

Article

Biotransformation of (–)- α -Bisabolol by *Absidia coerulea*

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Table S1. Screening for the microorganisms that transform (–)- α -bisabolol (**1**).

Microorganism	Capability [*]	Microorganism	Capability [*]
<i>A. alternata</i>	-	<i>H. resiniae</i>	-
<i>A. coerulea</i>	+++	<i>K. marxianus</i>	-
<i>A. fumigatus</i>	+	<i>M. hiemalis</i>	++
<i>C. elegans</i> var. <i>elegans</i>	++	<i>M. lacticum</i>	-
<i>F. neoformans</i>	-	<i>M. ramanniana</i> var. <i>angulispora</i>	-
<i>F. merismoides</i>	-	<i>P. chrysogenum</i>	-
<i>G. cingulata</i>	-	<i>T. koningii</i>	-
<i>G. deliquescens</i>	-		

^{*} Capability of transformation of (–)- α -bisabolol (**1**): (-) no transformation; (+) lower yield of metabolites; (++) higher yield of metabolites; (+++) highest yield of metabolites.

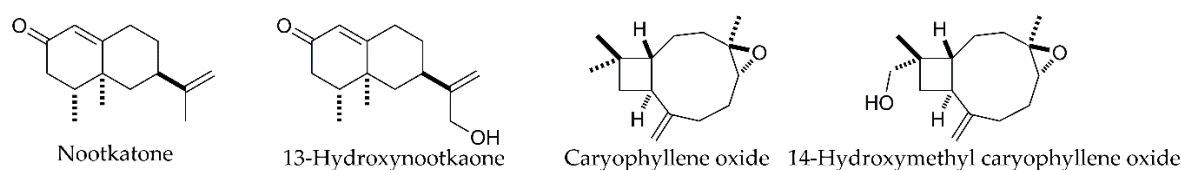


Figure S1. Chemical structures of nootkatone, 13-hydroxynootkatone, caryophyllene oxide and 14-hydroxymethyl caryophyllene oxide.

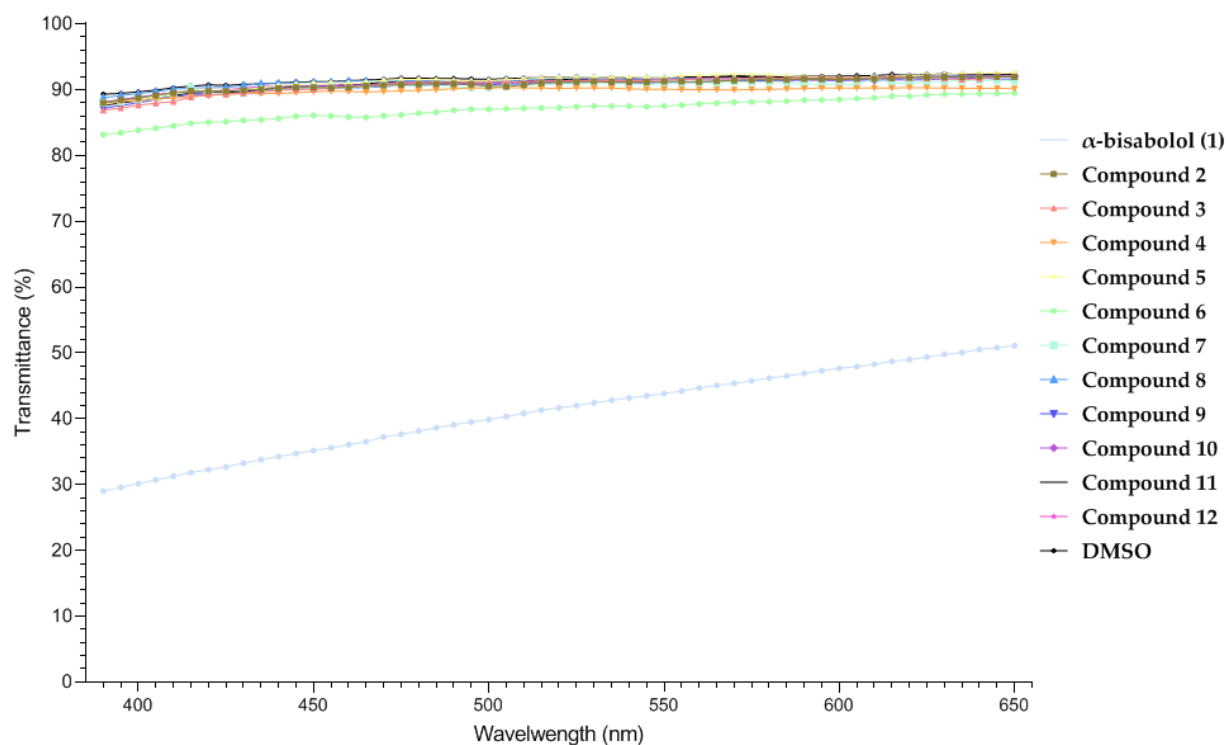


Figure S2. Light transmittance of the diluted solutions of (-)- α -bisabolol (1) and its metabolites in water.

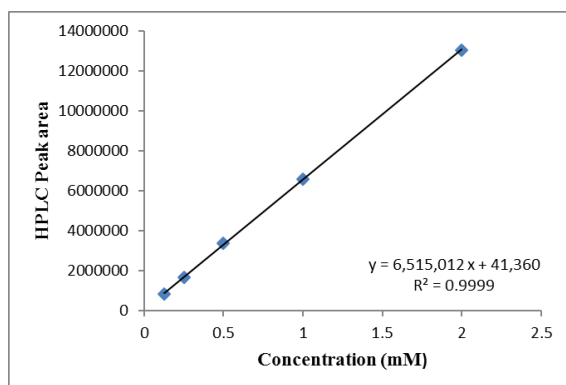


Figure S3. Calibration of measurement for solubility of (-)- α -bisabolol (1).

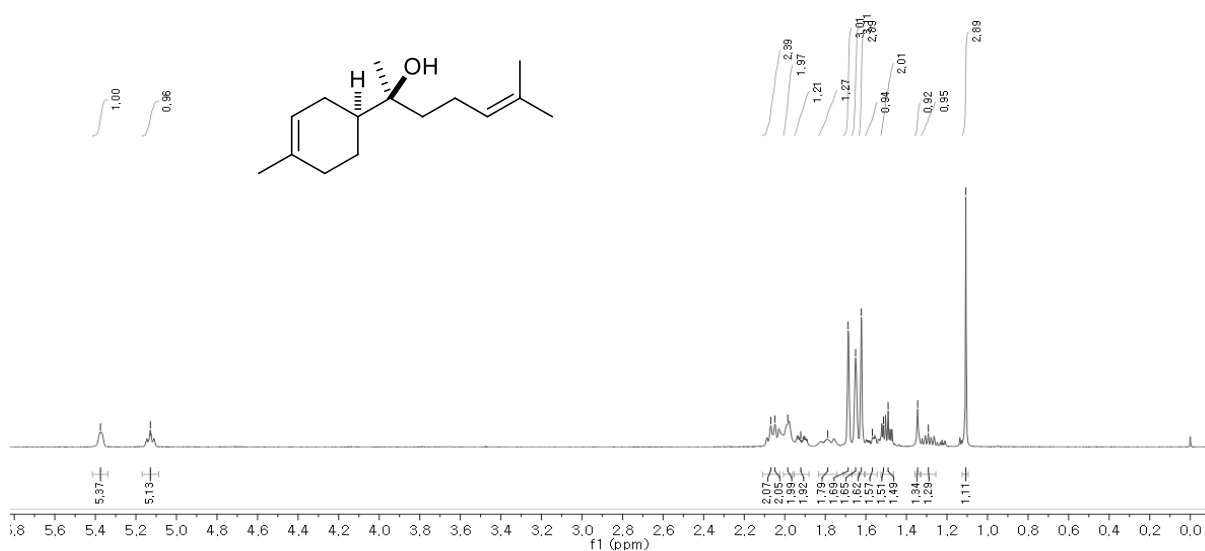


Figure S4. ^1H NMR spectrum of compound **1** recorded at 400 MHz in CDCl_3

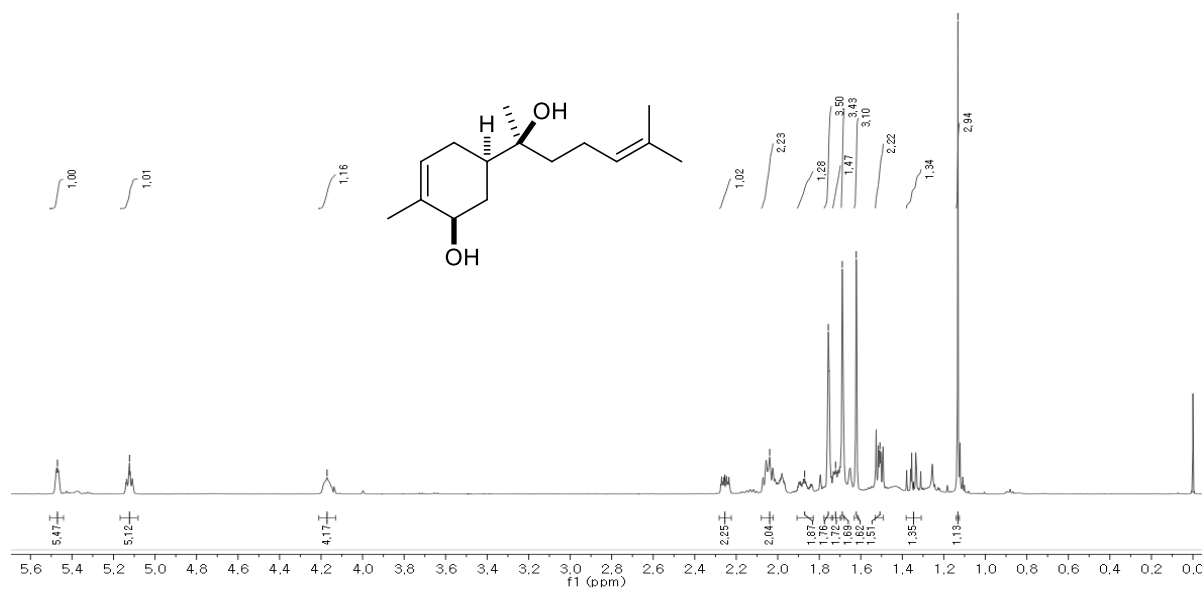


Figure S5. ^1H NMR spectrum of compound **2** recorded at 500 MHz in CDCl_3 .

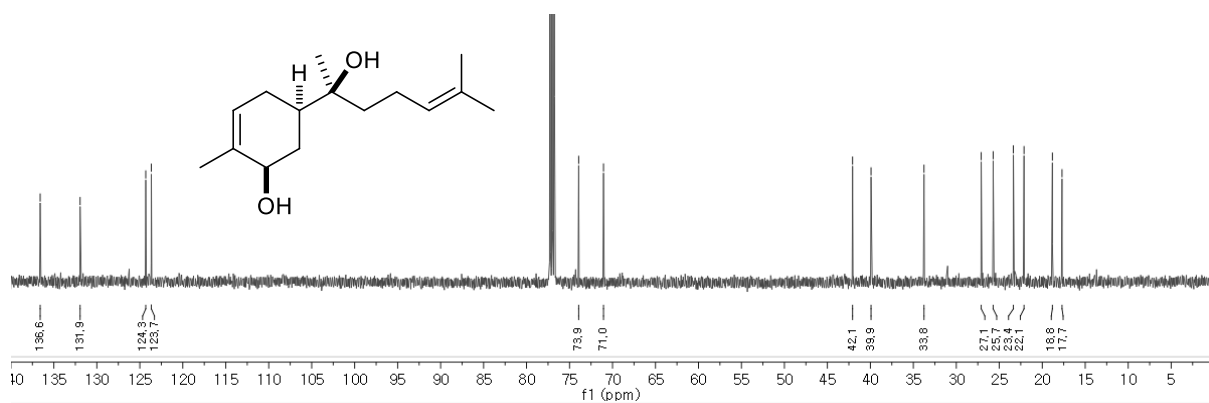


Figure S6. ^{13}C NMR spectrum of compound **2** recorded at 125 MHz in CDCl_3 .

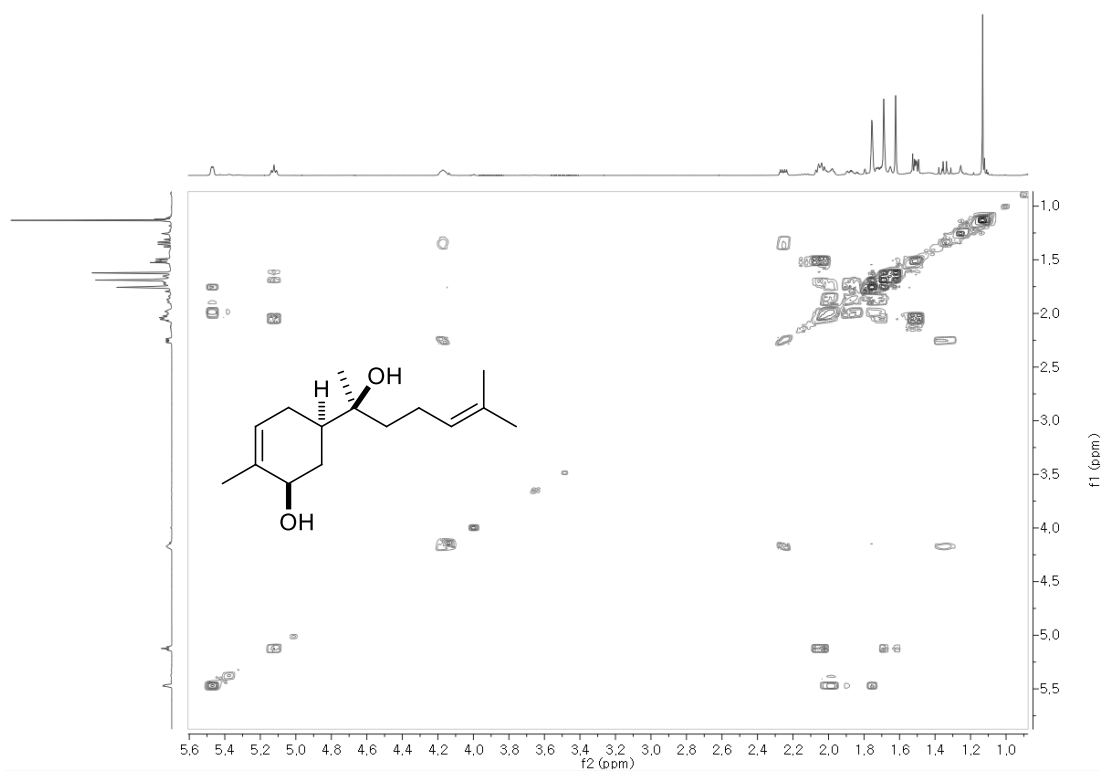


Figure S7. COSY spectrum of compound **2** recorded at 125 MHz in CDCl₃.



Figure S8. HSQC spectrum of compound **2** recorded at 500 MHz in CDCl₃.

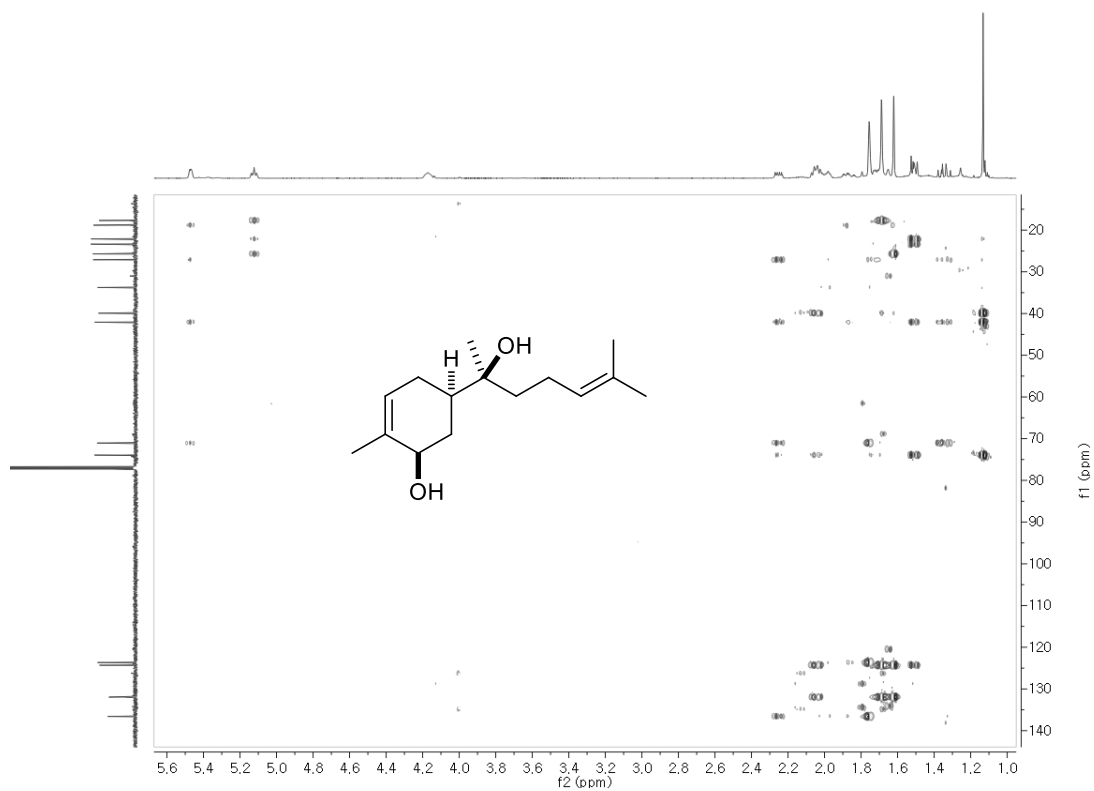


Figure S9. HMBC spectrum of compound **2** recorded at 500 MHz in CDCl₃.

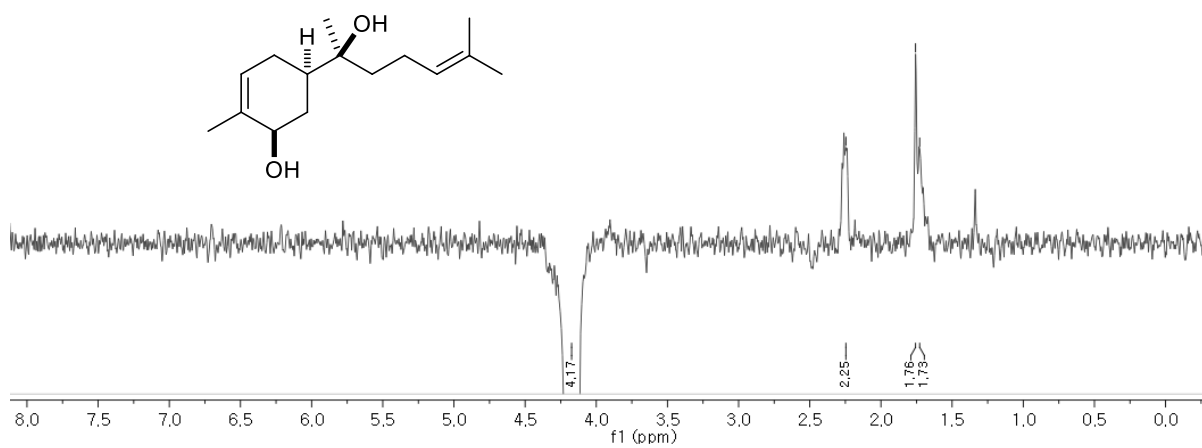


Figure S10. NOE spectrum of compound **2** recorded at 500 MHz in CDCl₃.

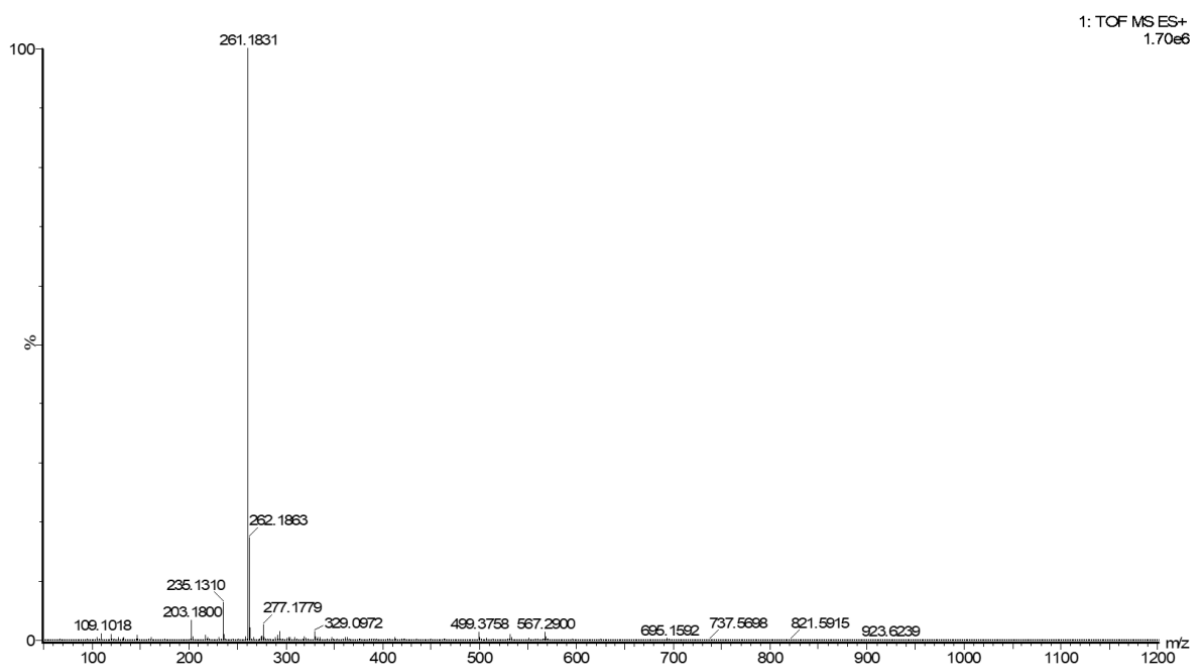


Figure S11. The HRESIMS spectroscopic data of compound 2.

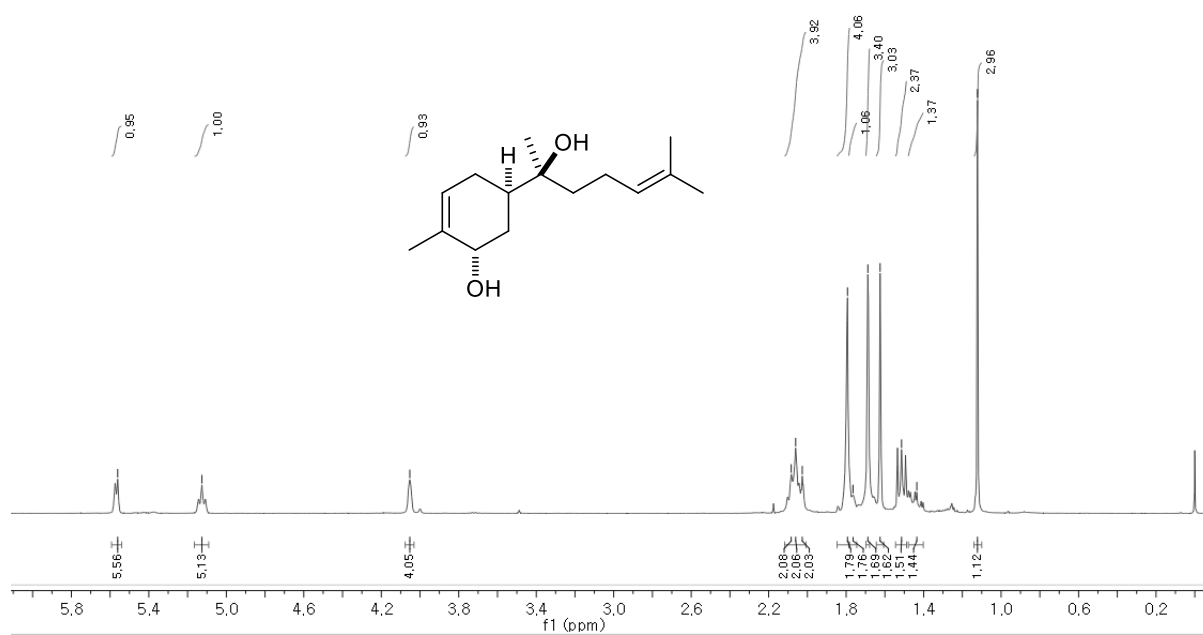


Figure S12. ^1H NMR spectrum of compound 3 recorded at 500 MHz in CDCl_3 .

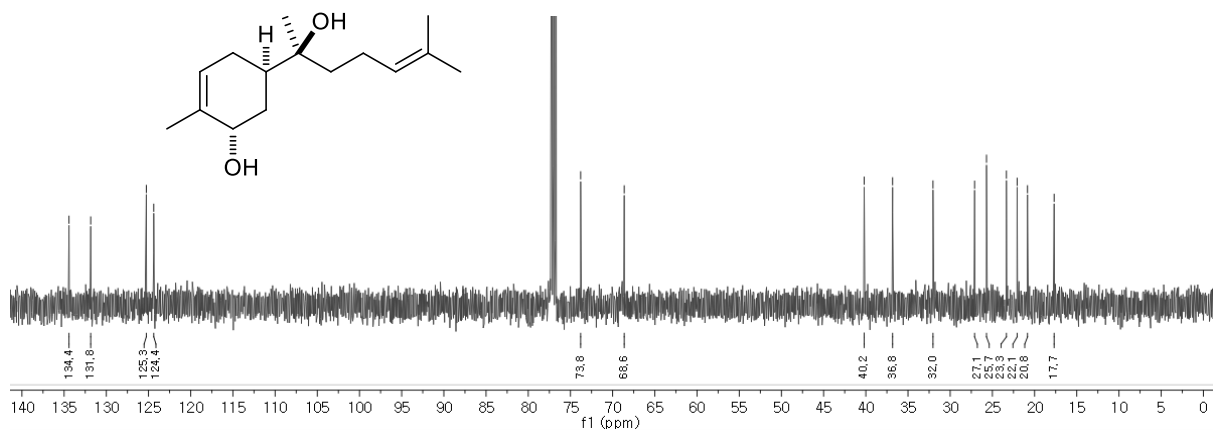


Figure S13. ^{13}C NMR spectrum of compound **3** recorded at 125 MHz in CDCl_3 .

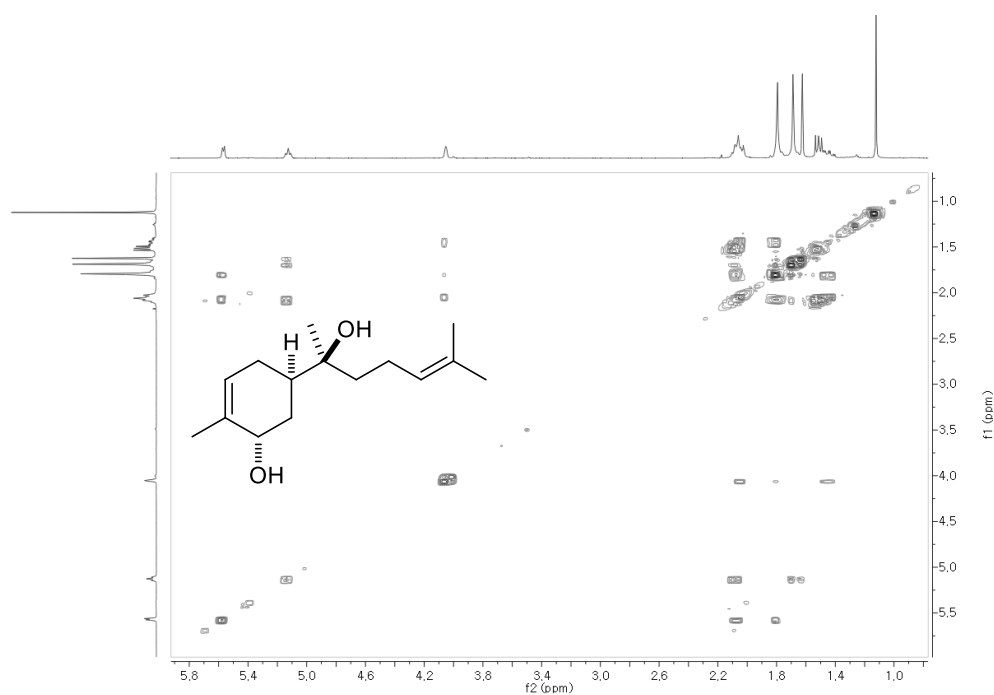


Figure S14. COSY spectrum of compound **3** recorded at 500 MHz in CDCl_3 .

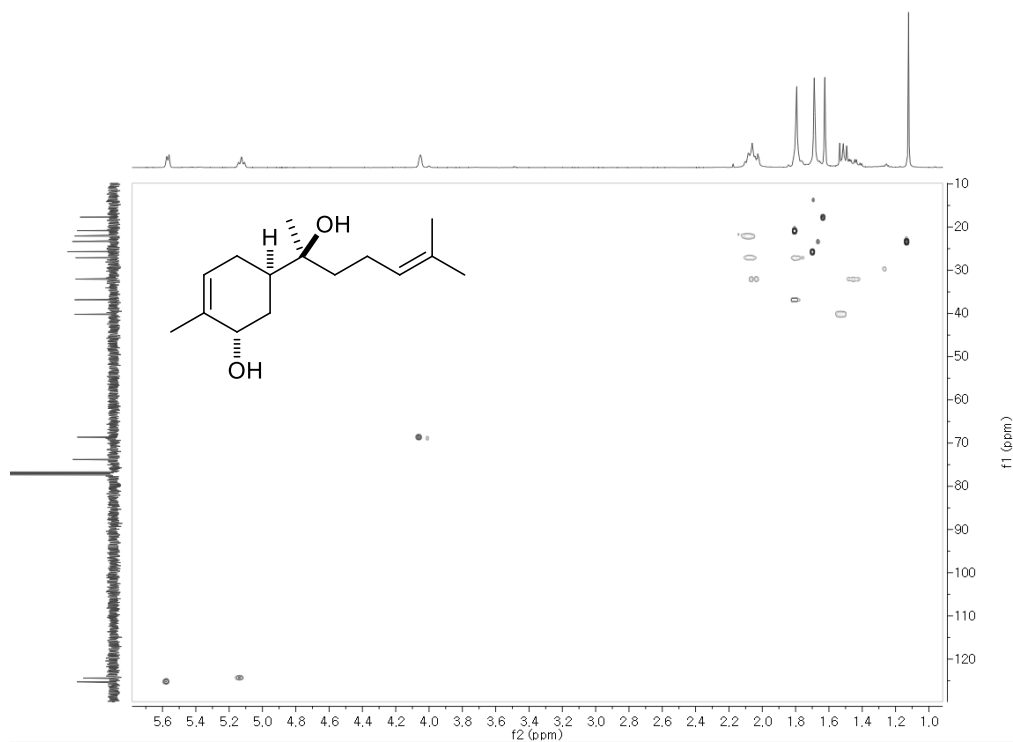


Figure S15. HSQC spectrum of compound **3** recorded at 500 MHz in CDCl₃.

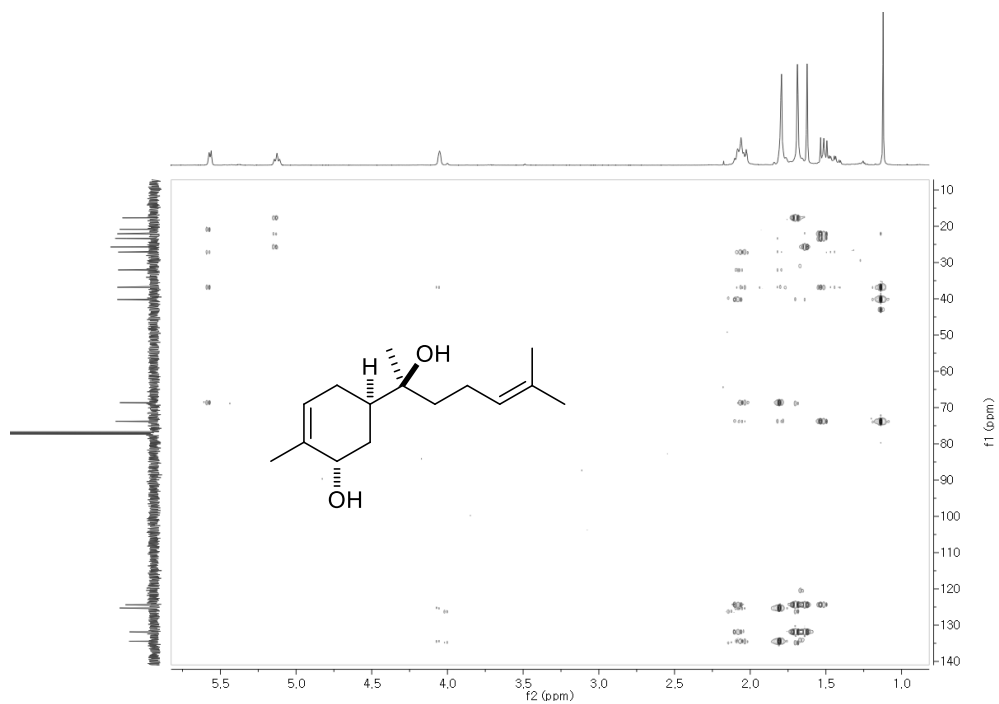


Figure S16. HMBC spectrum of compound **3** recorded at 500 MHz in CDCl₃.

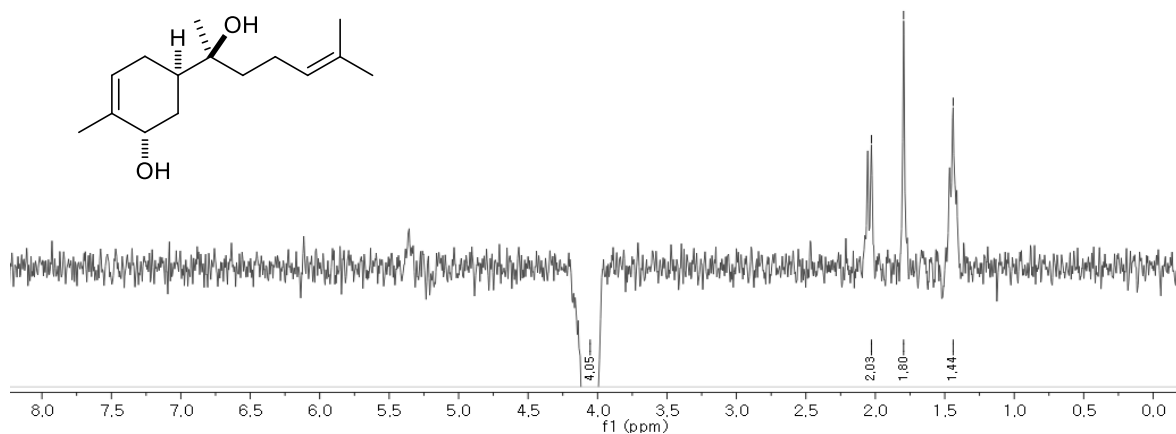


Figure S17. NOE spectrum of compound **3** recorded at 500 MHz in CDCl₃.

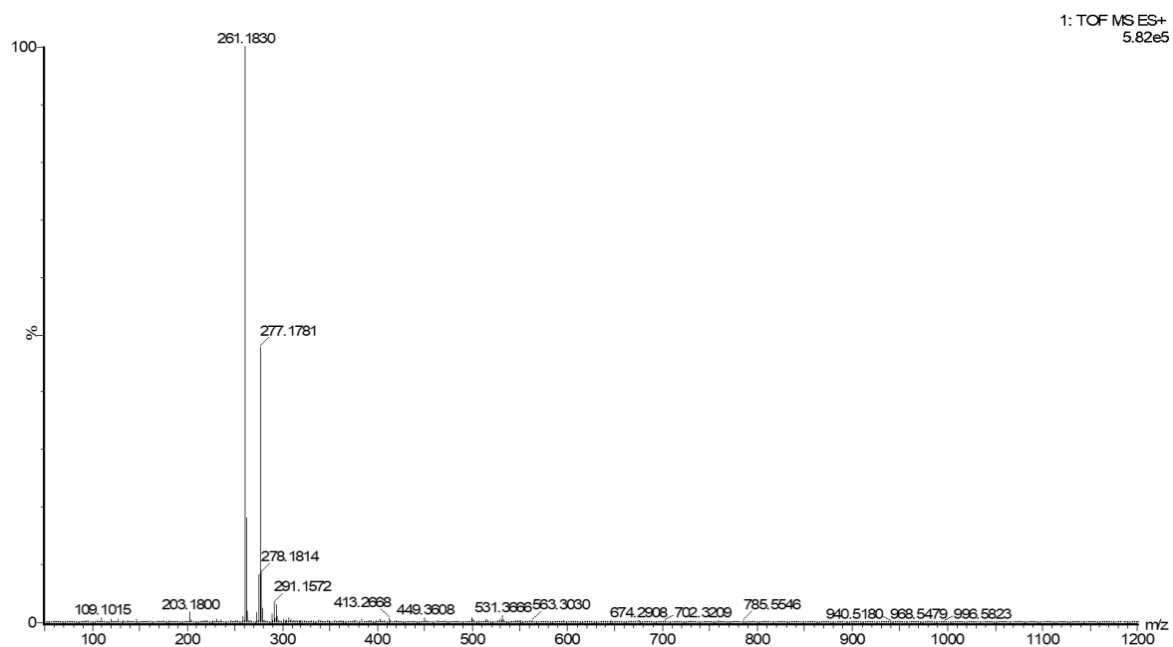


Figure S18. The HRESIMS spectroscopic data of compound **3**.

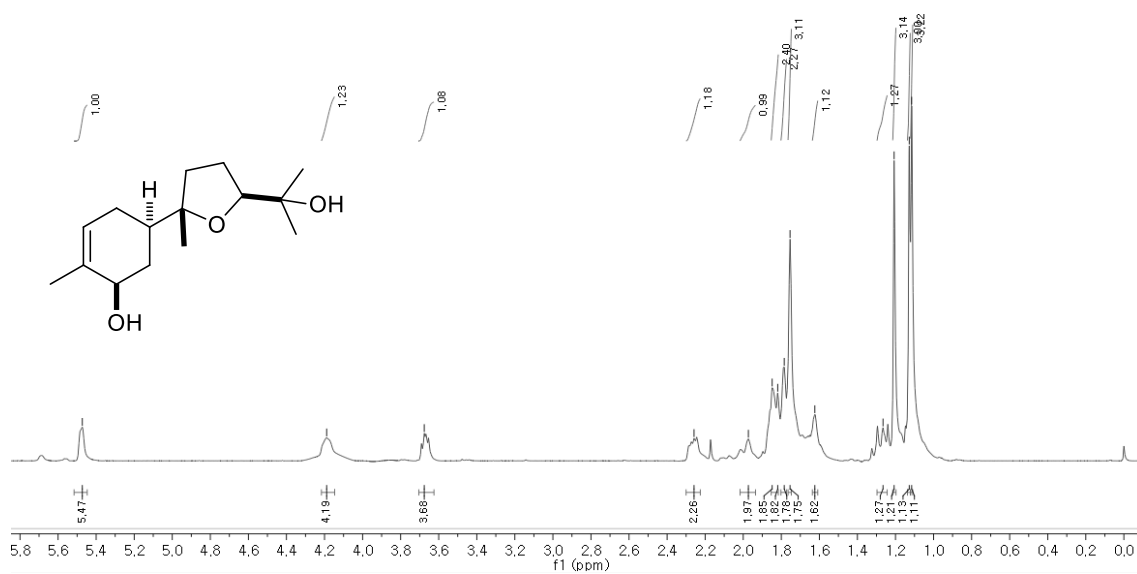


Figure S19. ¹H NMR spectrum of compound **4** recorded at 400 MHz in CDCl₃.

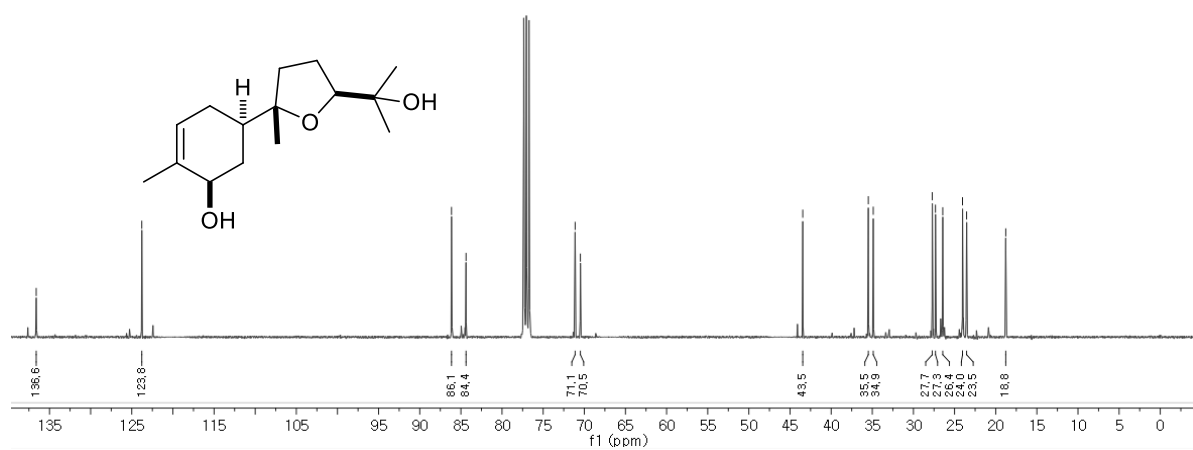


Figure S20. ¹³C NMR spectrum of compound **4** recorded at 100 MHz in CDCl₃.

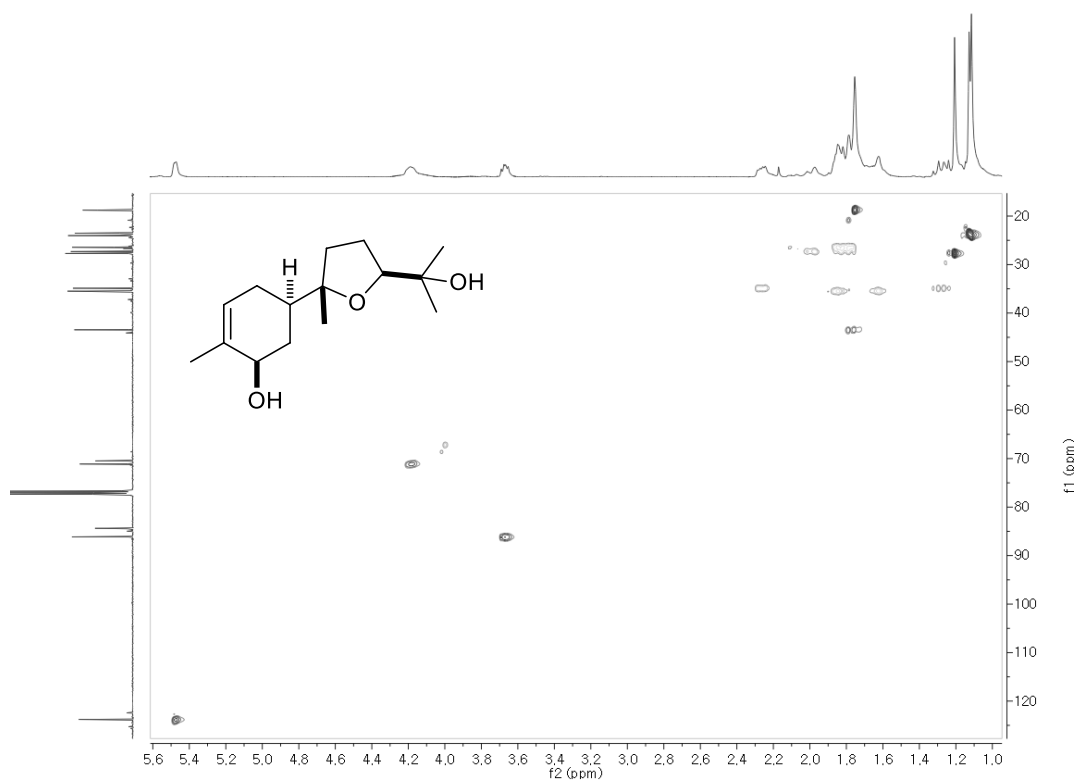


Figure S21. HSQC spectrum of compound **4** recorded at 400 MHz in CDCl₃.

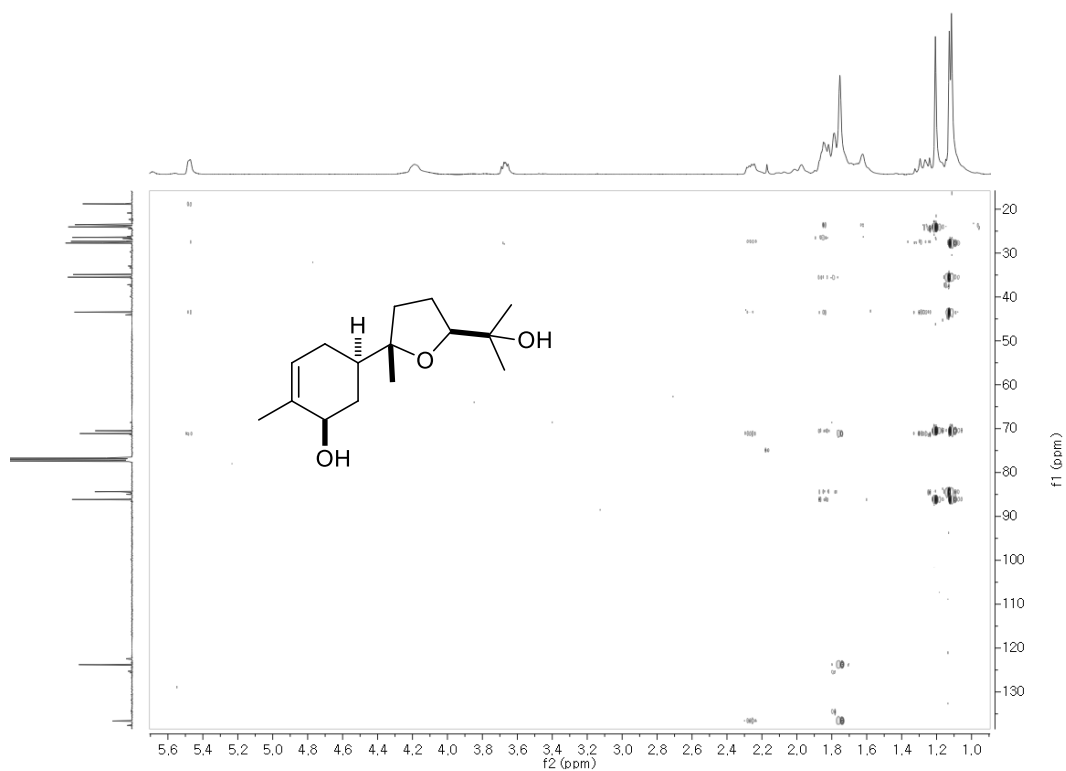


Figure S22. HMBC spectrum of compound **4** recorded at 400 MHz in CDCl₃.

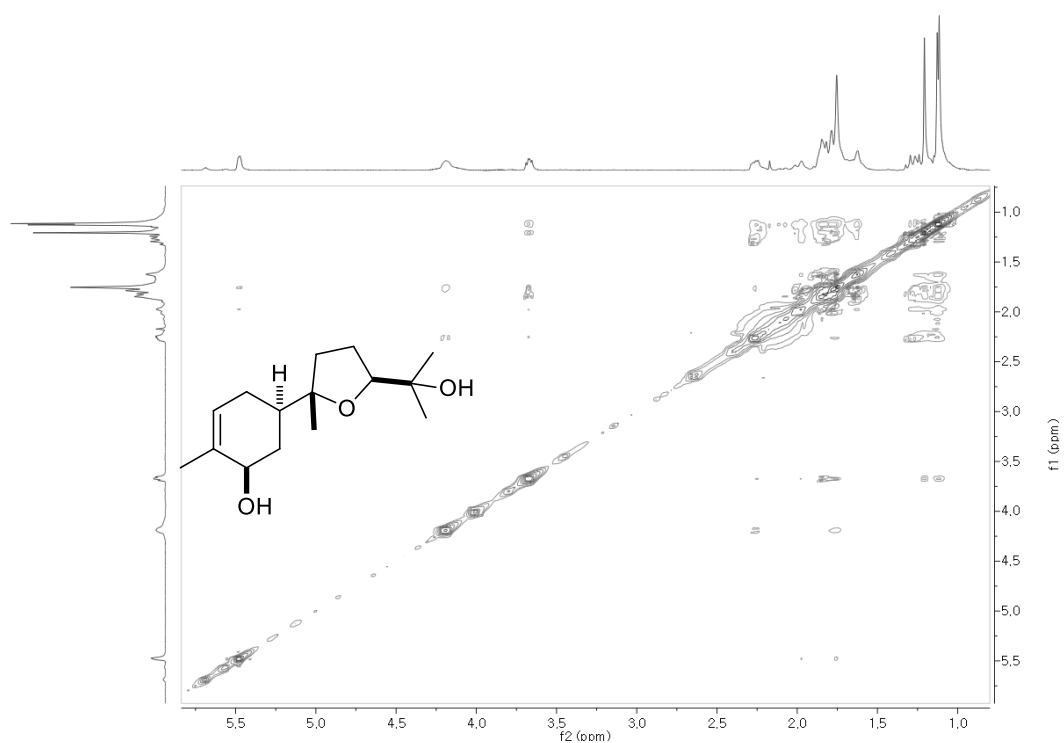


Figure S23. NOESY spectrum of compound **4** recorded at 400 MHz in CDCl₃.

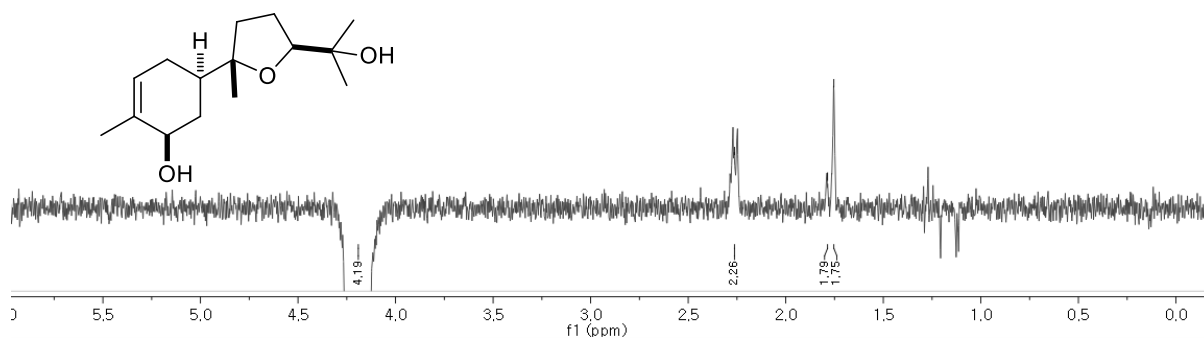


Figure S24. 1D ROESY spectrum of compound **4** recorded at 500 MHz in CDCl₃.

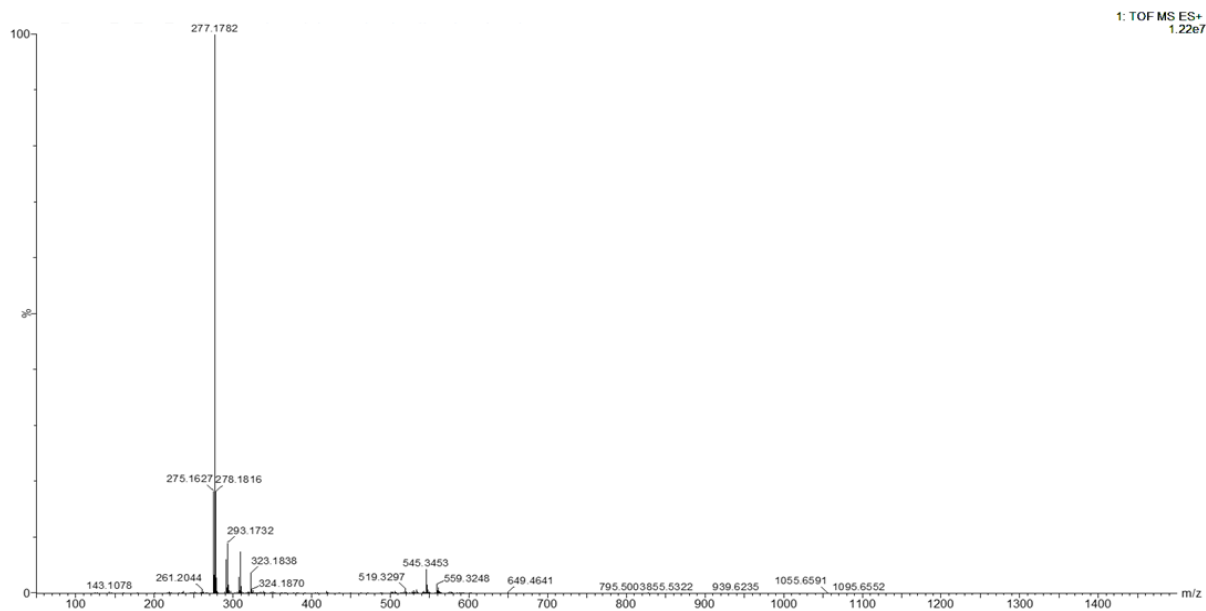


Figure S25. The HRESIMS spectroscopic data of compound **4**.

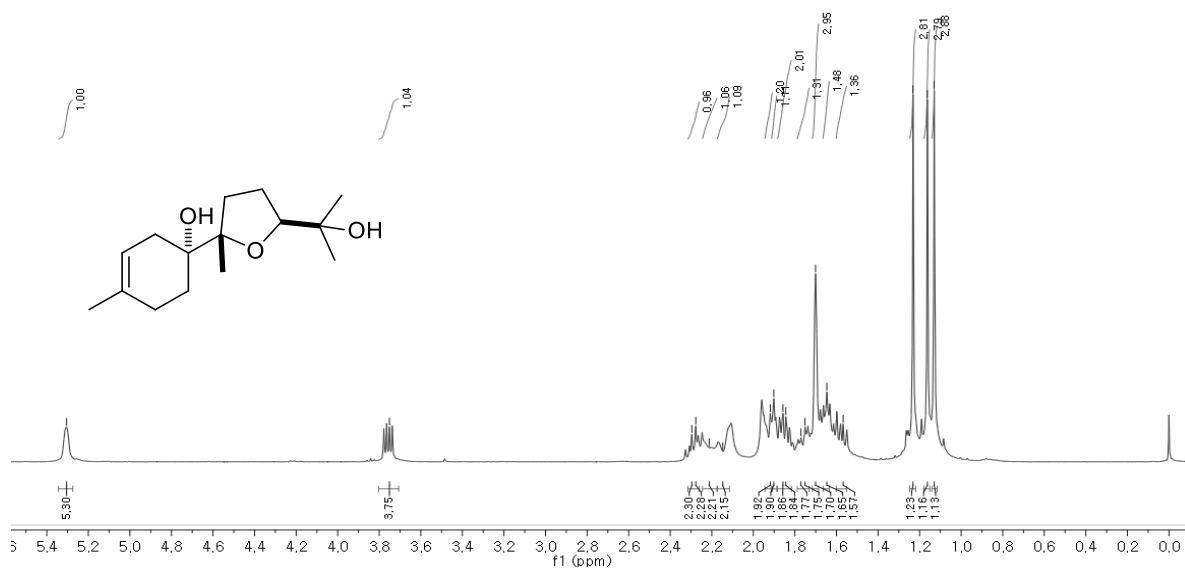


Figure S26. ¹H NMR spectrum of compound **5** recorded at 400 MHz in CDCl₃.

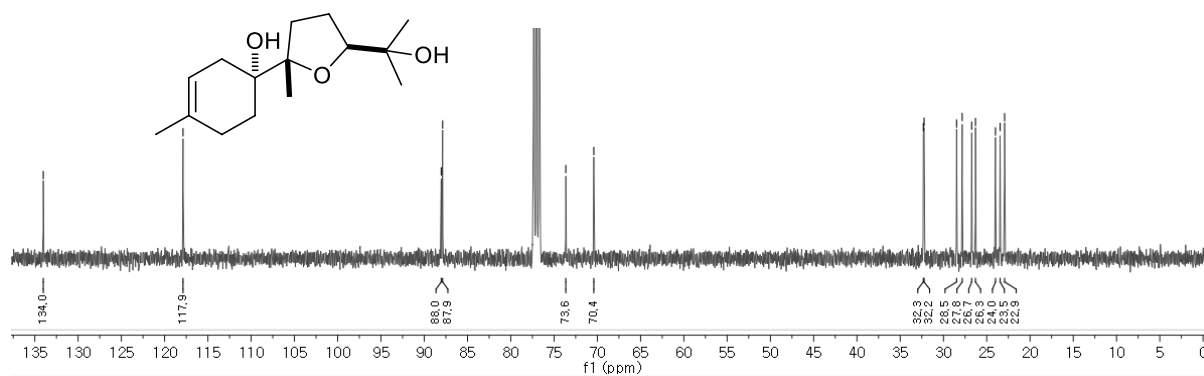


Figure S27. ¹³C NMR spectrum of compound **5** recorded at 100 MHz in CDCl₃.

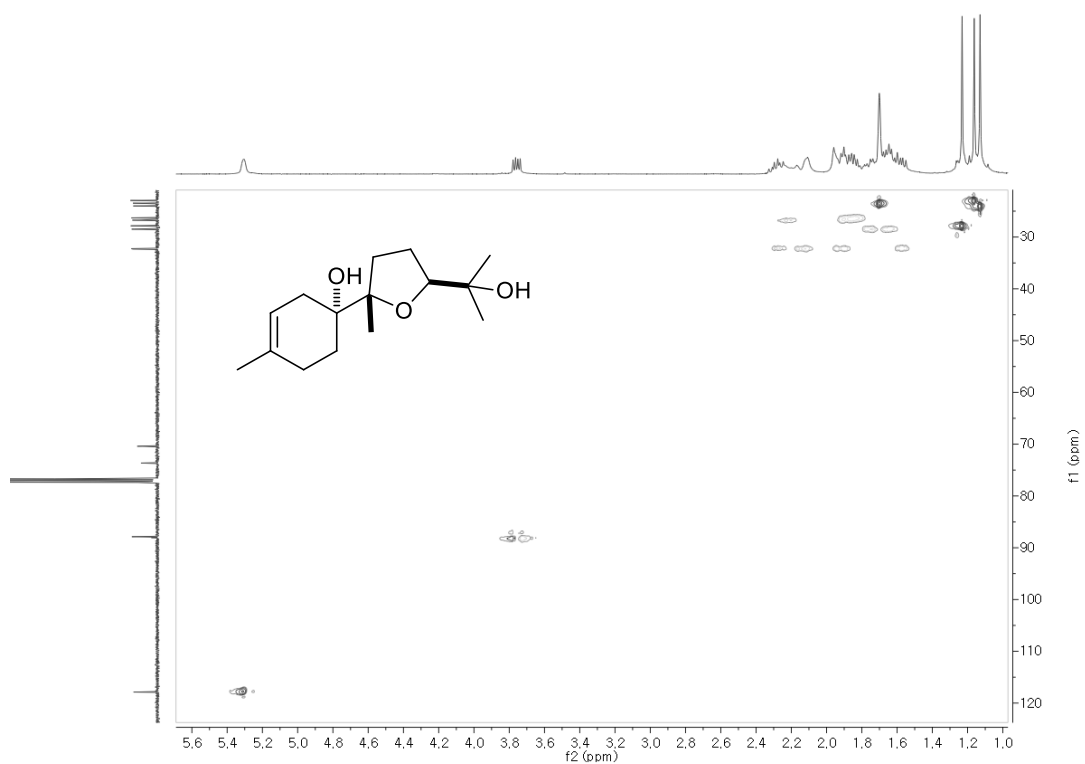


Figure S28. HSQC spectrum of compound **5** recorded at 400 MHz in CDCl₃.

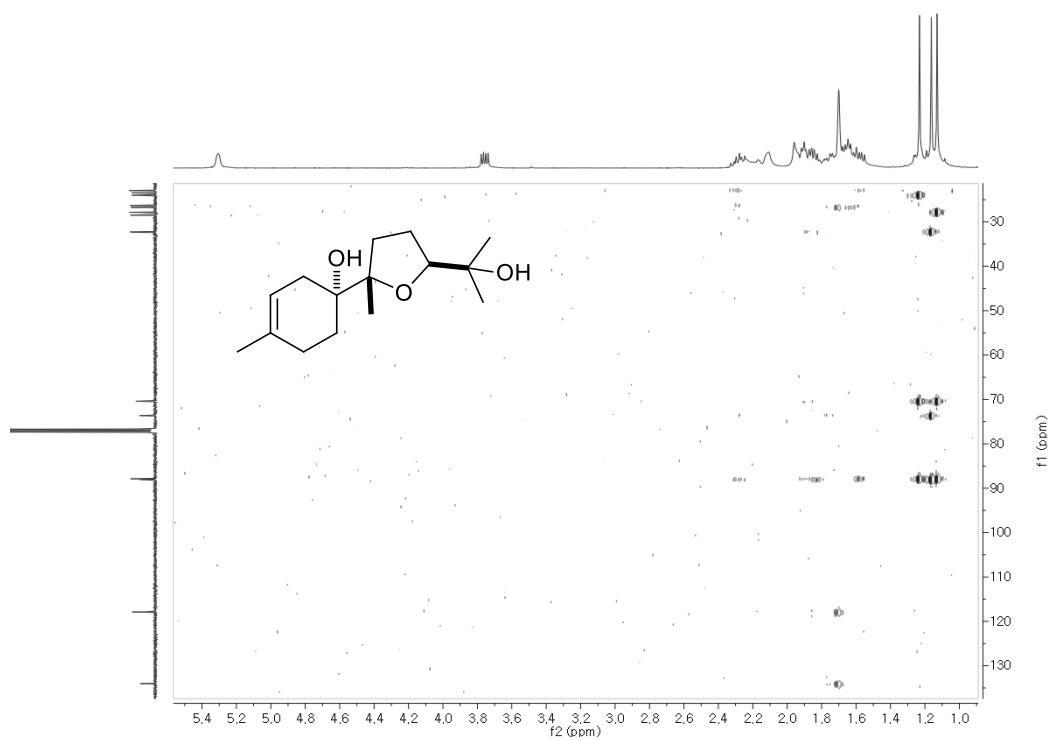


Figure S29. HMBC spectrum of compound **5** recorded at 400 MHz in CDCl₃.

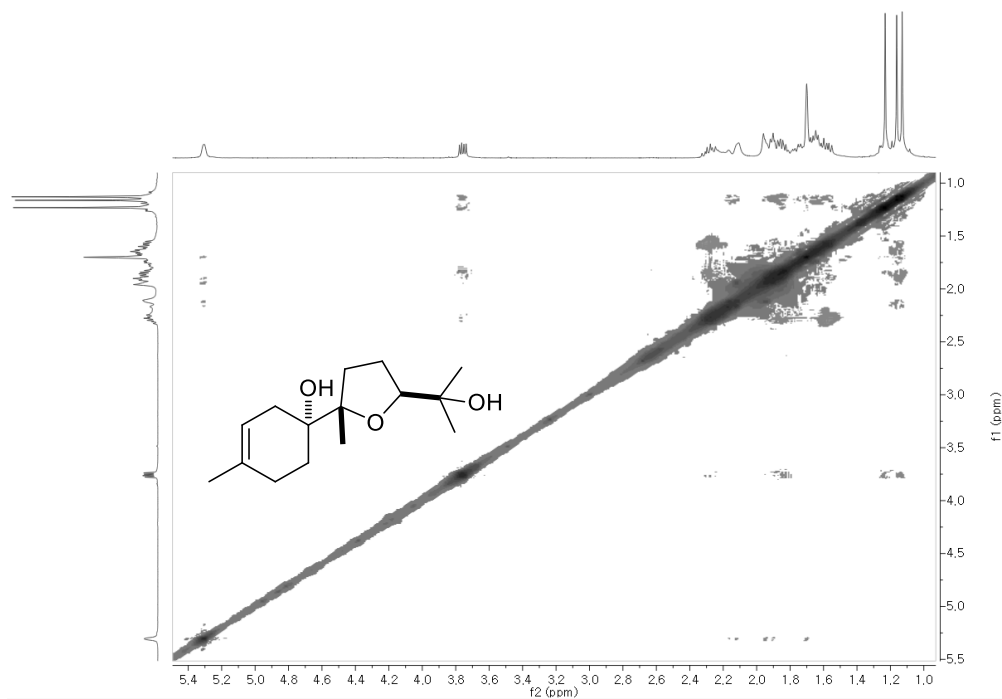


Figure S30. NOESY spectrum of compound **5** recorded at 400 MHz in CDCl₃.

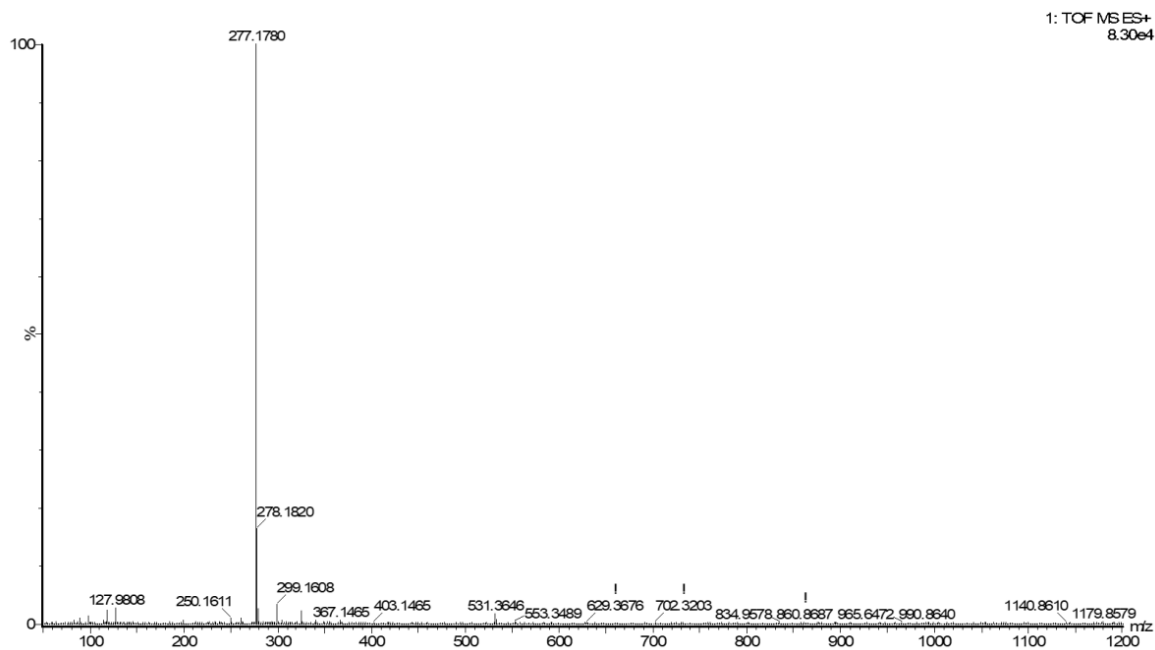


Figure S31. The HRESIMS spectrum of compound **5**.

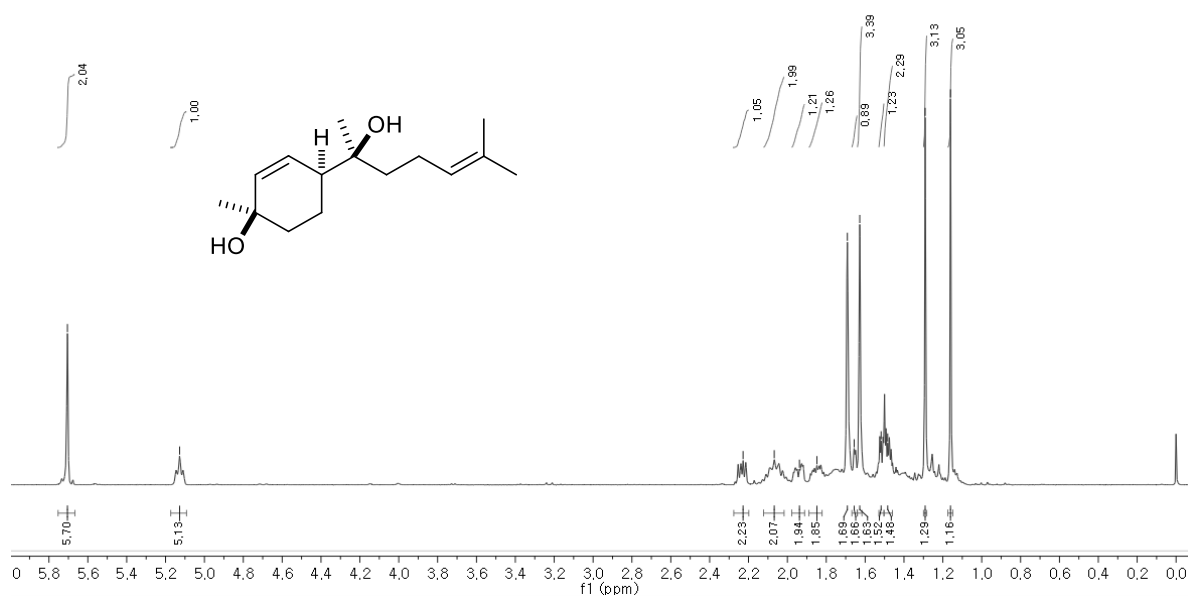


Figure S32. ^1H NMR spectrum of compound **6** recorded at 400 MHz in CDCl_3 .

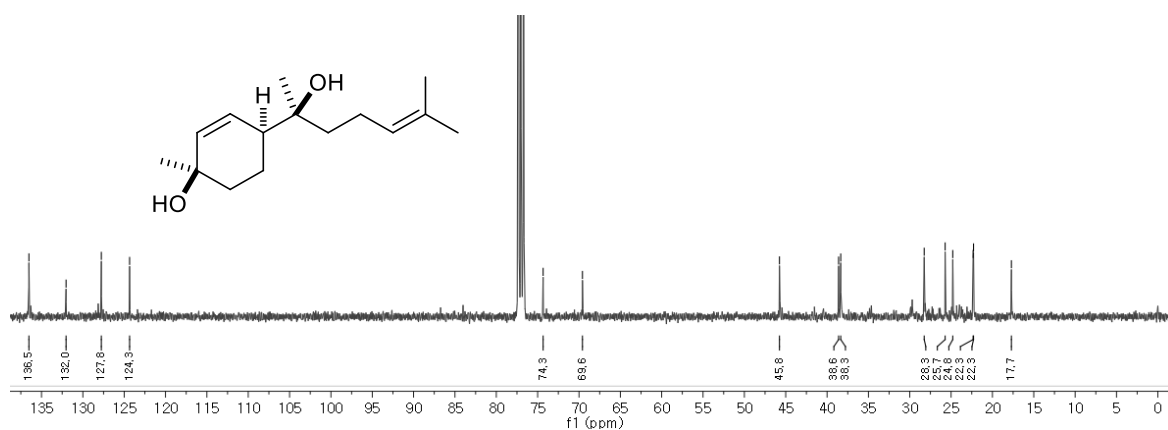


Figure S33. ^{13}C NMR spectrum of compound **6** recorded at 100 MHz in CDCl_3 .

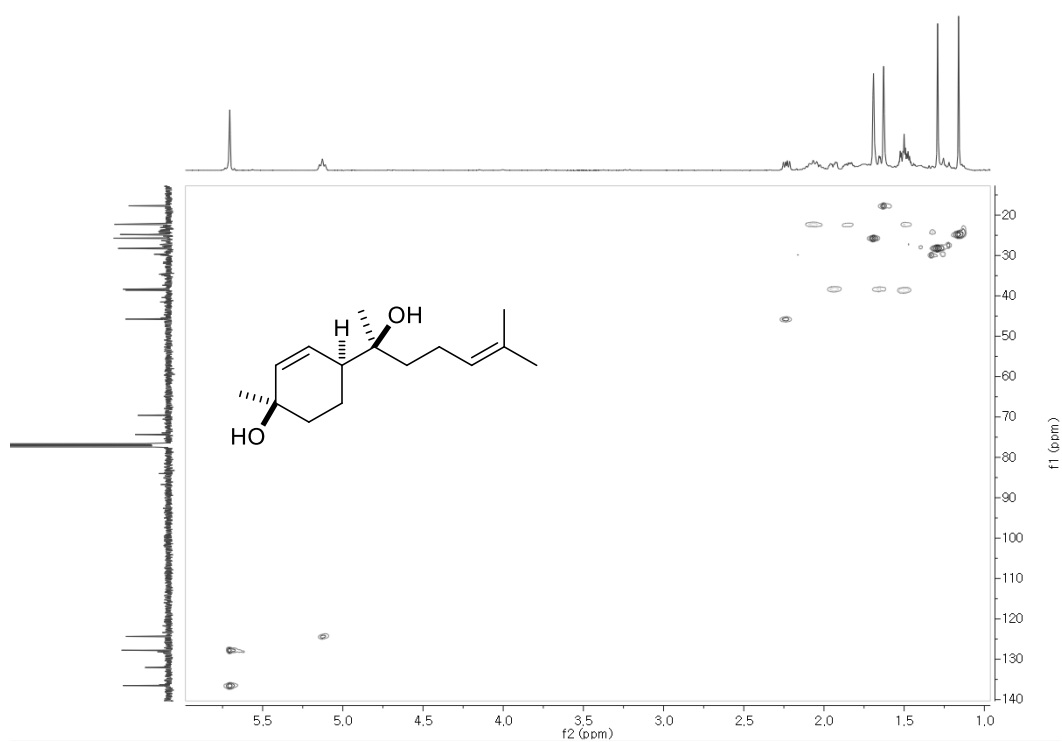


Figure S34. HSQC spectrum of compound **6** recorded at 400 MHz in CDCl_3 .



Figure S35. HMBC spectrum of compound **6** recorded at 400 MHz in CDCl₃.

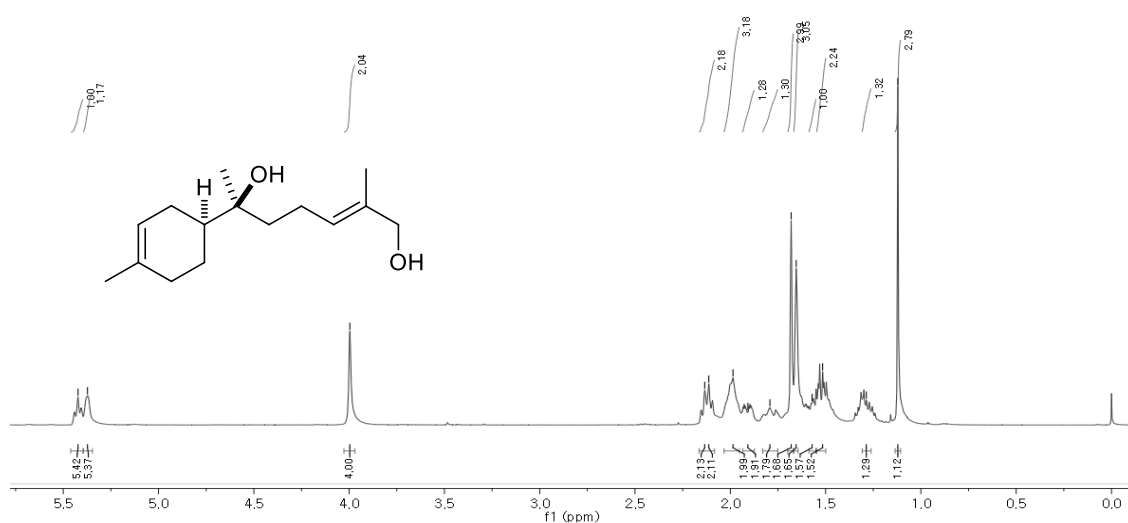


Figure S36. ¹H NMR spectrum of compound **7** recorded at 400 MHz in CDCl₃.

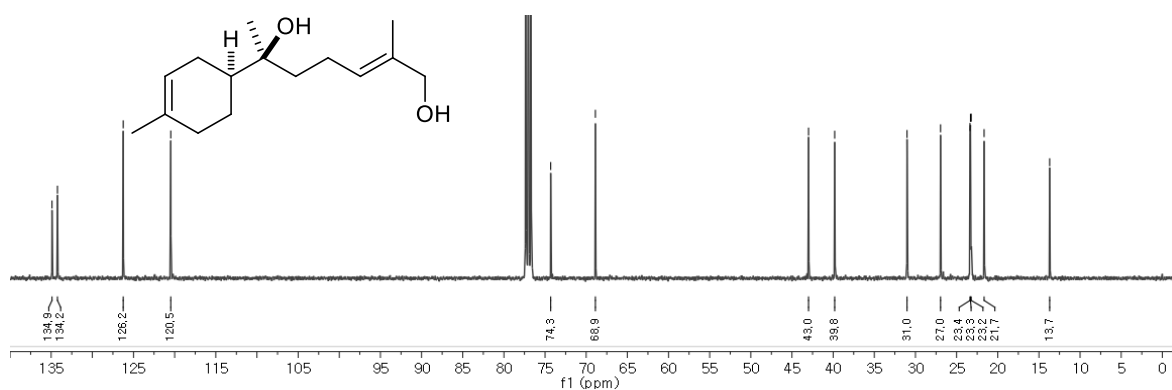


Figure S37. ¹³C NMR spectrum of compound **7** recorded at 100 MHz in CDCl₃.

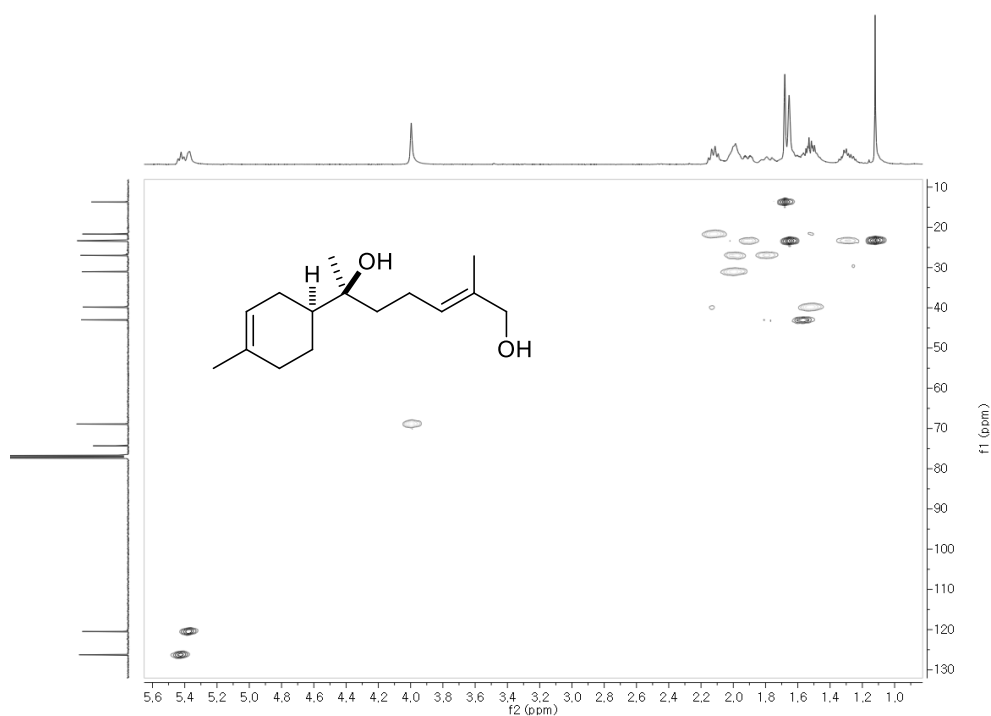


Figure S38. HSQC spectrum of compound 7 recorded at 400 MHz in CDCl₃.

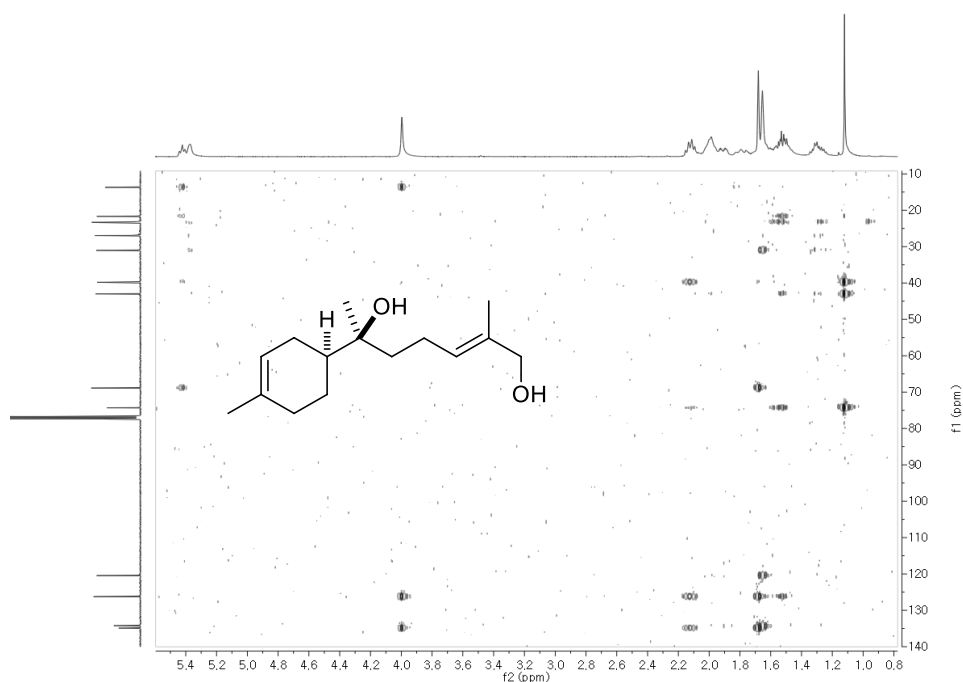


Figure S39. HMBC spectrum of compound 7 recorded at 400 MHz in CDCl₃.

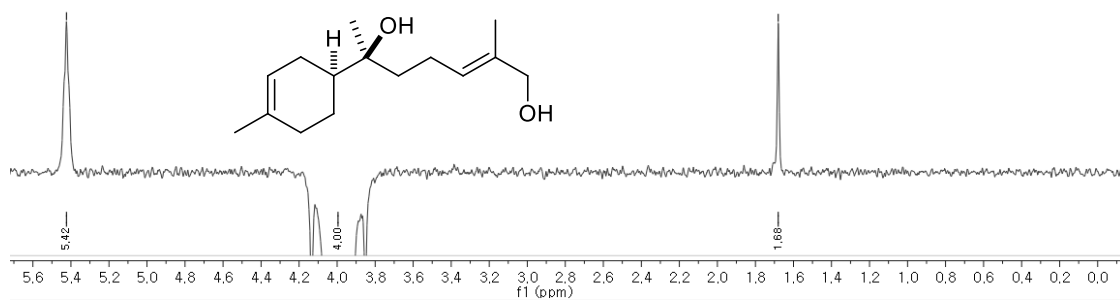


Figure S40. NOE spectrum of compound **7** recorded at 500 MHz in CDCl₃.

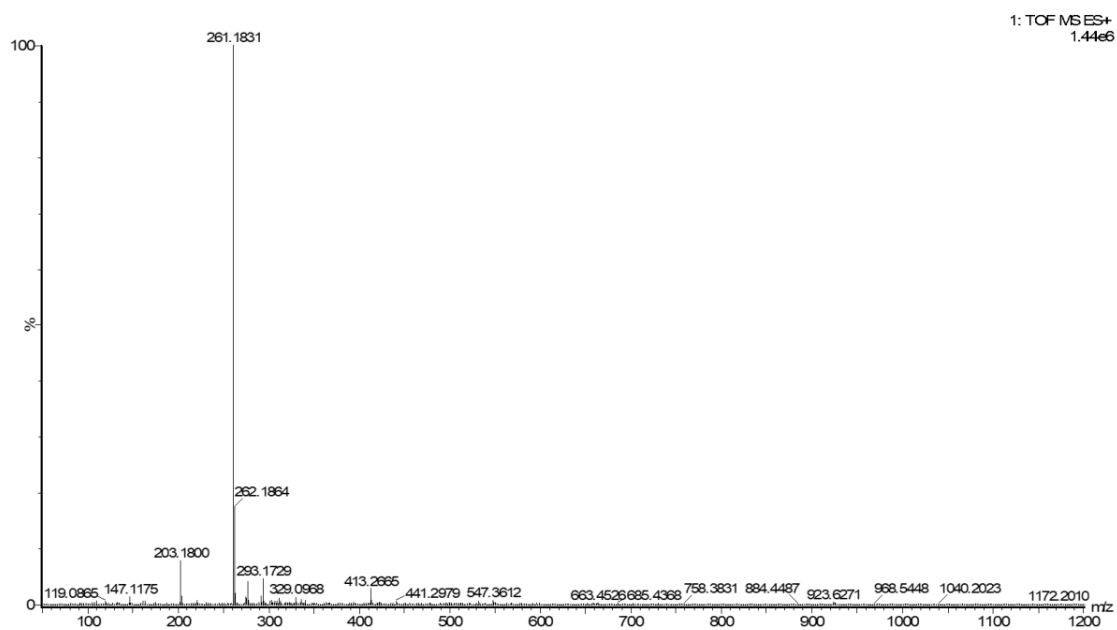


Figure S41. The HRESIMS spectroscopic data of compound **7**.

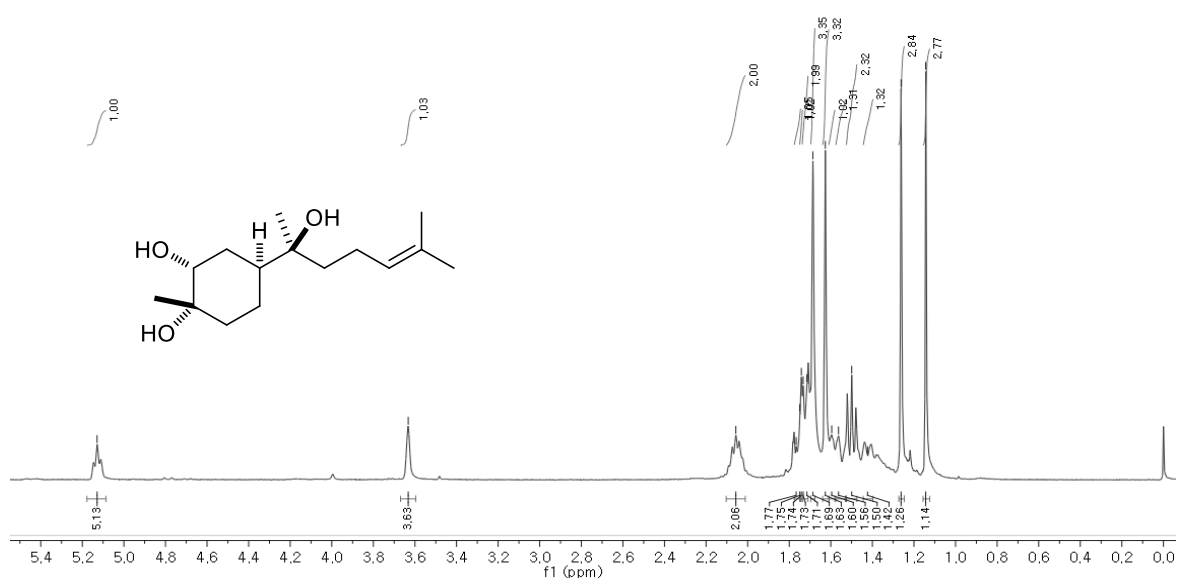


Figure S42. ¹H NMR spectrum of compound **8** recorded at 400 MHz in CDCl₃.

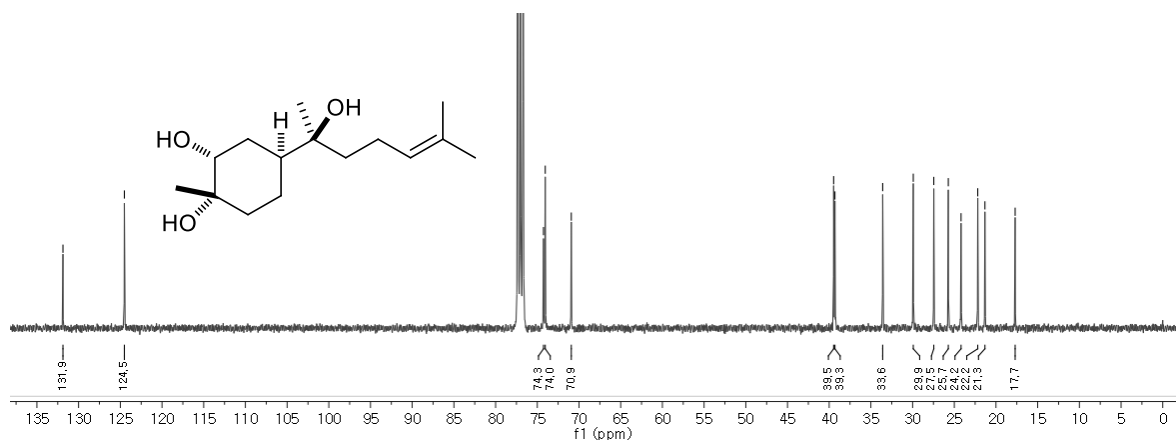


Figure S43. ¹³C NMR spectrum of compound **8** recorded at 100 MHz in CDCl₃.

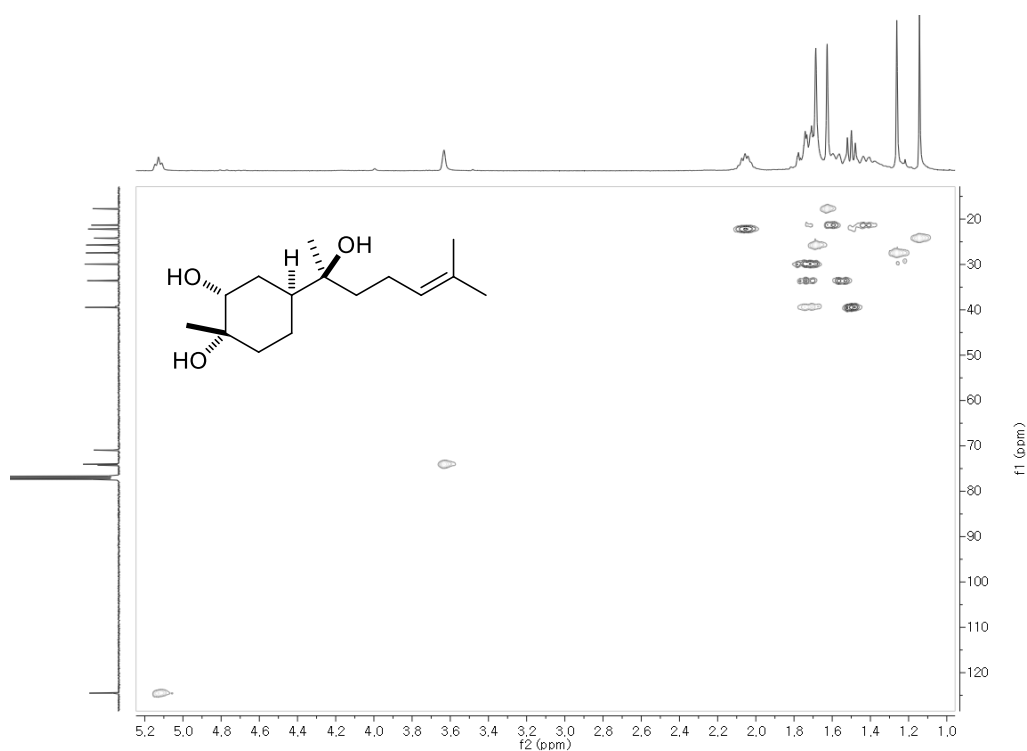


Figure S44. HSQC spectrum of compound **8** recorded at 400 MHz in CDCl₃.

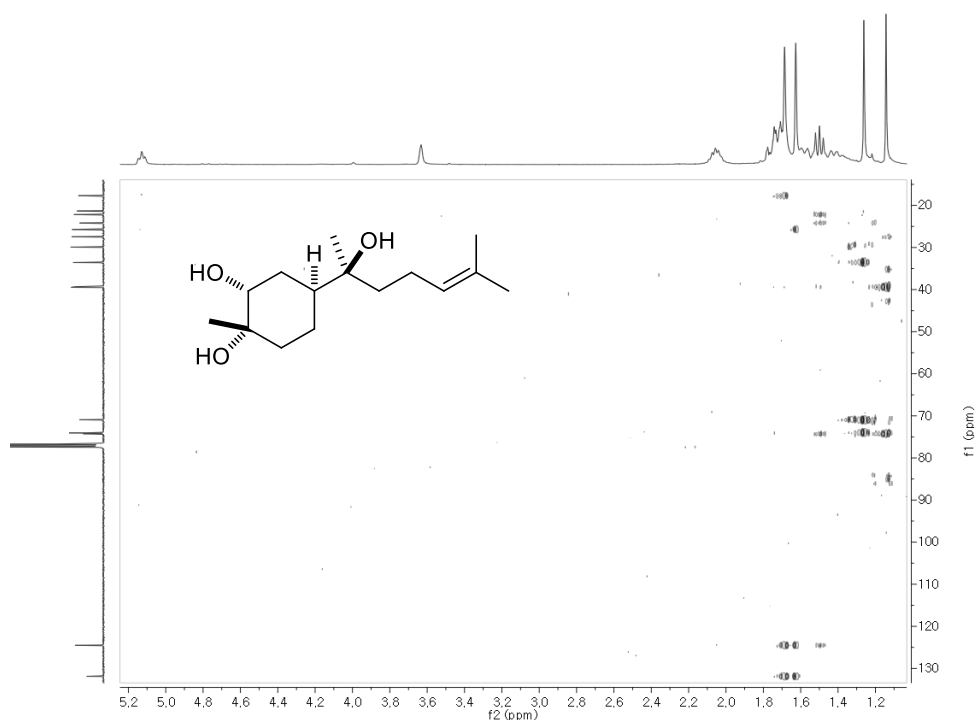


Figure S45. HMBC spectrum of compound **8** recorded at 400 MHz in CDCl₃.

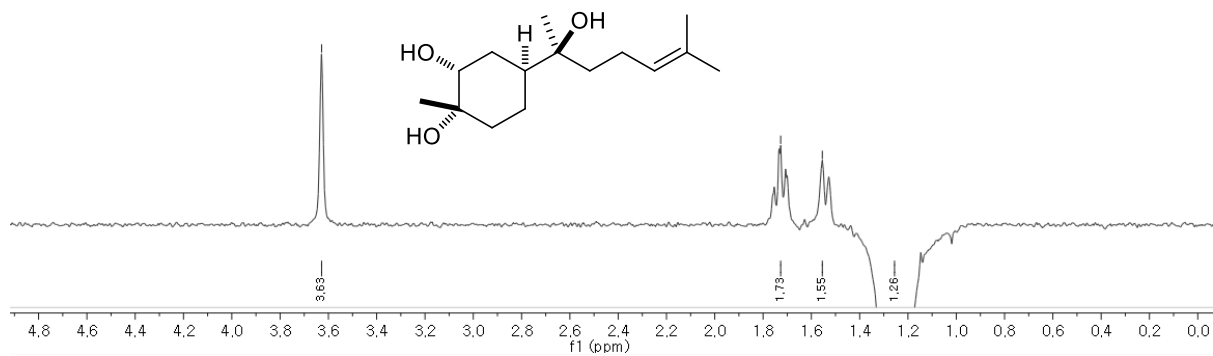


Figure S46. NOE spectrum of compound **8** recorded at 500 MHz in CDCl₃.

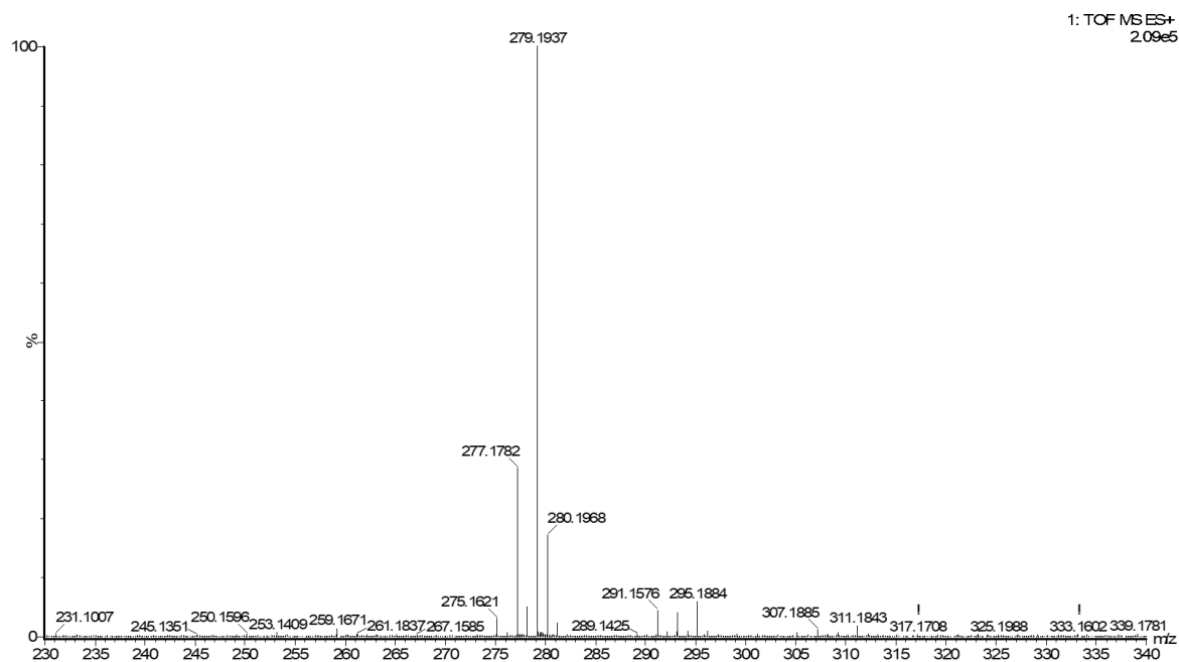


Figure S47. The HRESIMS spectroscopic data of compound 8.

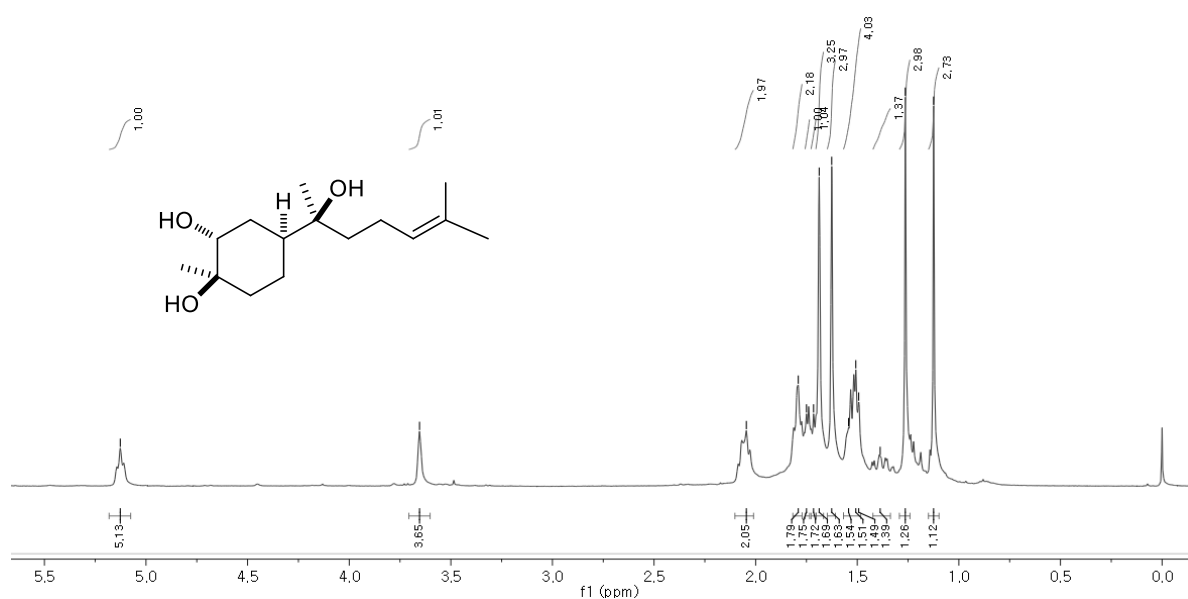


Figure S48. ¹H NMR spectrum of compound 9 recorded at 400 MHz in CDCl₃.

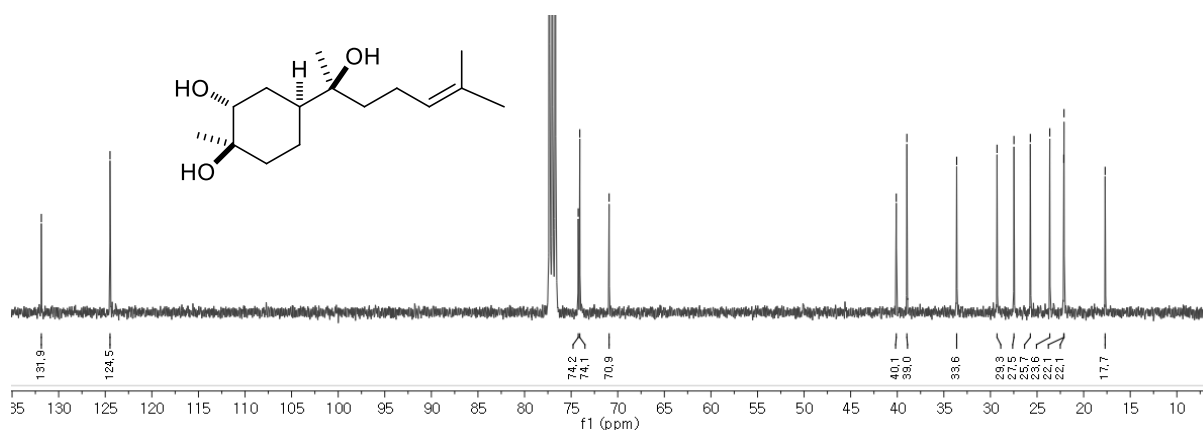


Figure S49. ^{13}C NMR spectrum of compound **9** recorded at 100 MHz in CDCl_3 .

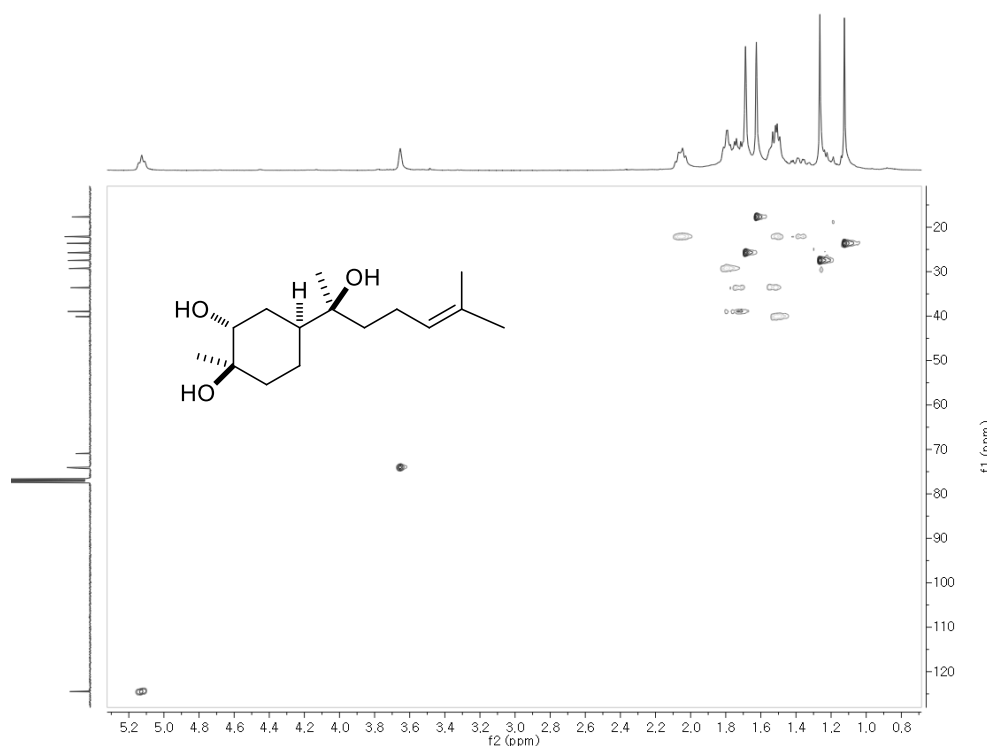


Figure S50. HSQC spectrum of compound **9** recorded at 400 MHz in CDCl_3 .

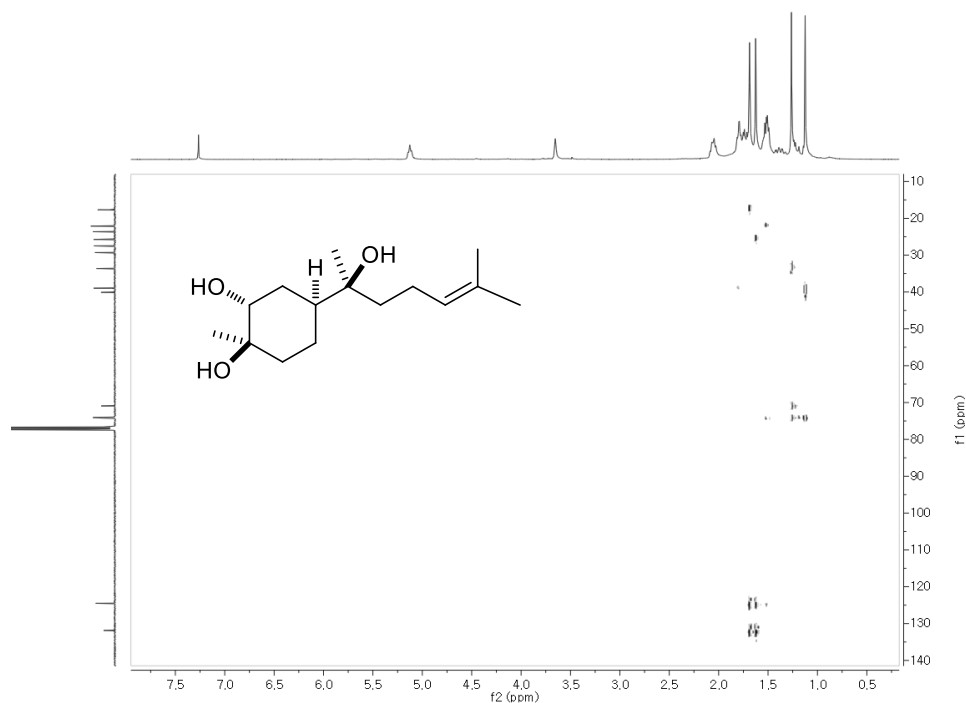


Figure S51. HMBC spectrum of compound **9** recorded at 400 MHz in CDCl_3 .

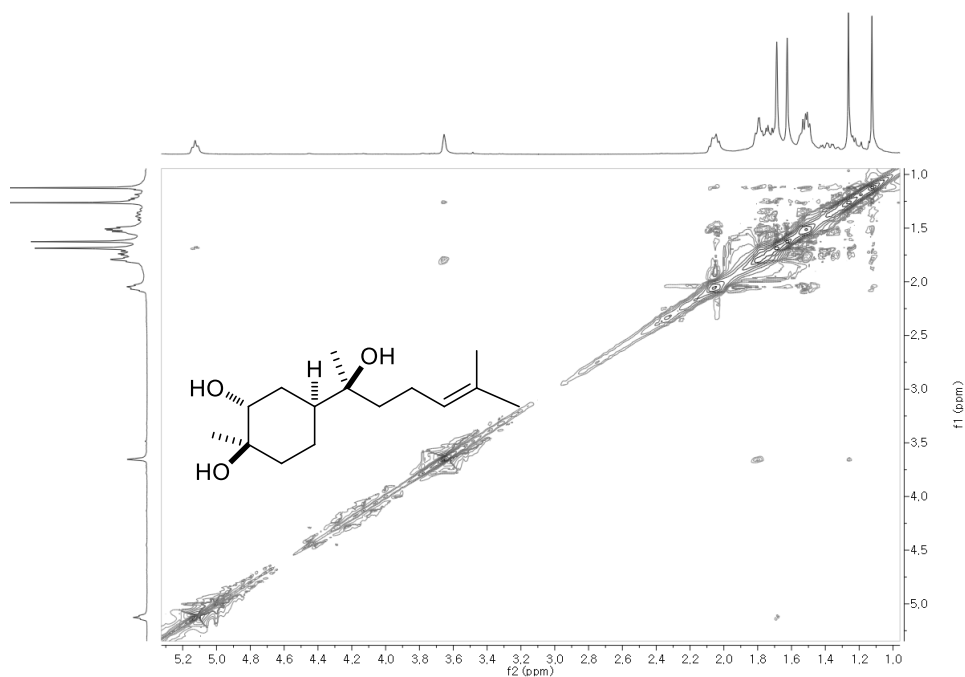


Figure S52. NOESY spectrum of compound **9** recorded at 400 MHz in CDCl_3 .

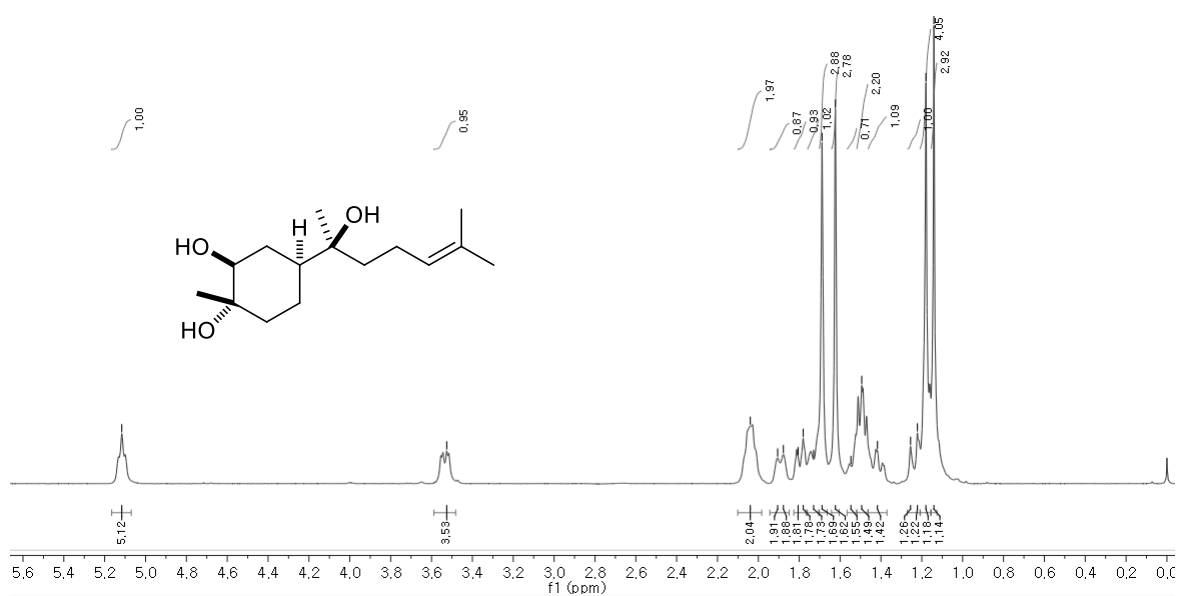


Figure S53. ^1H NMR spectrum of compound **10** recorded at 400 MHz in CDCl_3 .

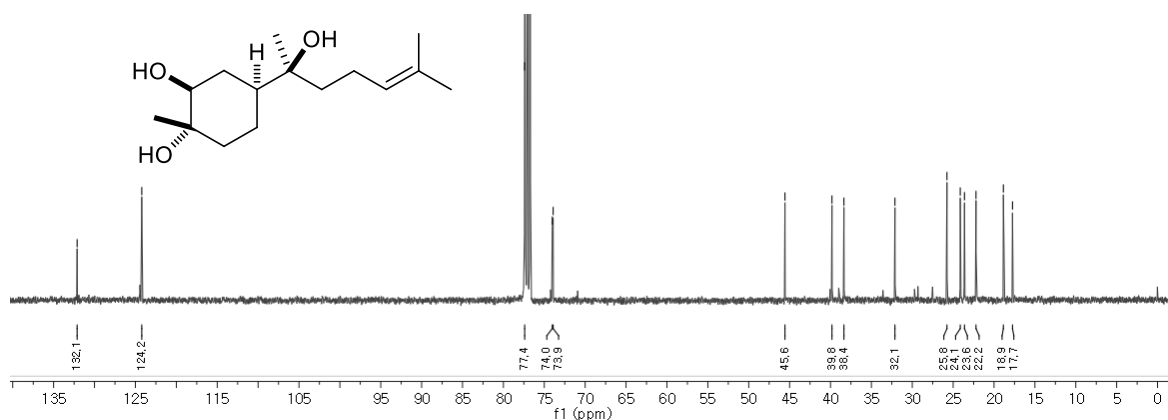


Figure S54. ^{13}C NMR spectrum of compound **10** recorded at 100 MHz in CDCl_3 .

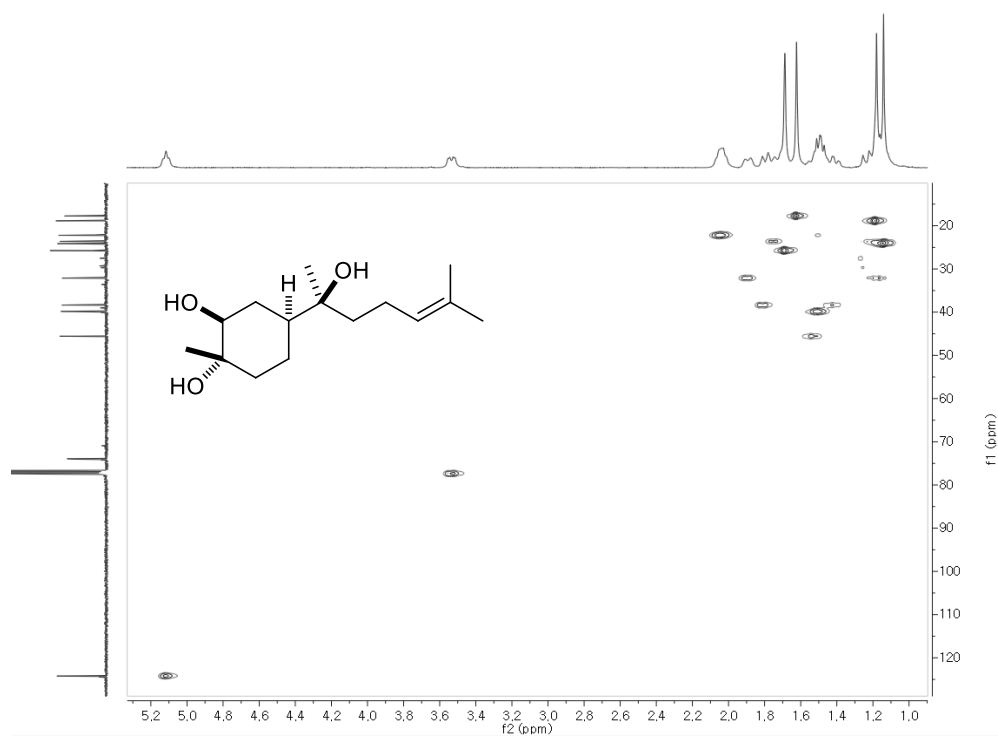


Figure S55. HSQC spectrum of compound **10** recorded at 400 MHz in CDCl_3 .

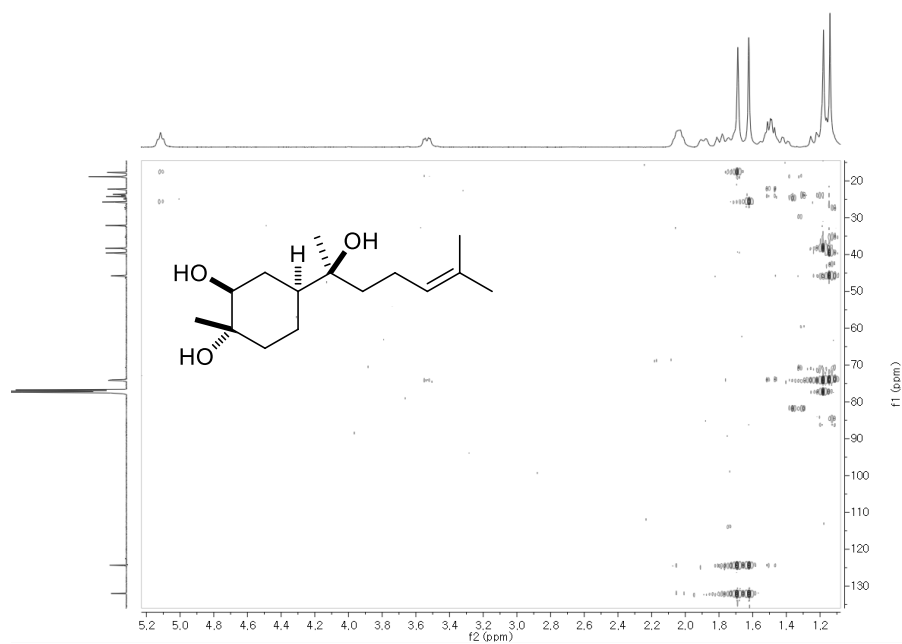


Figure S56. HMBC spectrum of compound **10** recorded at 400 MHz in CDCl_3 .

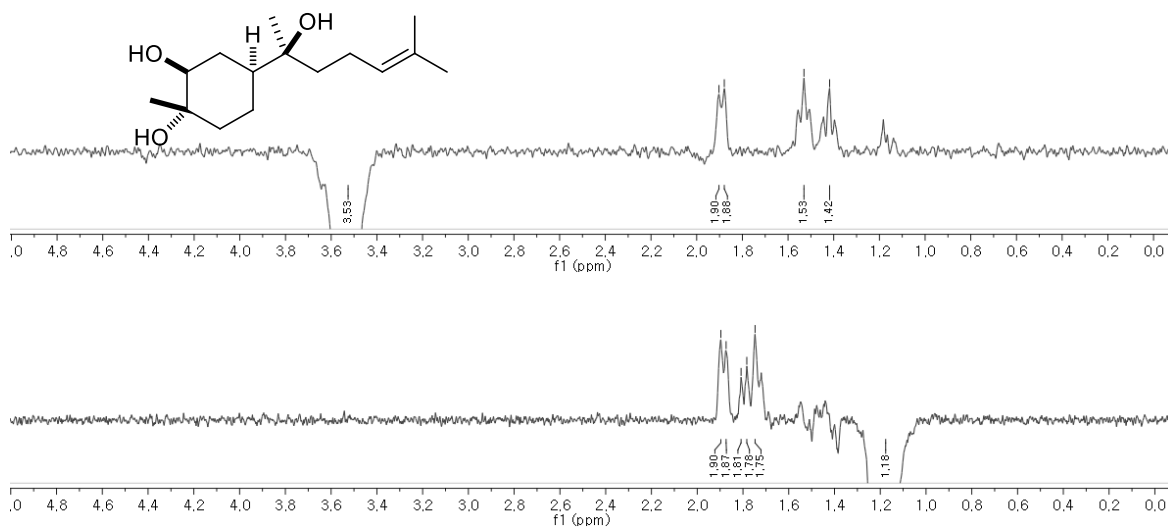


Figure S57. NOE spectrum of compound 10 recorded at 500 MHz in CDCl_3 .

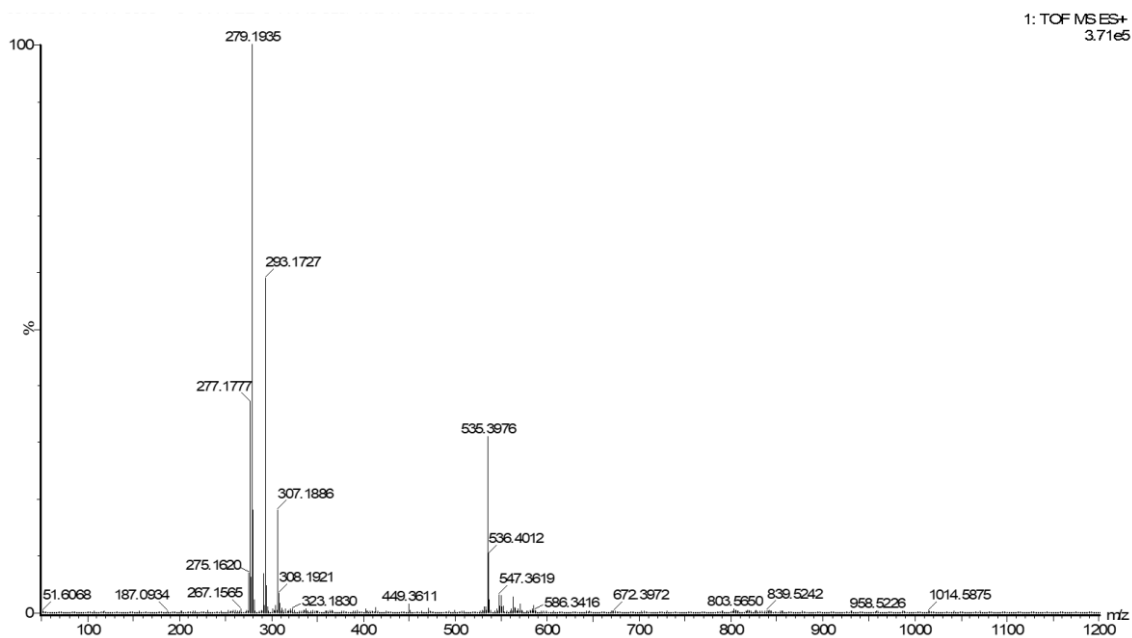


Figure S58. The HRESIMS spectroscopic data of compound 10.

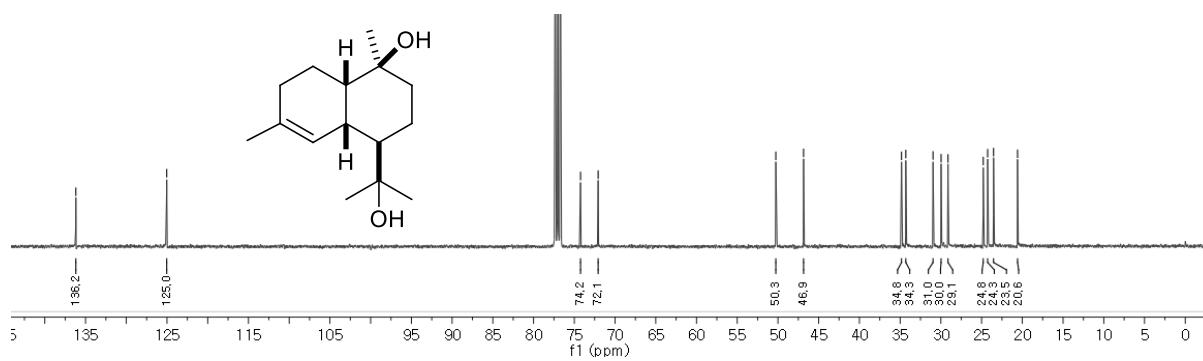


Figure S62. ¹³C NMR spectrum of compound **12** recorded at 100 MHz in CDCl₃.