

Supplementary Information for

A Potent Inhibitor to Drug-Resistant HIV-1 Strains Identified from the Medicinal Plant *Justicia gendarussa*

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Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data of compounds **1** in methanol- d_4 .

No	1	
	δ_{H} (J in Hz)	δ_{C}
1		128.84 C
2		131.79 C
3 ^a	6.971 s 6.951 s	106.80 CH
4		151.60 C
5		153.22 C
6 ^a	8.052 s 8.042 s	102.66 CH
7		146.33 C
8 ^a		132.22 C
9 ^a	5.537 d (15.2) 5.531 d (15.2) 5.410 d (15.2) 5.406 d (15.4)	69.10 CH ₂
1' ^a		129.89 C 129.86 C
2' ^a	6.730 d (1.6) 6.655 d (1.7)	111.75 CH
3'		148.94 S
4'		148.94 S
5' ^a	6.897 d (7.9)	108.94 CH 108.90 CH
6' ^a	6.682 dd (7.7, 1.8) 6.659 dd (7.8, 1.7)	124.75 CH 124.70 CH
7'		137.49 C
8' ^a		119.89 C 119.84 C
9'		172.15 C
1'' ^a	4.761 d (7.8) 4.760 d (7.9)	106.67 CH
2'' ^a	3.638 dd (9.2, 8.0) 3.634 dd (9.1, 7.9)	75.79 CH
3''	3.408 t (9.1)	77.80 CH
4''	3.136 t (9.1)	76.69 CH
5''	3.266 m	73.63 CH
6'' ^a	1.303 d (6.0) 1.299 d (6.1)	18.20 CH ₃
3'-OCH ₂ O-4' ^a	6.031 m 6.019 m	102.60 CH ₂
4-OCH ₃ ^a	3.670 s 3.664 s	55.97 CH ₃
5-OCH ₃ ^a	3.974 s 3.970 s	56.69 CH ₃

^a The NMR signals were shown to be doubling due to some degree of hindered rotation of the aryl-naphthalene bond.

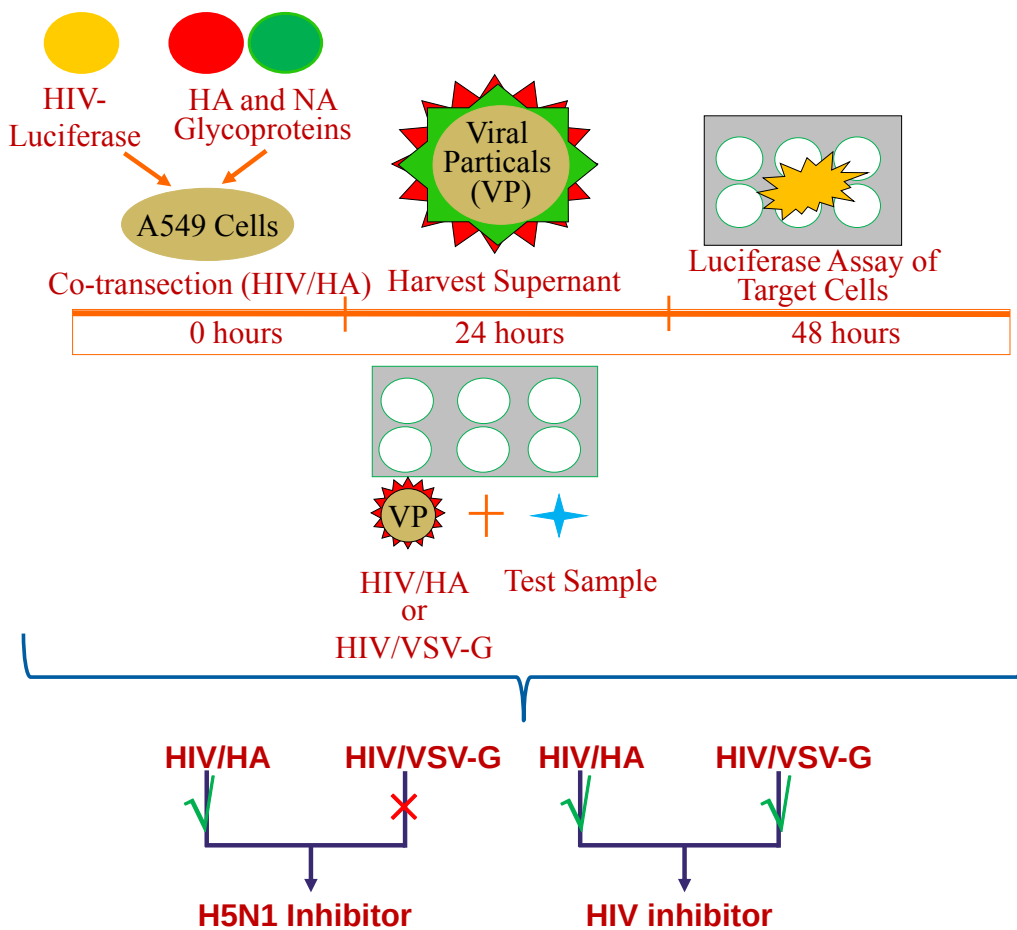


Figure S1. “One-Stone-Two-Birds” evaluation system. The HIV vector carrying luciferase gene is used as the reporter for viral replication. The HIV vector is co-transfected with bird flu H5N1 HA and NA constructs to generate HIV virions with bird flu HA on the viral surface (HIV/HA). The generated HIV/HA cells will then be placed in a 24 wells plate, incubated for 48 hours with samples or without samples. The cells will be harvested to measure the luciferase levels. In the assay system, we run HIV/HA and HIV/VSVG in parallel. HIV/VSV-G is VSV-G pseudotyped HIV virions without bird flu HA coated on the surface. When a sample is tested to inhibit HIV/HA but not HIV/VSV-G, we consider it as a potential bird flu inhibitor. However, when a sample is tested to inhibit both HIV/HA and HIV/VSV-G, we consider it as a potential HIV inhibitor.

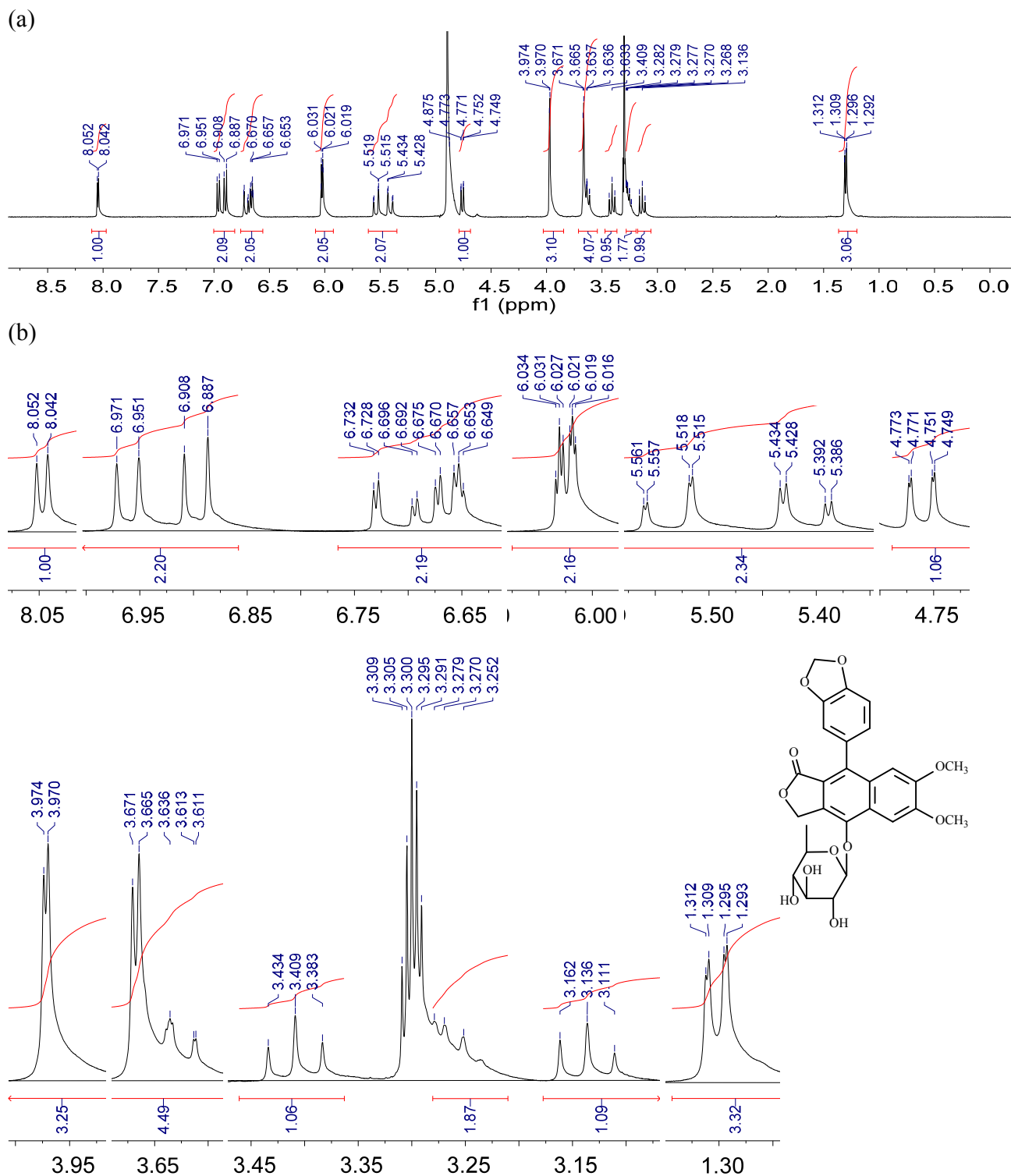


Figure S2. ^1H NMR (360 MHz) spectrum of patentiflorin A (**1**) in CD_3OD . (a) Full view; (b) Expansion.

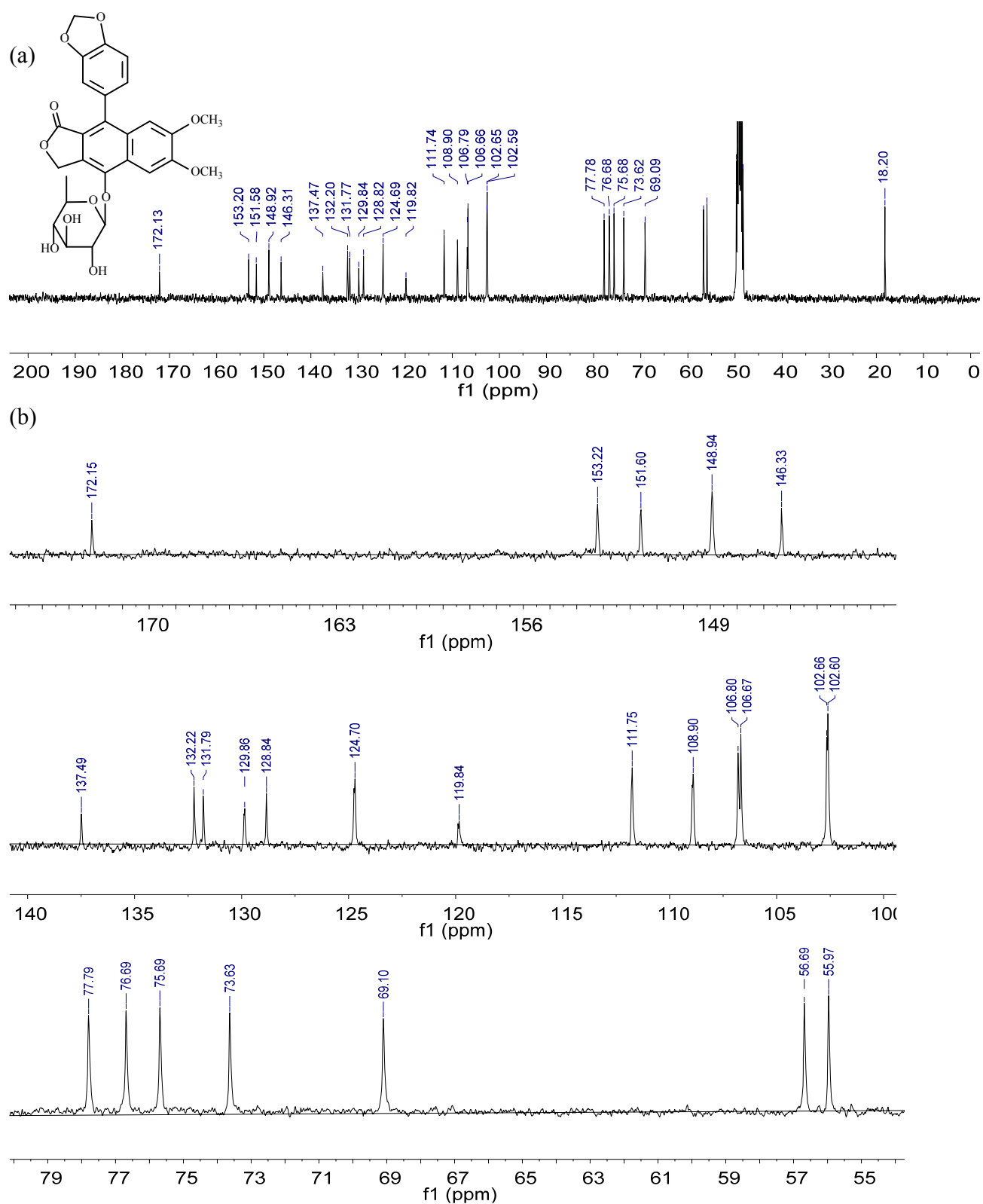


Figure S3. ¹³C NMR (90 MHz) spectrum of patentiflorin A (1) in CD₃OD. (a) Full view; (b) Expansion.

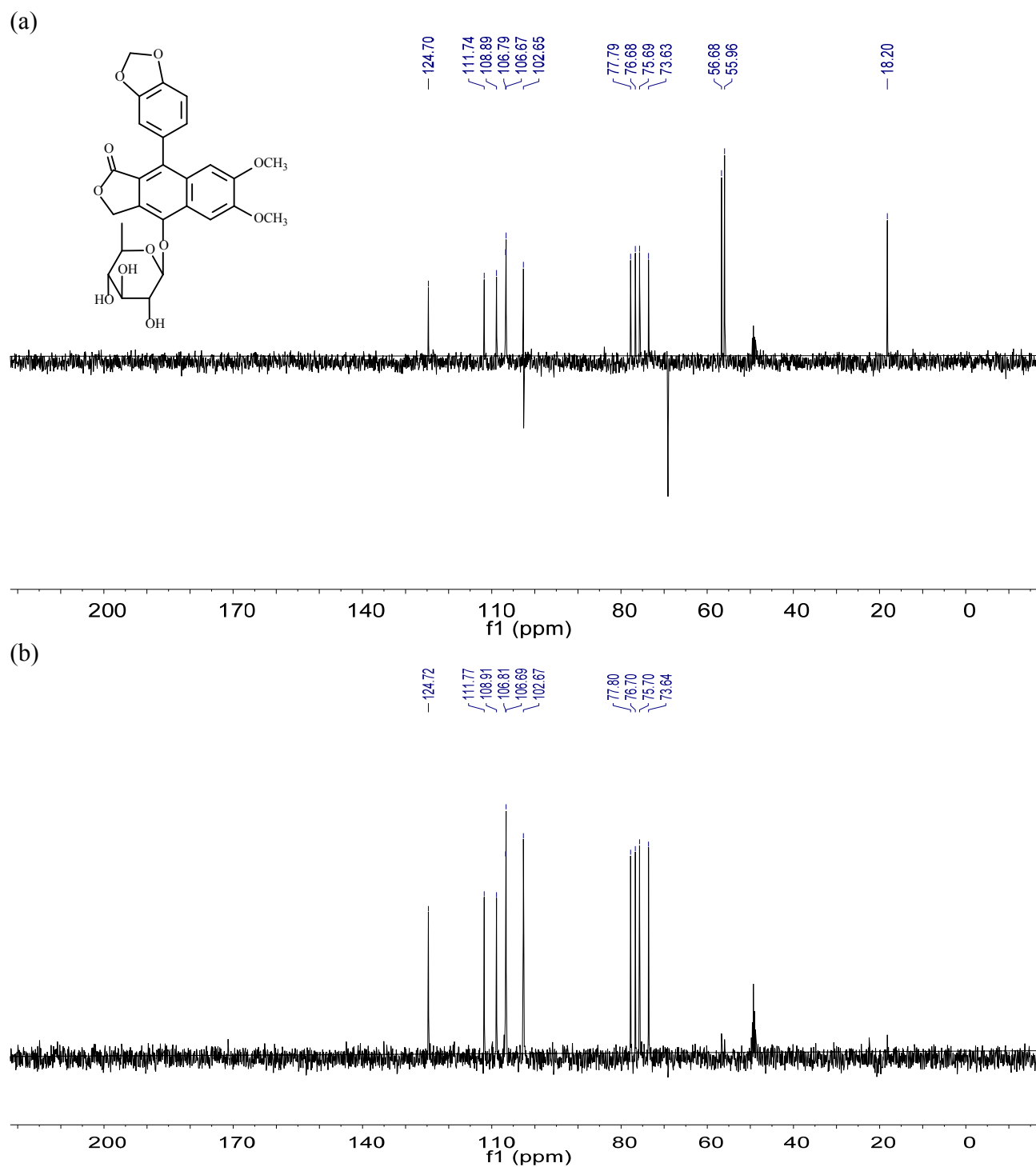
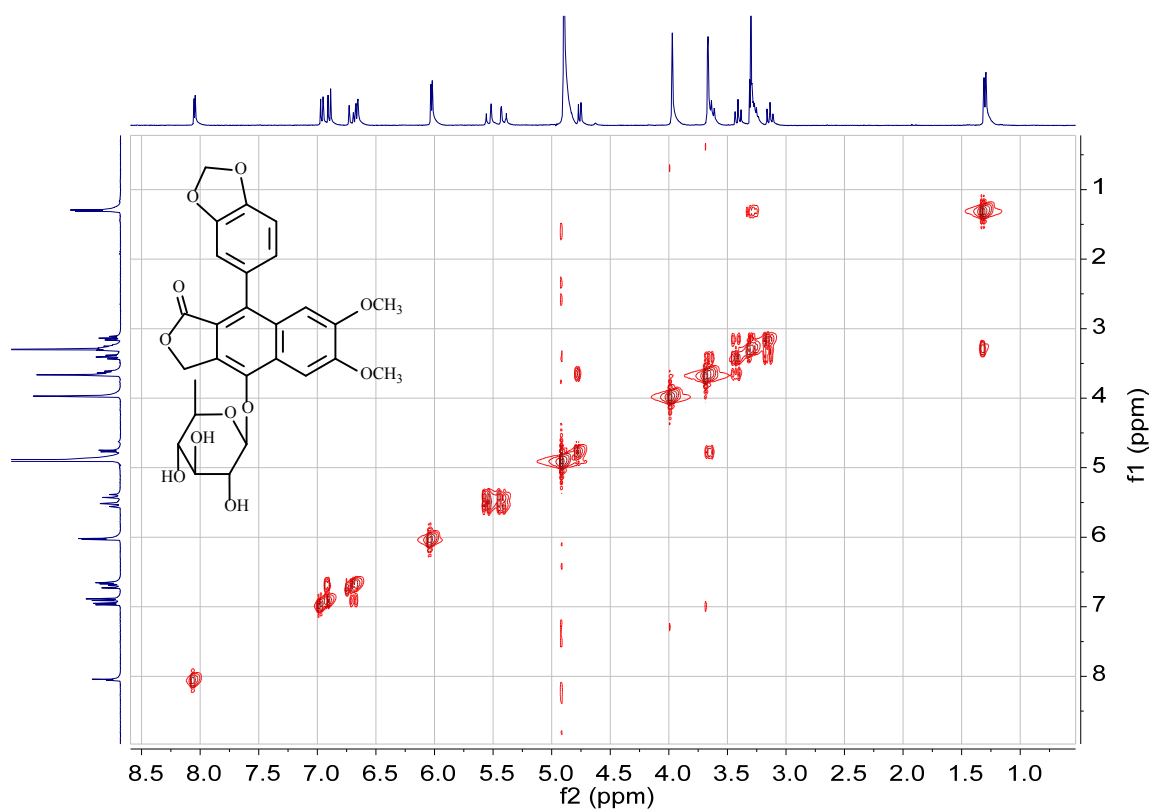


Figure S4. DEPT NMR (90 MHz) spectra of patentiflorin A (**1**) in CD₃OD. (a) DEPT-135; (b) DEPT-90.

(a)



(a)

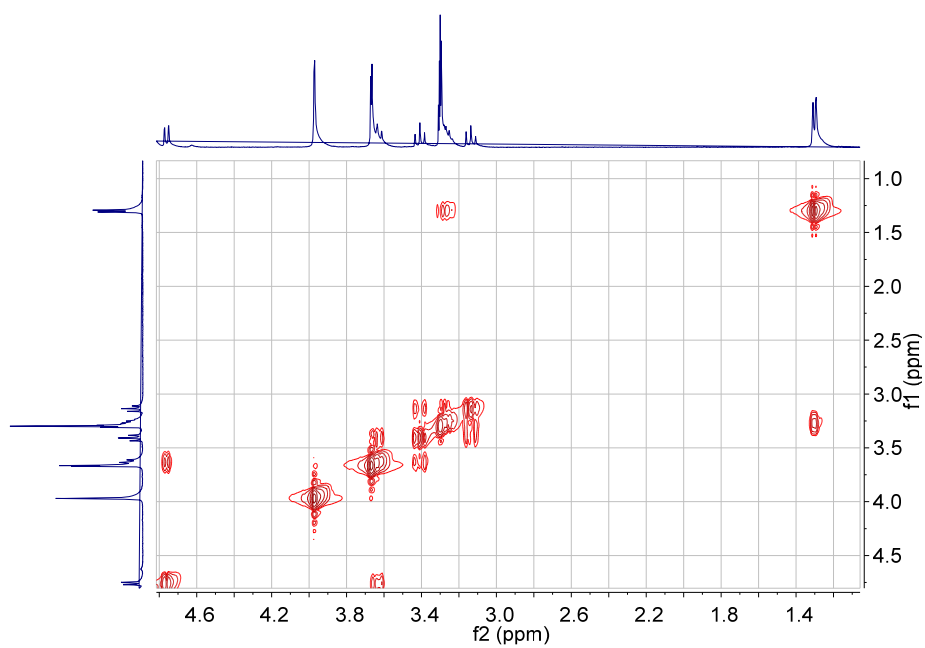
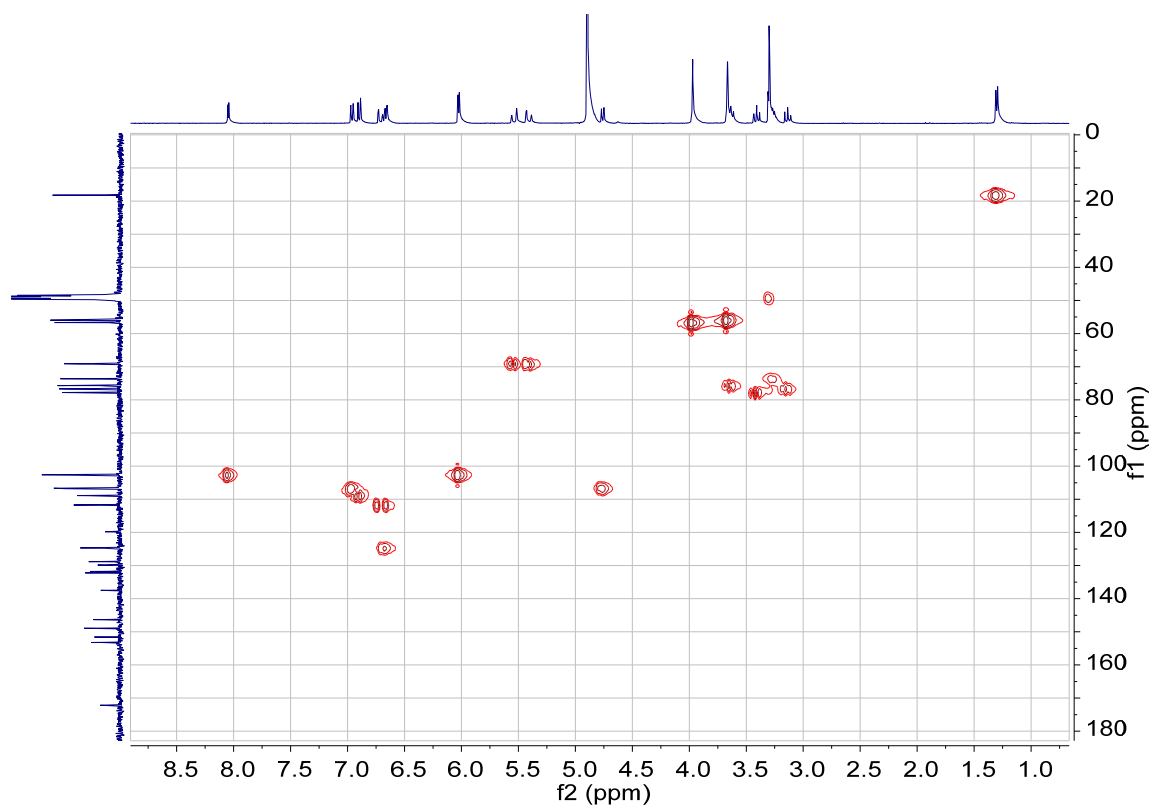


Figure S5. ^1H - ^1H COSY (360 MHz) spectrum of patentiflorin A (**1**) in CD_3OD . (a) Full view; (b) Expansion.

(a)



(b)

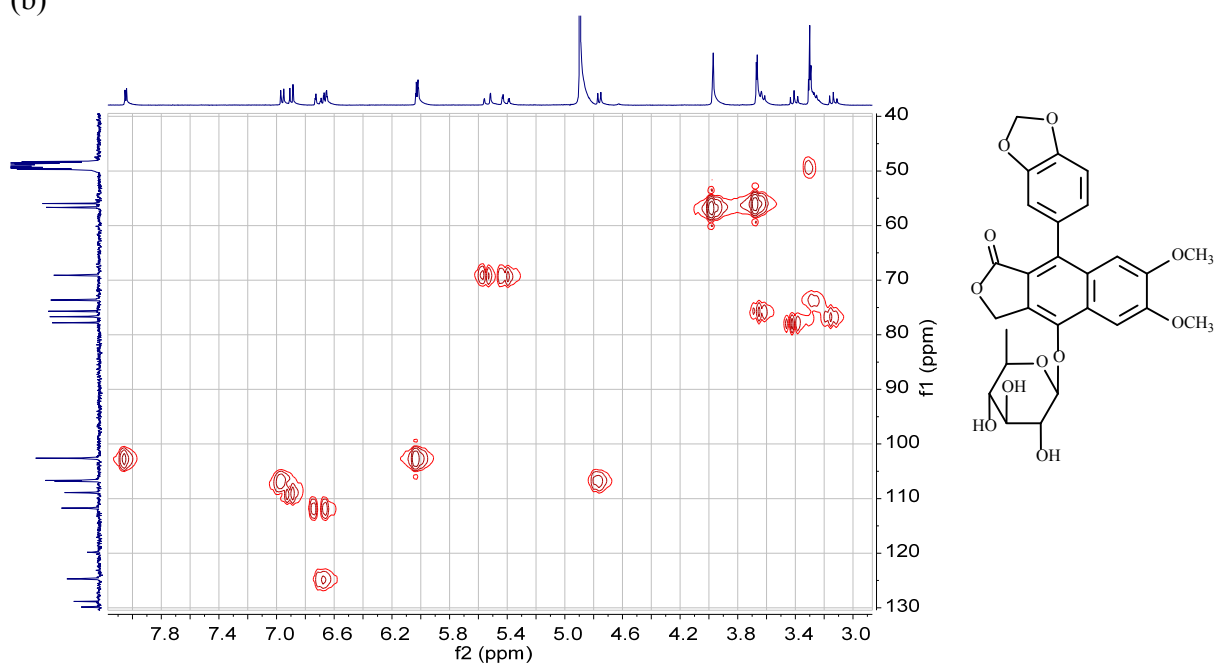
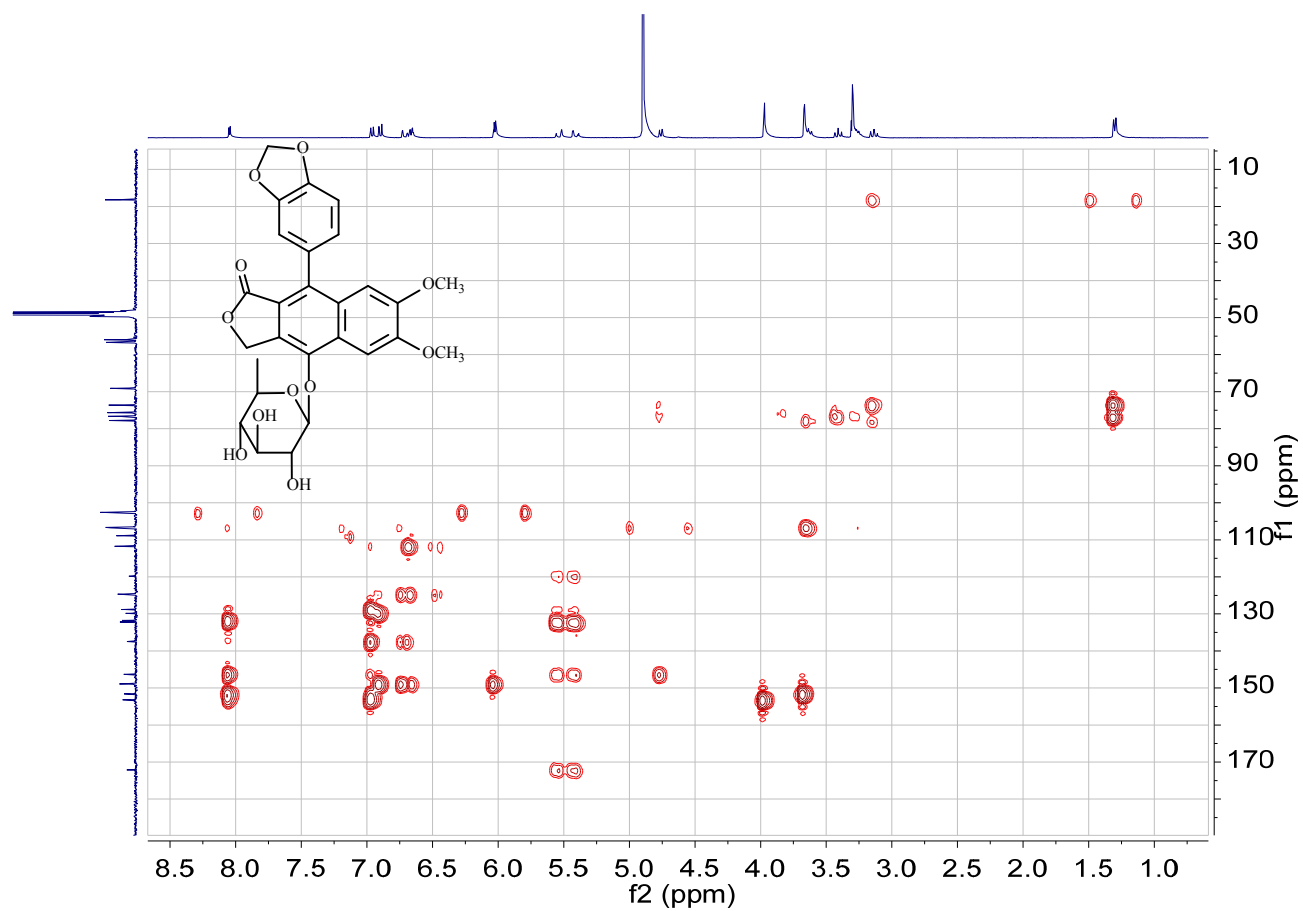


Figure S6. HMQC (360 MHz) spectrum of patentiflorin A (**1**) in CD₃OD. (a) Full view; (b) Expansion.

(a)



(b)

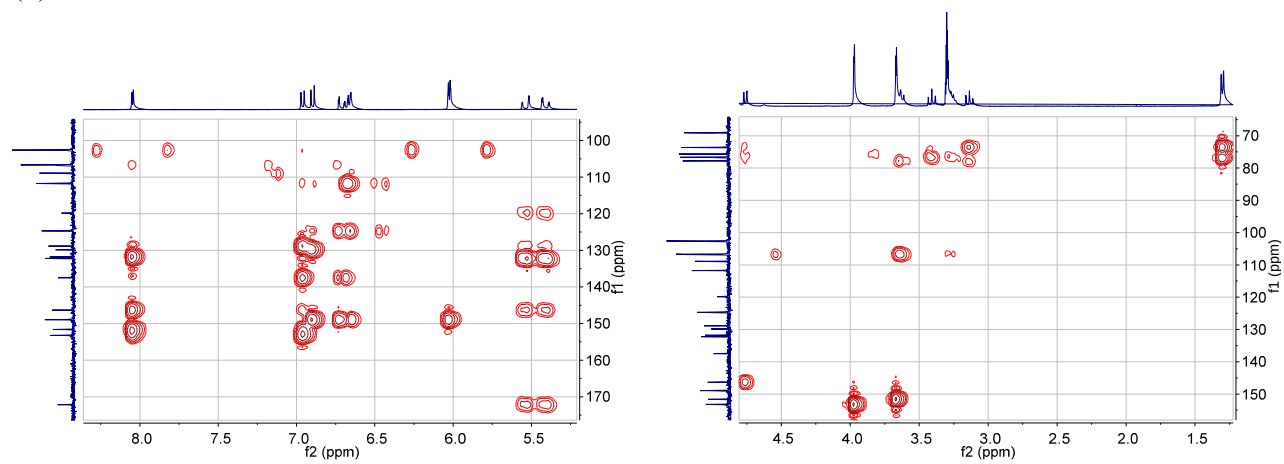


Figure S7. HMBC (360 MHz) spectrum of patentiflorin A (**1**) in CD₃OD. (a) Full view; (b) Expansion.

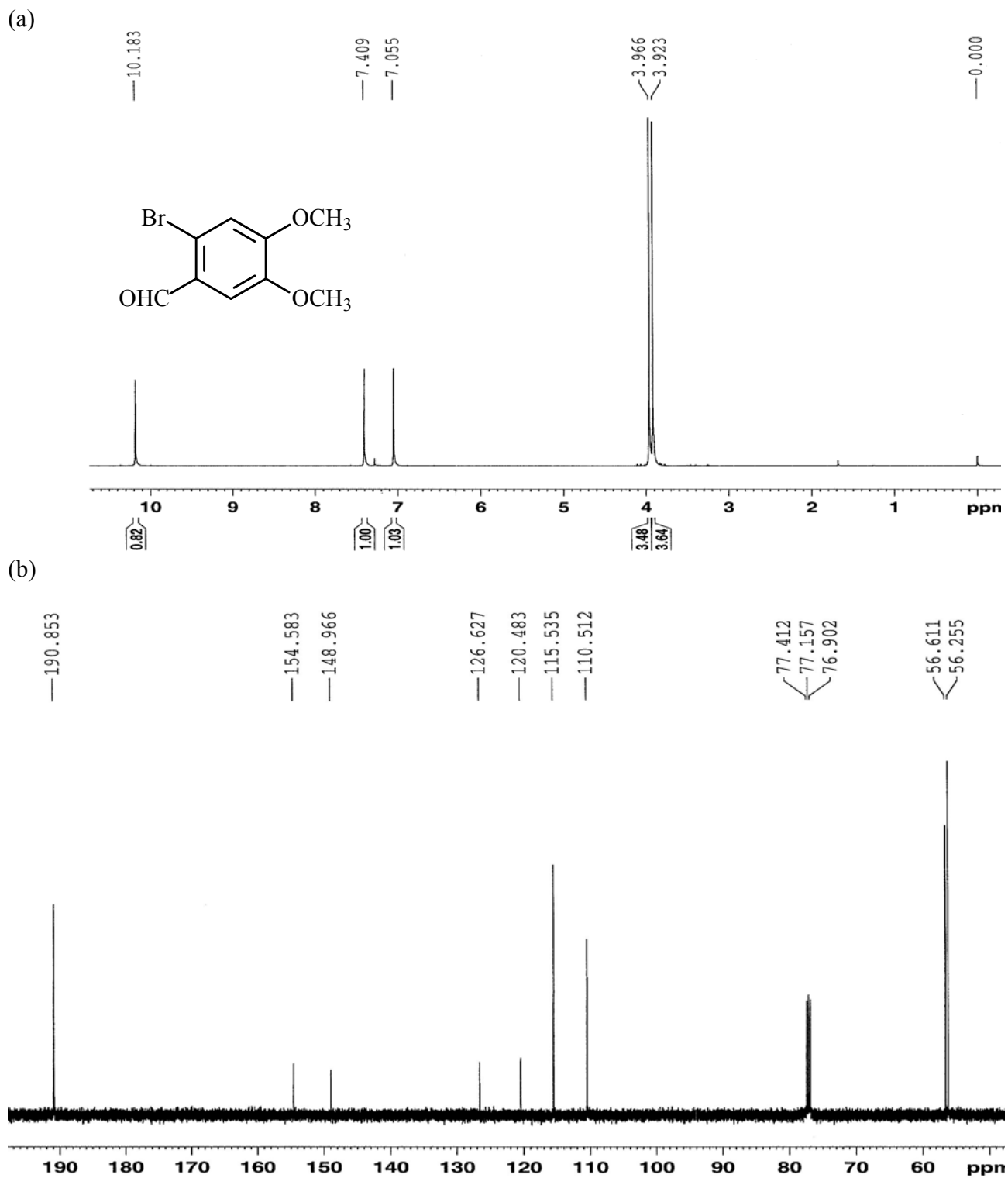


Figure S8. NMR spectrum of the synthetic **3** in CDCl₃. (a) ¹H NMR (500 MHz); (b) ¹³C NMR (125 MHz).

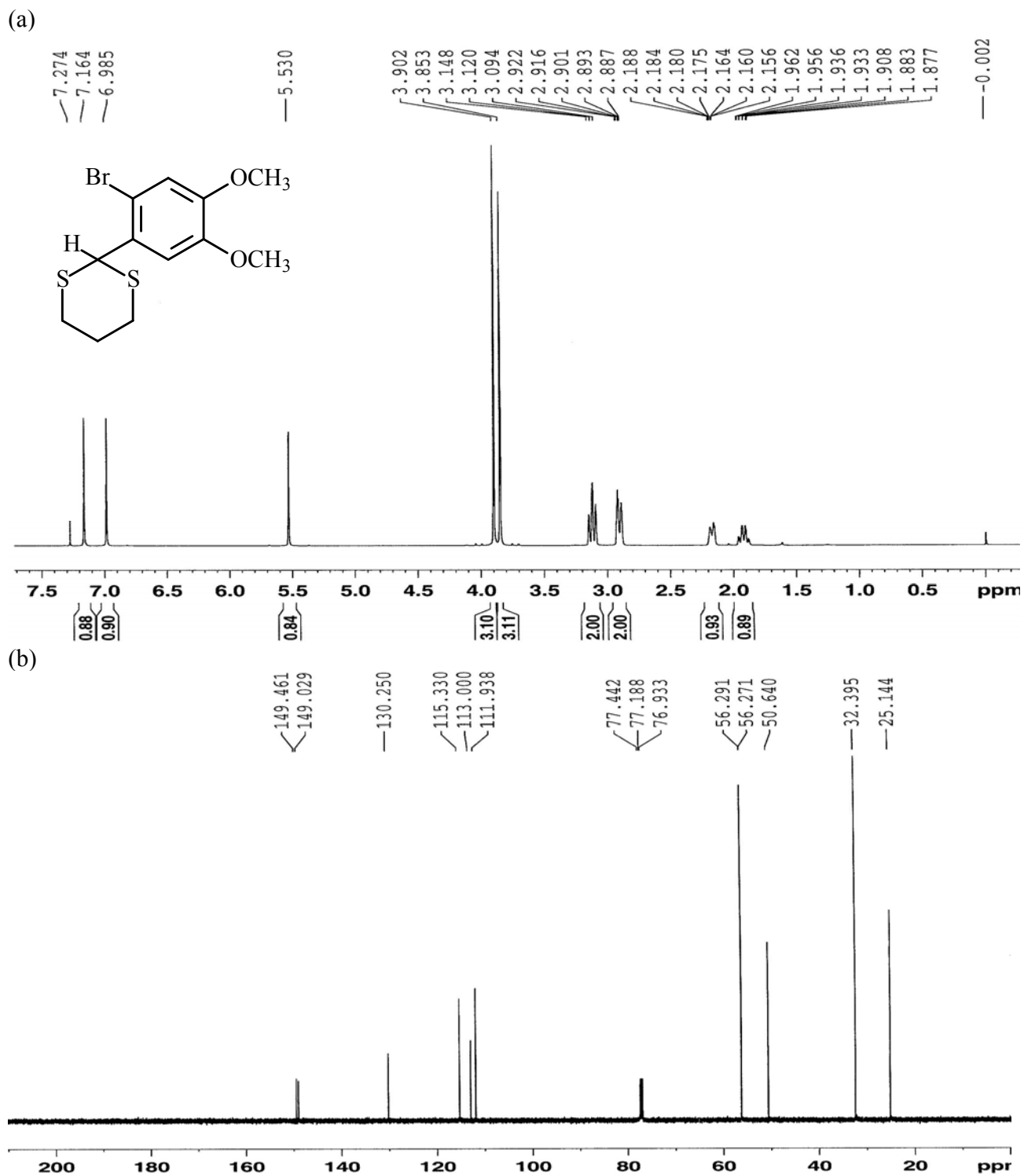


Figure S9. NMR spectrum of the synthetic **4** in CDCl₃. (a) ¹H NMR (500 MHz); (b) ¹³C NMR (125 MHz).

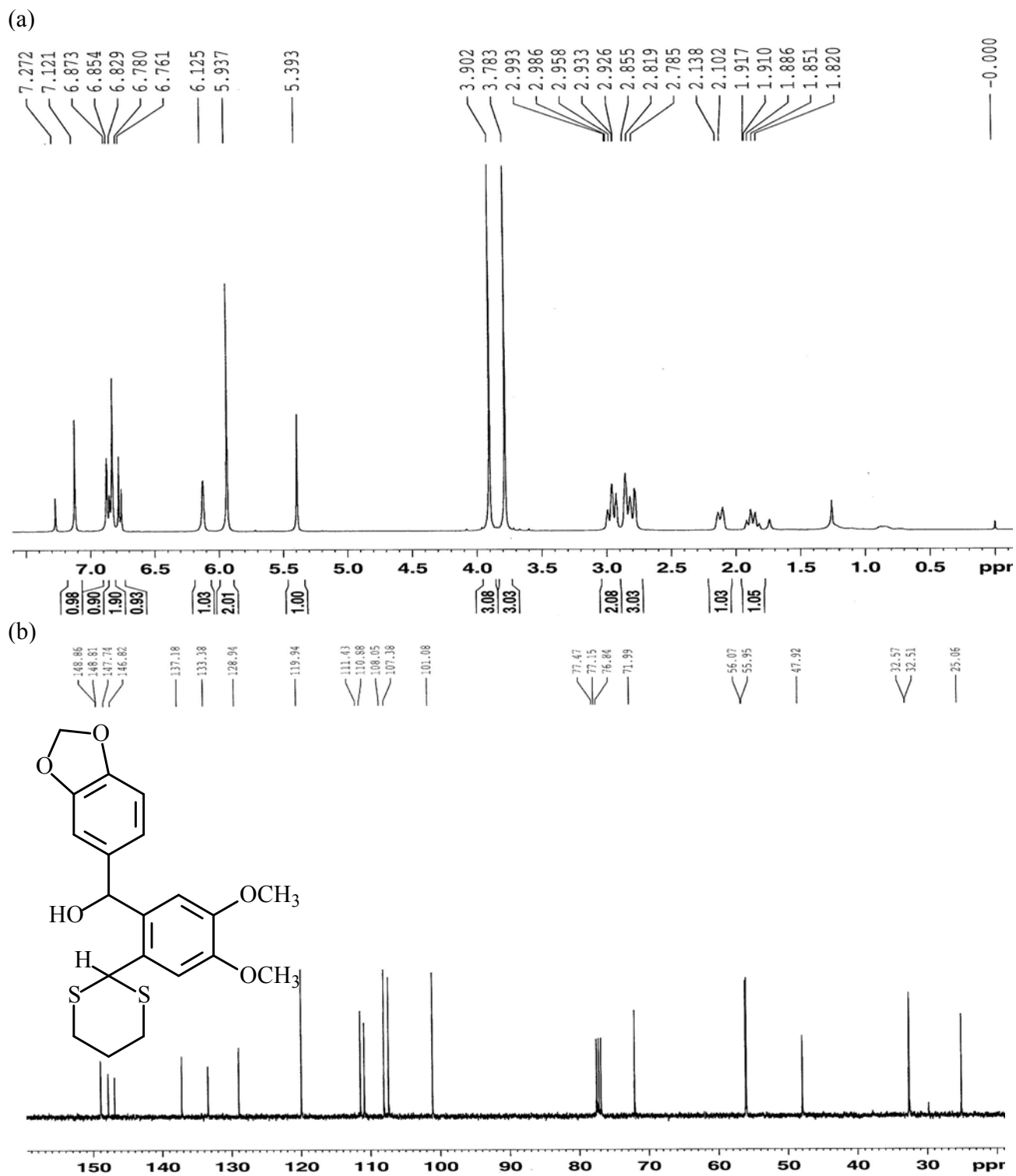


Figure S10. NMR spectrum of the synthetic 5 in CDCl₃. (a) ¹H NMR (400 MHz); (b) ¹³C NMR (100 MHz).

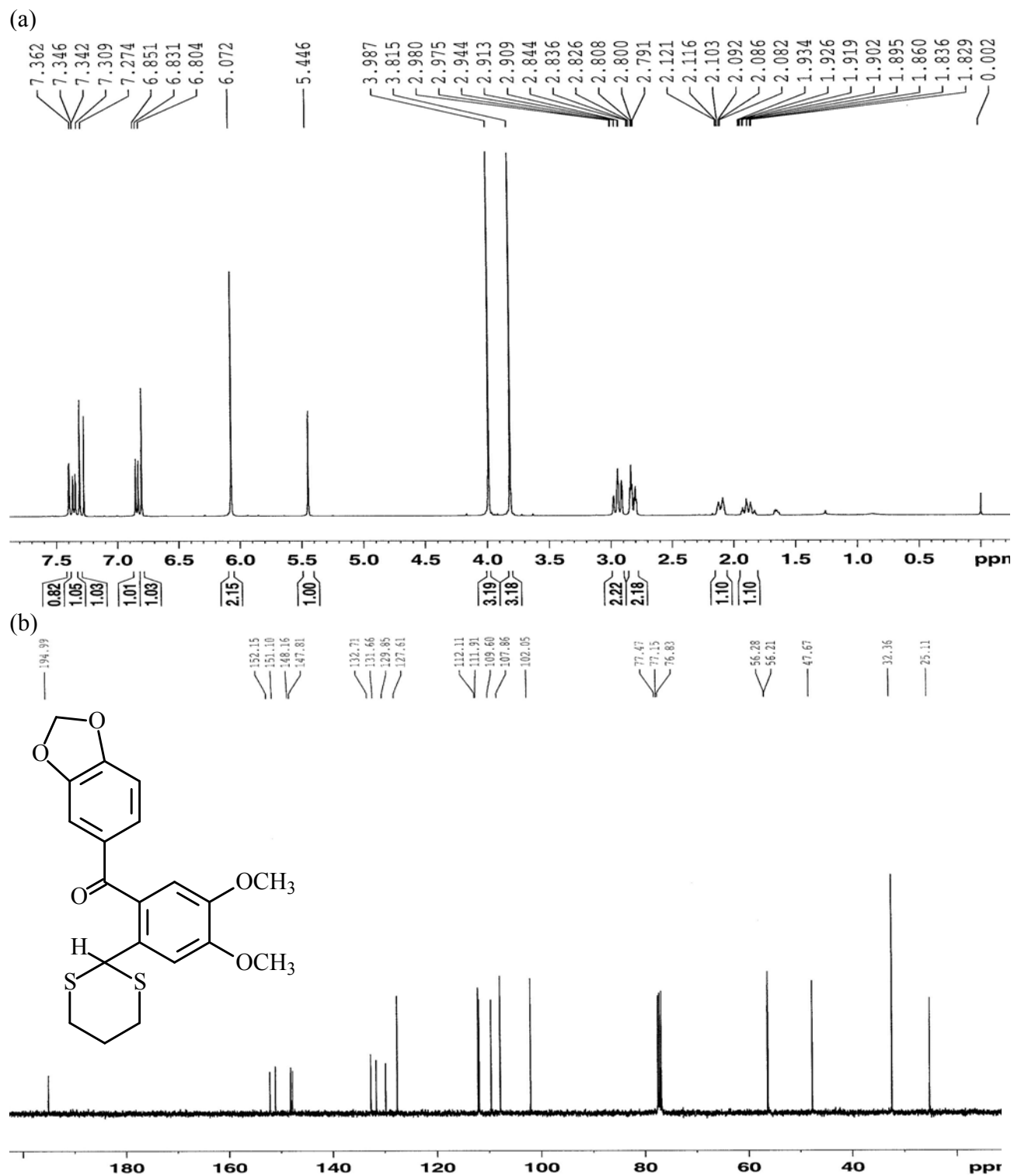


Figure S11. NMR spectrum of the synthetic **6** in CDCl_3 . (a) ^1H NMR (400 MHz); (b) ^{13}C NMR (100 MHz).

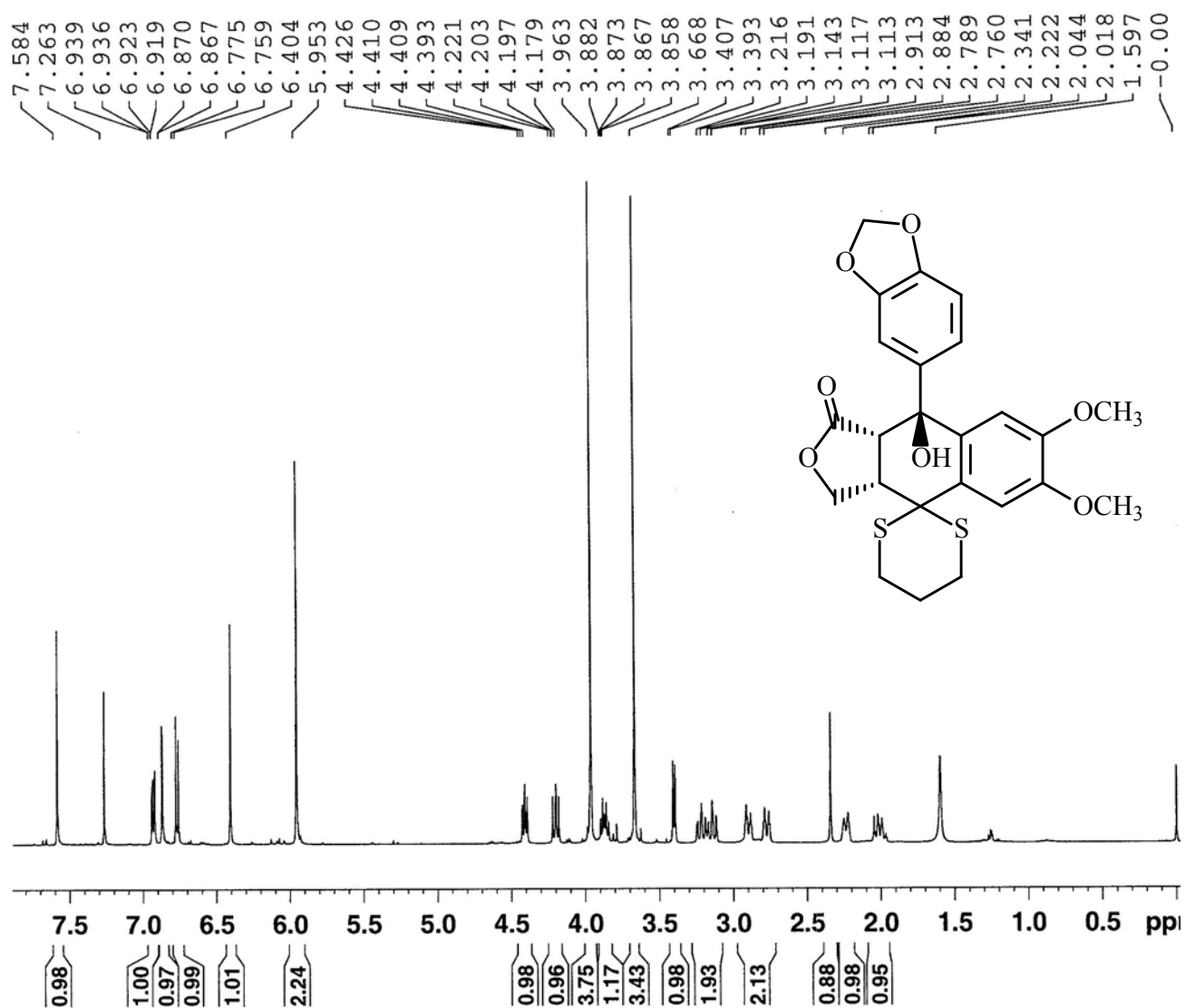


Figure S12. ¹H NMR (500 MHz) spectrum of the synthetic **8** in CDCl₃.

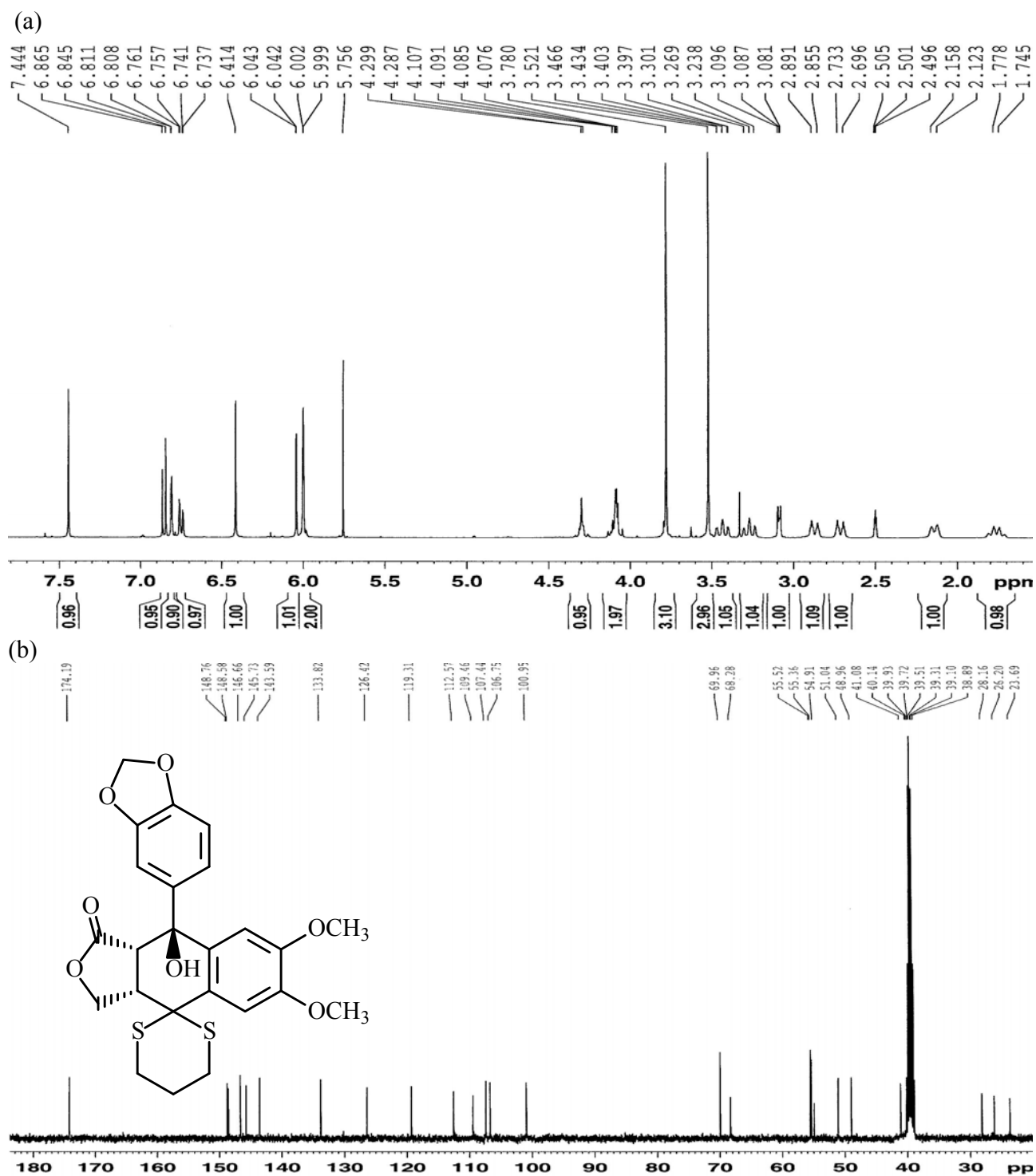


Figure S13. NMR spectrum of the synthetic **8** in DMSO- d_6 . (a) ^1H NMR (400 MHz); (b) ^{13}C NMR (100 MHz).

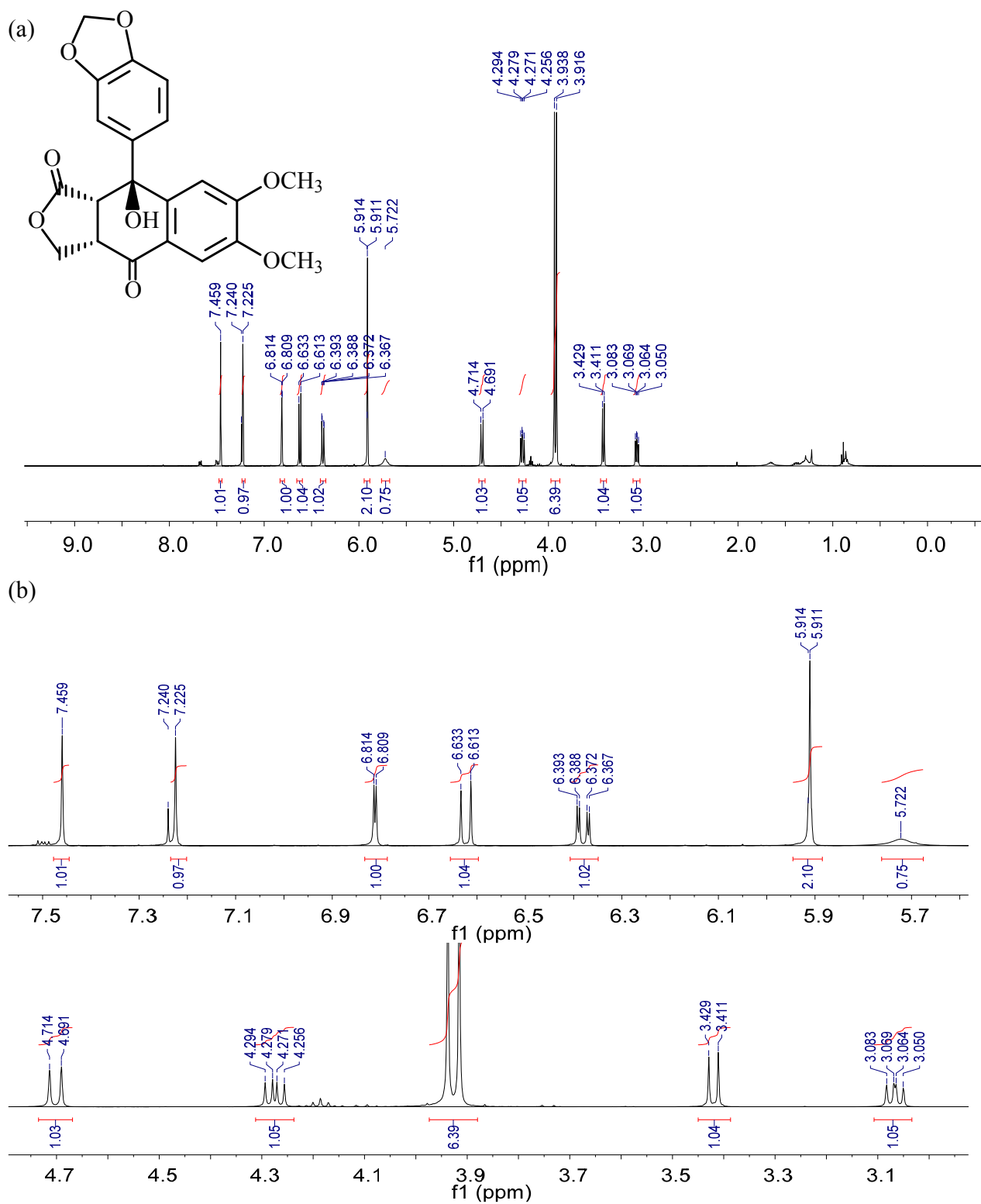


Figure S14. ^1H NMR (400 MHz) spectrum of the synthetic **9** in CDCl_3 . (a) Full view; (b) Expansion.

(a)

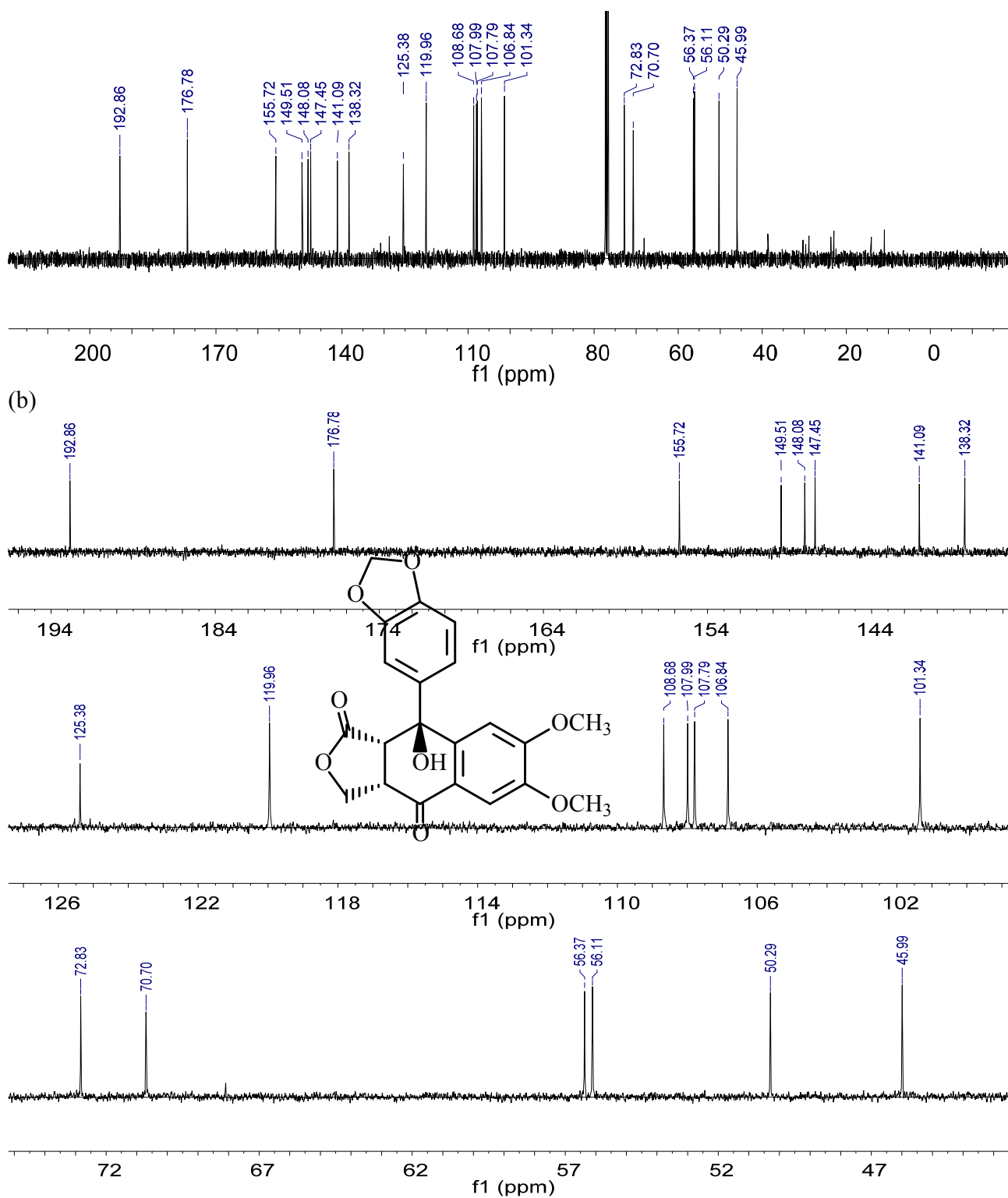


Figure S15. ^{13}C NMR (100 MHz) spectrum of the synthetic **9** in CDCl_3 . (a) Full view; (b) Expansion.

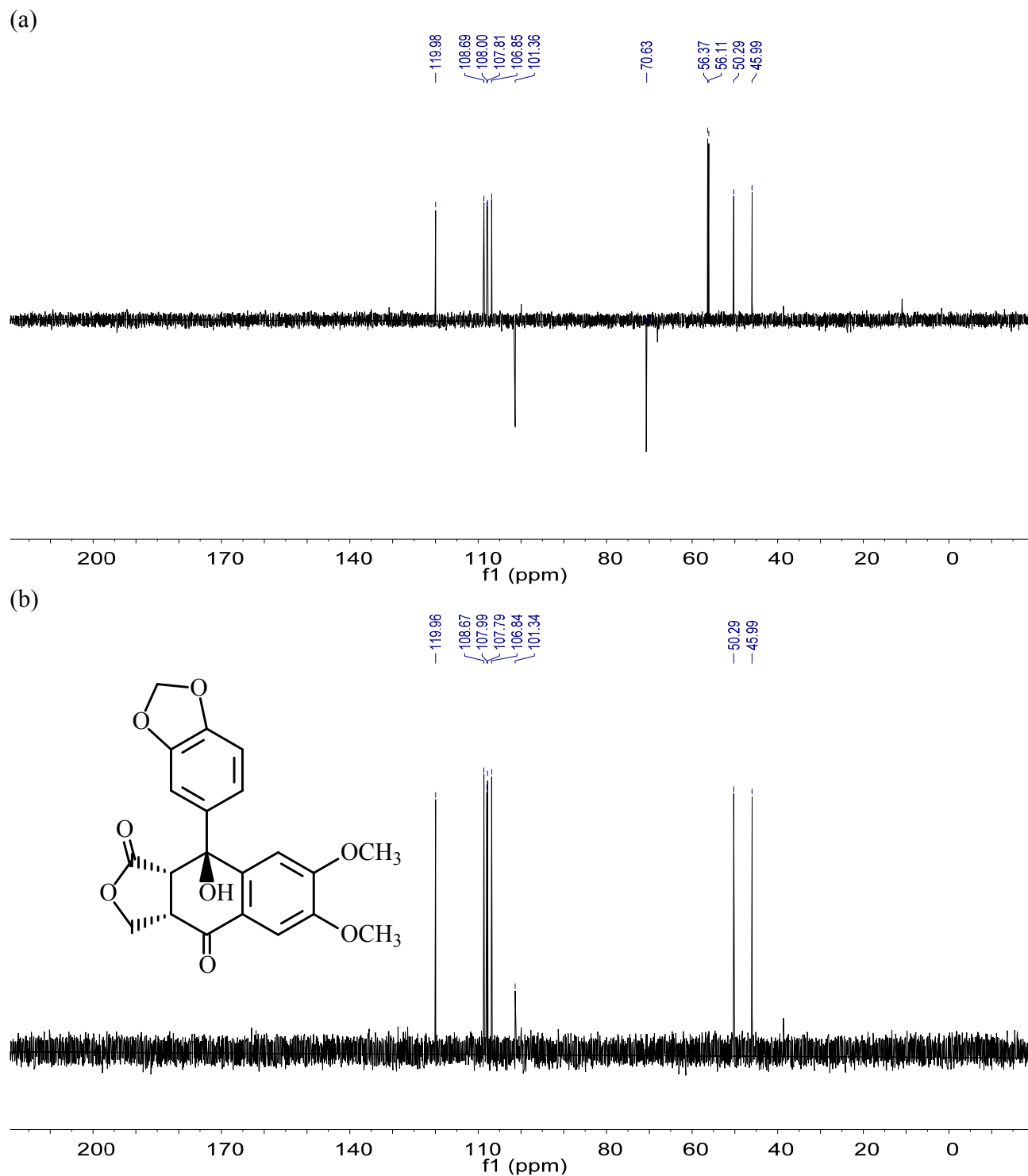


Figure S16. DEPT NMR (100 MHz) spectra of synthetic **9** in CDCl₃. (a) DEPT-135; (b) DEPT-90.

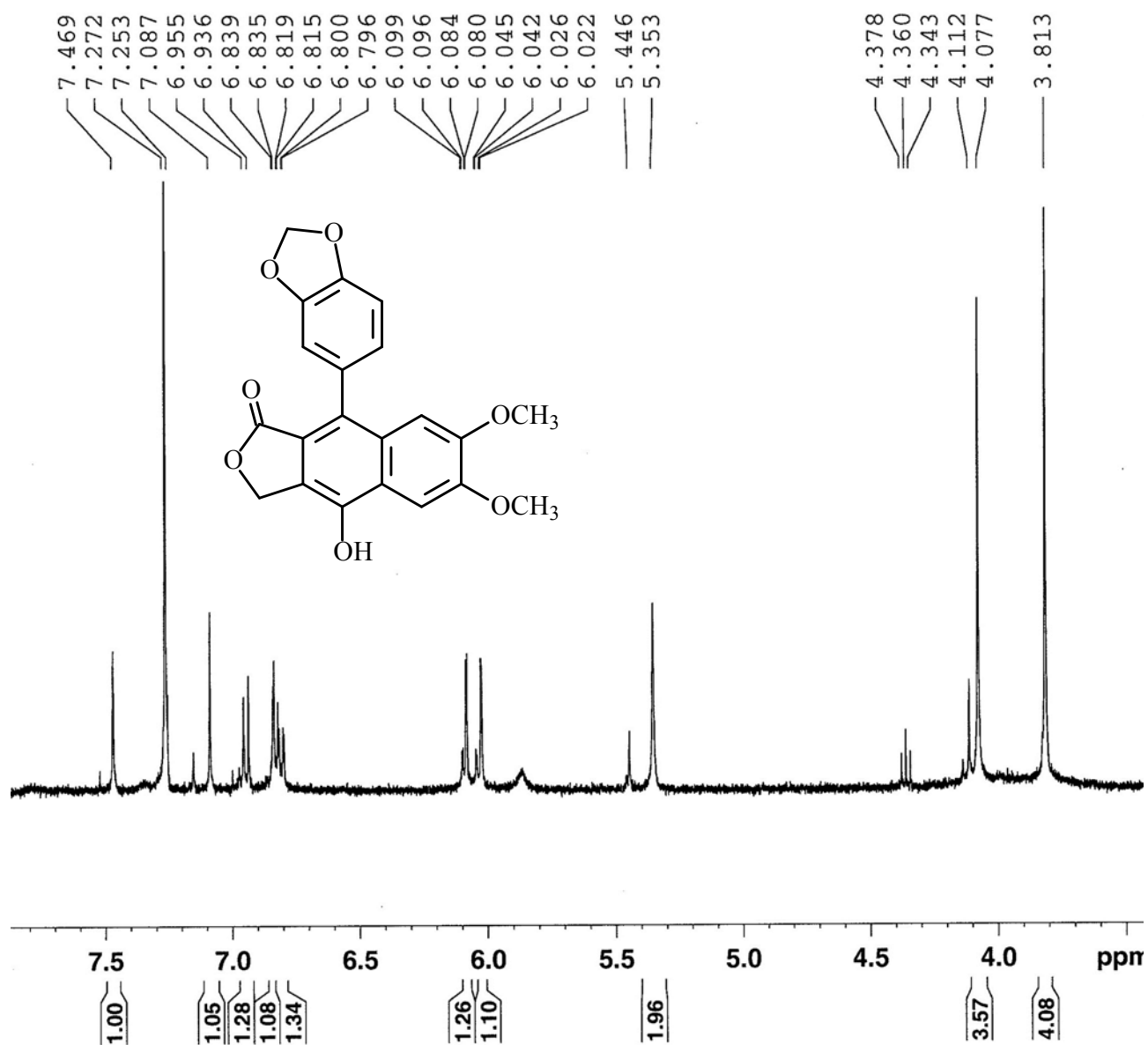


Figure S17. ¹H NMR (400 MHz) spectrum of diphyllin (**10**) in CDCl₃.

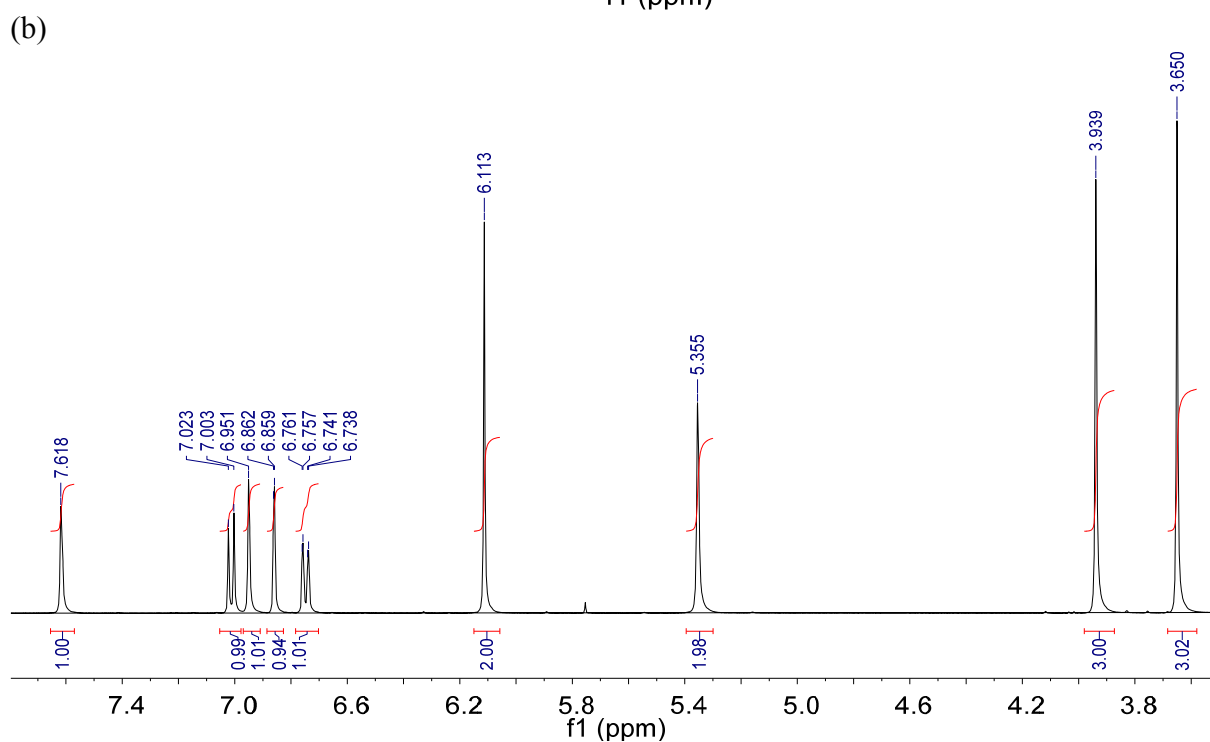
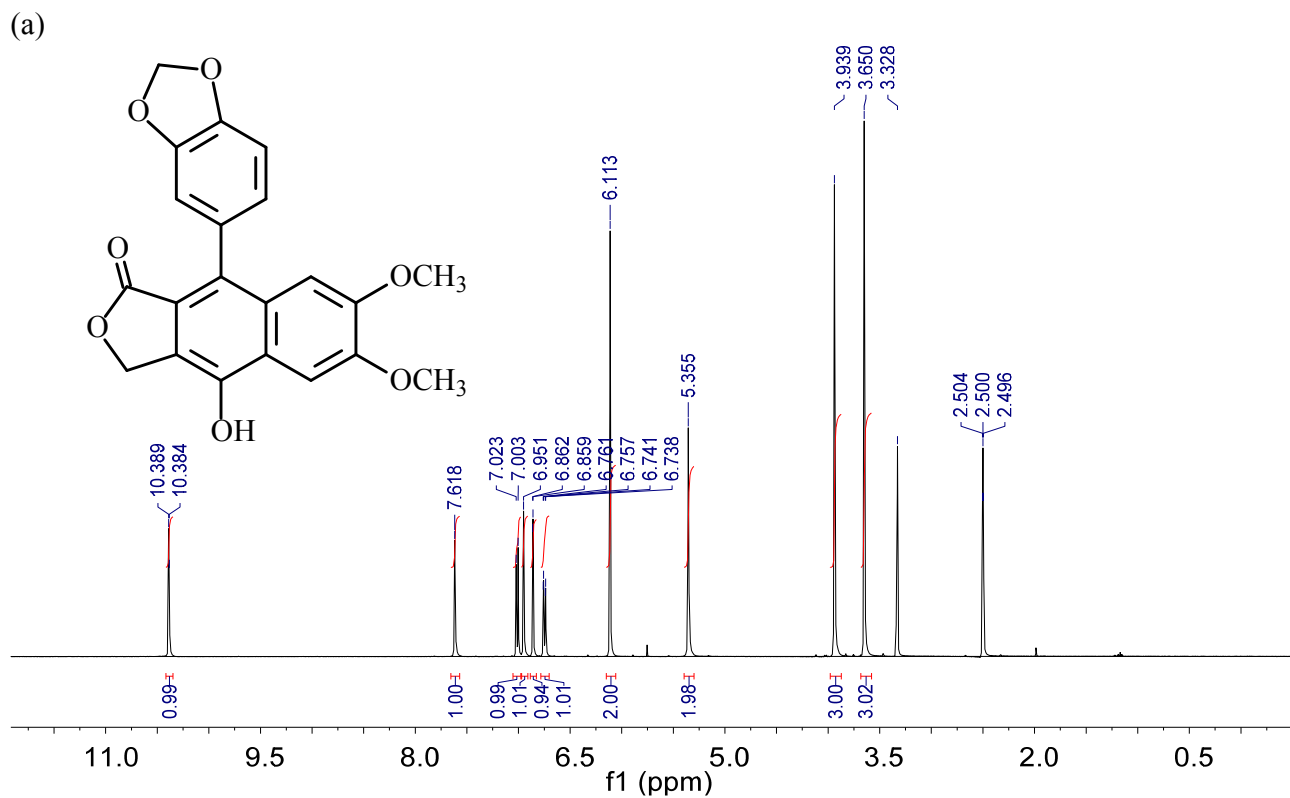


Figure S18. ¹H NMR (400 MHz) spectrum of diphyllin (**10**) in DMSO-d₆. (a) Full view; (b) Expansion.

(a)

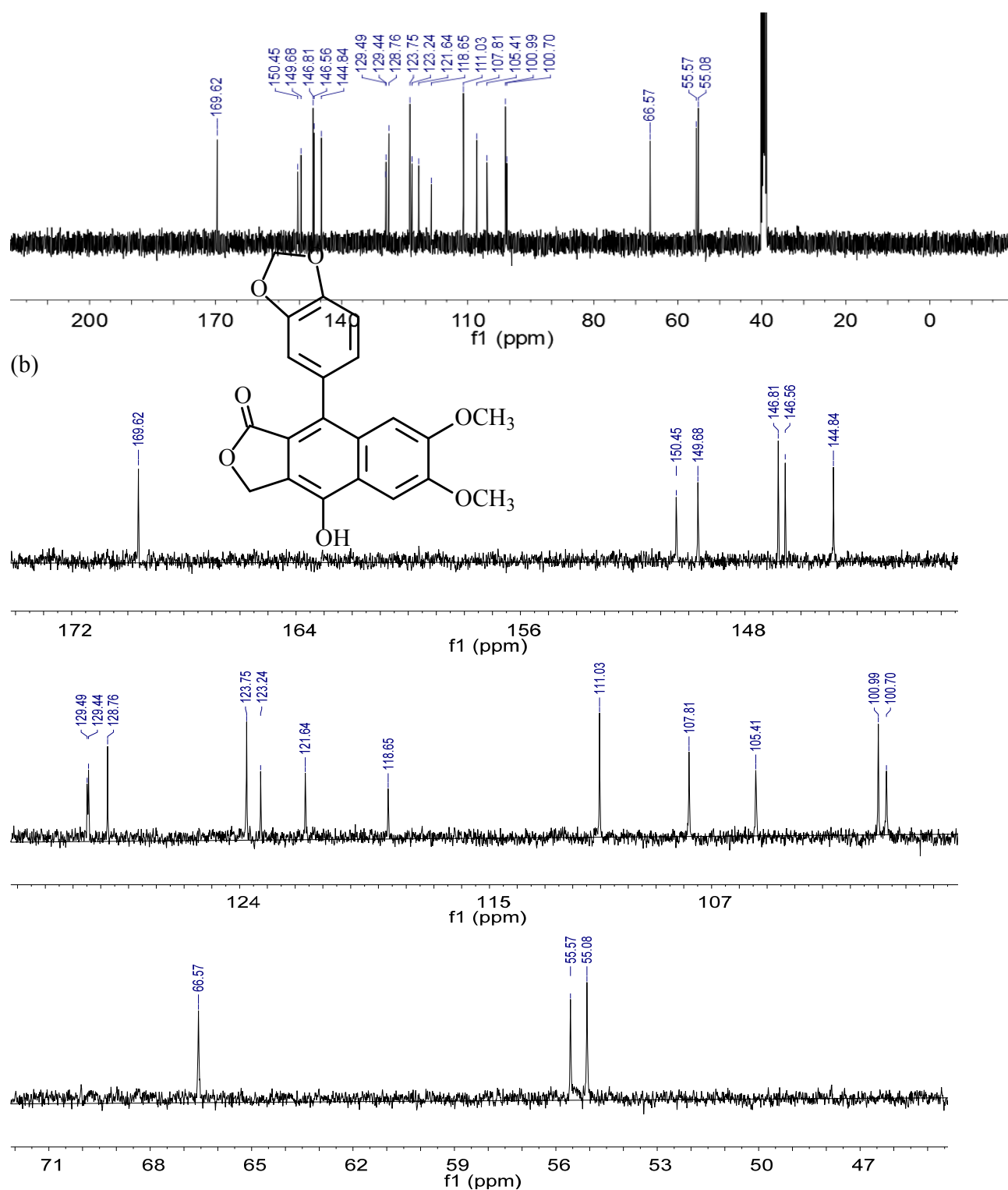
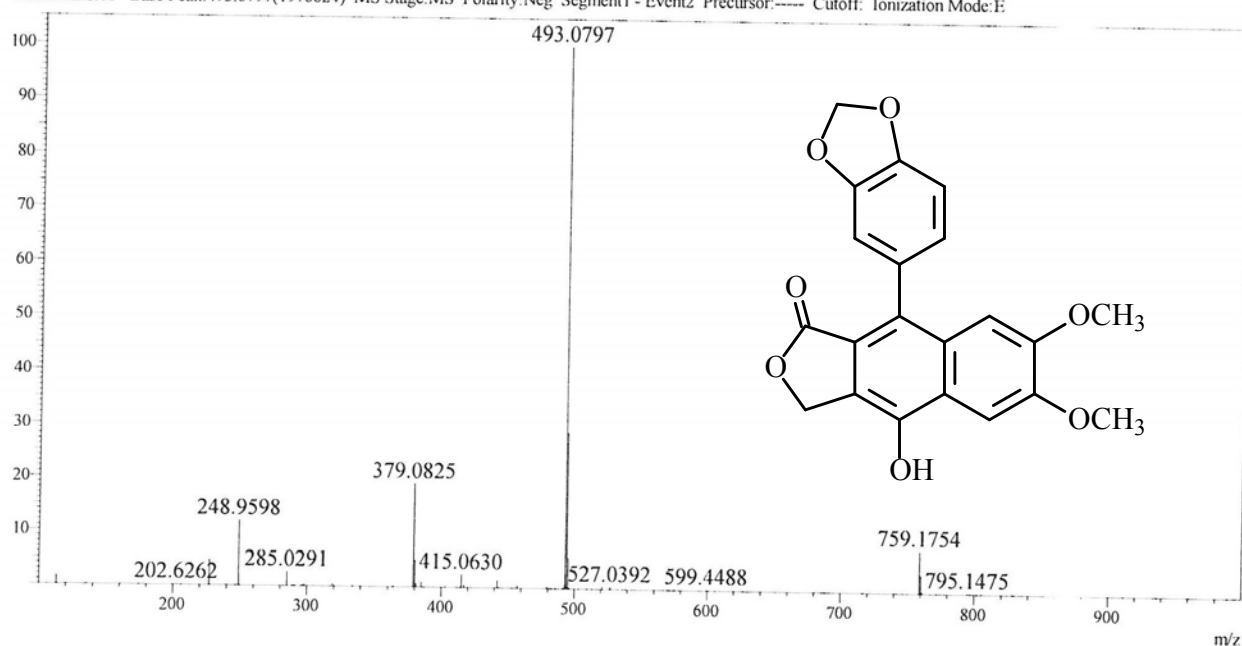


Figure S19. ¹³C NMR (100 MHz) spectrum of diphyllin (10) in DMSO-d₆. (a) Full view; (b) Expansion.

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Figure S20. HRMS spectrum of diphyllin (**10**).

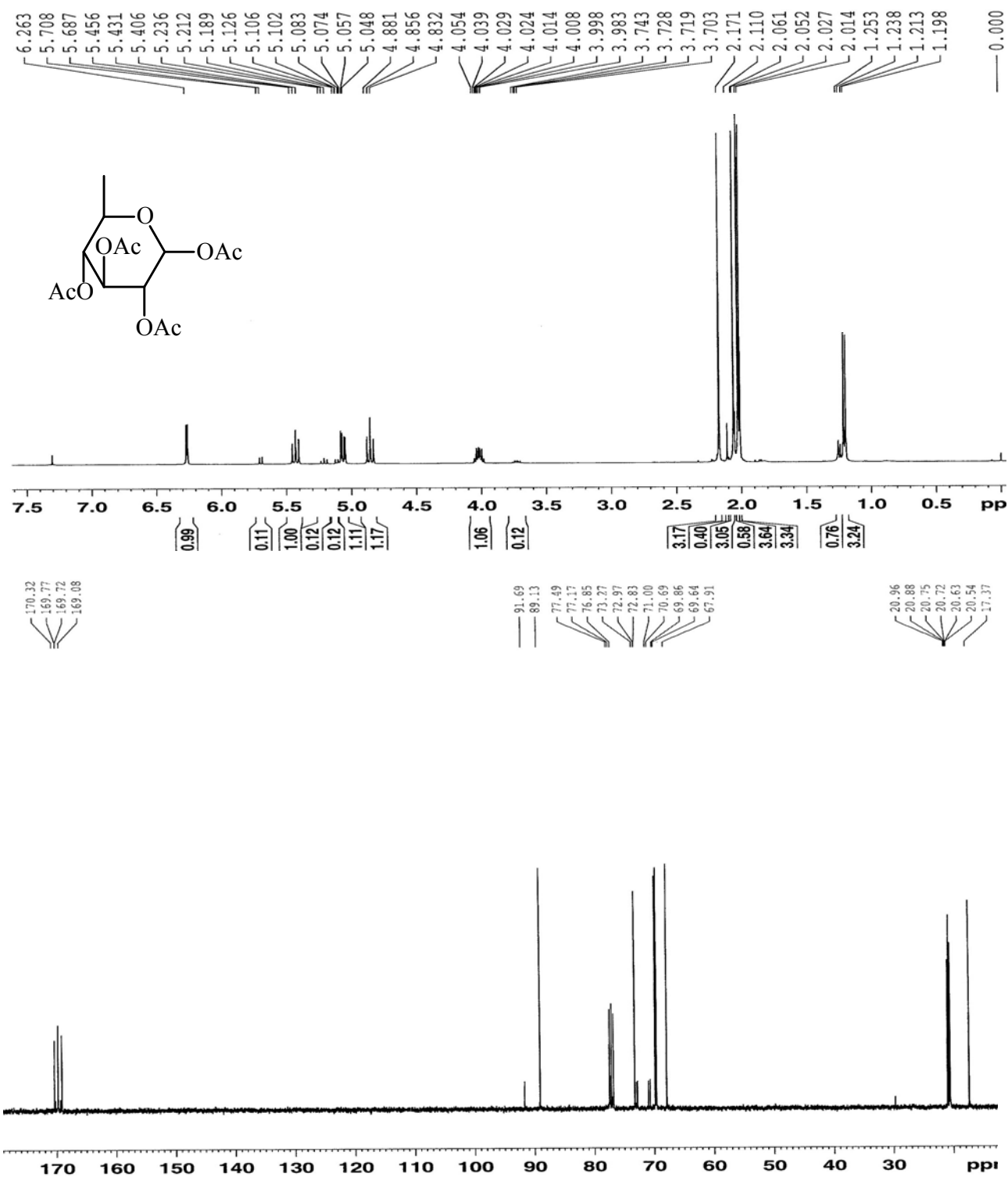


Figure S21. NMR spectrum of the synthetic **13** in CDCl_3 . (a) ^1H NMR (400 MHz); (b) ^{13}C NMR (100 MHz).

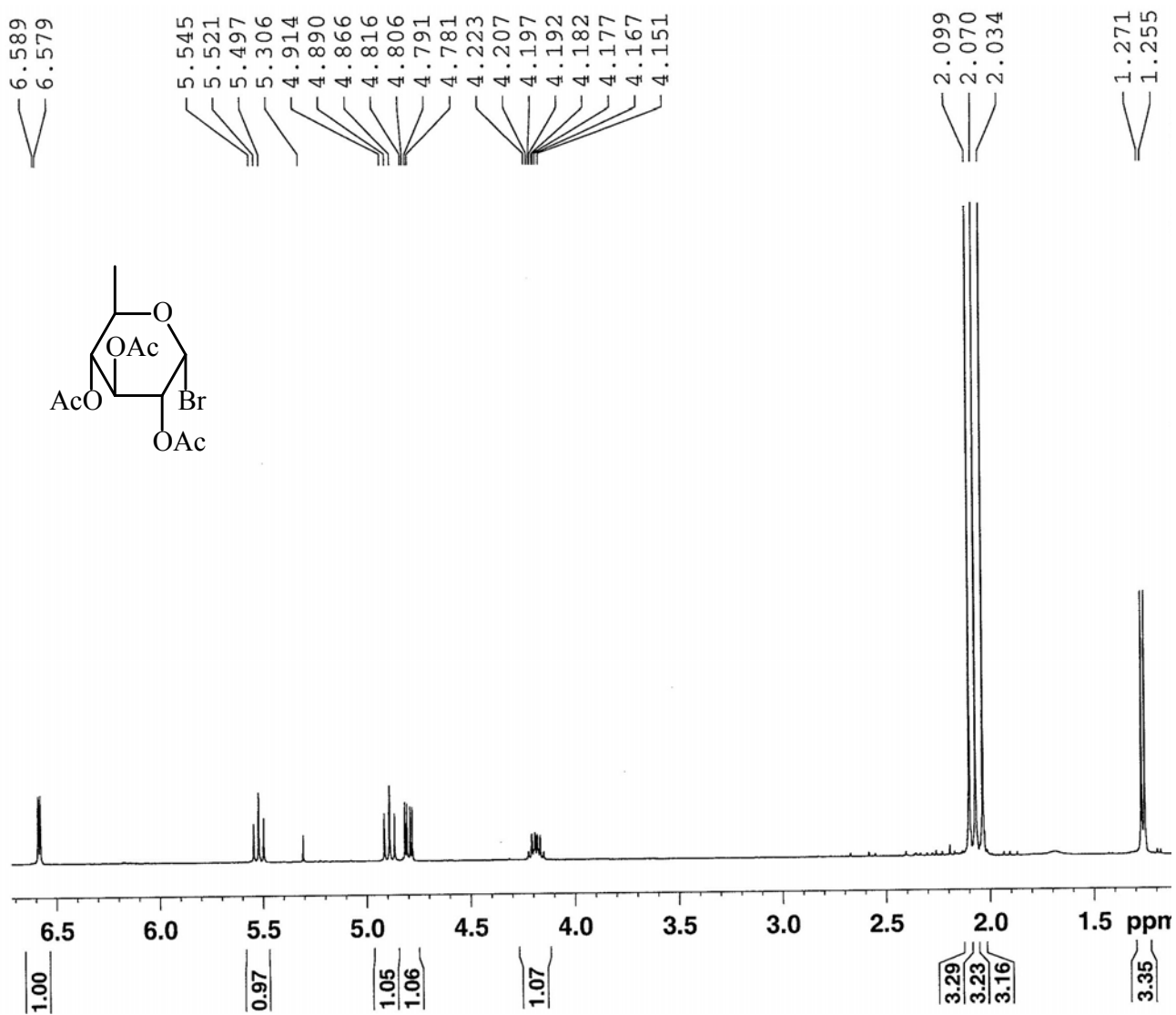


Figure S22. ¹H NMR (400 MHz) spectrum of the synthetic **13** in CDCl₃.

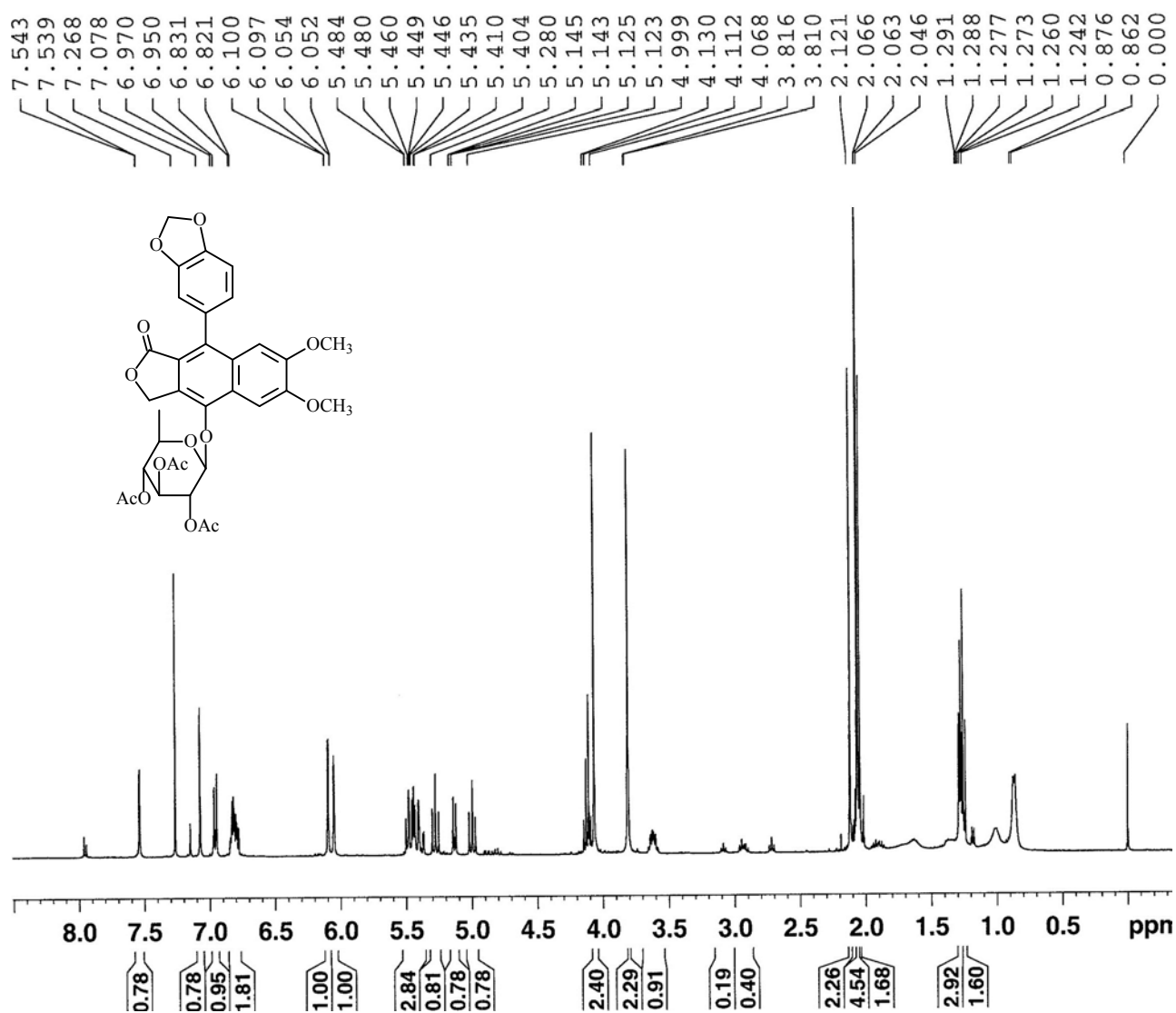


Figure S23. ^1H NMR (400 MHz) spectrum of the synthetic **14** in CDCl_3 .

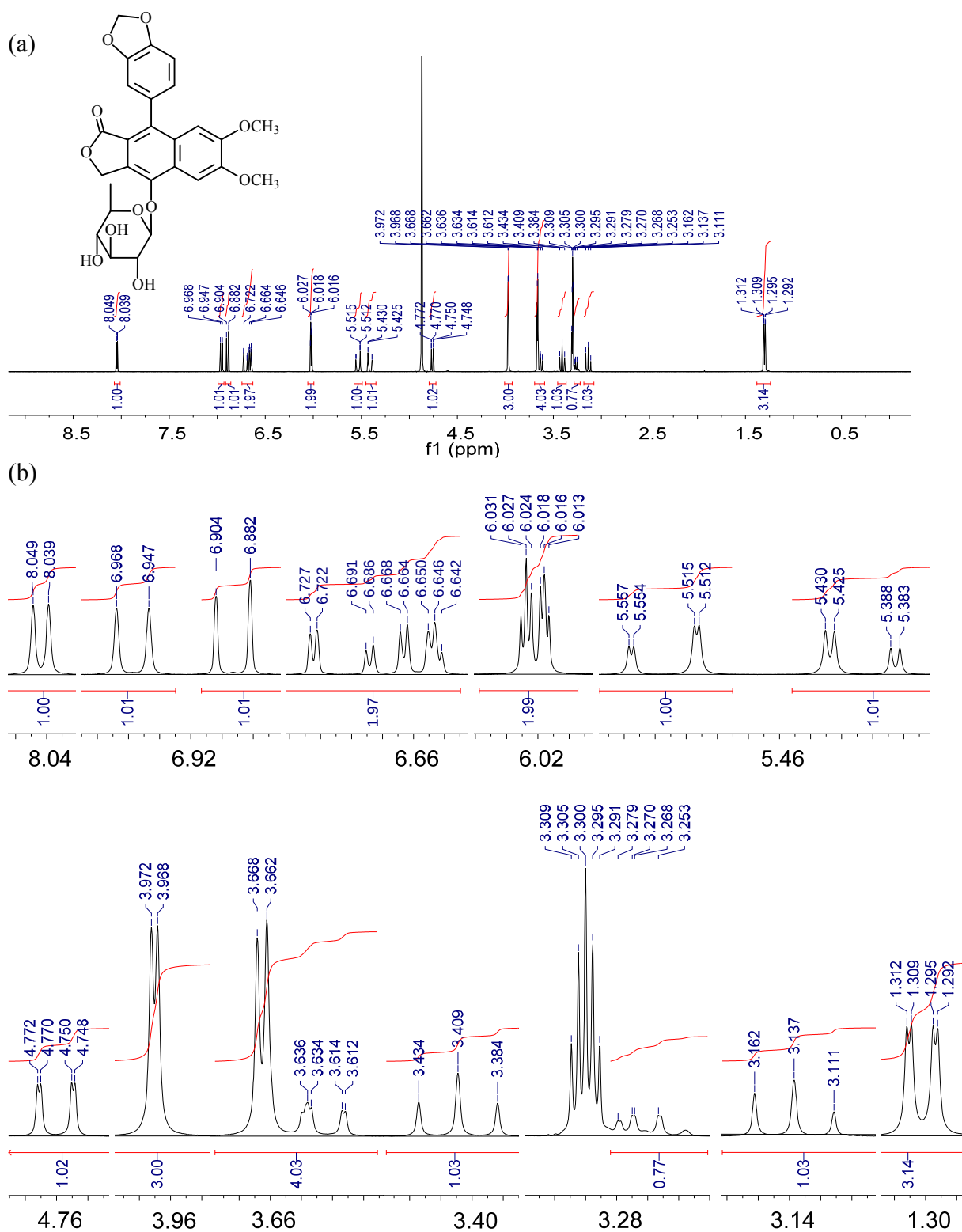


Figure S24. ^1H NMR (360 MHz) spectrum of the synthetic patentiflorin A (**1**) in CD_3OD . (a) Full view; (b) Expansion.

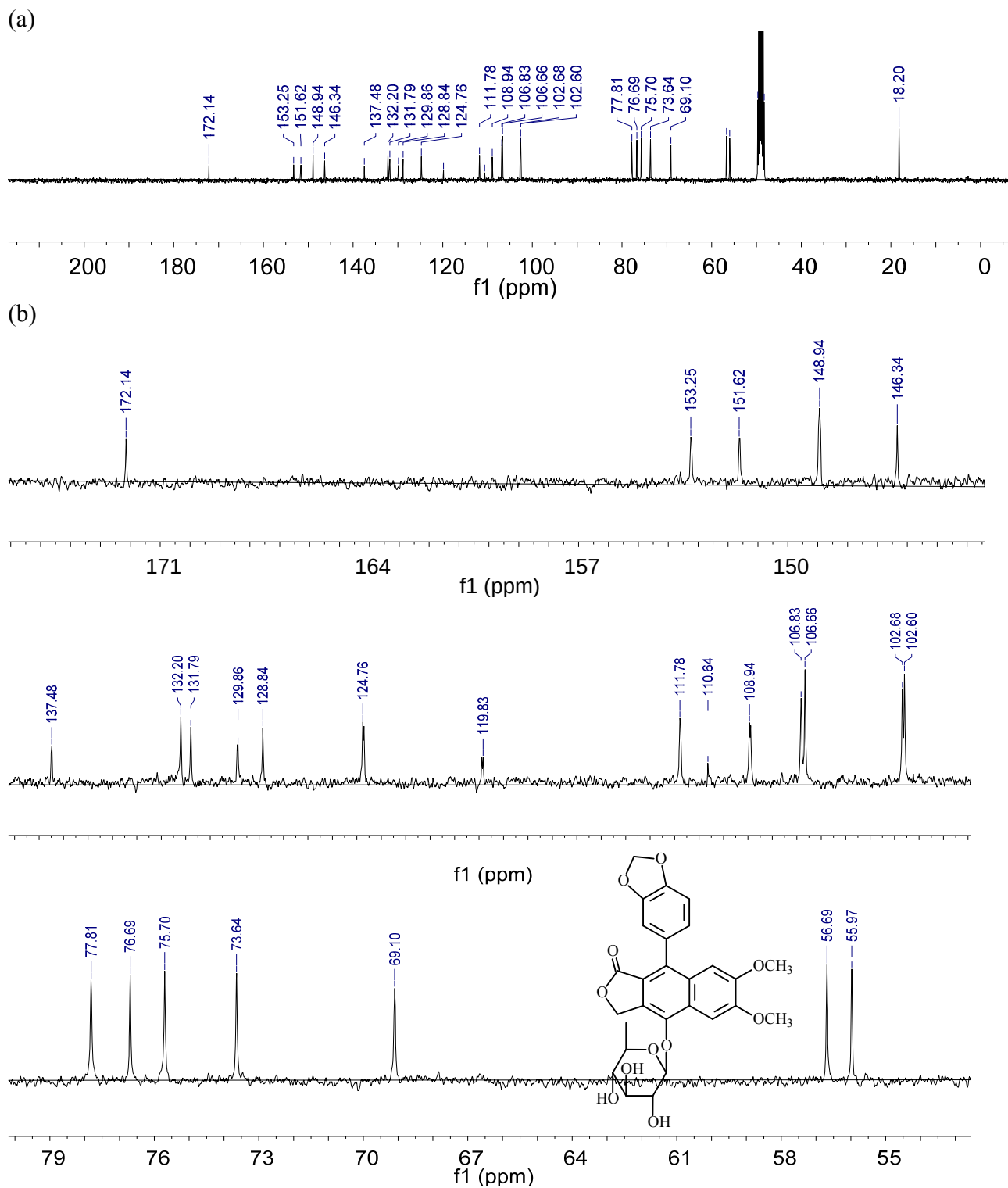


Figure S25. ^{13}C NMR (90 MHz) spectrum of the synthetic patentiflorin A (**1**) in CD_3OD . (a) Full view; (b) Expansion.

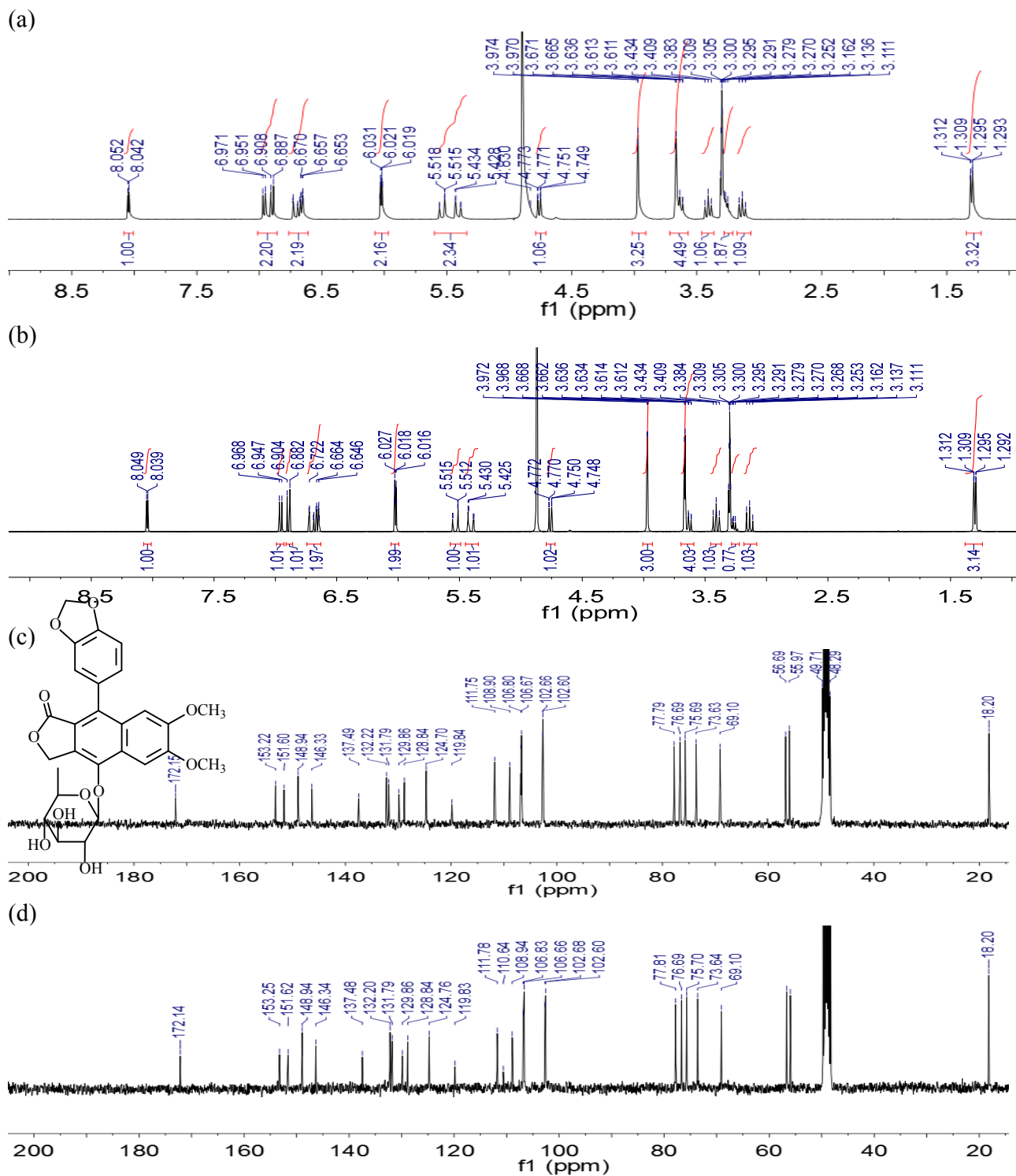


Figure S26. Comparison of the NMR data of the natural and synthetic patentiflorin A (**1**) in CD_3OD . (a) ^1H NMR (360 MHz) of the natural; (b) ^1H NMR (360 MHz) of the synthetic; (c) ^{13}C NMR (90 MHz) of the natural; (d) ^{13}C NMR (90 MHz) of the synthetic.

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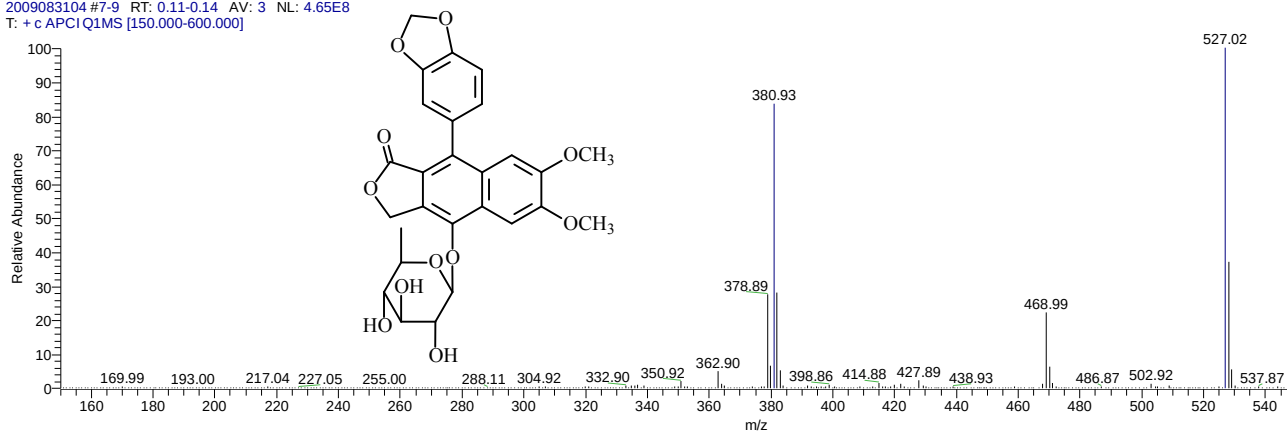


Figure S27. MS spectrum of the synthetic patentiflorin A (**1**).

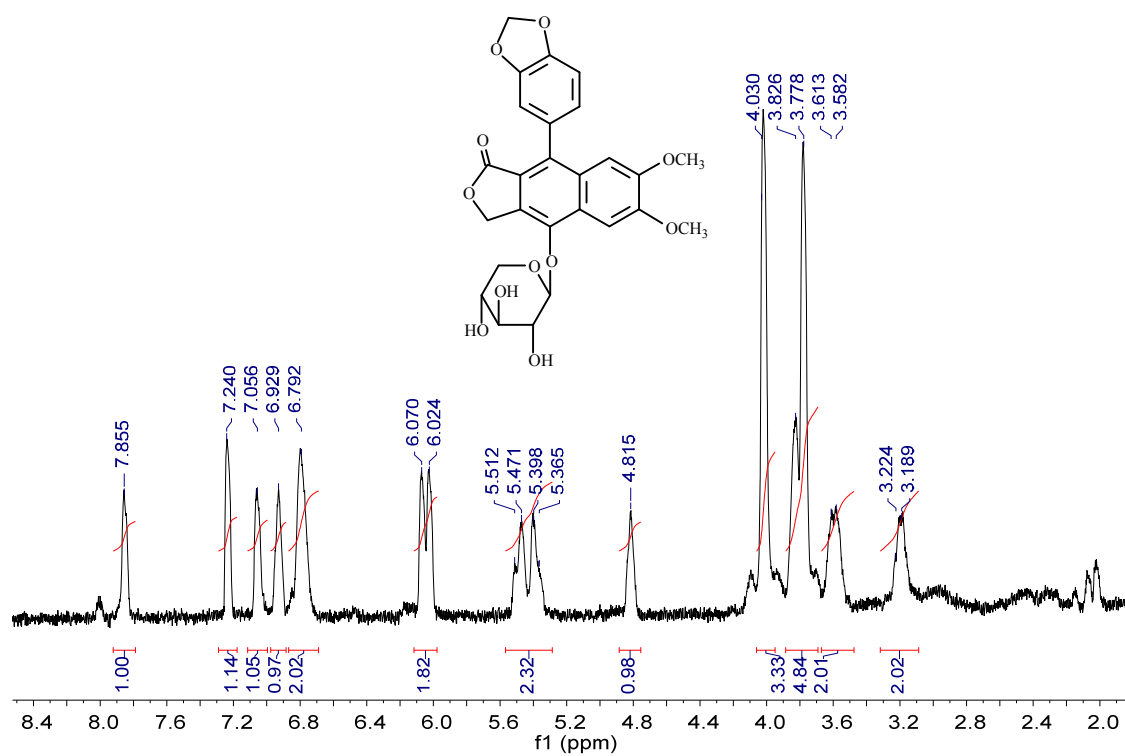


Figure S28. ¹H NMR (400 MHz) spectrum of 7-O-β-D-xylosyldiphyllin (**15**) in CDCl₃.

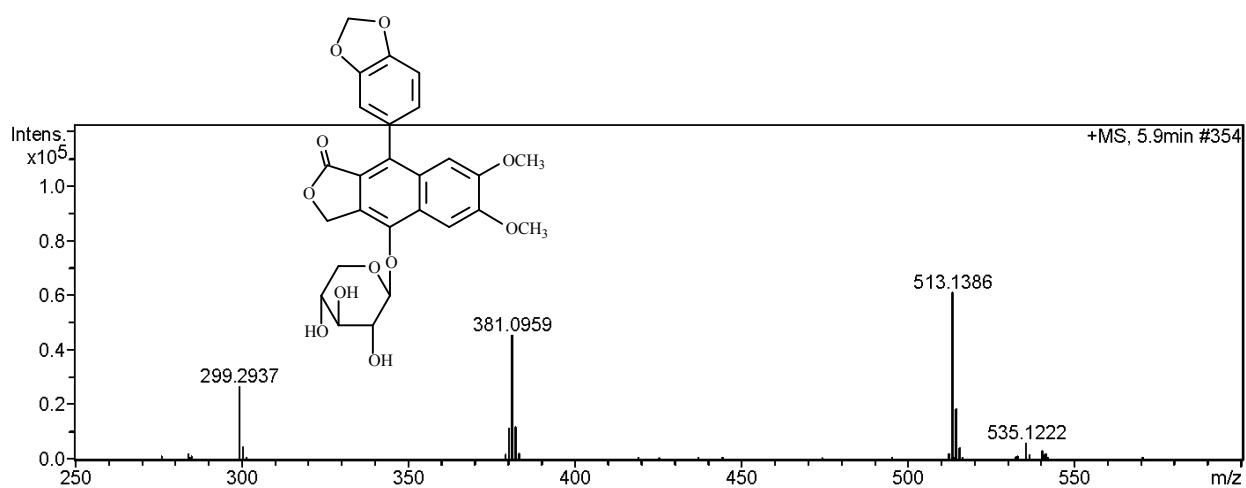


Figure S29. MS spectrum of the synthetic 7-O- β -D-xylosydiphyllin (15).

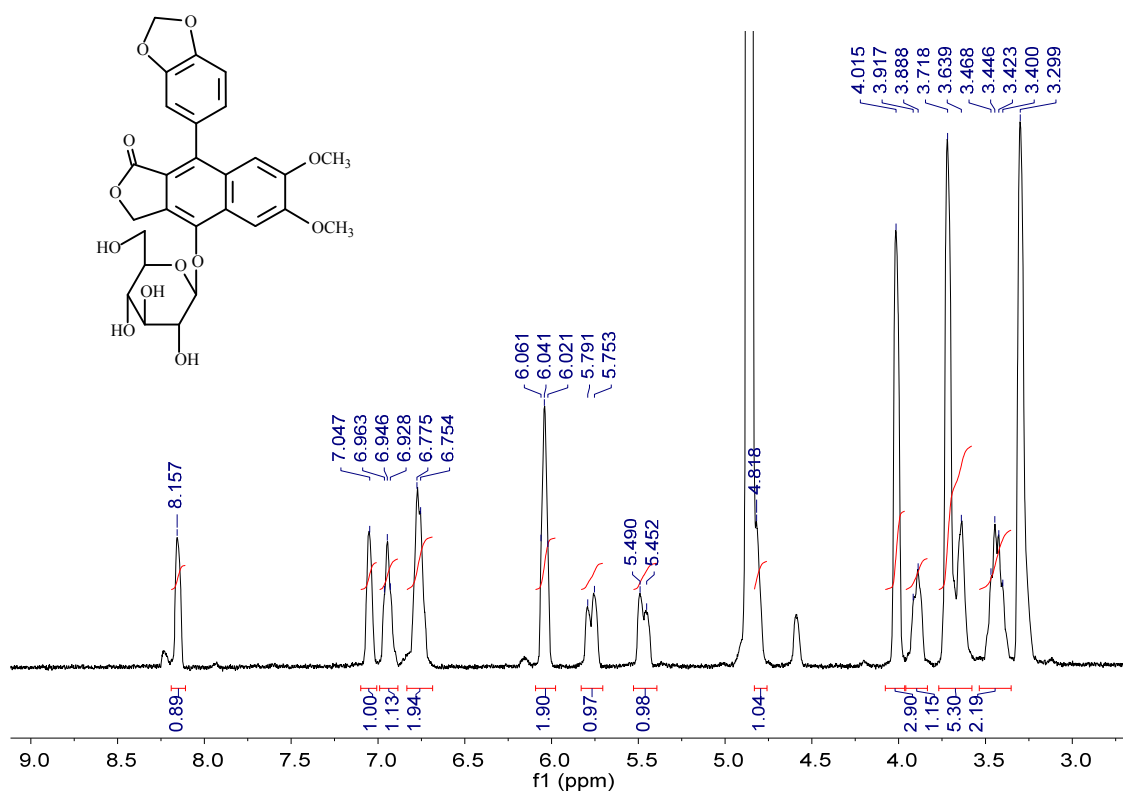


Figure S30. ¹H NMR (400 MHz) spectrum of 7-O-β-D-glucopyranosyldiphyllin (**16**) in CD₃OD.

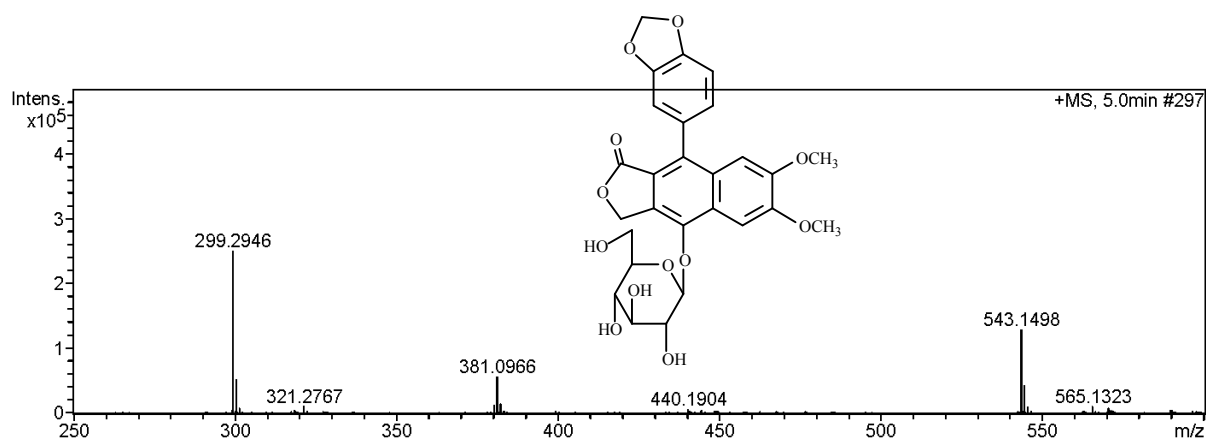


Figure S31. MS spectrum of the synthetic 7-O-β-D-glucopyranosyldiphyllin (16).