

Supporting Information

Chromium Complexes Supported by NNO-Tridentate Ligands: An Unprecedented Activity with the Requirement of a small amount of MAO

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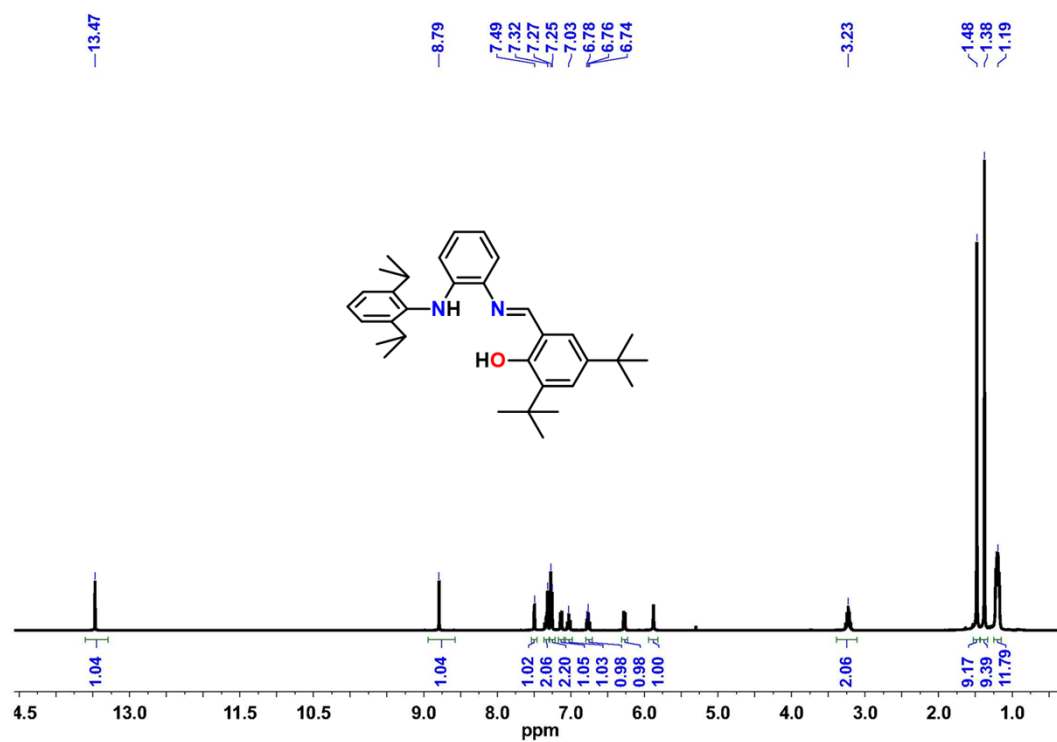


Figure S1. ¹H NMR spectrum of L1 in CDCl₃.

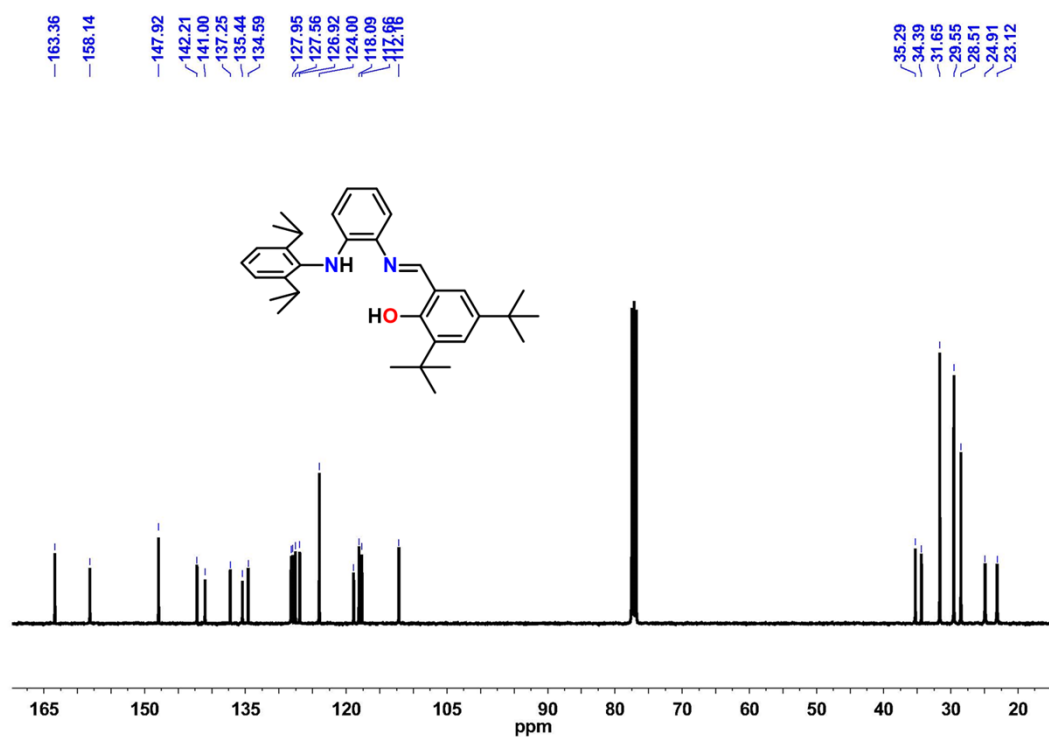


Figure S2. ¹³C NMR spectrum of L1 in CDCl₃.

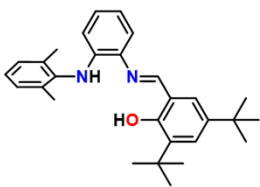


Figure S3. ^1H NMR spectrum of **L2** in CDCl_3 .

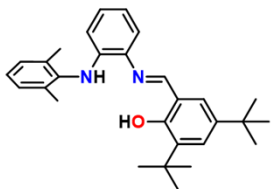


Figure S4. ^{13}C NMR spectrum of **L2** in CDCl_3 .

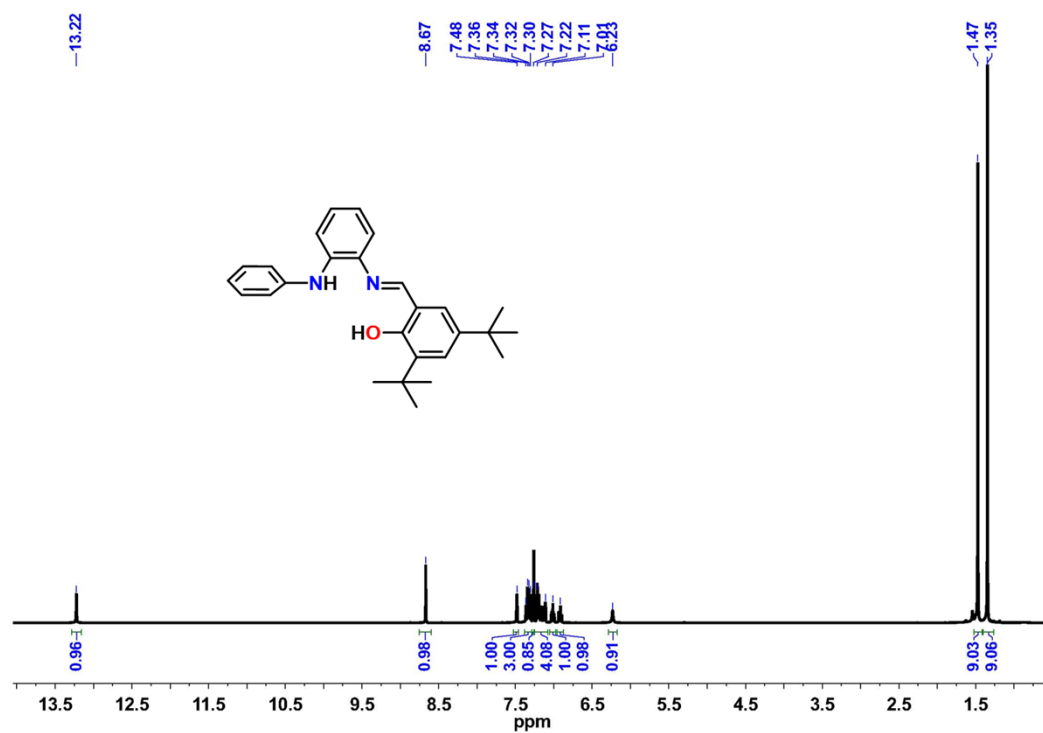


Figure S5. ¹H NMR spectrum of L3 in CDCl₃.

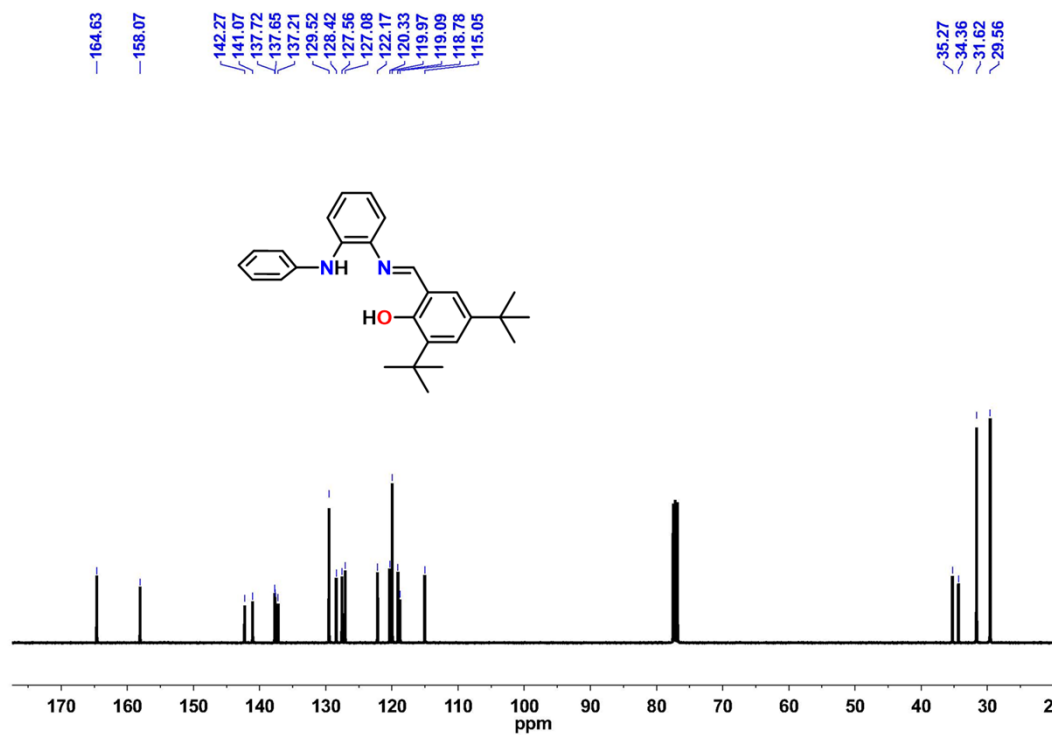


Figure S6. ¹³C NMR spectrum of L3 in CDCl₃.

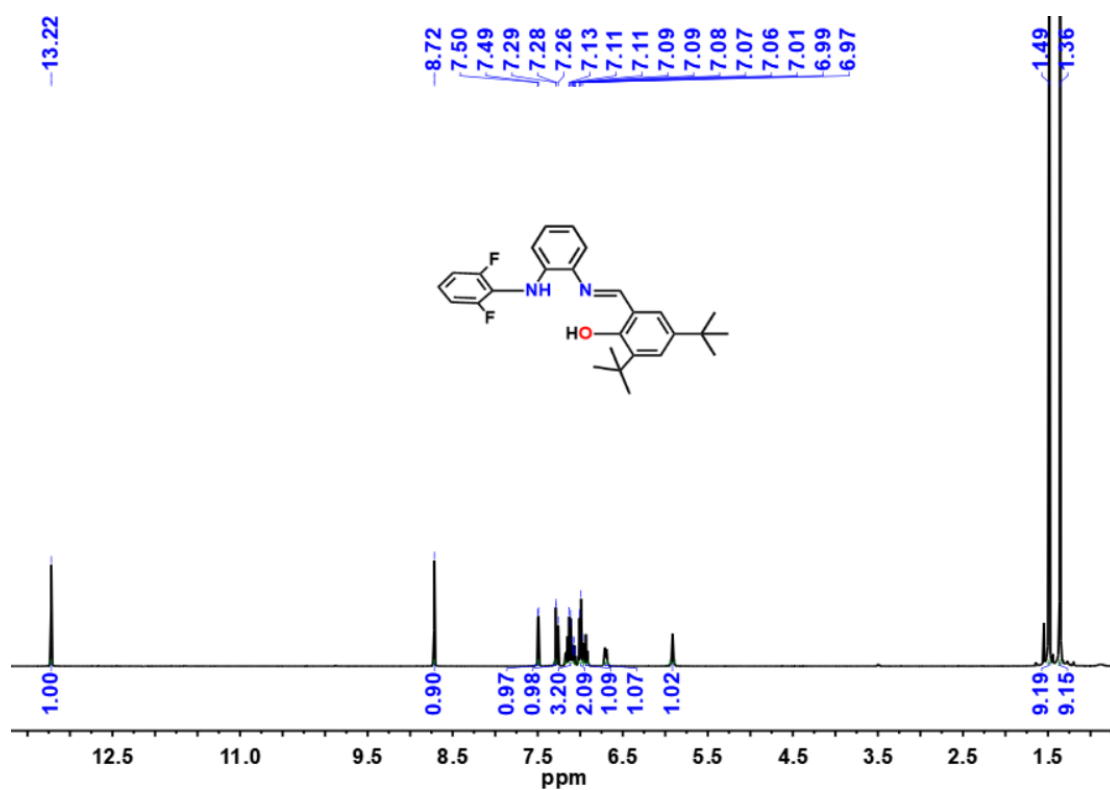


Figure S7. ¹H NMR spectrum of L4 in CDCl₃.

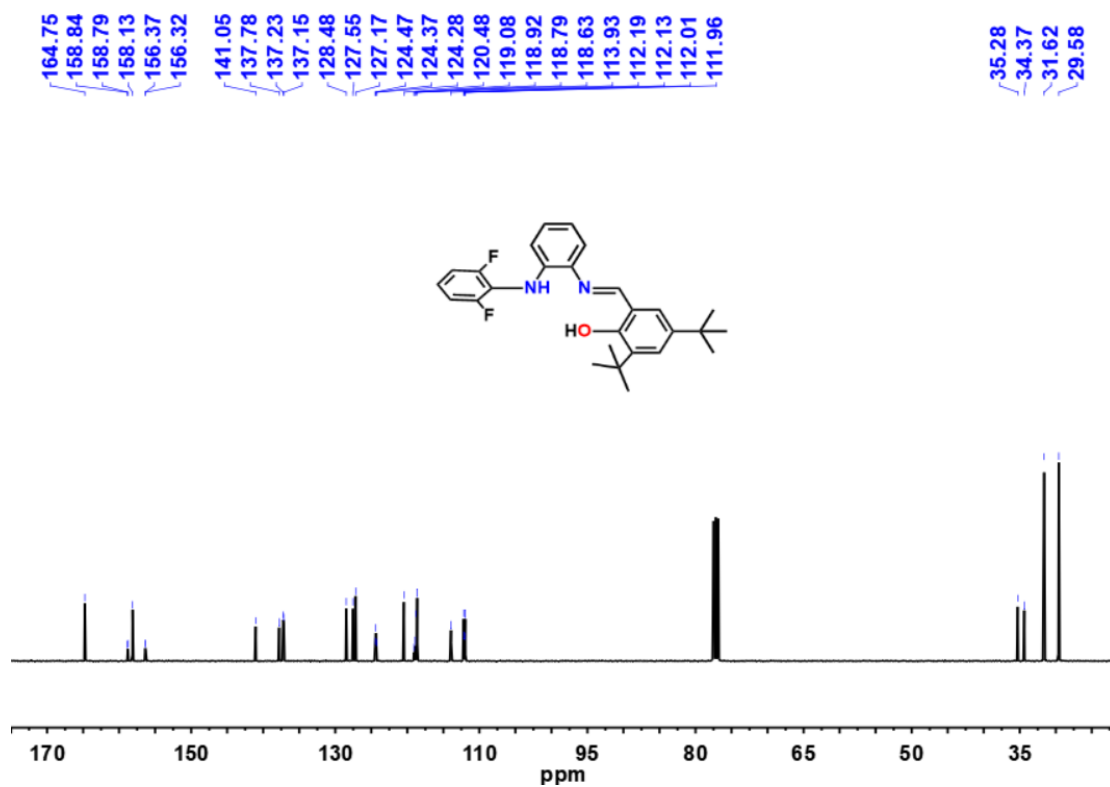


Figure S8. ¹³C NMR spectrum of L4 in CDCl₃.

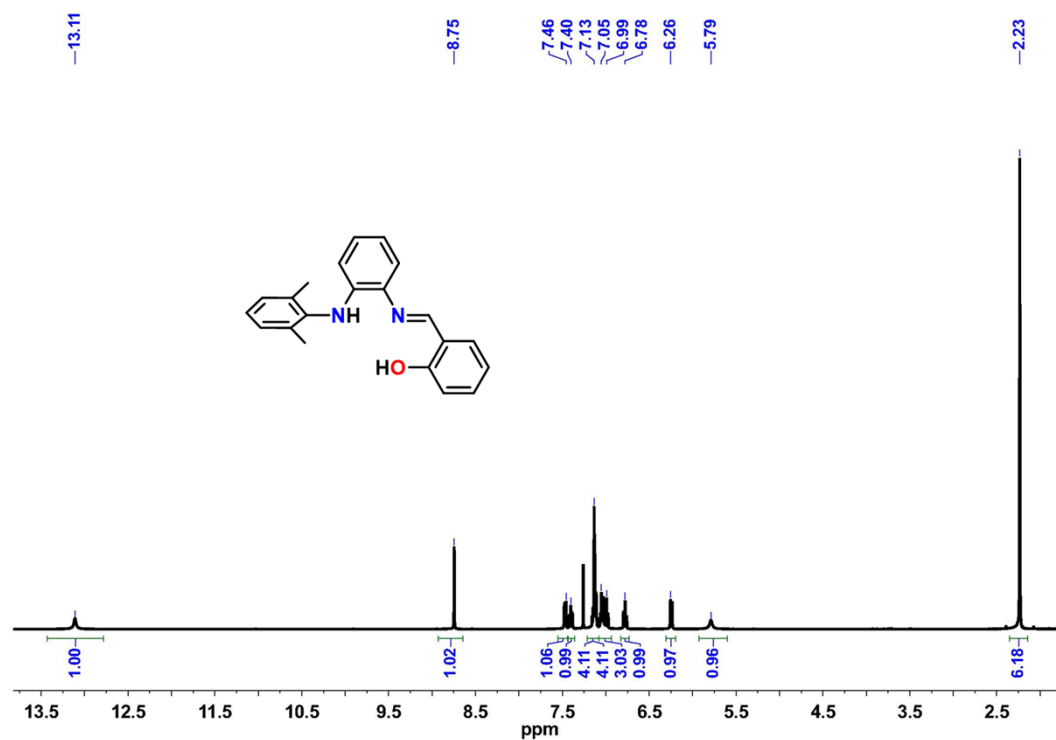


Figure S9. ¹H NMR spectrum of **L5** in CDCl₃.

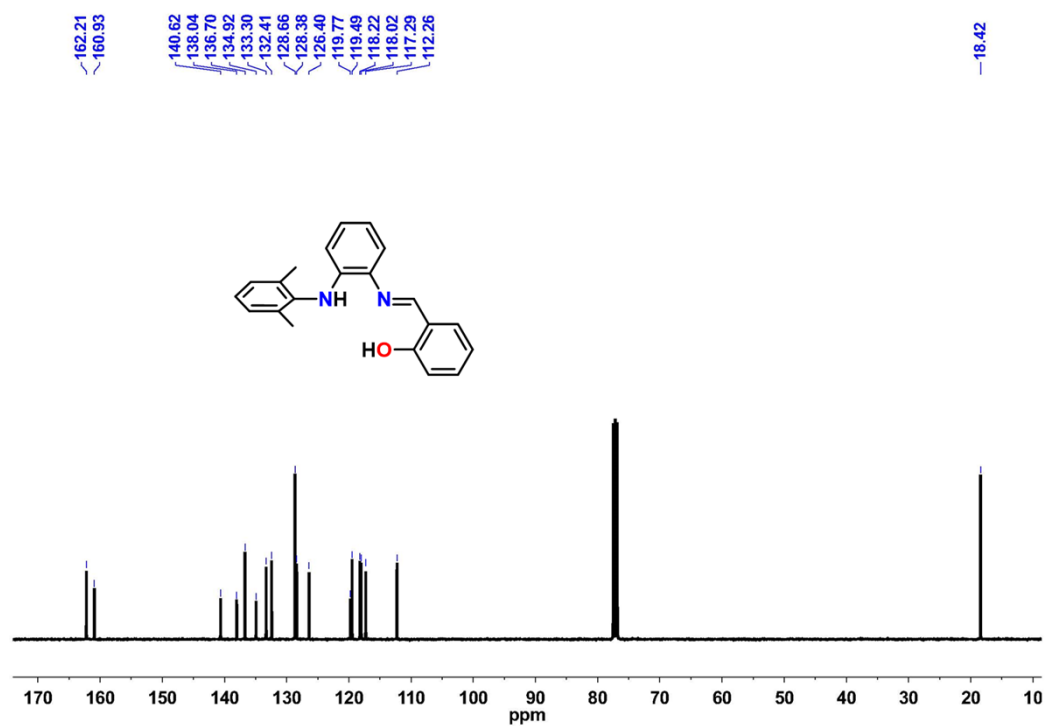


Figure S10. ¹³C NMR spectrum of **L5** in CDCl₃.

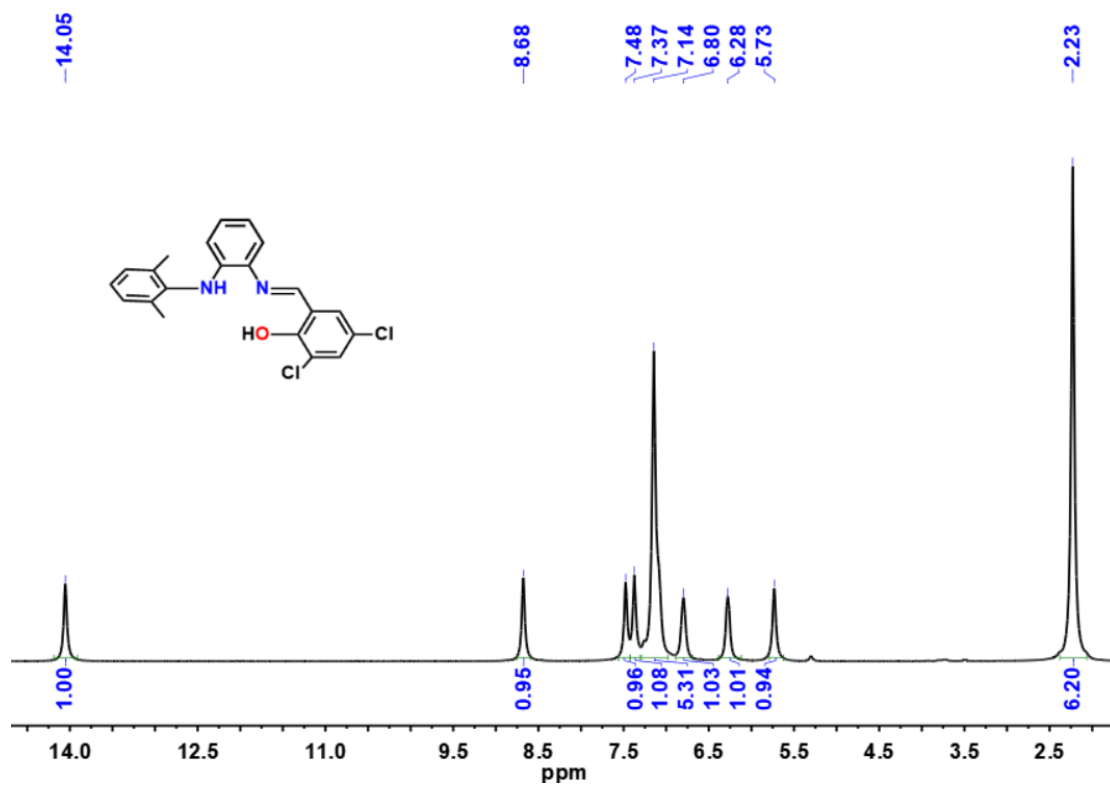


Figure S11. ^1H NMR spectrum of L6 in CDCl_3 .

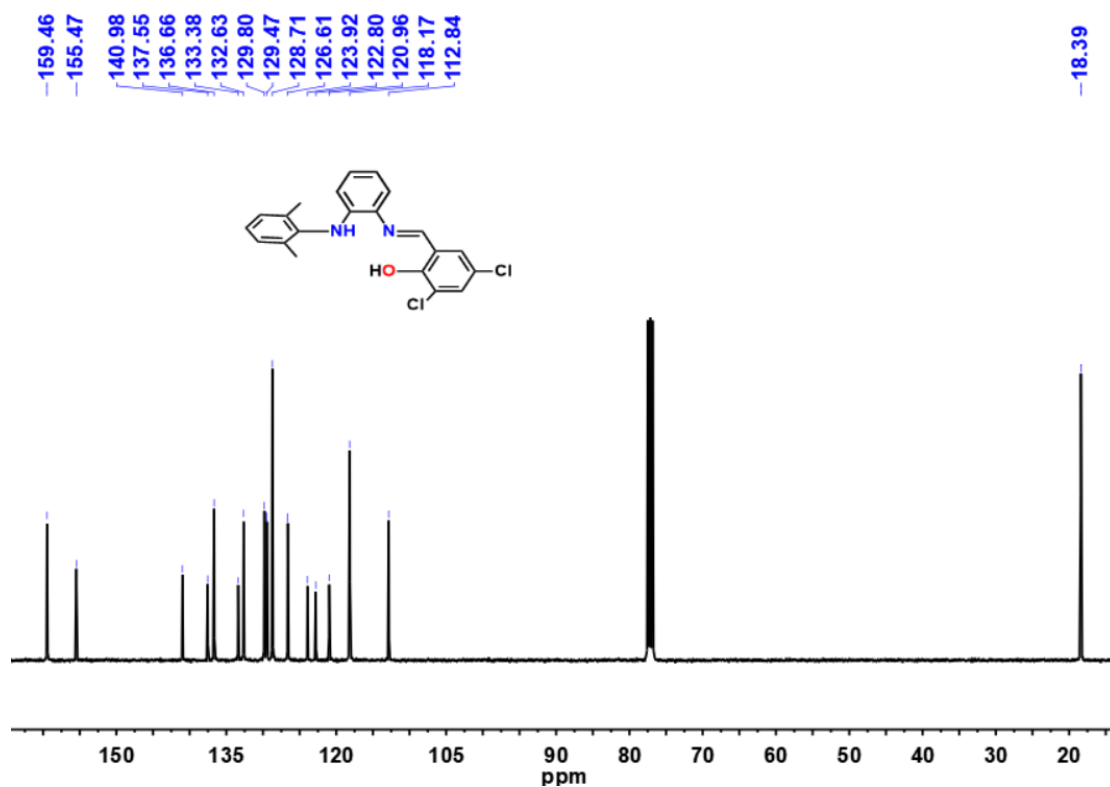


Figure S12. ^{13}C NMR spectrum of L6 in CDCl_3 .

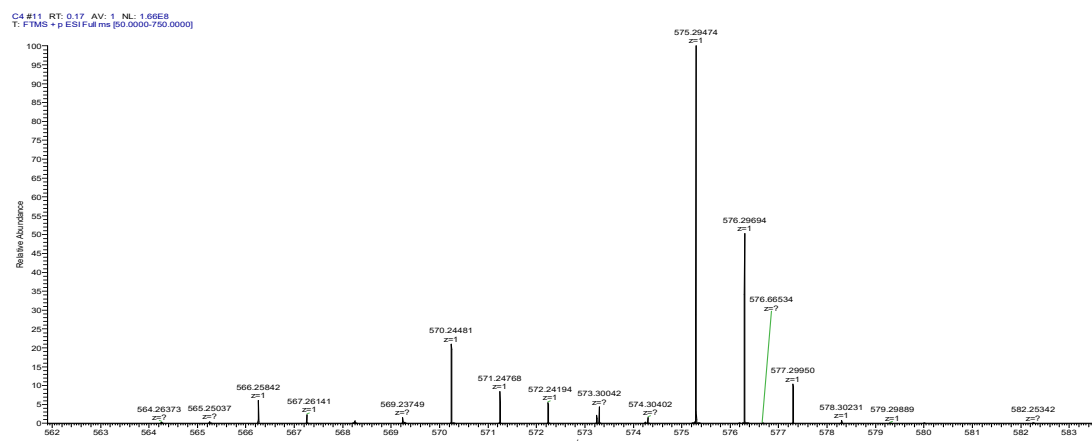


Figure S13. HRMS spectrum of Cr1(THF) (m/z 575.27, $[M-2Cl-THF+OH+Na]^+$).

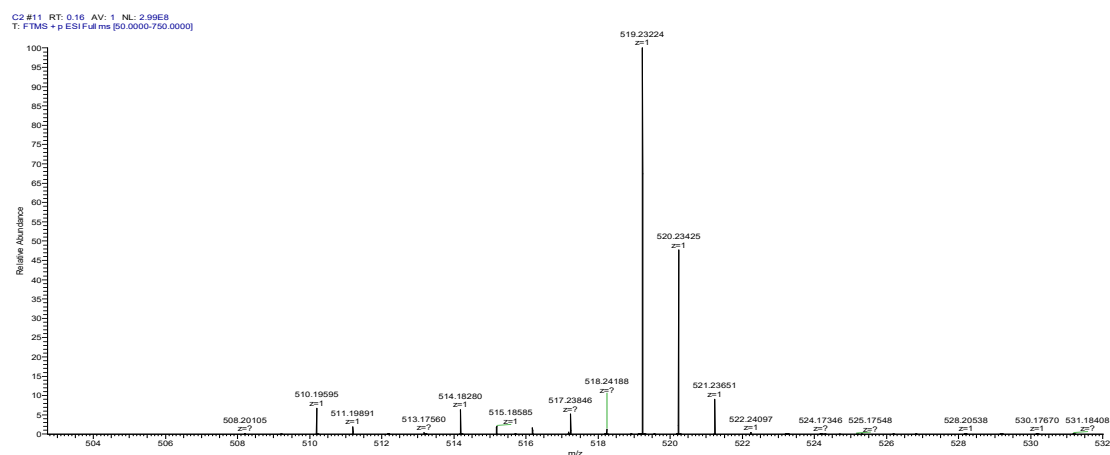


Figure S14. HRMS spectrum of Cr2(THF) (m/z 519.21, $[M-2Cl-THF+OH+Na]^+$).

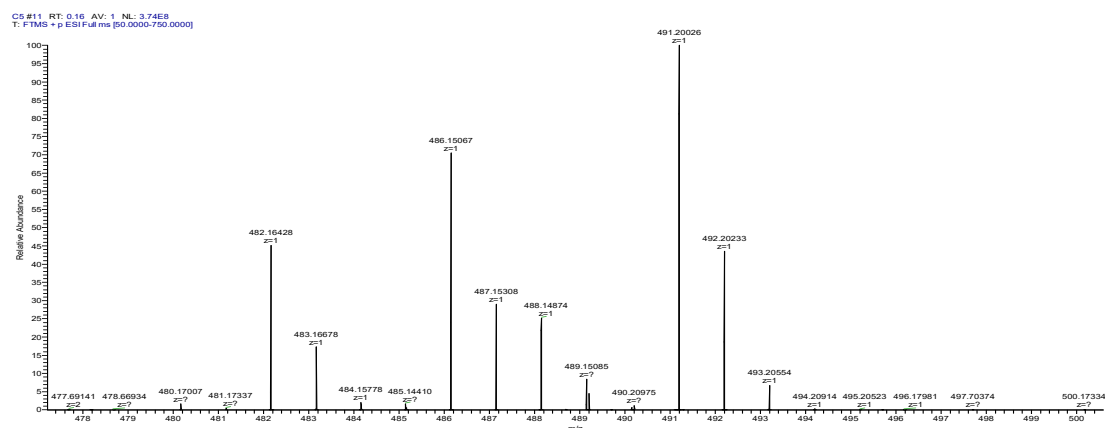


Figure S15. HRMS spectrum of Cr3(THF) (m/z 491.18, $[M-2Cl-THF+OH+Na]^+$).

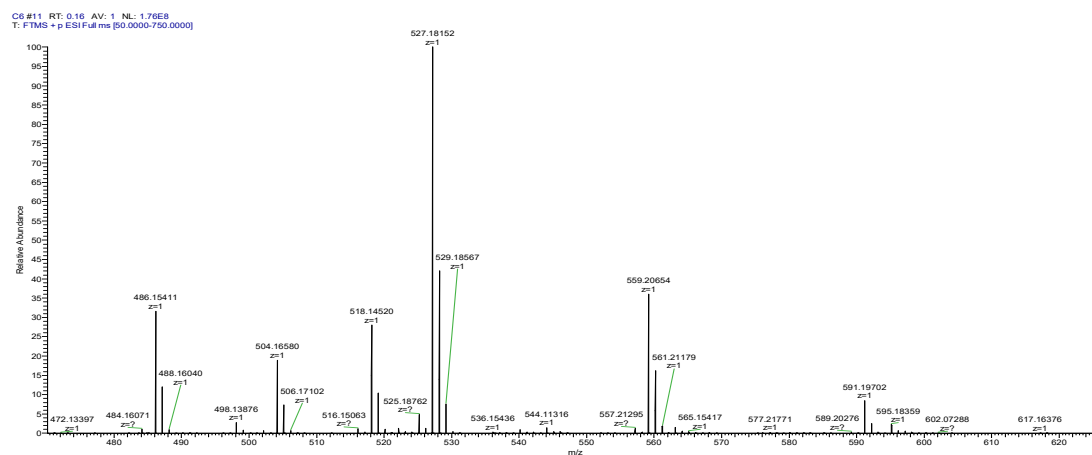


Figure S16. HRMS spectrum of Cr4(THF) (m/z 527.16, $[M-2Cl-THF+OH+Na]^+$).

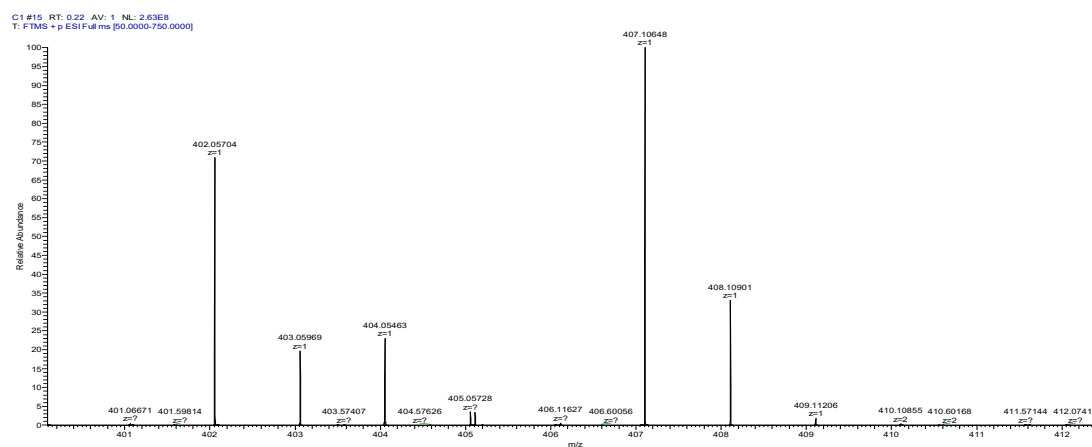


Figure S17. HRMS spectrum of Cr5(THF) (m/z 407.08, $[M-2Cl-THF+OH+Na]^+$).

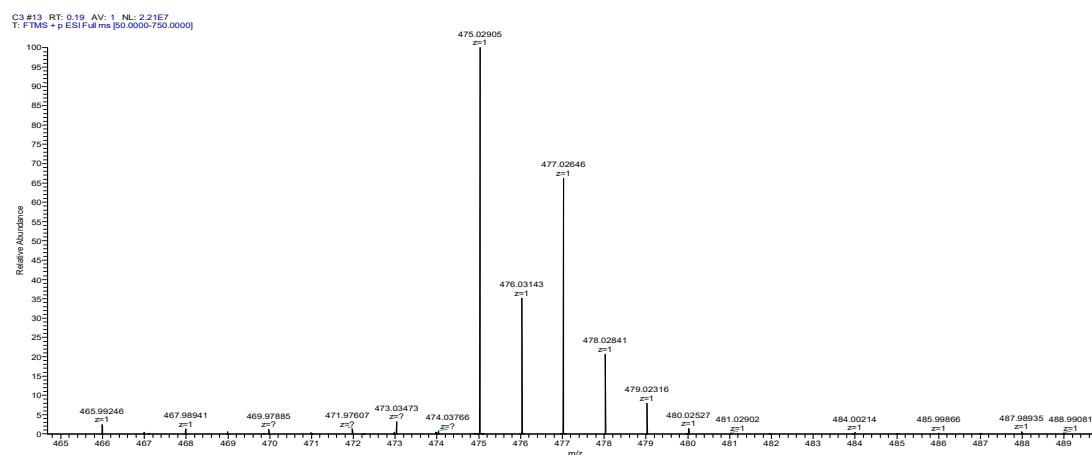


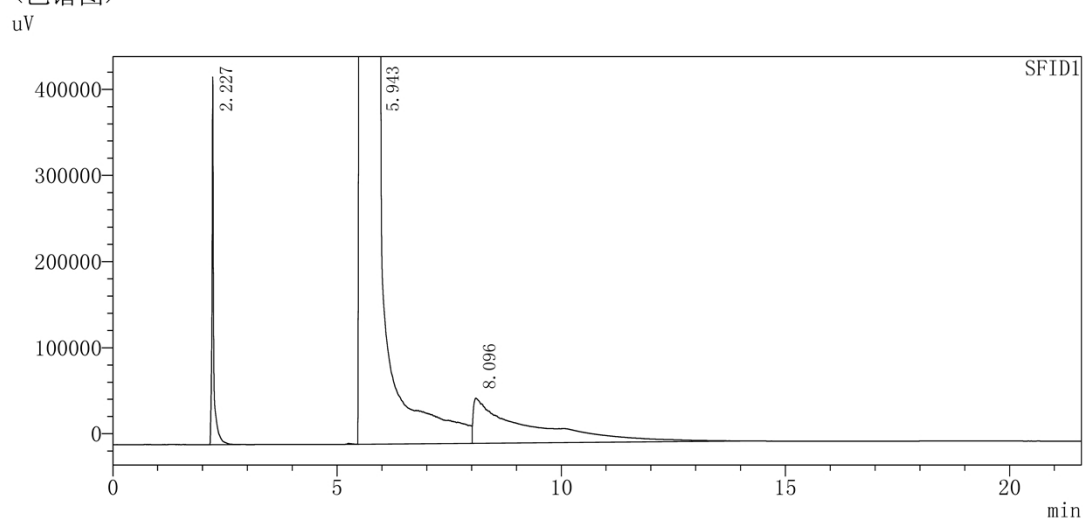
Figure S18. HRMS spectrum of Cr6(THF) (m/z 475.01, $[M-2Cl-THF+OH+Na]^+$).

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 方法文件名 : fcy-1. gcm
 批处理文件名 :
 样品瓶号 : 1
 进样体积 : 1 uL
 分析日期 : 2022/1/12 0:45:02
 处理日期 : 2022/1/12 1:11:43

样品类型 : 未知
 分析者 : System Administrator
 处理者 : System Administrator

<色谱图>



<峰表>

SFID1

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	2.227	1069715	418452	1.006	%	M	C2H4
2	5.943	100980908	5301357	94.930	%	M	Tol
3	8.096	4323008	52432	4.064	%	V M	C6H5C1
总计		106373632	5772241				

Figure S19. GC analysis of the liquid fraction obtained from polymerization in Table

1 run 1.

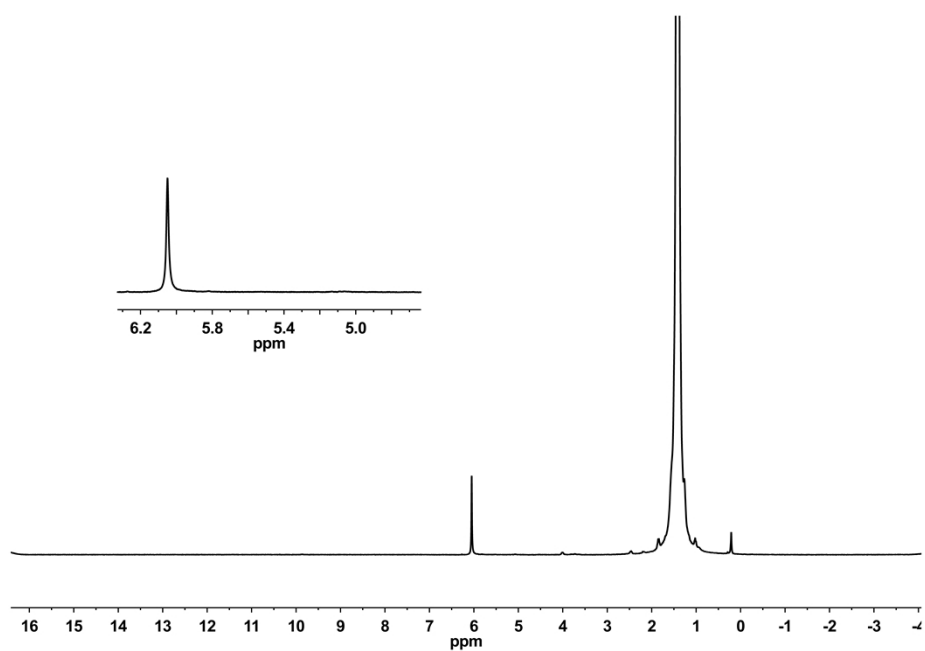


Figure S20. ^1H NMR spectrum of polyethylene sample obtained in Table 2 run 10 (120 °C in $\text{C}_2\text{D}_2\text{Cl}_4$).

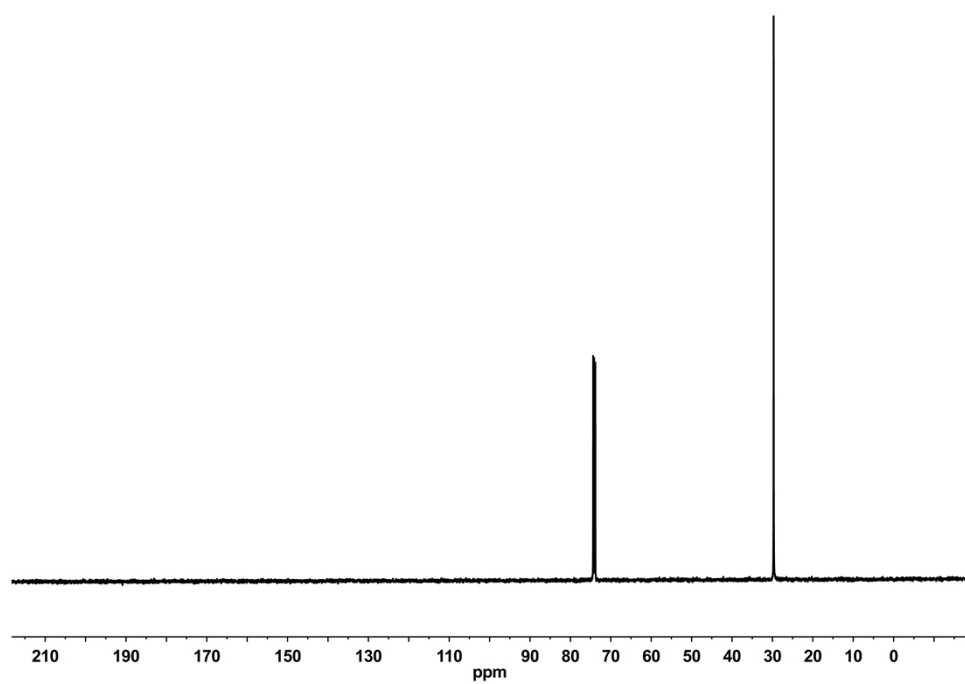


Figure S21. ^{13}C NMR spectrum of polyethylene sample obtained in Table 2 run 10 (120 °C in $\text{C}_2\text{D}_2\text{Cl}_4$).

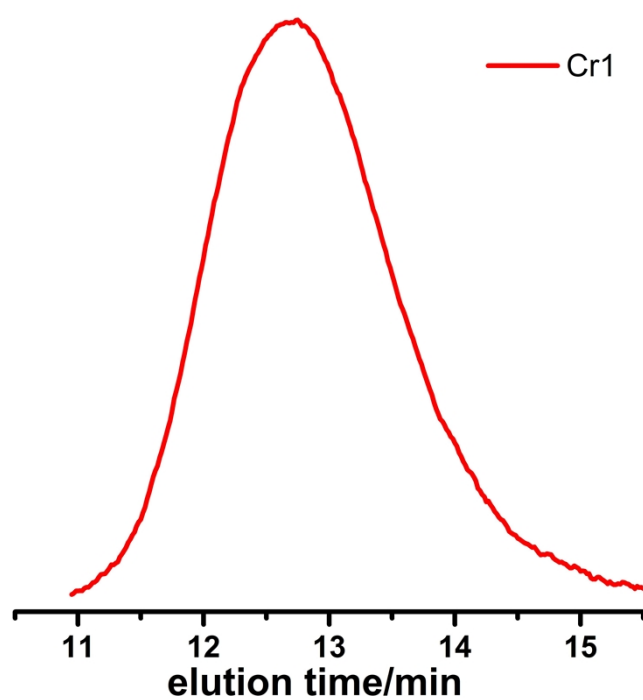


Figure S22. GPC curve of polyethylene obtained in Table 3 run 1 ($M_w = 14.4 \times 10^4$ g·mol⁻¹, $D = 2.3$).

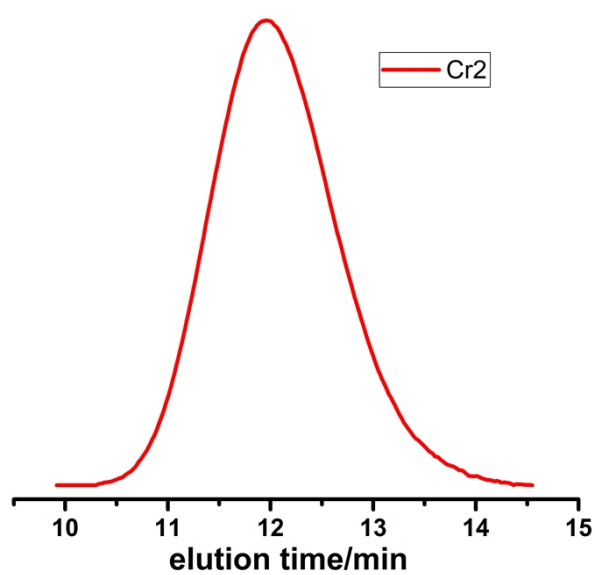


Figure S23. GPC curve of polyethylene obtained in Table 3 run 2 ($M_w = 38.9 \times 10^4$ g·mol⁻¹, $D = 1.5$).

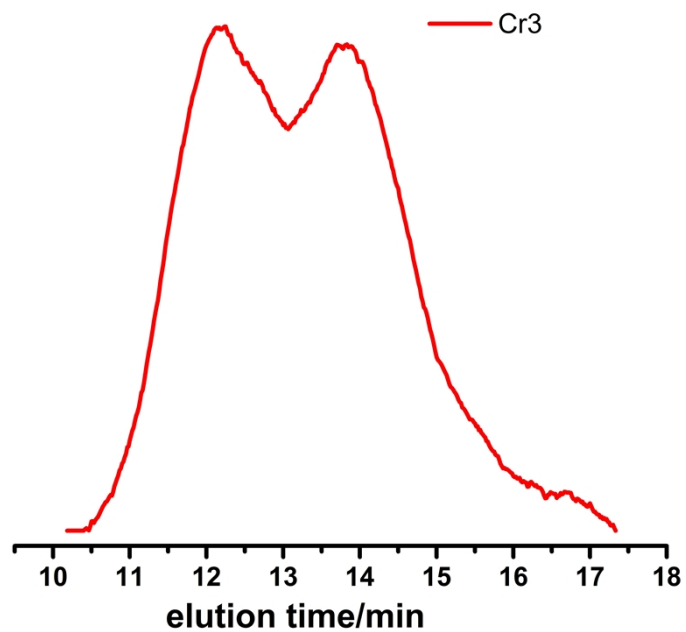


Figure S24. GPC curve of polyethylene obtained in Table 3 run 3 ($M_w = 22.3 \times 10^4$ g·mol⁻¹, $D = 4.2$).

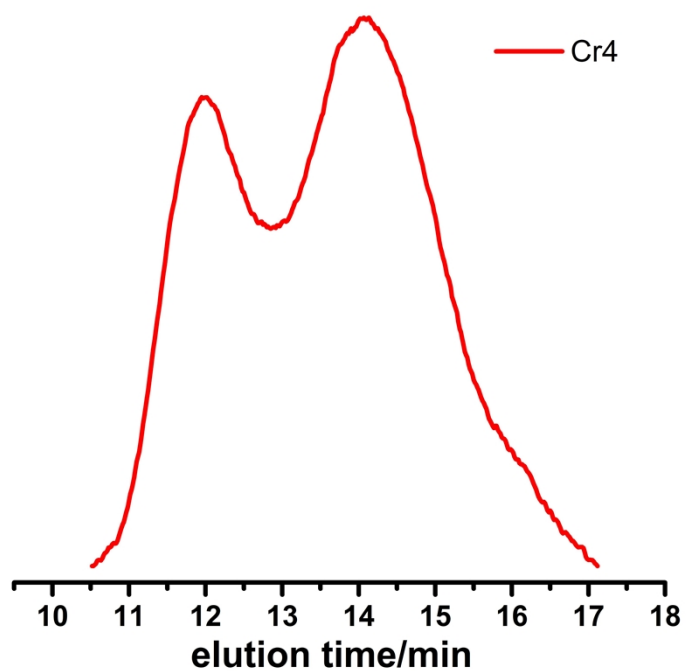


Figure S25. GPC curve of polyethylene obtained in Table 3 run 4 ($M_w = 18.0 \times 10^4$ g·mol⁻¹, $D = 10$).

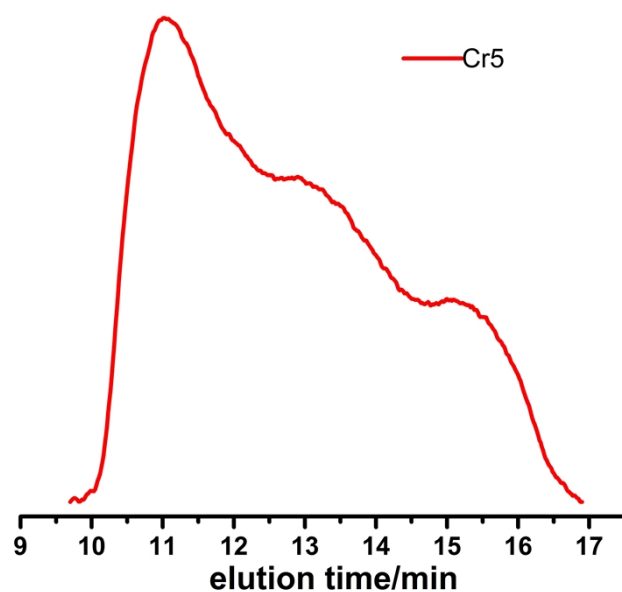


Figure S26. GPC curve of polyethylene obtained in Table 3 run 5 ($M_w = 45.6 \times 10^4$ g·mol⁻¹, $D = 19$).

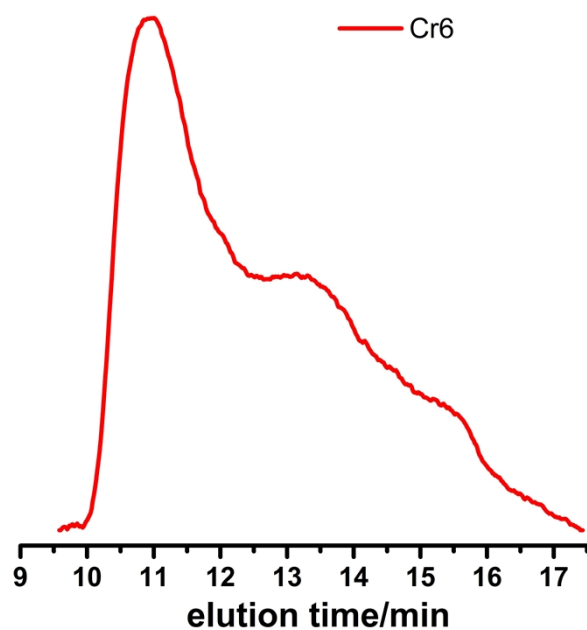


Figure S27. GPC curve of polyethylene obtained in Table 3 run 6 ($M_w = 53.4 \times 10^4$ g·mol⁻¹, $D = 19$).

Table S1. Crystal data and structure refinement for **Cr2**(THF) and **Cr4**(THF).

Complex	Cr2 (THF)	Cr4 (THF)
Empirical formula	C ₃₃ H ₄₃ Cl ₂ CrN ₂ O ₂	C ₃₁ H ₃₇ Cl ₂ CrF ₂ N ₂ O ₂
Formula weight	622.59	630.52
Temperature / K	193	213
Crystal system	triclinic	monoclinic
Space group	P-1	P2 ₁ /c
a / Å, b / Å, c / Å	16.326(3), 16.389(3), 16.464(3)	14.4764(4), 14.5398(4), 15.5208(4)
α /°, β /°, γ /°	70.953(7), 89.935(10), 71.859(7)	90, 109.5390(10), 90
Volume / Å ³	3932.1(13)	3078.75(15)
Z	4	4
ρ_{calc} / mg mm ⁻³	1.052	1.360
μ / mm ⁻¹	2.591	3.395
F(000)	1316.0	1316.0
Crystal size / mm ³	0.05 × 0.03 × 0.03	0.07 × 0.07 × 0.05
2 Θ range for data collection	5.866 to 110.332	8.222 to 110.554
Index ranges	-19 ≤ h ≤ 17, -20 ≤ k ≤ 19, -20 ≤ l ≤ 20	-17 ≤ h ≤ 17, -17 ≤ k ≤ 11, -18 ≤ l ≤ 18
Reflections collected	56466	26800
Independent reflections	14951 [R _{int} = 0.0787]	5858 [R _{int} = 0.0458]
Data/restraints/parameters	14951/0/737	5858/18/367
Goodness-of-fit on F ²	1.054	1.072
Final R indexes [I > 2 σ (I)]	R ₁ = 0.0736, wR ₂ = 0.2105	R ₁ = 0.0518, wR ₂ = 0.1382
Final R indexes [all data]	R ₁ = 0.1177, wR ₂ = 0.2400	R ₁ = 0.0664, wR ₂ = 0.1507
Largest diff. peak/hole / e Å ⁻³	0.35/-0.67	0.78/-0.56