

SUPPORTING INFORMATION

Isopimarane Diterpenoids from the Rhizomes of *Kaempferia marginata* and Their Potential Anti-inflammatory Activities

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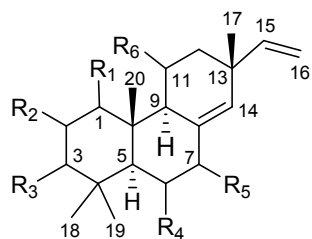
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- 7**, $R_1 = \alpha\text{-OH}$, $R_2 = R_3 = R_4 = R_5 = R_6 = \text{H}$
8, $R_1 = \alpha\text{-OH}$, $R_2 = R_3 = R_4 = R_6 = \text{H}$, $R_5 = \text{=O}$
9, $R_1 = R_6 = \alpha\text{-OH}$, $R_2 = R_3 = R_4 = R_5 = \text{H}$
10, $R_1 = \alpha\text{-OAc}$, $R_2 = \alpha\text{-OH}$, $R_3 = R_4 = R_5 = R_6 = \text{H}$
11, $R_1 = R_2 = \alpha\text{-OH}$, $R_3 = R_4 = R_5 = R_6 = \text{H}$
12, $R_1 = R_3 = R_4 = R_6 = \text{H}$, $R_2 = \alpha\text{-OH}$, $R_5 = \text{=O}$
13, $R_1 = R_2 = \alpha\text{-OH}$, $R_3 = R_4 = R_6 = \text{H}$, $R_5 = \beta\text{-OH}$
14, $R_1 = R_5 = R_6 = \alpha\text{-OH}$, $R_2 = R_3 = R_4 = \text{H}$

Figure S1. The structure of known compounds **7–14**.

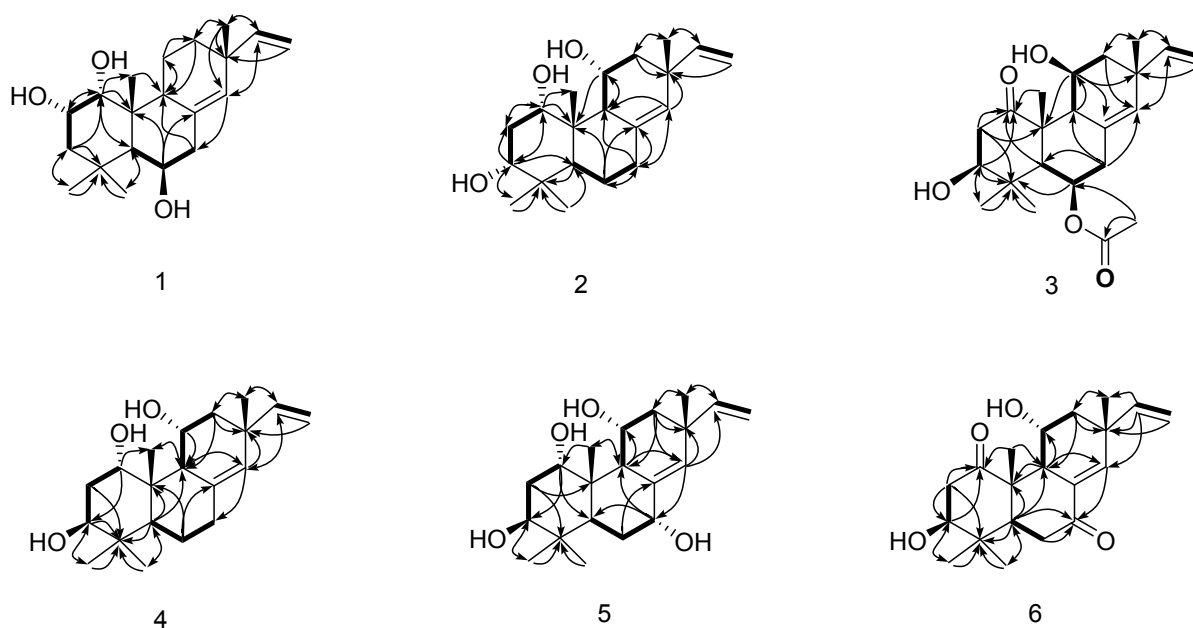


Figure S2. The COSY and key HMBC ($^1\text{H} \rightarrow ^{13}\text{C}$) correlations of compounds **1–6**.

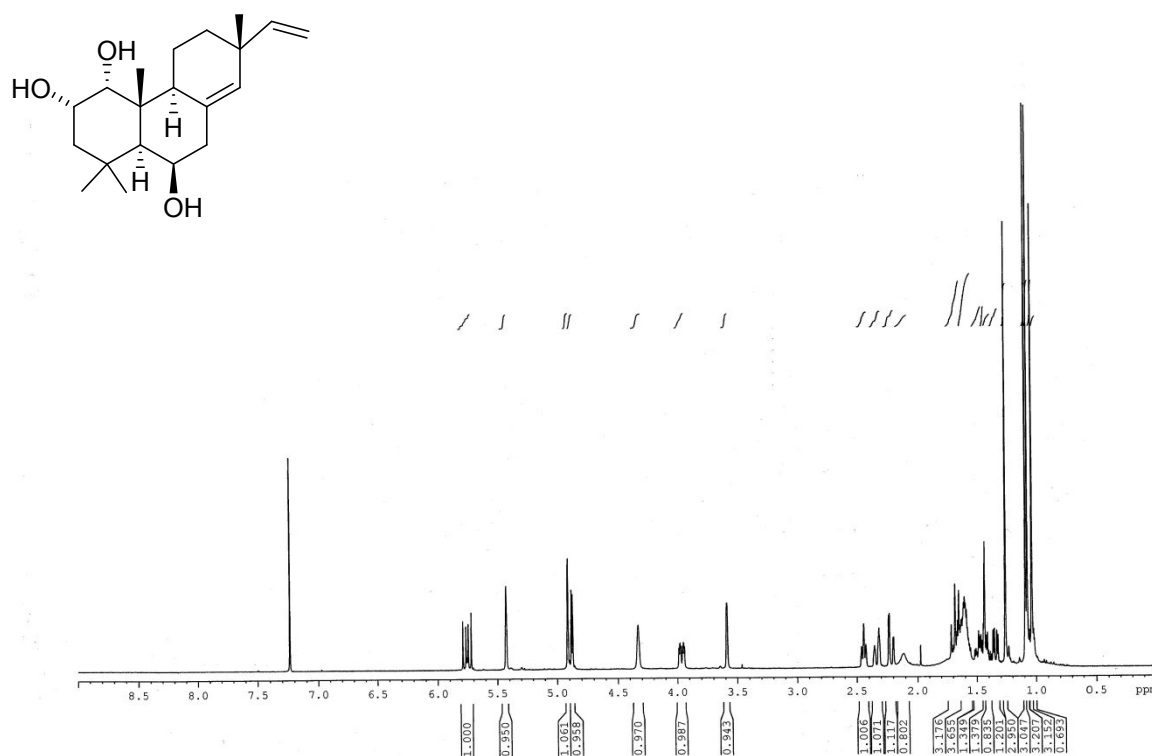


Figure S3. ¹H NMR spectrum (CDCl₃, 400 MHz) of marginaol A (1)

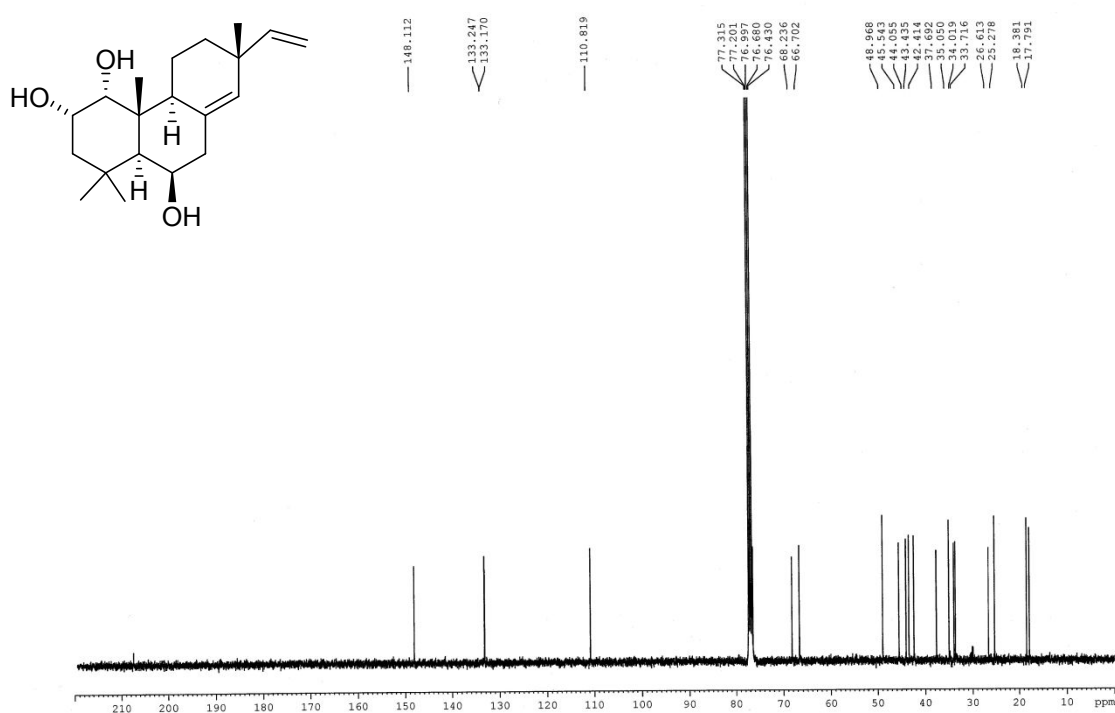


Figure S4. ¹³C NMR spectrum (CDCl₃, 100 MHz) of marginaol A (1)

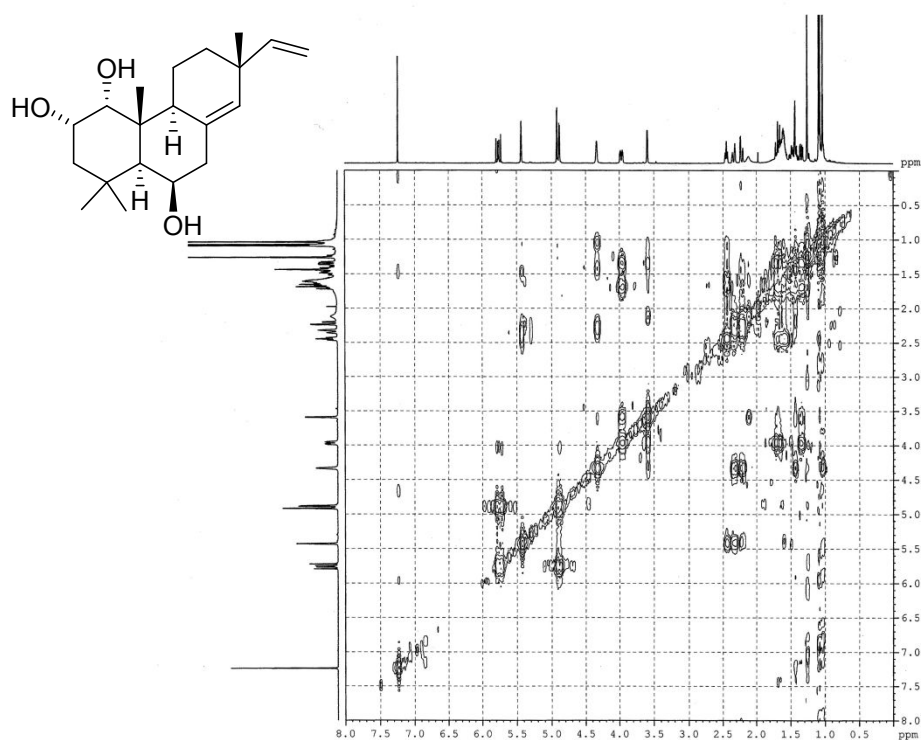


Figure S5. COSY spectrum of marginaol A (**1**) in CDCl₃

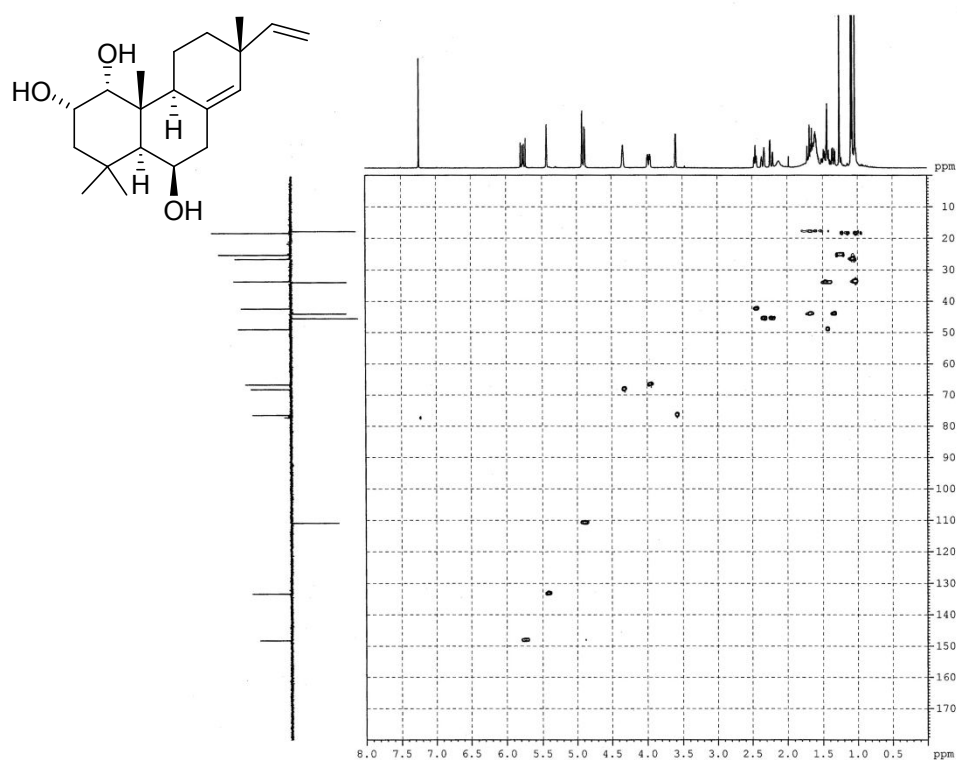


Figure S6. HMQC spectrum of marginaol A (**1**) in CDCl₃

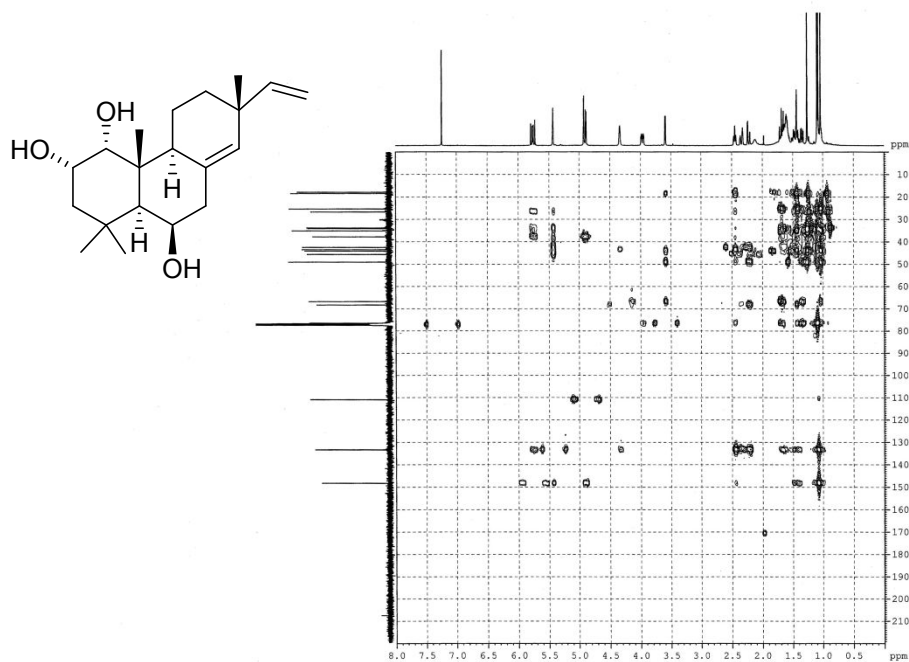


Figure S7. HMBC spectrum of marginaol A (**1**) in CDCl_3

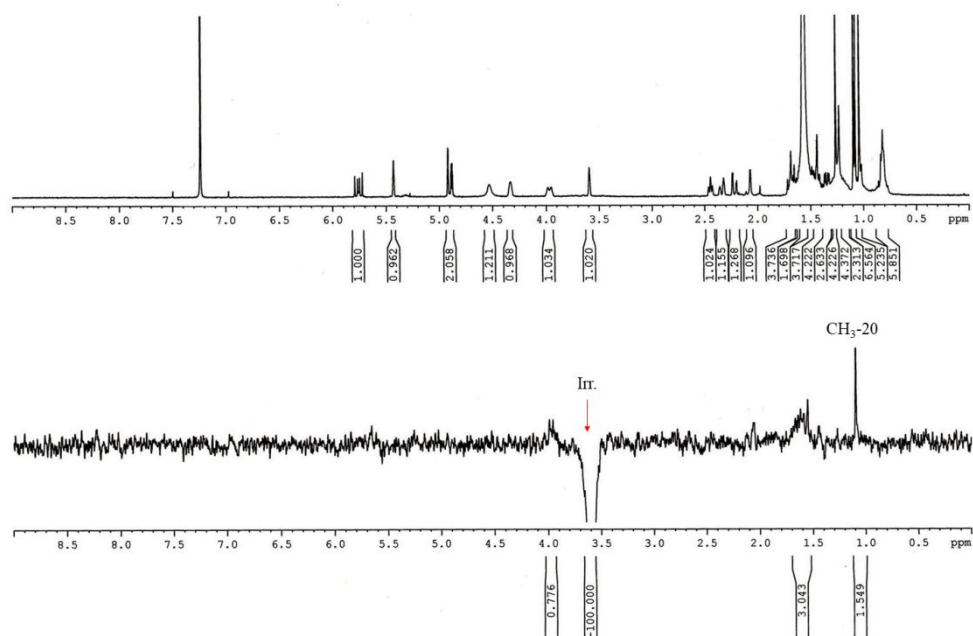


Figure S8. Difference NOE of **1** irradiating H-1 in CDCl_3

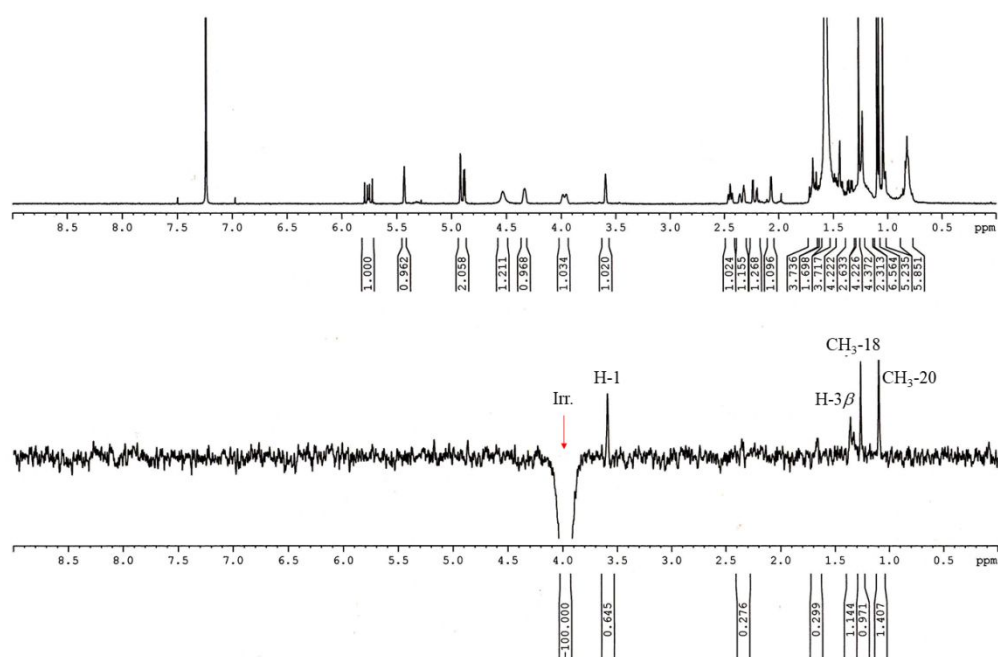


Figure S9. Difference NOE of **1** irradiating H-2 in CDCl_3

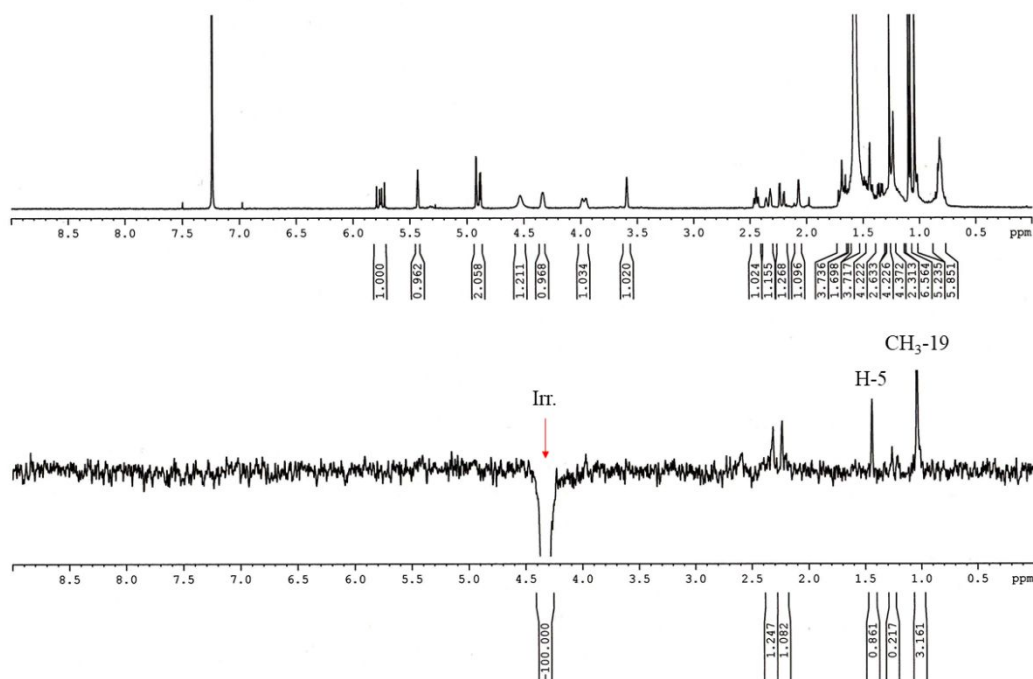


Figure S10. Difference NOE of **1** irradiating H-6 in CDCl_3

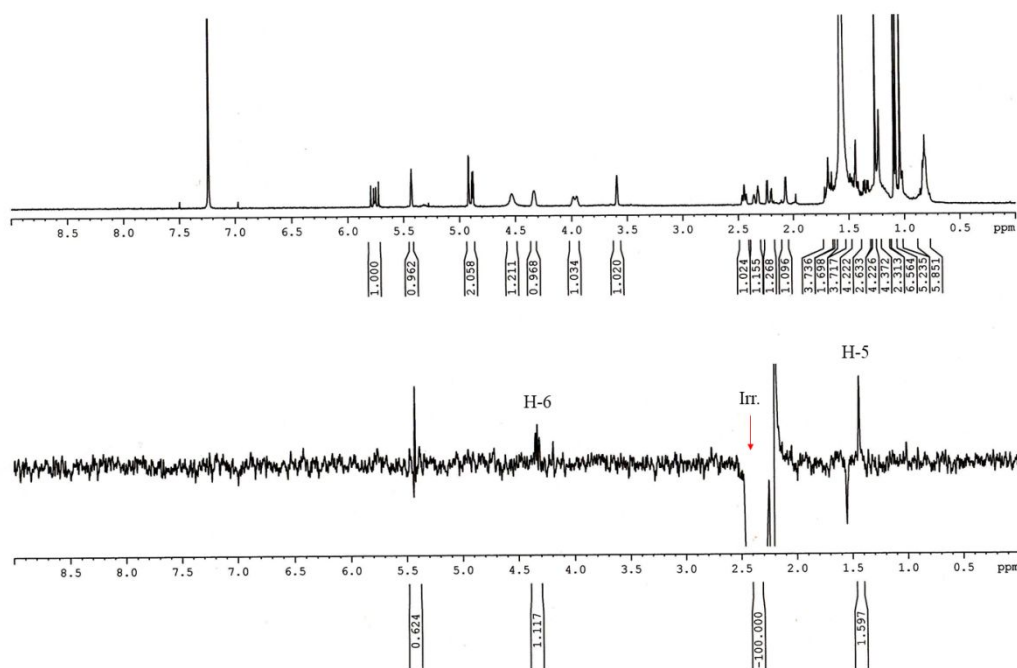


Figure S11. Difference NOE of **1** irradiating H-7 α in CDCl_3

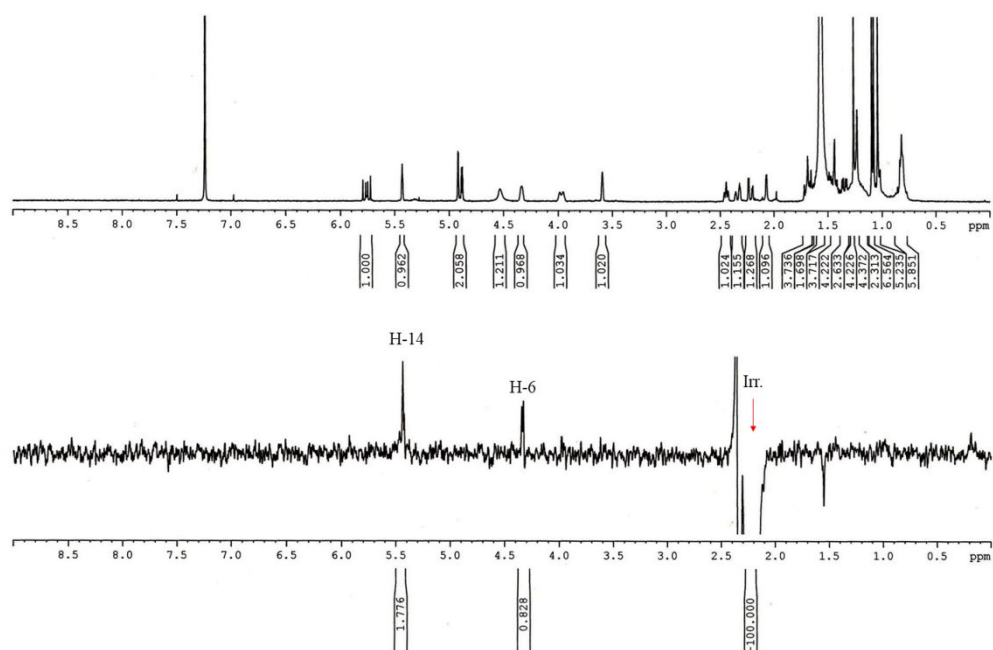


Figure S12. Difference NOE of **1** irradiating H-7 β in CDCl_3

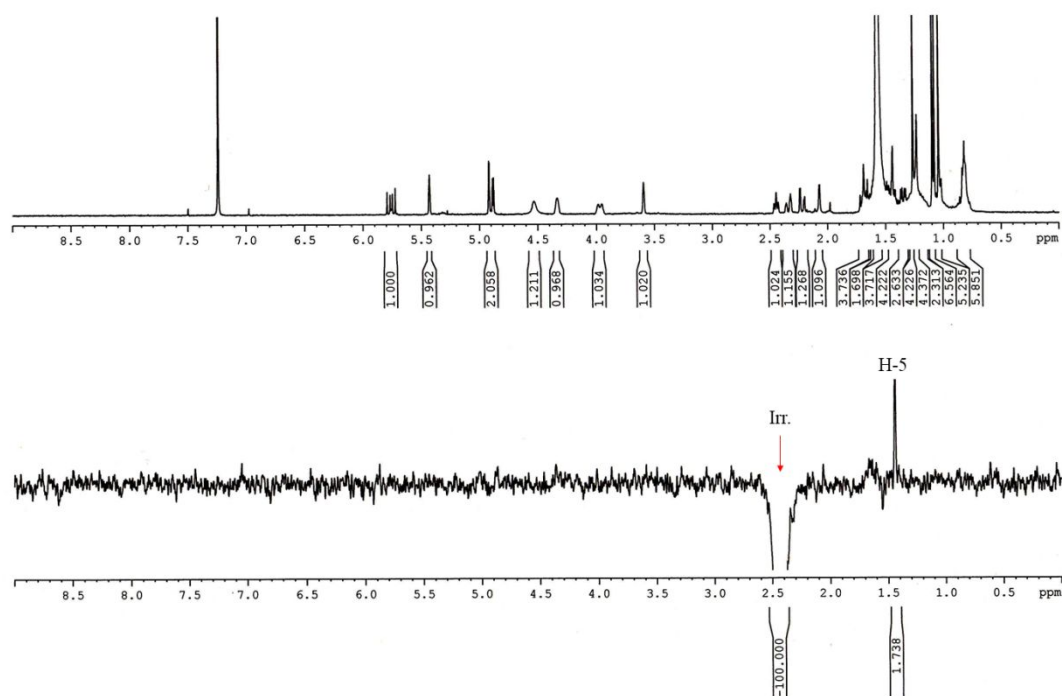


Figure S13. Difference NOE of **1** irradiating H-9 in CDCl_3

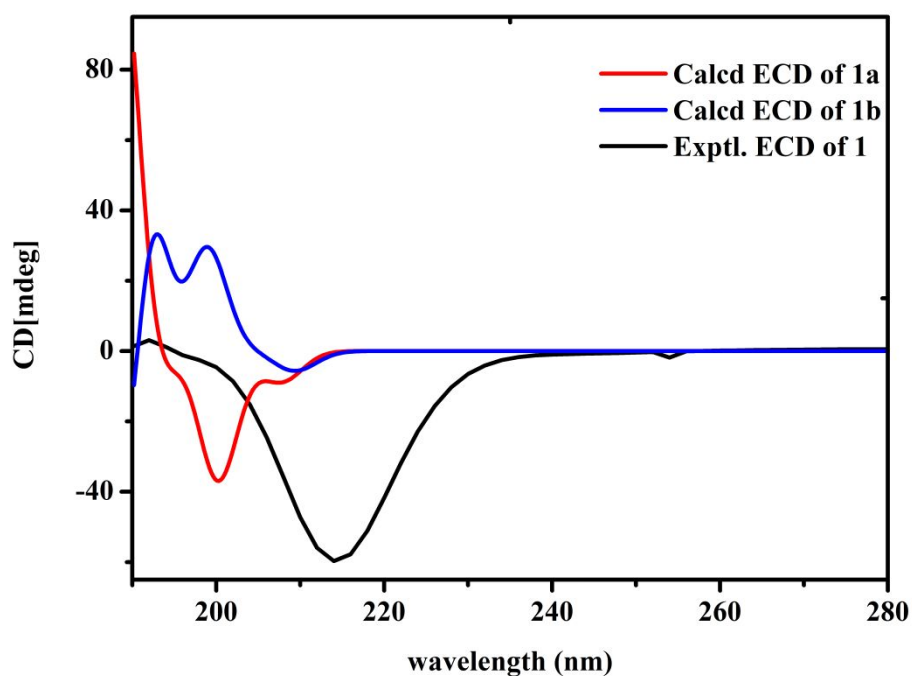


Figure S14. Calculated ECD spectra of (1*R*, 2*S*, 5*S*, 6*R*, 9*S*, 10*R*, 13*R*)-**1a** and (1*S*, 2*R*, 5*R*, 6*S*, 9*R*, 10*S*, 13*S*)-**1b** isomers and the experimental ECD spectrum of **1** in MeOH

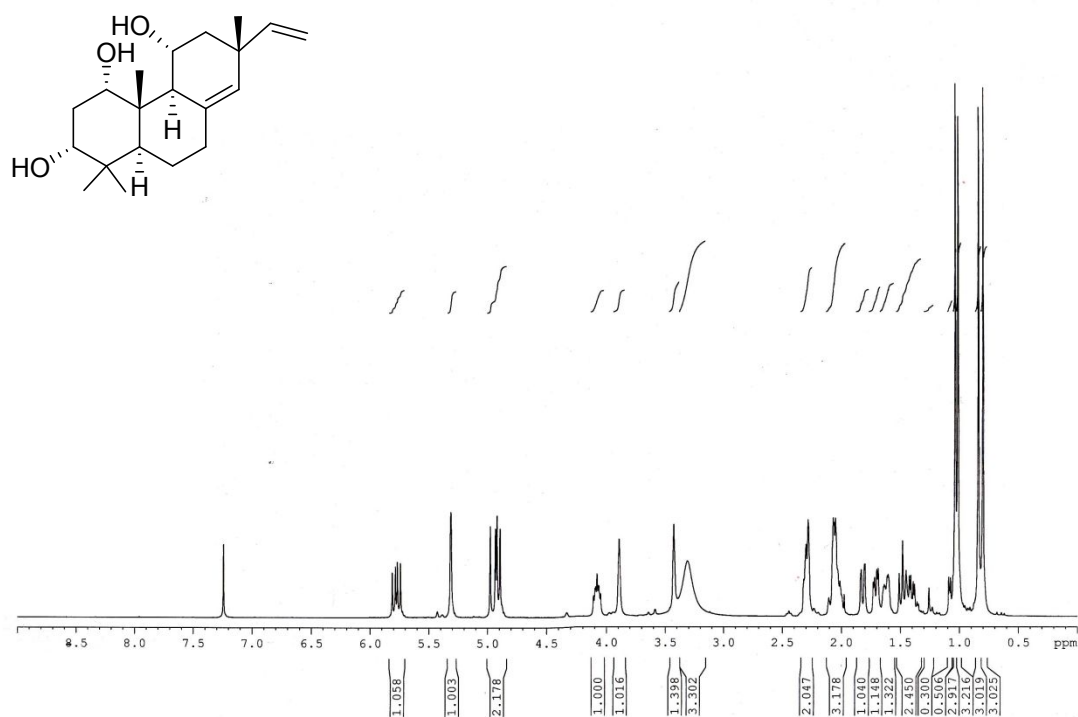


Figure S15. ¹H NMR spectrum (CDCl₃, 400 MHz) of marginaol B (2)

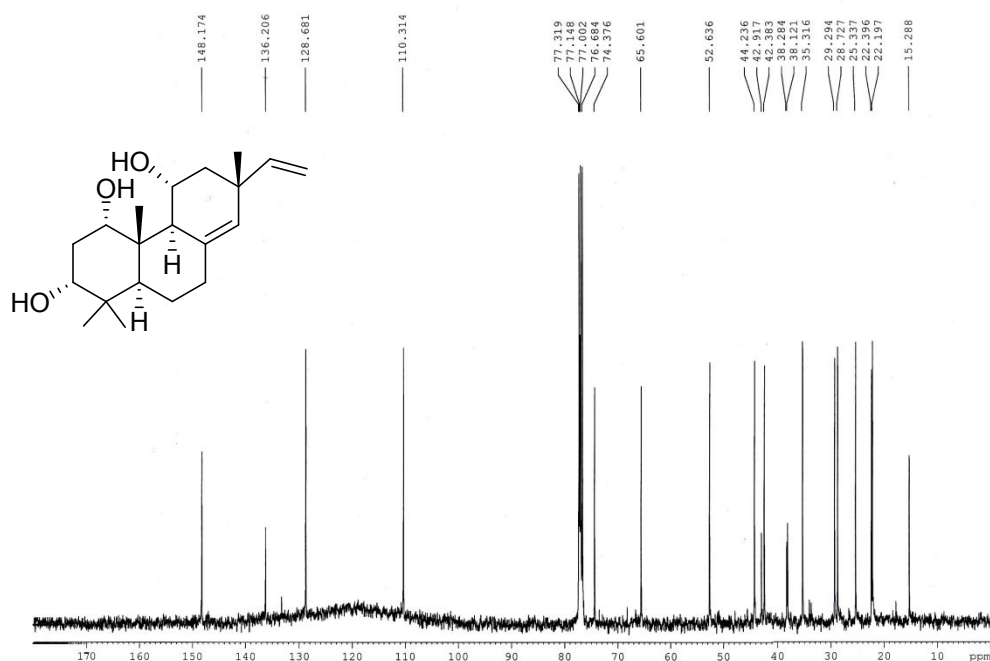


Figure S16. ¹³C NMR spectrum (CDCl₃, 100 MHz) of marginaol B (2)

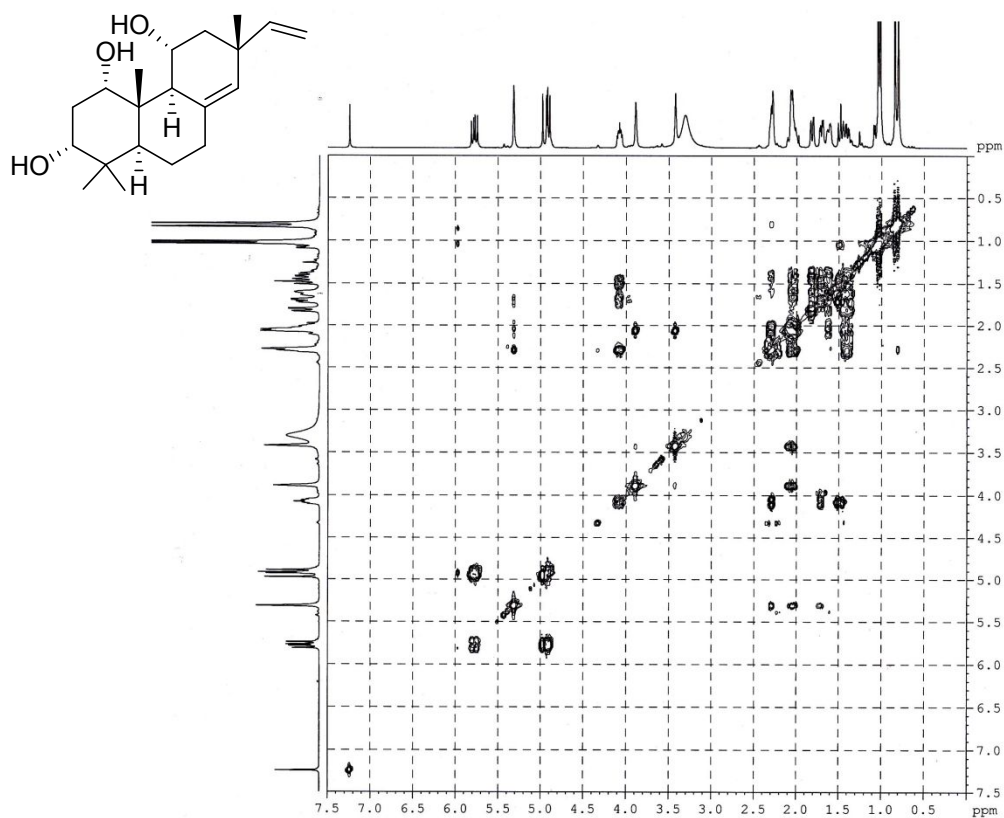


Figure S17. COSY spectrum of marginaol B (2) in CDCl₃

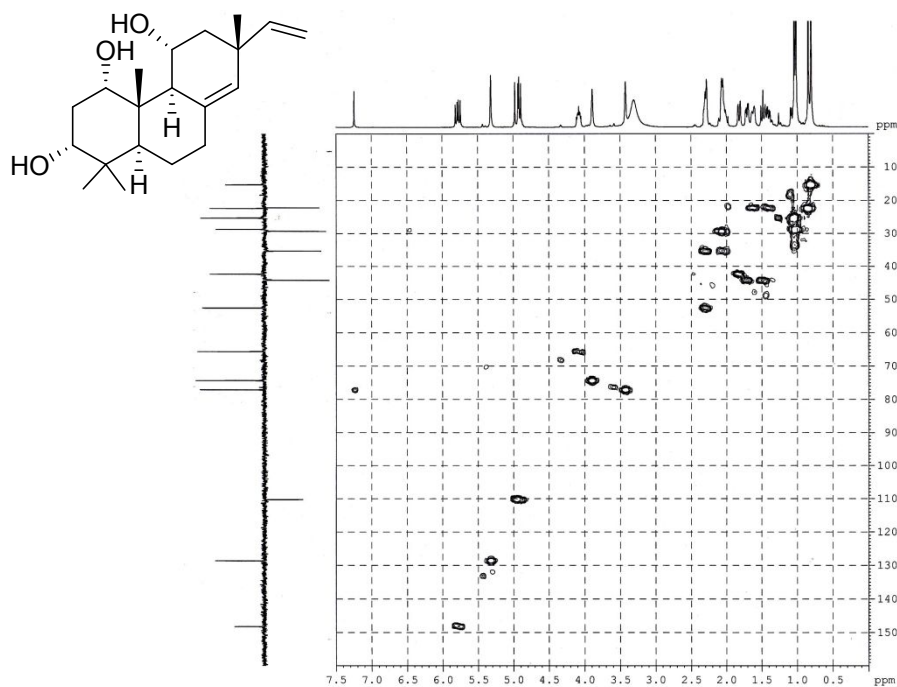


Figure S18. HMQC spectrum of marginaol B (2) in CDCl₃

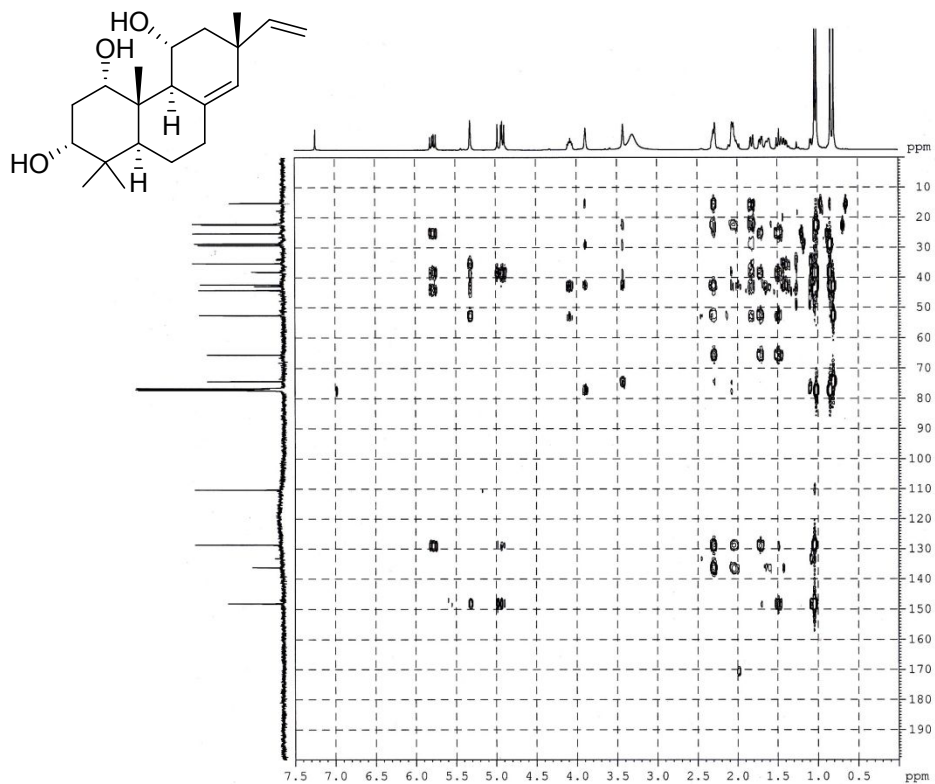


Figure S19. HMBC spectrum of marginaol B (**2**) in CDCl_3

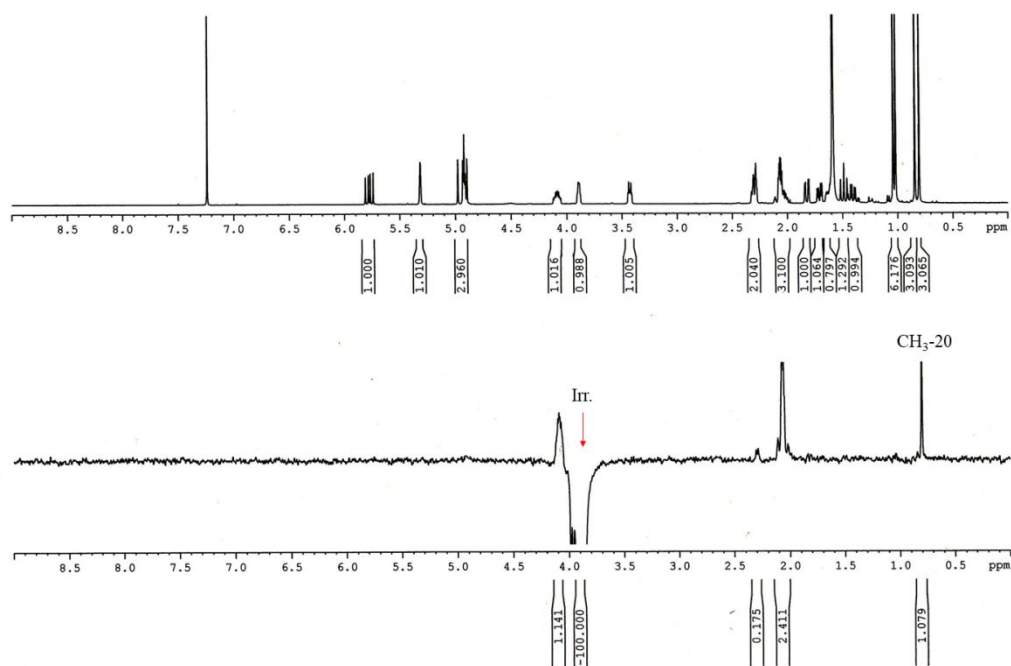


Figure S20. Difference NOE of **2** irradiating H-1 in CDCl_3

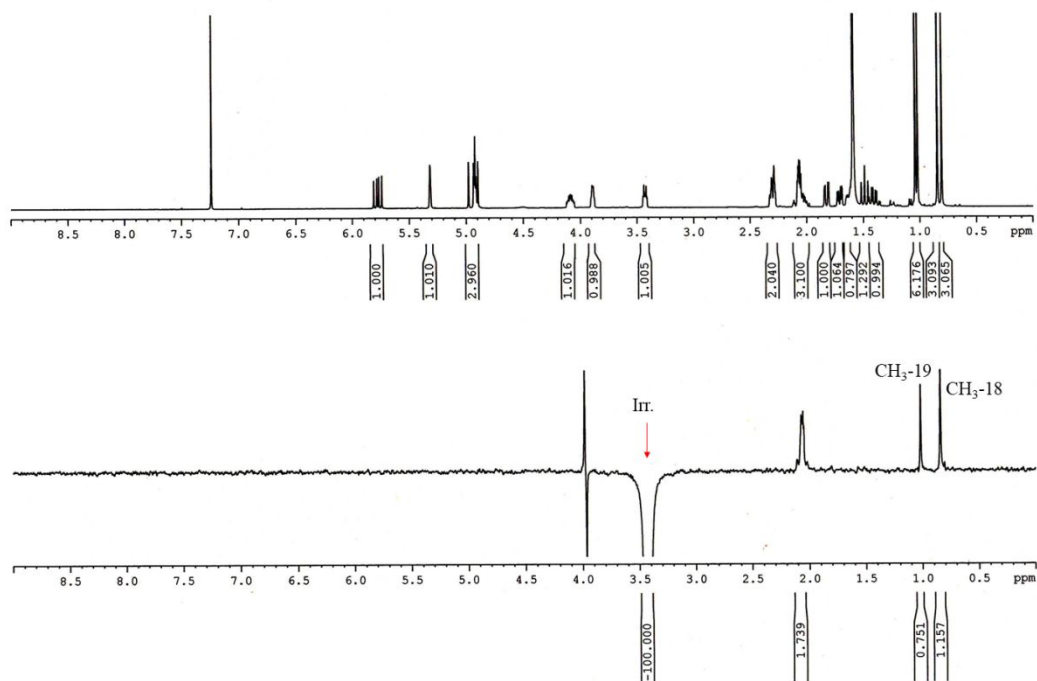


Figure S21. Difference NOE of **2** irradiating H-3 in CDCl_3

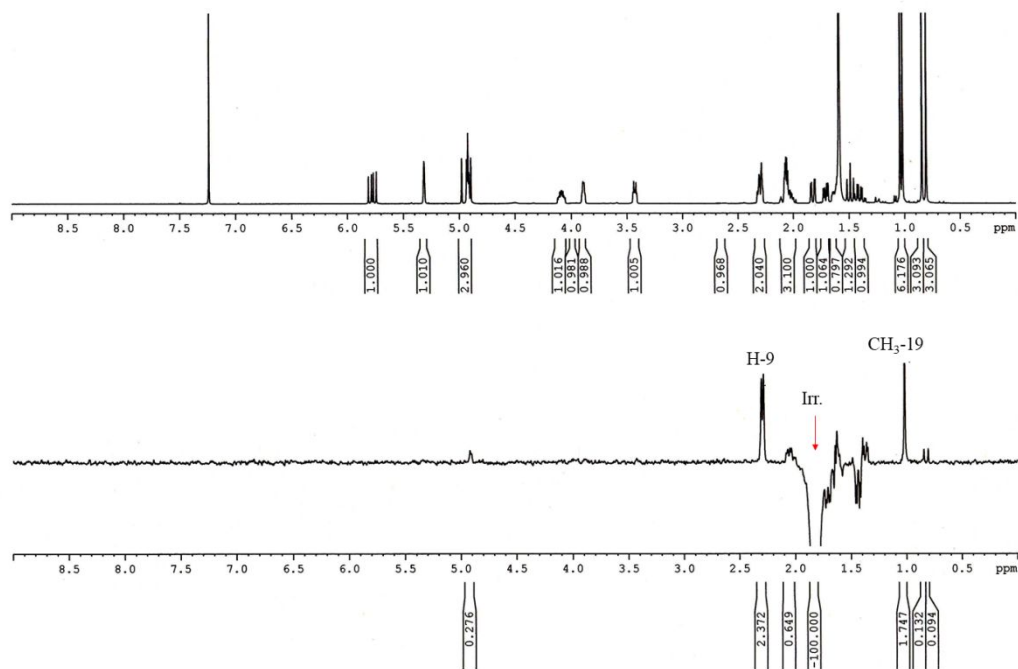


Figure S22. Difference NOE of **2** irradiating H-5 in CDCl_3

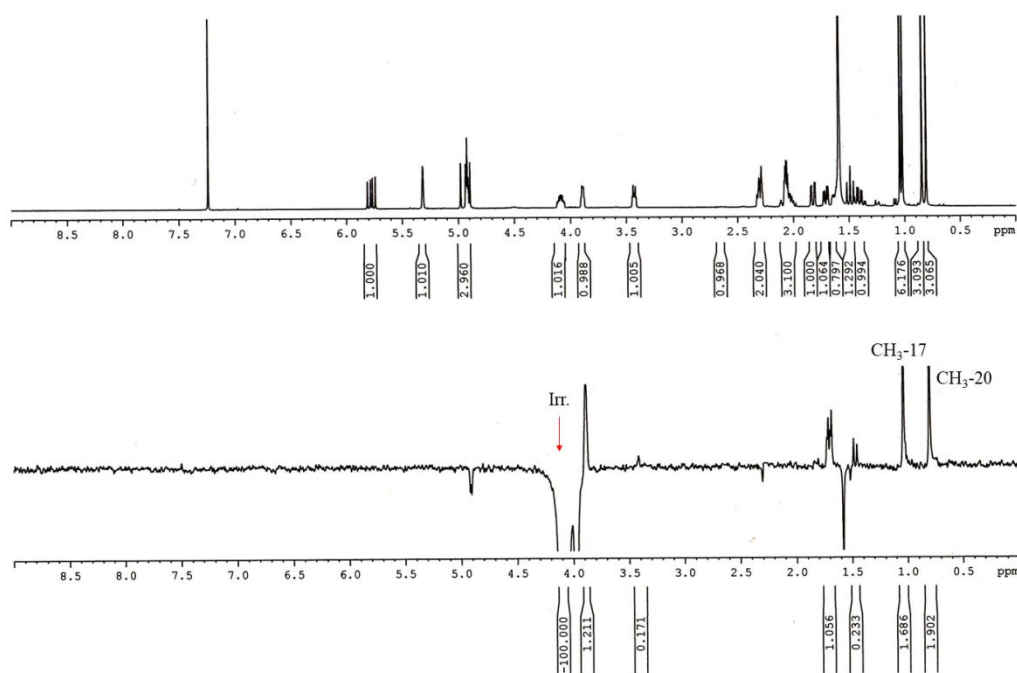


Figure S23. Difference NOE of **2** irradiating H-11 in CDCl_3

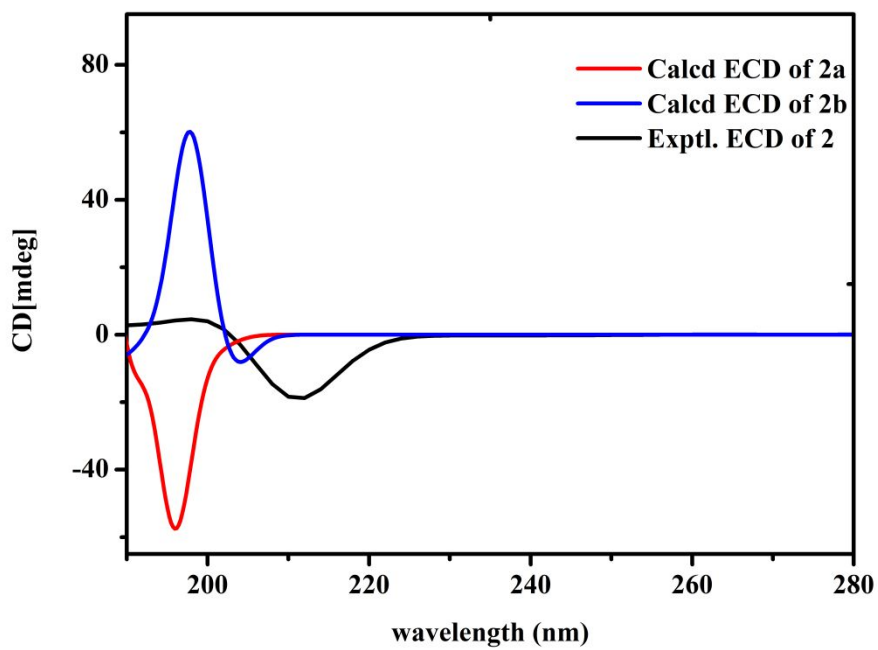


Figure S24. Calculated ECD spectra of (1*S*, 3*R*, 5*S*, 9*S*, 10*S*, 11*R*, 13*R*)-**2a** and (1*R*, 3*S*, 5*R*, 9*R*, 10*R*, 11*S*, 13*S*)-**2b** isomers and the experimental ECD spectrum of **2** in MeOH

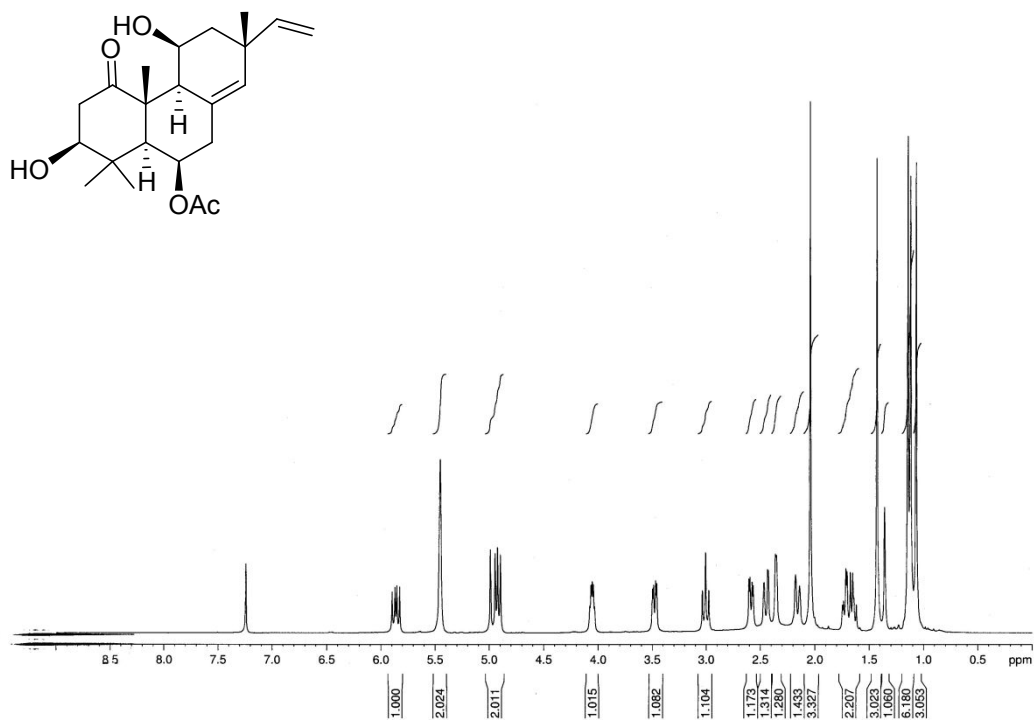


Figure S25. ¹H NMR spectrum (CDCl₃, 400 MHz) of marginaol C (3)

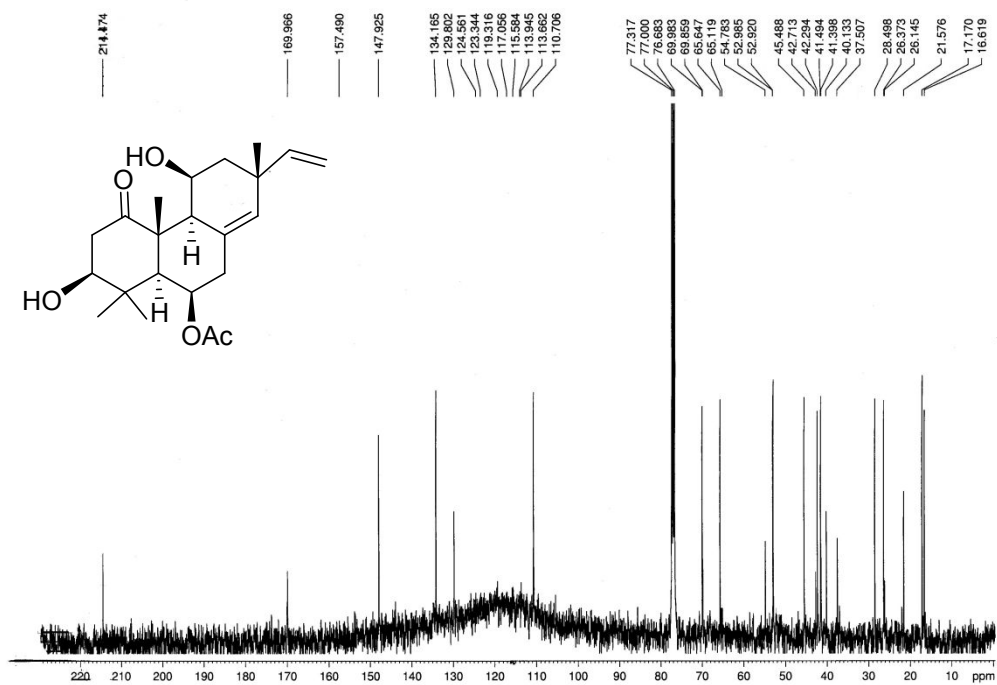


Figure S26. ¹³C NMR spectrum (CDCl₃, 100 MHz) of marginaol C (3)

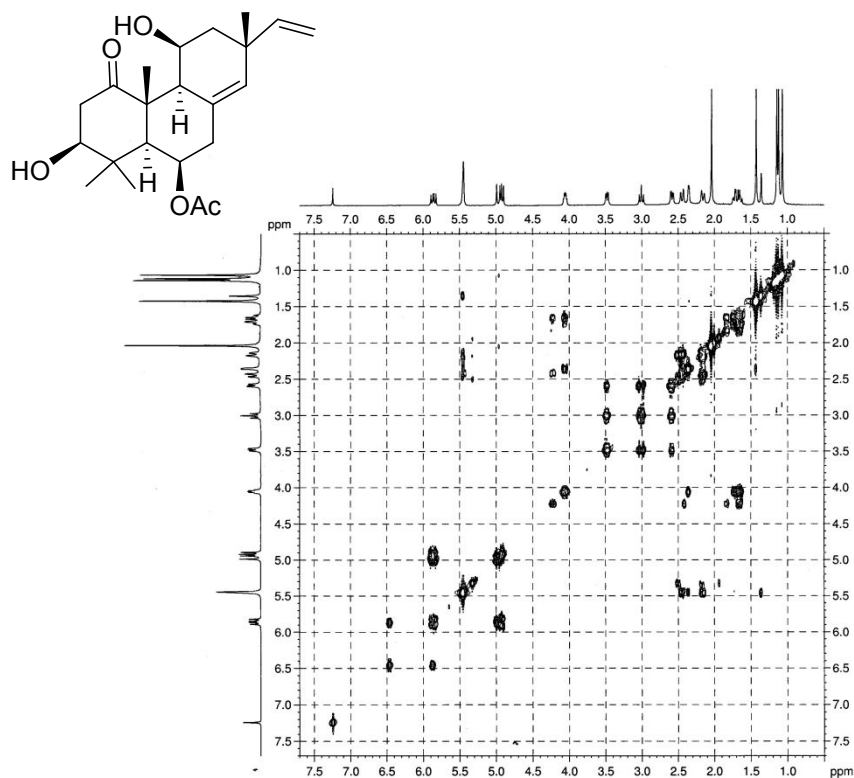


Figure S27. COSY spectrum of marginaol C (3) in CDCl₃

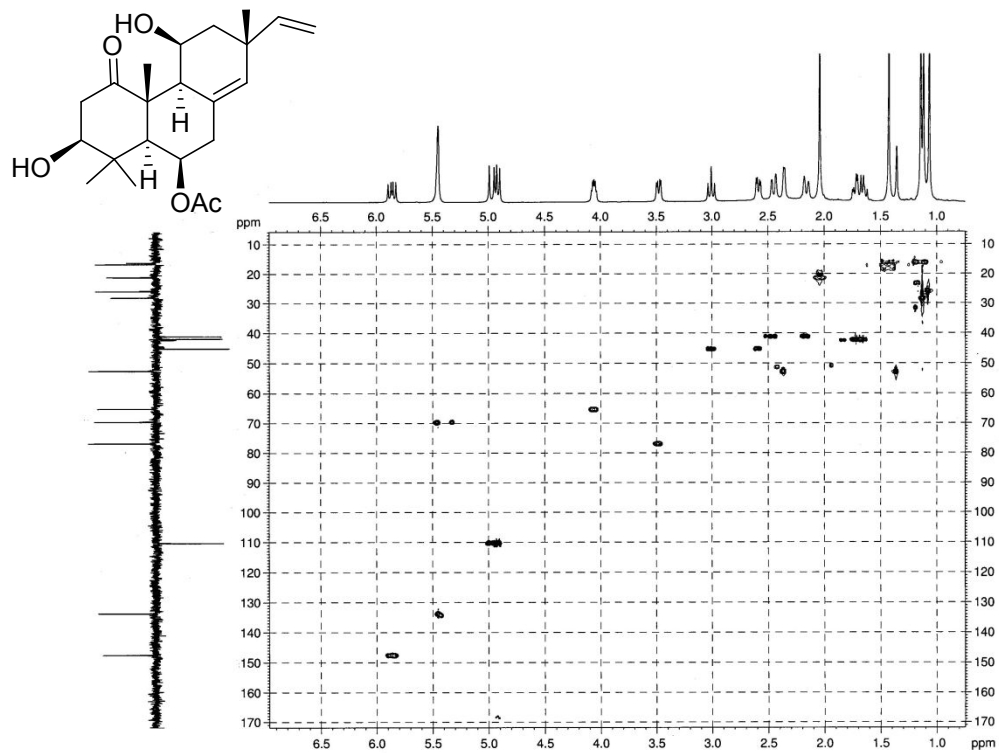


Figure S28. HMQC spectrum of marginaol C (3) in CDCl₃

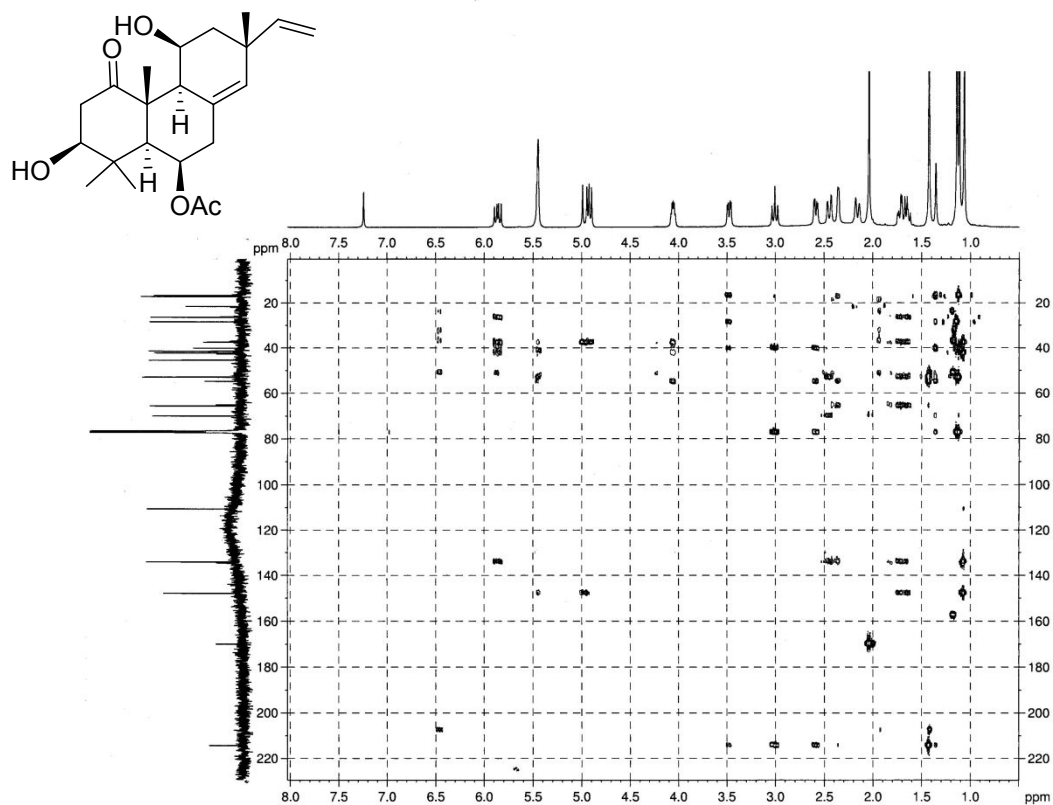


Figure S29. HMBC spectrum marginaol C (**3**) in CDCl_3

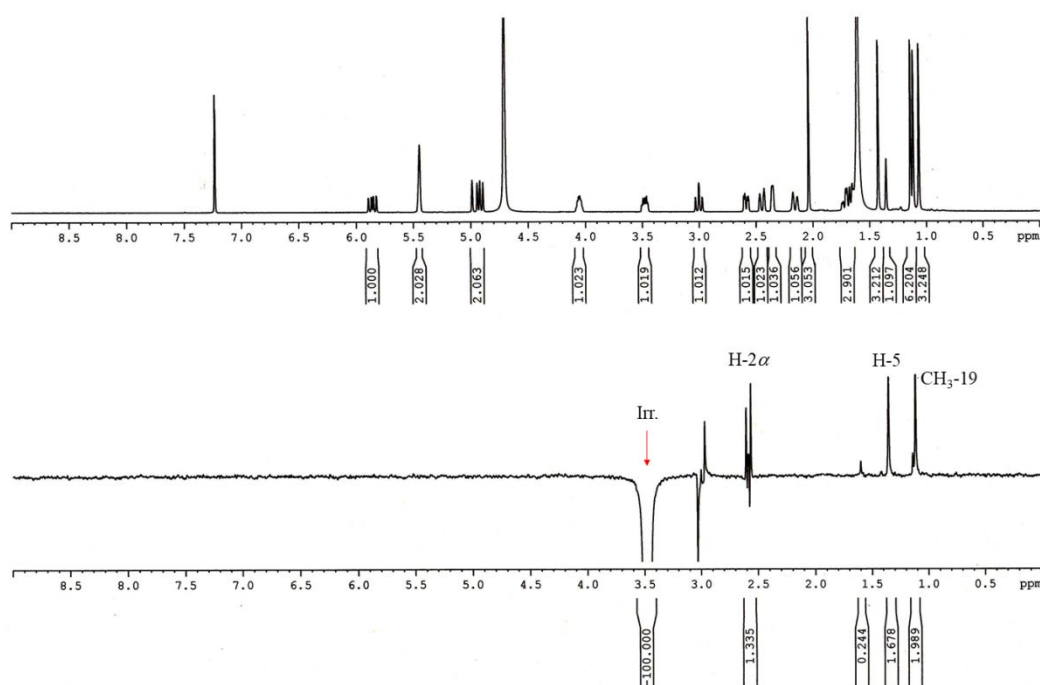


Figure S30. Difference NOE of **3** irradiating H-3 in CDCl_3

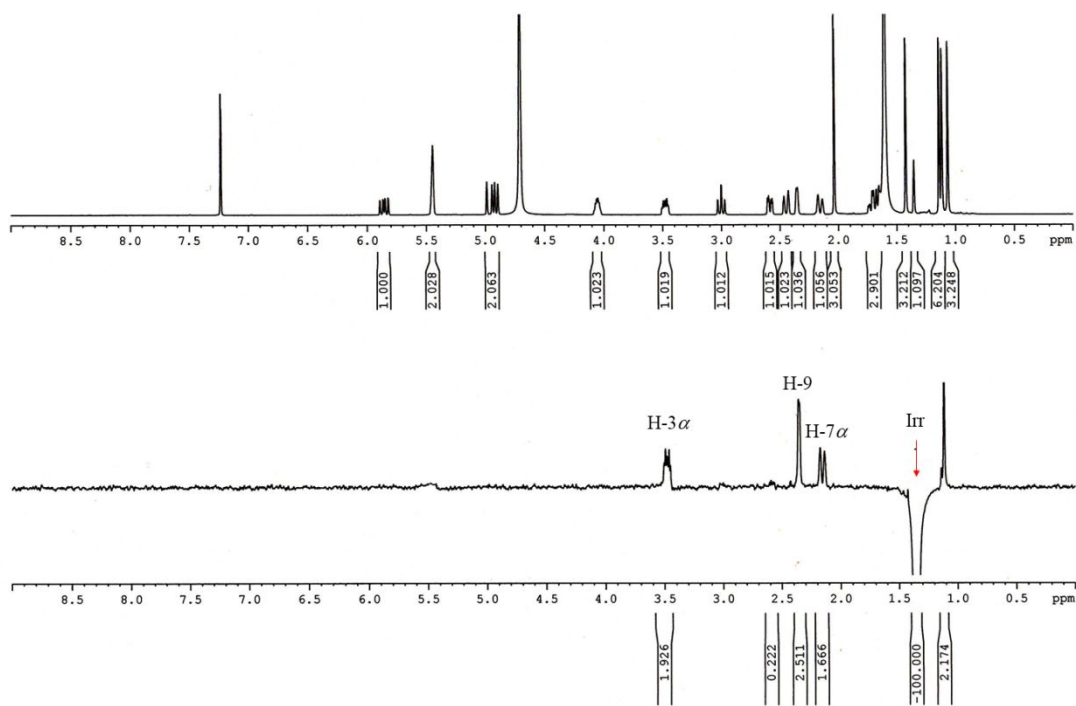


Figure S31. Difference NOE of **3** irradiating H-5 in CDCl_3

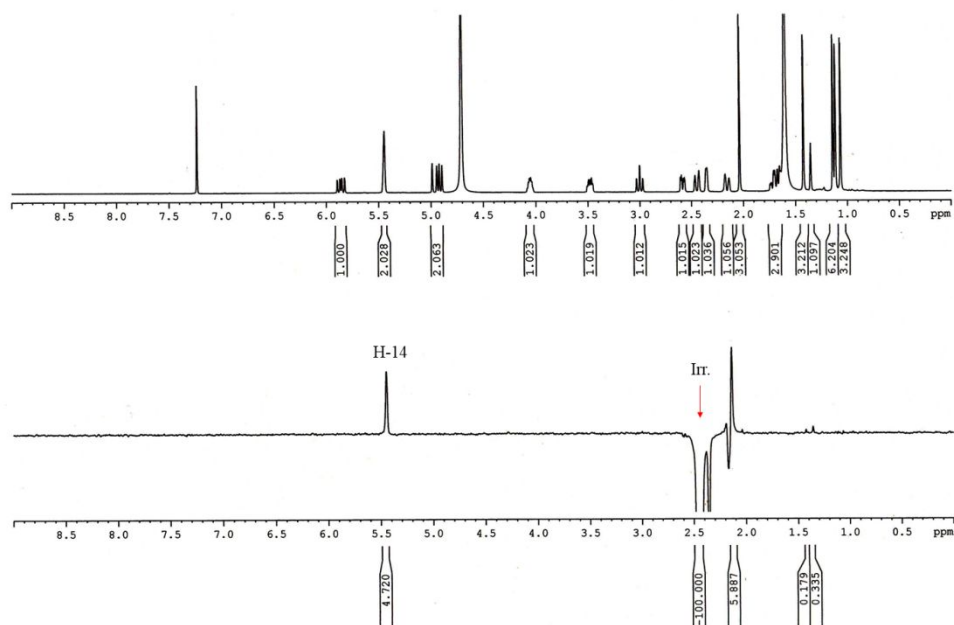


Figure S32. Difference NOE of **3** irradiating H-7 β in CDCl_3

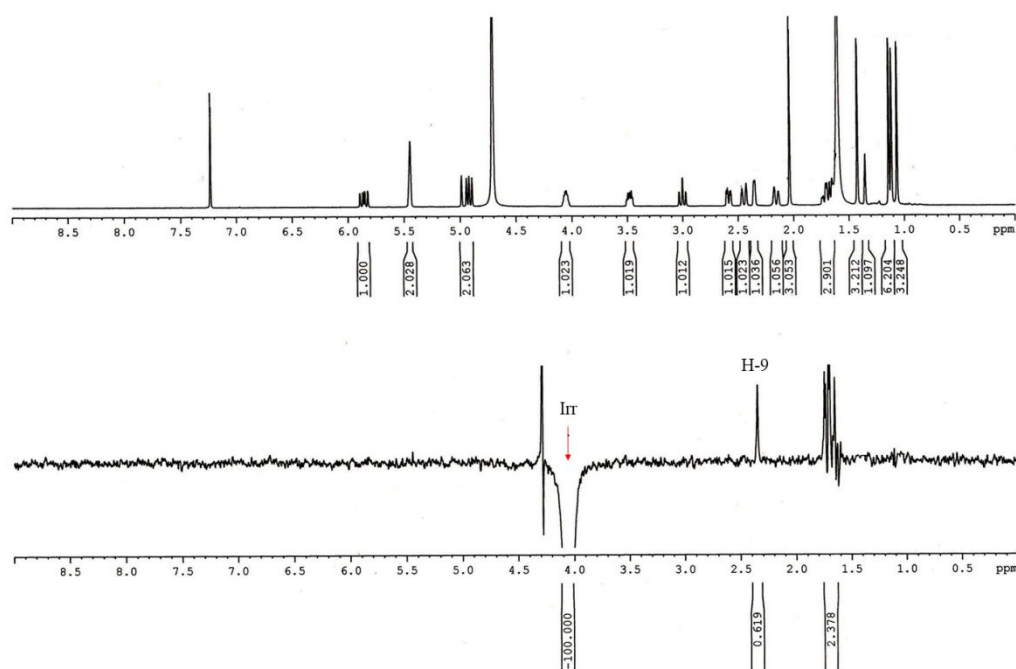


Figure S33. Difference NOE of **3** irradiating H-11 in CDCl_3

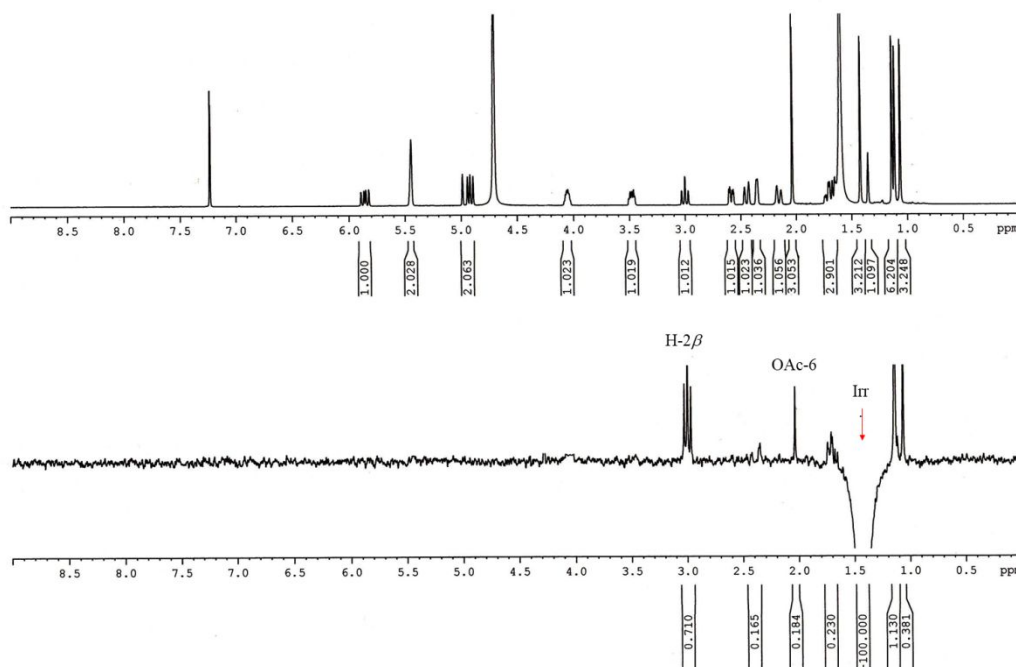


Figure S34. Difference NOE of **3** irradiating H₃-20 in CDCl_3

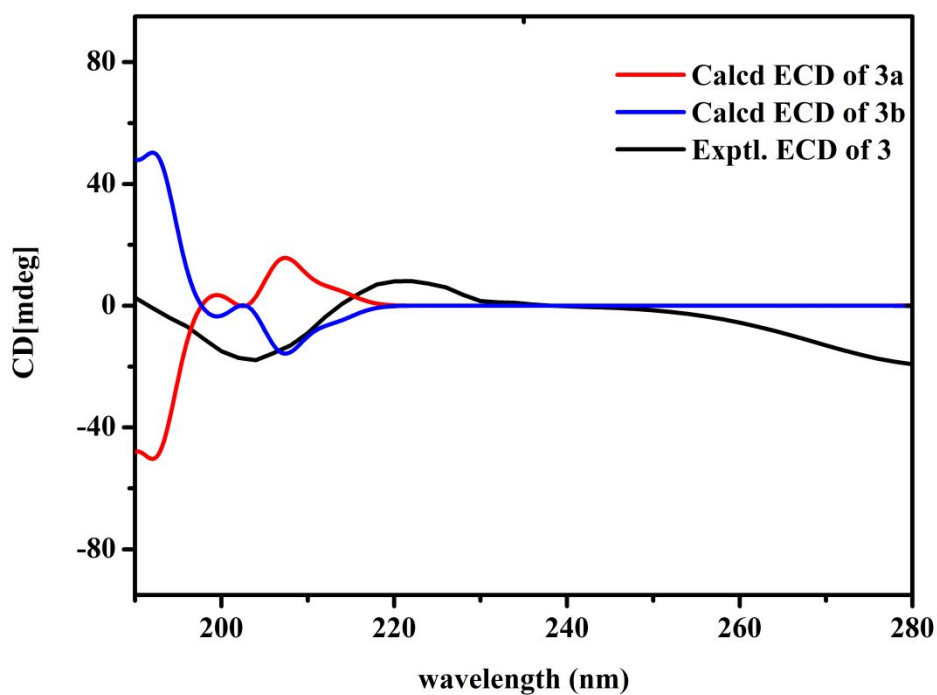


Figure S35. Calculated ECD spectra of (3*S*, 5*S*, 6*R*, 9*S*, 10*R*, 11*S*, 13*R*)-**3a** and (3*R*, 5*R*, 6*S*, 9*R*, 10*S*, 11*R*, 13*S*)-**3b** isomers and the experimental ECD spectrum of **3** in MeOH

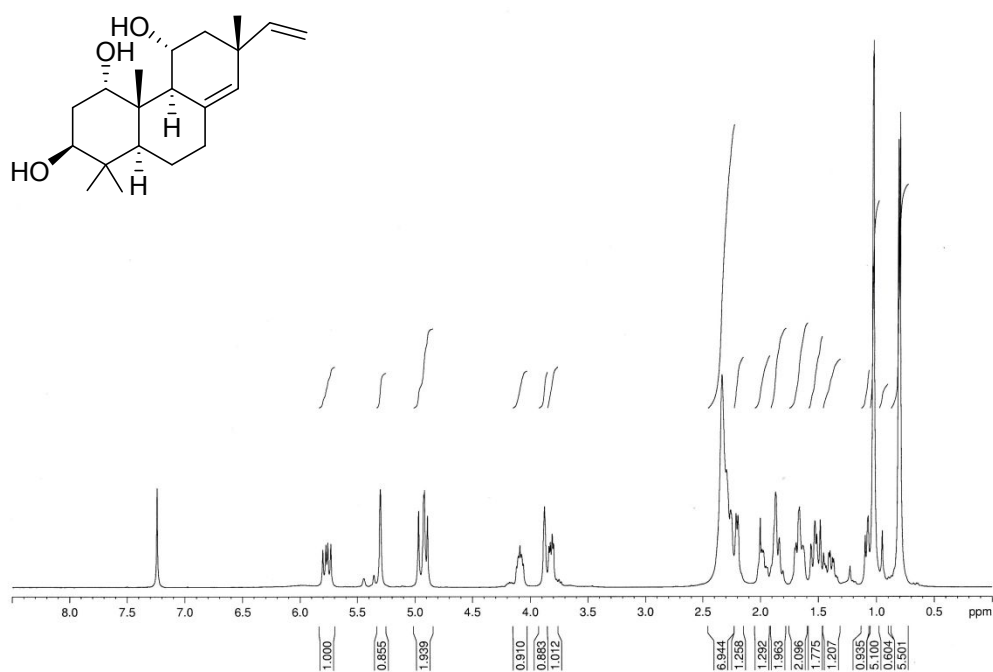


Figure S36. ^1H NMR spectrum (CDCl_3 , 400 MHz) of marginaol D (**4**)

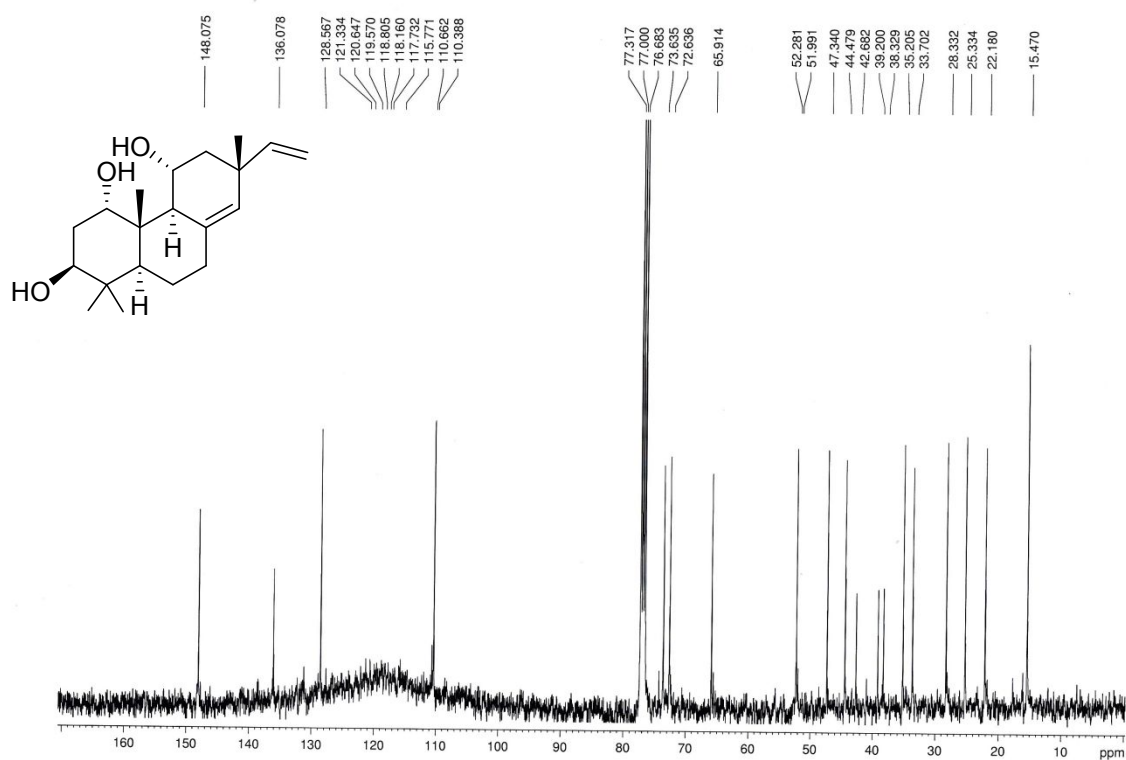


Figure S37. ¹³C NMR spectrum (CDCl₃, 100 MHz) of marginaol D (4)

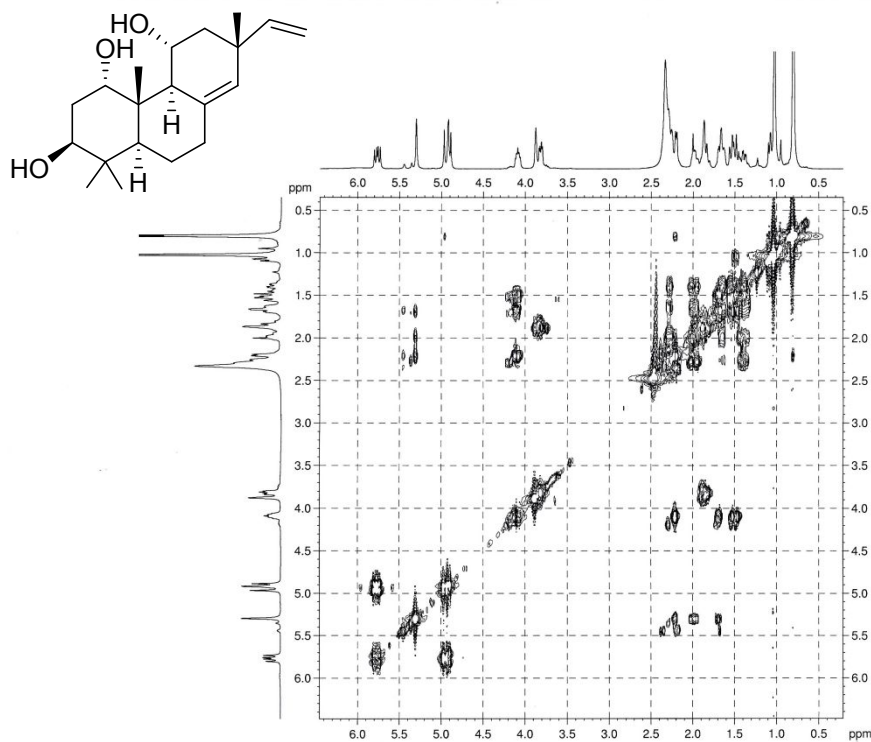


Figure S38. COSY spectrum of marginaol D (4) in CDCl₃

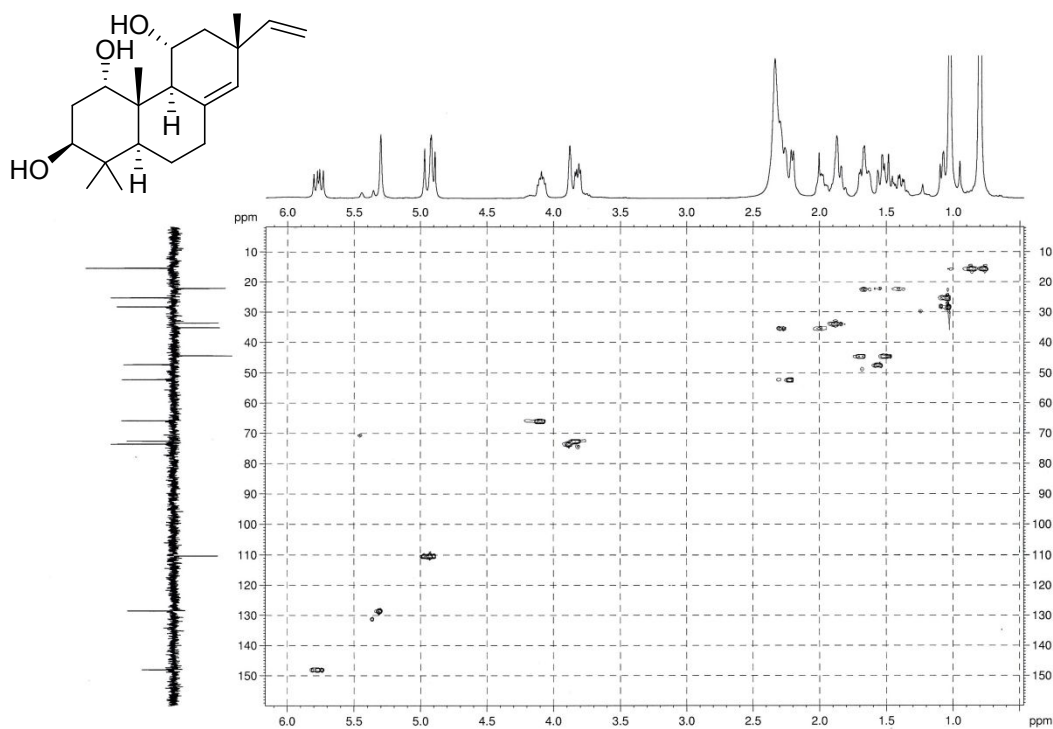


Figure S39. HMQC spectrum of marginaol D (4) in CDCl₃

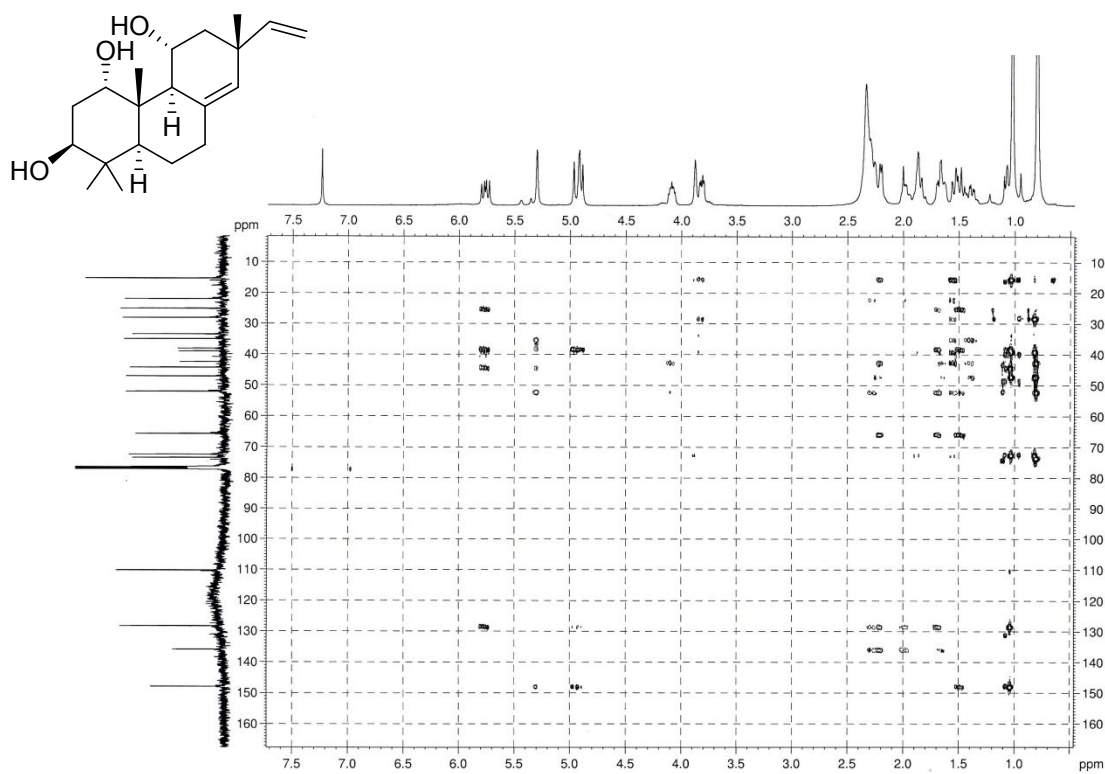


Figure S40. HMBC spectrum of marginaol D (4) in CDCl₃

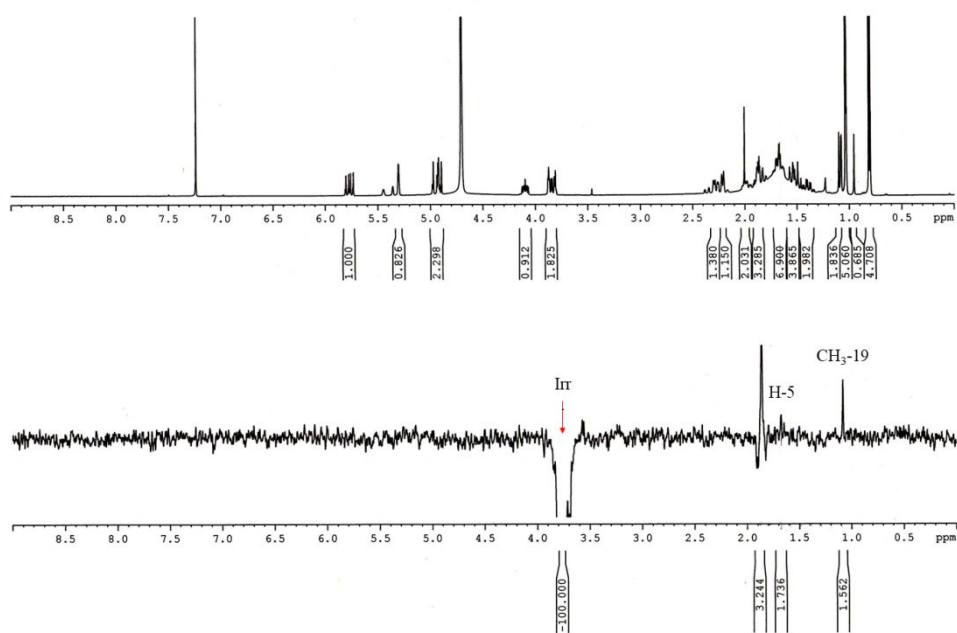


Figure S41. Difference NOE of **4** irradiating H-3 in CDCl_3

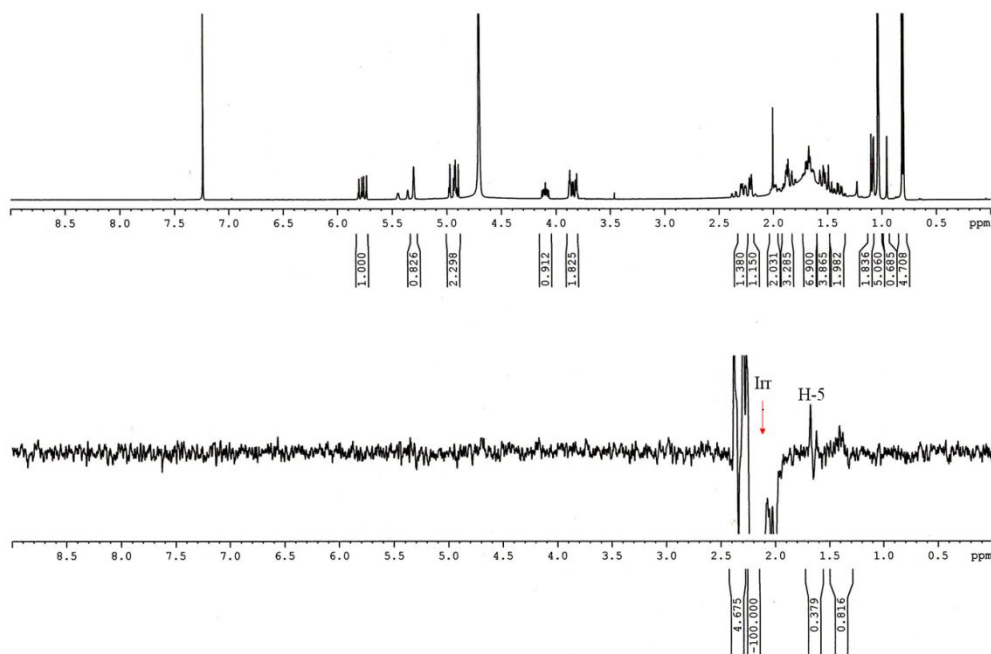


Figure S42. Difference NOE of **4** irradiating H-9 in CDCl_3

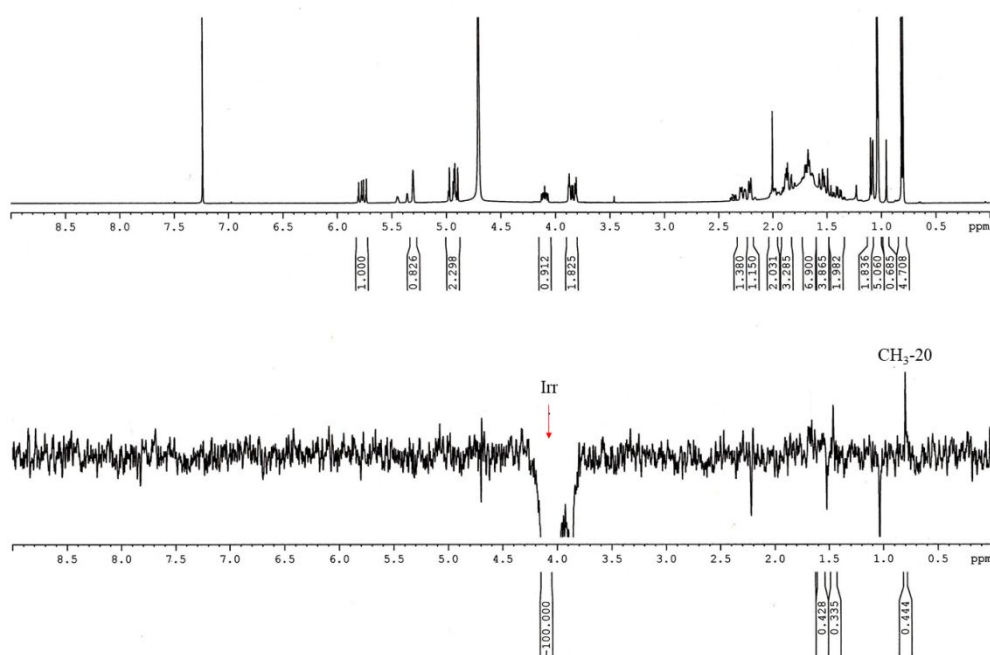


Figure S43. Difference NOE of **4** irradiating H-11 in CDCl_3

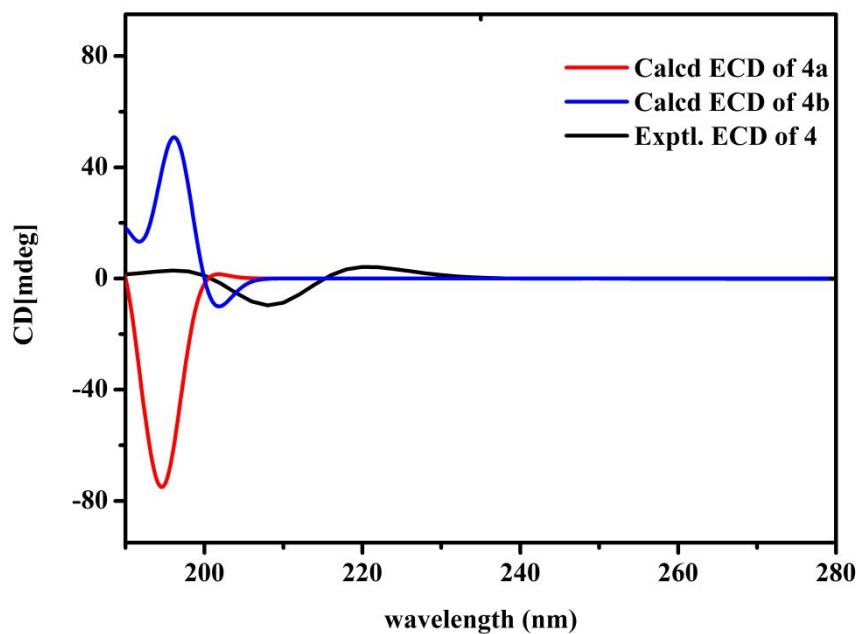


Figure S44. Calculated ECD spectra of (1*S*, 3*S*, 5*S*, 9*S*, 10*S*, 11*R*, 13*R*)-**4a** and (1*R*, 3*R*, 5*R*, 9*R*, 10*R*, 11*S*, 13*S*)-**4b** isomers and the experimental ECD spectrum of **4** in MeOH

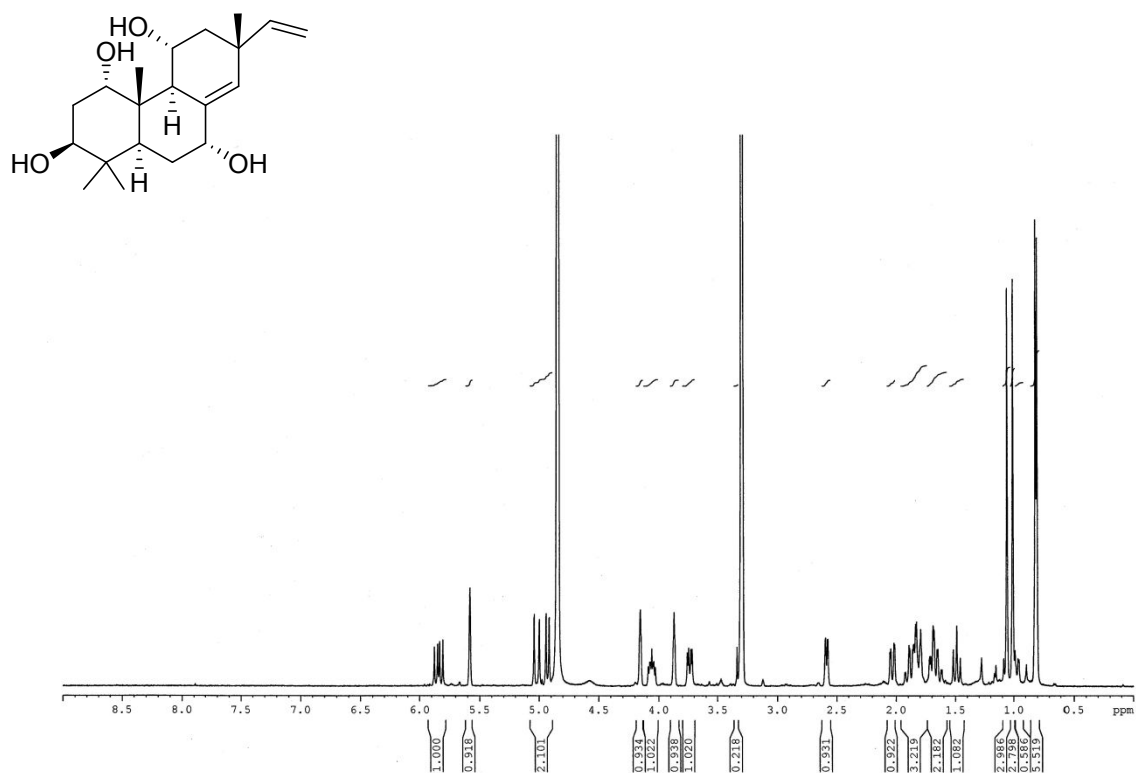


Figure S45. ¹H NMR spectrum (CD₃OD, 400 MHz) of marginaol E (5)

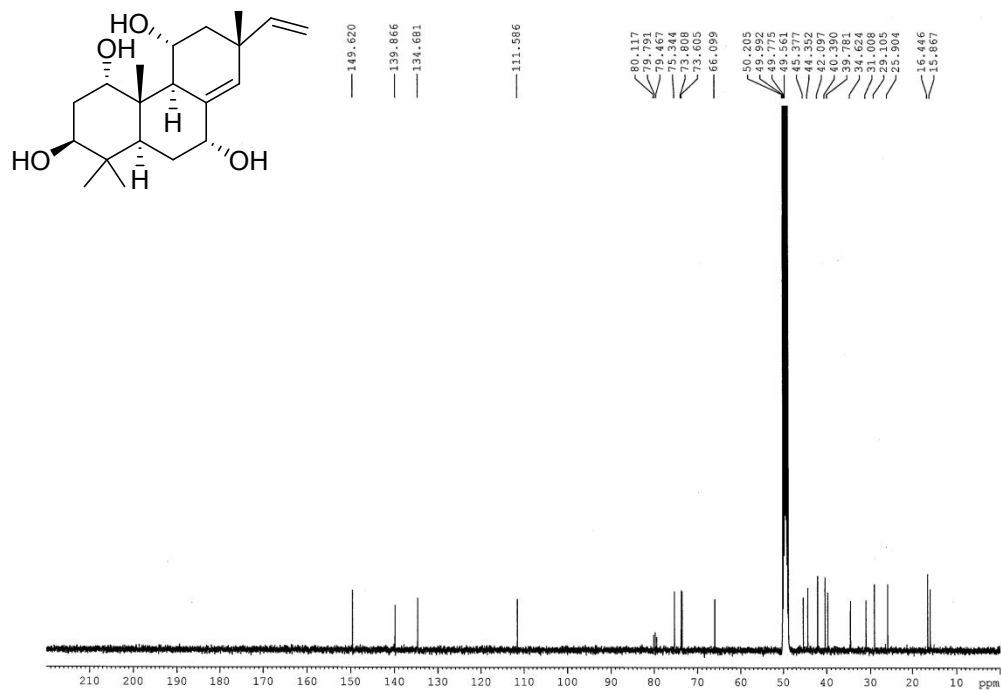


Figure S46. ¹³C NMR spectrum (CD₃OD, 100 MHz) of marginaol E (5)

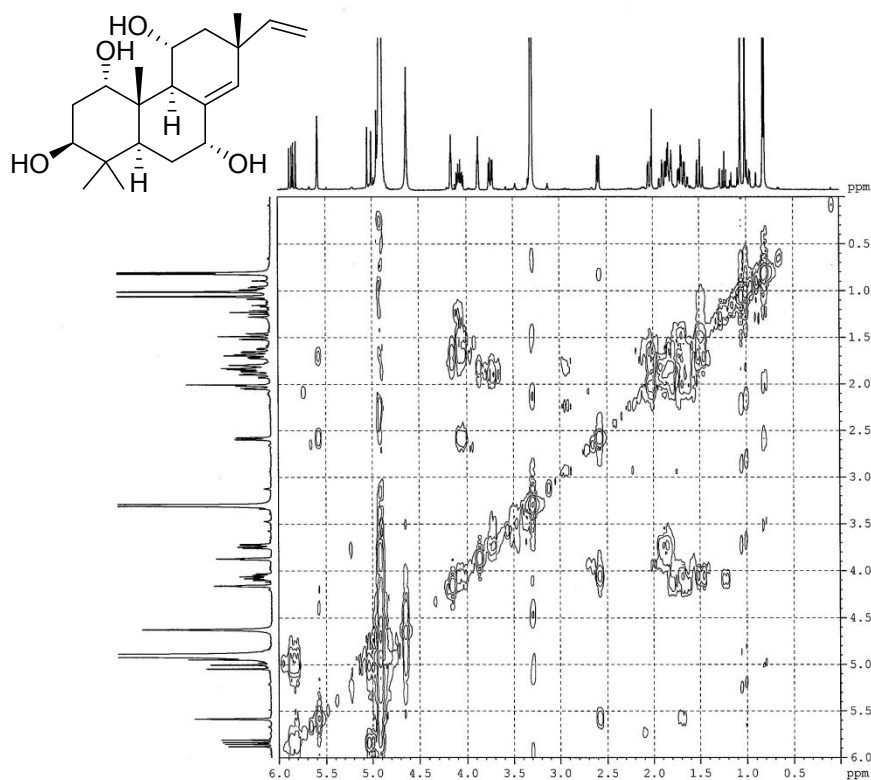


Figure S47. COSY spectrum of marginaol E (5) in CD₃OD

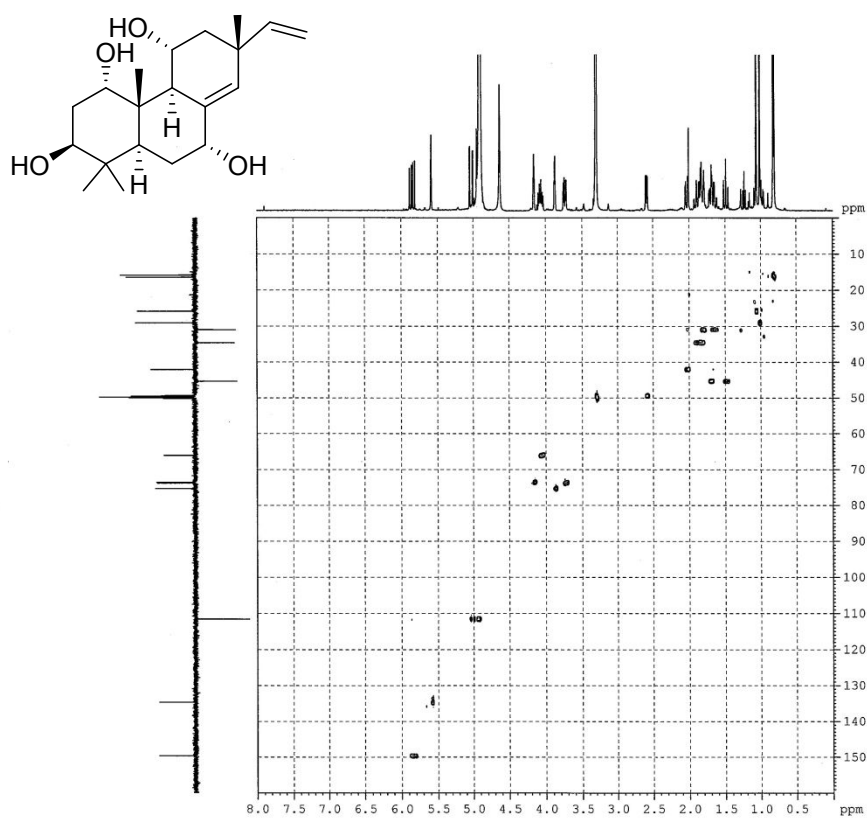


Figure S48. HMQC spectrum of marginaol E (5) in CD₃OD

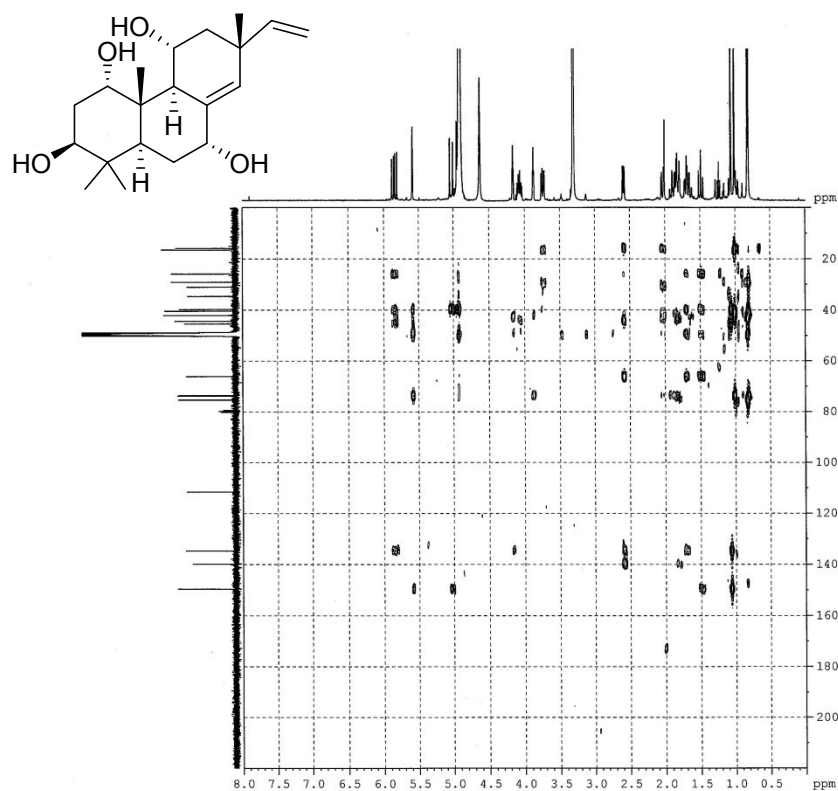


Figure S49. HMBC spectrum of marginaol E (**5**) in CD₃OD

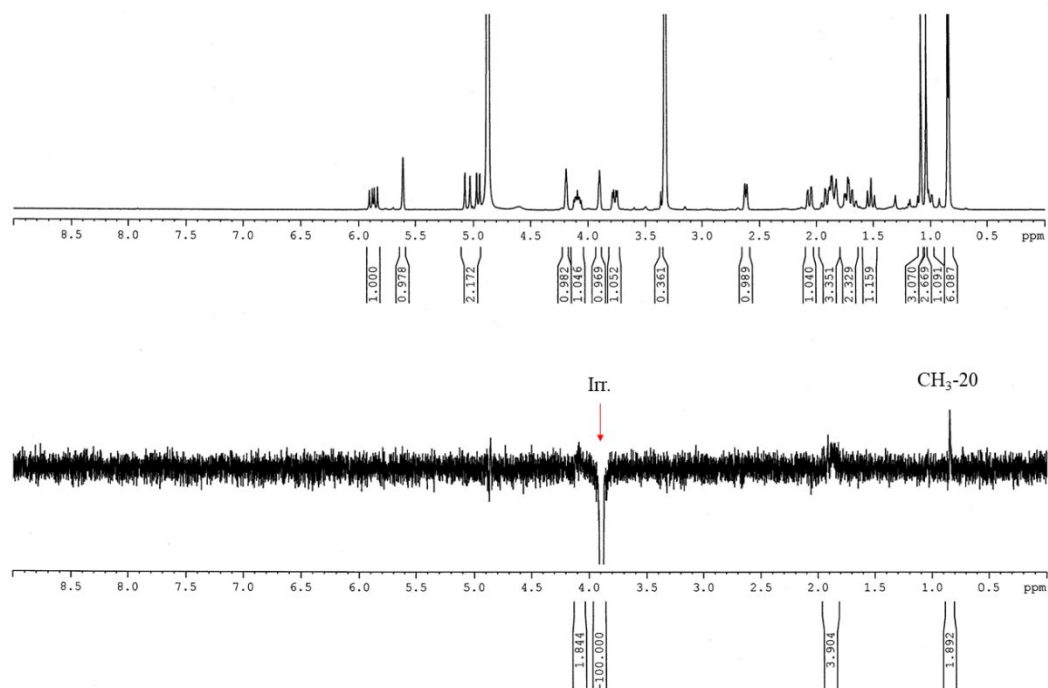


Figure S50. Difference NOE of **5** irradiating H-1 in CD₃OD

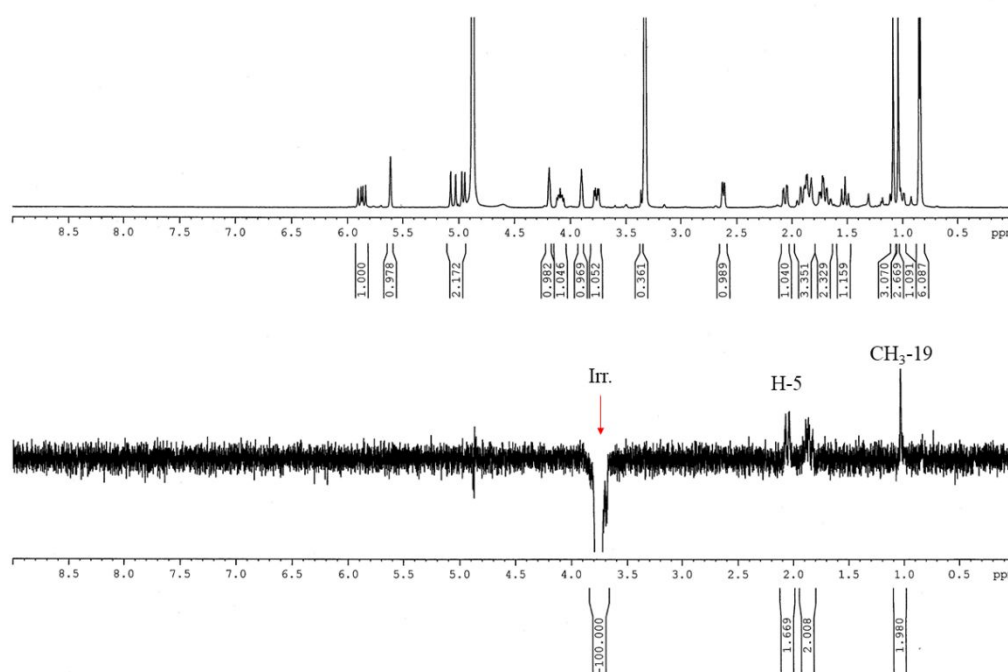


Figure S51. Difference NOE of **5** irradiating H-3 in CD₃OD

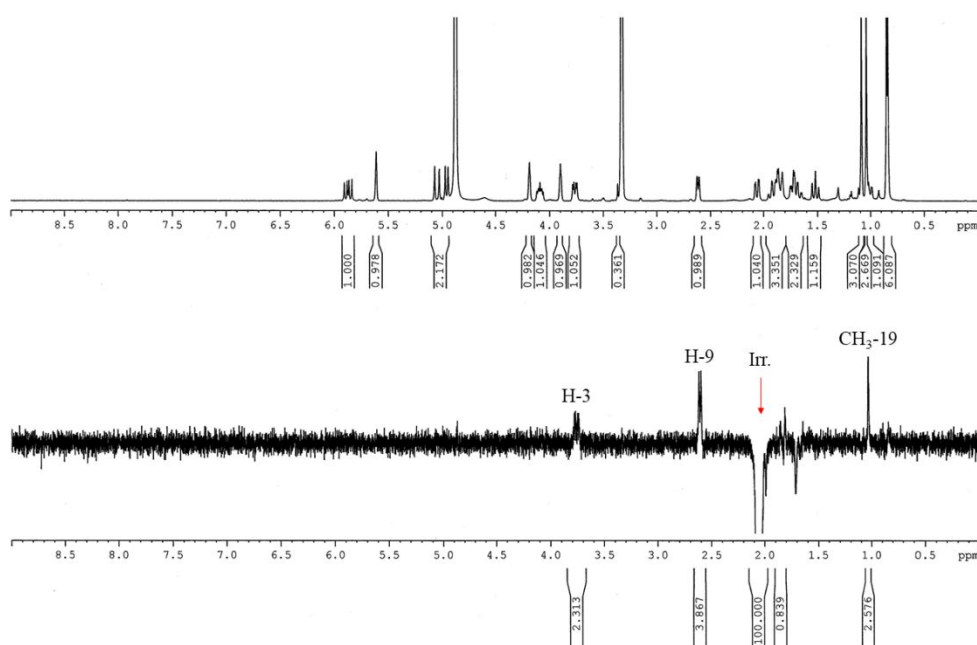


Figure S52. Difference NOE of **5** irradiating H-5 in CD₃OD

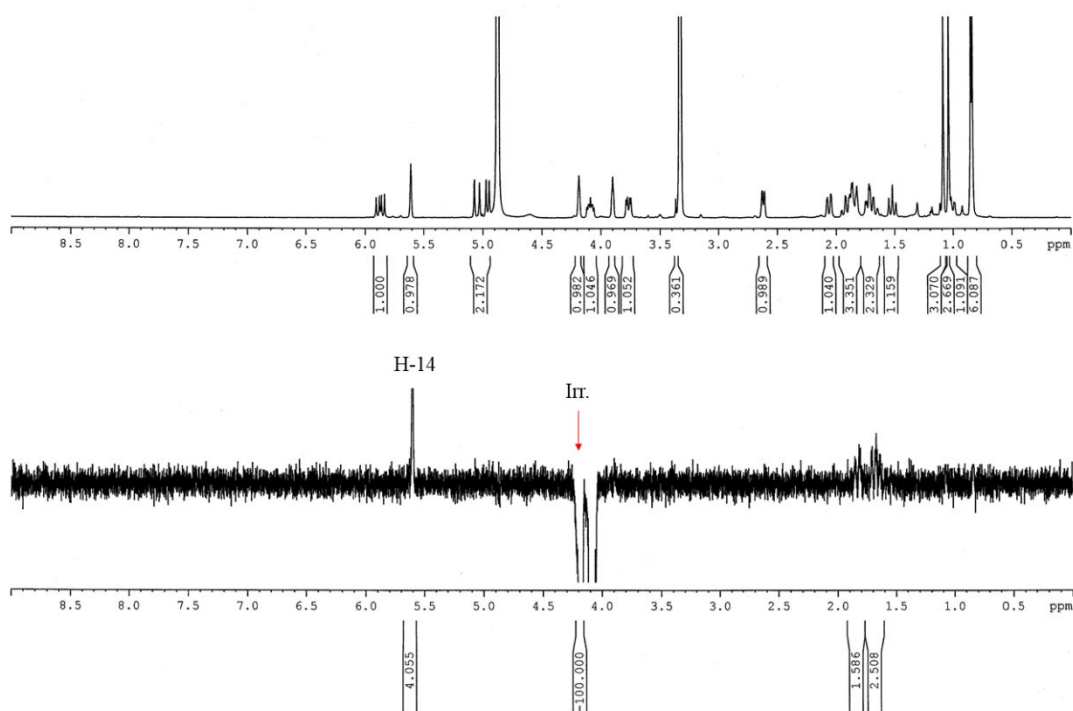


Figure S53. Difference NOE of **5** irradiating H-7 in CD_3OD

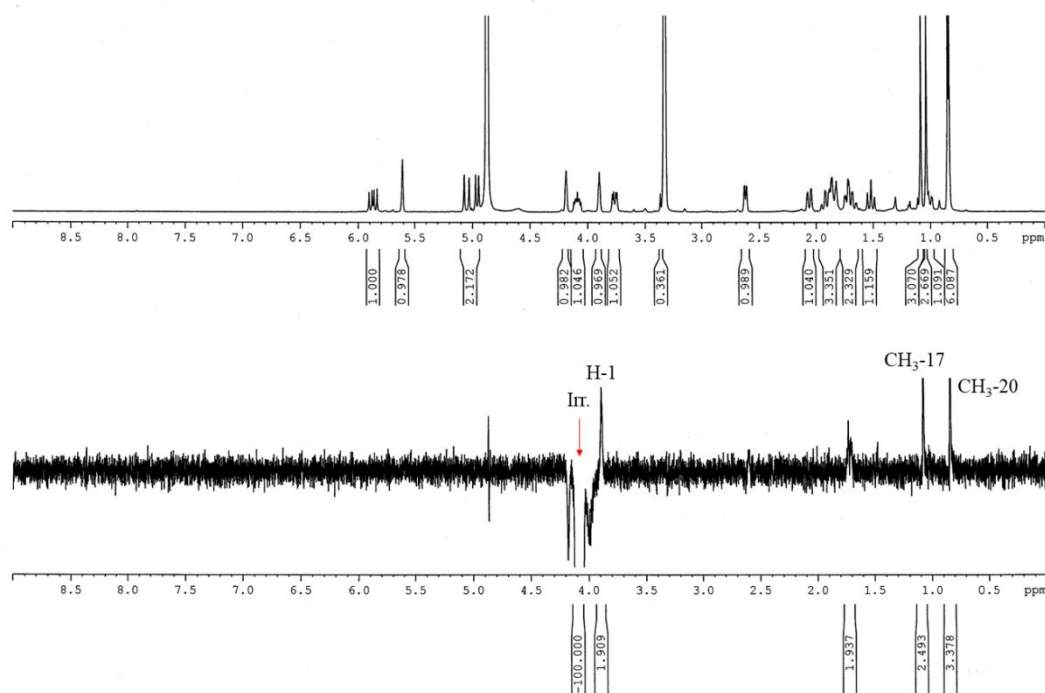


Figure S54. Difference NOE of **5** irradiating H-11 in CD_3OD

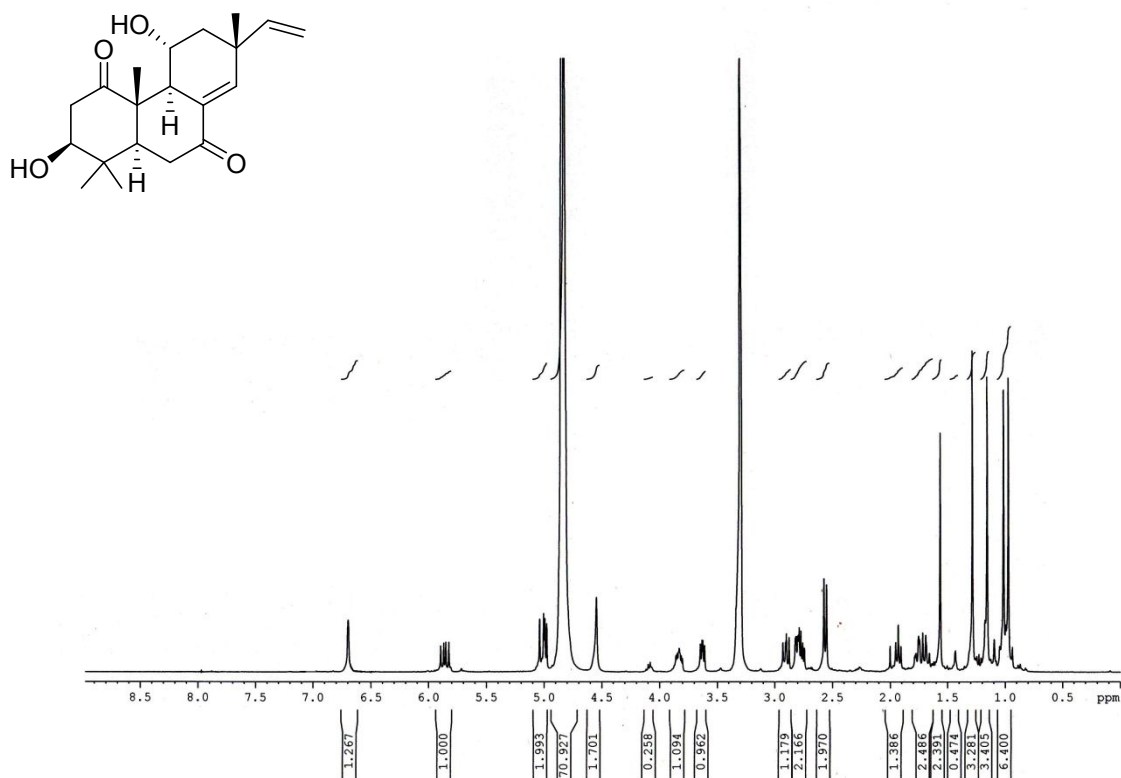


Figure S55. ¹H NMR spectrum (CD₃OD, 400 MHz) of marginaol F (6)

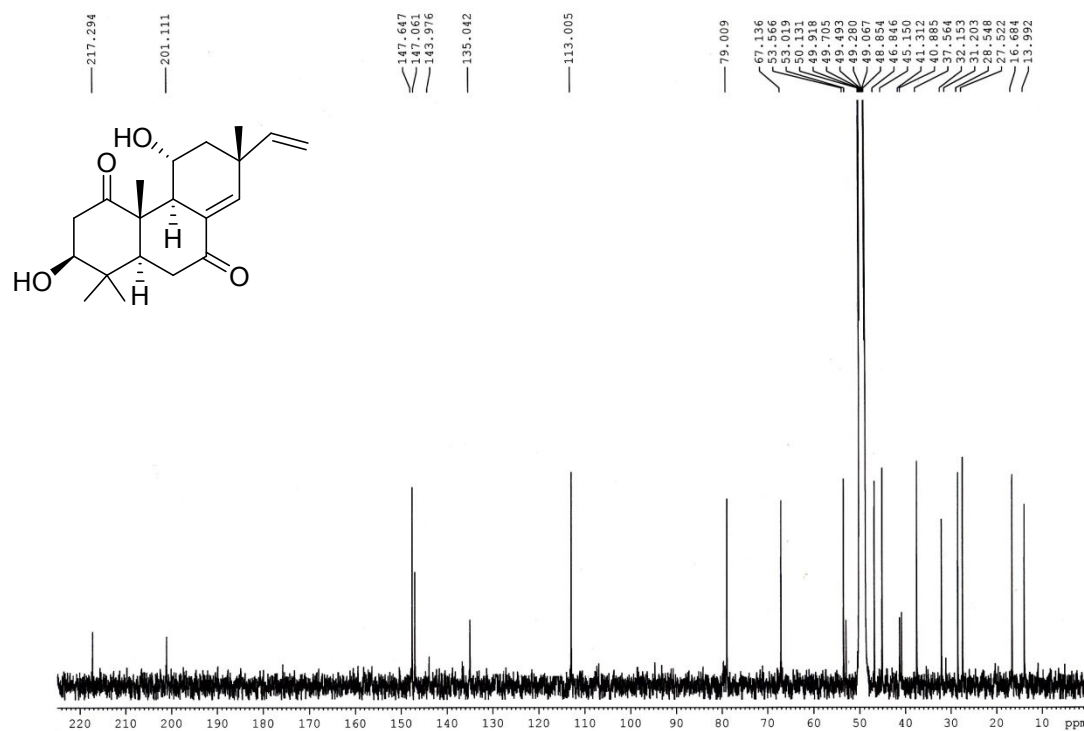


Figure S56. ¹³C NMR spectrum (CD₃OD, 100 MHz) of marginaol E (6)

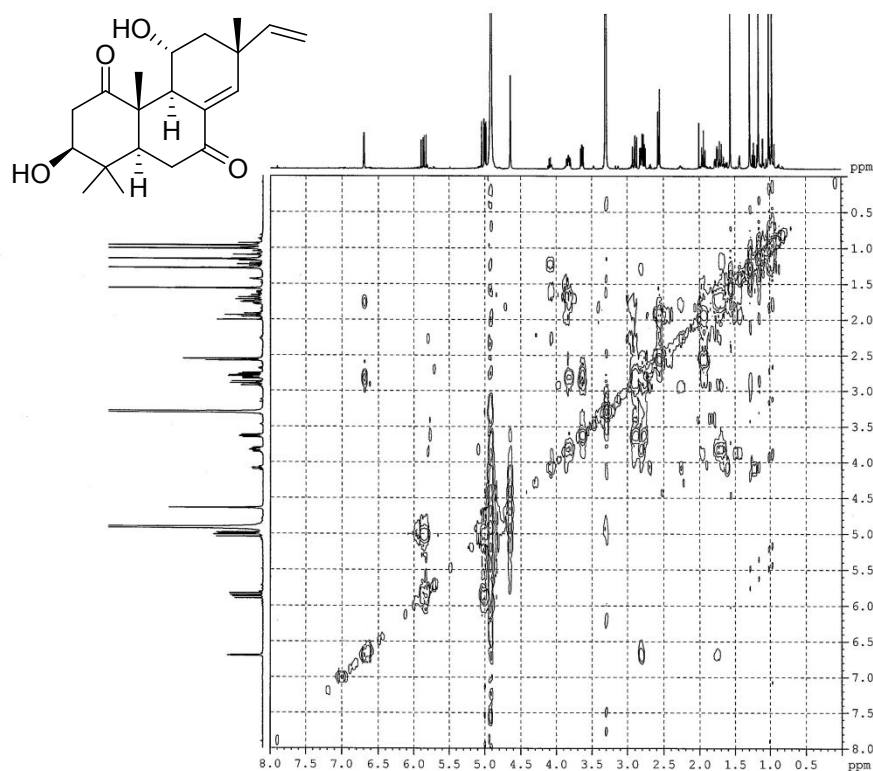


Figure S57. COSY spectrum of marginaol E (6) in CD₃OD

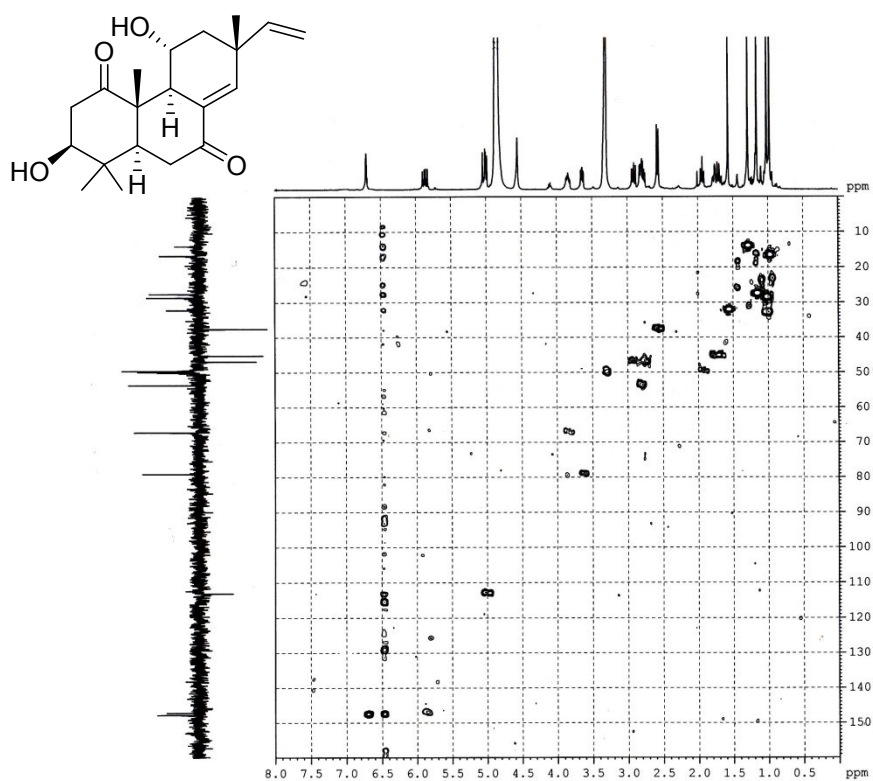


Figure S58. HMQC spectrum of marginaol E (6) in CD₃OD

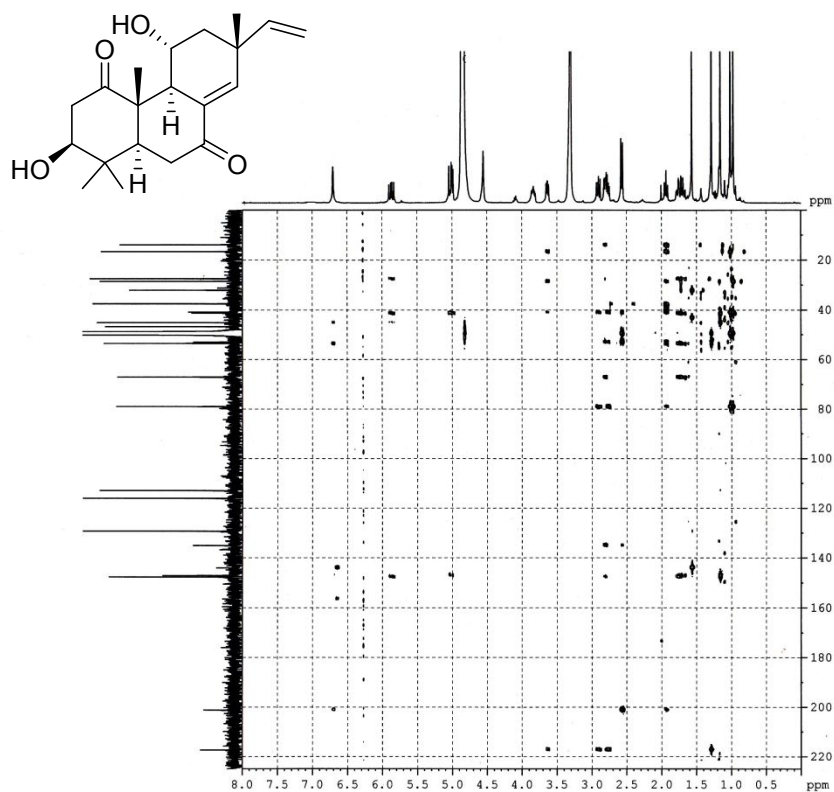


Figure S59. HMBC spectrum of marginaol E (**6**) in CD₃OD

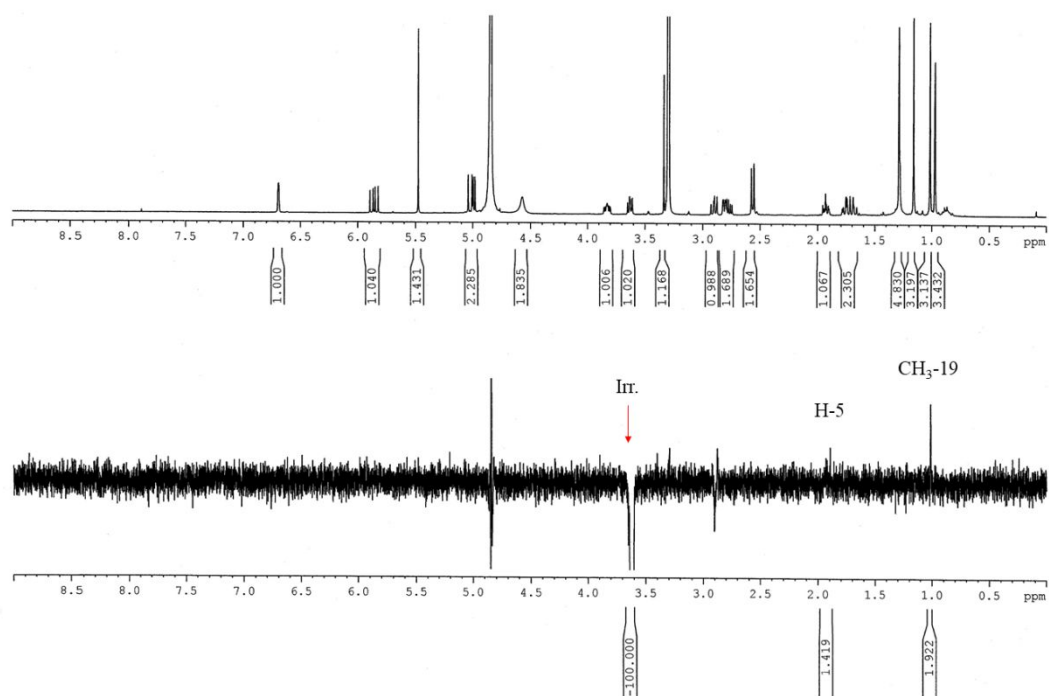


Figure S60. Difference NOE of **6** irradiating H-3 in CD₃OD

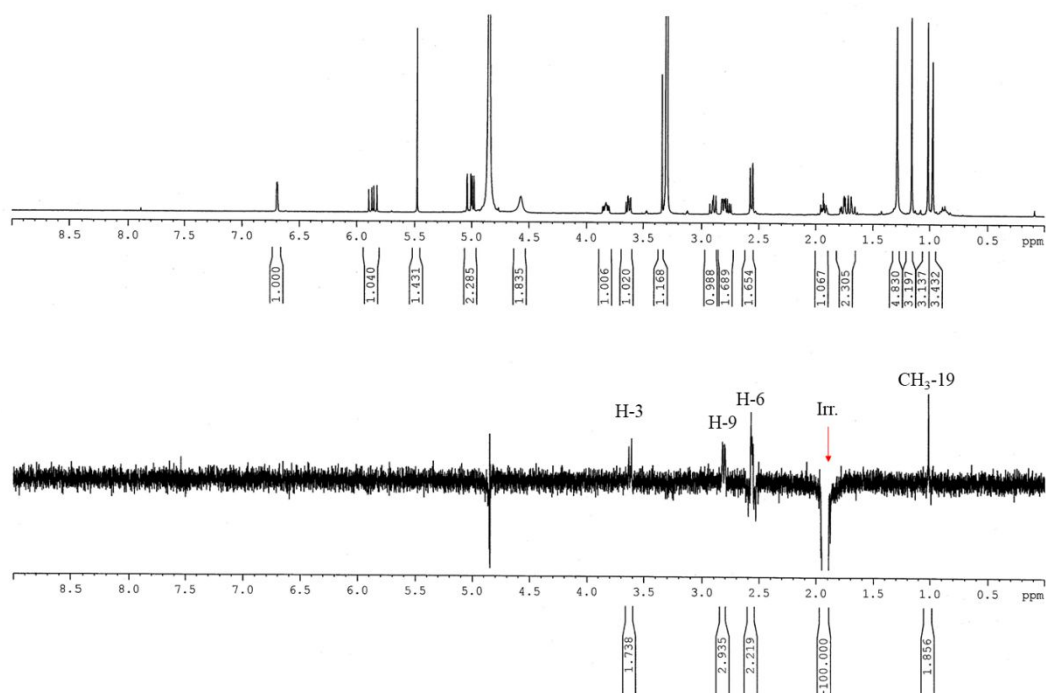


Figure S61. Difference NOE of **6** irradiating H-5 in CD_3OD

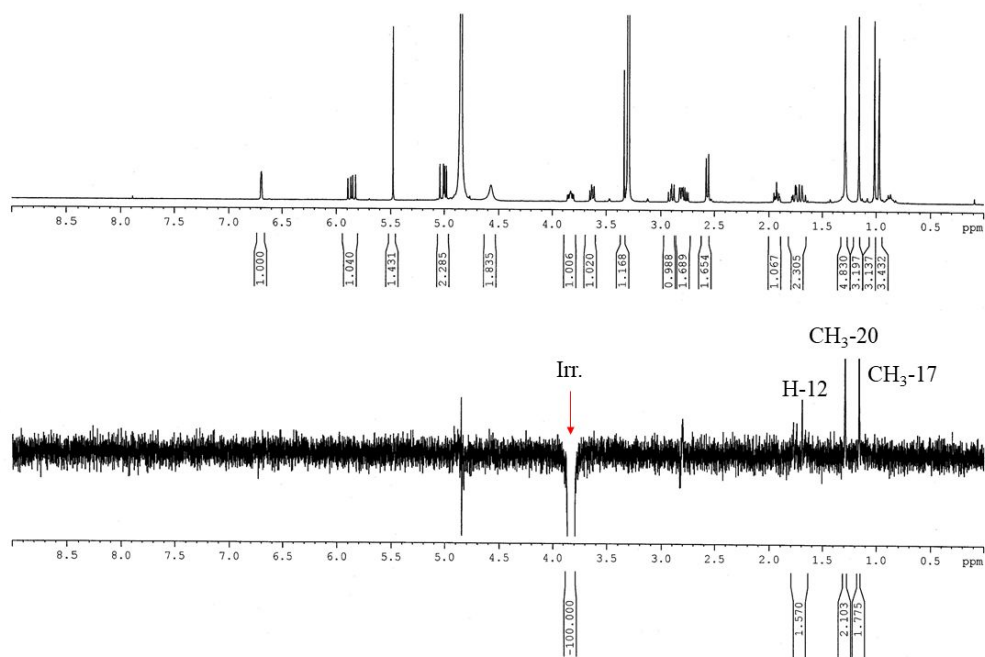


Figure S62. Difference NOE of **6** irradiating H-11 in CD_3OD