

Supplementary Materials

Synthesis, fungitoxic activity against *Botrytis cinerea* and phytotoxicity of alkoxyclovanols and alkoxyisocaryolanols

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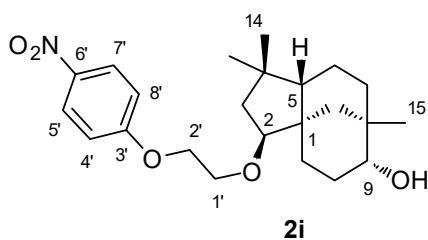
These authors contributed equally to this work.

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(2*S*,9*R*)-2-(2'-(*p*-nitrophenoxy)ethoxy)clovan-9-ol (**2i**):¹ ¹H NMR (CDCl₃, 400 MHz), see Table S1; ¹³C NMR (CDCl₃, 100 MHz), see Table S1; HMBC (selected correlations): C-1 → H-2 α , H-3 α , H-5 β , H-12a, H-12b; C-2 → H-3 α , H-3 β , H-12a, H-12b, H-1'a,b; C-9 → H-7a, H-7b, H-11a, H-12a, H-12b, H₃-15 β ; C-1' → H-2 α , H₂-2'; C-2' → H-1'a,b; C-3' → H₂-2', H-4', H-8', H-5', H-7'; C-6' → H-4', H-8', H-5', H-7'.

¹ Saiz-Urra, L.; Racero, J. C.; Macias-Sanchez, A. J.; Hernandez-Galan, R.; Hanson, J. R.; Perez- Gonzalez, M.; Collado, I. G. *J. Agric. Food Chem.* **2009**, *57*, 2420–2428.

Table S1. ¹H NMR (CDCl₃, 400 MHz) and ¹³C NMR (CDCl₃, 100 MHz)**Spectroscopic Data for Compound 2i**

Position	2i	
	δ_{H} , mult (<i>J</i> in Hz)	δ_{C} , type
2 α	3.47, dd (10.0, 5.6)	44.38, C
3 α	1.67, dd (11.5, 5.6)	89.27, CH
3 β	1.51 dd (11.5, 10.5)	44.45, CH ₂
4		37.10, C
5 β	1.41, m	50.46, CH
6a	1.40, m	20.52, CH ₂
6b	1.30, m	
7a	1.37, m	33.00, CH ₂
7b	1.10, m	
8		34.65, C
9 β	3.29, brs	75.04, CH
10 α	1.59, m	26.00, CH ₂
10 β	1.94, tdd (14.3, 4.6, 3.4)	
11a	1.69, m	26.70, CH ₂
11b	1.11, m	
12a	1.57, d (12.8)	36.41, CH ₂
12b	0.96, brd (12.8)	
13 α	0.84, ^a s	25.35, ^b CH ₃
14 β	1.00, ^a s	31.22, ^b CH ₃
15	0.92, s	28.30, CH ₃
1'a,b	3.87-3.79	68.57, CH ₂
2'	4.17, t (5.0)	68.48, CH ₂
3'		164.03, C
4', 8'	6.96, d (9.3)	114.65, 2CH
5', 7'	8.16, d (9.3)	125.77, 2CH
6'		141.41, C

^{a-b} Interchangeable signals

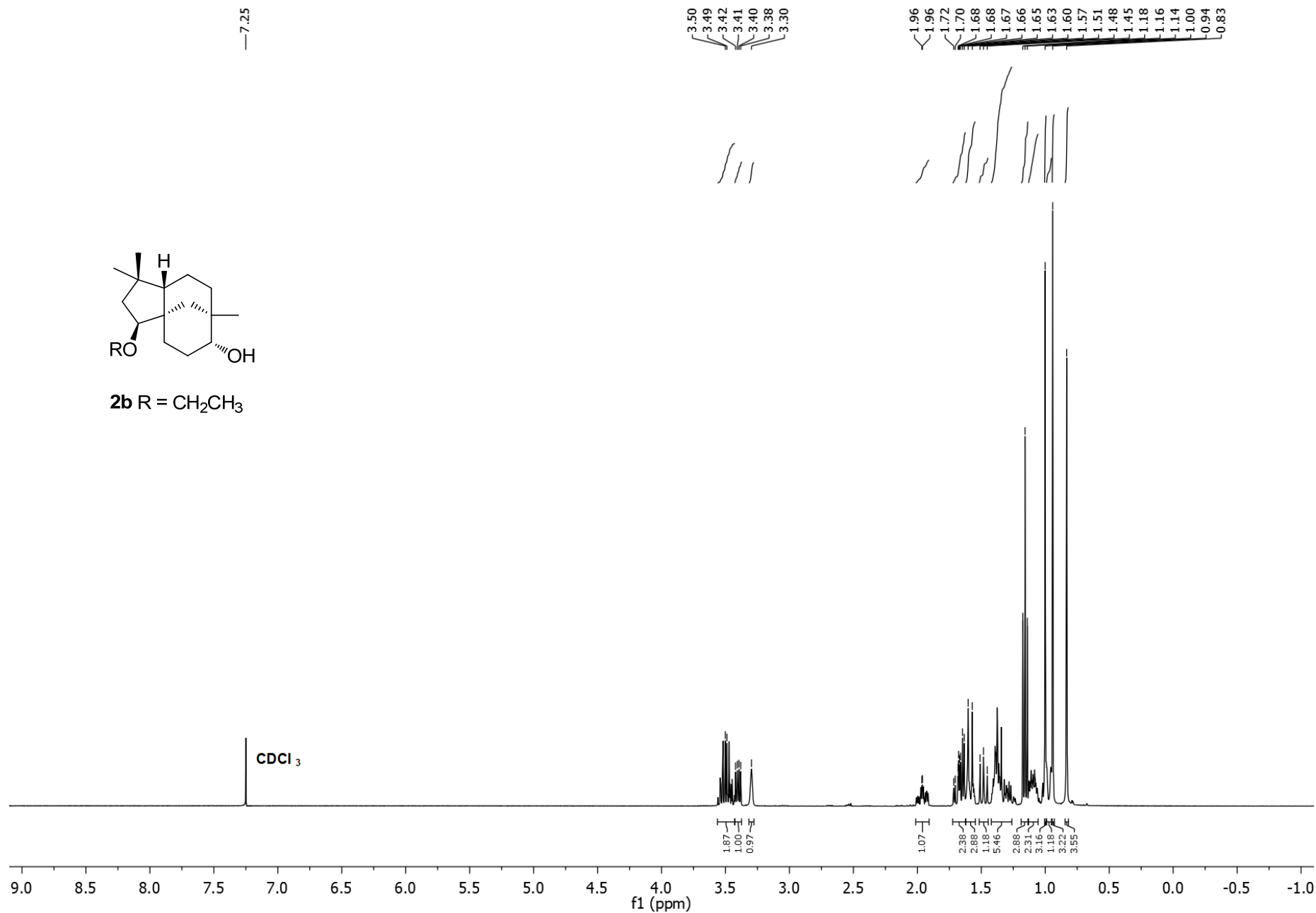


Figure S1. ^1H NMR spectrum of compound **2b** in CDCl_3 (400 MHz).

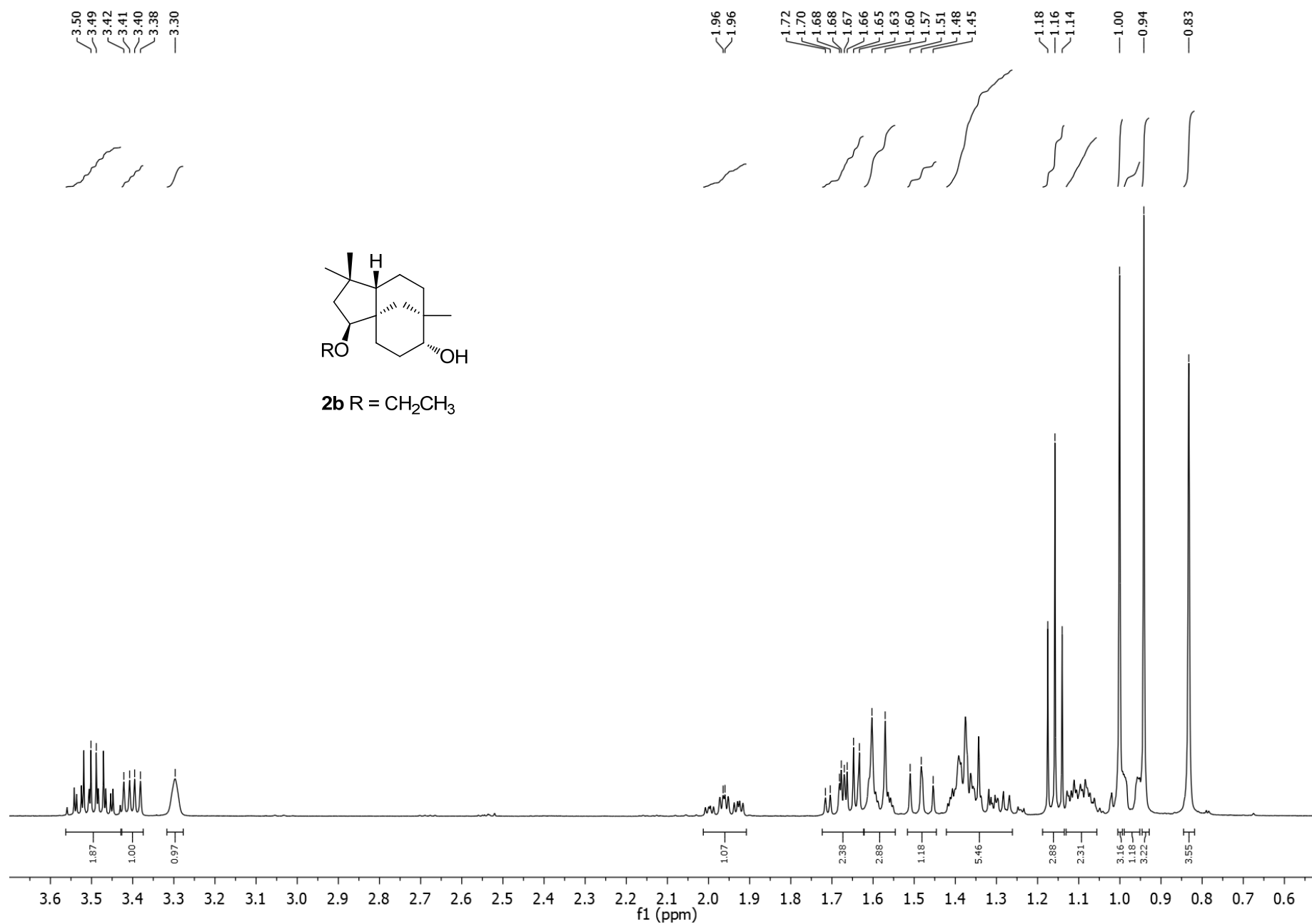
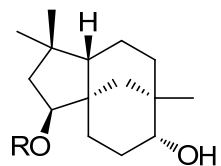


Figure S1a. Expansion (δ_{H} 3.7-0.5) of ^1H NMR spectrum of compound **2b** in CDCl_3 (400 MHz).



2b R = CH₂CH₃

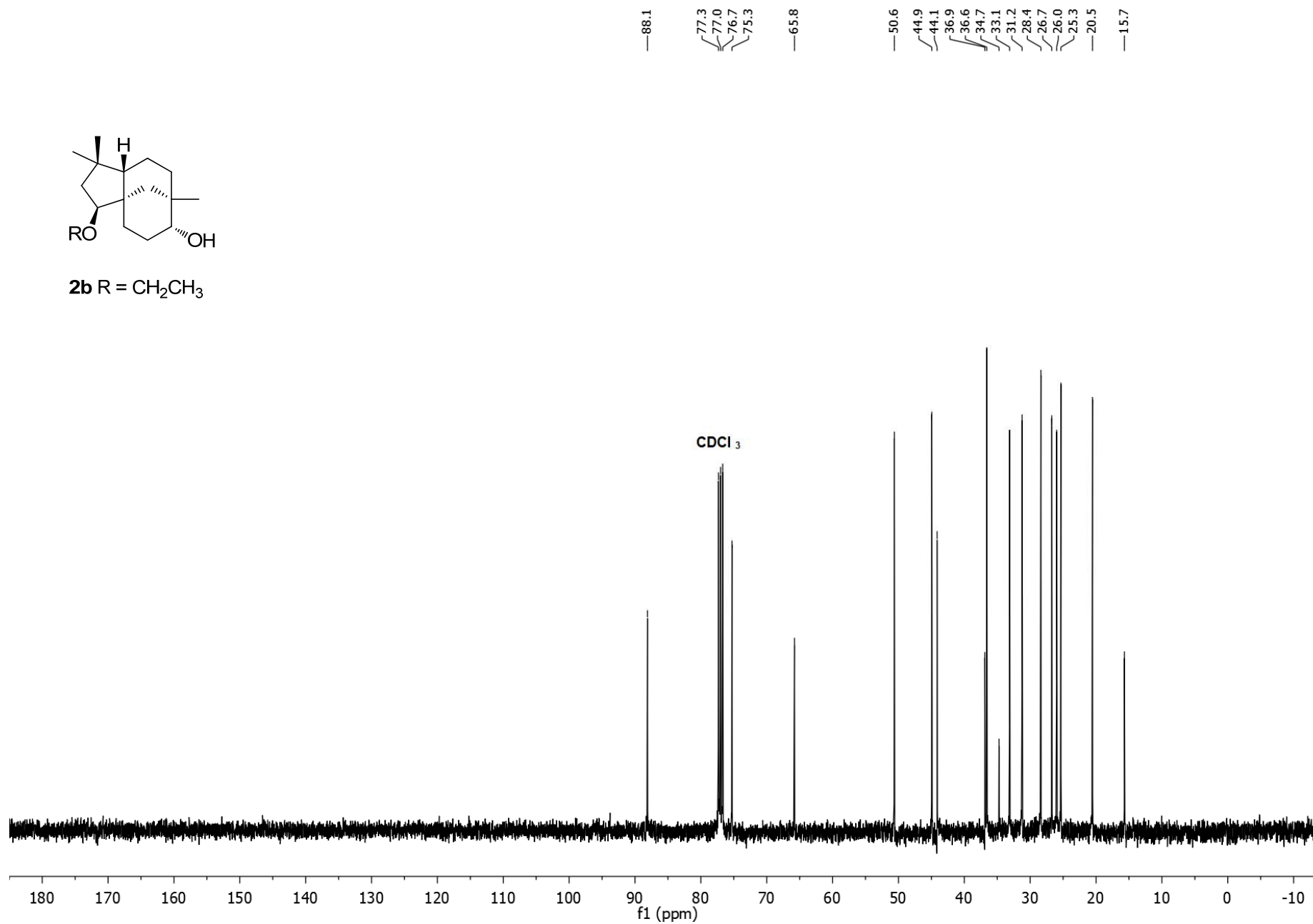


Figure S2. ¹³C NMR spectrum of compound **2b** in CDCl₃ (100 MHz).

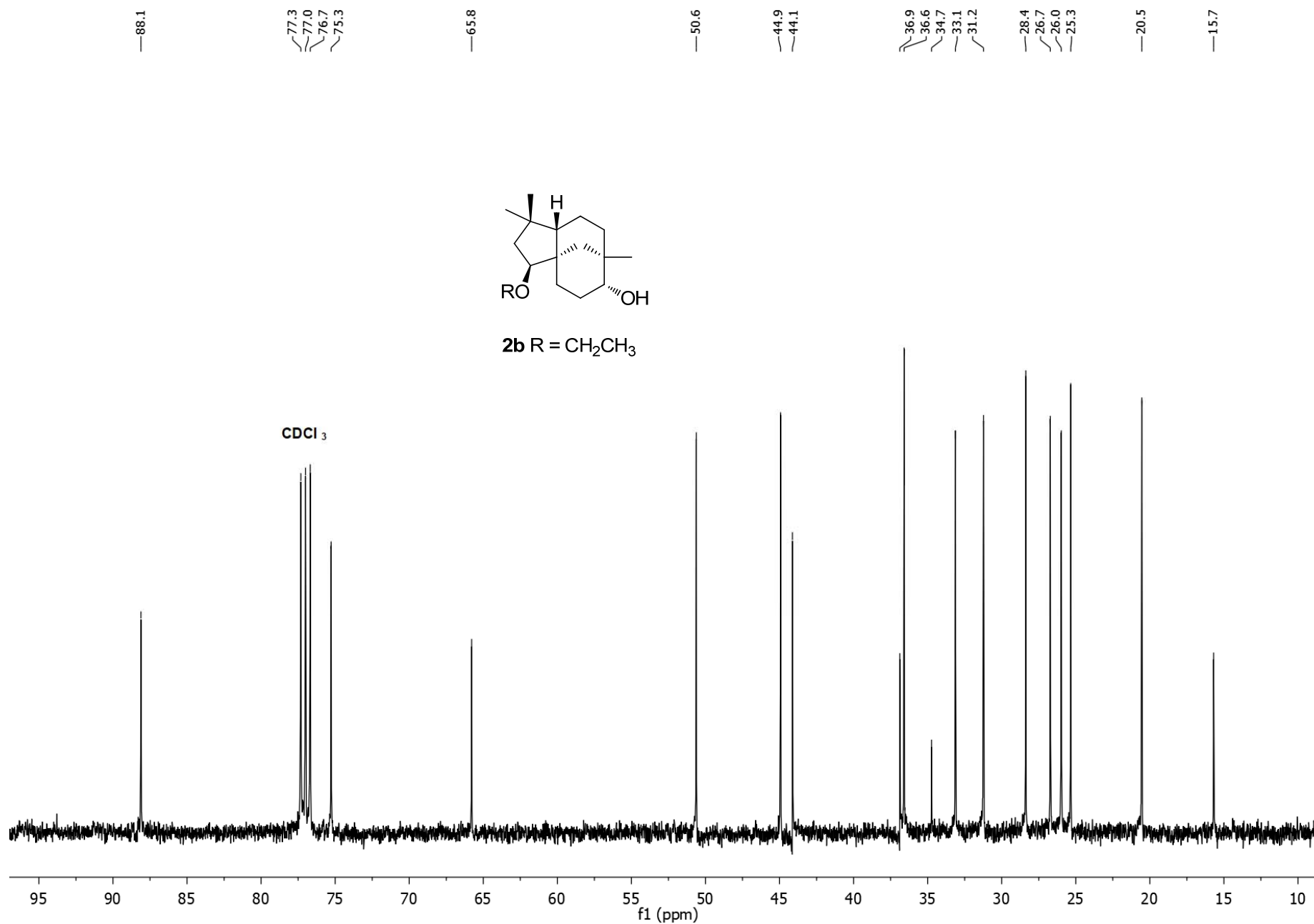


Figure S2a. Expansion (δ_{C} 95-10) of ^{13}C NMR spectrum of compound **2b** in CDCl_3 (100 MHz).

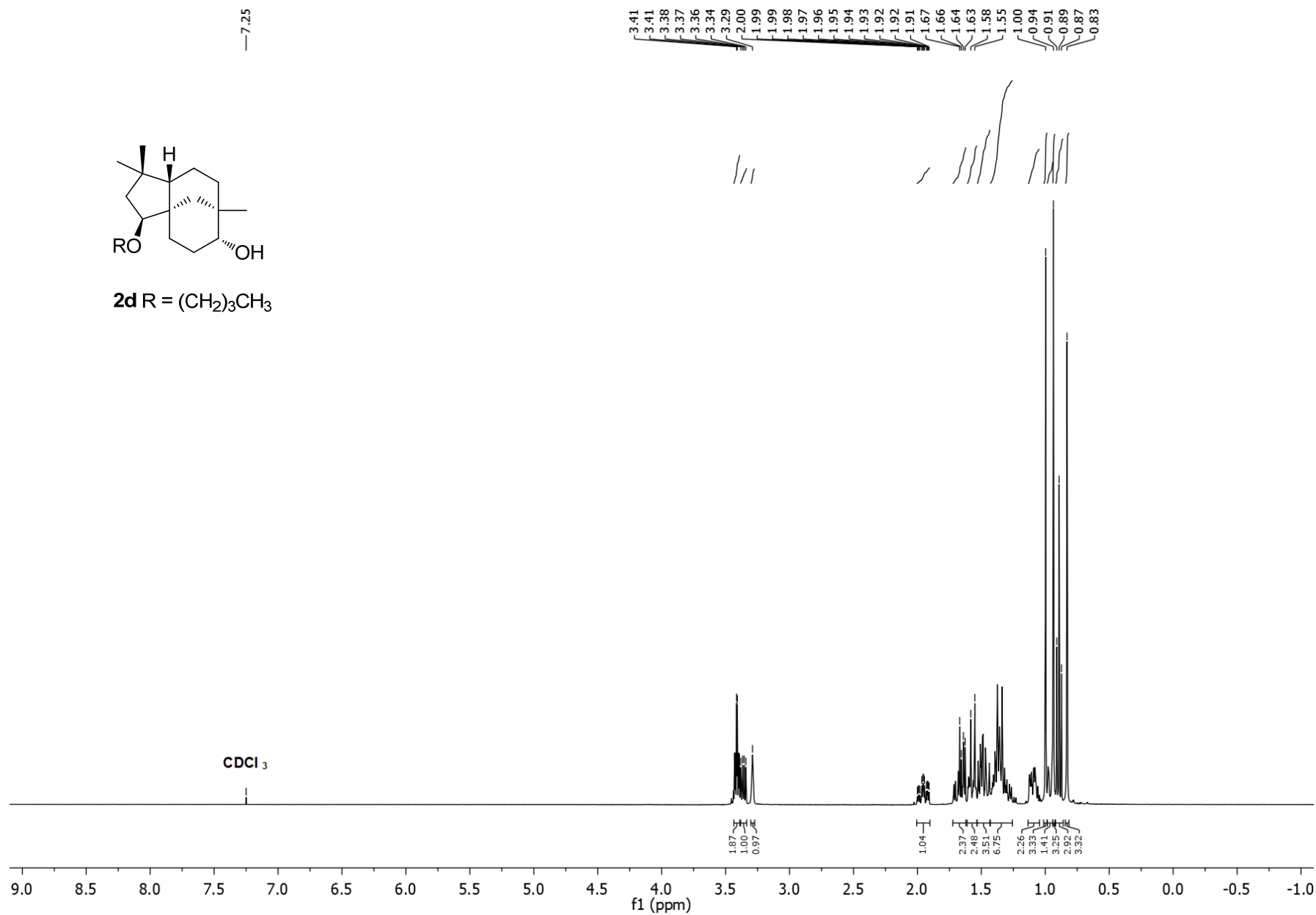


Figure S3. 1H NMR spectrum of compound **2d** in $CDCl_3$ (400 MHz).

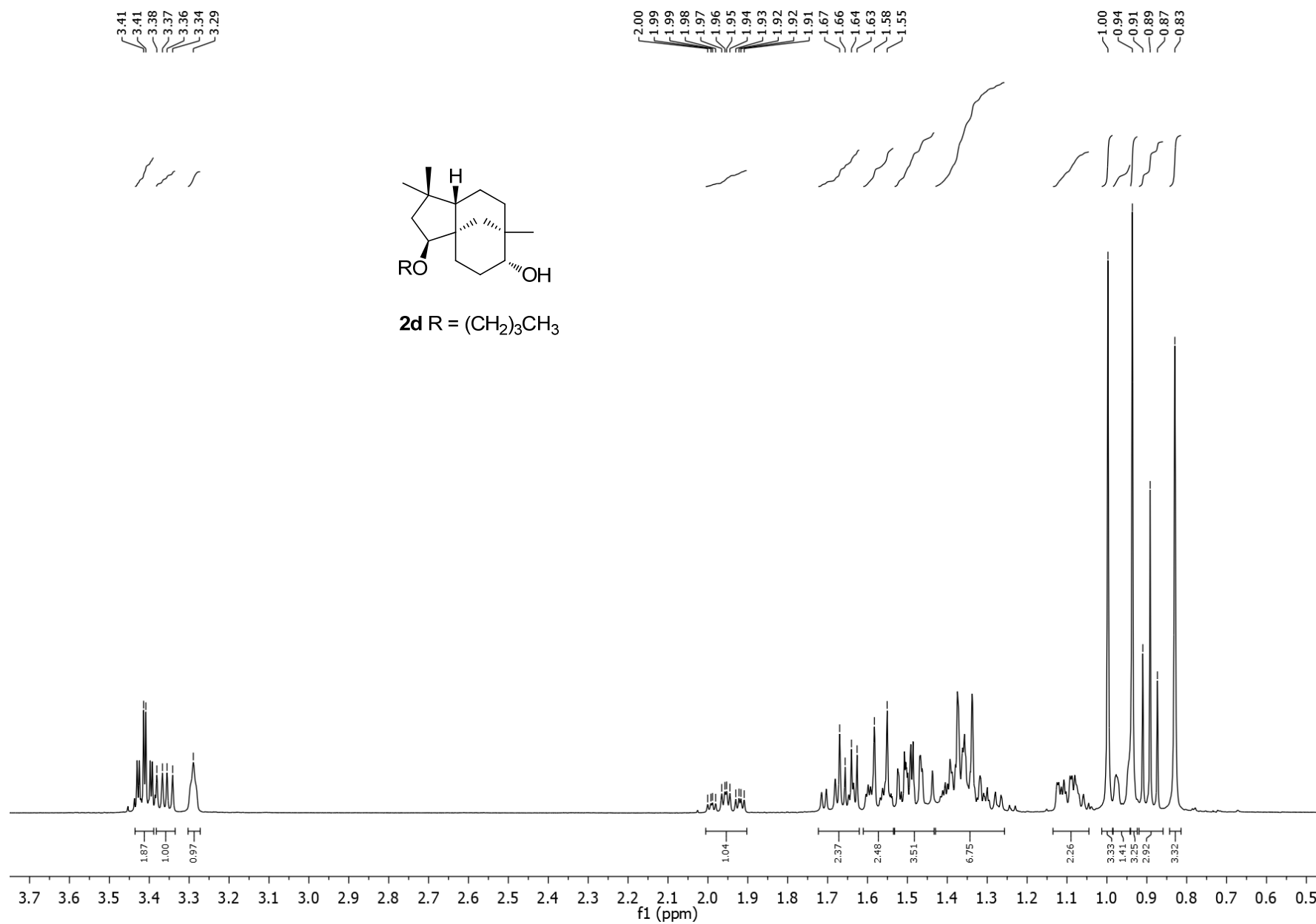
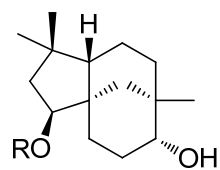


Figure S3a. Expansion (δ_H 3.7-0.5) of 1H NMR spectrum of compound **2d** in $CDCl_3$ (400 MHz).



2d R = (CH₂)₃CH₃

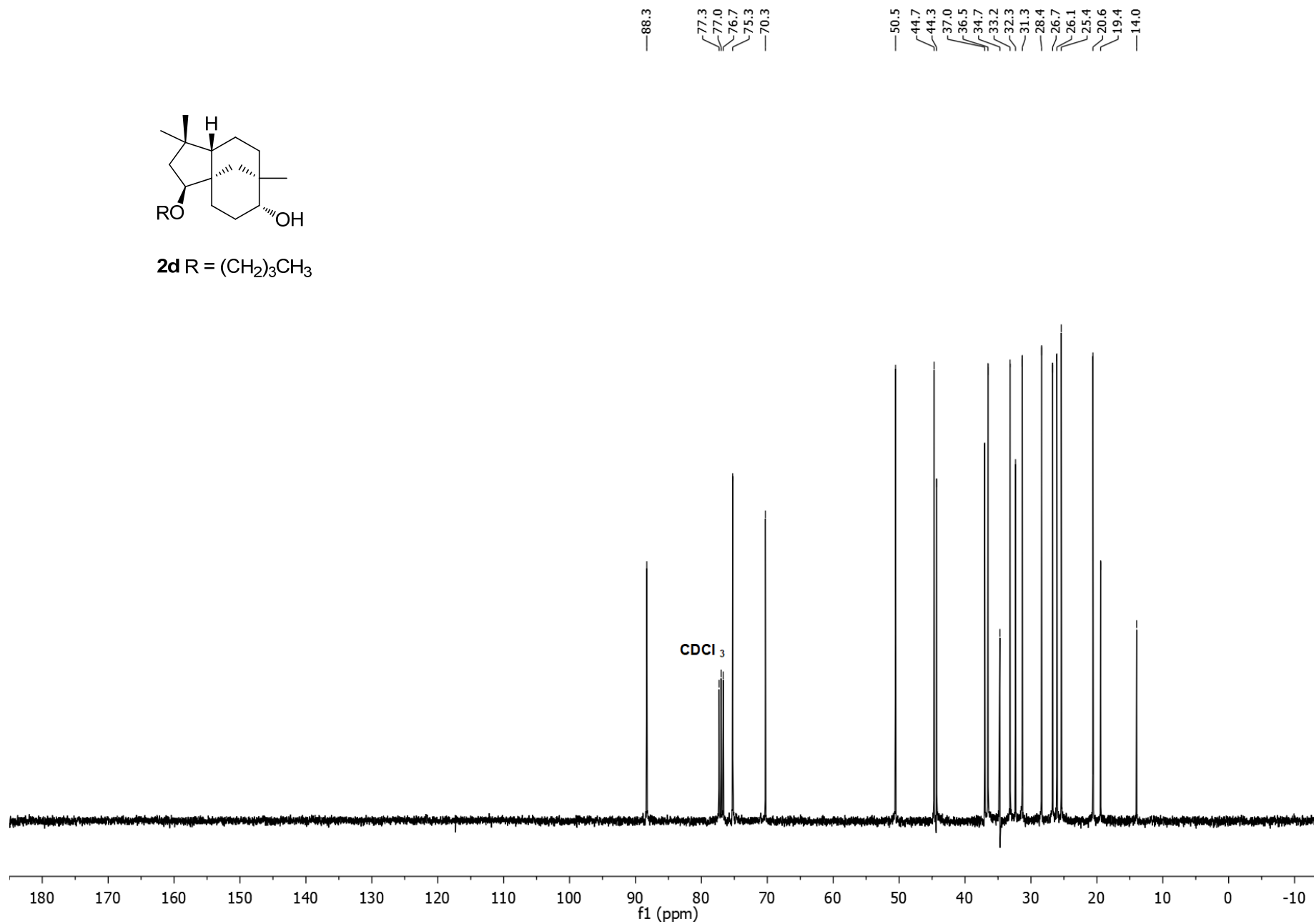


Figure S4. ¹³C NMR spectrum of compound **2d** in CDCl₃ (100 MHz).

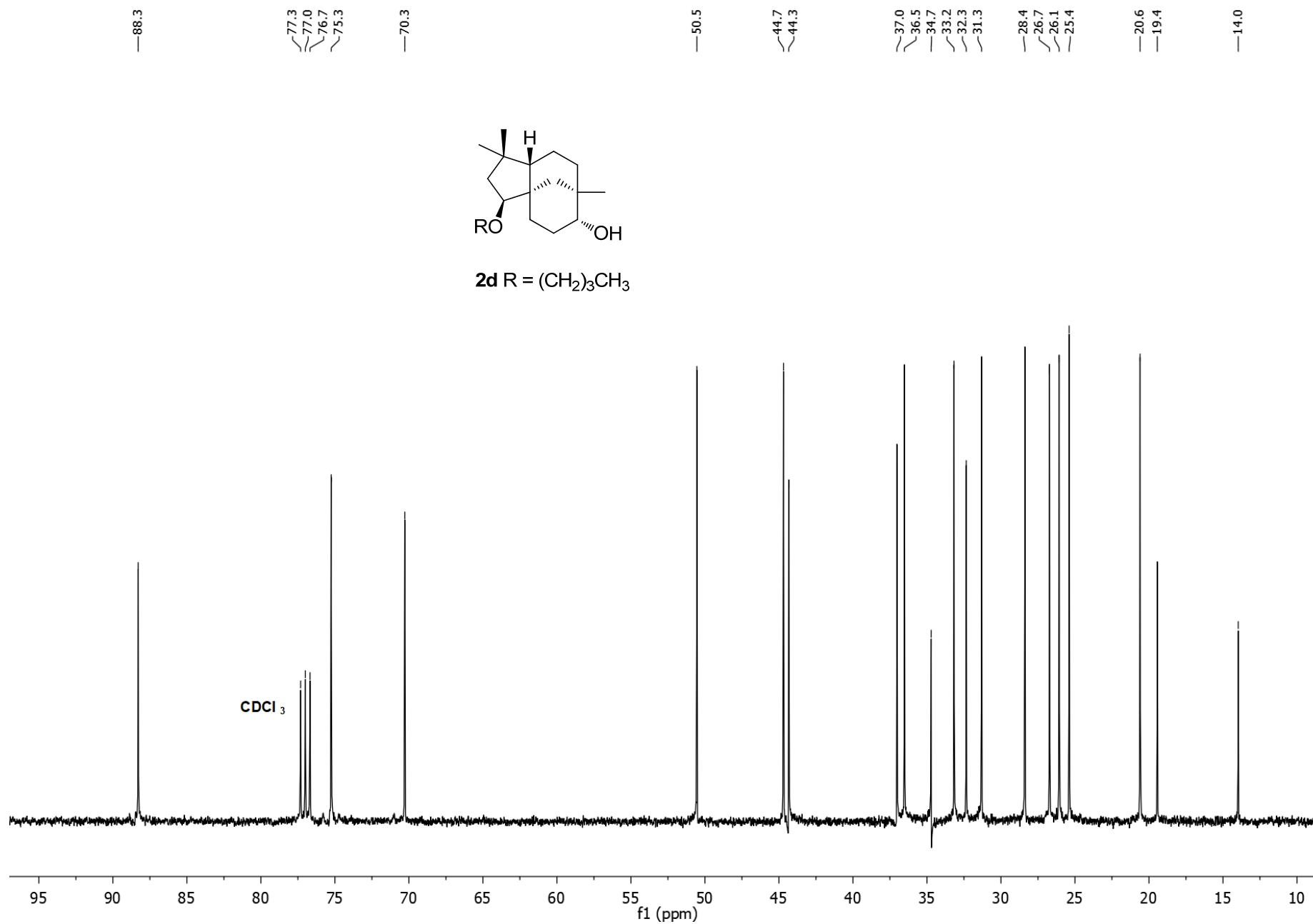


Figure S4a. Expansion (δ_{C} 95-10) of ^{13}C NMR spectrum of compound **2d** in CDCl_3 (100 MHz).

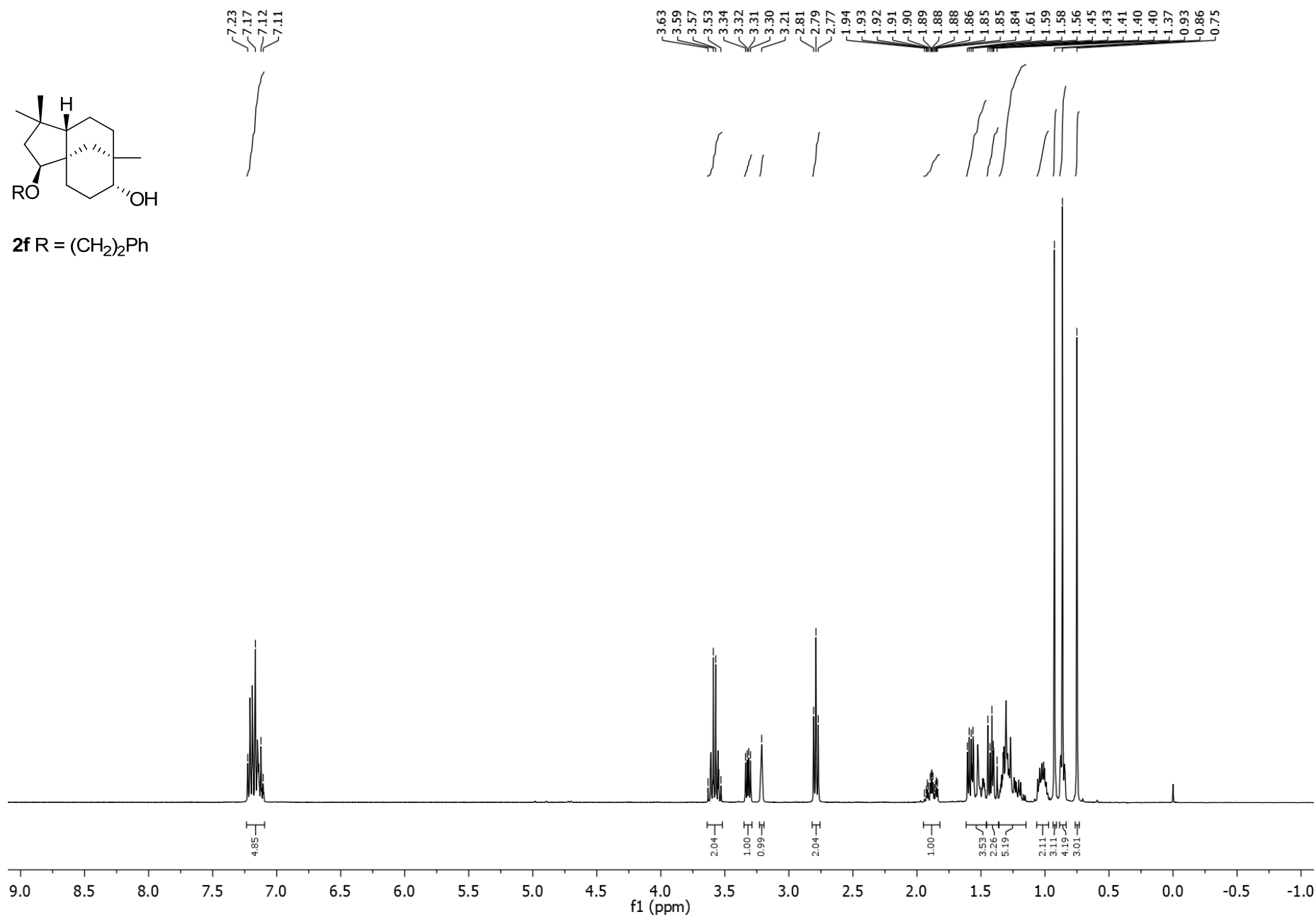


Figure S5. 1H NMR spectrum of compound **2f** in $CDCl_3$ (400 MHz).

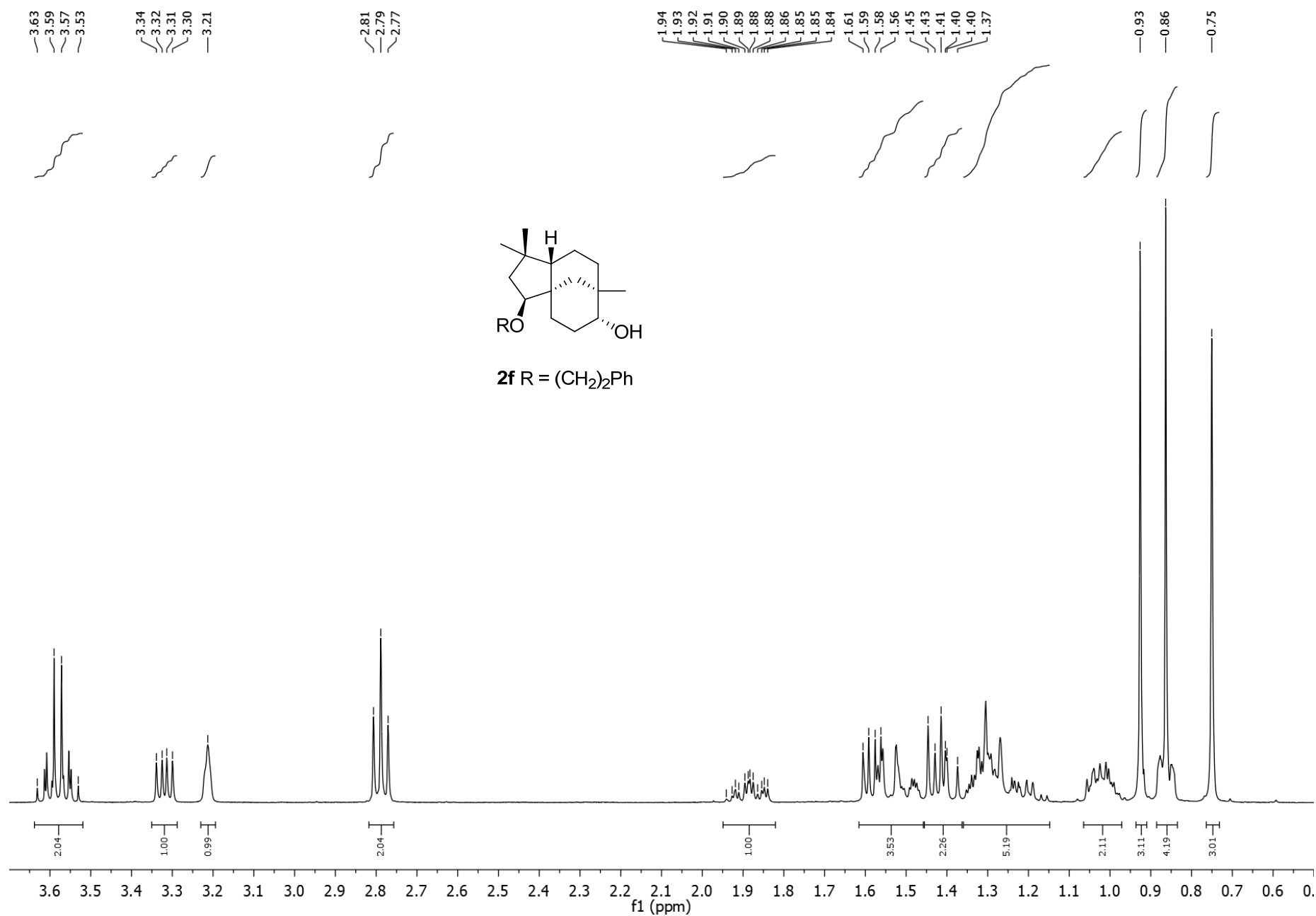


Figure S5a. Expansion (δ_H 3.7-0.5) of 1H NMR spectrum of compound **2f** in $CDCl_3$ (400 MHz).

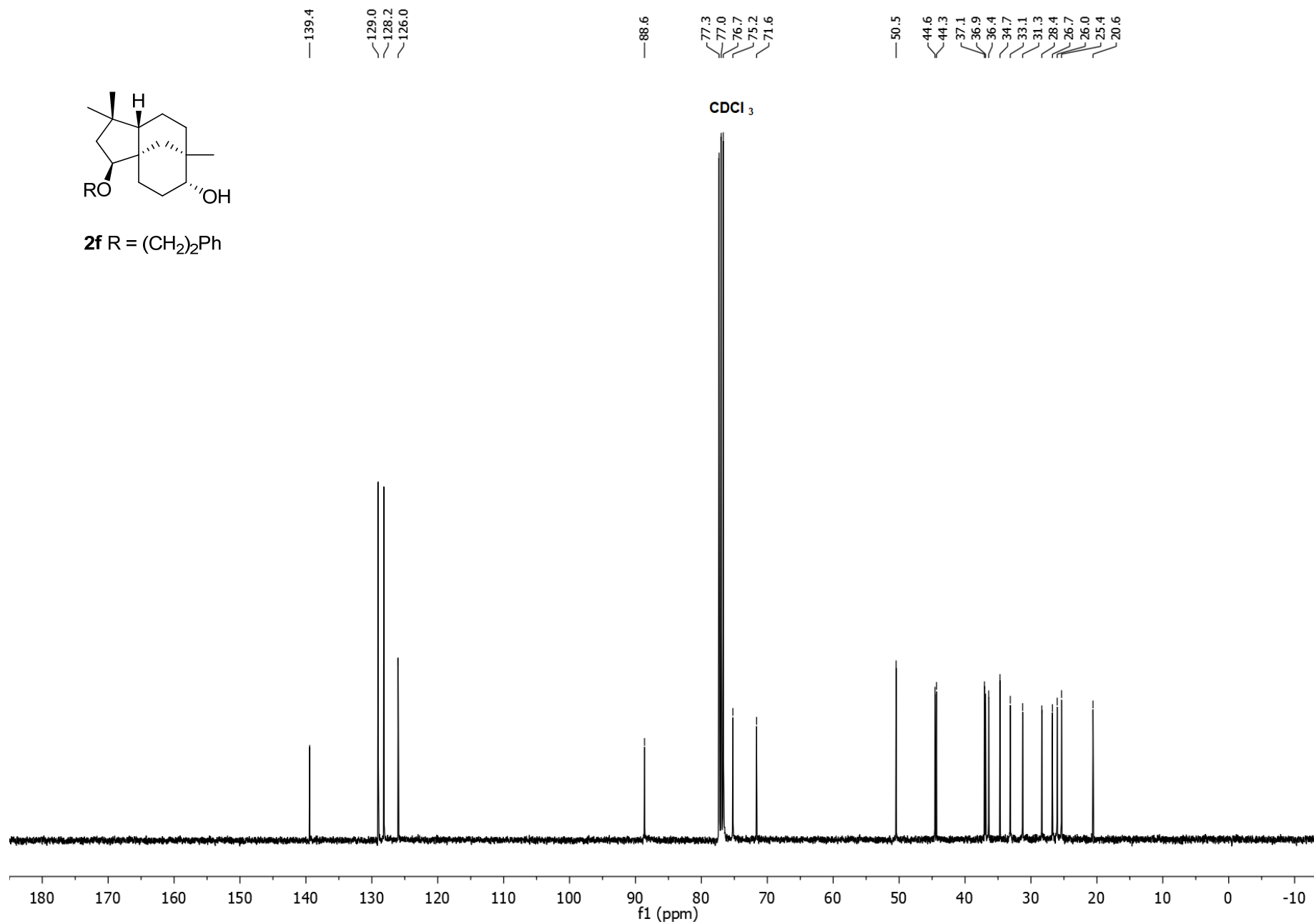


Figure S6. ¹³C NMR spectrum of compound **2f** in CDCl₃ (100 MHz).

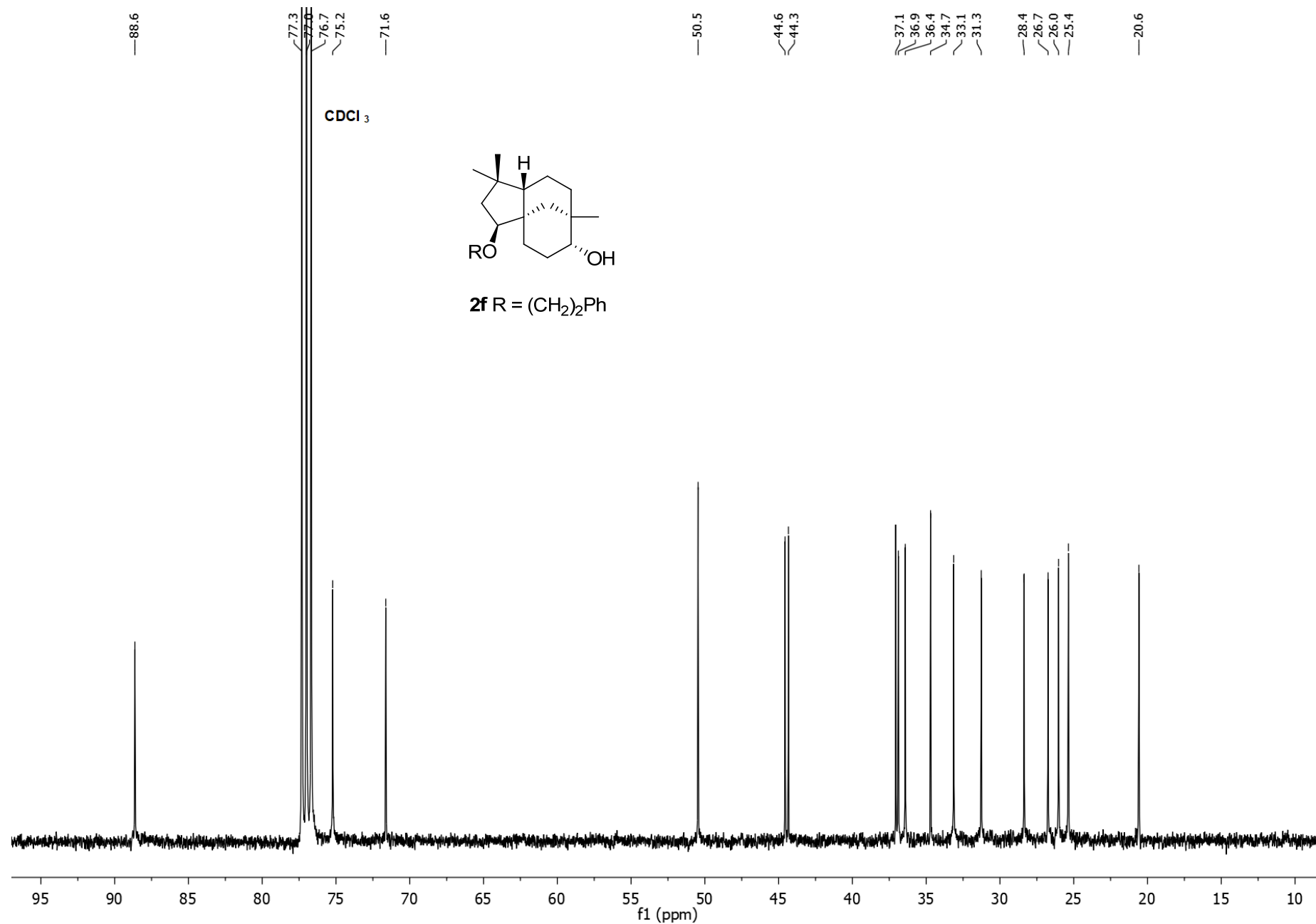


Figure S6a. Expansion (δ_c 95-10) of ^{13}C NMR spectrum of compound **2f** in $CDCl_3$ (100 MHz).

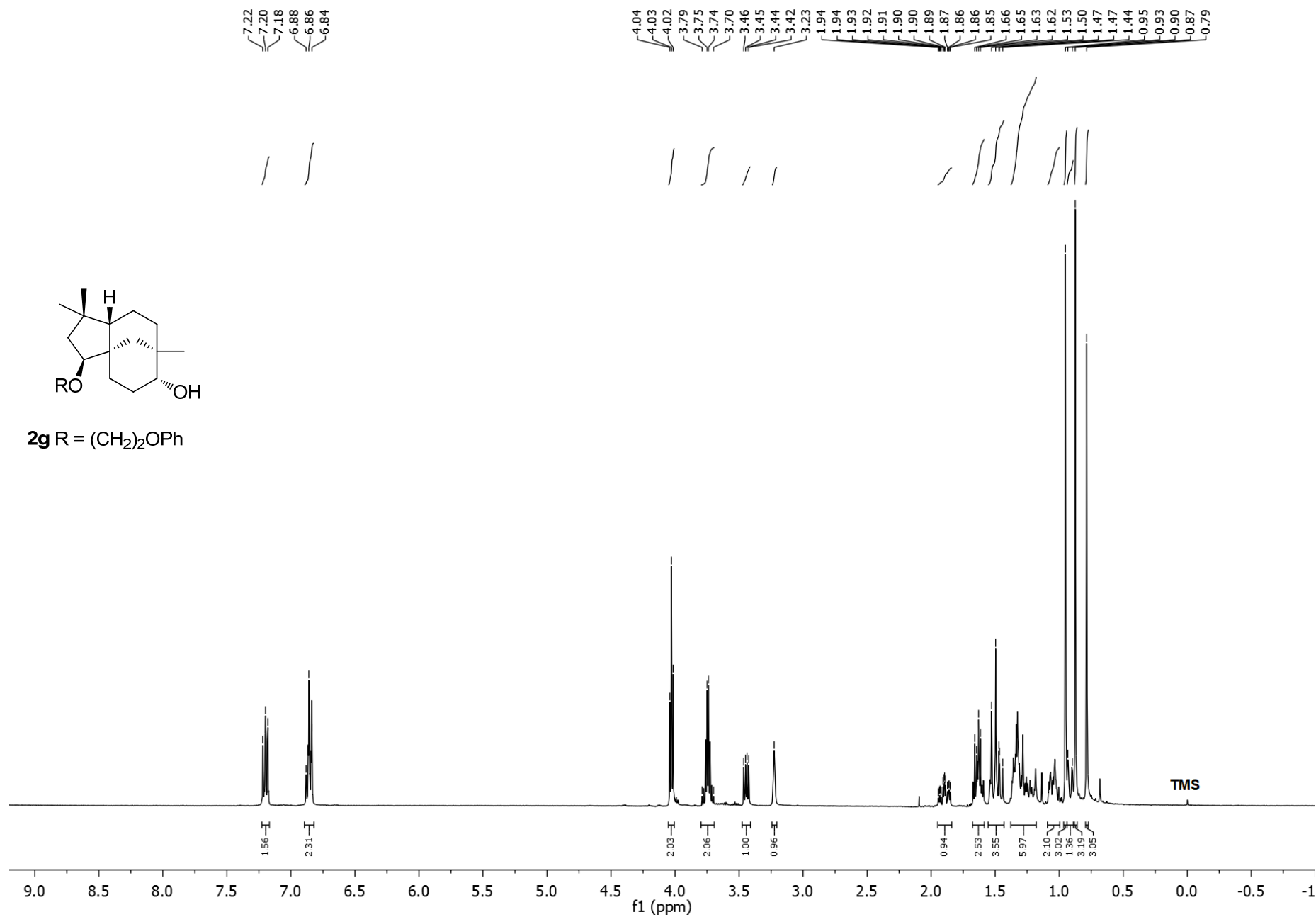


Figure S7. 1H NMR spectrum of compound **2g** in $CDCl_3$ (400 MHz).

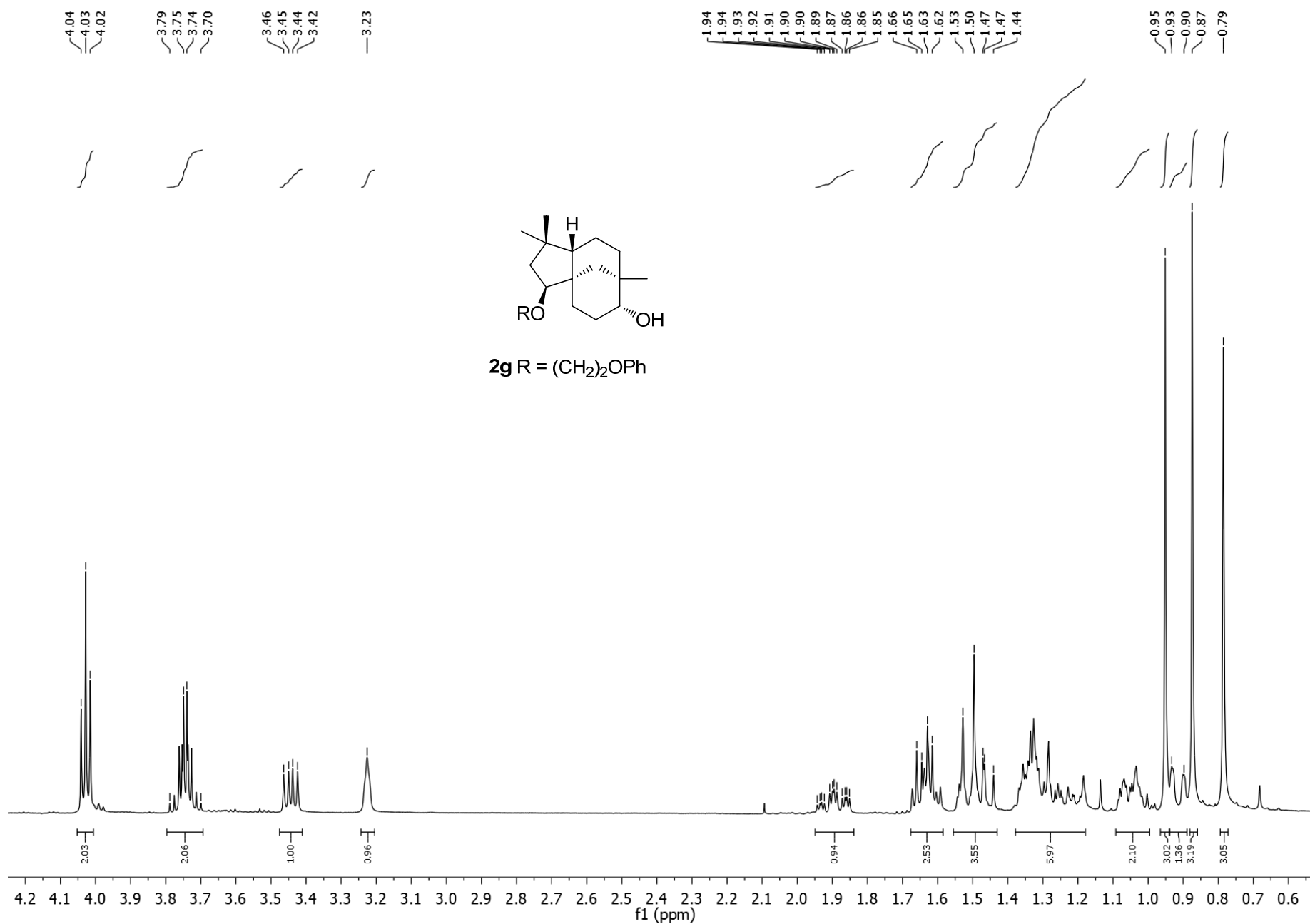


Figure S7a. Expansion (δ_H 4.2-0.5) of 1H NMR spectrum of compound **2g** in $CDCl_3$ (400 MHz).

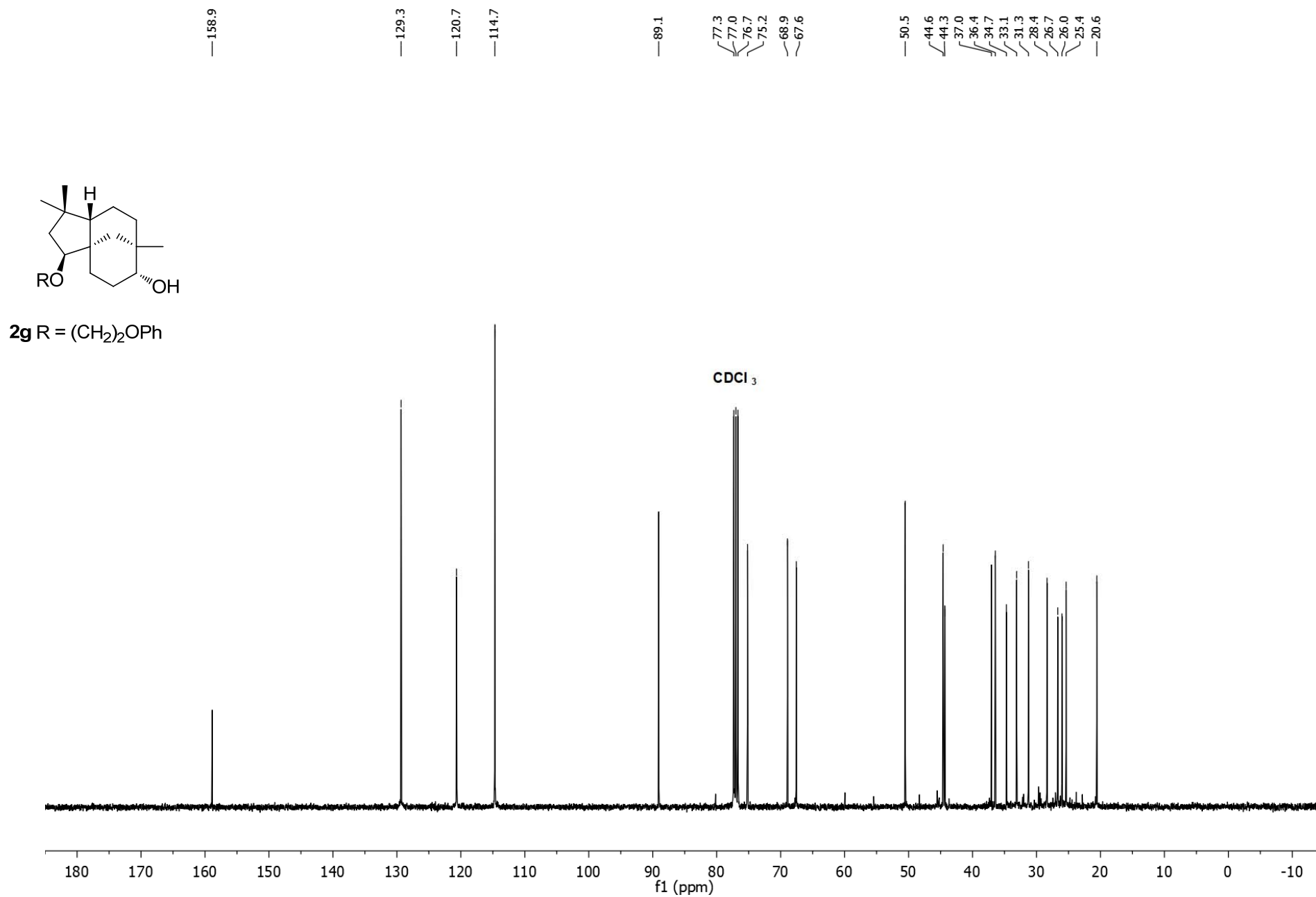


Figure S8. ¹³C NMR spectrum of compound **2g** in CDCl₃ (100 MHz).

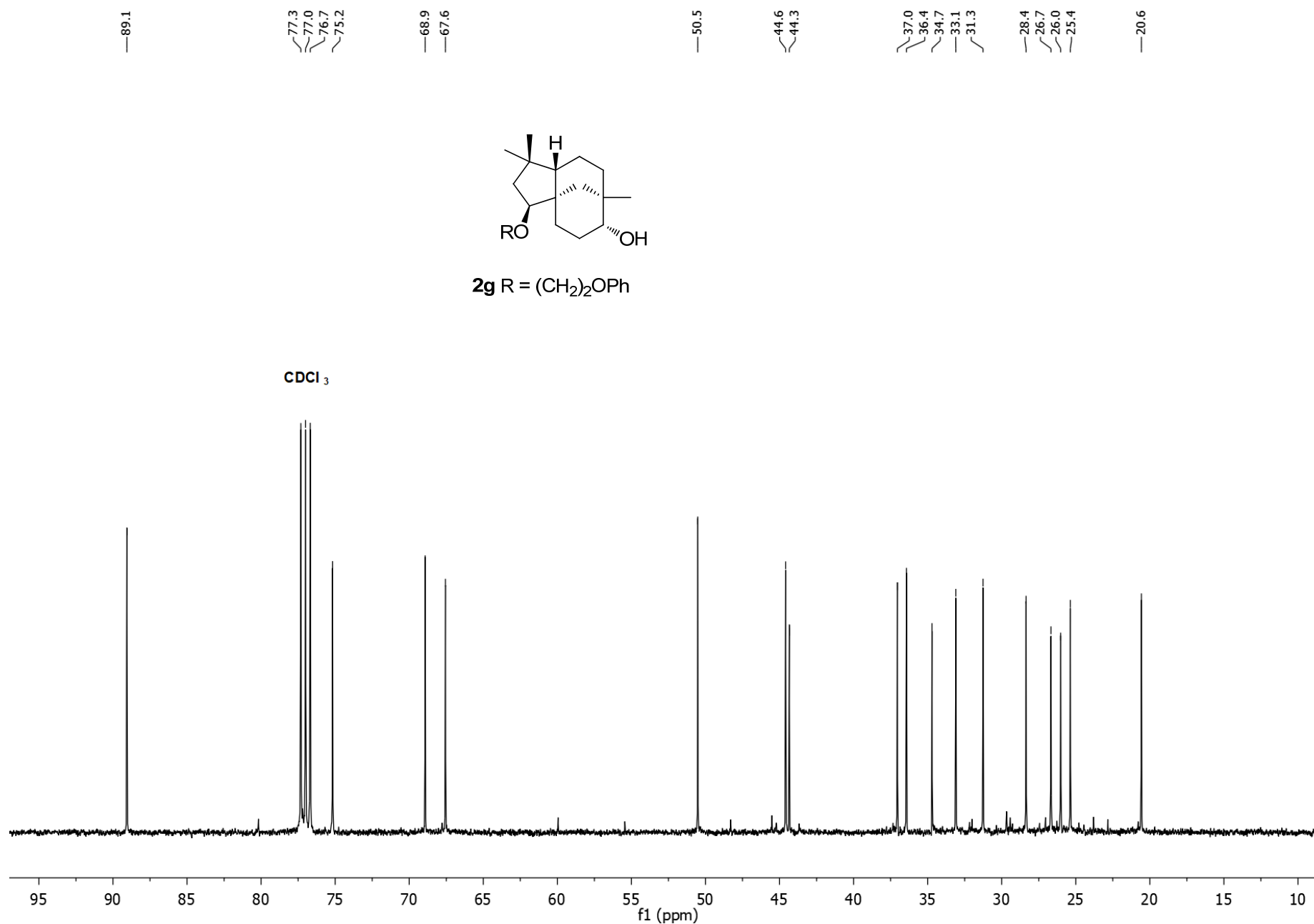


Figure S8a. Expansion (δ_c 95-10) of ¹³C NMR spectrum of compound **2g** in CDCl₃ (100 MHz).

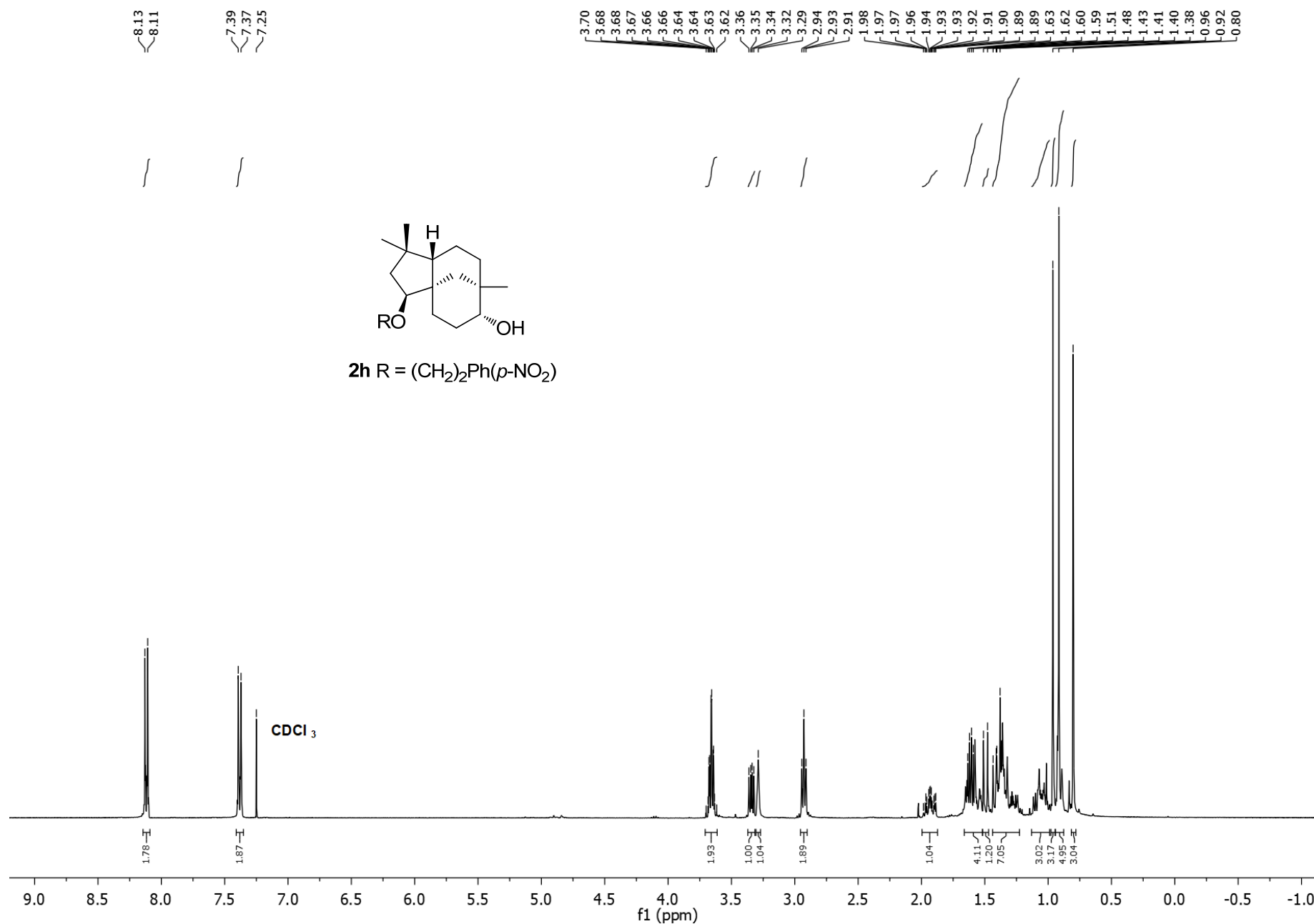


Figure S9. ¹H NMR spectrum of compound **2h** in CDCl₃ (400 MHz).

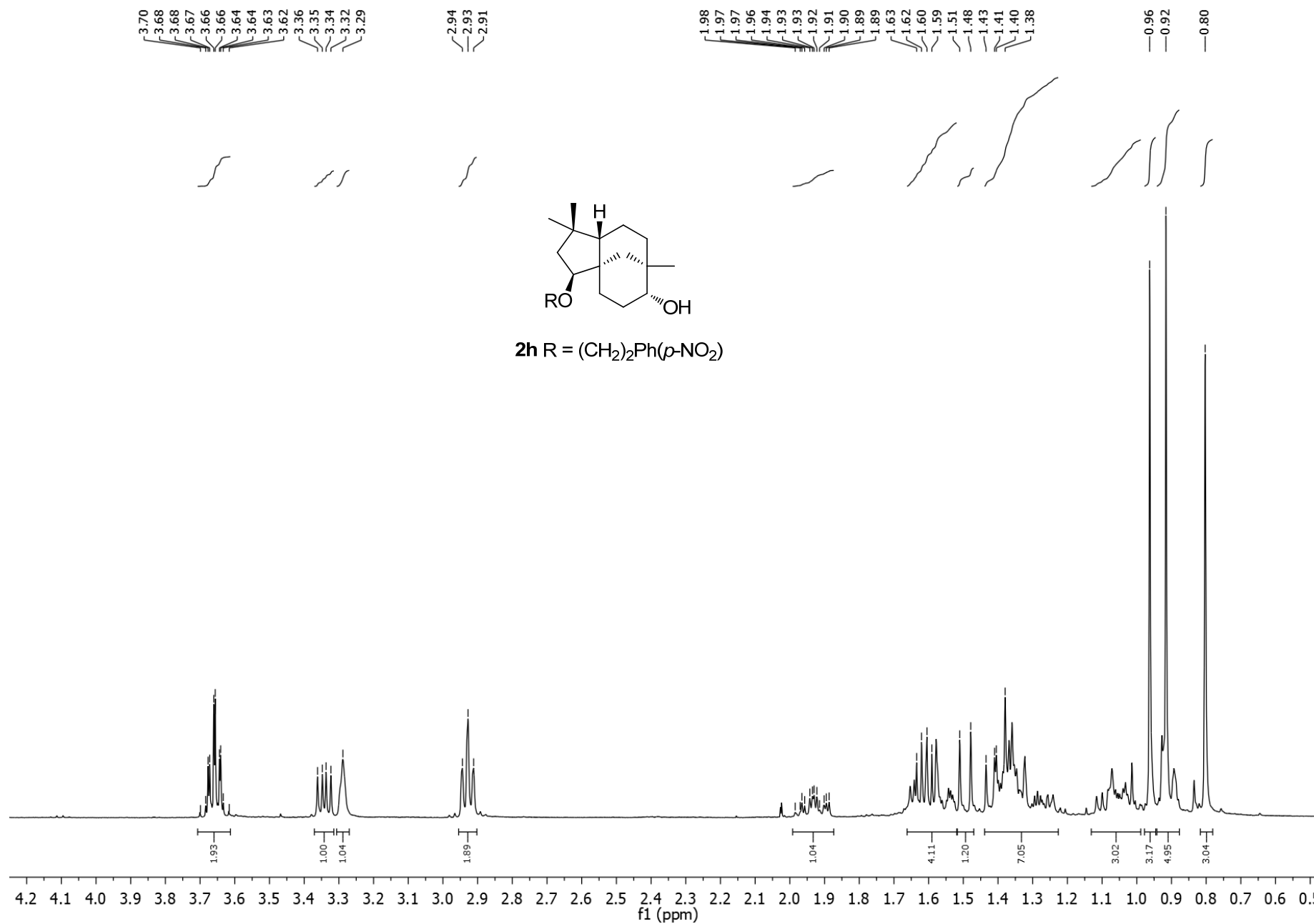


Figure S9a. Expansion (δ_{H} 4.2-0.5) of ^1H NMR spectrum of compound **2h** in CDCl_3 (400 MHz).

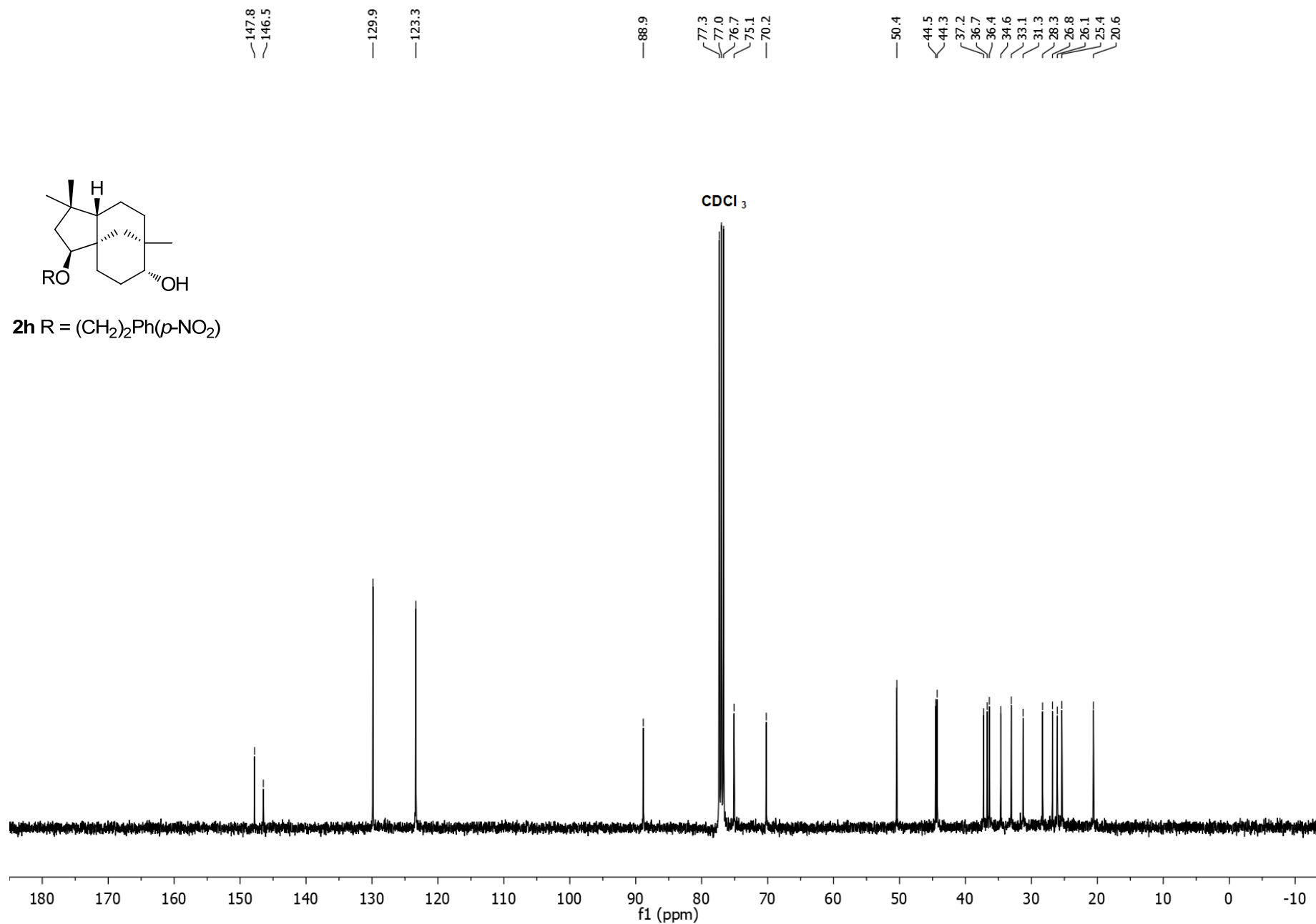


Figure S10. ¹³C NMR spectrum of compound **2h** in CDCl₃ (100 MHz).

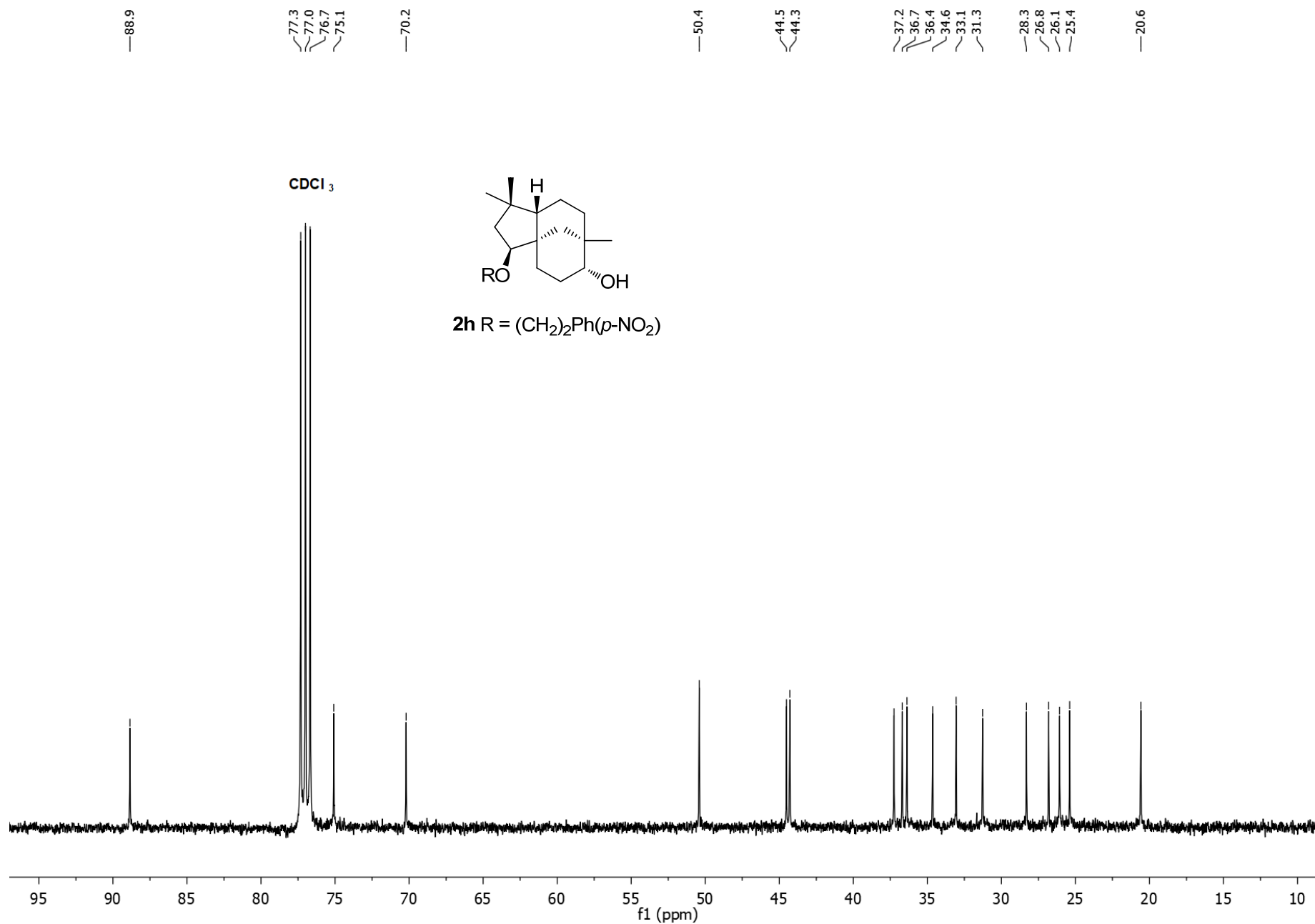


Figure S10a. Expansion (δ_C 95-10) of ^{13}C NMR spectrum of compound **2h** in $CDCl_3$ (100 MHz).

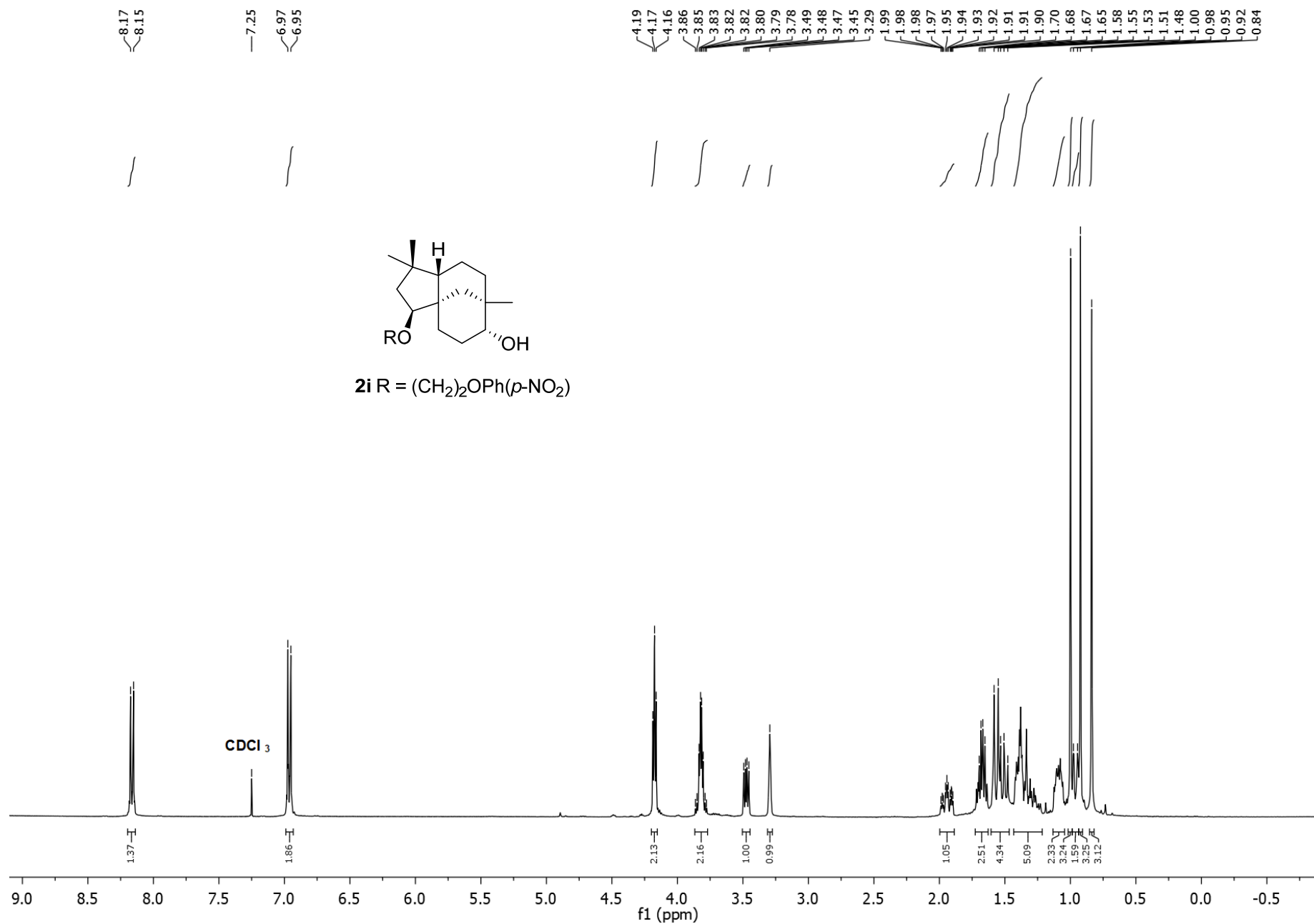


Figure S11. 1H NMR spectrum of compound **2i** in $CDCl_3$ (400 MHz).

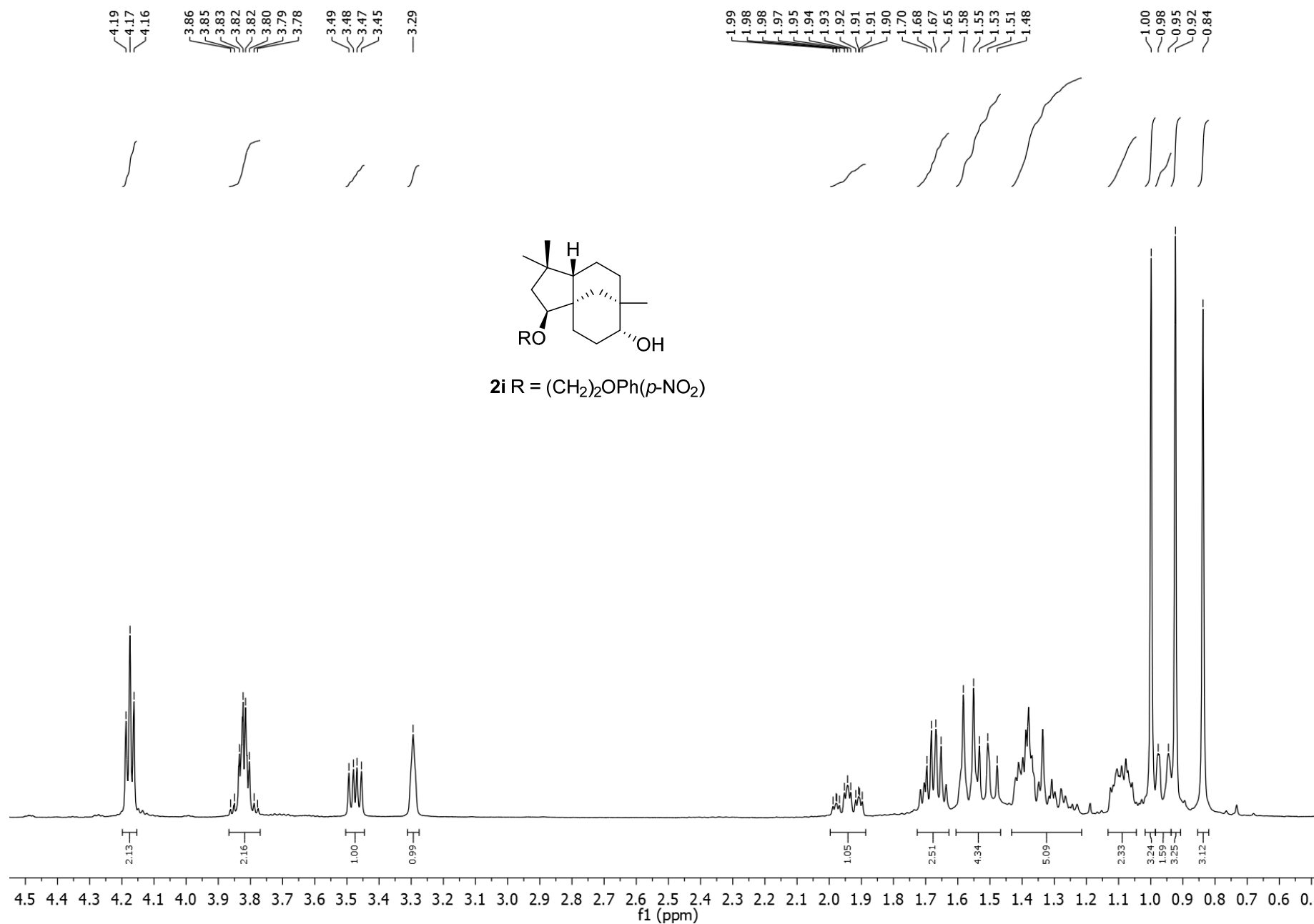


Figure S11a. Expansion (δ_H 4.5-0.5) of 1H NMR spectrum of compound **2i** in $CDCl_3$ (400 MHz).

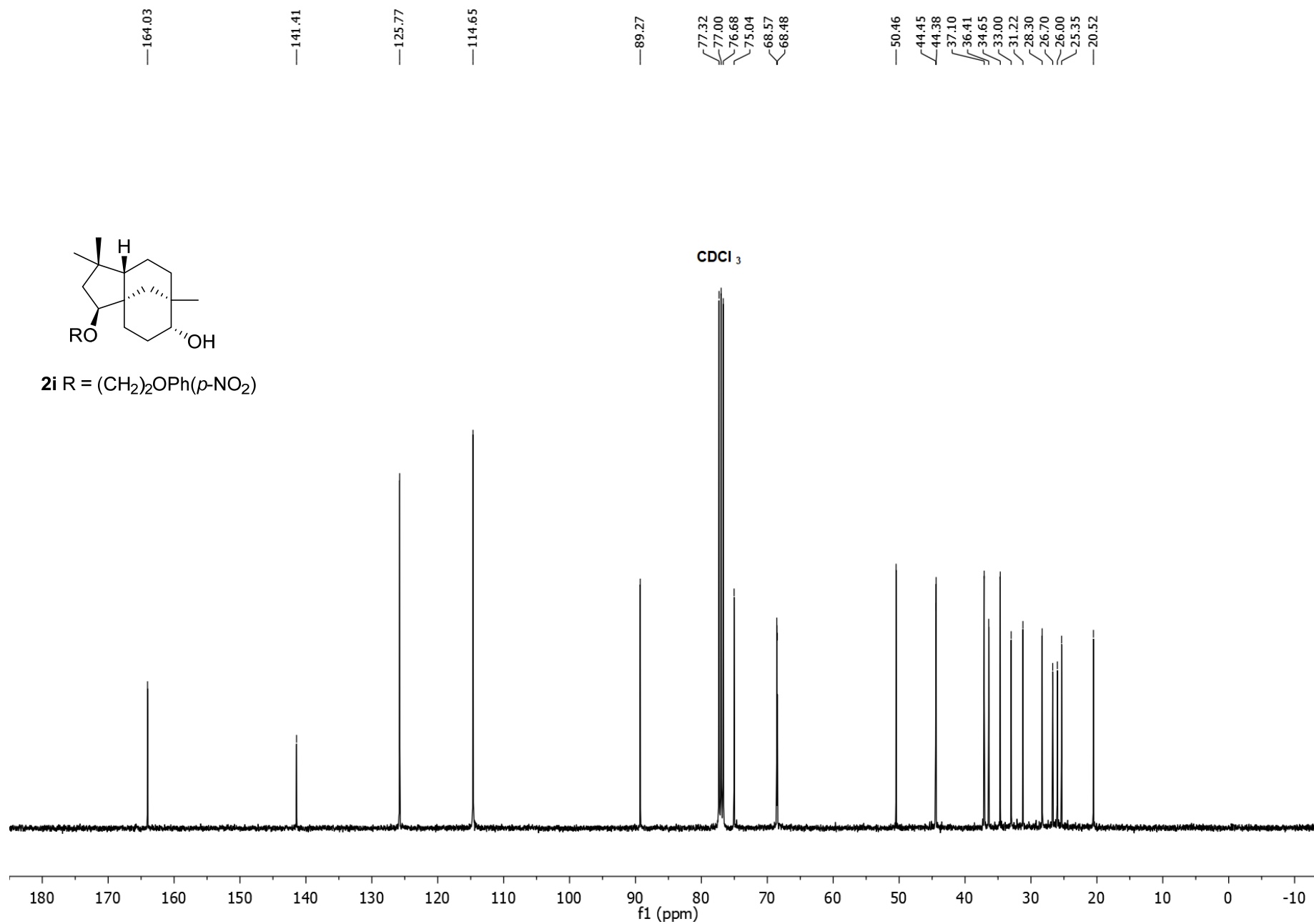


Figure S12. ^{13}C NMR spectrum of compound **2i** in $CDCl_3$ (100 MHz).

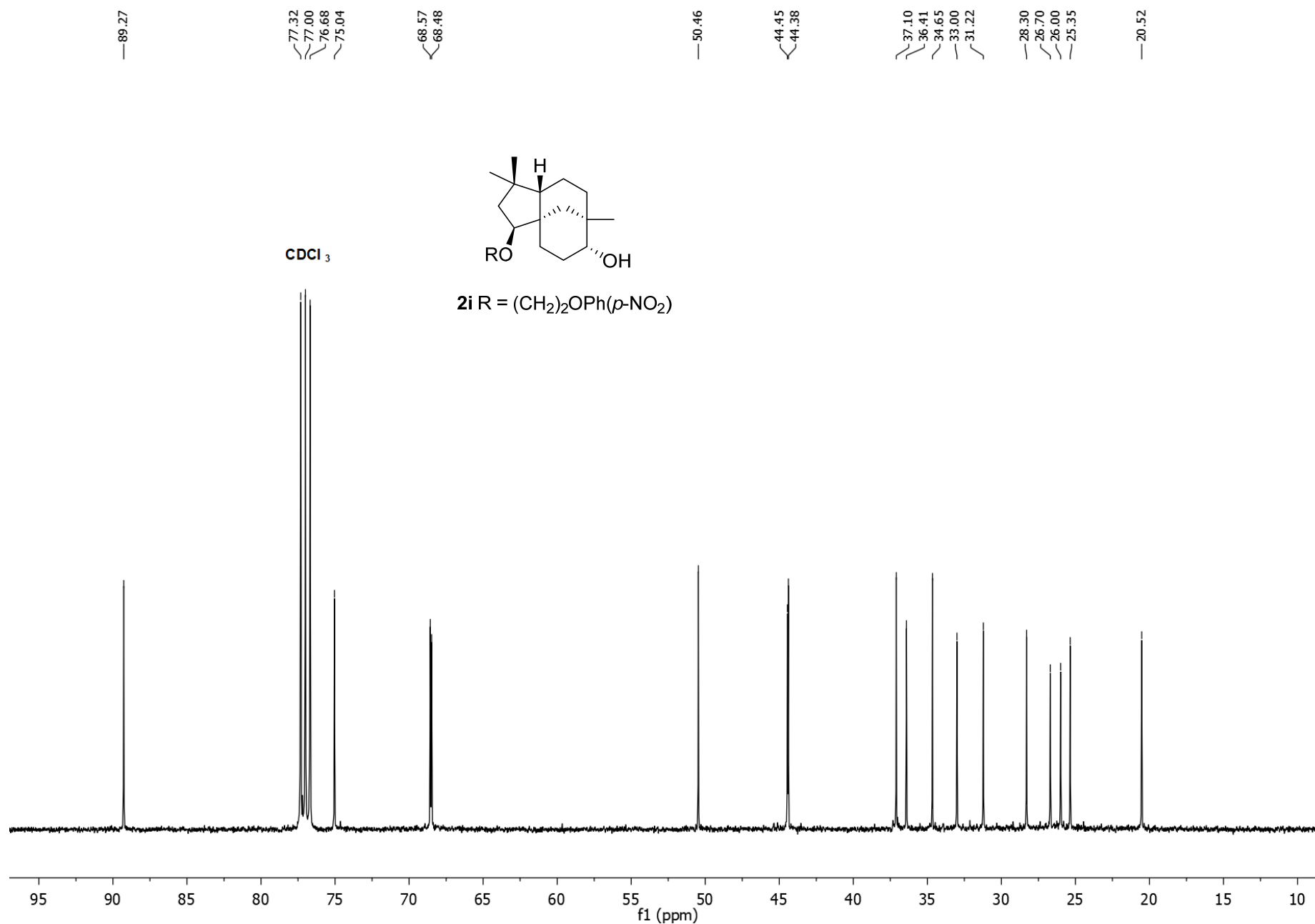


Figure S12a. Expansion (δ_C 95-10) of ^{13}C NMR spectrum of compound **2i** in $CDCl_3$ (100 MHz).

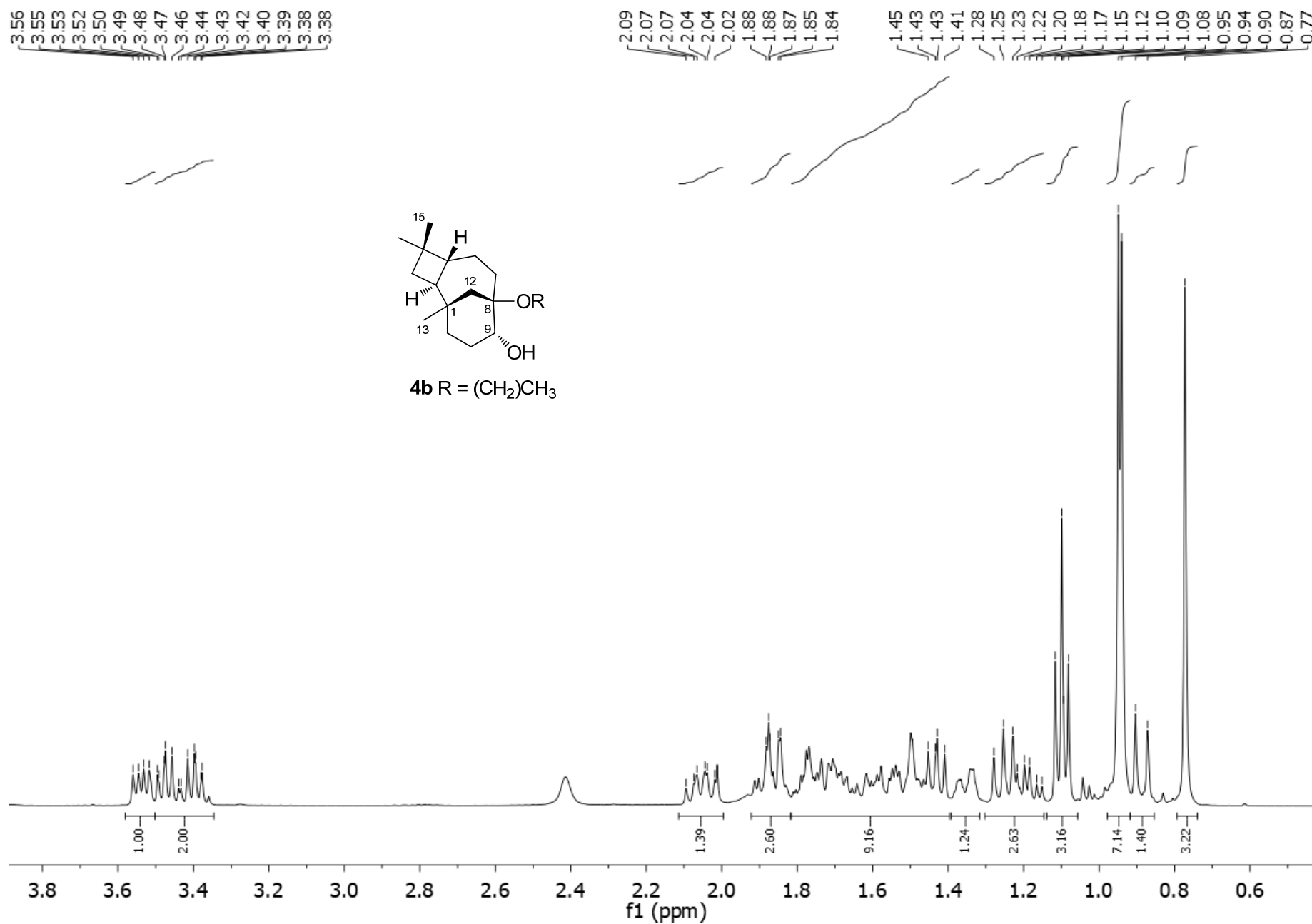


Figure S13a. Expansion (δ_H 3.8-0.5) of 1H NMR spectrum of compound **4b** in $CDCl_3$ (400 MHz).

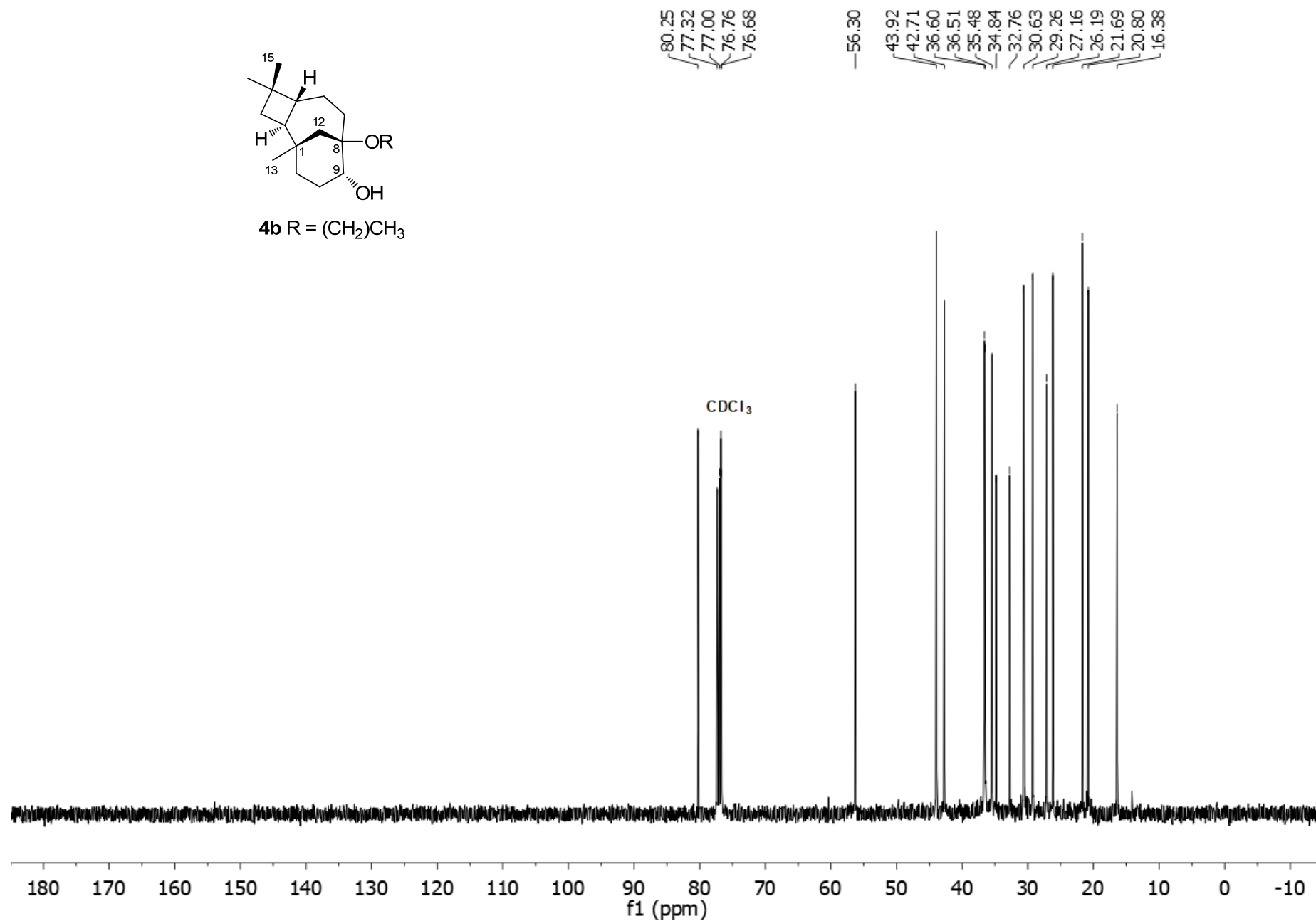


Figure S14. ^{13}C NMR spectrum of compound **4b** in $CDCl_3$ (100 MHz).

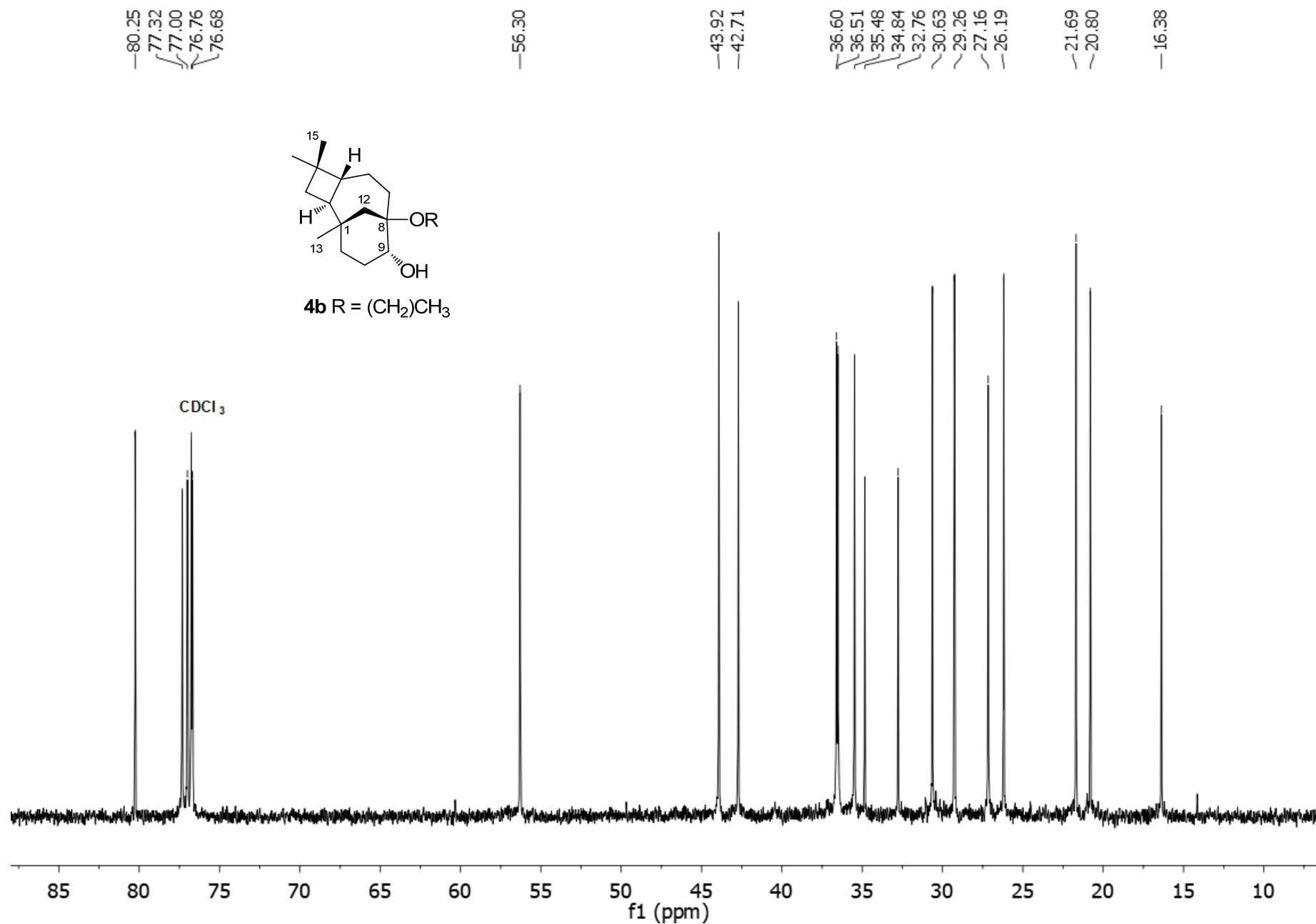


Figure S14a. Expansion (δ_C 95-10) of ^{13}C NMR spectrum of compound **4b** in CDCl₃ (100 MHz).

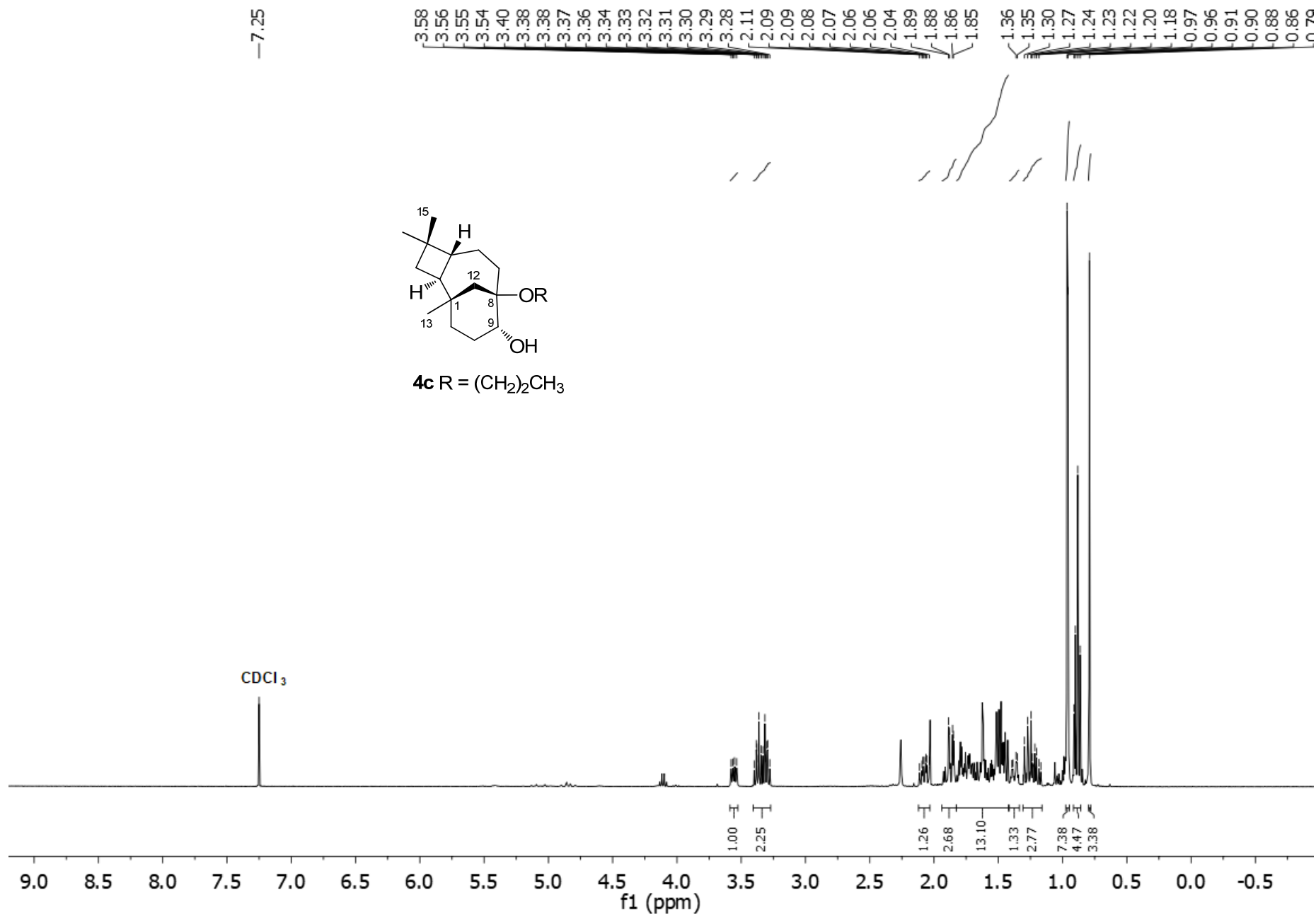


Figure S15. ¹H NMR spectrum of compound **4c** in CDCl₃ (400 MHz).

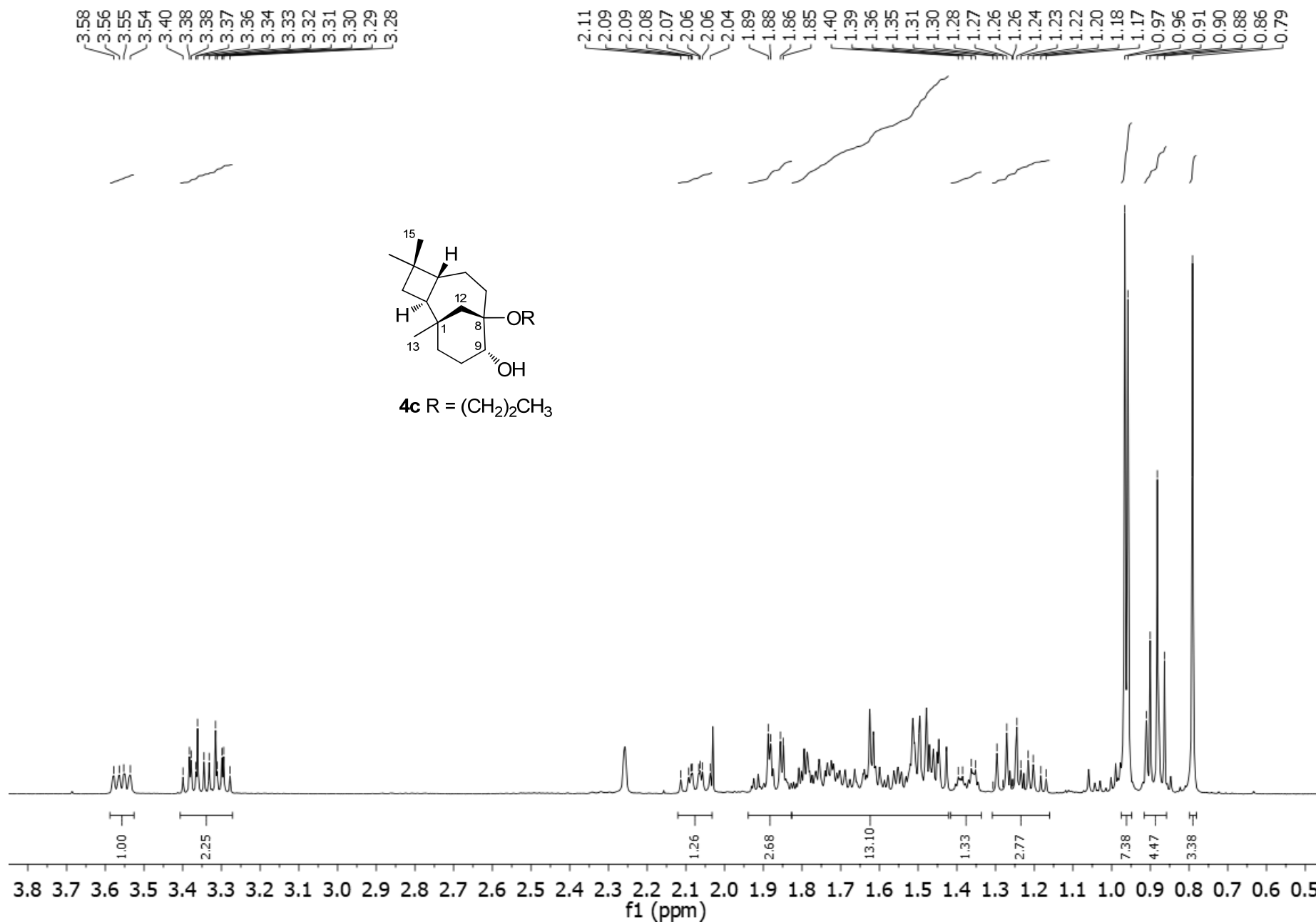


Figure S15a. Expansion (δ_H 3.8-0.5) of 1H NMR spectrum of compound **4c** in CDCl₃ (400 MHz).

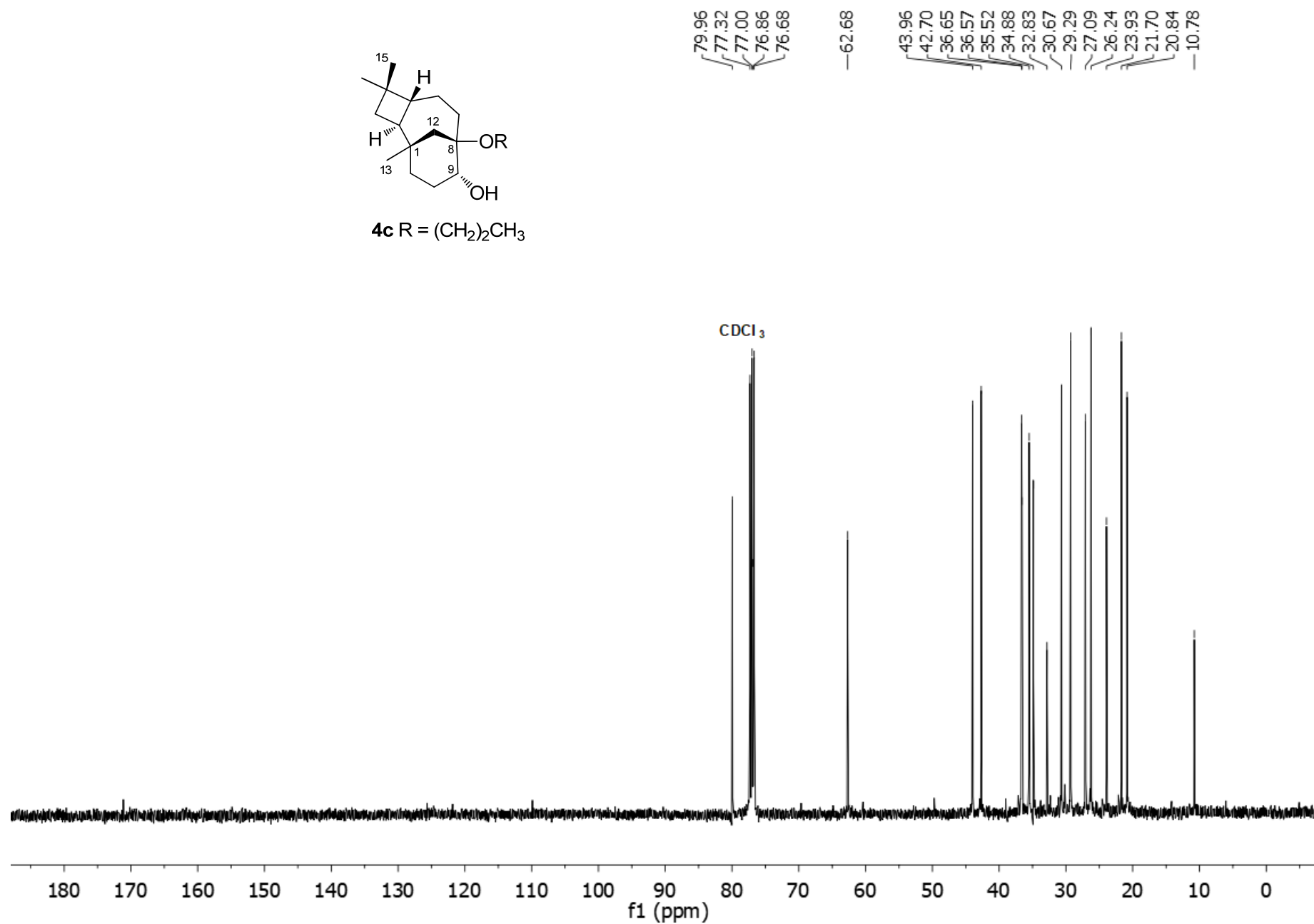


Figure S16. ^{13}C NMR spectrum of compound **4c** in $CDCl_3$ (100 MHz).

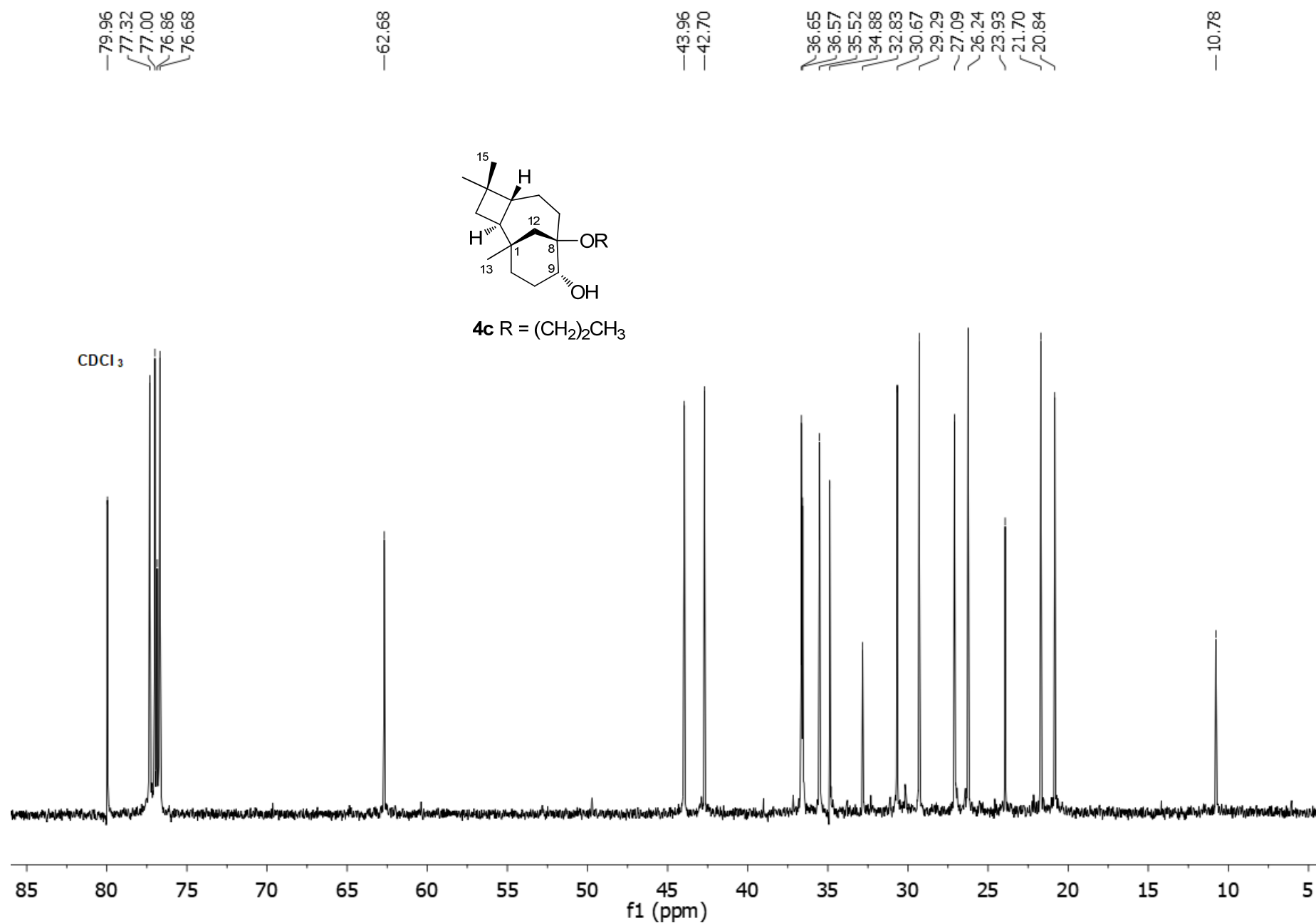


Figure S16a. Expansion (δ 85-5) of ^{13}C NMR spectrum of compound **4c** in $CDCl_3$ (100 MHz).

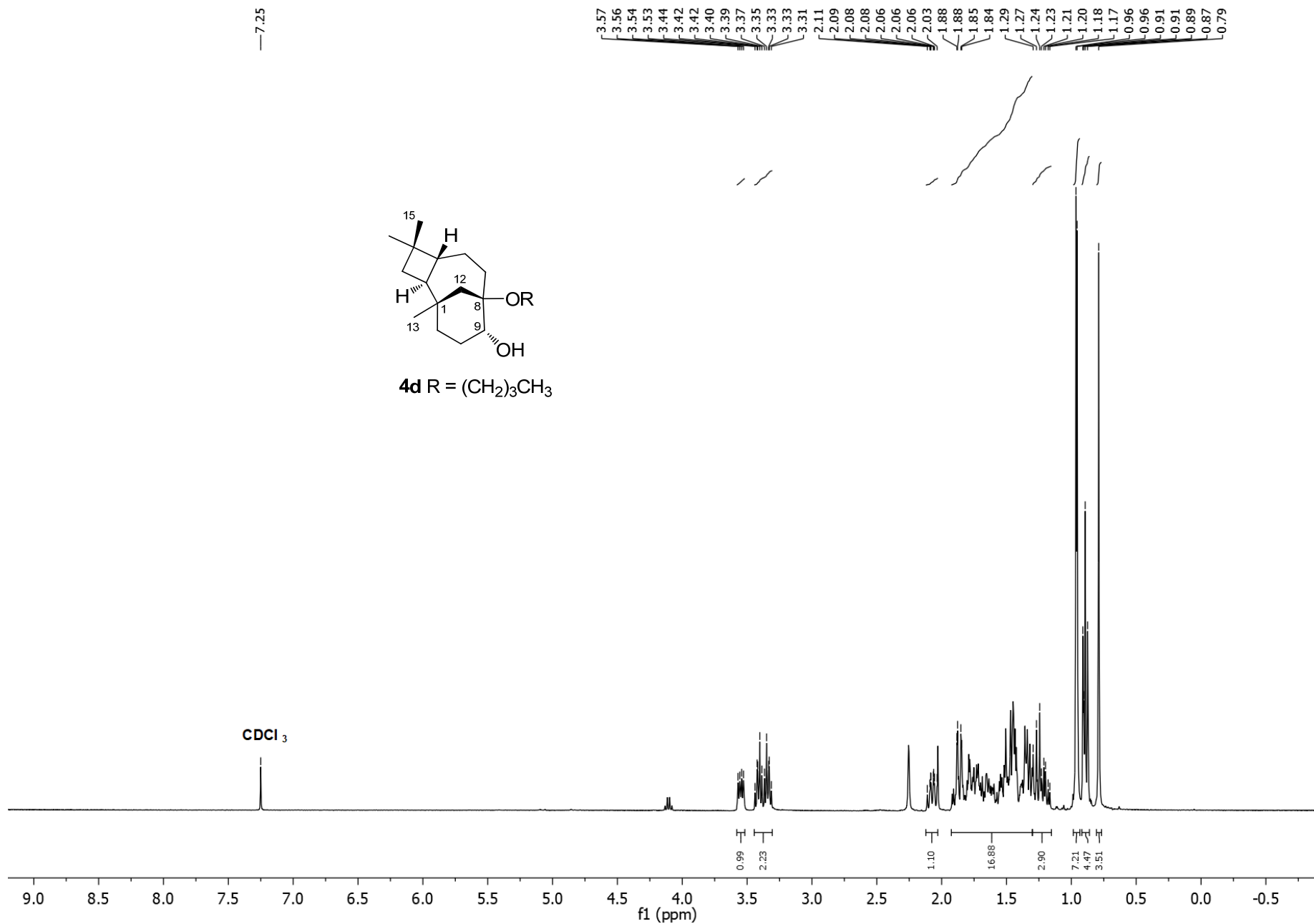


Figure S17. 1H NMR spectrum of compound **4d** in $CDCl_3$ (400 MHz).

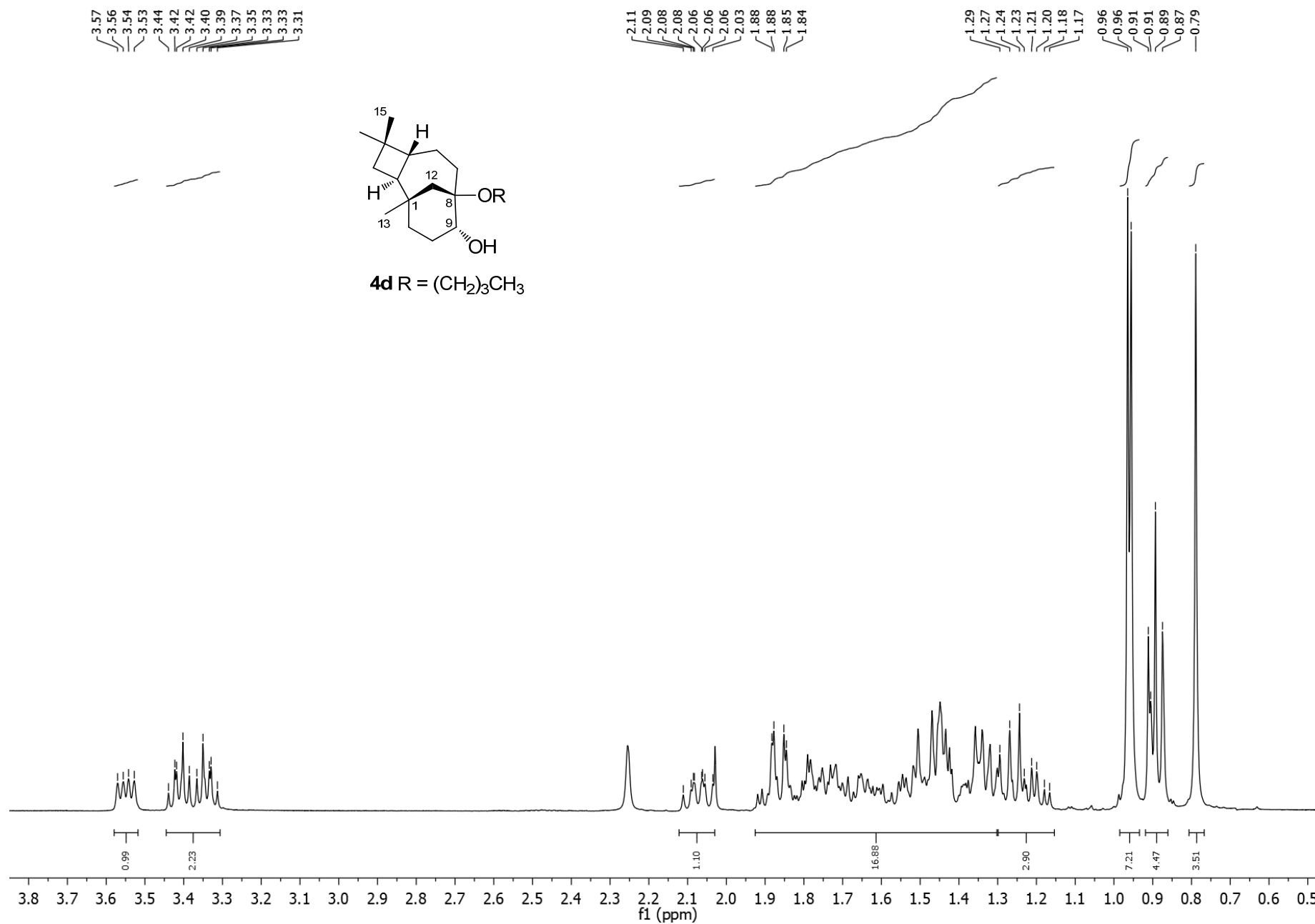


Figure S17a. Expansion (δ_H 3.8-0.5) of 1H NMR spectrum of compound **4d** in $CDCl_3$ (400 MHz).

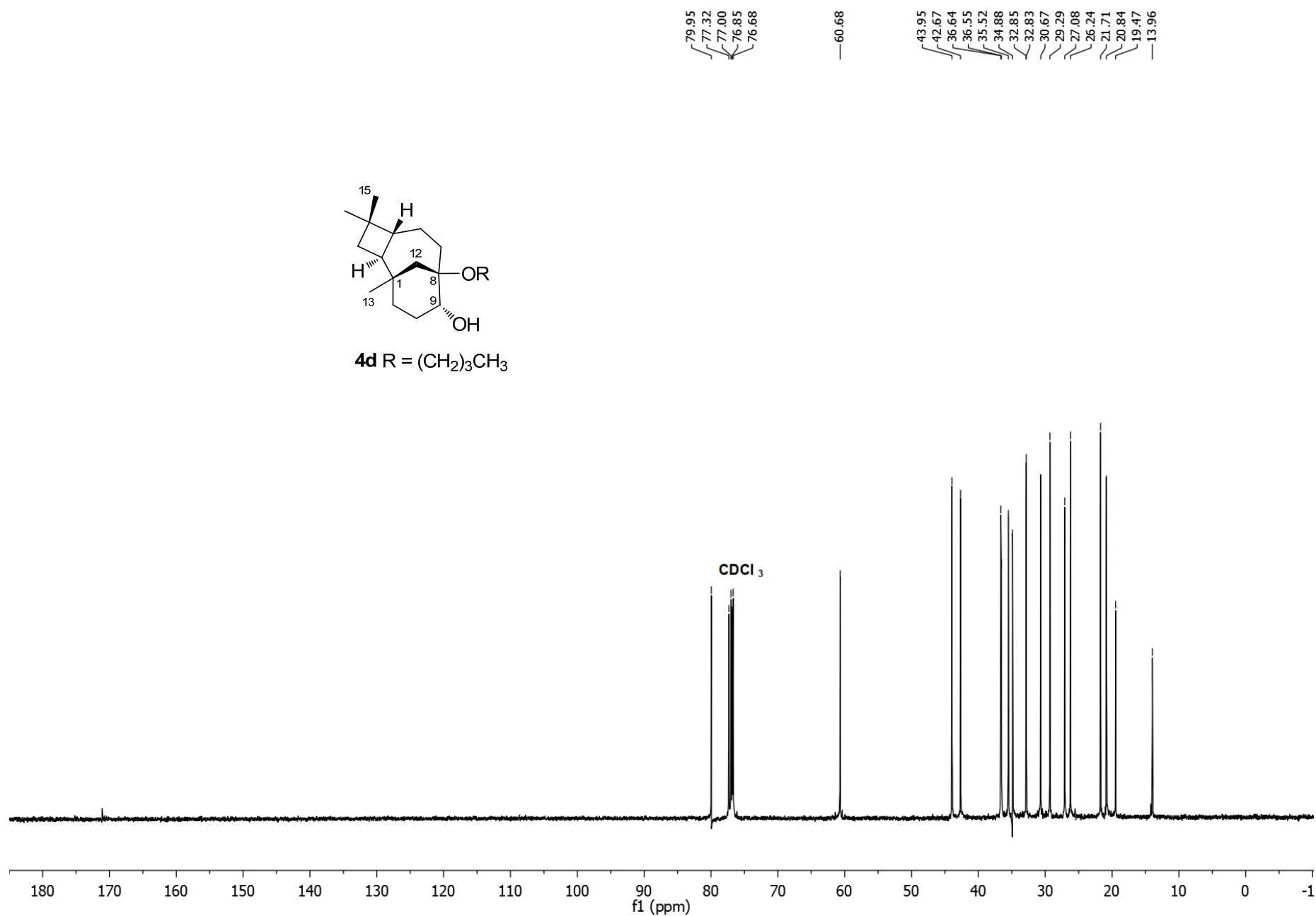


Figure S18. ¹³C NMR spectrum of compound **4d** in CDCl₃ (100 MHz).

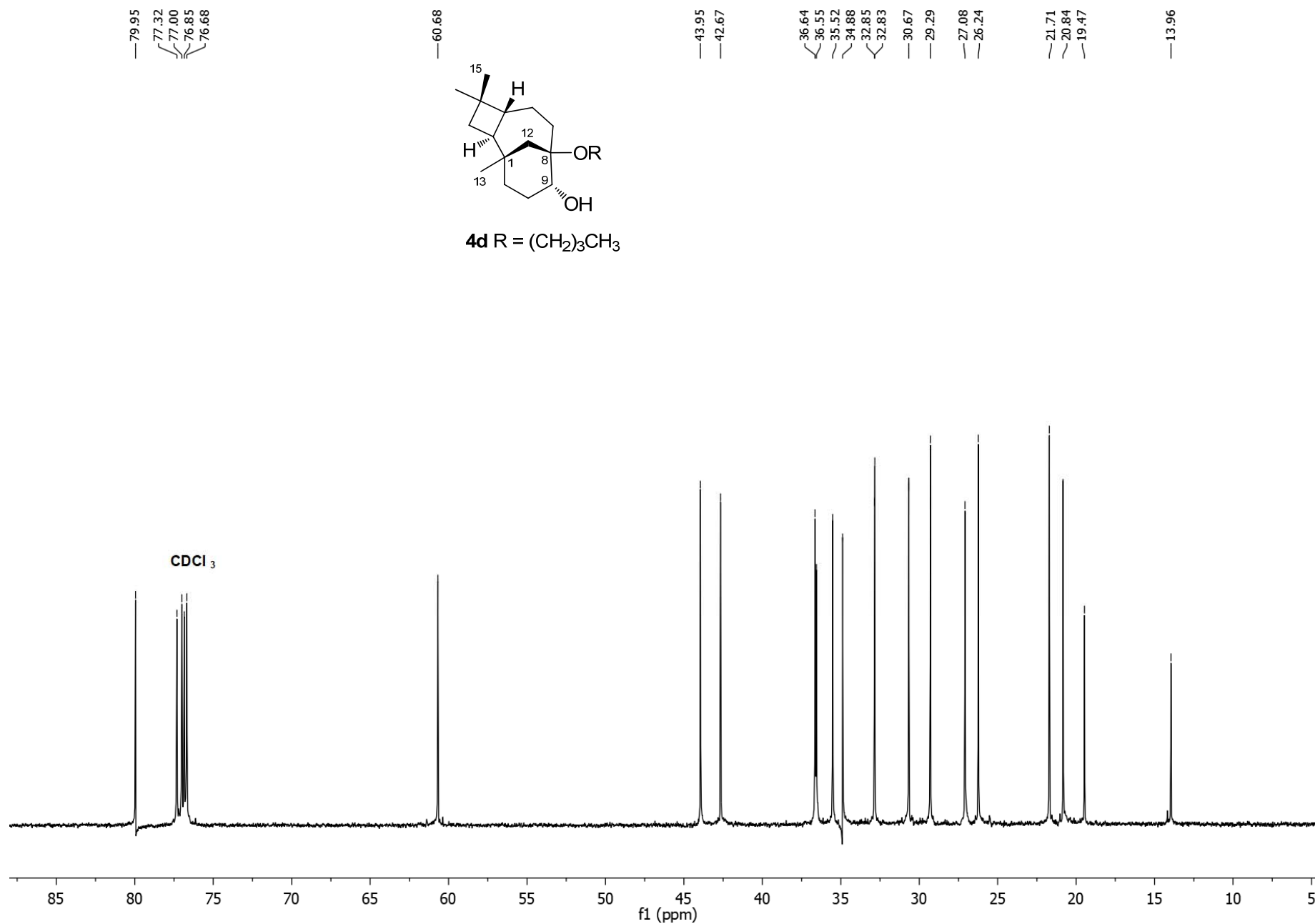


Figure S18a. Expansion (δ_C 85-5) of ^{13}C NMR spectrum of compound **4d** in $CDCl_3$ (100 MHz).

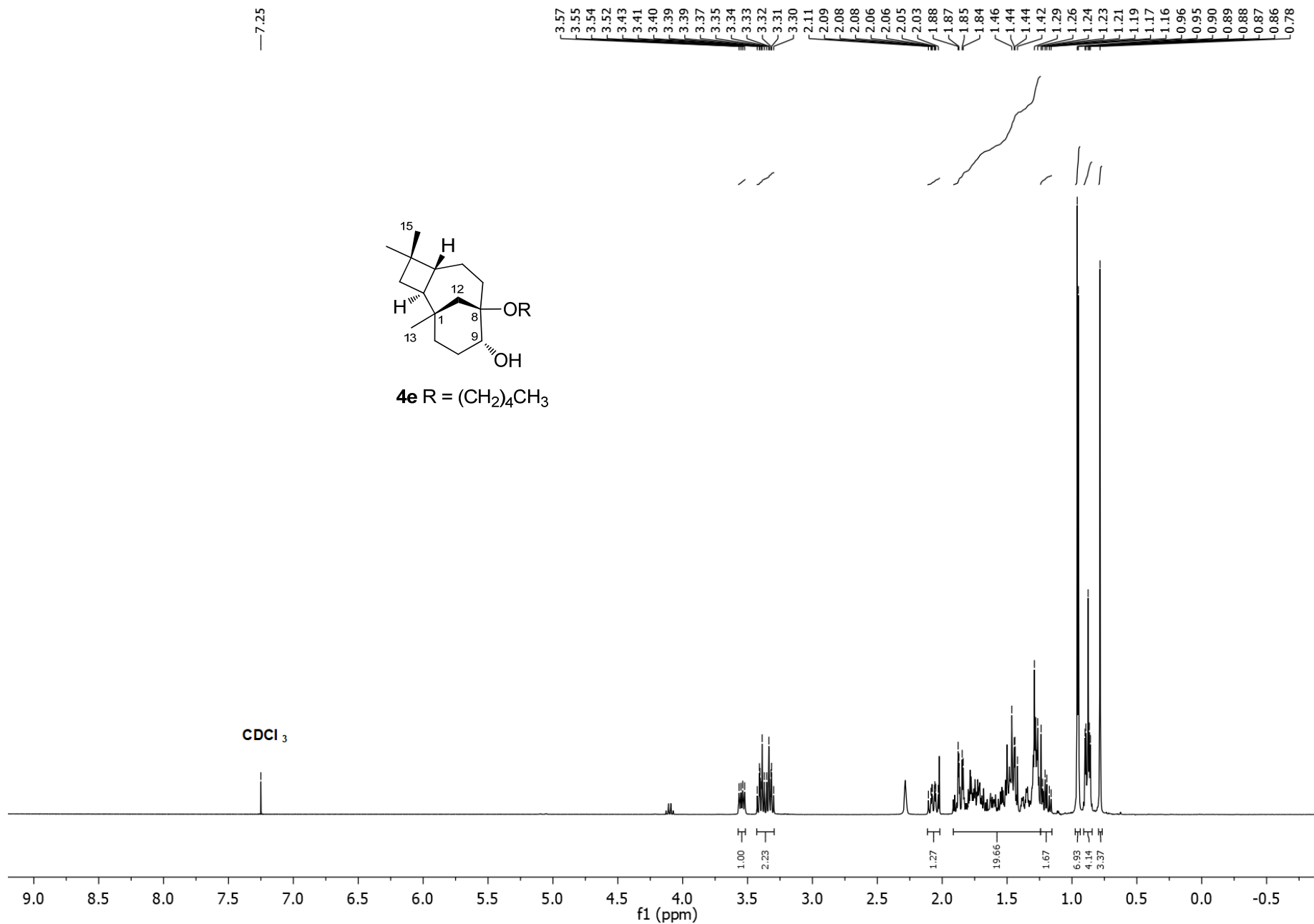


Figure S19. 1H NMR spectrum of compound **4e** in $CDCl_3$ (400 MHz).

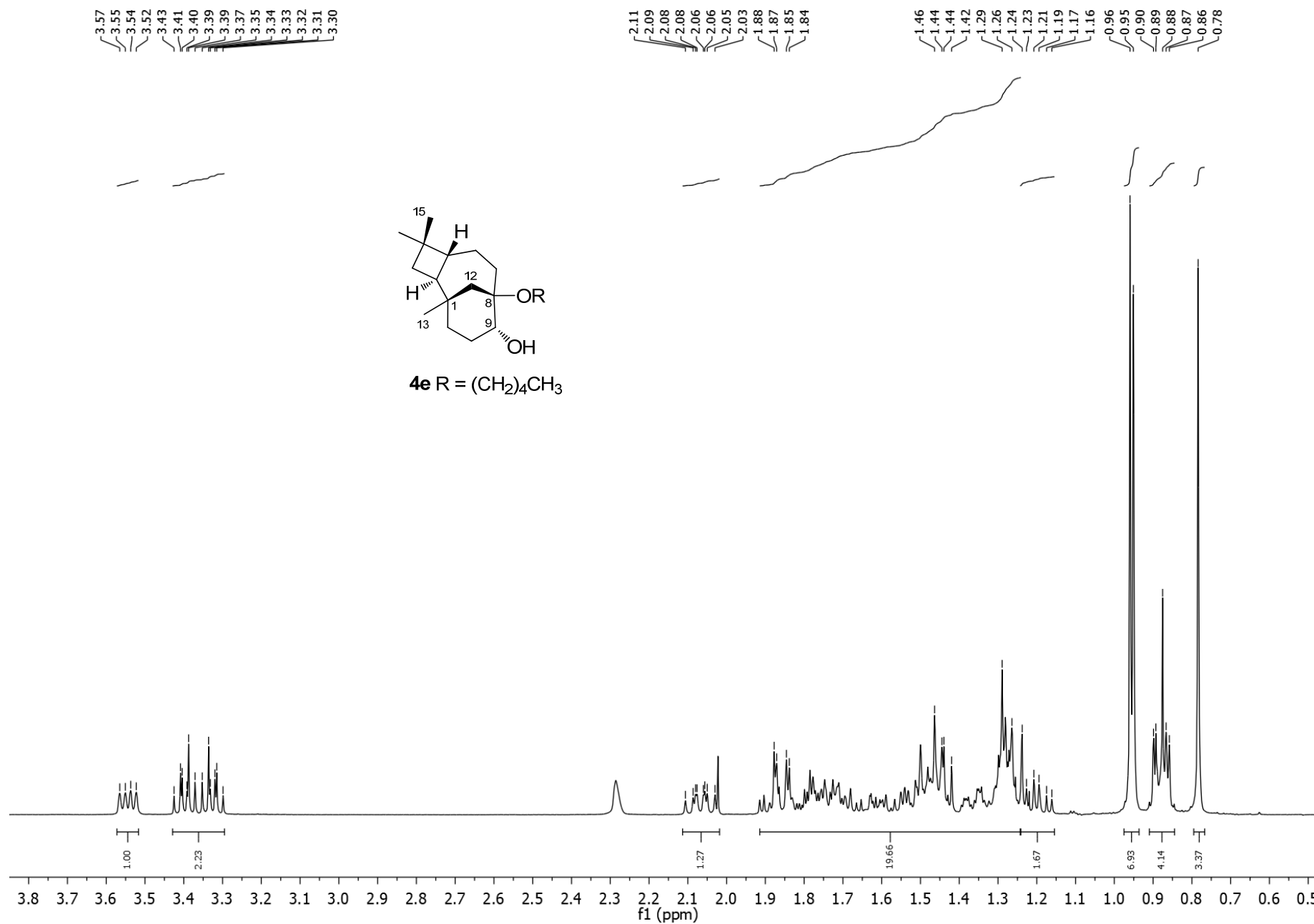


Figure S19a. Expansion (δ_H 3.8-0.5) of 1H NMR spectrum of compound **4e** in $CDCl_3$ (400 MHz).

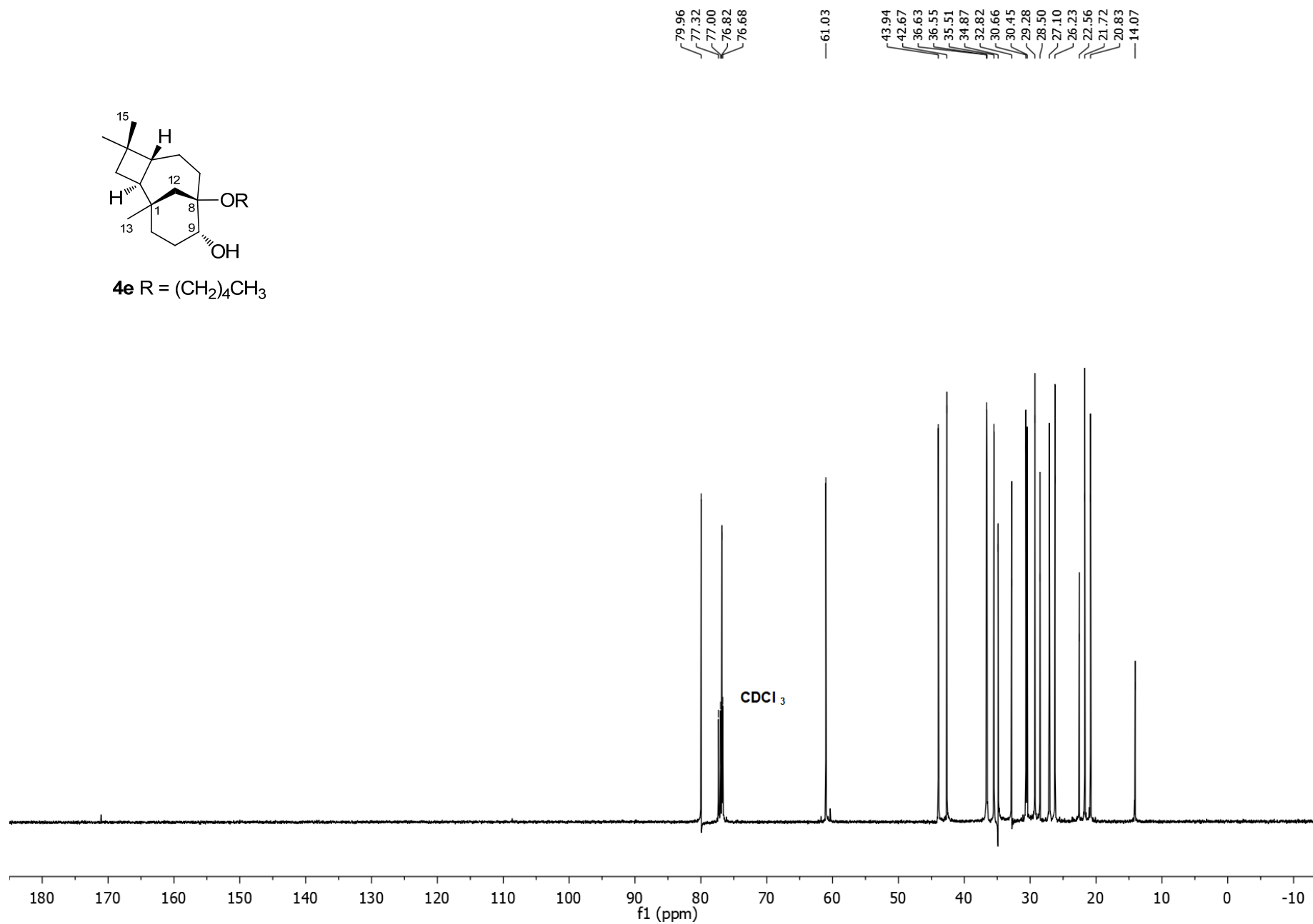


Figure S20. ¹³C NMR spectrum of compound **4e** in CDCl₃ (100 MHz).

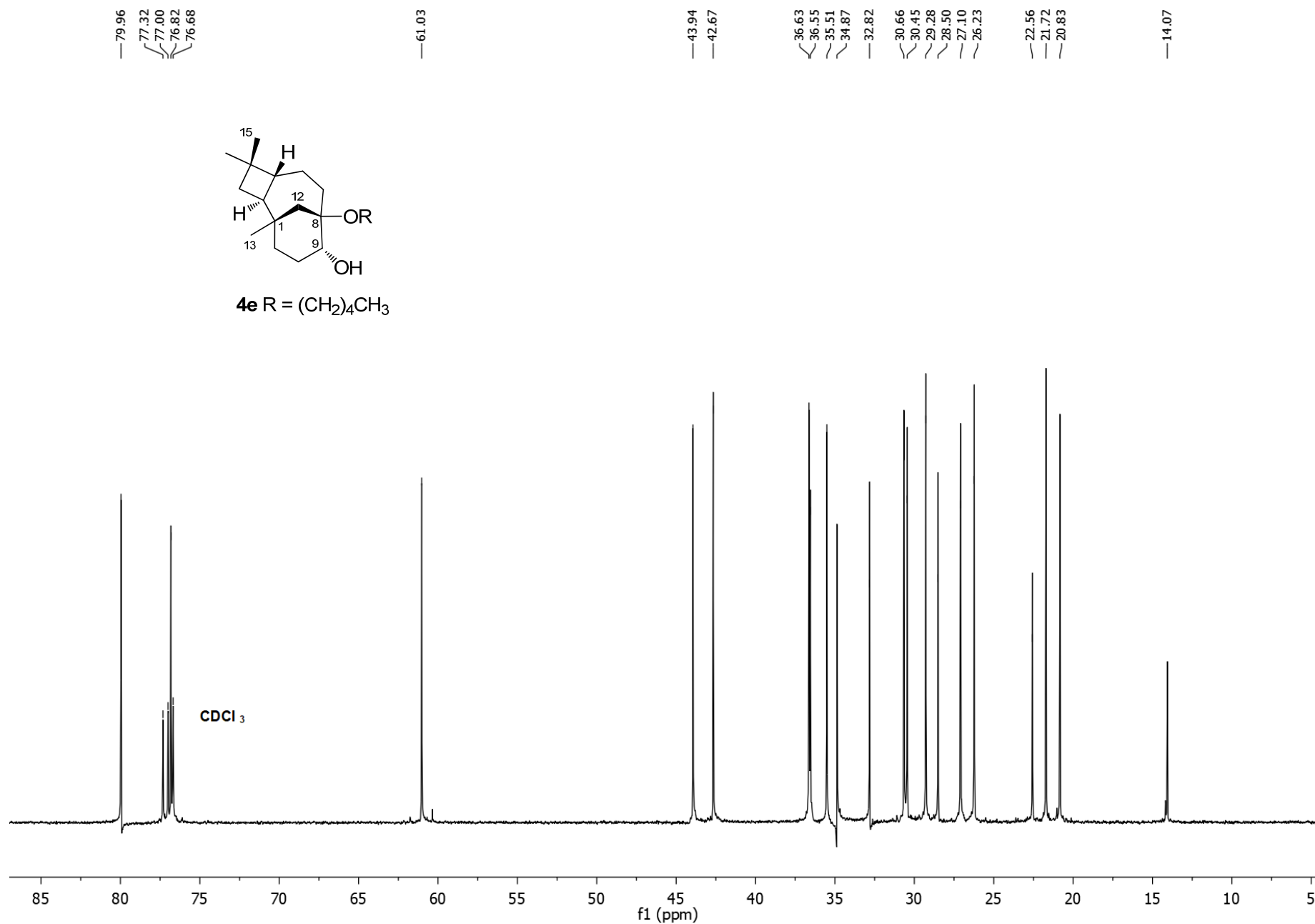


Figure S20a. Expansion (δ_c 85-5) of ^{13}C NMR spectrum of compound **4e** in $CDCl_3$ (100 MHz).