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Sesquiterpenes and lignans from the flower buds of *Daphne genkwa* and their nitric oxide inhibitory activities.

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SUPPLEMENTARY MATERIAL

Sesquiterpenes and lignans from the flower buds of *Daphne genkwa* and their nitric oxide inhibitory activities

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Abstract: Chemical investigation of the *Daphne genkwa* has led to the isolation of four sesquiterpenes (**1a/1b**, **2**, and **3**), including one pair of sesquiterpene enantiomers (**1a/1b**), **1a** is a new compound (+)-4-Hydroxy-10-epirotundone, and twelve lignans (**4–15**). Their structures were elucidated by spectroscopic analysis, and the absolute configurations of **1a/1b** were determined by CD analysis. All compounds were examined for their inhibitory effects on the nitric oxide (NO) production induced by lipopolysaccharide (LPS) in BV-2 microglial cells, and compounds **7–10** exhibited pronounced inhibition on NO production with IC₅₀ values in the range of 5.8–10.2 μM, being more active than the positive control, quercetin (IC₅₀ = 17.0 μM).

Keywords: *Daphne genkwa*; Sesquiterpene; Lignan; Nitric Oxide

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Table S1. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data of compound **1** in CDCl_3 (δ_{C} in ppm, J in Hz).

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No.	δ_{H}	δ_{C}	No.	δ_{H}	δ_{C}
1		145.0, C	8b	1.61, m	
2		204.8, C	9a	1.97, m	29.1, CH_2
3a	2.54, 1H, d (3.5)	51.5, CH	9b	1.70, m	
3b	2.55, 1H, d (3.5)		10	2.80, m	29.1, CH
4		76.4, C	11		149.4, C
5		173.8, C	12a	4.78, d (1.4)	110.2, CH_2
6a	2.63, m	28.6, CH_2	12b	4.75, d (1.4, 1.4)	
6b	2.50, m		13	1.76, s	21.0, CH_3
7a	2.51, m	44.5, CH	14	1.12, d (7.2)	18.1, CH_3
8a	1.86, m	29.0, CH_2	15	1.46, s	26.9, CH_3

Figure S1. Selected ^1H - ^1H COSY (—) and HMBC (\rightarrow) correlations of **1**

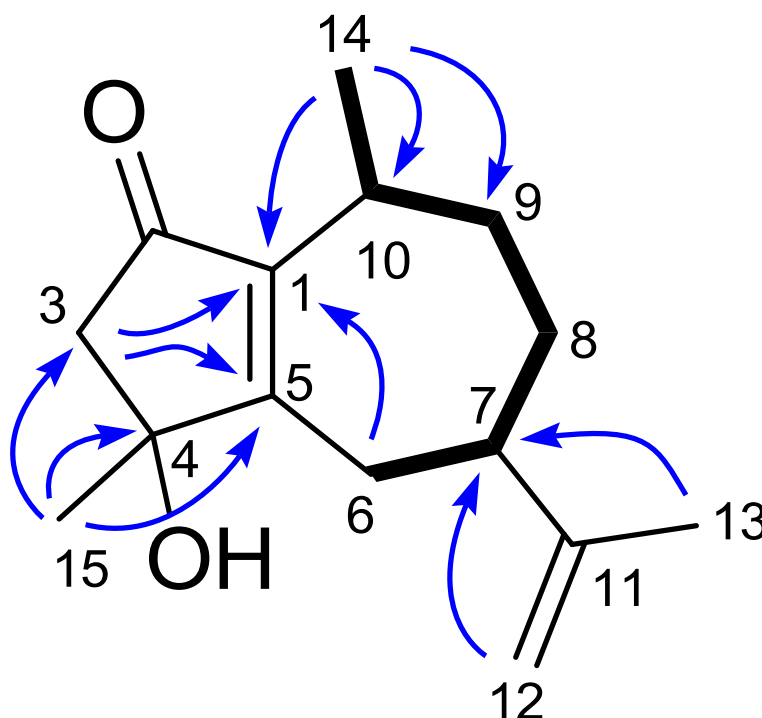


Figure S2. Key NOE correlations ($\leftarrow \cdots \rightarrow$) of **1**.

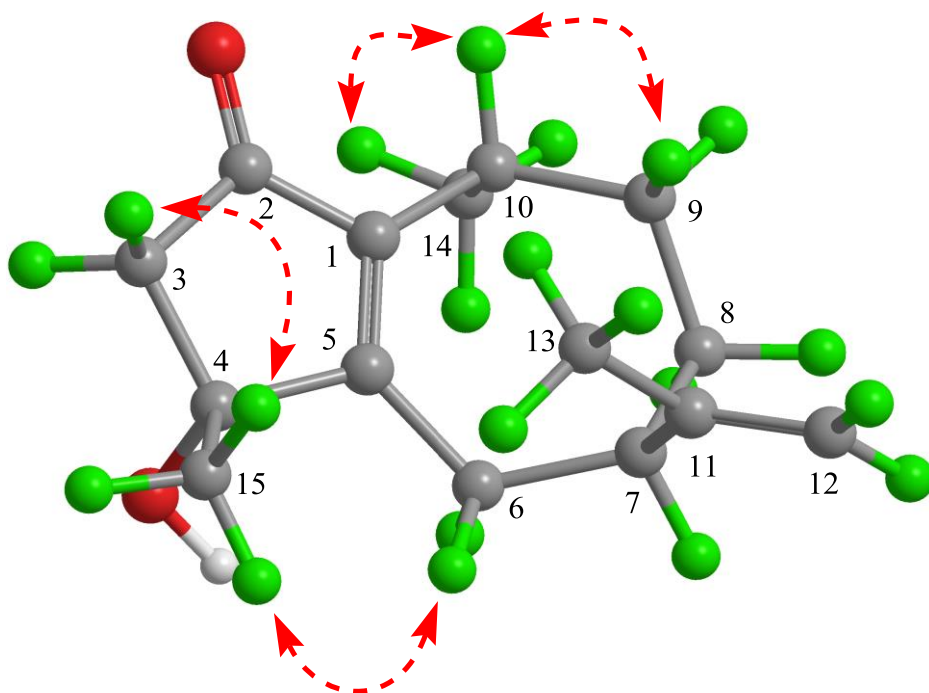


Figure S3. The CD spectrum of **1a** and **1b**

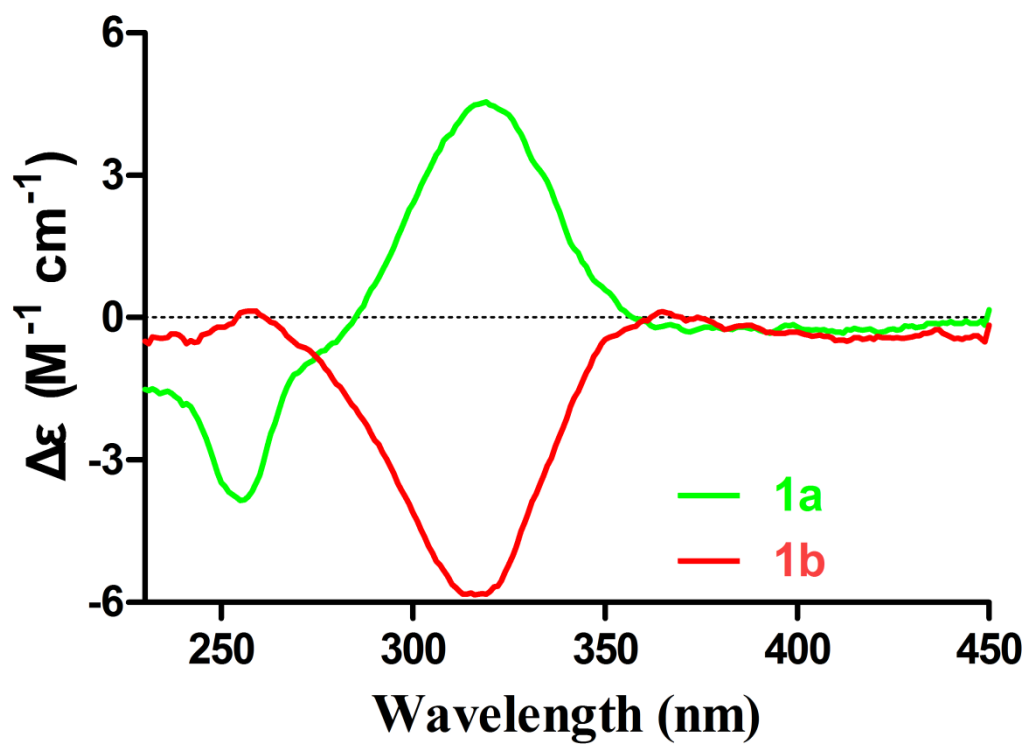


Figure S4. ^1H NMR (400 MHz, CDCl_3) spectrum of **1**

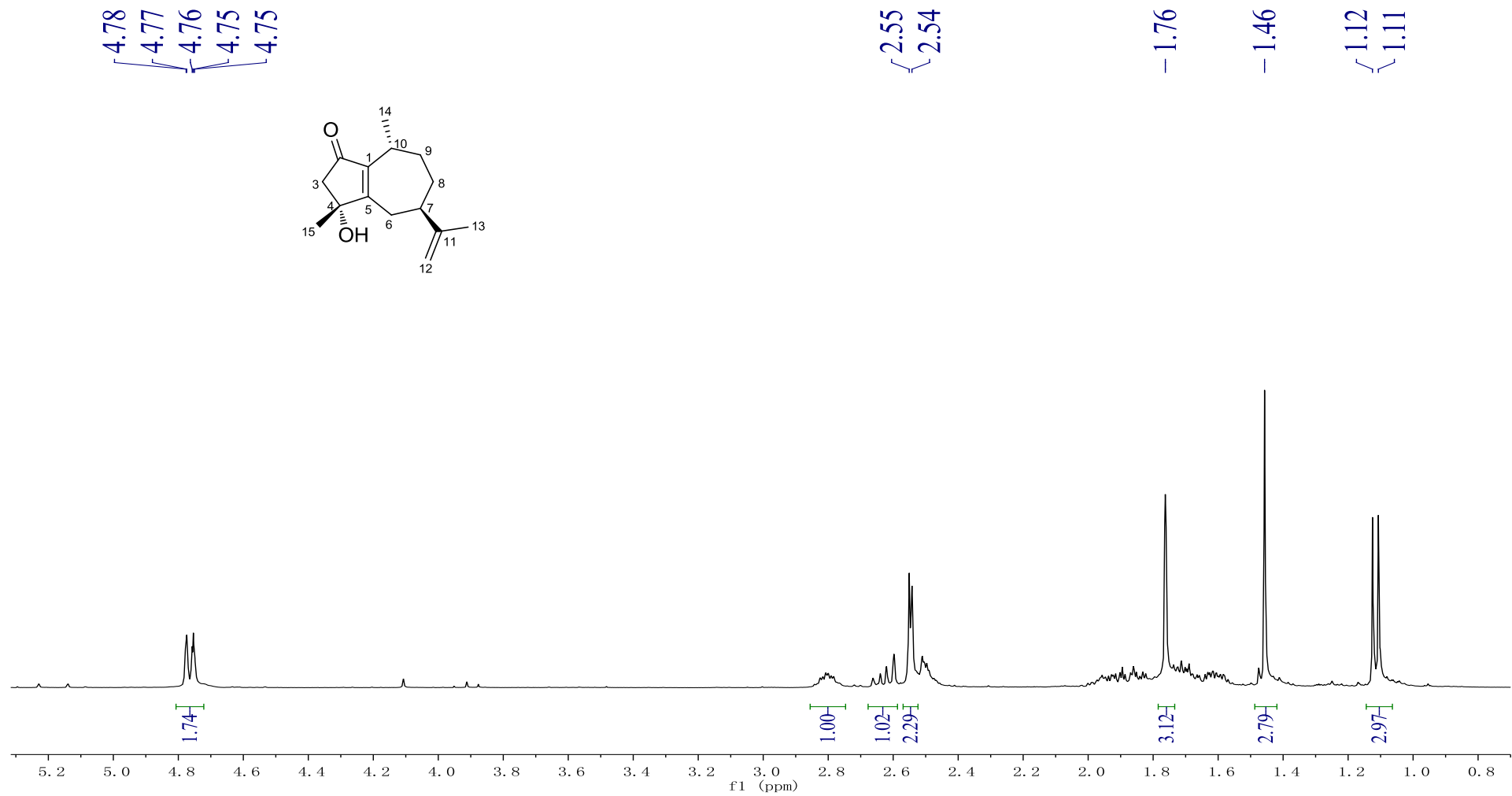


Figure S5. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **1**

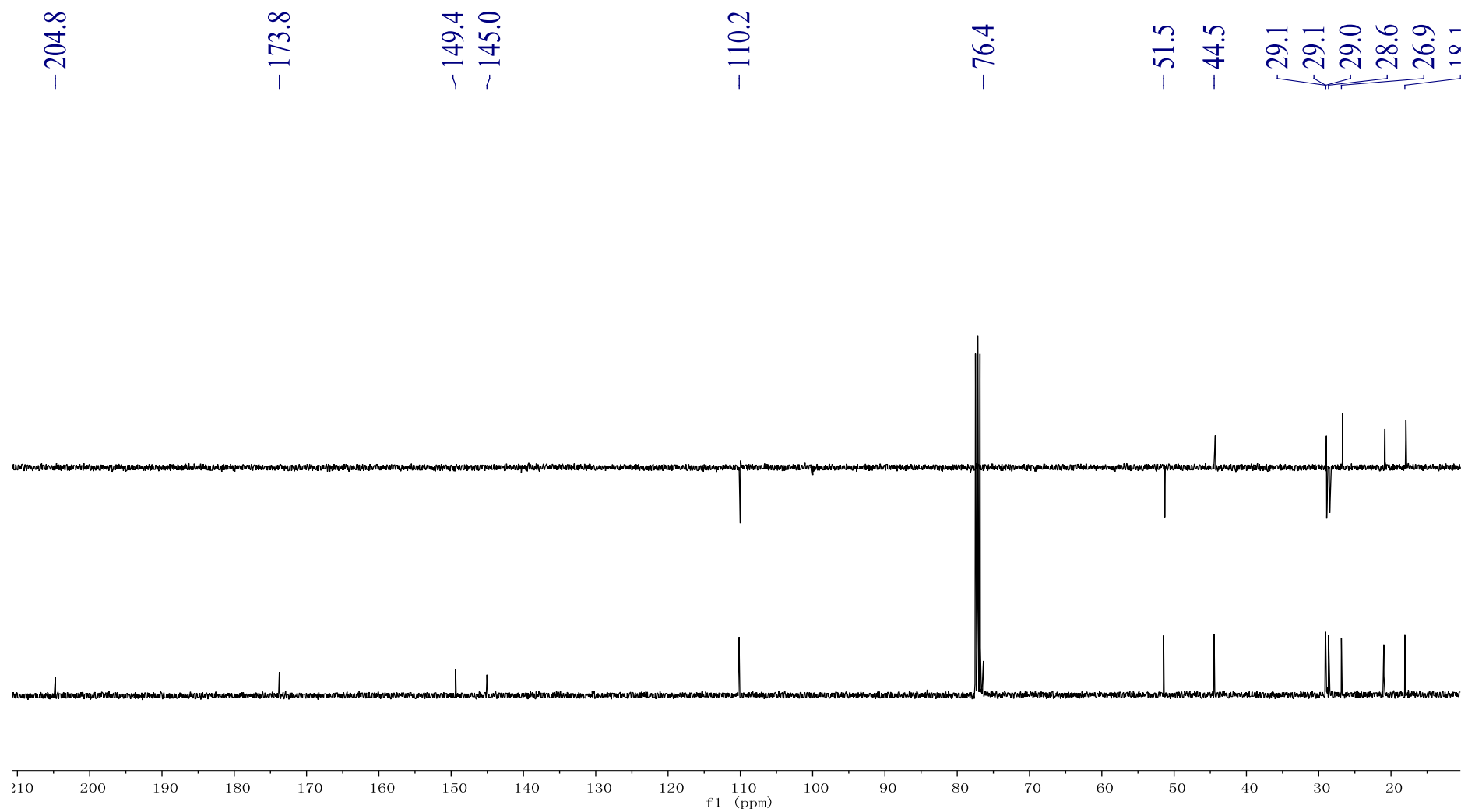


Figure S6. ^1H - ^1H COSY spectrum of **1** in CDCl_3

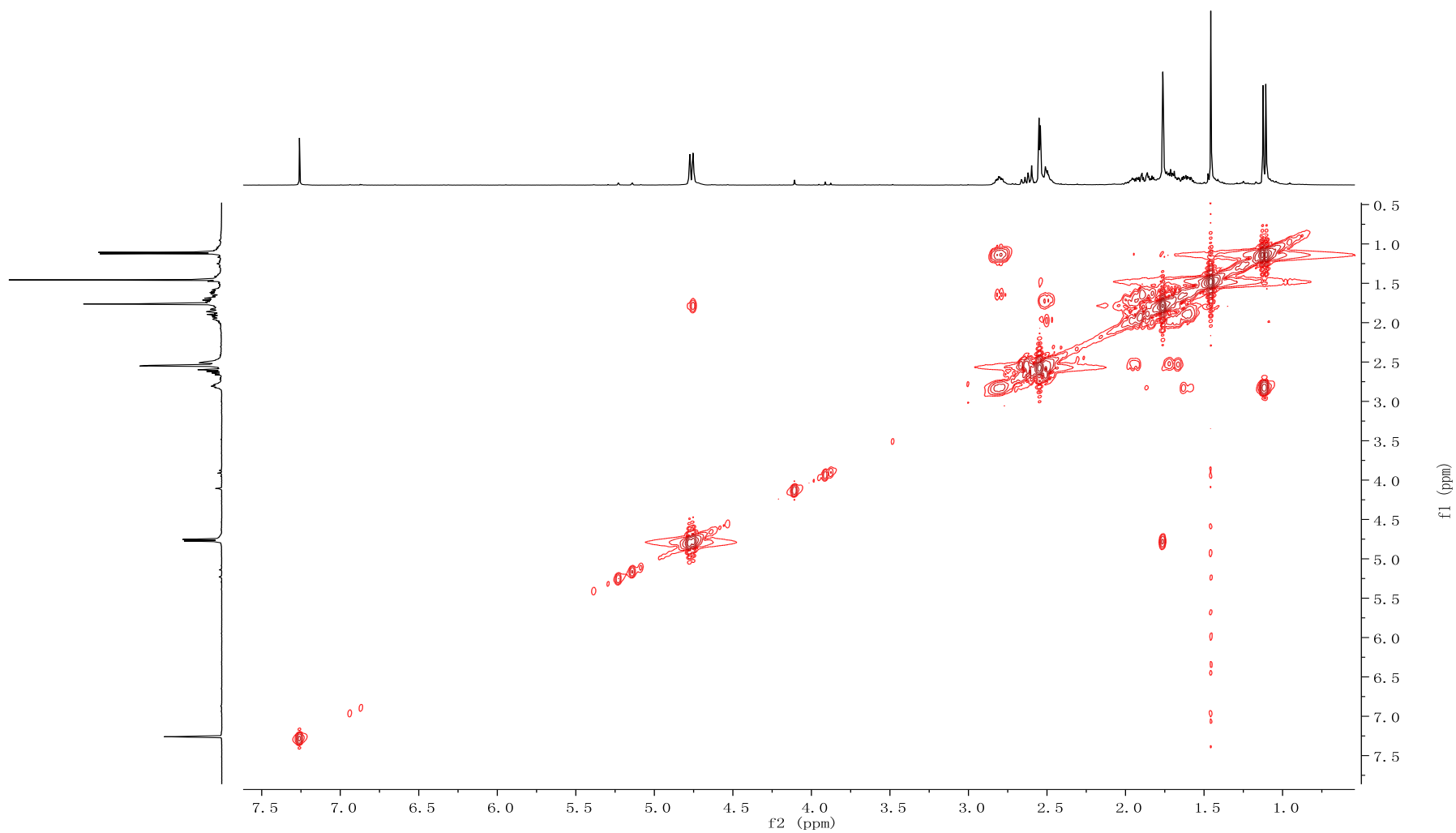


Figure S7. HSQC spectrum of **1** in CDCl₃

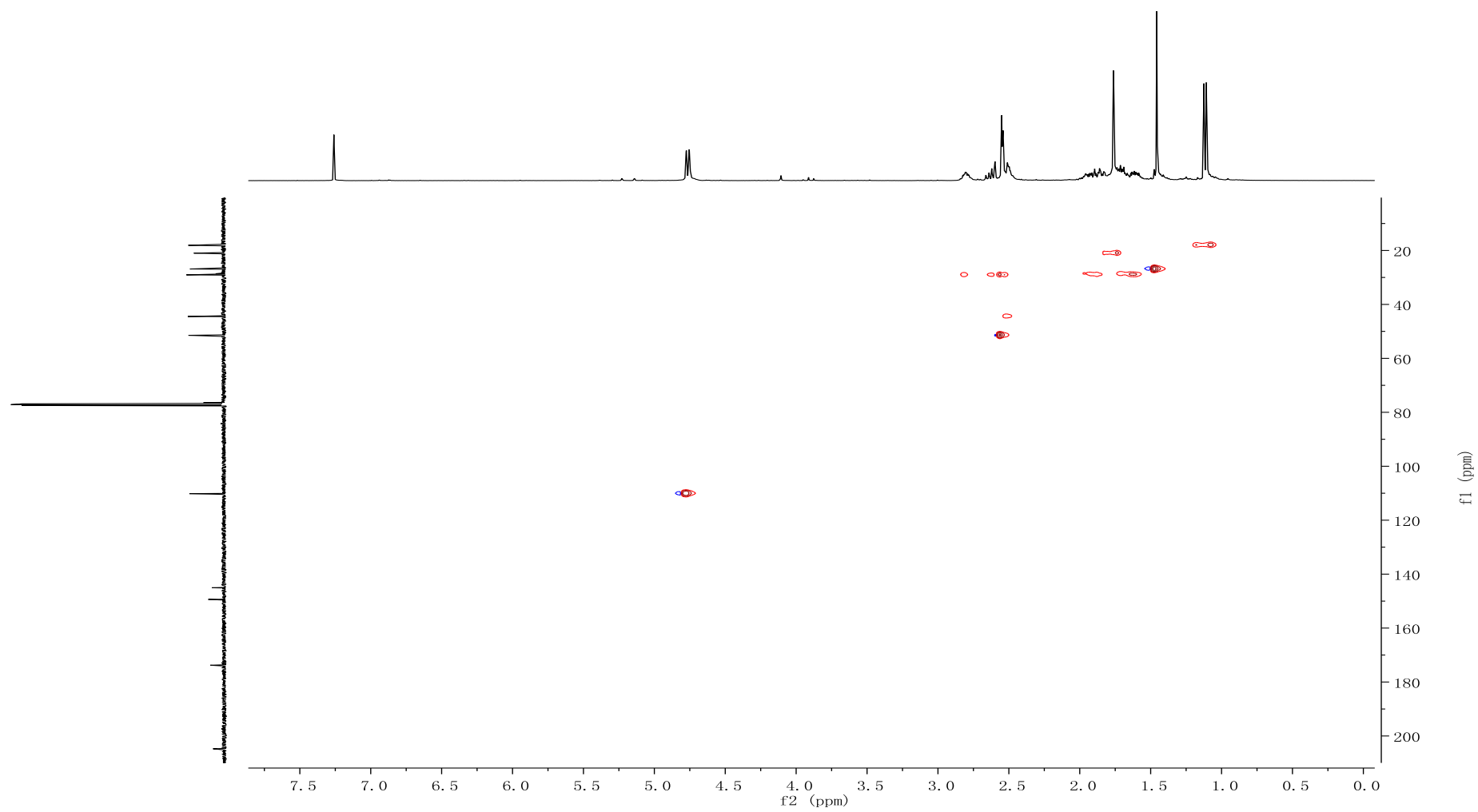


Figure S8. HMBC spectrum of **1** in CDCl₃

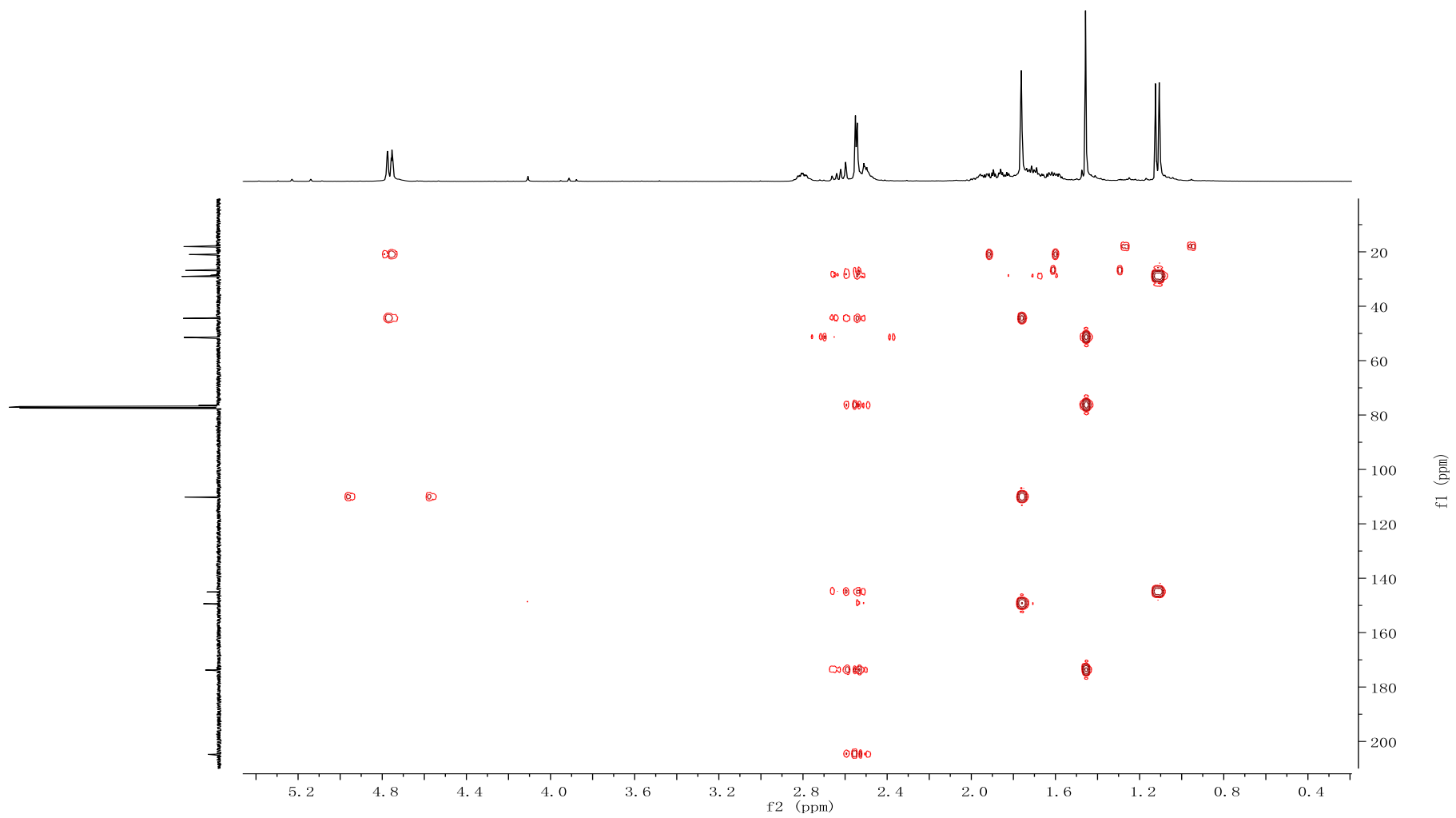


Figure S9. NOESY spectrum of **1** in CDCl₃

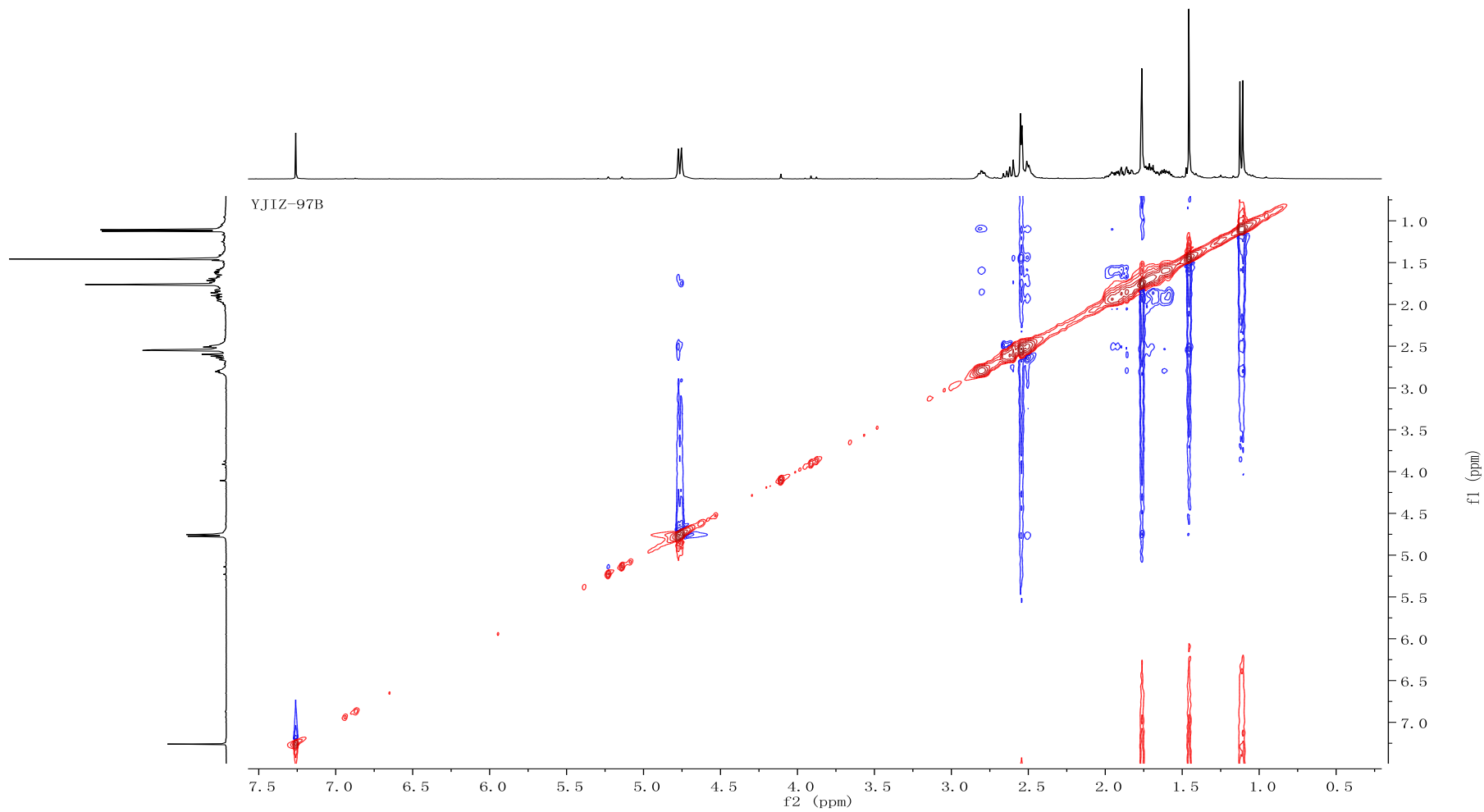


Figure S10. HRESIMS spectrum of **1**

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T: FTMS + p ESI Full ms [220.00-850.00]

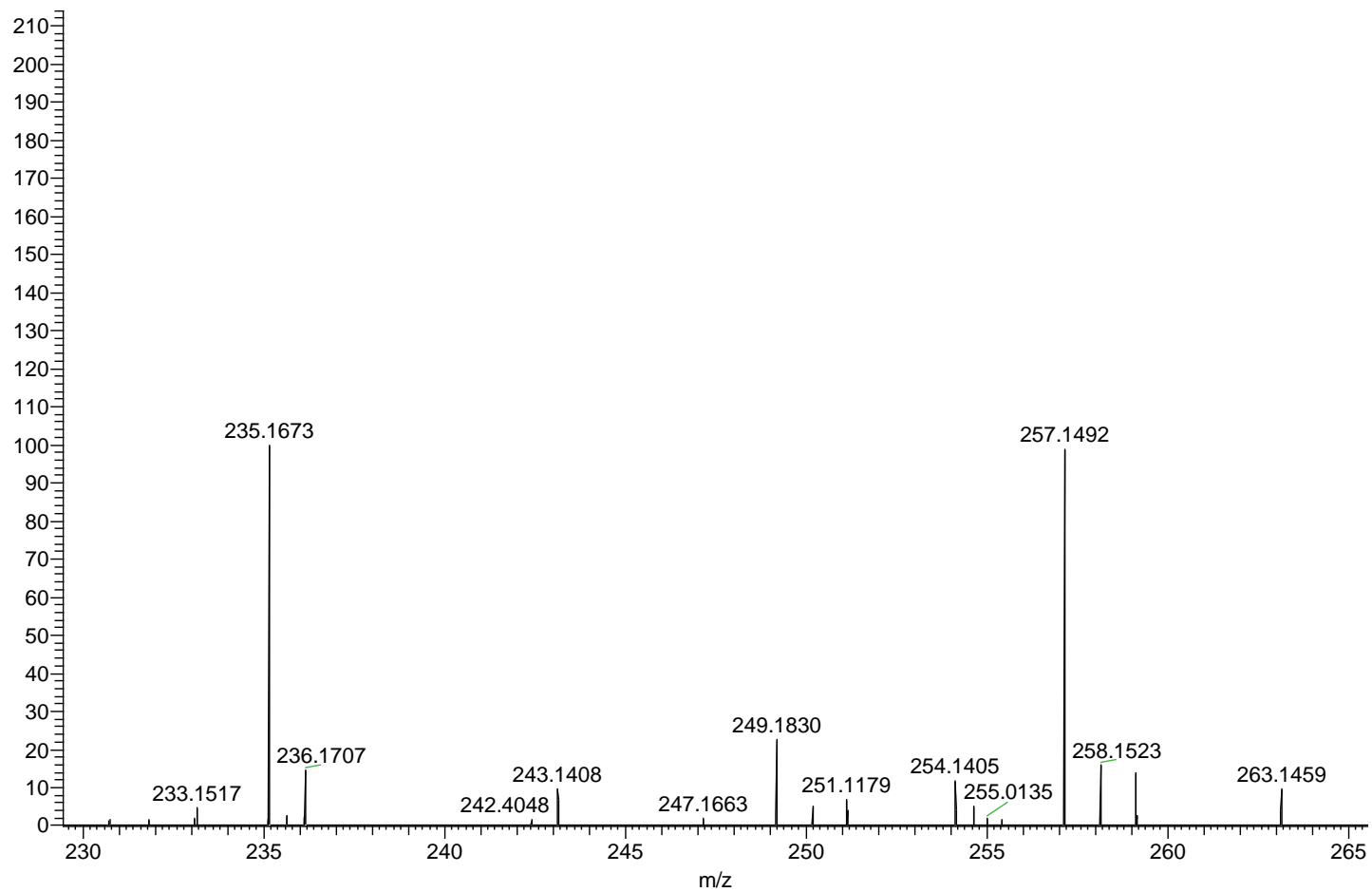
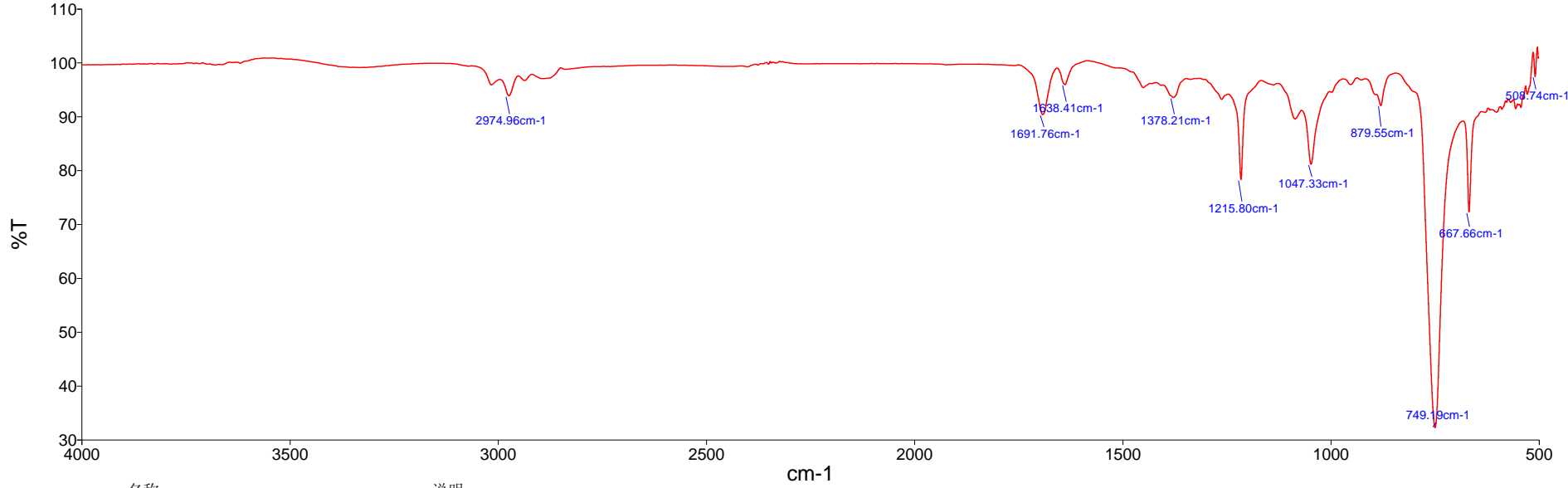


Figure S11. IR (KBr disc) spectrum of **1**



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Figure S12. ^1H NMR (600 MHz, CDCl_3) spectrum of **2**

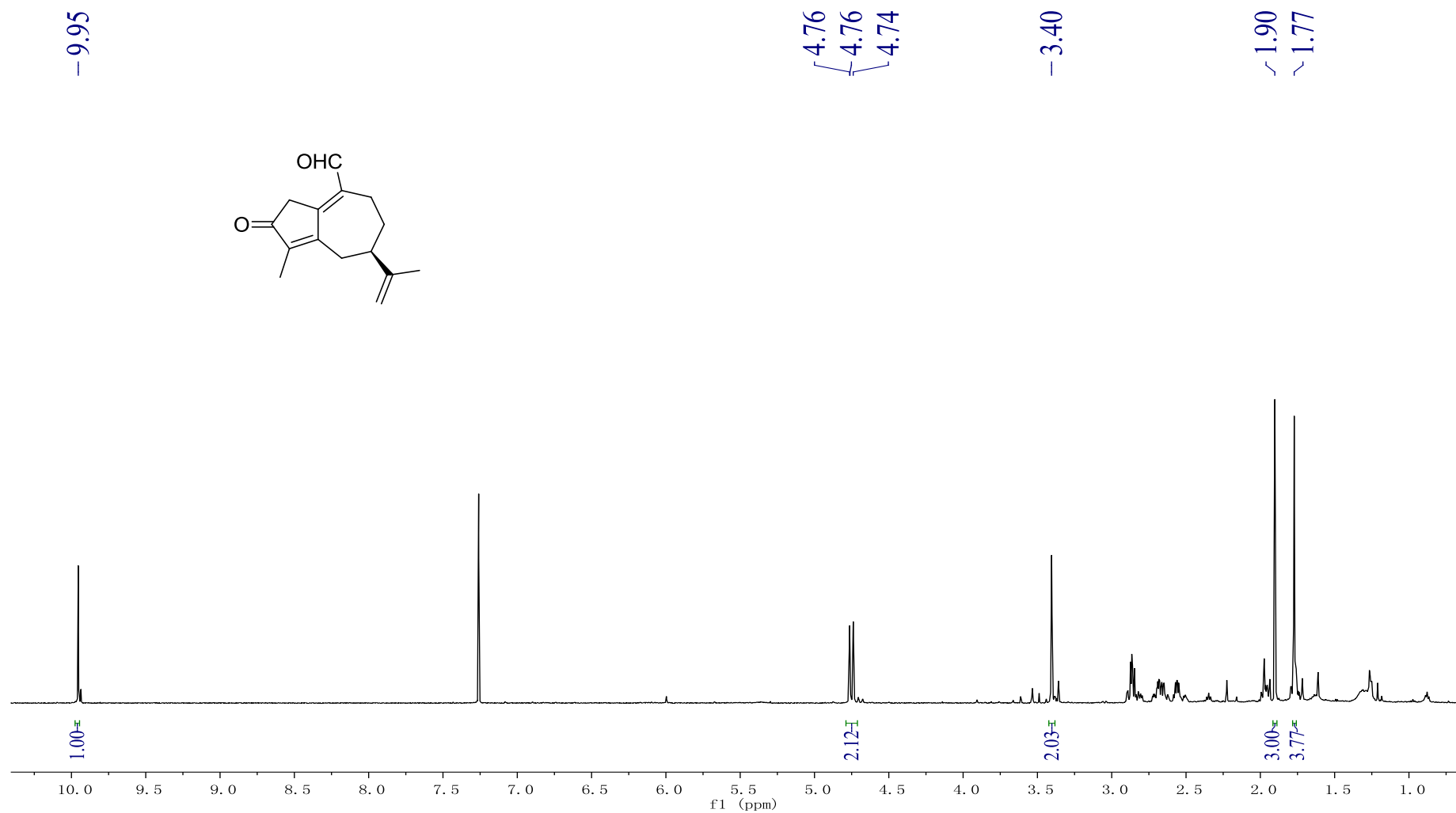


Figure S13. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **2**

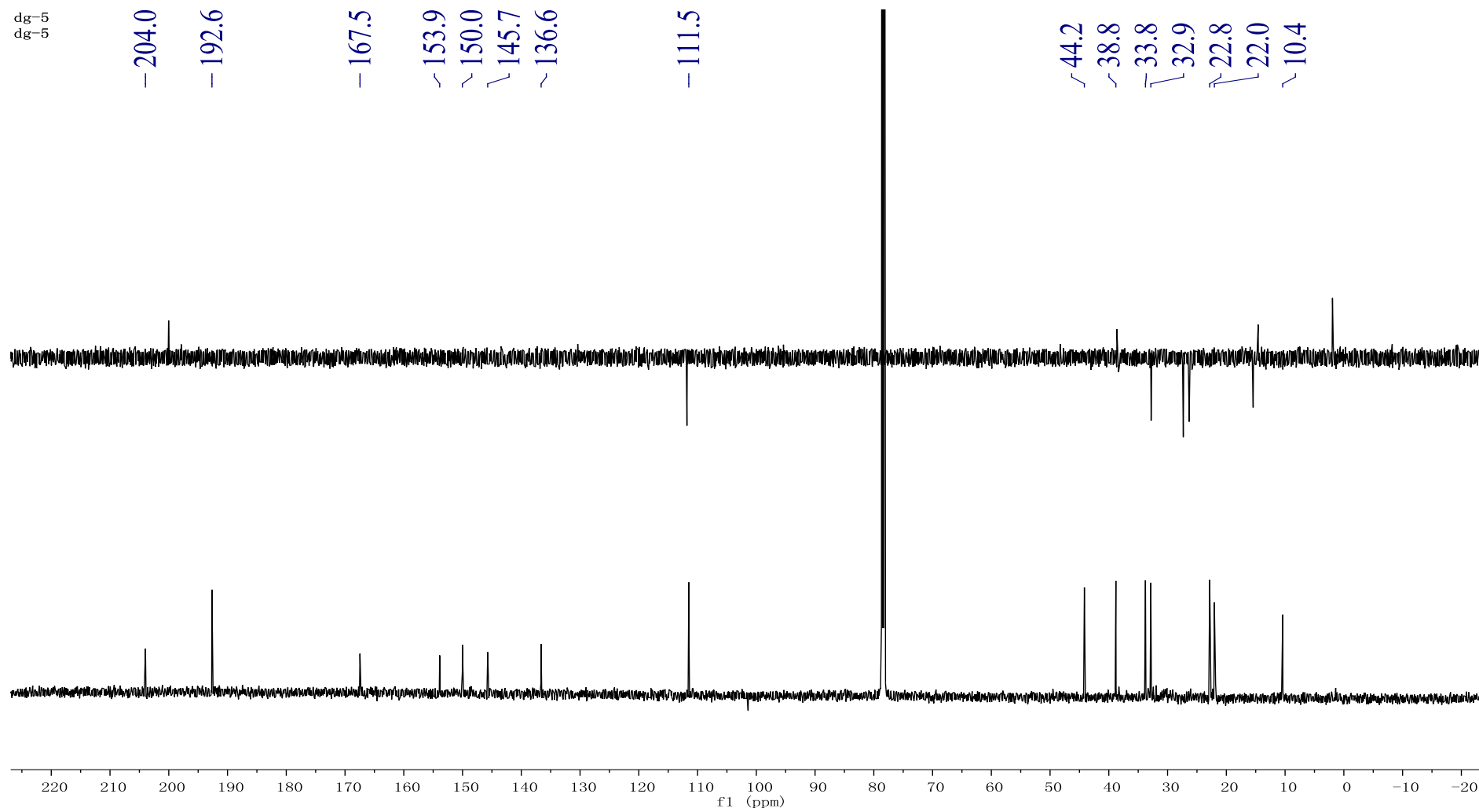


Figure S14. ^1H NMR (400 MHz, CDCl_3) spectrum of **3**

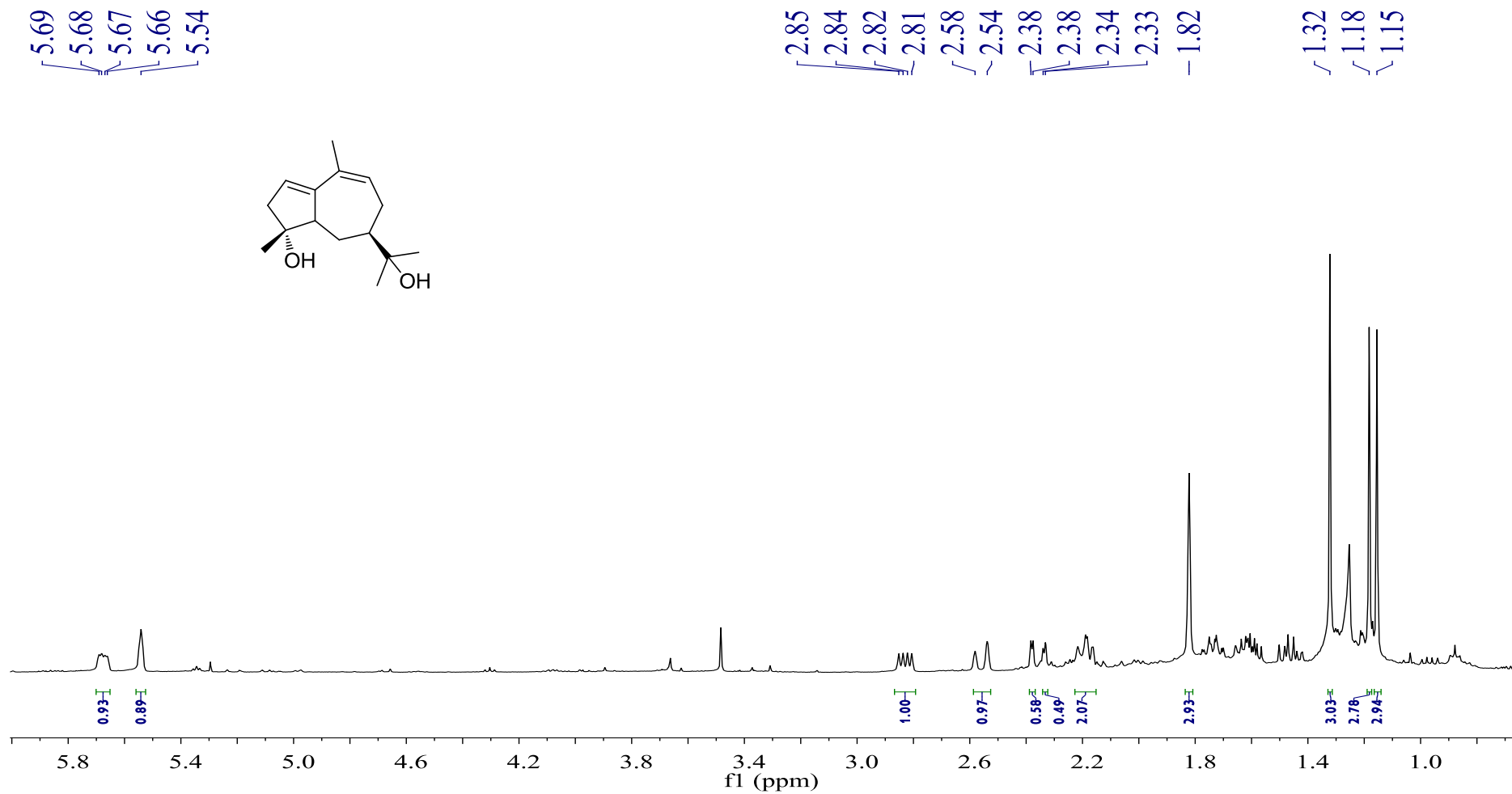


Figure S15. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **3**

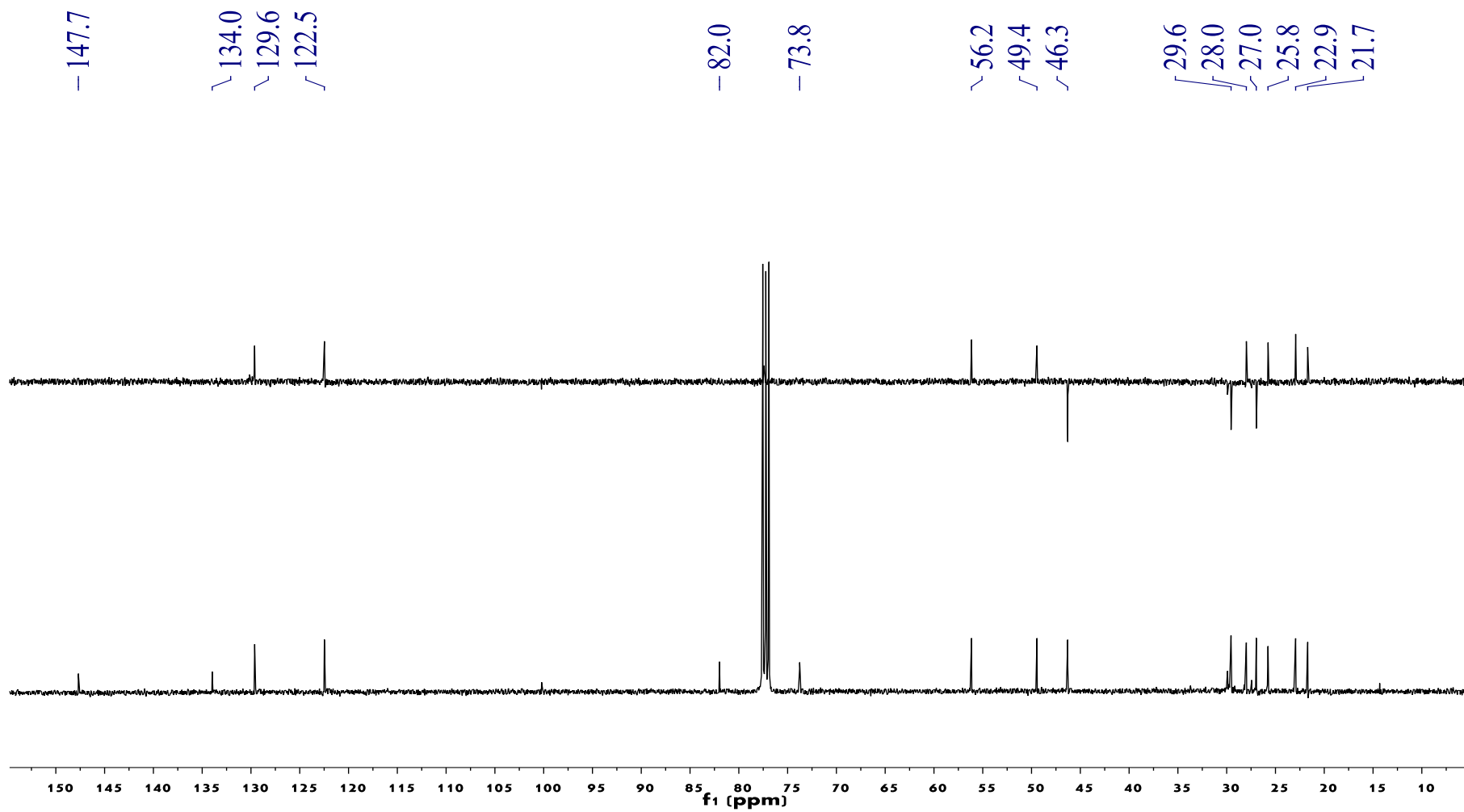


Figure S16. ^1H NMR (600 MHz, CD_3OD) spectrum of **4**

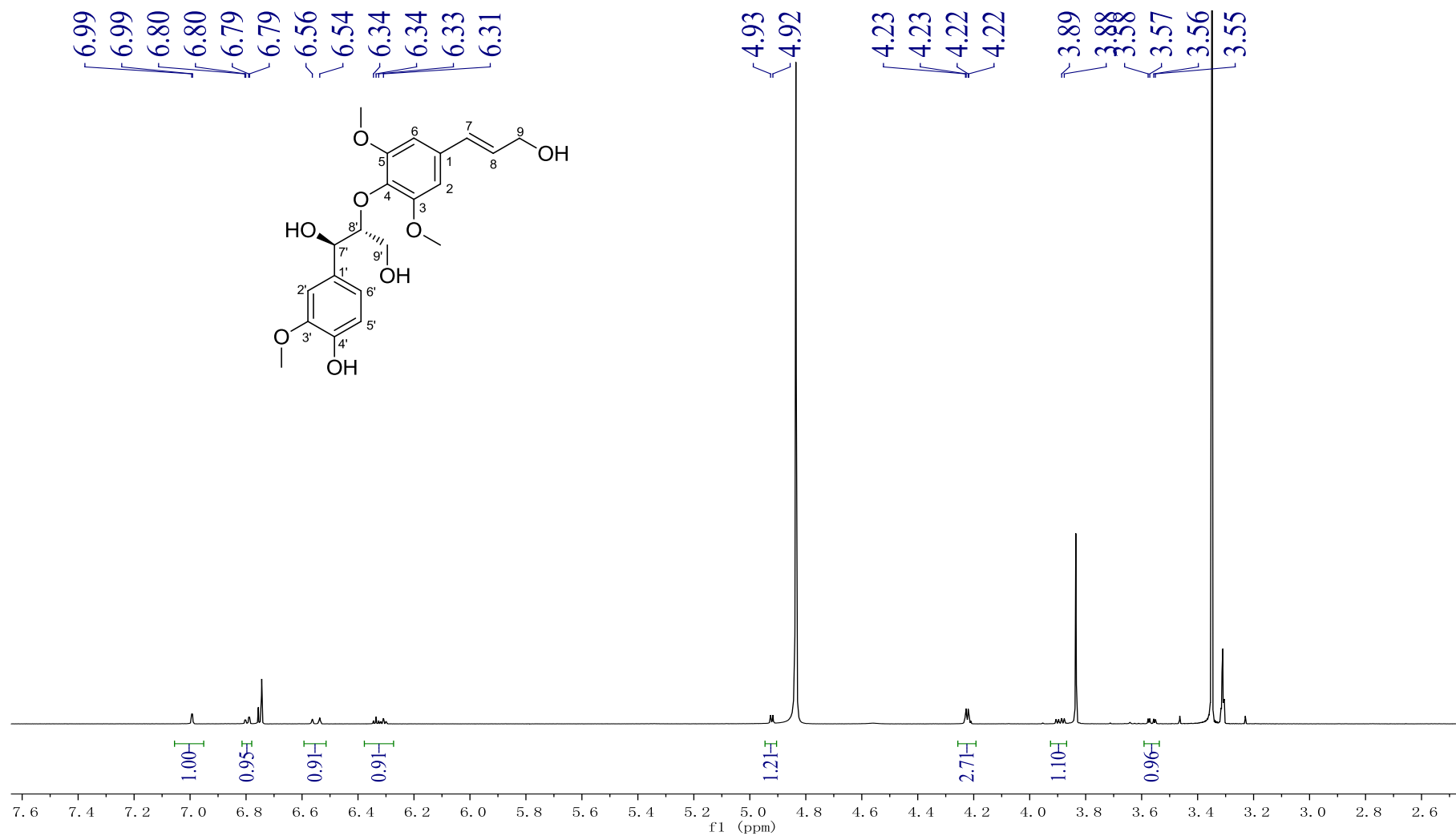


Figure S17. ^{13}C NMR (150 MHz, CD_3OD) spectrum of **4**

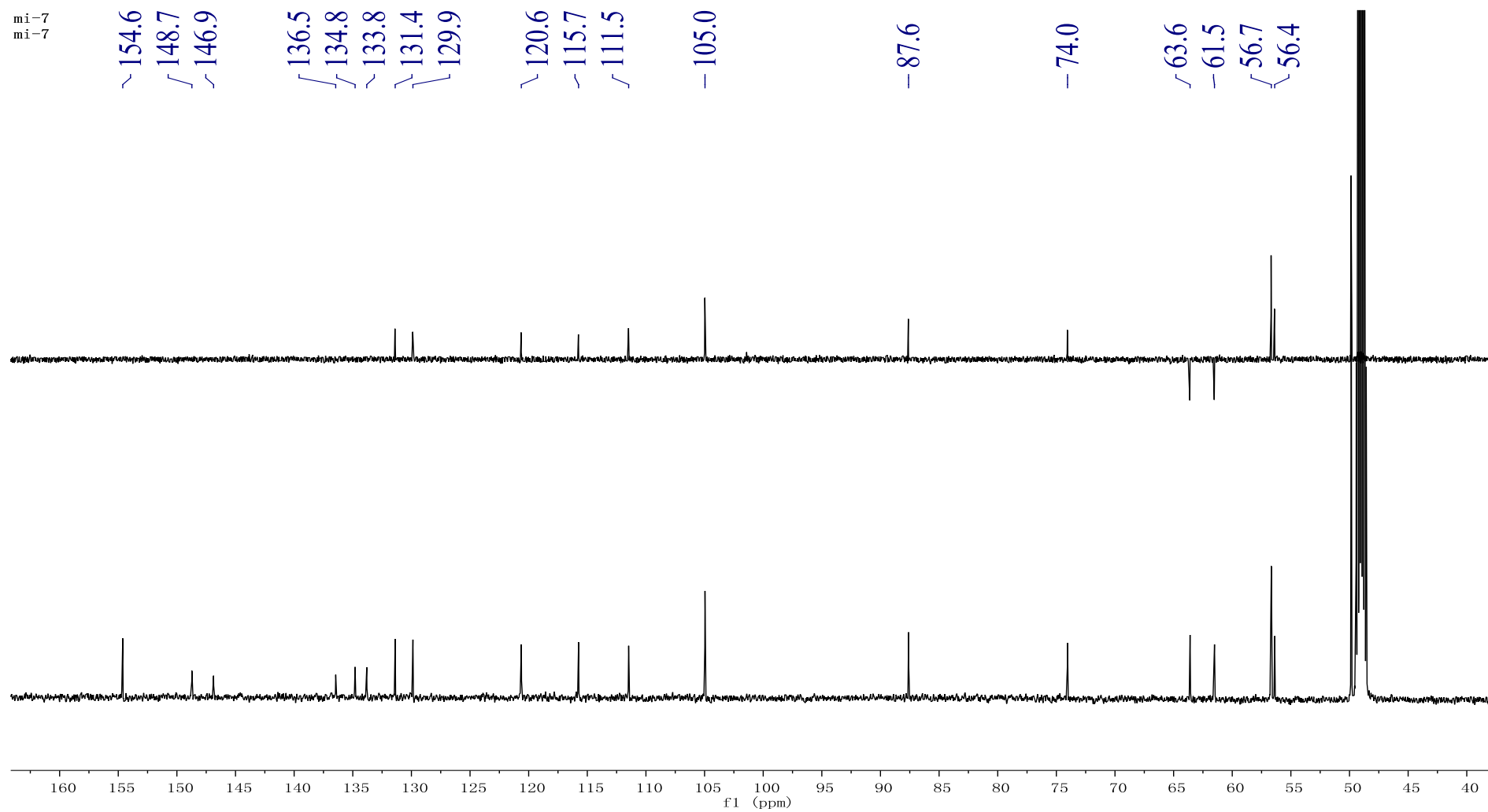


Figure S18. ^1H NMR (600 MHz, CDCl_3) spectrum of **5**

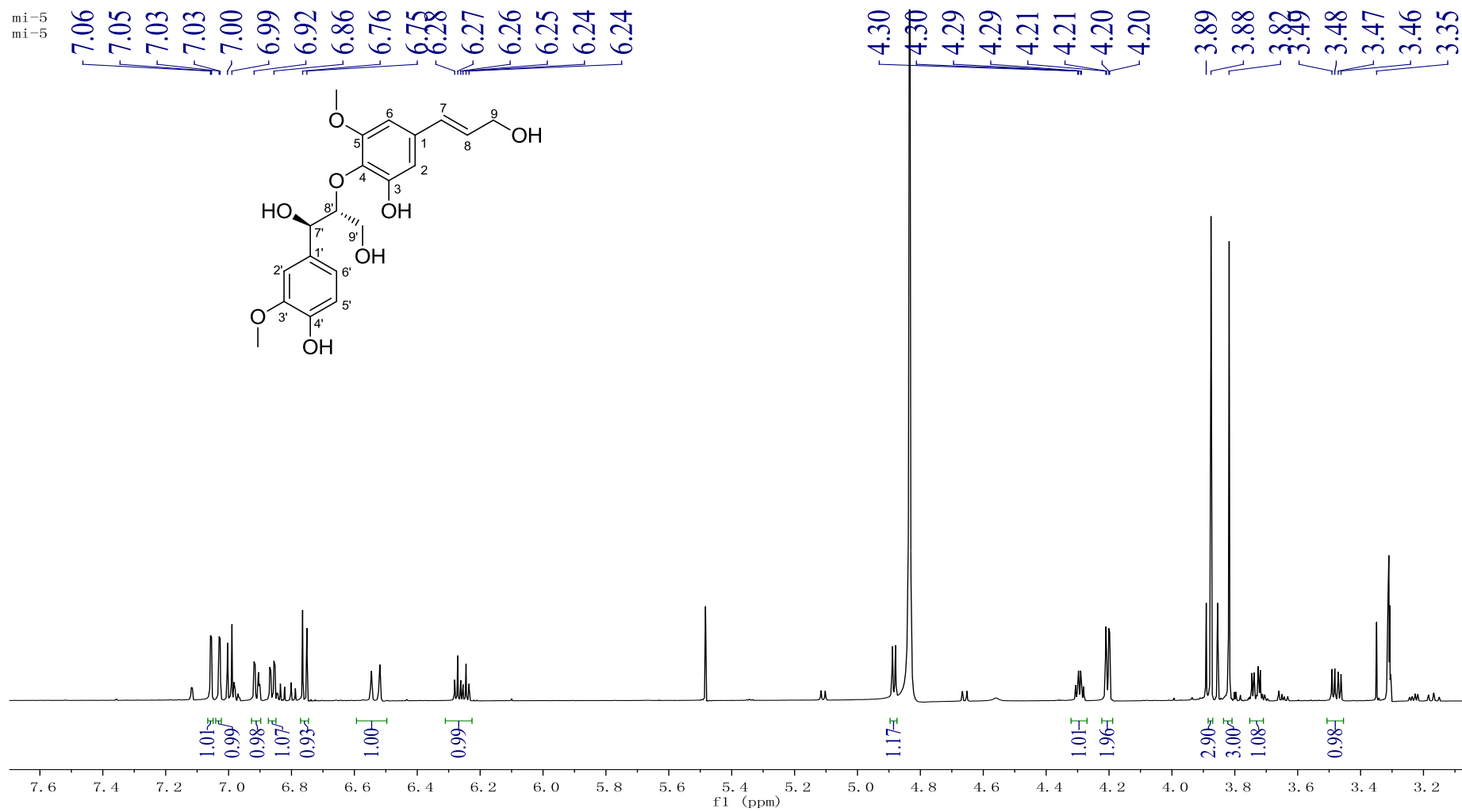


Figure S19. ^{13}C NMR (600 MHz, CDCl_3) spectrum of **5**

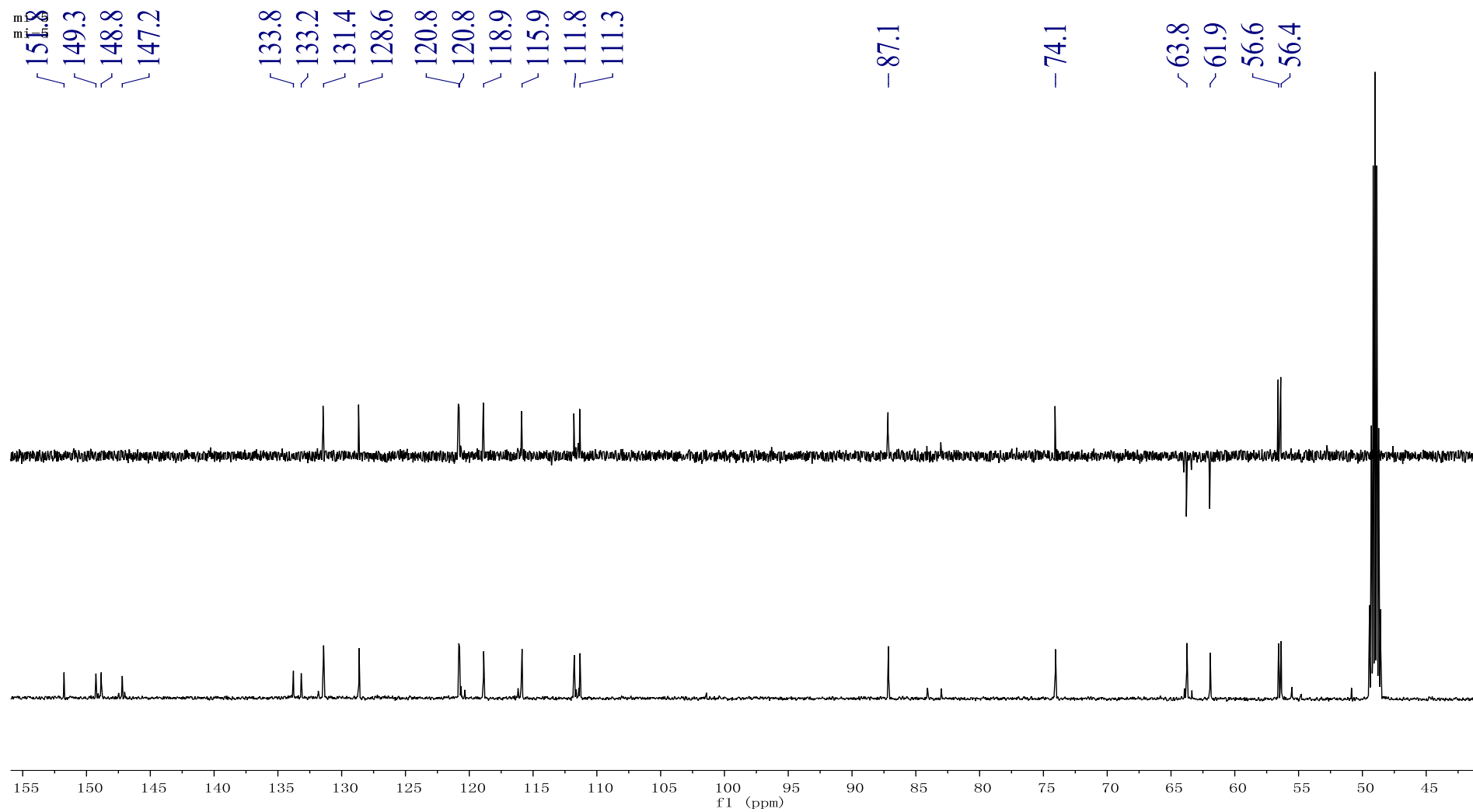


Figure S20. ^1H NMR (150 MHz, CDCl_3) spectrum of **6**

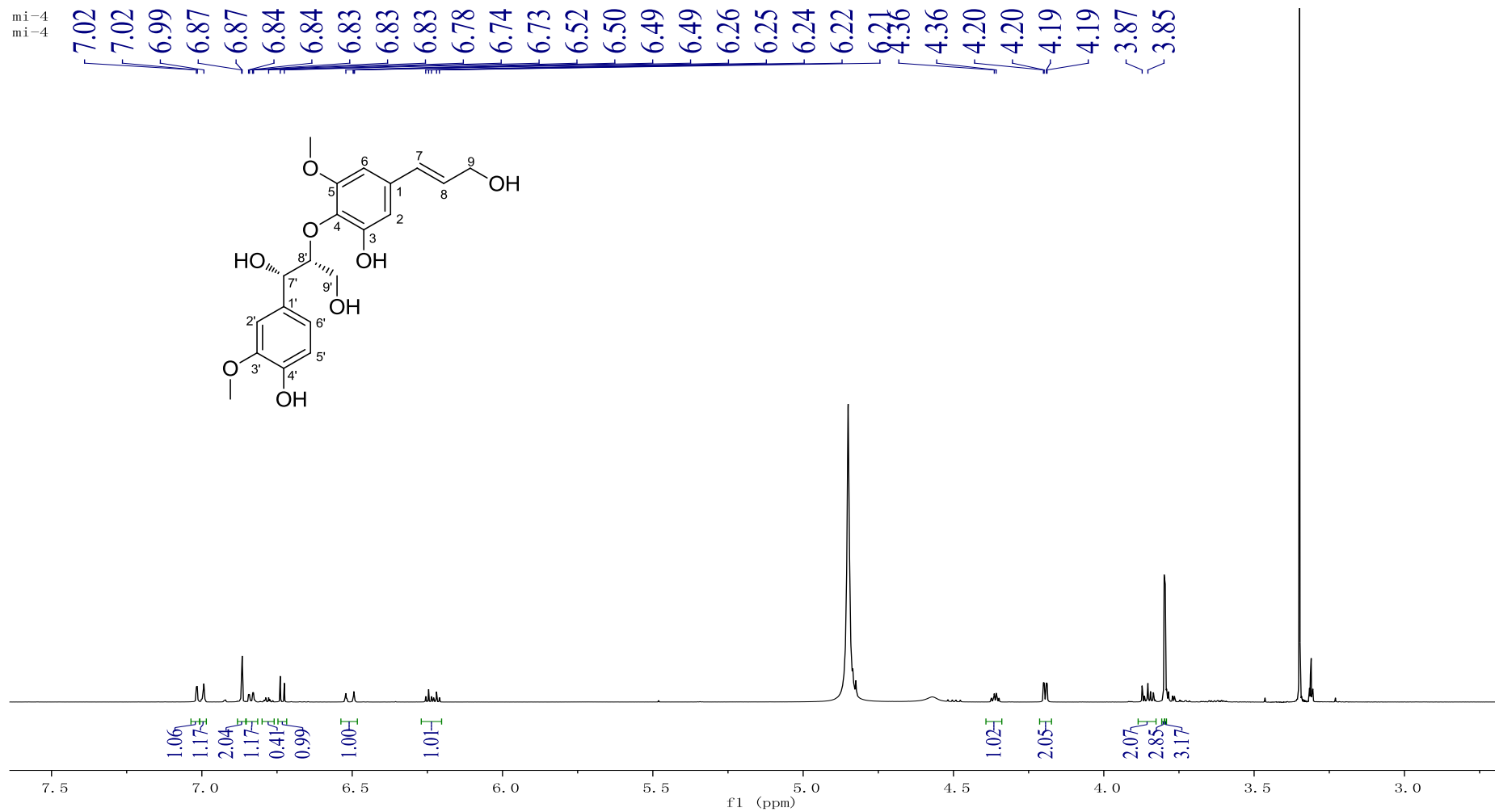


Figure S21. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **6**

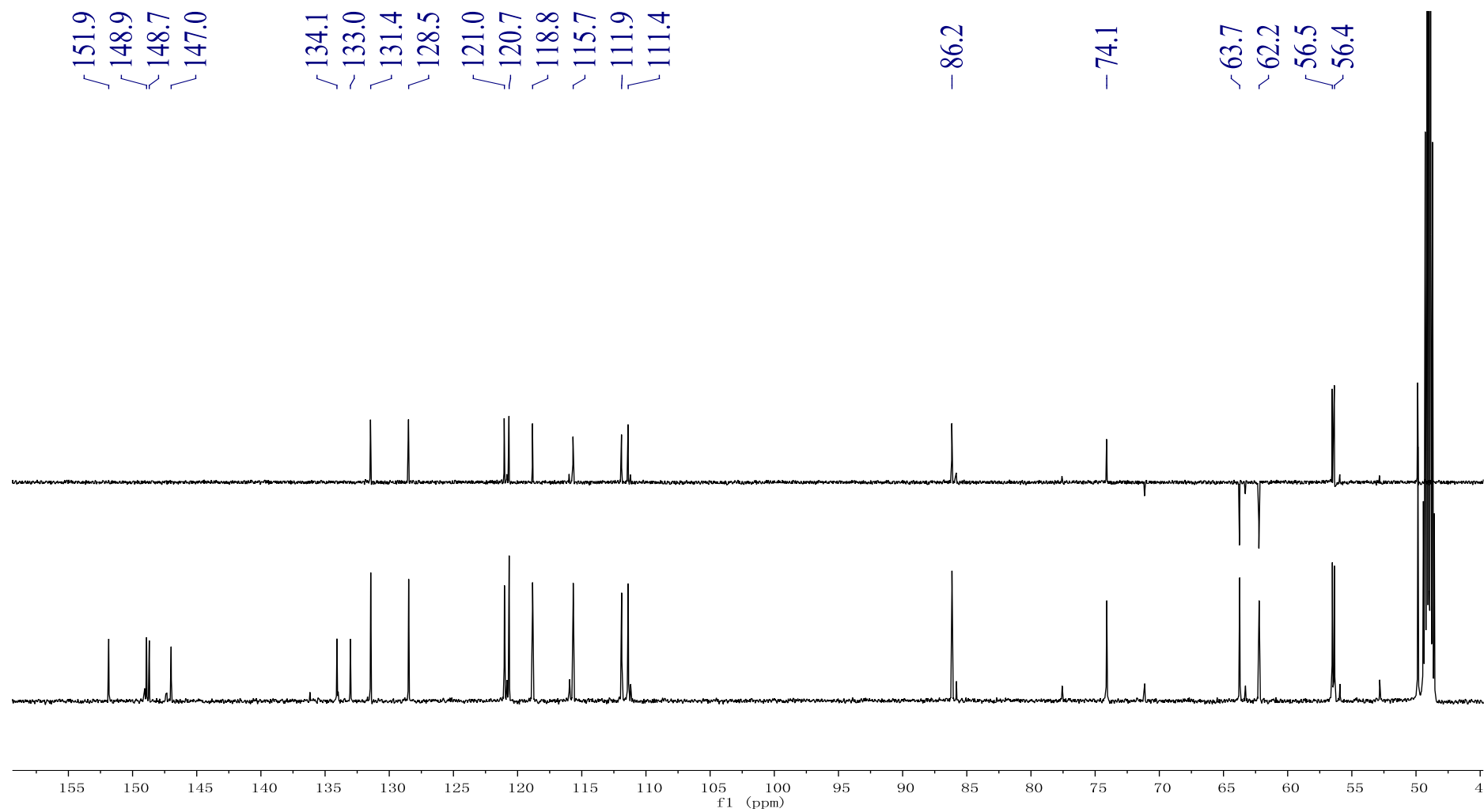


Figure S22. ^1H NMR (600 MHz, CDCl_3) spectrum of **7**

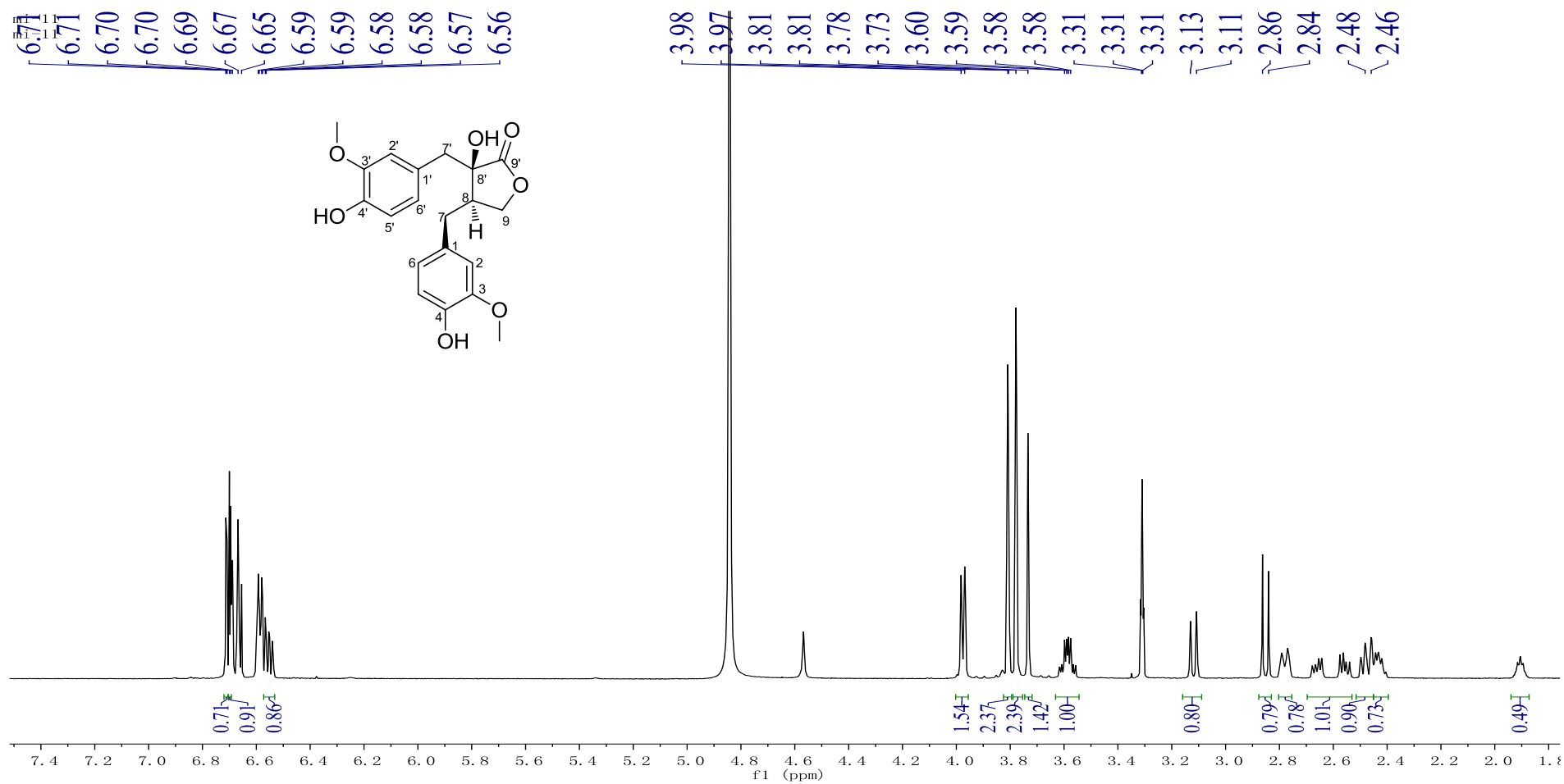


Figure S23. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **7**

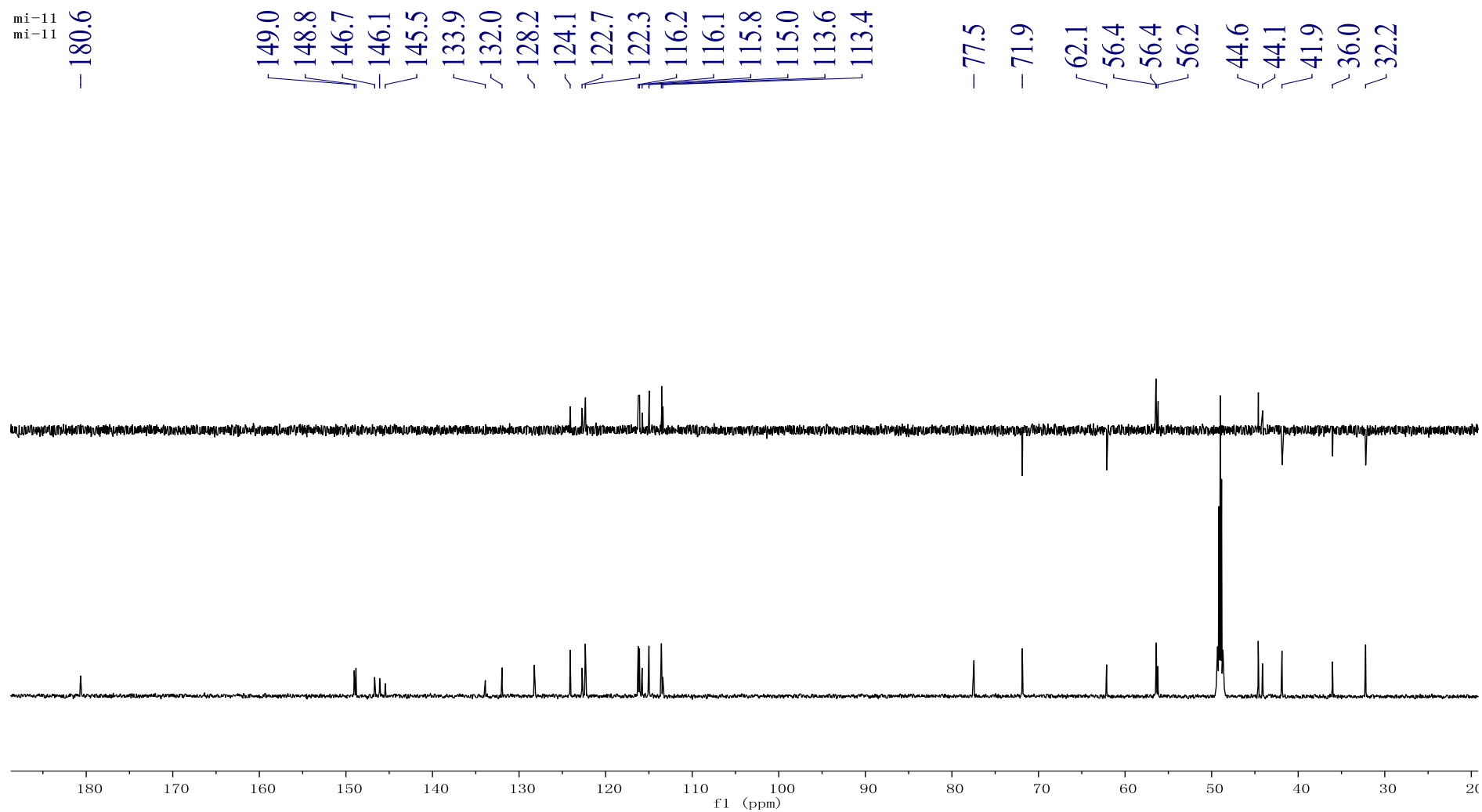


Figure S24. ^1H NMR (600 MHz, CDCl_3) spectrum of **8**

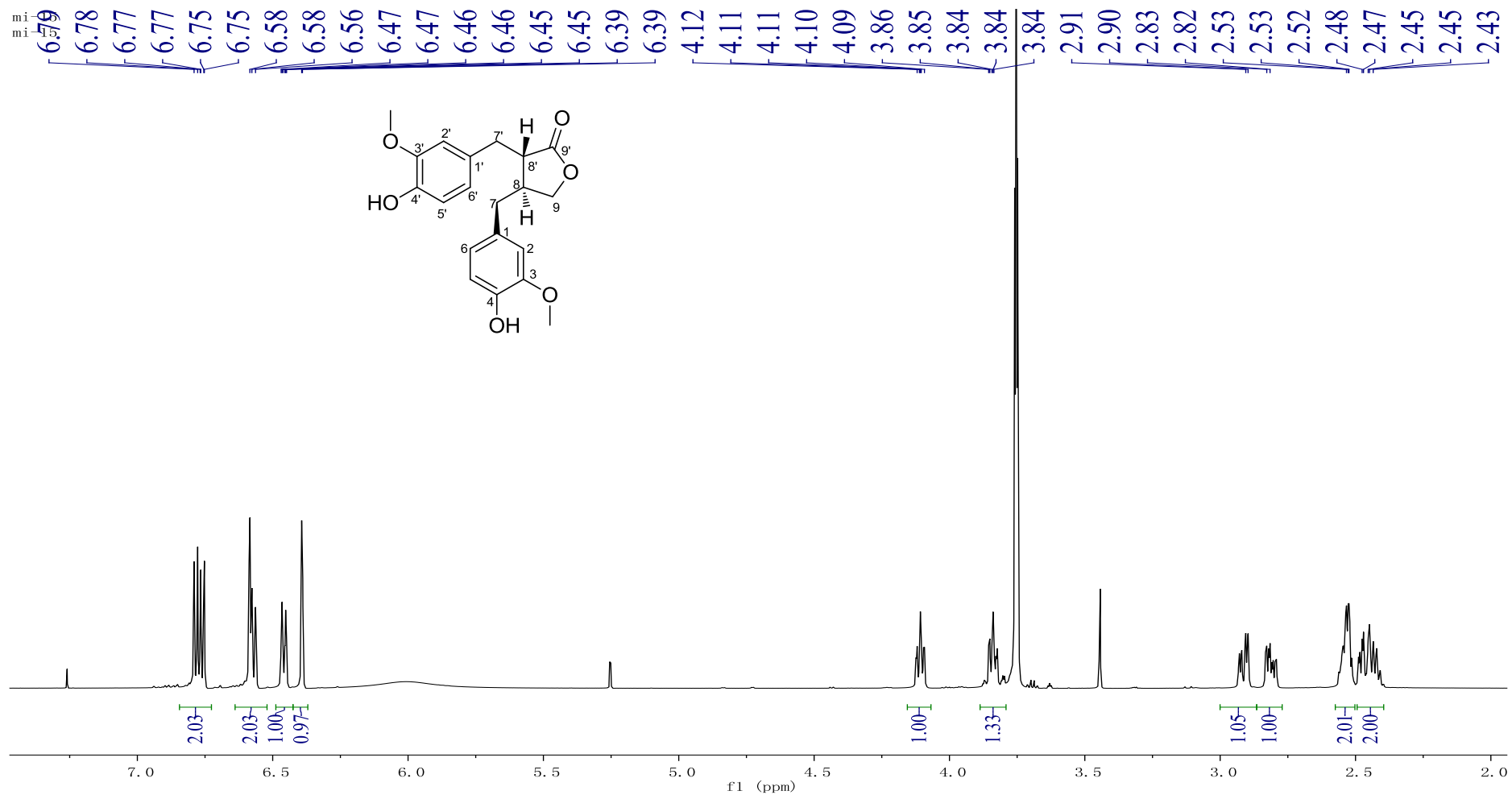


Figure S25. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **8**

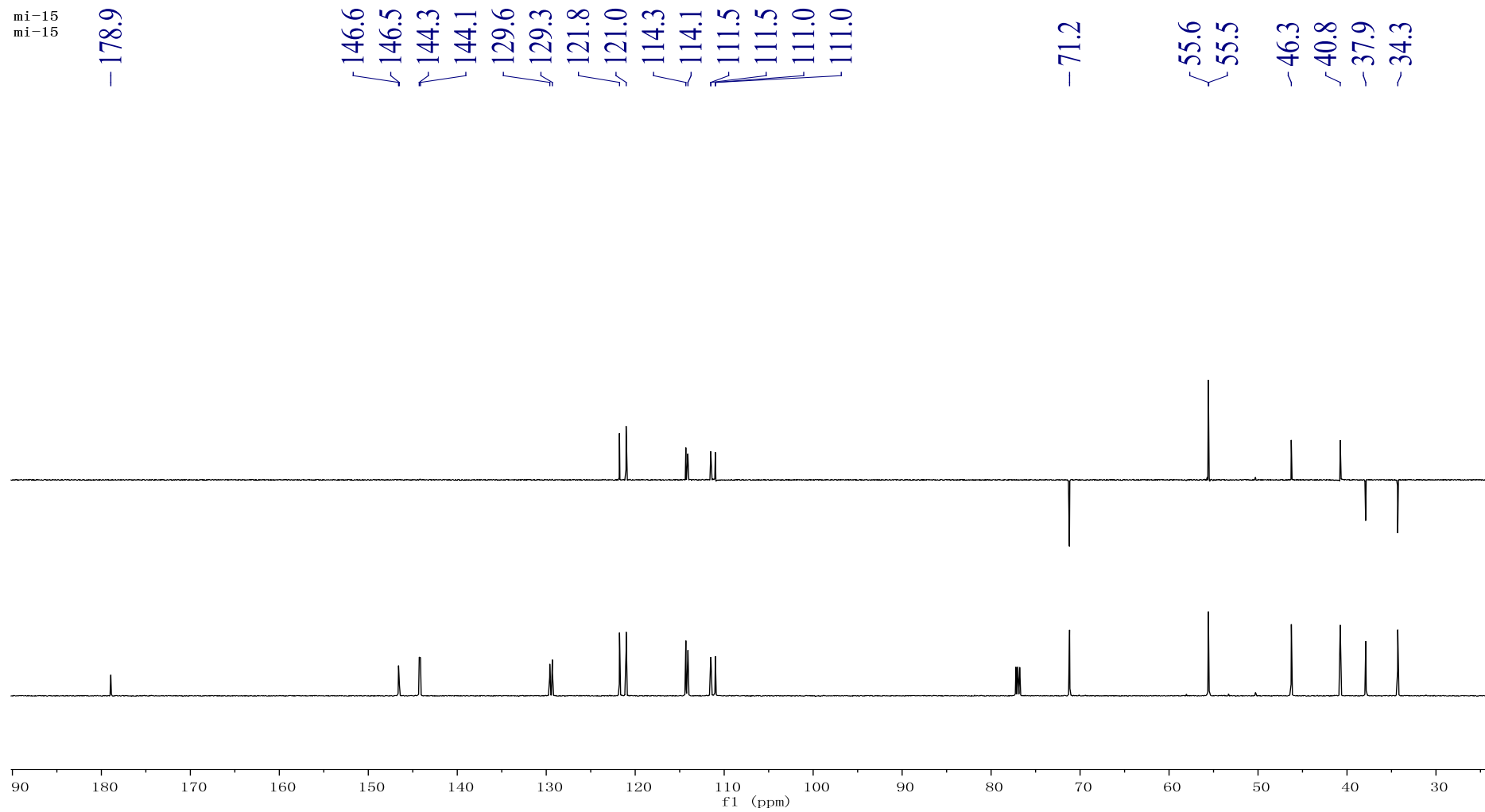


Figure S26. ^1H NMR (600 MHz, CDCl_3) spectrum of **9**

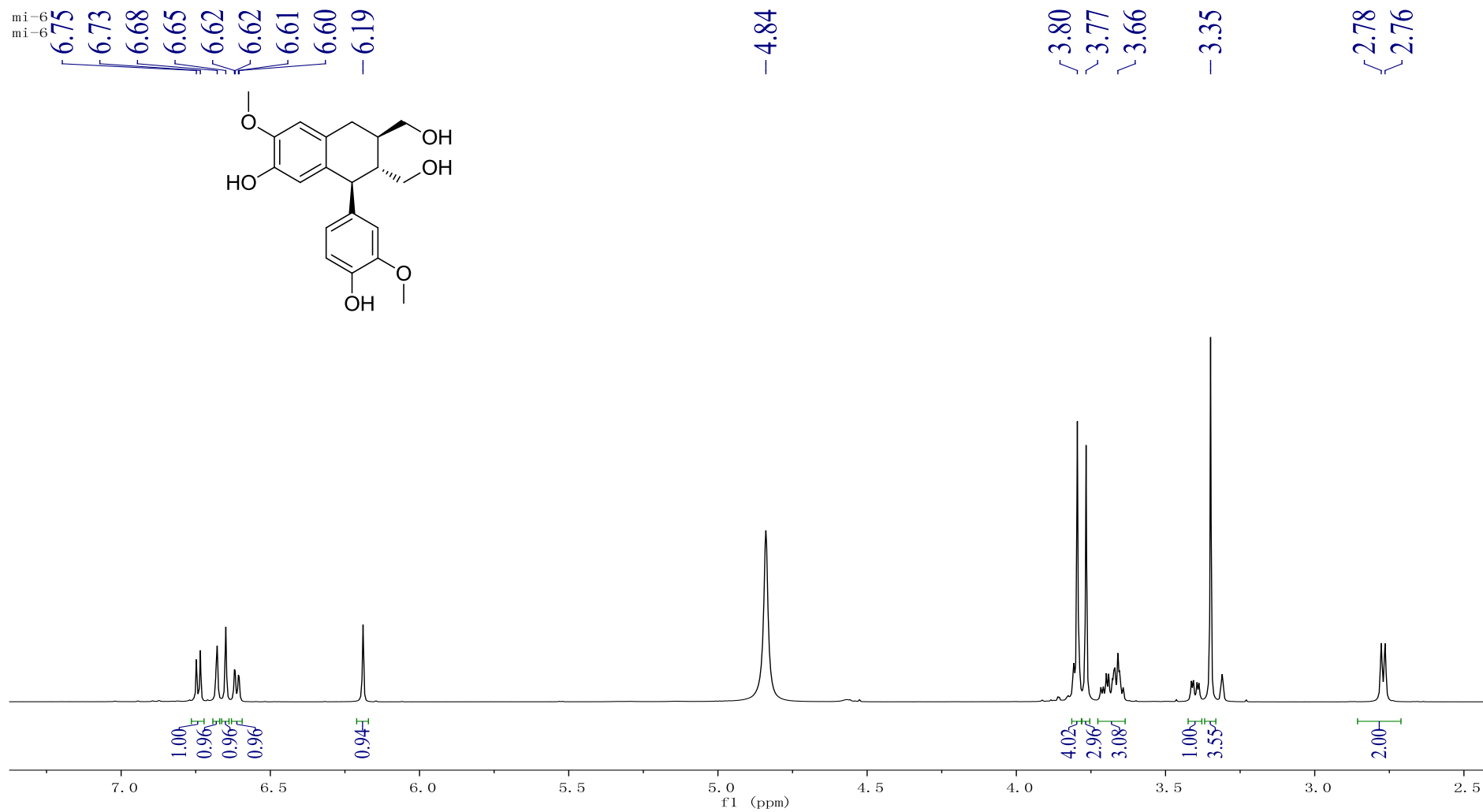


Figure S27. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **9**

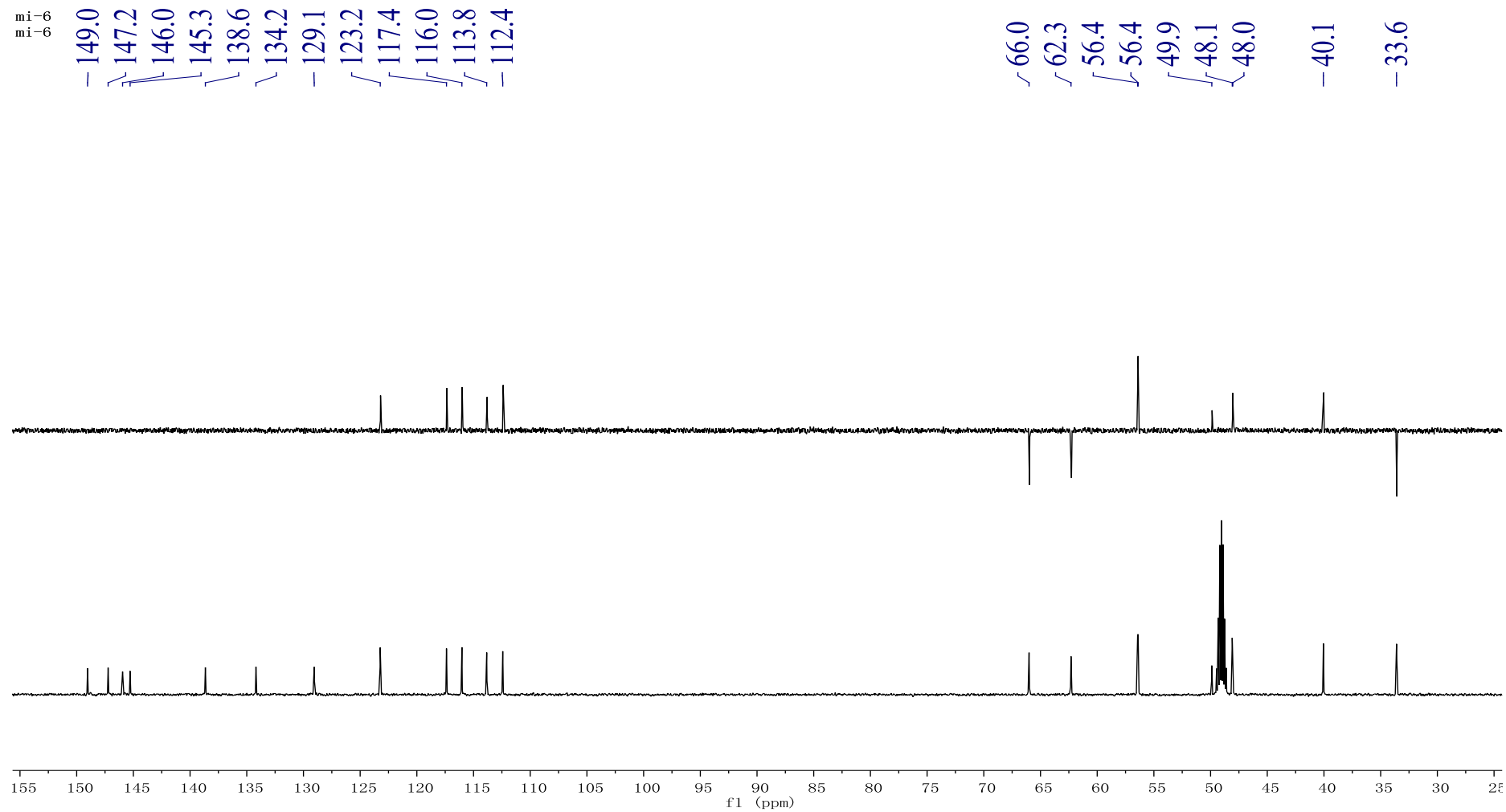


Figure S28. ^1H NMR (600 MHz, CDCl_3) spectrum of **10**

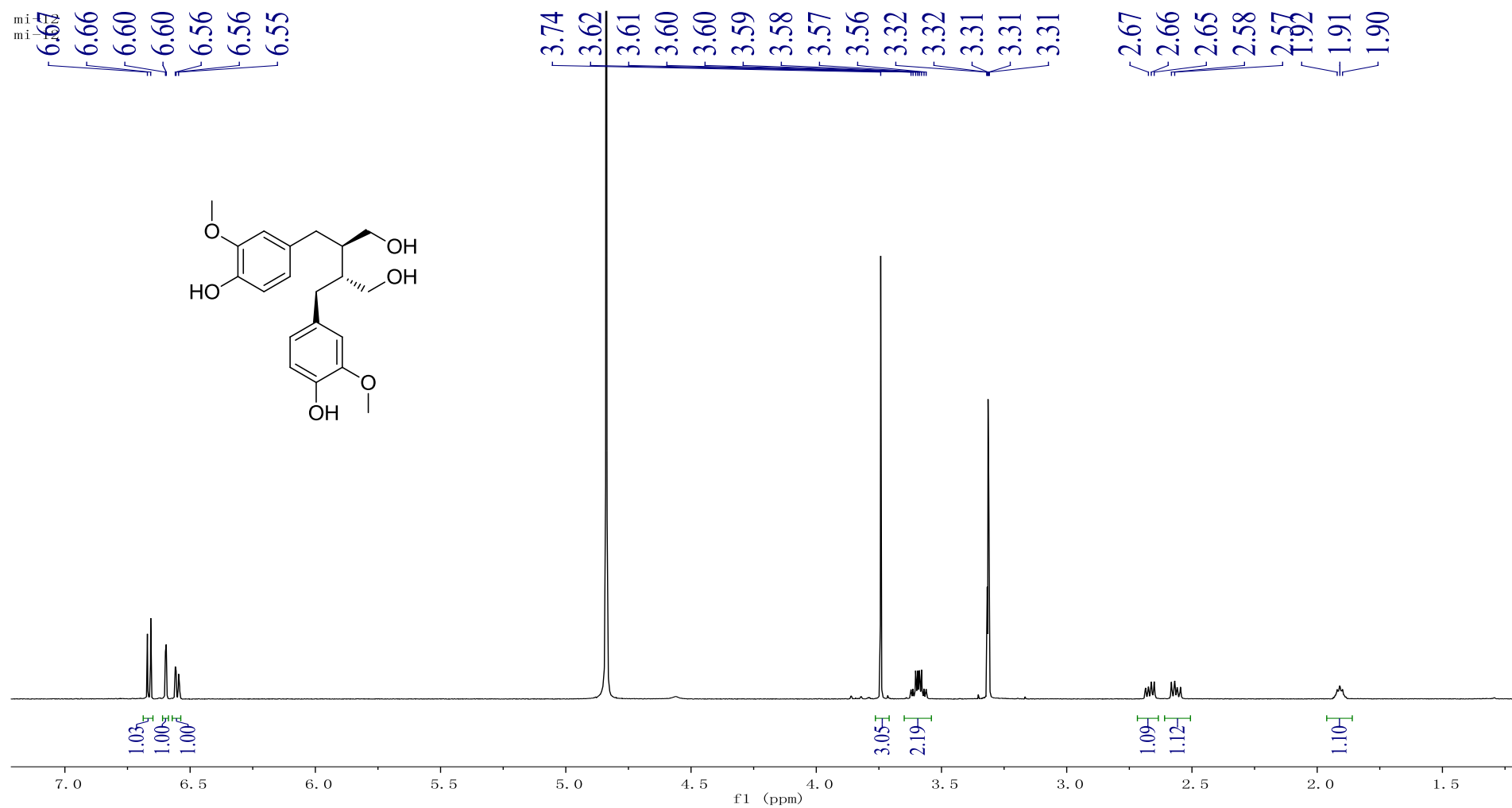


Figure S29. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **10**

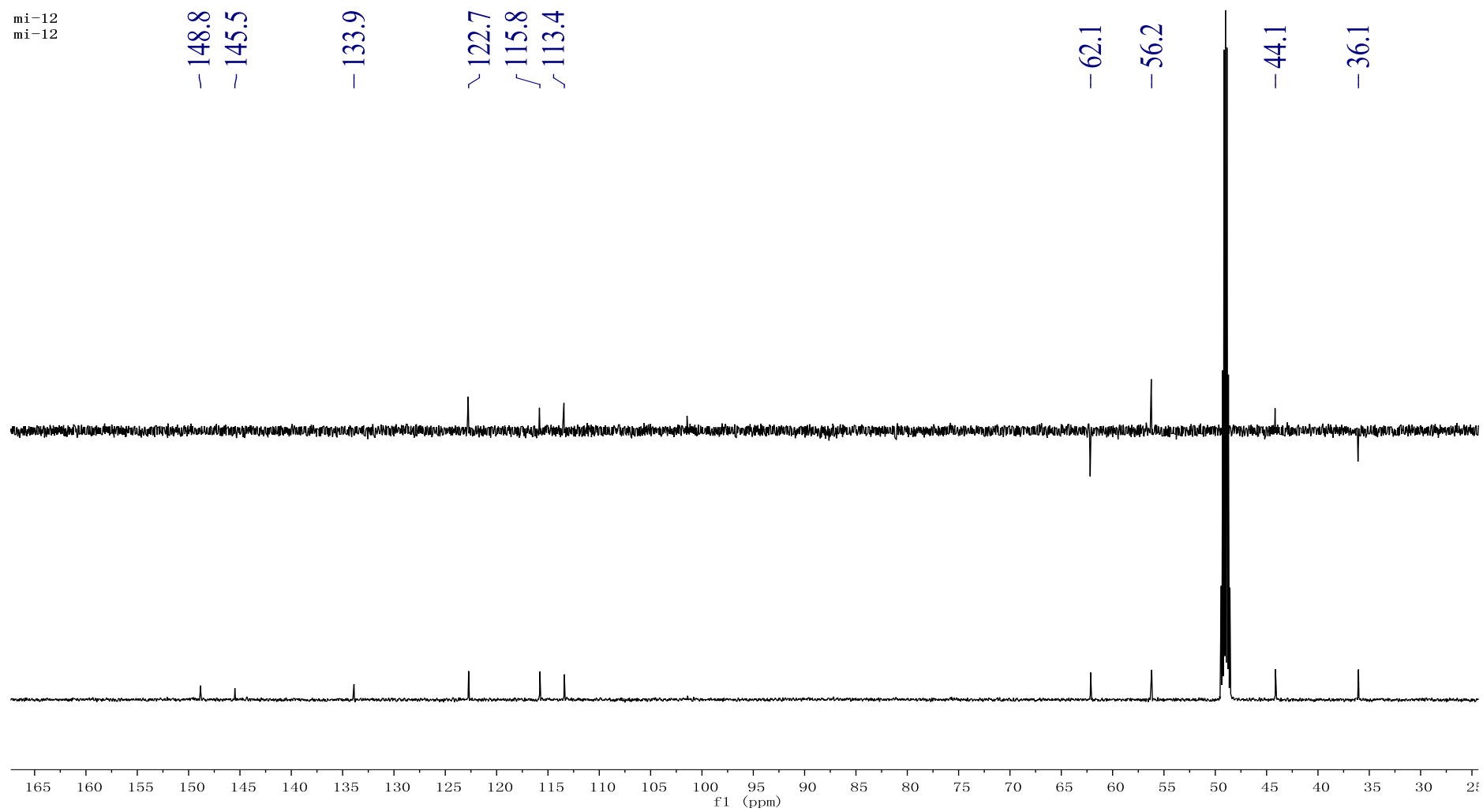


Figure S30. ^1H NMR (600 MHz, CDCl_3) spectrum of **11**

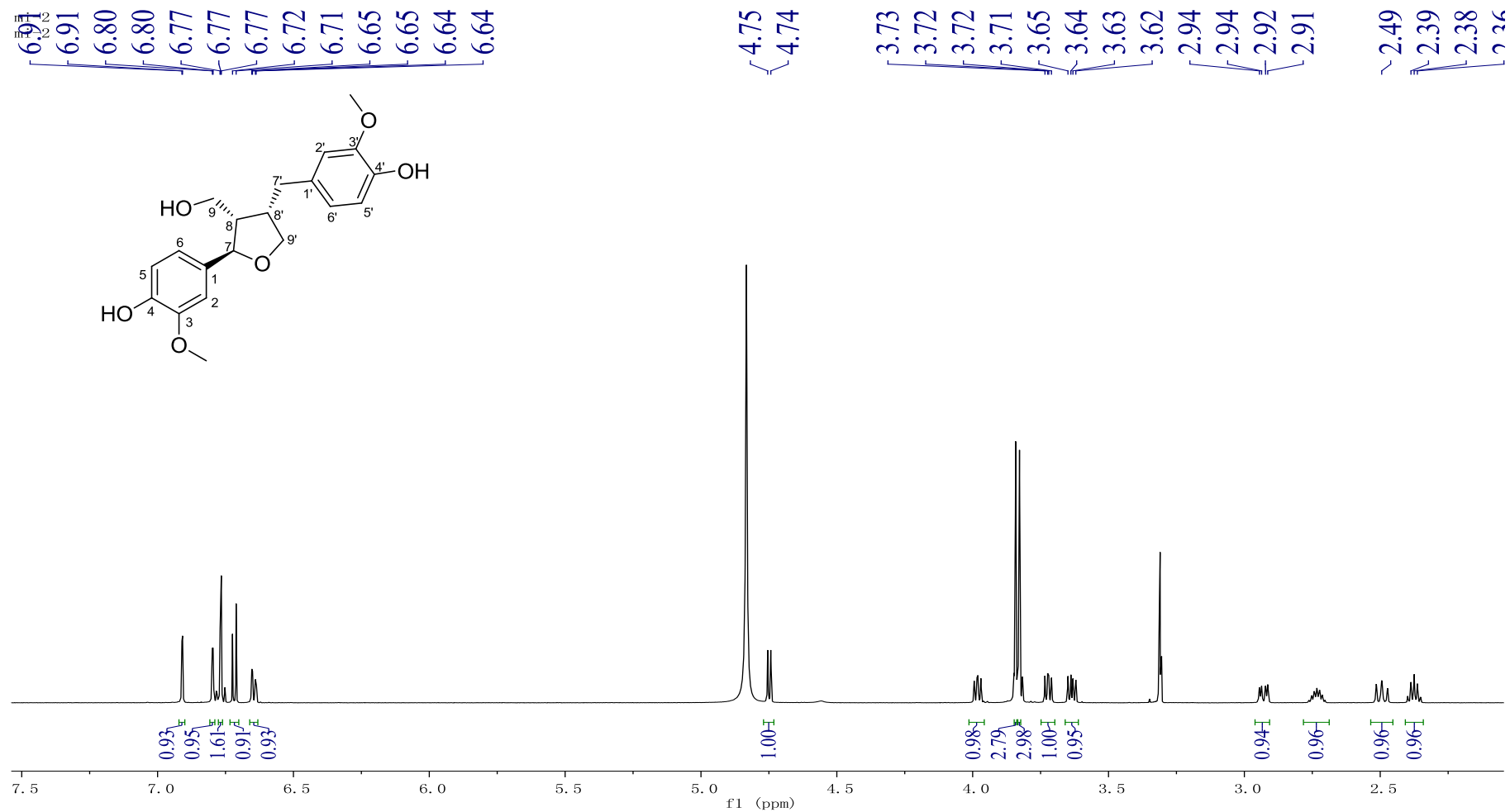


Figure S31. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **11**

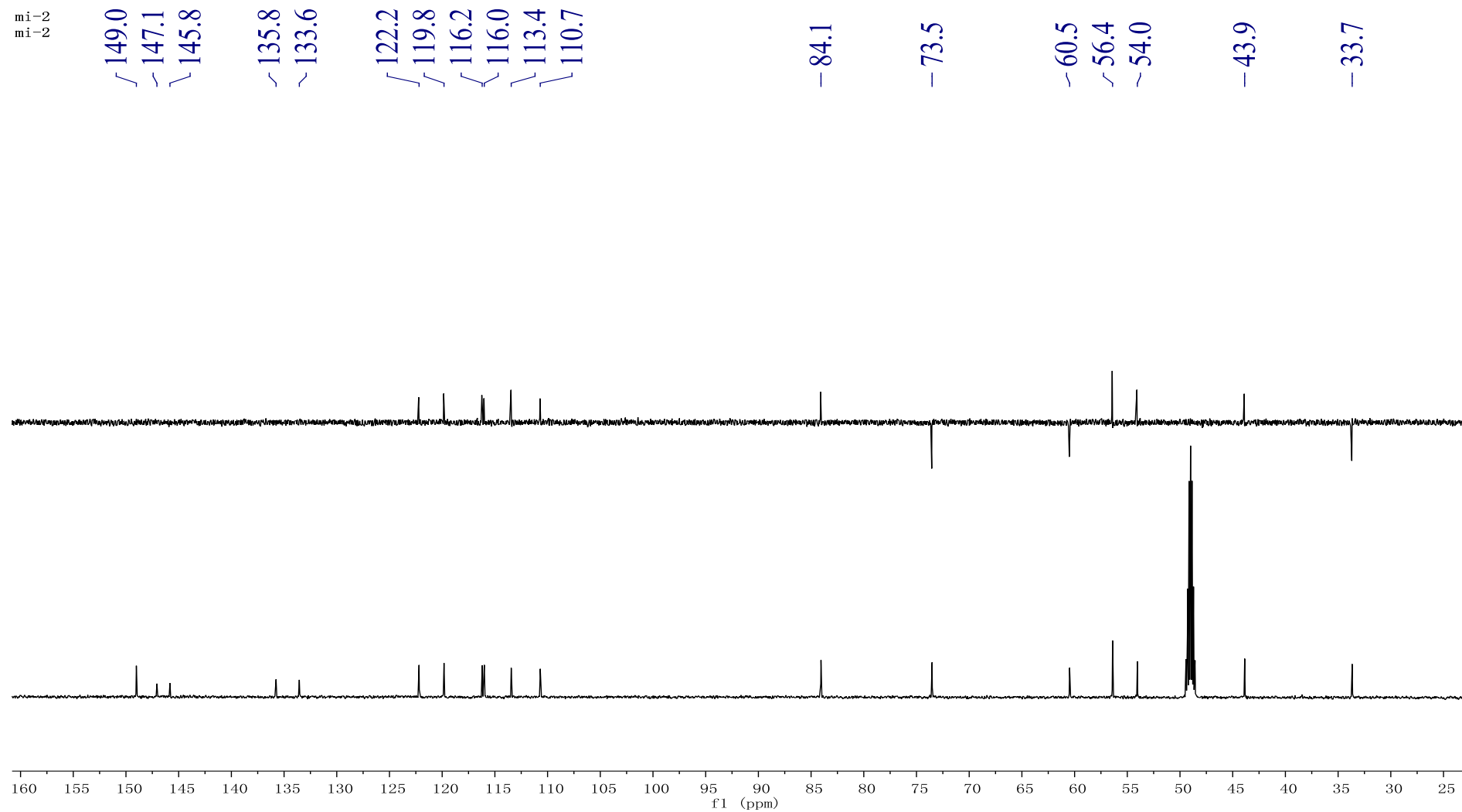


Figure S32. ^1H NMR (600 MHz, CDCl_3) spectrum of **12**

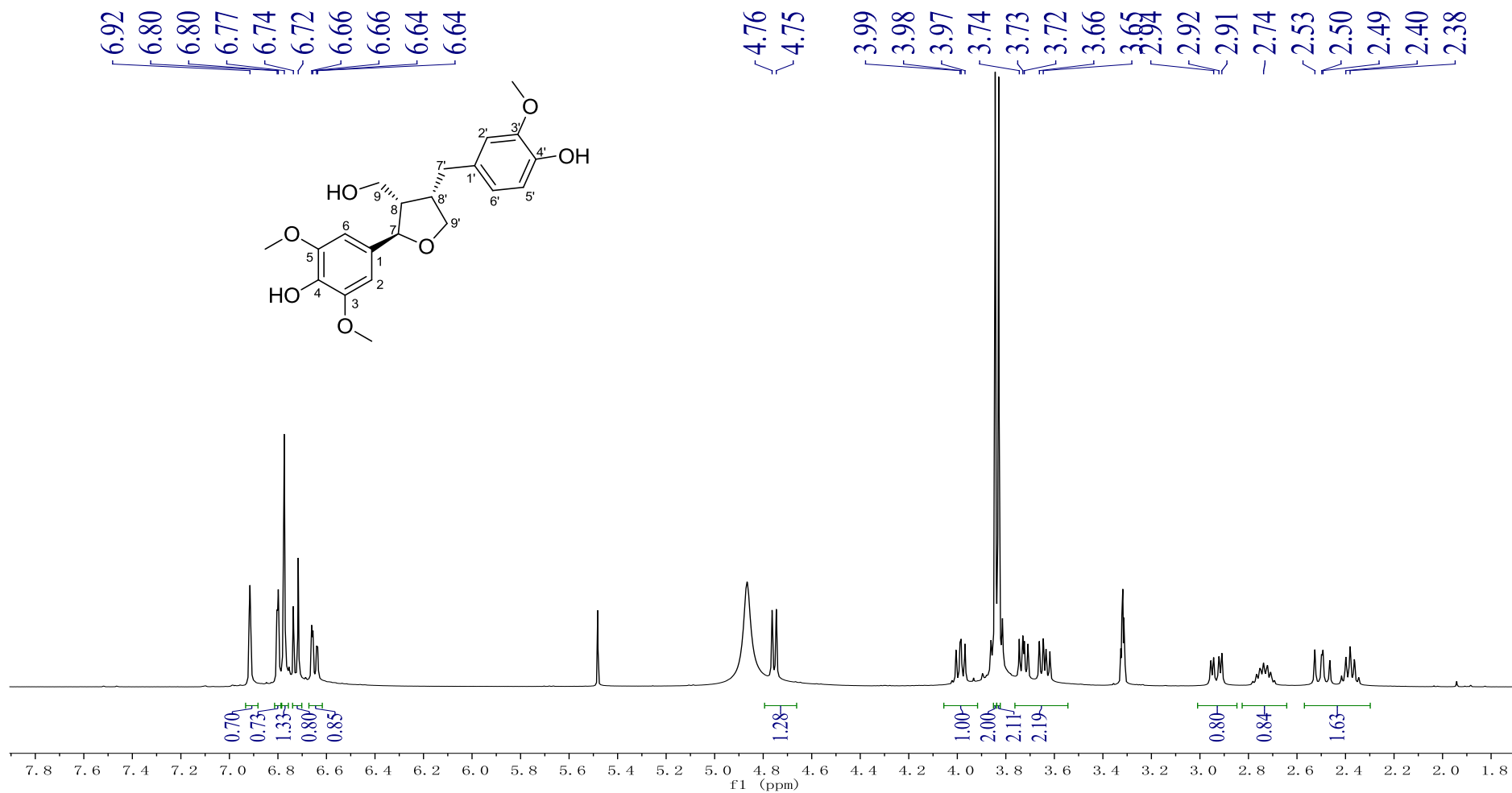


Figure S33. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **12**

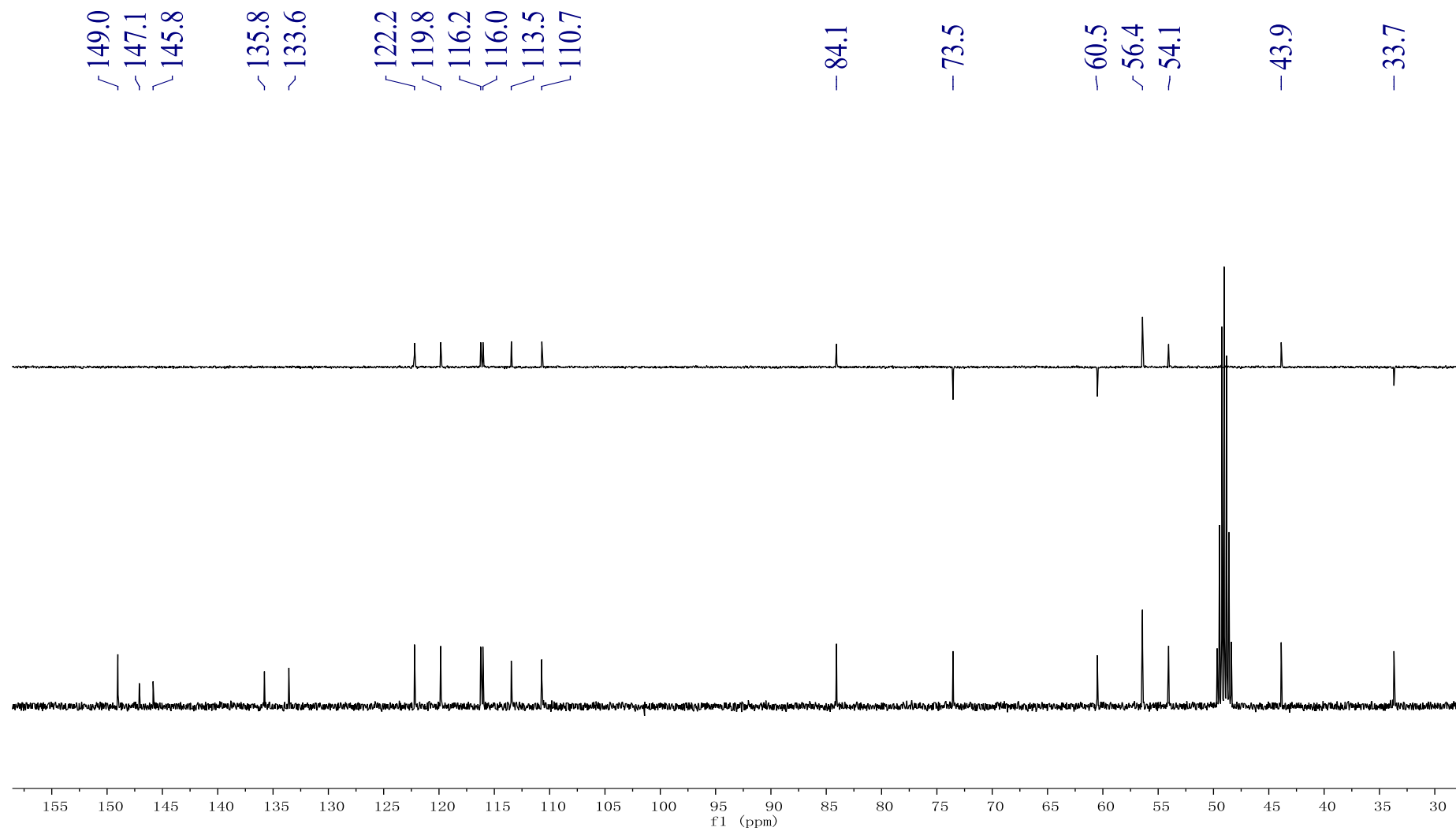


Figure S34. ^1H NMR (600 MHz, CDCl_3) spectrum of **13**

mi-13
mi-13

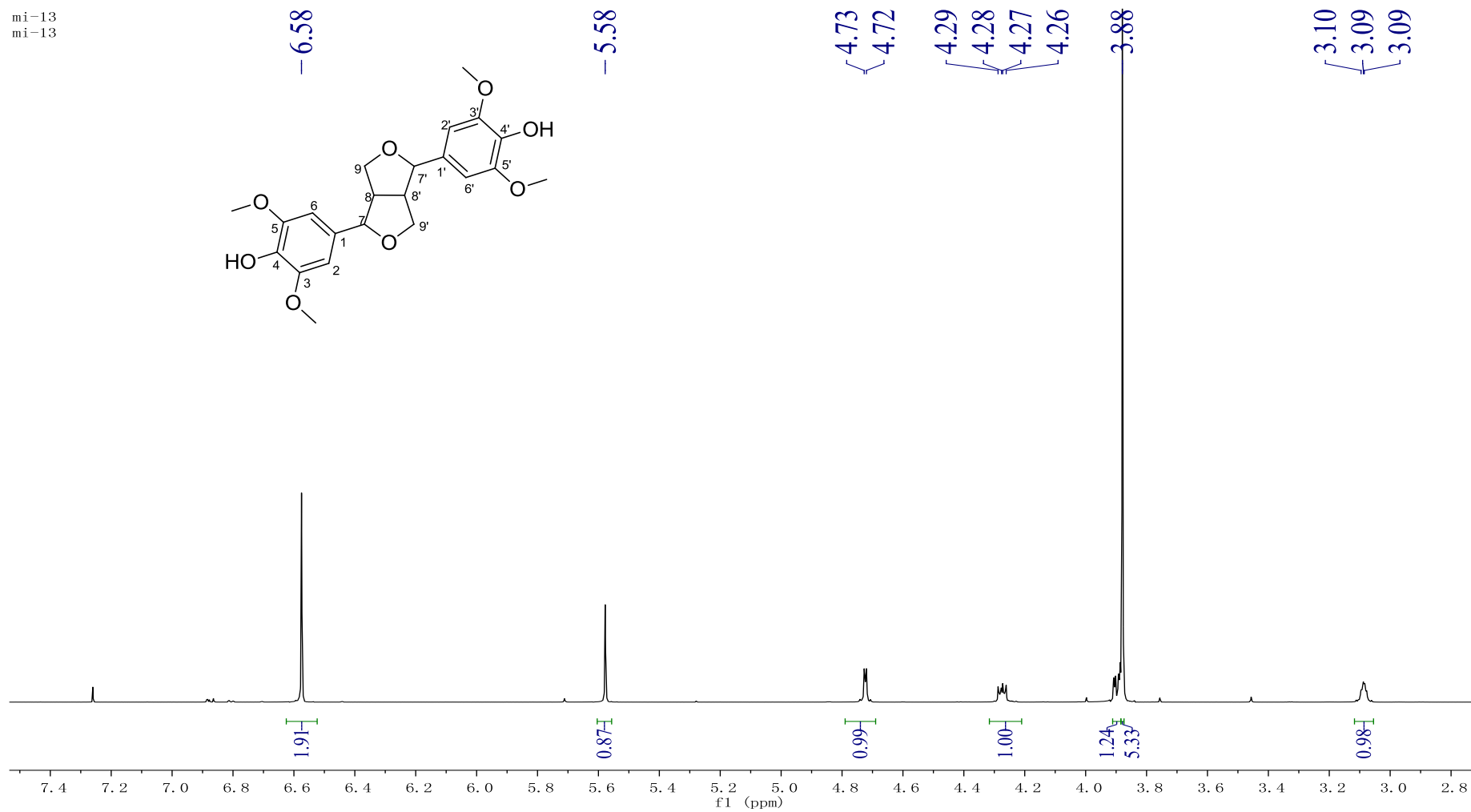


Figure S35. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **13**

mi-13
mi-13

-147.3

~134.4

~132.2

-102.8

-86.2

-71.9

~56.5

~54.4

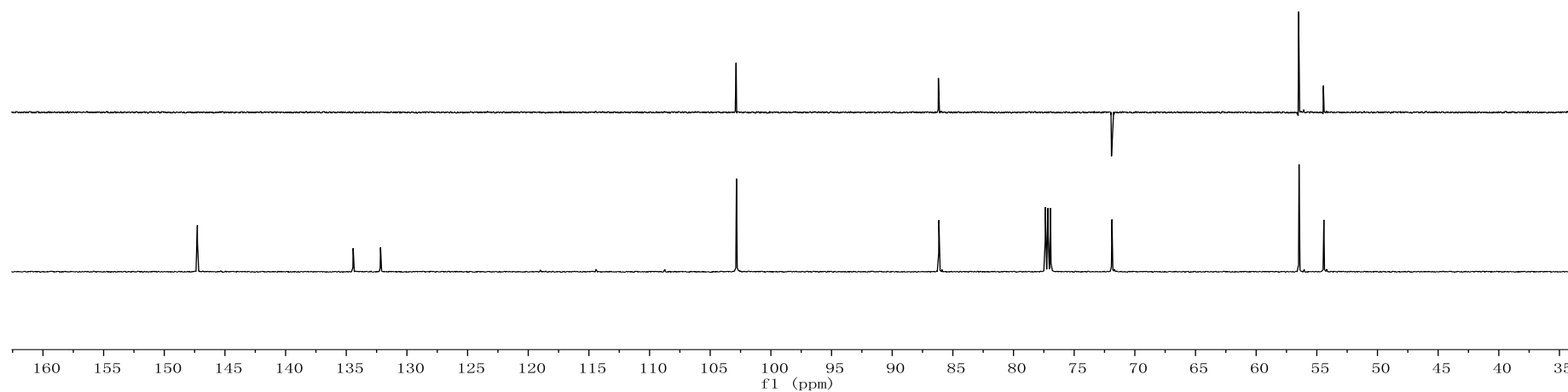


Figure S36. ^1H NMR (600 MHz, CDCl_3) spectrum of **14**

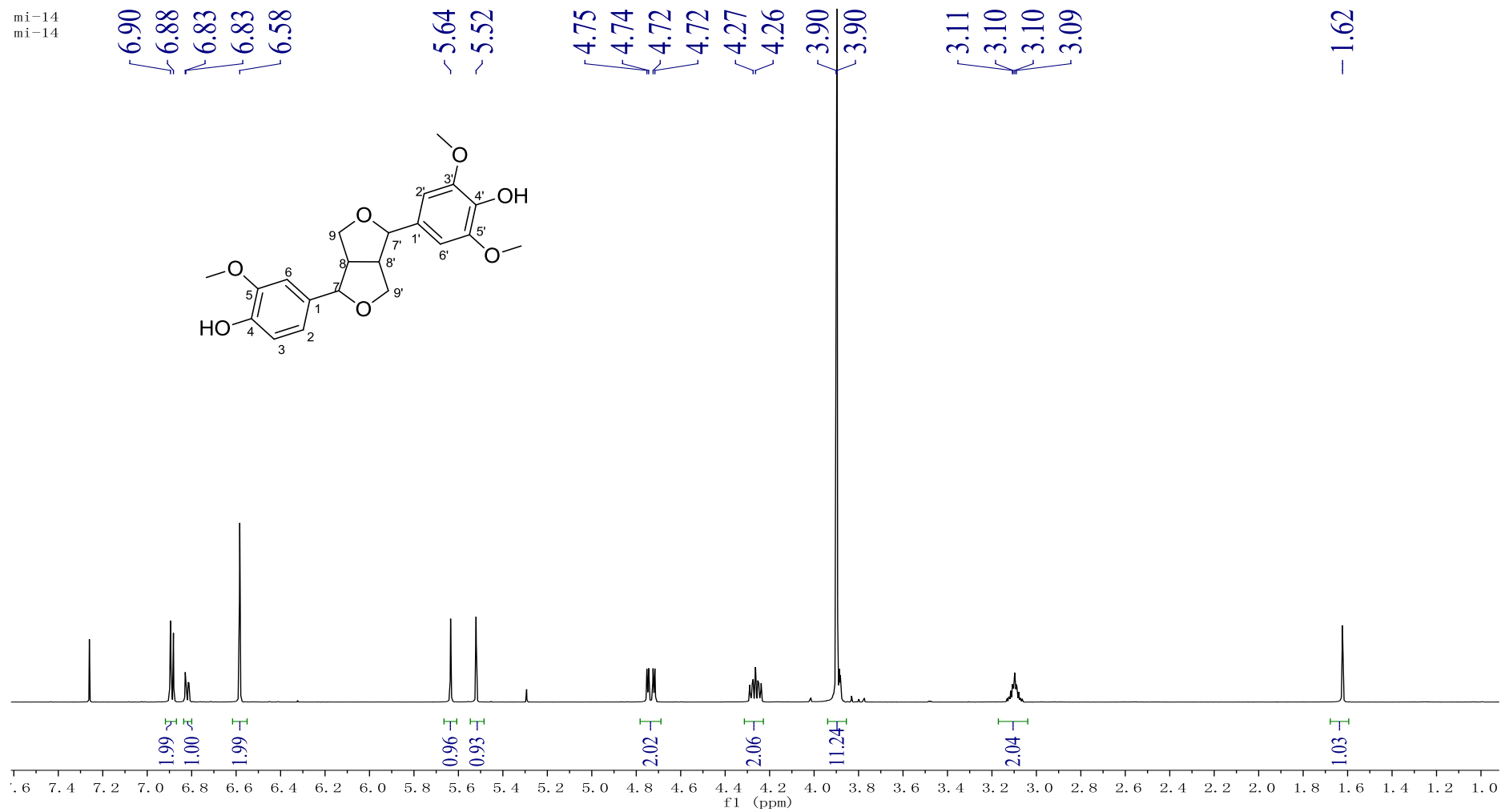


Figure S37. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **14**

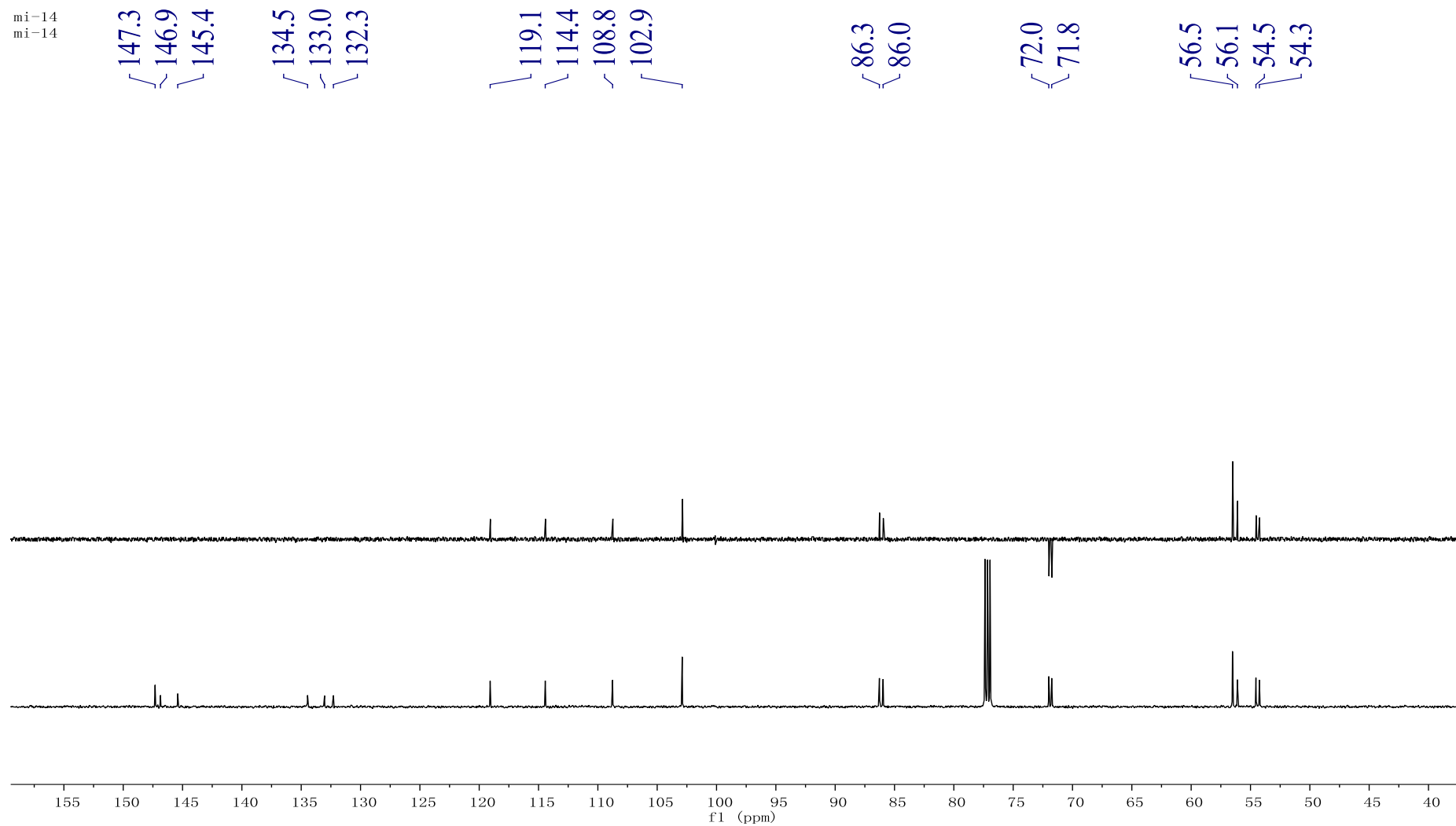


Figure S38. ^1H NMR (600 MHz, CDCl_3) spectrum of **15**

mi-17
mi-17

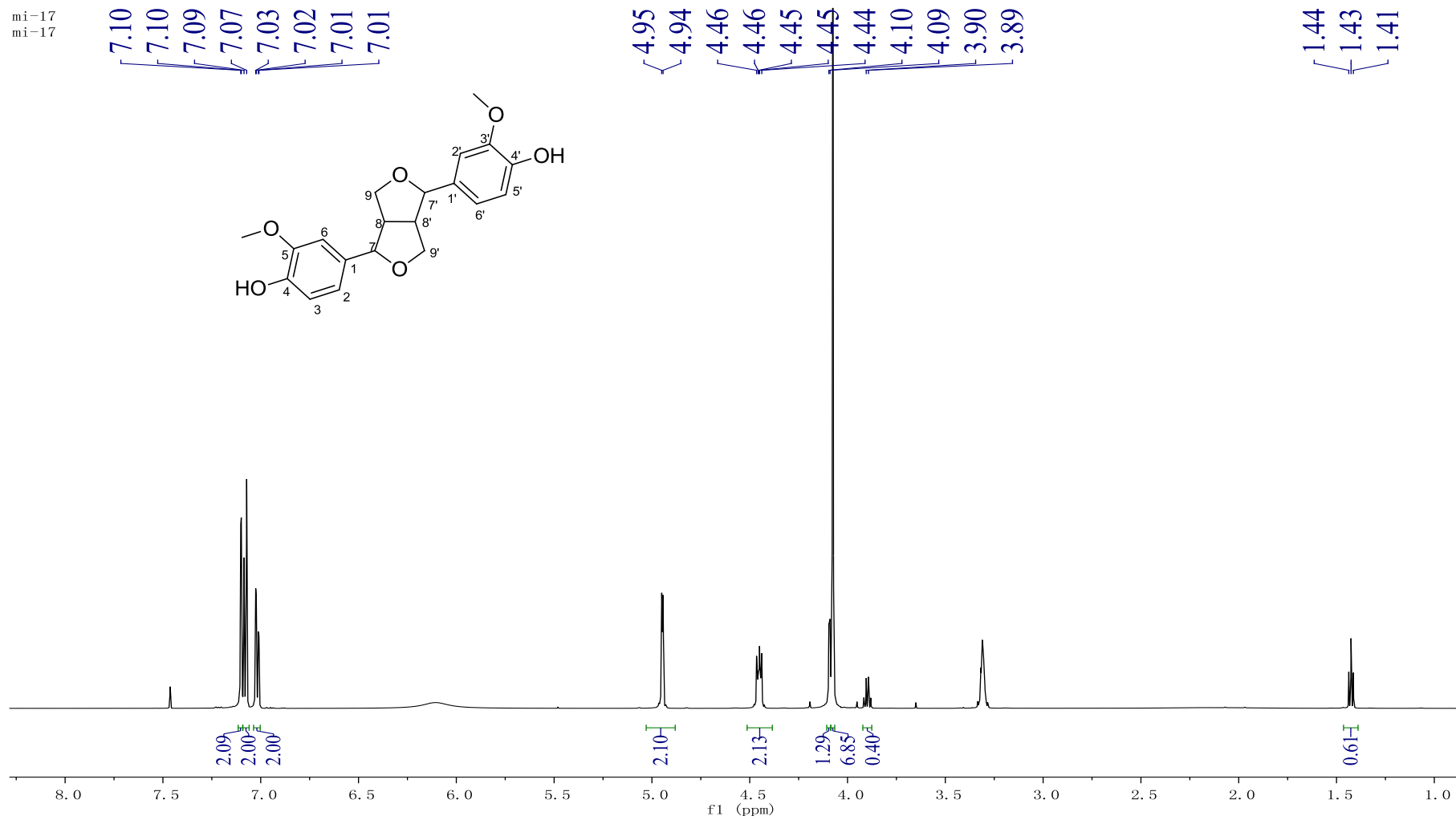


Figure S39. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **15**

