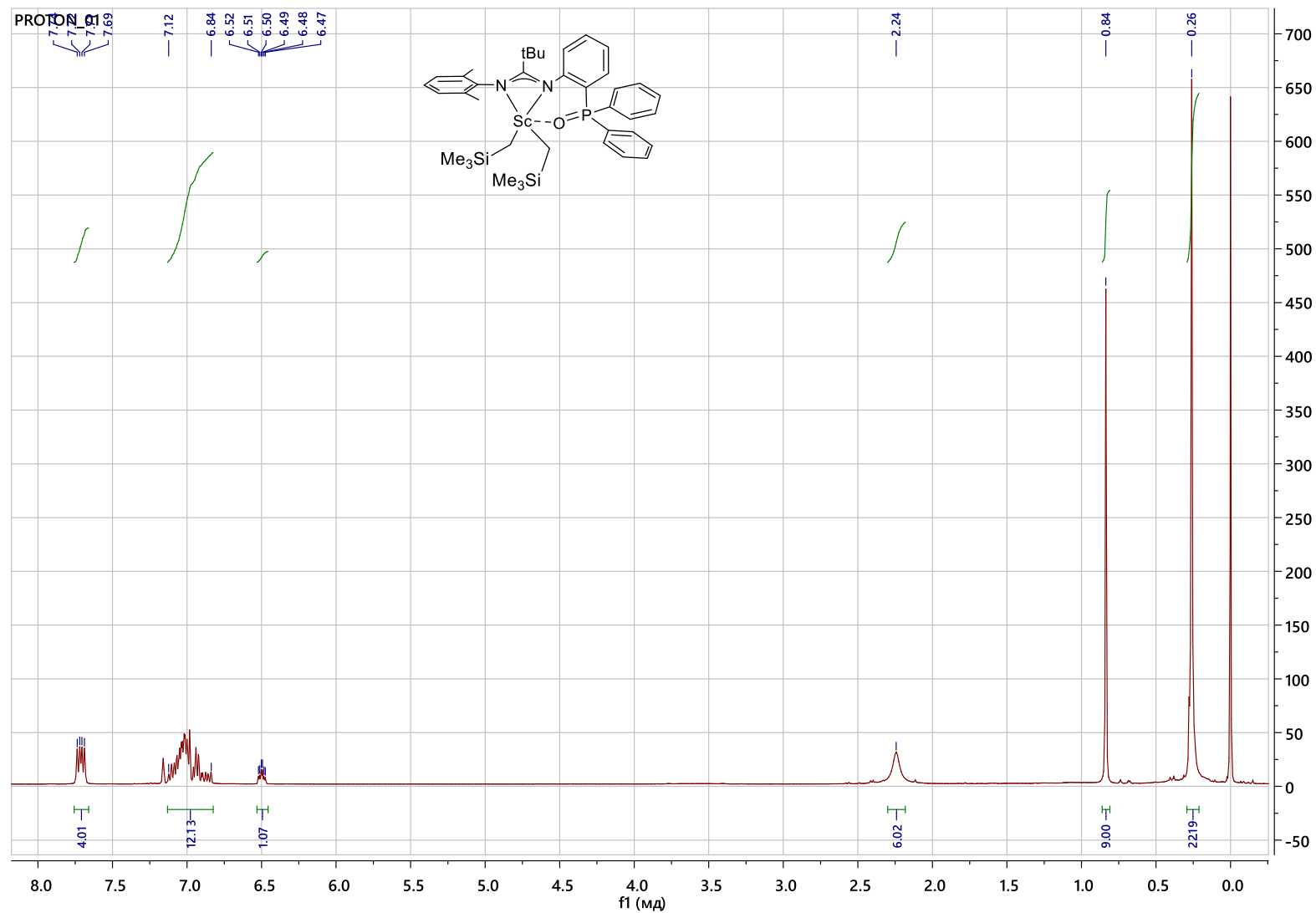


Figure S7. ^1H NMR spectrum (400 MHz, C_6D_6 , 20 °C) of $\{2\text{-}[\text{Ph}_2\text{P}(\text{O})]\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2$ (**3**).

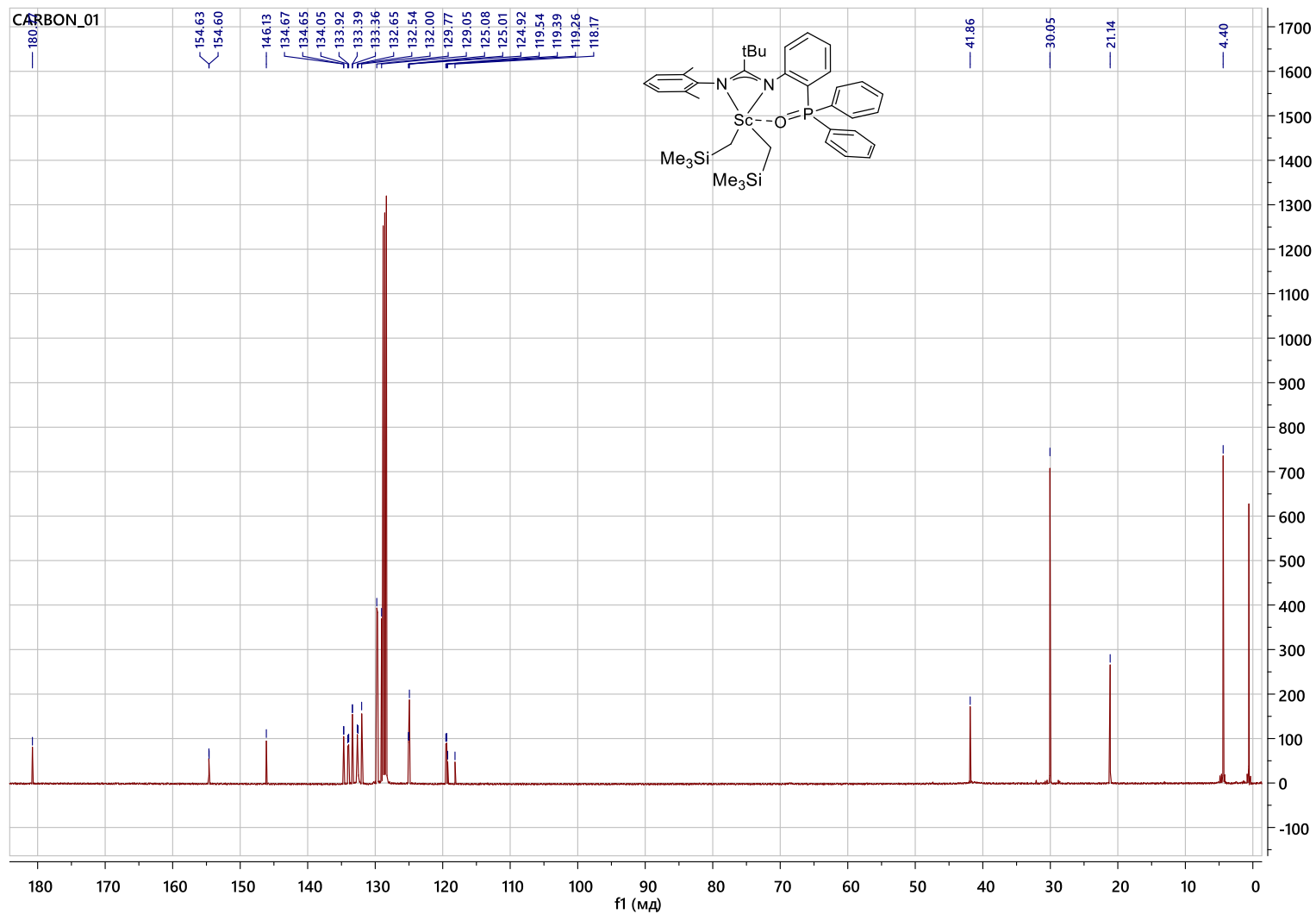


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.62 MHz, C_6D_6 , 20 °C) of $\{2\text{-}[\text{Ph}_2\text{P}(\text{O})\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)]\text{Sc}(\text{CH}_2\text{SiMe}_3)_2\}$ (**3**).

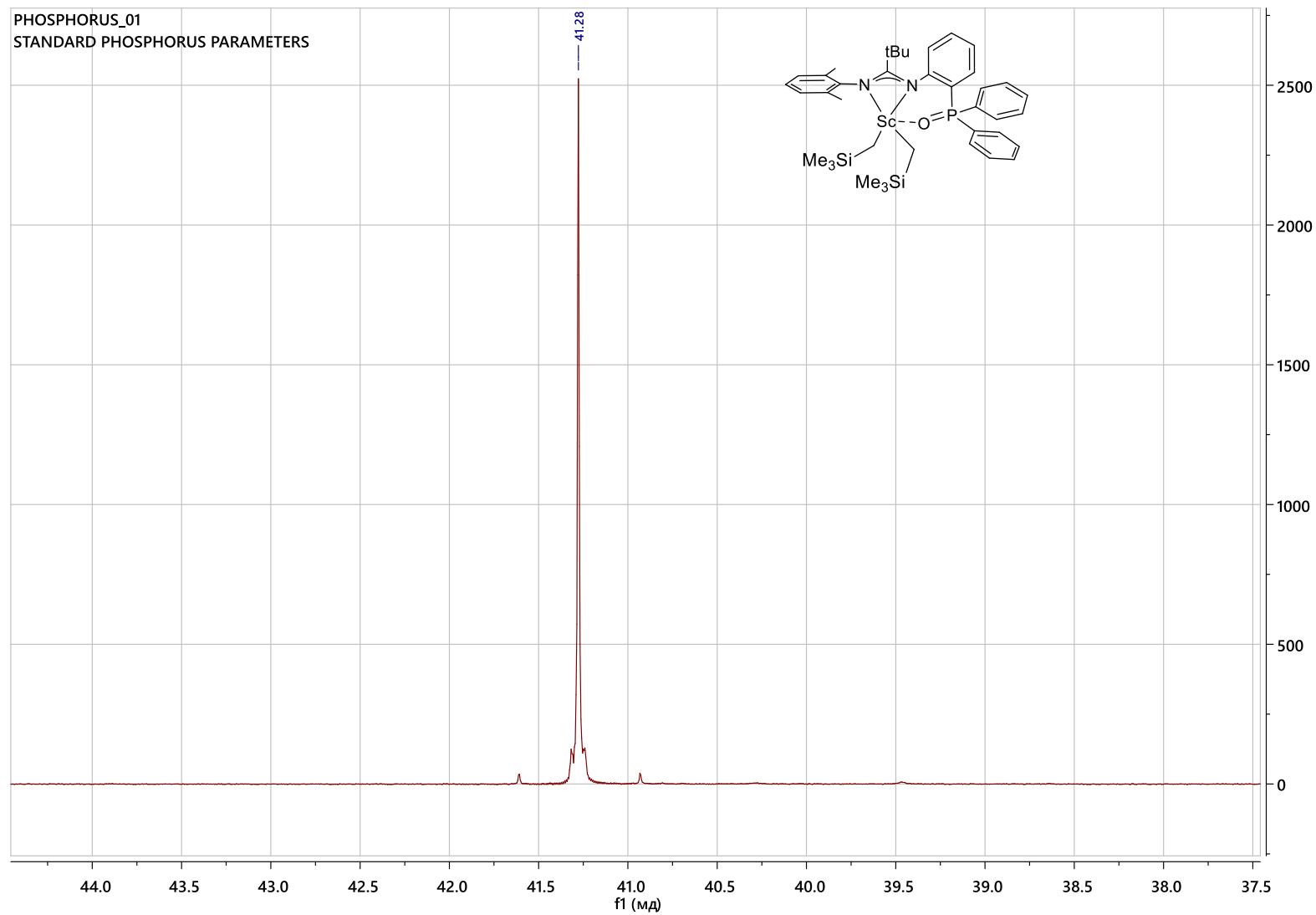


Figure S9. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, C_6D_6 , 20 °C) of $\{2\text{-}[\text{Ph}_2\text{P}(\text{O})]\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2$ (**3**).

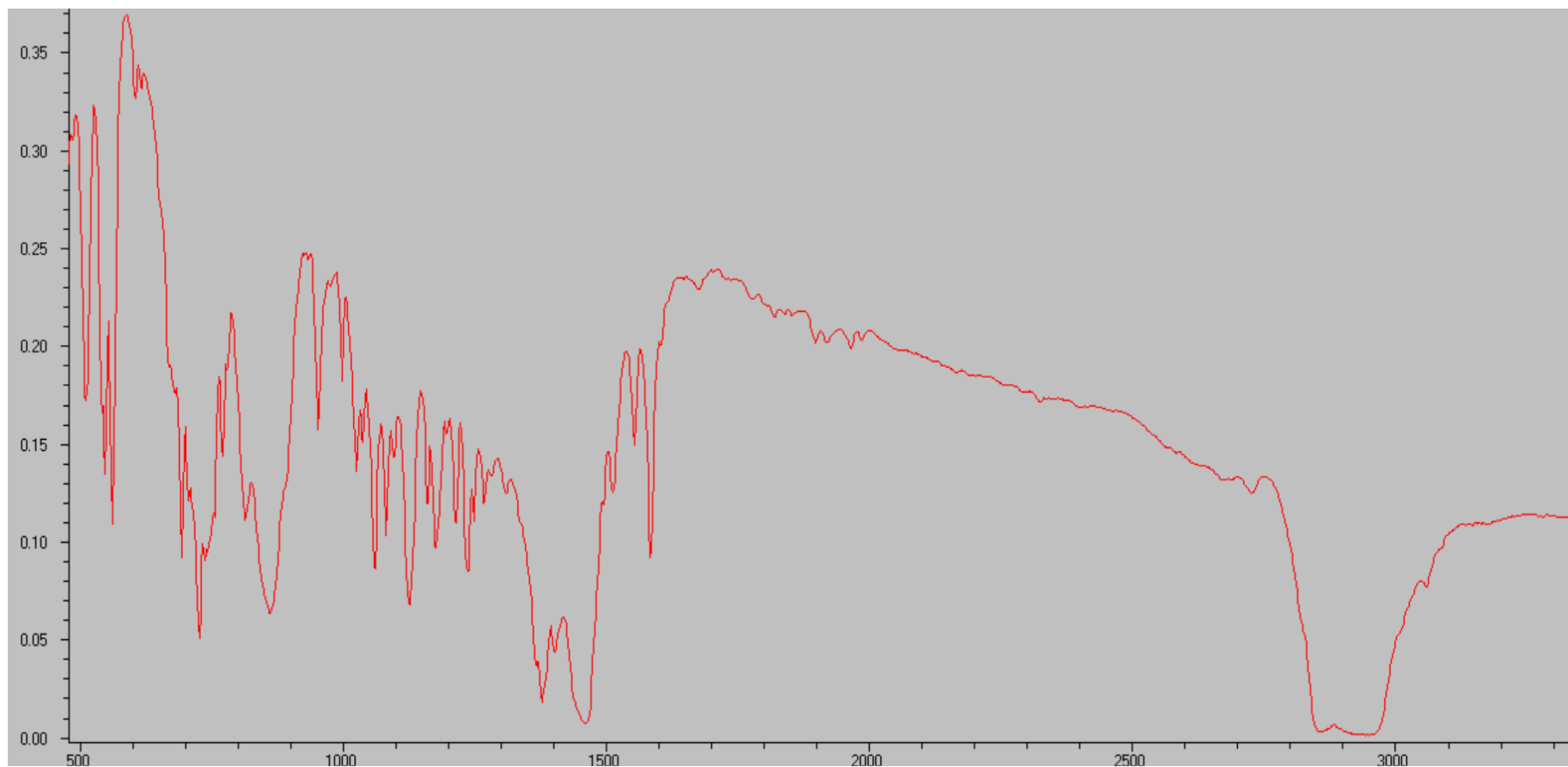


Figure S10. IR spectrum of $\{2\text{-[Ph}_2\text{P(O)]C}_6\text{H}_4\text{NC(tBu)N(2,6-Me}_2\text{C}_6\text{H}_3)\}\text{Sc(CH}_2\text{SiMe}_3)_2$ (**3**).

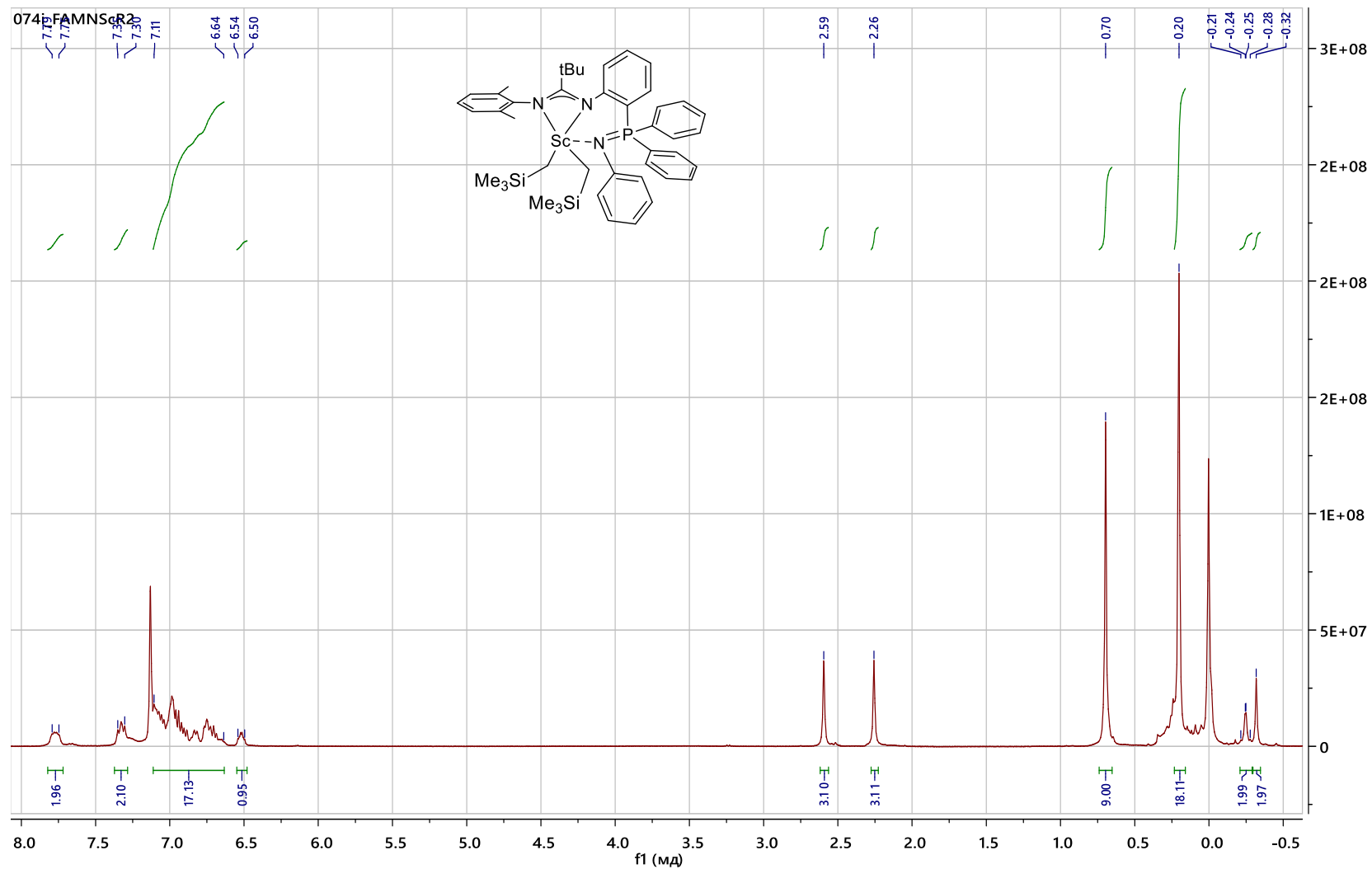


Figure S11. ^1H NMR spectrum (400 MHz, C_6D_6 , 20 °C) of $\{2\text{-}[\text{Ph}_2\text{P}(\text{NPh})\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)]\text{Sc}(\text{CH}_2\text{SiMe}_3)_2\}$ (**4**).

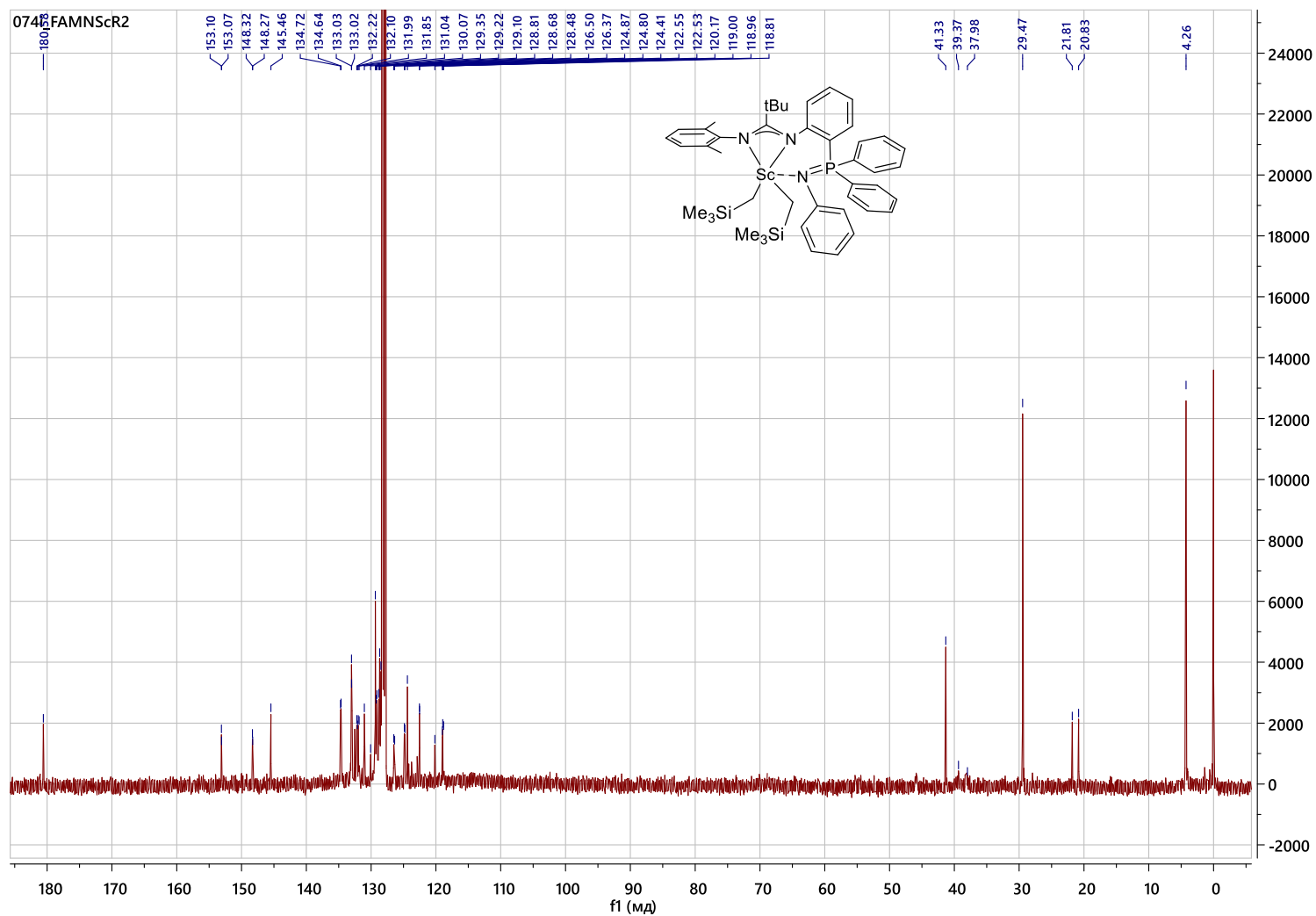


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.62 MHz, C_6D_6 , 20 °C) of $\{2\text{-}[\text{Ph}_2\text{P}(\text{NPh})]\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2$ (**4**).

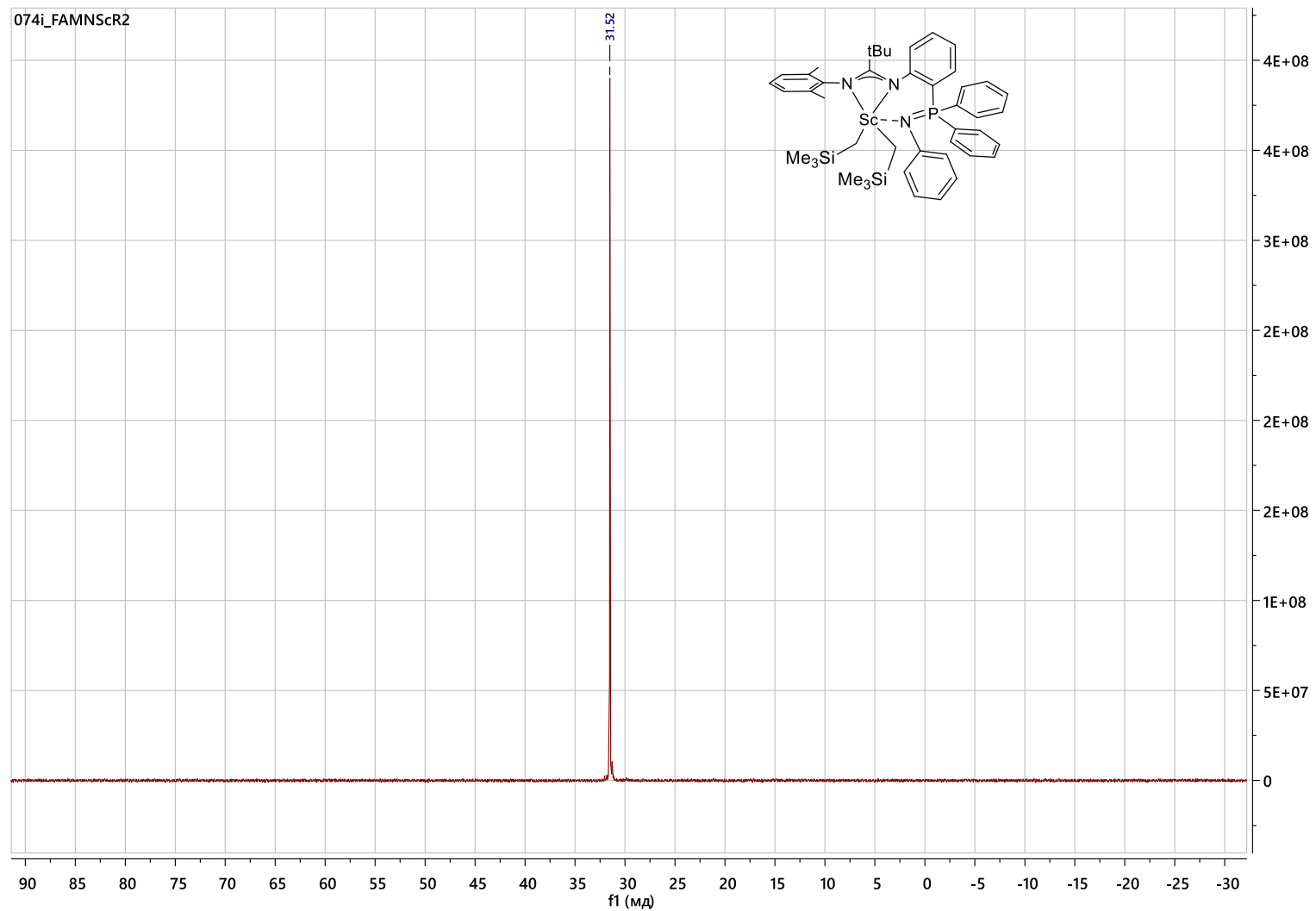


Figure S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, C_6D_6 , 20 °C) of $\{2\text{-}[\text{Ph}_2\text{P}(\text{NPh})]\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)\}\text{Sc}(\text{CH}_2\text{SiMe}_3)_2$ (**4**).

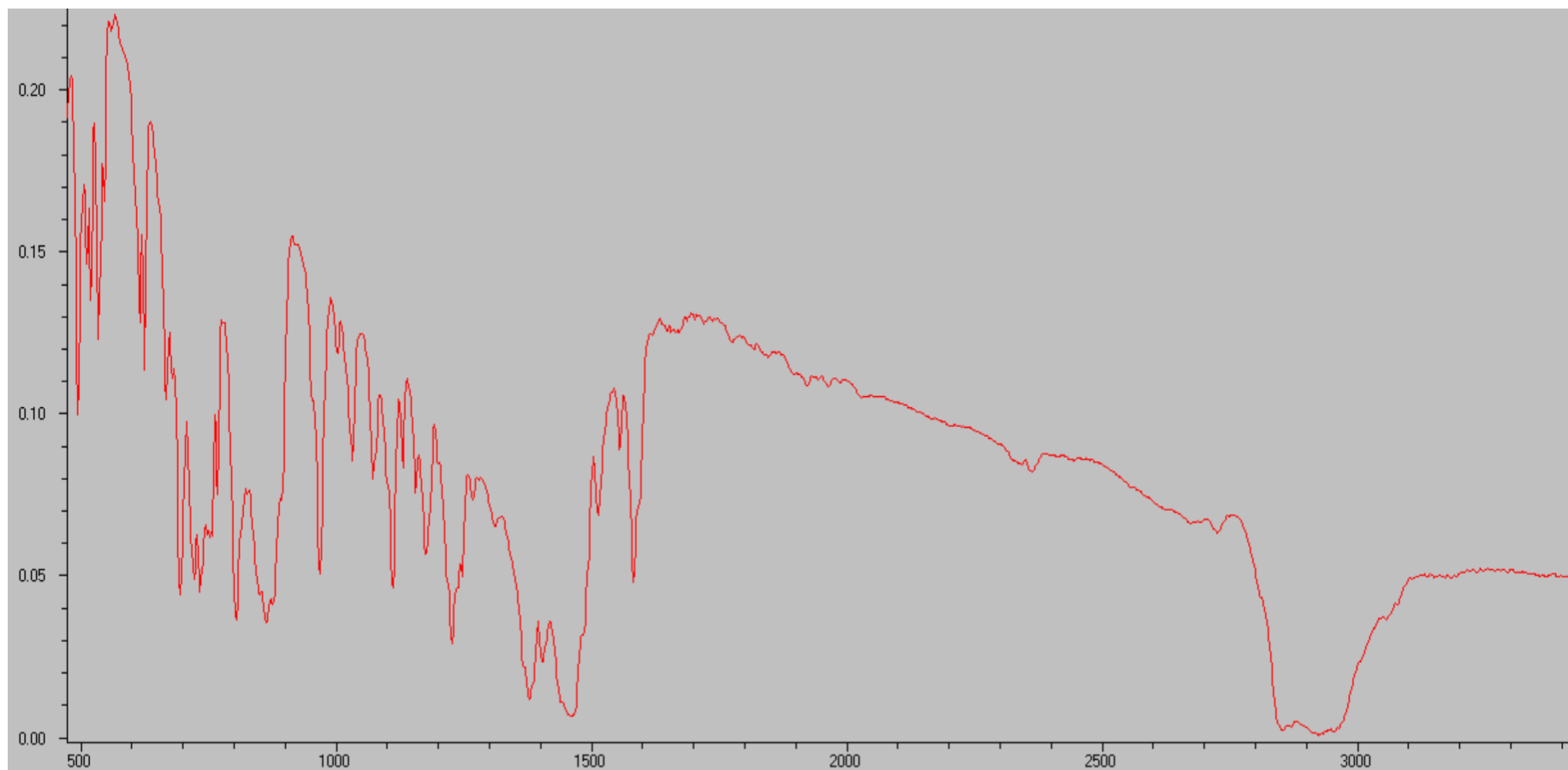


Figure S14. IR spectrum of $\{2\text{-}[\text{Ph}_2\text{P}(\text{NPh})\text{C}_6\text{H}_4\text{NC}(\text{tBu})\text{N}(2,6\text{-Me}_2\text{C}_6\text{H}_3)]\text{Sc}(\text{CH}_2\text{SiMe}_3)_2\}$ (**4**).

SEC Summary information

S 2300/S 2400

Processing Start Time (min) = 5,943

Processing Stop Time (min) = 10,907

Number of Slices = 298

Weight Average Molecular Weight = 90864

Number Average Molecular Weight = 29792

Z Average Molecular Weight = 629457

Z+1 Average Molecular Weight = 3265914

Polydispersity index = 3,050

Peak Molecular Weight = 56292

Z Average / Weight Average = 6,927

Z+1 Average / Weight Average = 35,943

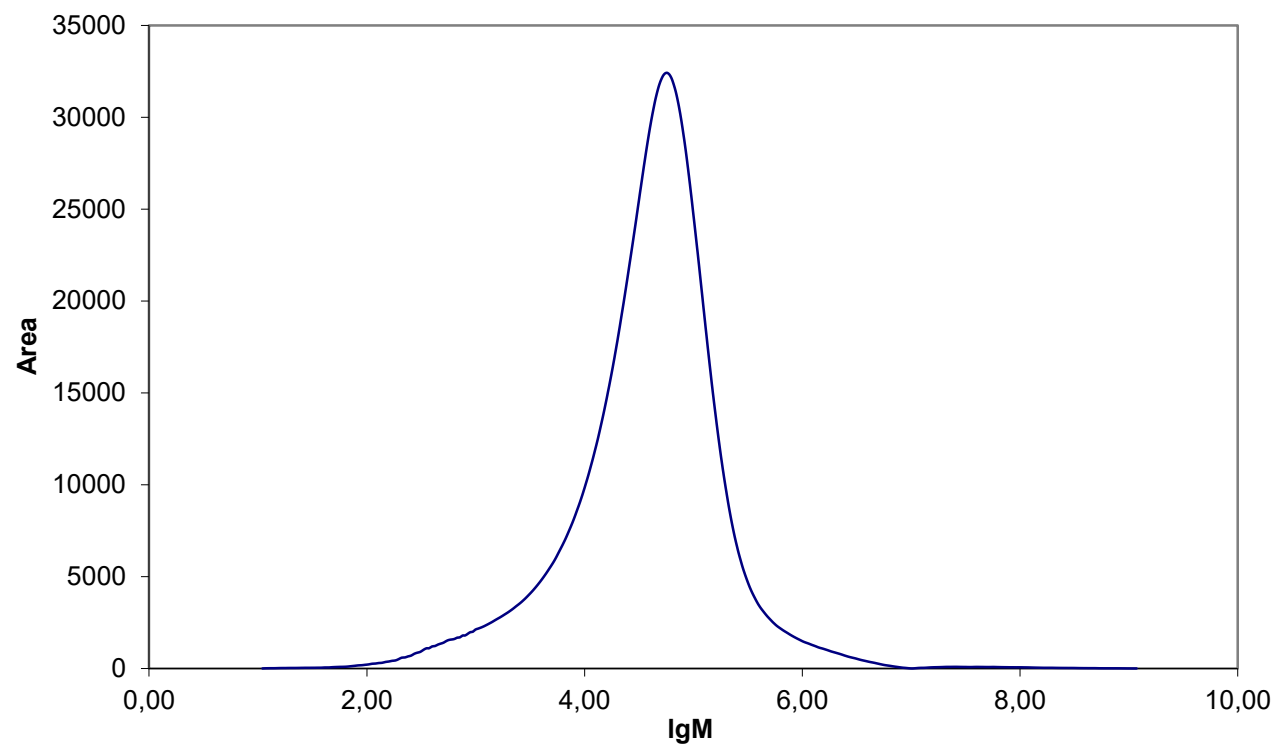


Figure S 15. GPC of PIP sample (Table 1, entry 1).

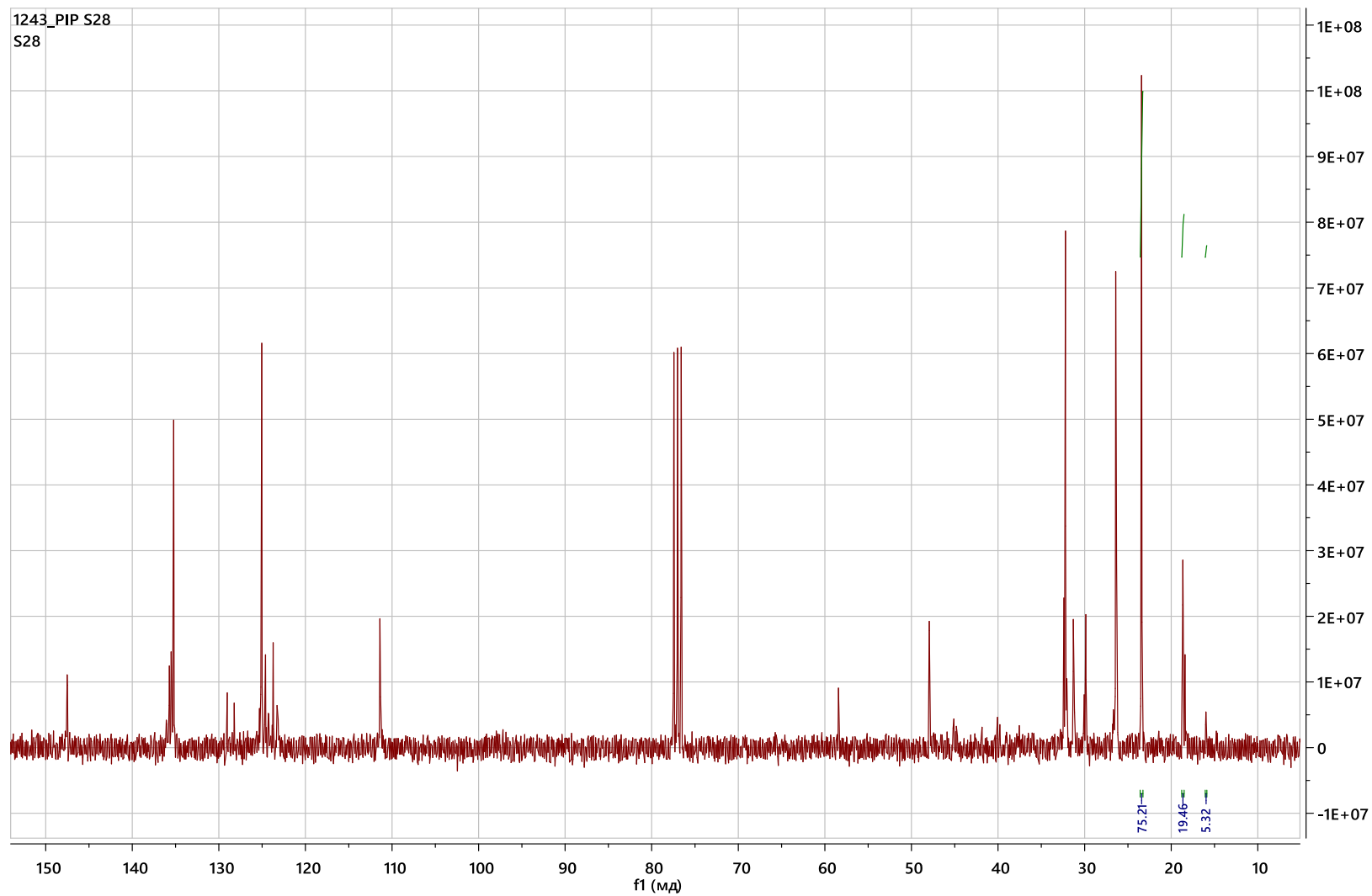


Figure S 16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 1).

SEC Summary information

S 2300/S 2400

Processing Start Time(min) = 6,391

Processing Stop Time(min) = 10,668

Number of Slices = 257

Weight Average Molecular Weight = 232774

Number Average Molecular Weight = 83781

Z Average Molecular Weight = 515104

Z+1 Average Molecular Weight = 938324

Polydispersity index = 2,778

Peak Molecular Weight = 159264

Z Average / Weight Average = 2,213

Z+1 Average / Weight Average = 4,031

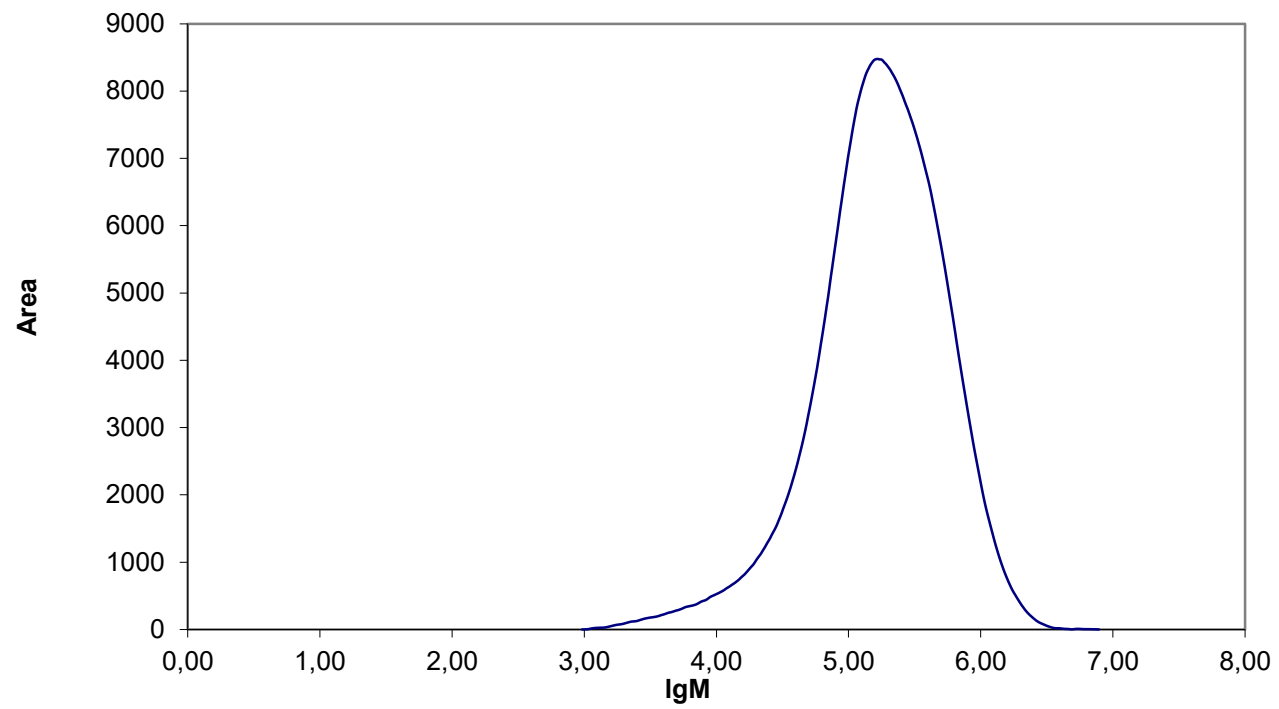


Figure S 17. GPC of PIP sample (Table 1, entry 2).

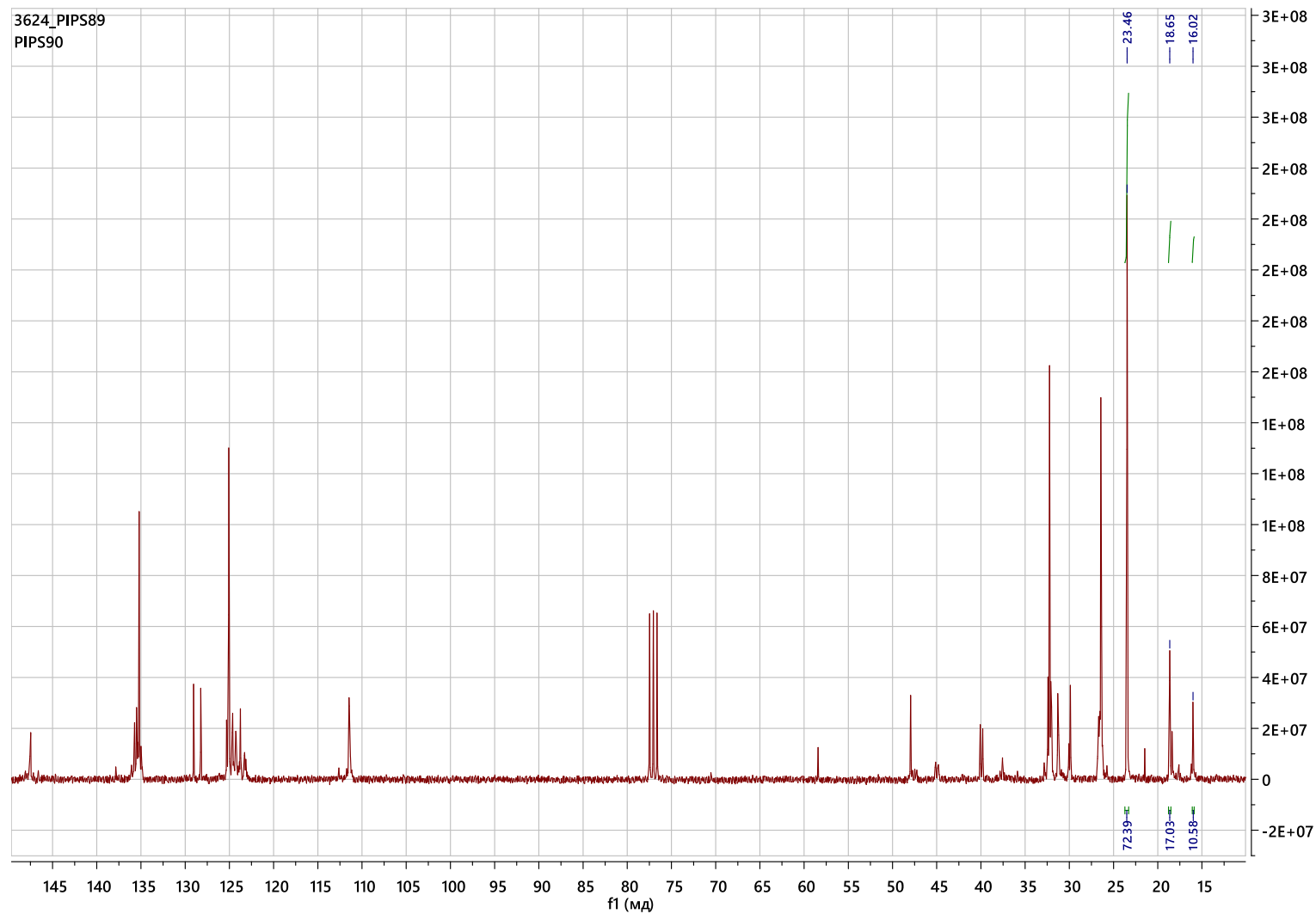


Figure S 18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 2).

SEC Summary information

S 2300/S 2400

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Processing Stop Time(min) = 15,029

Number of Slices = 212

Weight Average Molecular Weight = 3422

Number Average Molecular Weight = 1903

Z Average Molecular Weight = 6218

Z+1 Average Molecular Weight = 11922

Polydispersity index = 1,798

Peak Molecular Weight = 2615

Z Average / Weight Average = 1,817

Z+1 Average / Weight Average = 3,484

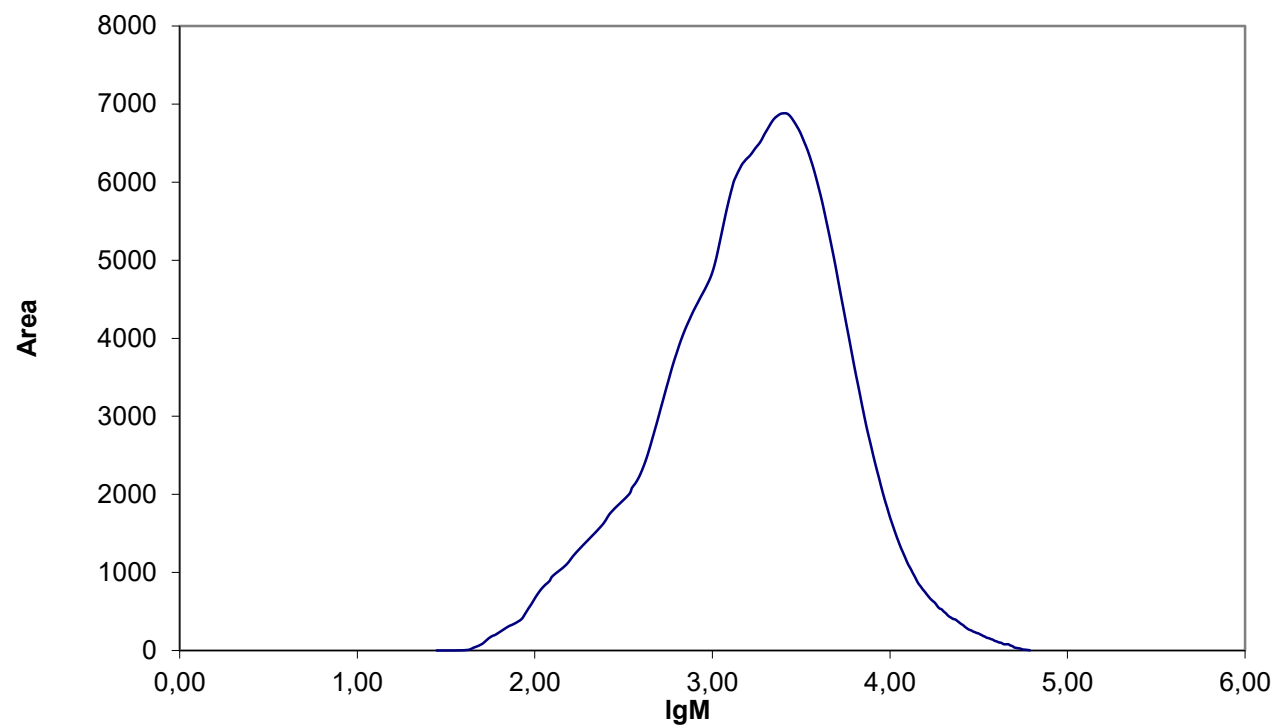


Figure S 19. GPC of PIP sample (Table 1, entry 5).

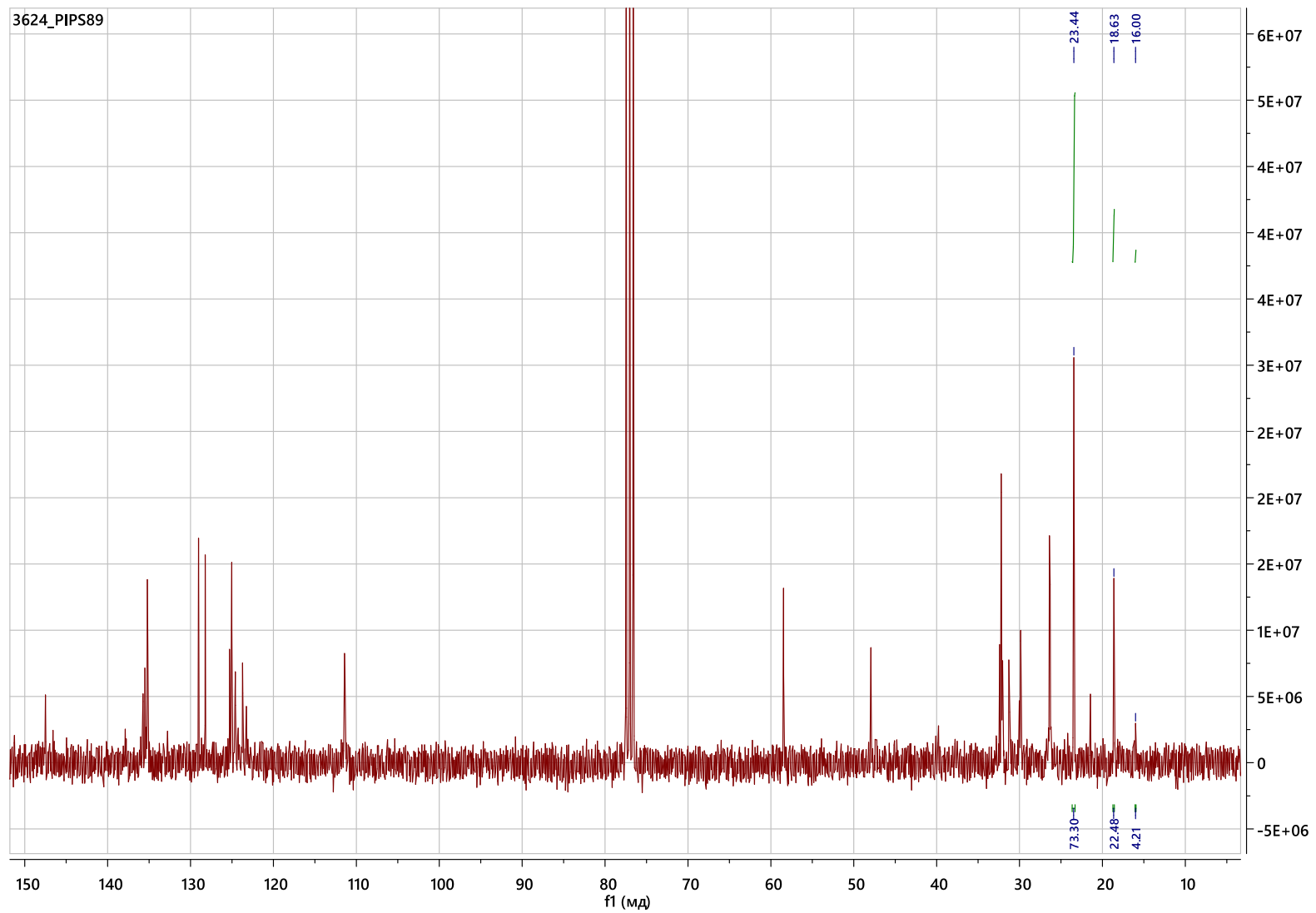


Figure S 20. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 5).

SEC Summary information

S 2300/S 2400

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Processing Stop Time (min) = 8,600

Number of Slices = 188

Weight Average Molecular Weight = 8264602

Number Average Molecular Weight = 976555

Z Average Molecular Weight = 35667725

Z+1 Average Molecular Weight = 62126591

Polydispersity index = 8,463

Peak Molecular Weight = 3293592

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Z+1 Average / Weight Average = 7,517

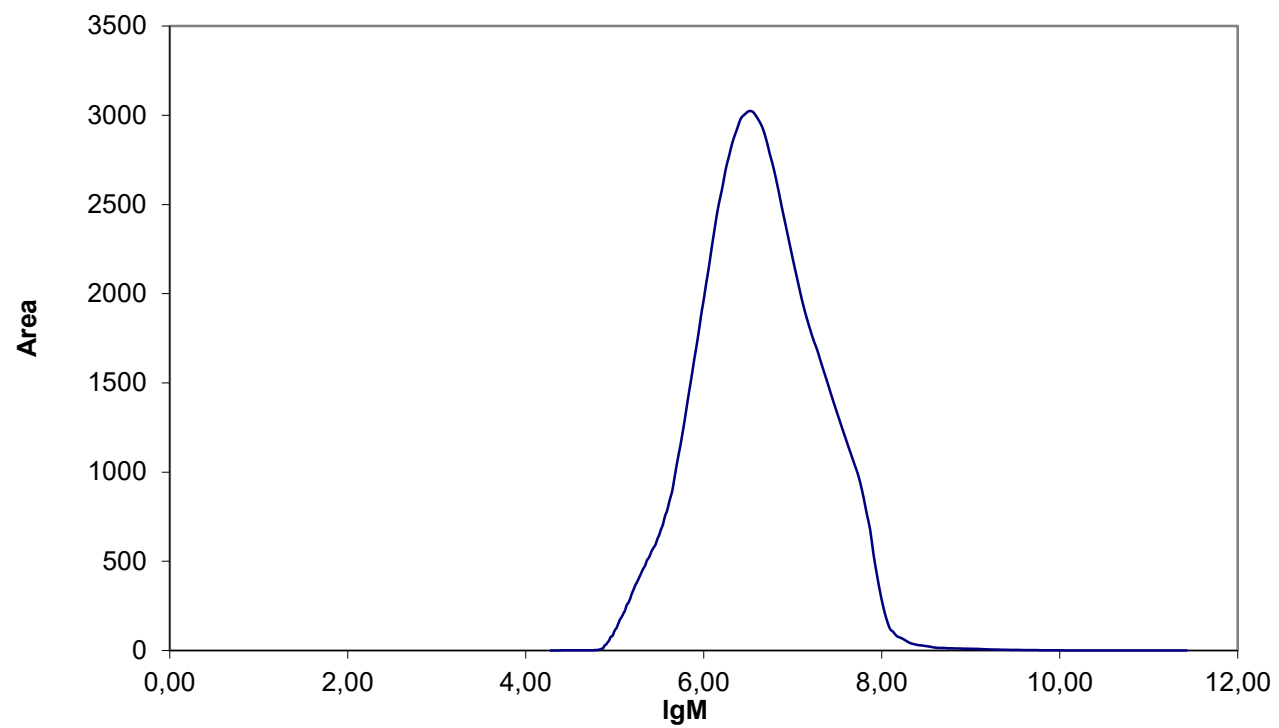


Figure S 21. GPC of PIP sample (Table 1, entry 7).

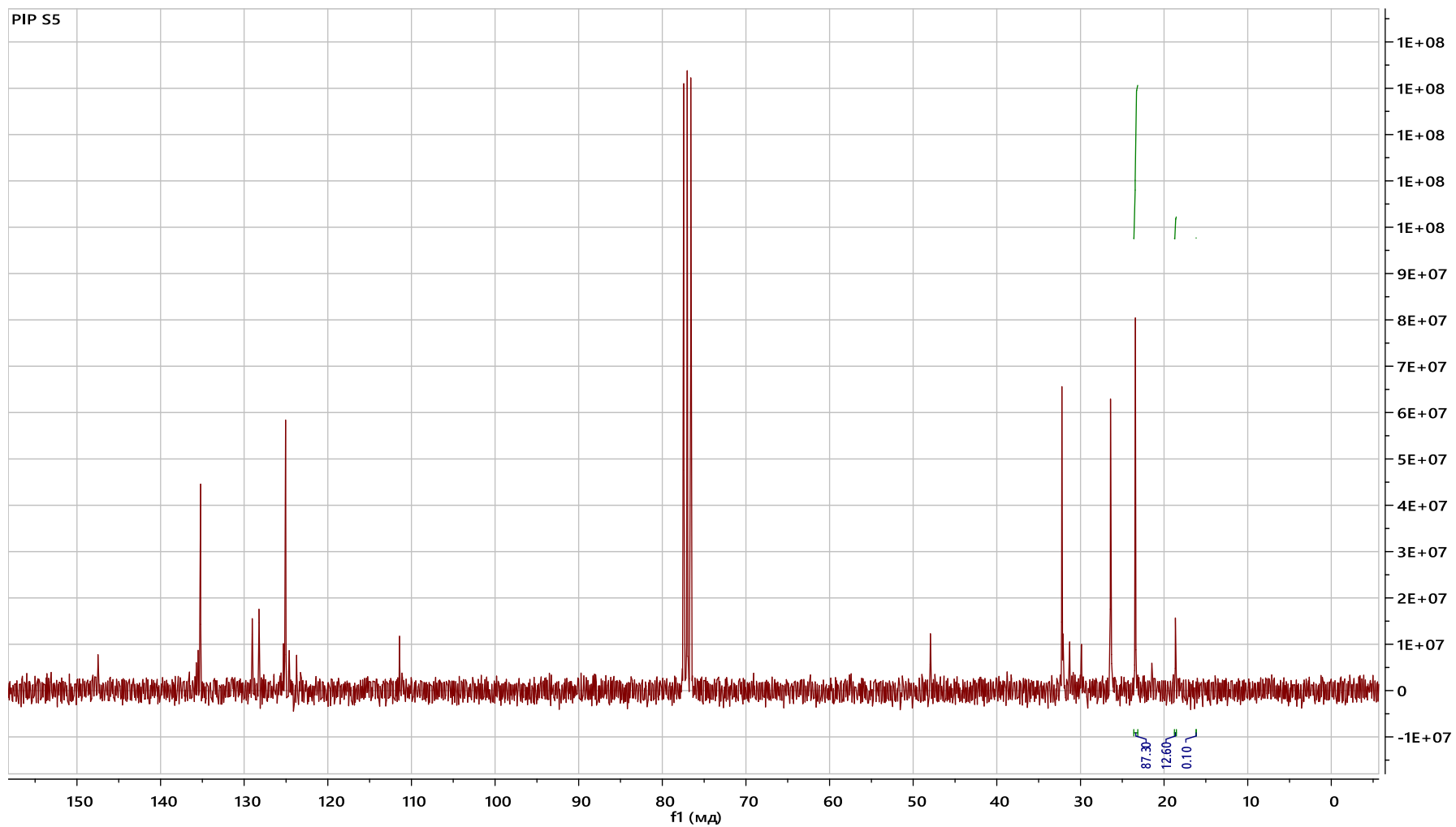


Figure S 22. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 7).

SEC Summary information

S 2300/S 2400

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Processing Stop Time (min) = 9,058

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Number Average Molecular Weight = 990610

Z Average Molecular Weight = 20115327

Z+1 Average Molecular Weight = 3131020

Polydispersity index = 7,810

Peak Molecular Weight = 3451922

Z Average / Weight Average = 2,600

Z+1 Average / Weight Average = 4,047

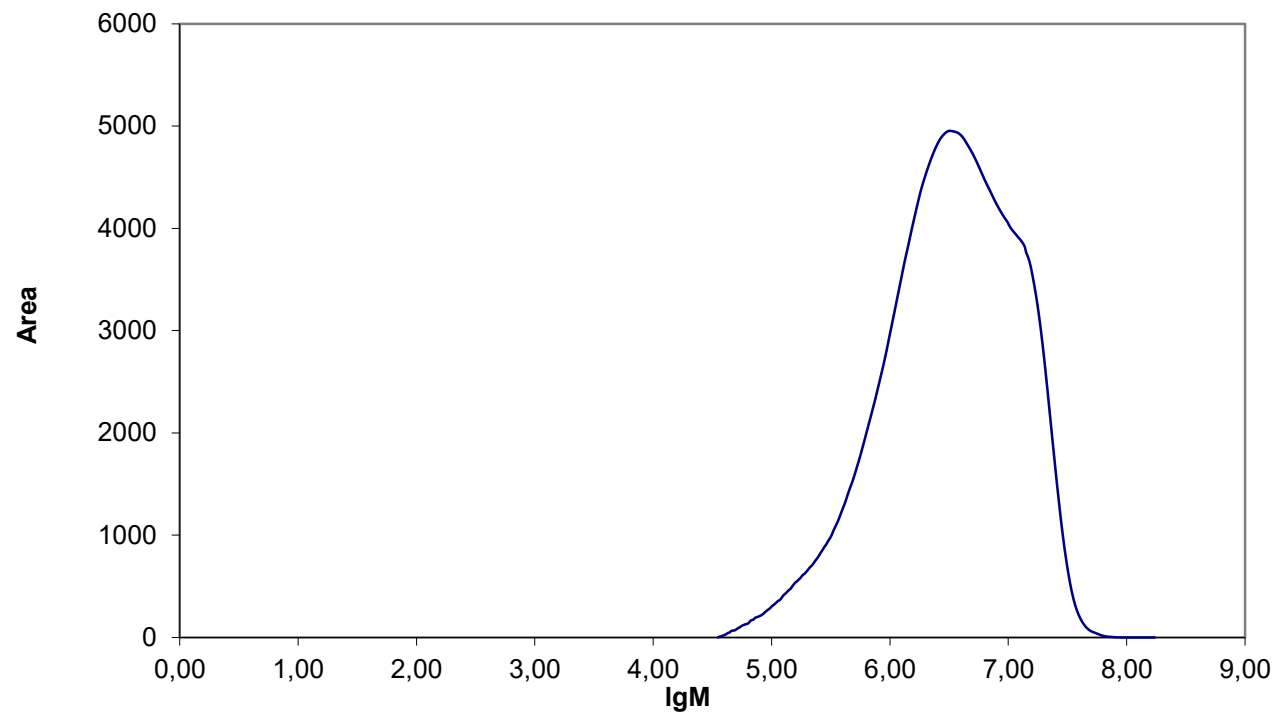


Figure S 23. GPC of PIP sample (Table 1, entry 8).

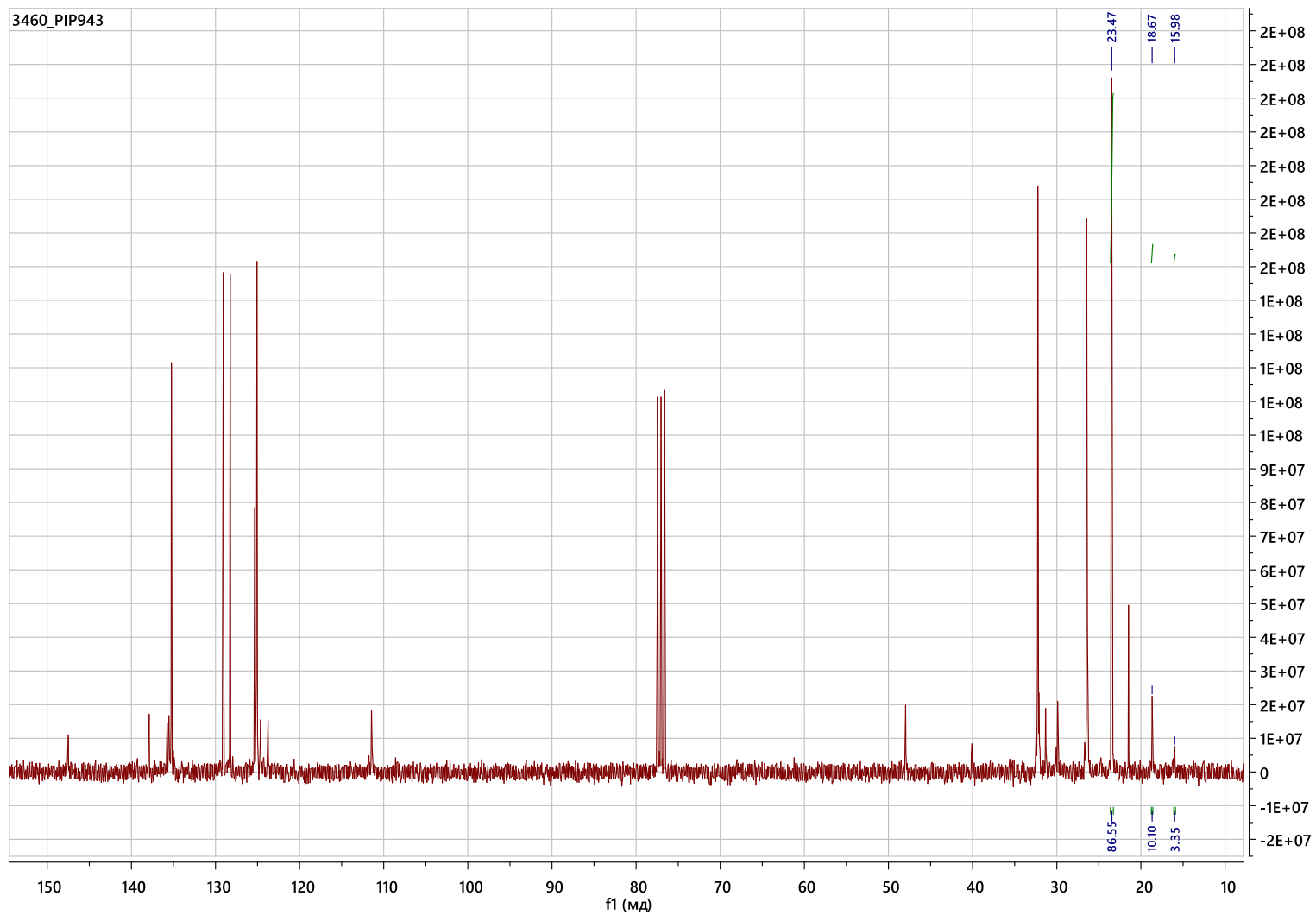


Figure S 24. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 8).

SEC Summary information

S 2300/S 2400

Processing Start Time (min) = 7,479

Processing Stop Time (min) = 11,385

Number of Slices = 234

Weight Average Molecular Weight = 23491

Number Average Molecular Weight = 6231

Z Average Molecular Weight = 42446

Z+1 Average Molecular Weight = 60975

Polydispersity index = 3,770

Peak Molecular Weight = 19589

Z Average / Weight Average = 1,807

Z+1 Average / Weight Average = 2,596

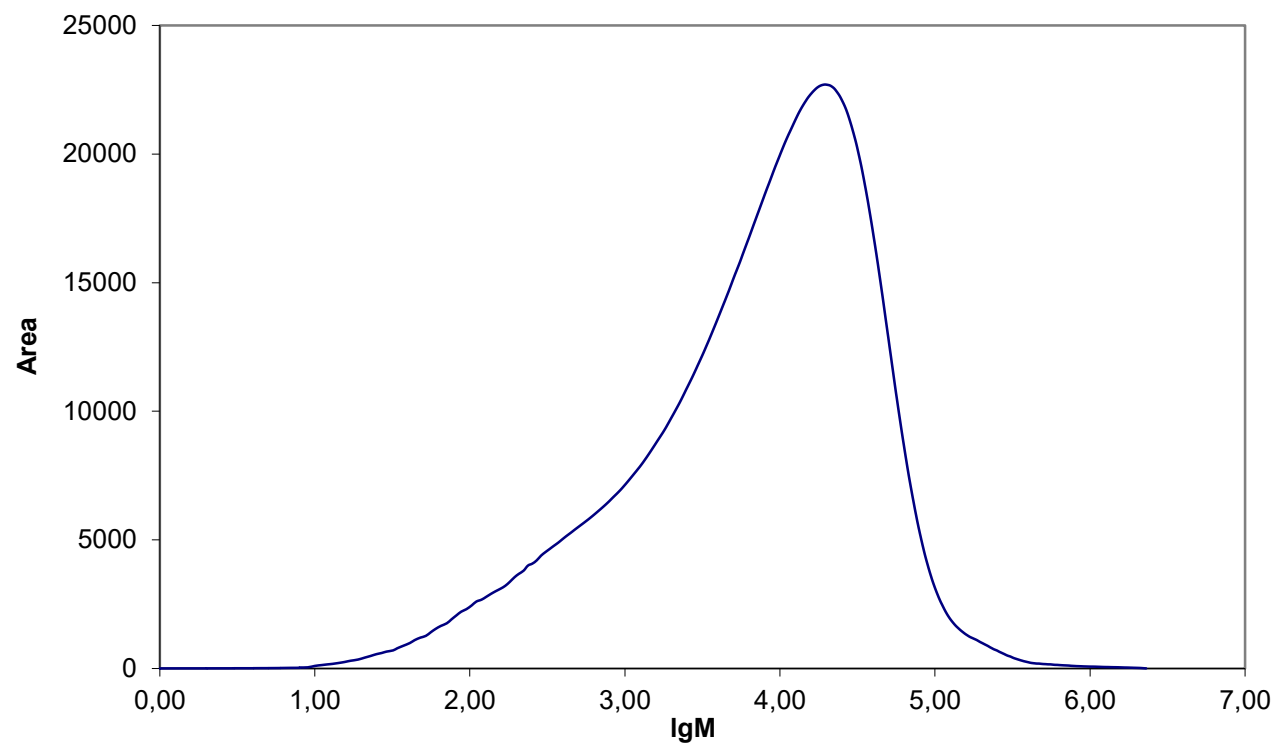


Figure S 25. GPC of PIP sample (Table 1, entry 10).

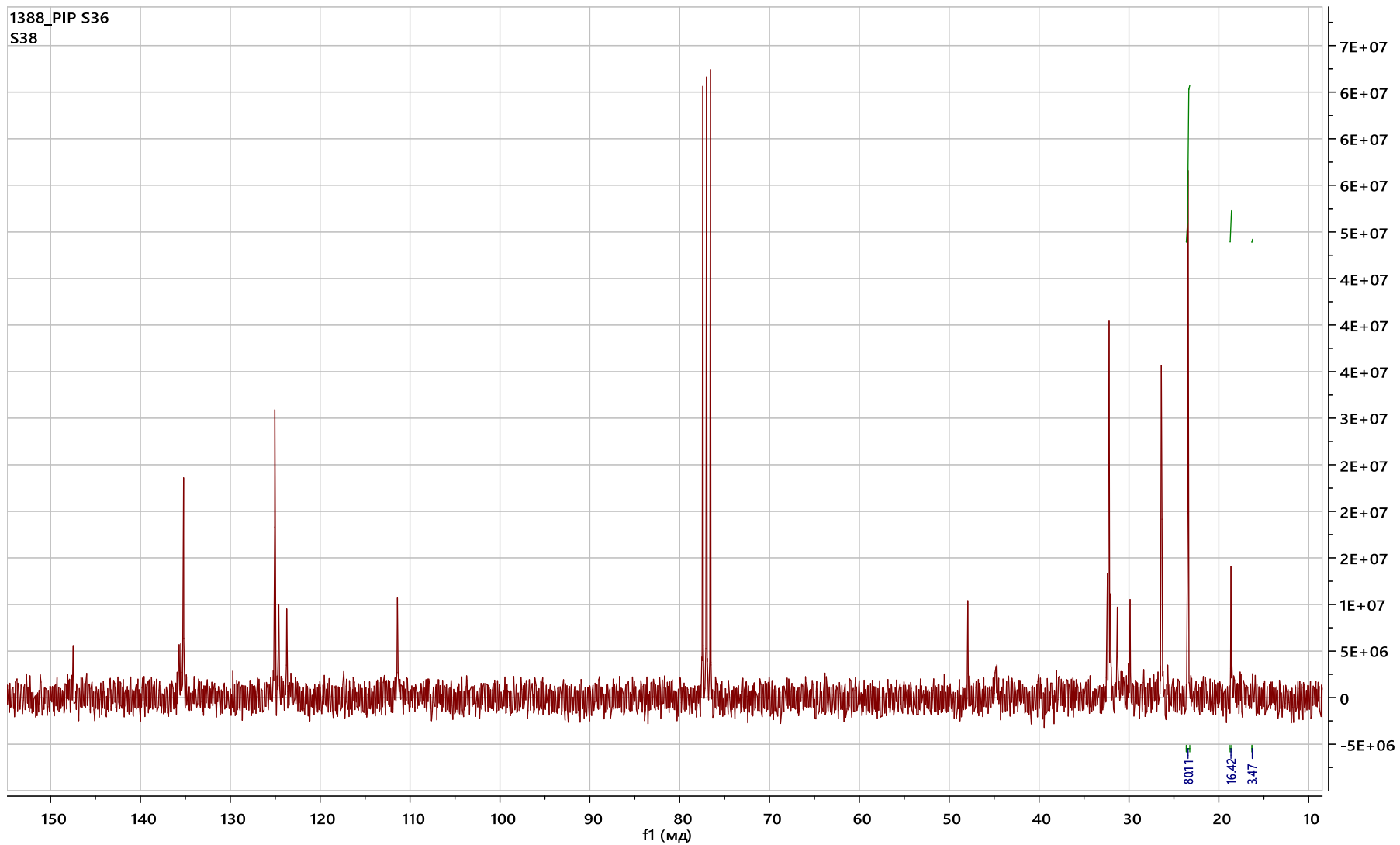


Figure S 26. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 10).

SEC Summary information

S 2300/S 2400

Processing Start Time (min) = 12,012

Processing Stop Time (min) = 15,099

Number of Slices = 185

Weight Average Molecular Weight = 9030

Number Average Molecular Weight = 5596

Z Average Molecular Weight = 12564

Z+1 Average Molecular Weight = 15905

Polydispersity index = 1,614

Peak Molecular Weight = 7507

Z Average / Weight Average = 1,391

Z+1 Average / Weight Average = 1,761

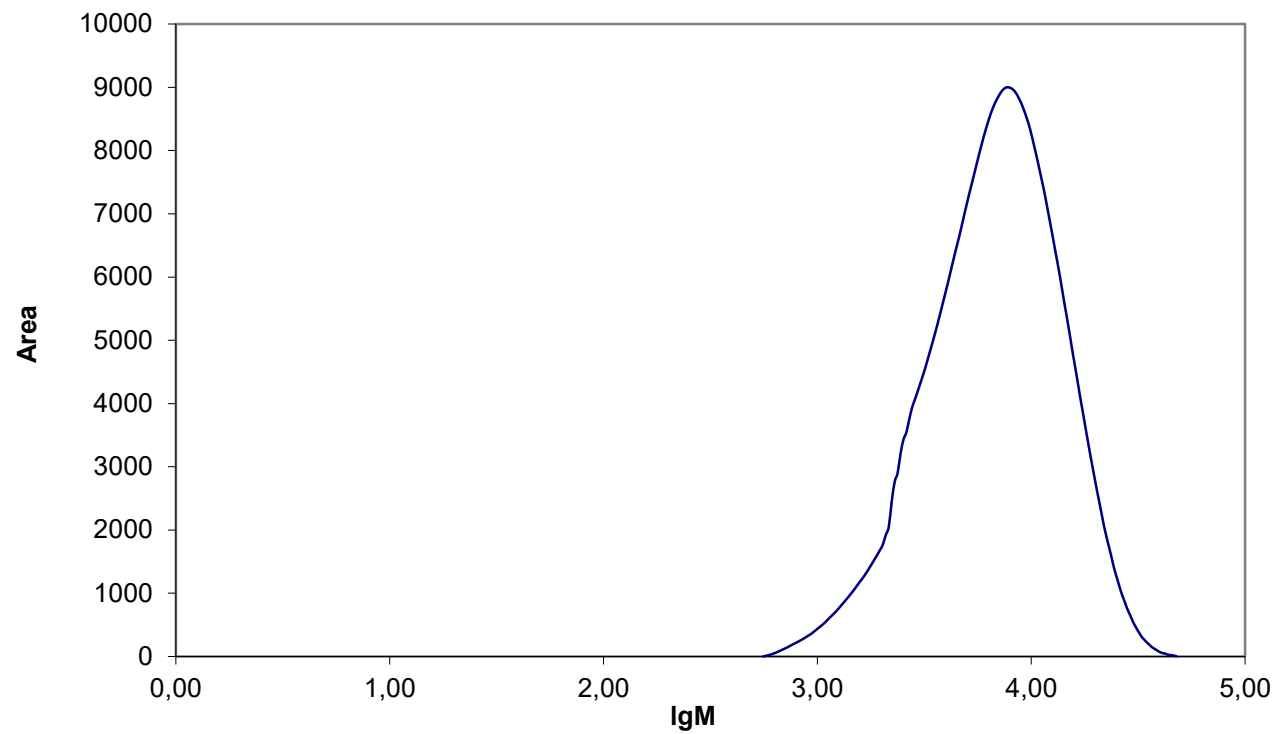


Figure S 27. GPC of PIP sample (Table 1, entry 11).

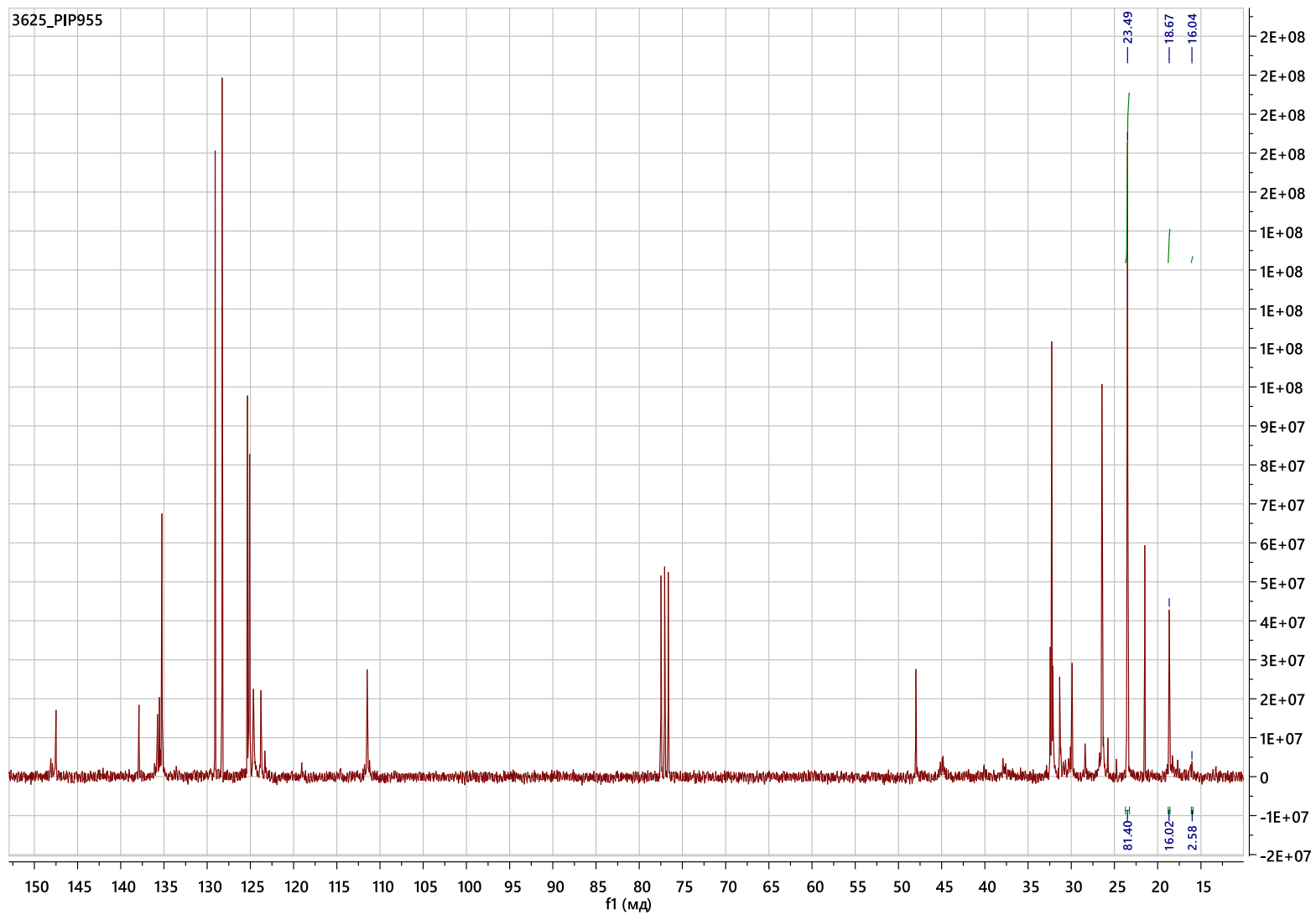


Figure S 28. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 11).

SEC Summary information

S 2300/S 2400

Processing Start Time (min) = 5,435

Processing Stop Time (min) = 8,301

Number of Slices = 172

Weight Average Molecular Weight = 3169399

Number Average Molecular Weight = 668809

Z Average Molecular Weight = 13965628

Z+1 Average Molecular Weight = 31120891

Polydispersity index = 4,739

Peak Molecular Weight = 1403981

Z Average / Weight Average = 4,406

Z+1 Average / Weight Average = 9,819

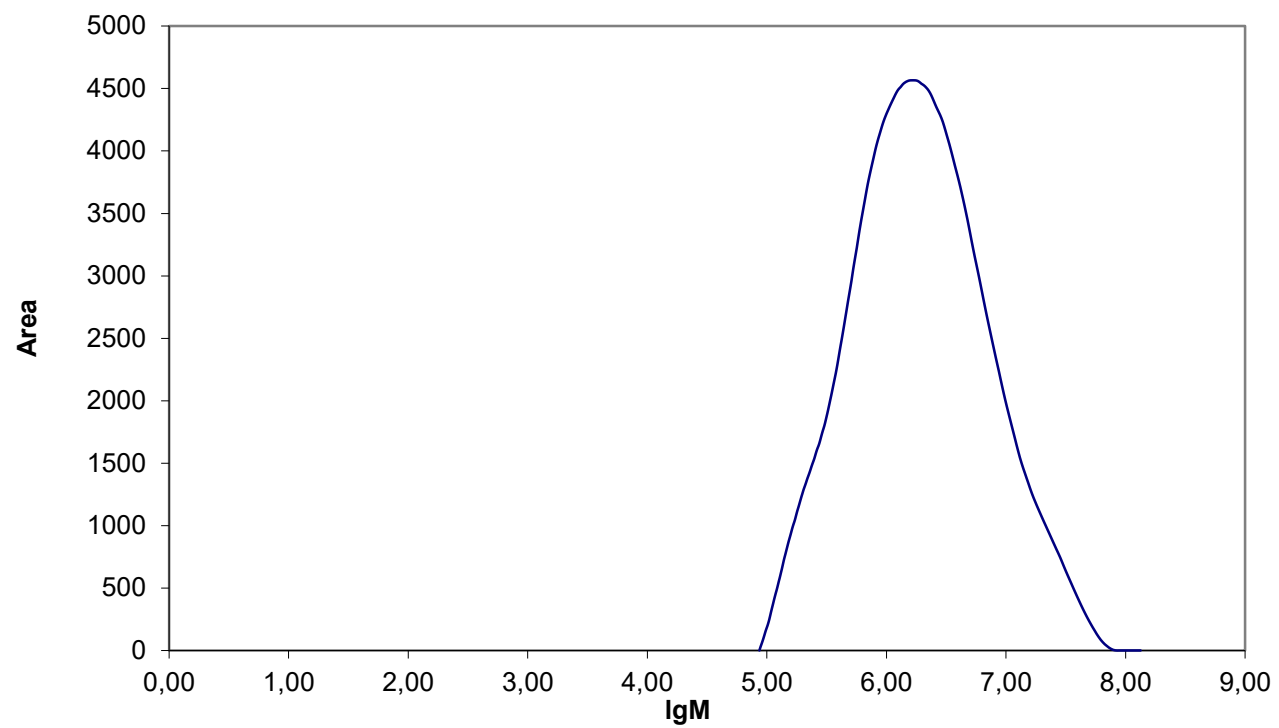


Figure S 29. GPC of PIP sample (Table 1, entry 15).

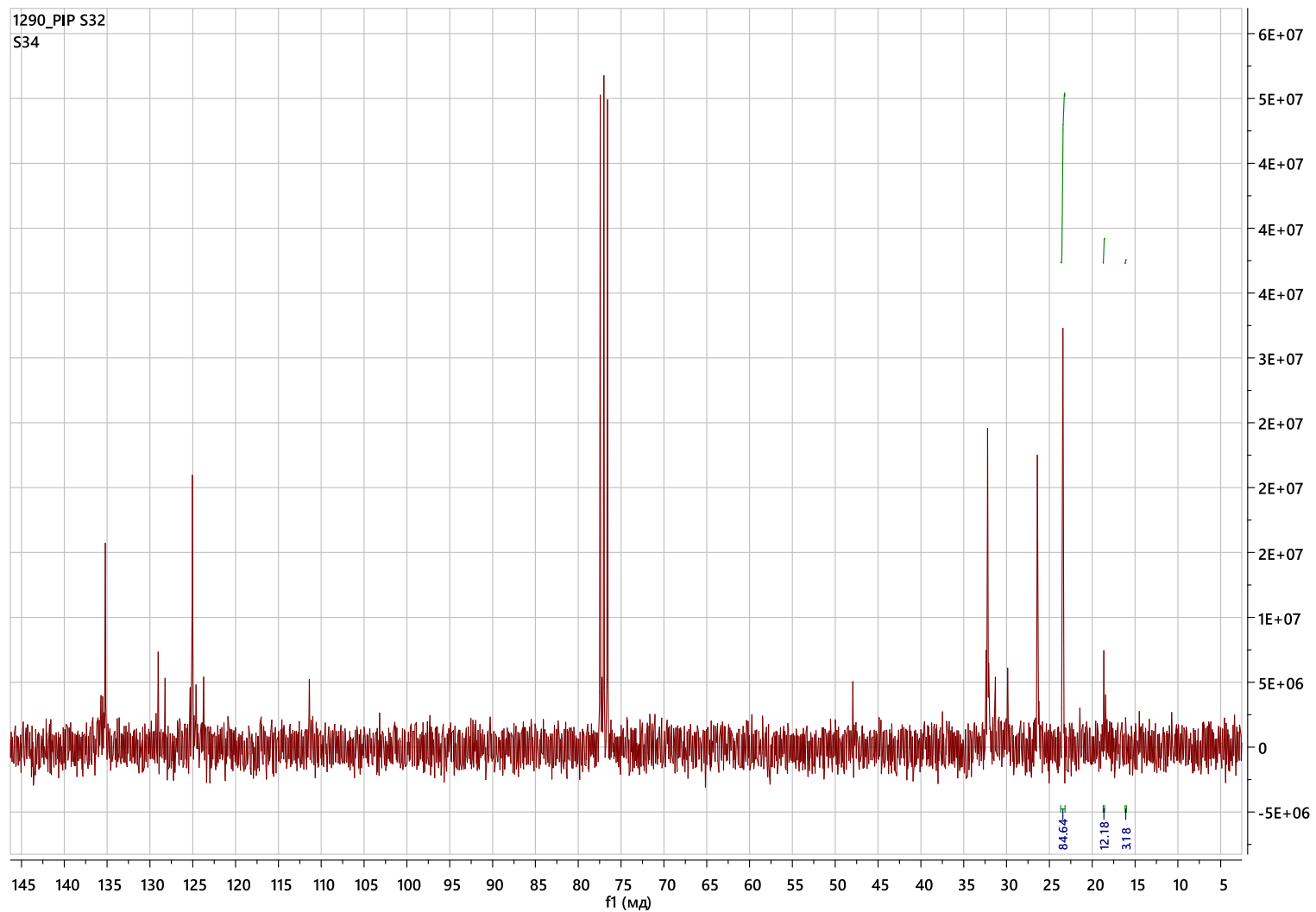


Figure S 30. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 15).

SEC Summary information

S 2300/S 2400

Processing Start Time (min) = 5,685

Processing Stop Time (min) = 8,182

Number of Slices = 150

Weight Average Molecular Weight = 1909911

Number Average Molecular Weight = 690318

Z Average Molecular Weight = 5114144

Z+1 Average Molecular Weight = 10492767

Polydispersity index = 2,767

Peak Molecular Weight = 1344801

Z Average / Weight Average = 2,678

Z+1 Average / Weight Average = 5,494

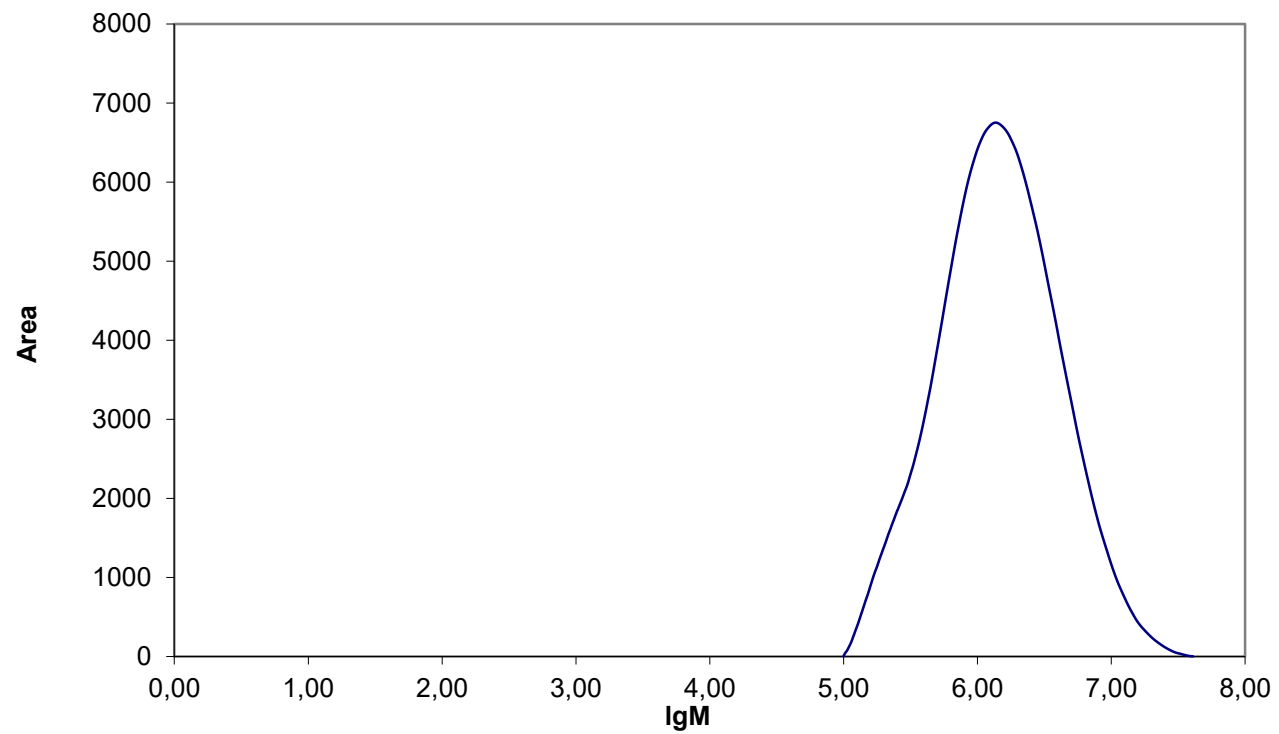


Figure S 31. GPC of PIP sample (Table 1, entry 16).

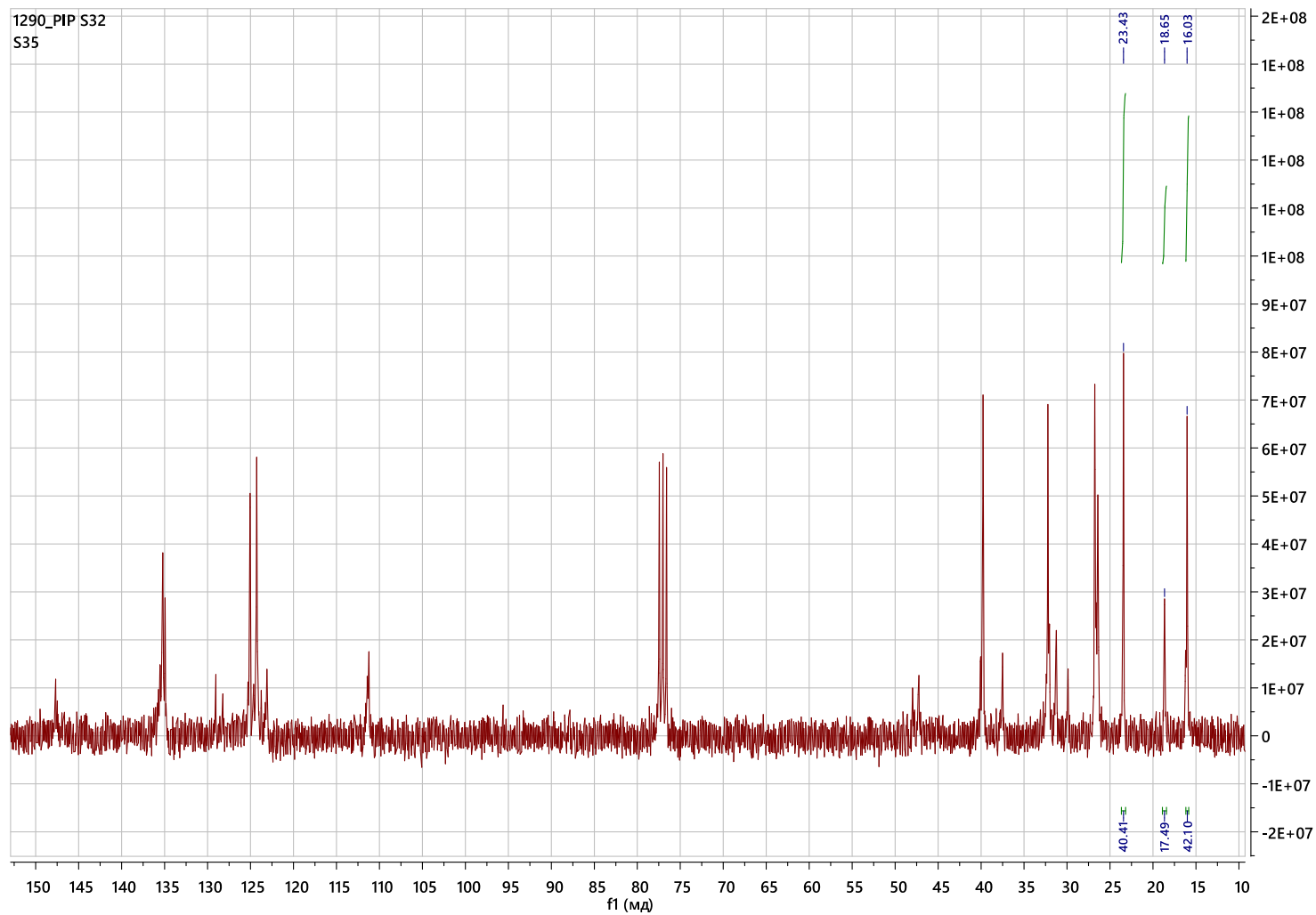


Figure S 32. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 16).

SEC Summary information

S 2300/S 2400

Processing Start Time (min) = 5,387

Processing Stop Time (min) = 8,863

Number of Slices = 209

Weight Average Molecular Weight = 2939503

Number Average Molecular Weight = 535126

Z Average Molecular Weight = 13569322

Z+1 Average Molecular Weight = 34839903

Polydispersity index = 5,493

Peak Molecular Weight = 1920848

Z Average / Weight Average = 4,616

Z+1 Average / Weight Average = 11,852

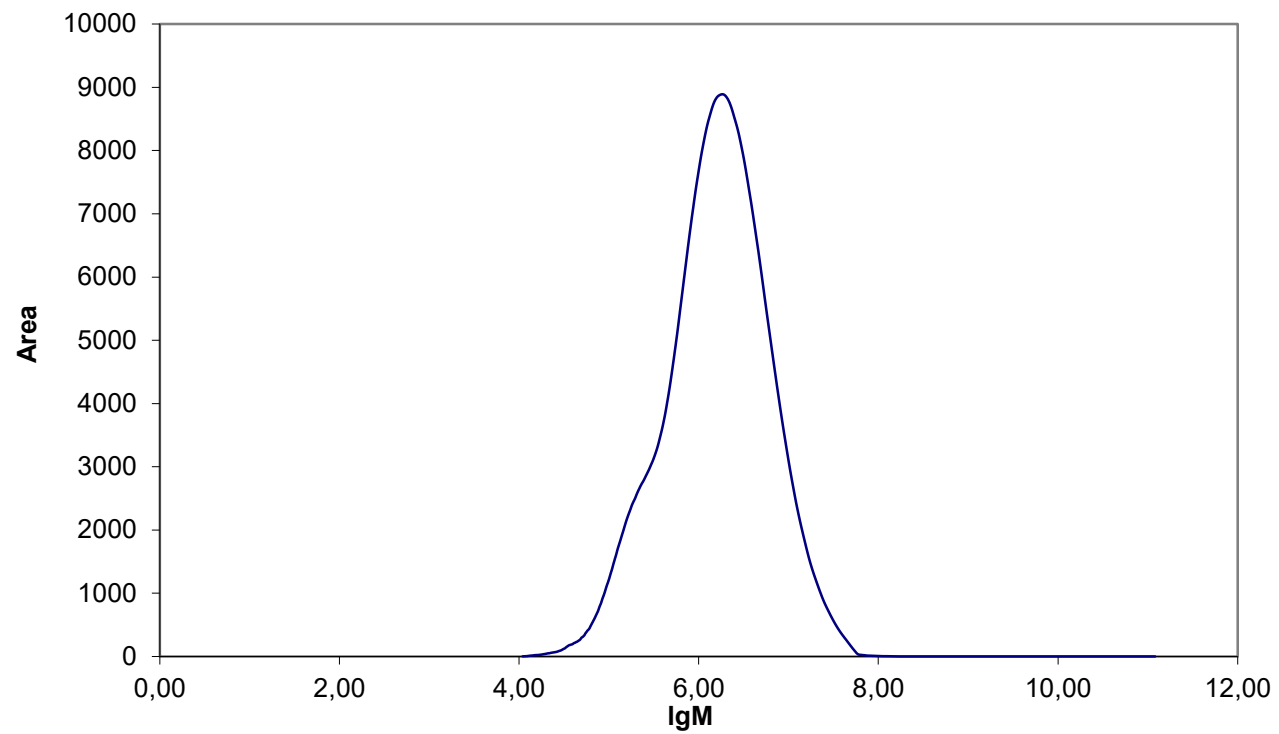


Figure S 33. GPC of PIP sample (Table 1, entry 17).

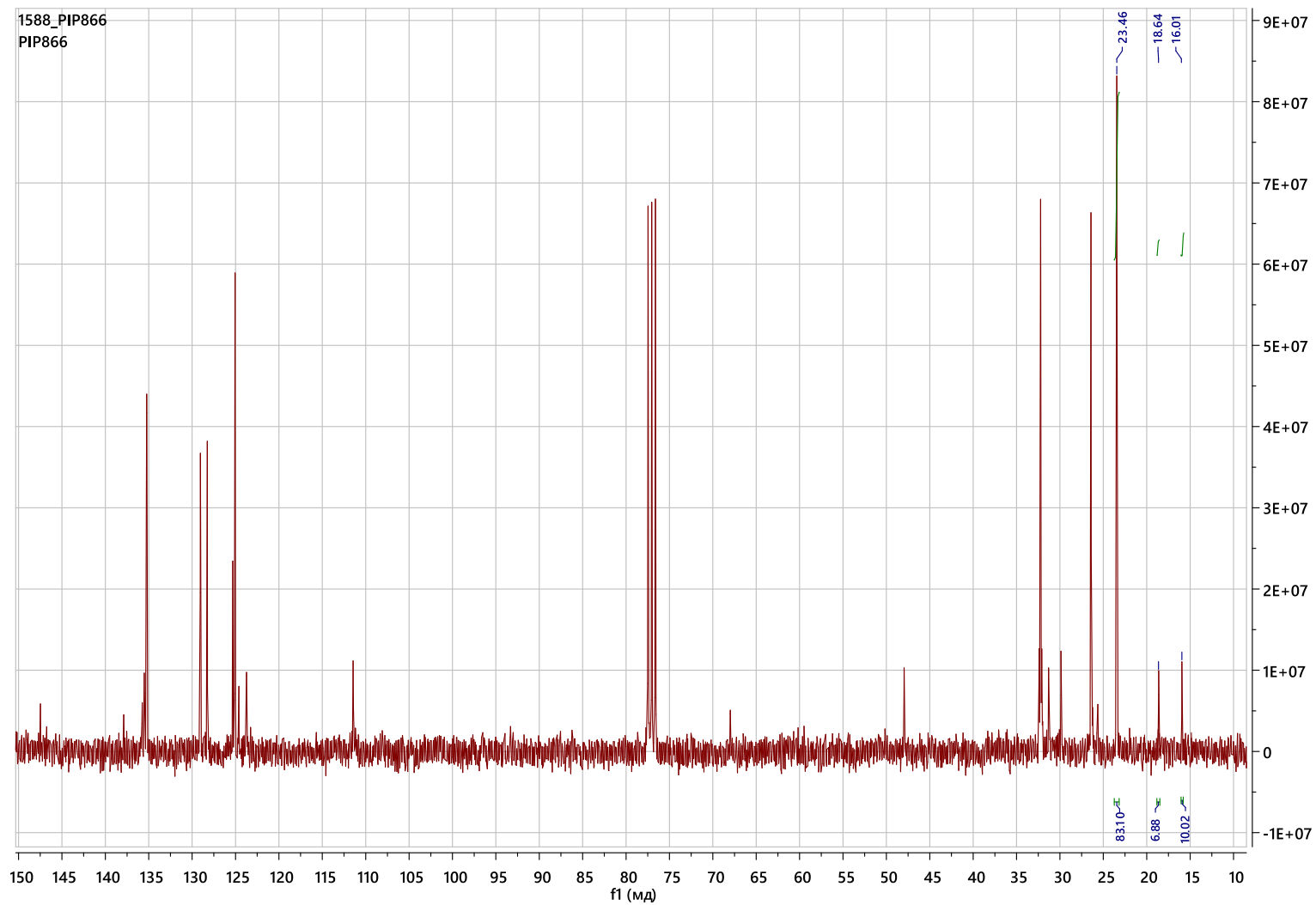


Figure S 34. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of PIP sample (Table 1, entry 17).

SEC Summary information

S 2300/S 2400

Processing Start Time (min) = 8,363

Processing Stop Time (min) = 10,704

Number of Slices = 141

Weight Average Molecular Weight = 24500

Number Average Molecular Weight = 11690

Z Average Molecular Weight = 35305

Z+1 Average Molecular Weight = 42916

Polydispersity index = 2,096

Peak Molecular Weight = 3230

Z Average / Weight Average = 1,441

Z+1 Average / Weight Average = 1,752

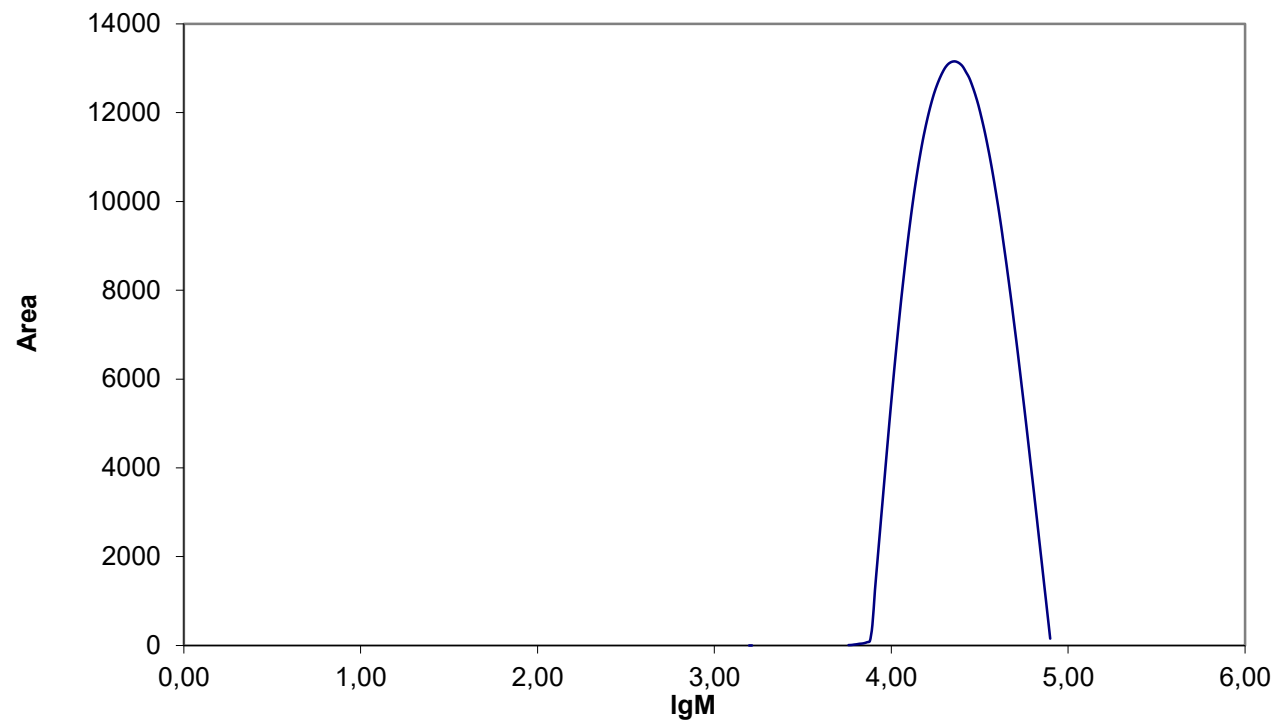


Figure S 35. GPC of polyheptene sample (Table 2, entry 2).

SEC Summary information

S 2300/S 2400

Processing Start Time(min) = 5,782

Processing Stop Time(min) = 9,986

Number of Slices = 252

Weight Average Molecular Weight = 720588

Number Average Molecular Weight = 156512

Z Average Molecular Weight = 2953846

Z+1 Average Molecular Weight = 6810021

Polydispersity index = 4,604

Peak Molecular Weight = 519817

Z Average / Weight Average = 4,099

Z+1 Average / Weight Average = 9,451

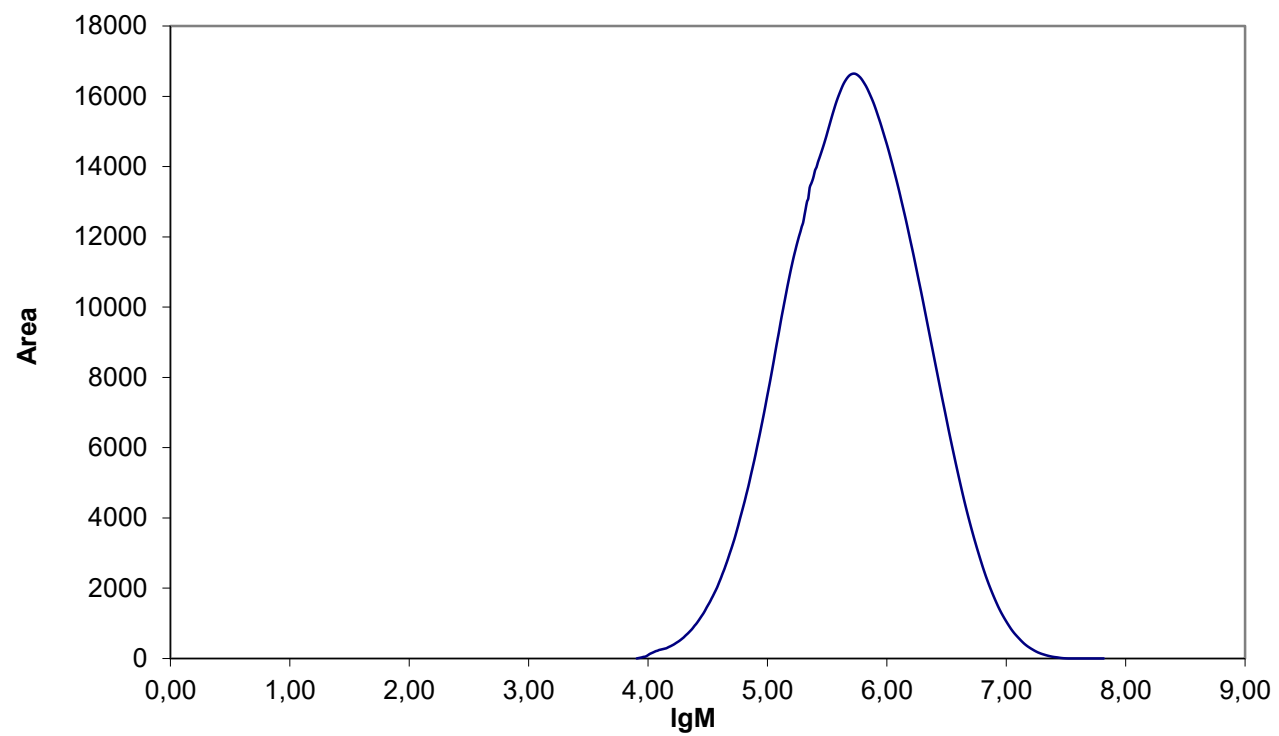


Figure S 36. GPC of polyheptene sample (Table 2, entry 3).

S 2300/S 2400

Processing Start Time (min) = 5,698

Processing Stop Time (min) = 9,616

Number of Slices = 235

Weight Average Molecular Weight = 737535

Number Average Molecular Weight = 190201

Z Average Molecular Weight = 2636200

Z+1 Average Molecular Weight = 7636250

Polydispersity index = 3,878

Peak Molecular Weight = 617365

Z Average / Weight Average = 3,574

Z+1 Average / Weight Average = 10,354

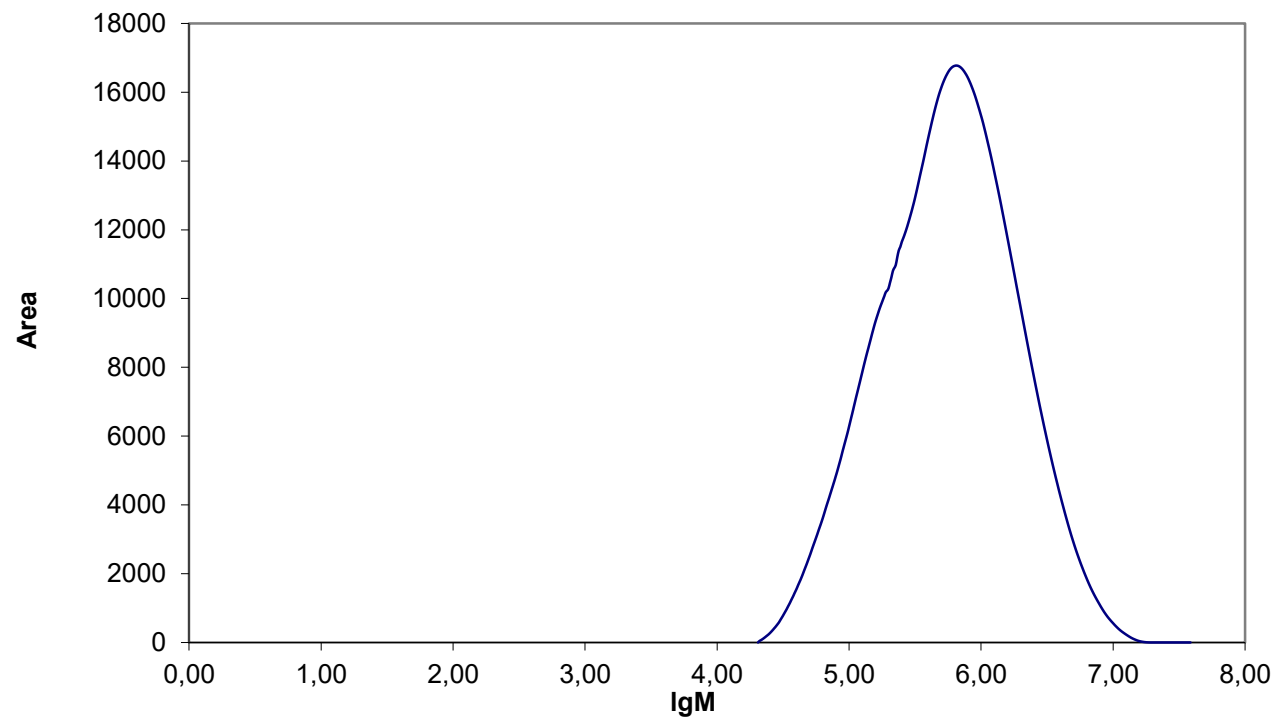


Figure S 37. GPC of polyheptene sample (Table 2, entry 4).

S 2300/S 2400

Processing Start Time (min) = 10,727

Processing Stop Time (min) = 12,293

Number of Slices = 94

Weight Average Molecular Weight = 2693

Number Average Molecular Weight = 1736

Z Average Molecular Weight = 4732

Z+1 Average Molecular Weight = 7131

Polydispersity index = 1,551

Peak Molecular Weight = 1486

Z Average / Weight Average = 1,757

Z+1 Average / Weight Average = 2,648

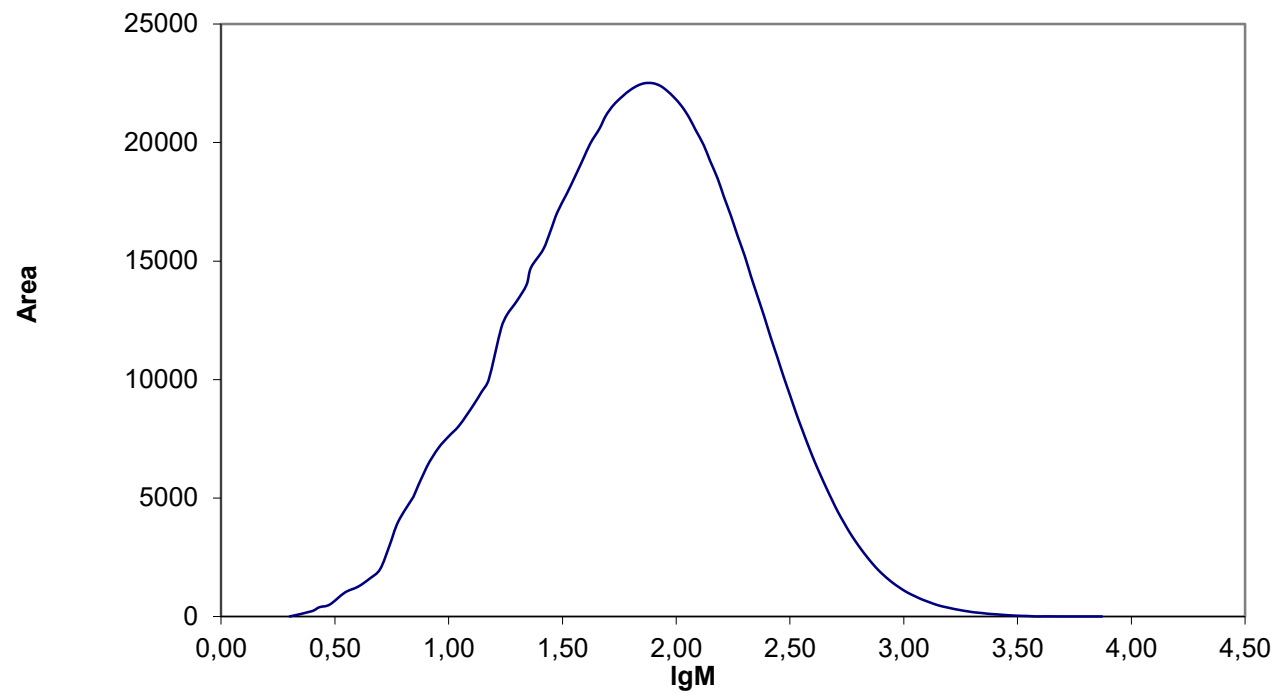


Figure S 38. GPC of polyheptene sample (Table 2, entry 6).

SEC Summary information

S 2300/S 2400

Processing Start Time(min) =	9,128
Processing Stop Time(min) =	12,487
Number of Slices =	202
Weight Average Molecular Weight =	8485
Number Average Molecular Weight =	3705
Z Average Molecular Weight =	16067
Z+1 Average Molecular Weight =	25478
Polydispersity index =	2,290
Peak Molecular Weight =	4406
Z Average / Weight Average =	1,893
Z+1 Average / Weight Average =	3,003

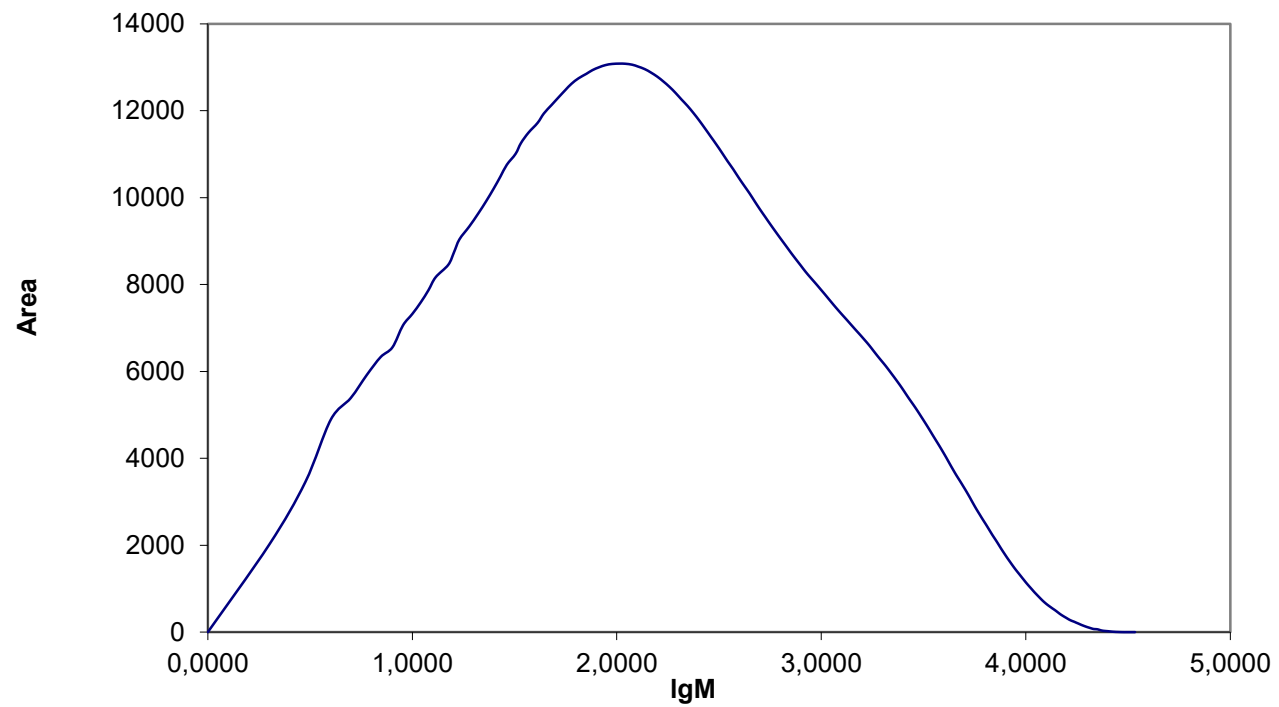


Figure S 39. GPC of polyheptene sample (Table 2, entry 8).