

Supplementary Information

Sesquiterpenoids of Diverse Types from the Rhizomes of *Acorus calamus*

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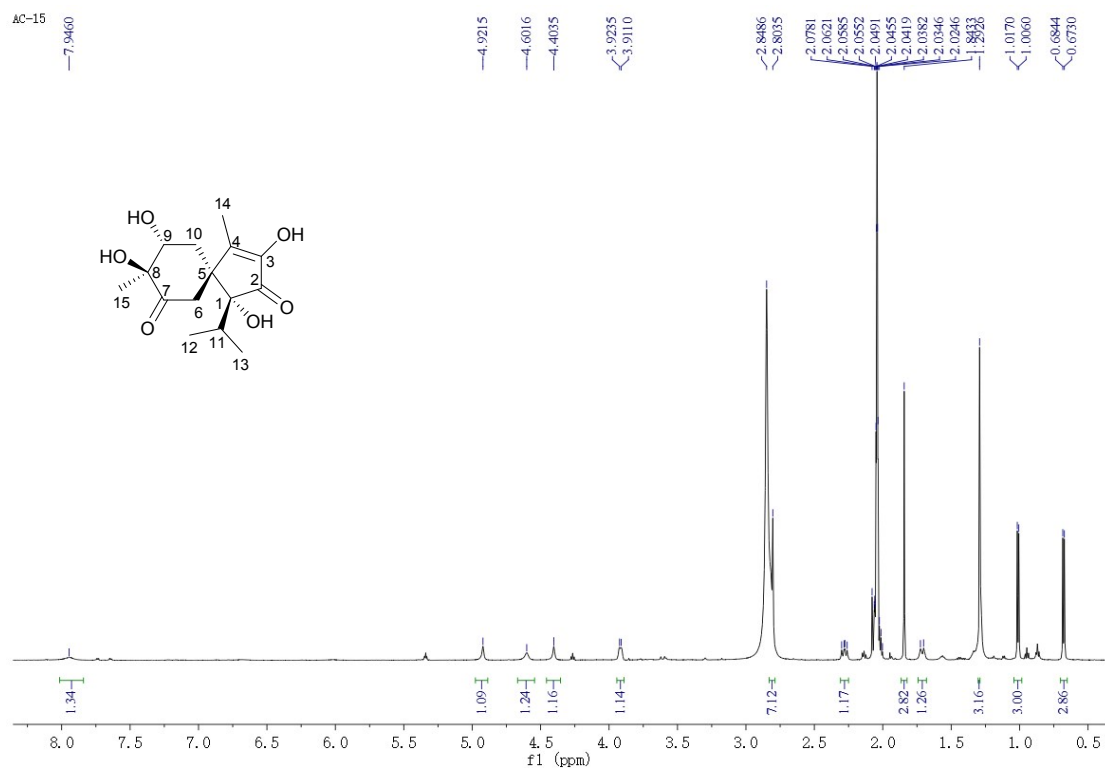


Figure S1. ^1H NMR of compound **1** (600 MHz, CD_3COCD_3)

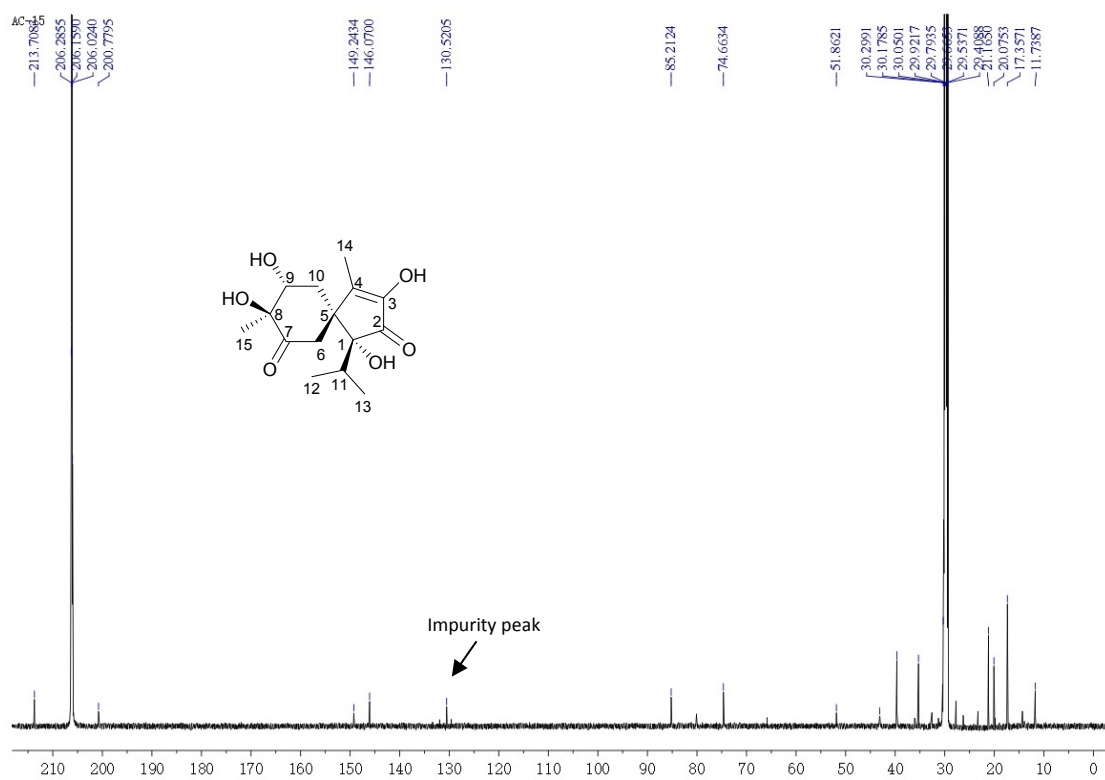


Figure S2. ^{13}C NMR of compound **1** (150 MHz, CD_3COCD_3)

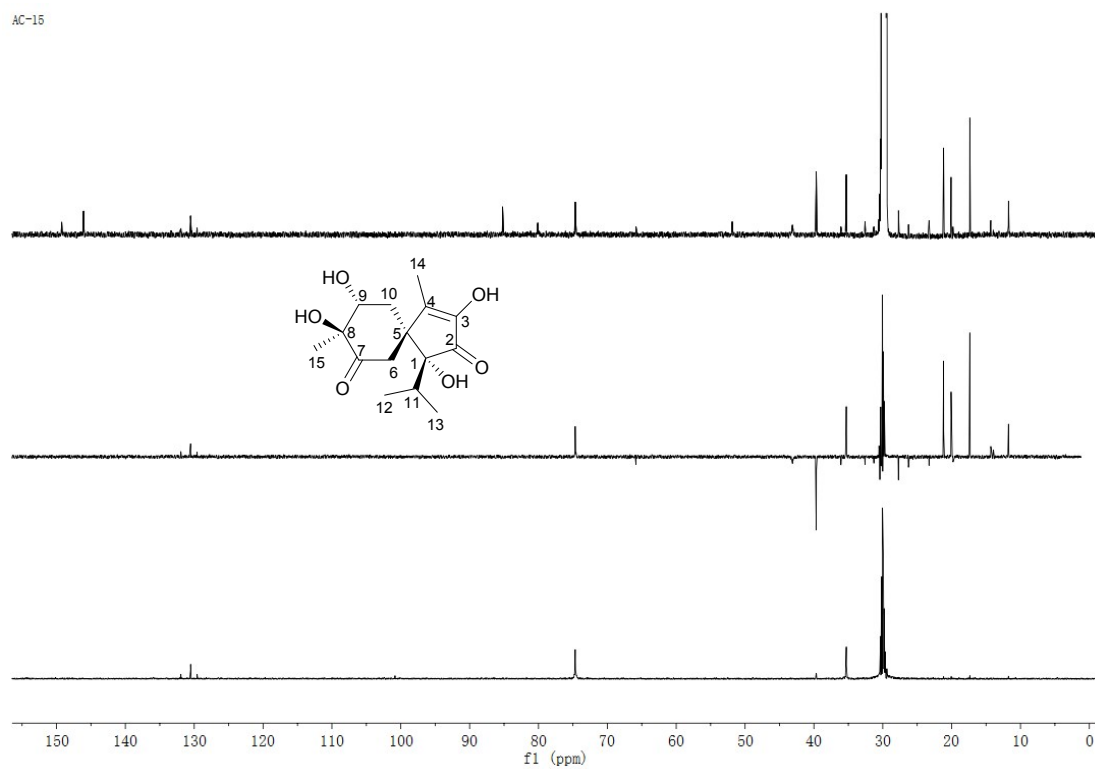
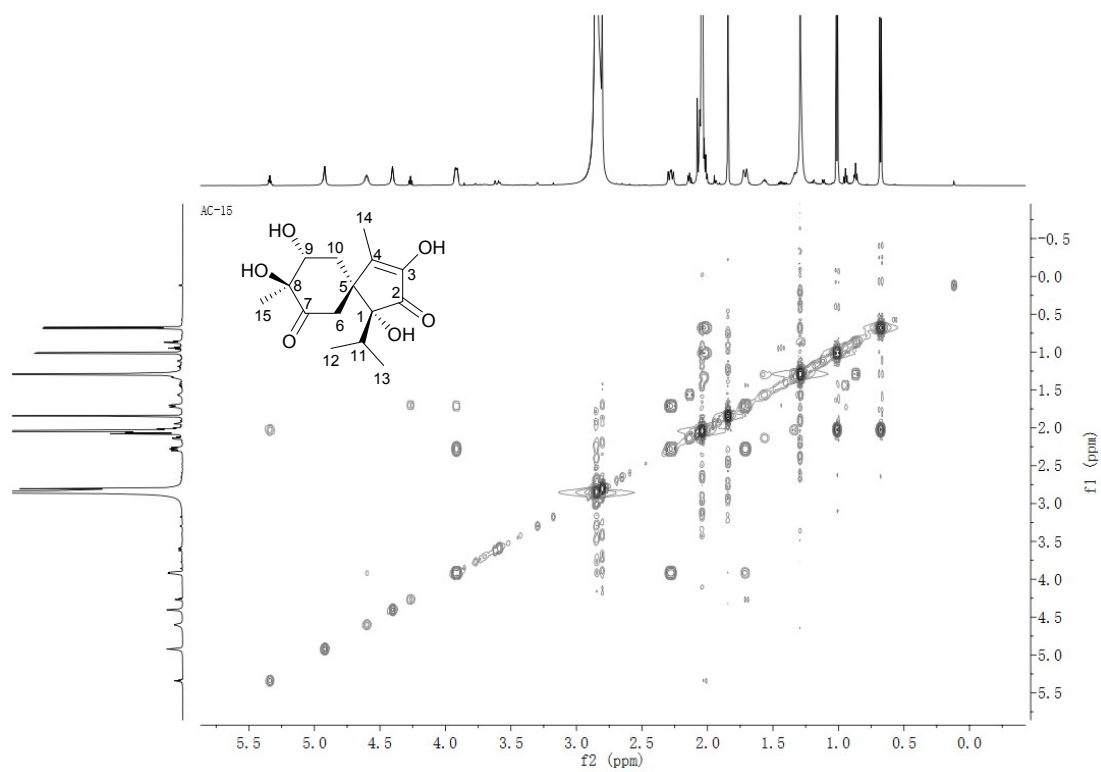


Figure S3. DEPT spectrum of compound 1

Figure S4. ^1H - ^1H COSY spectrum of compound 1

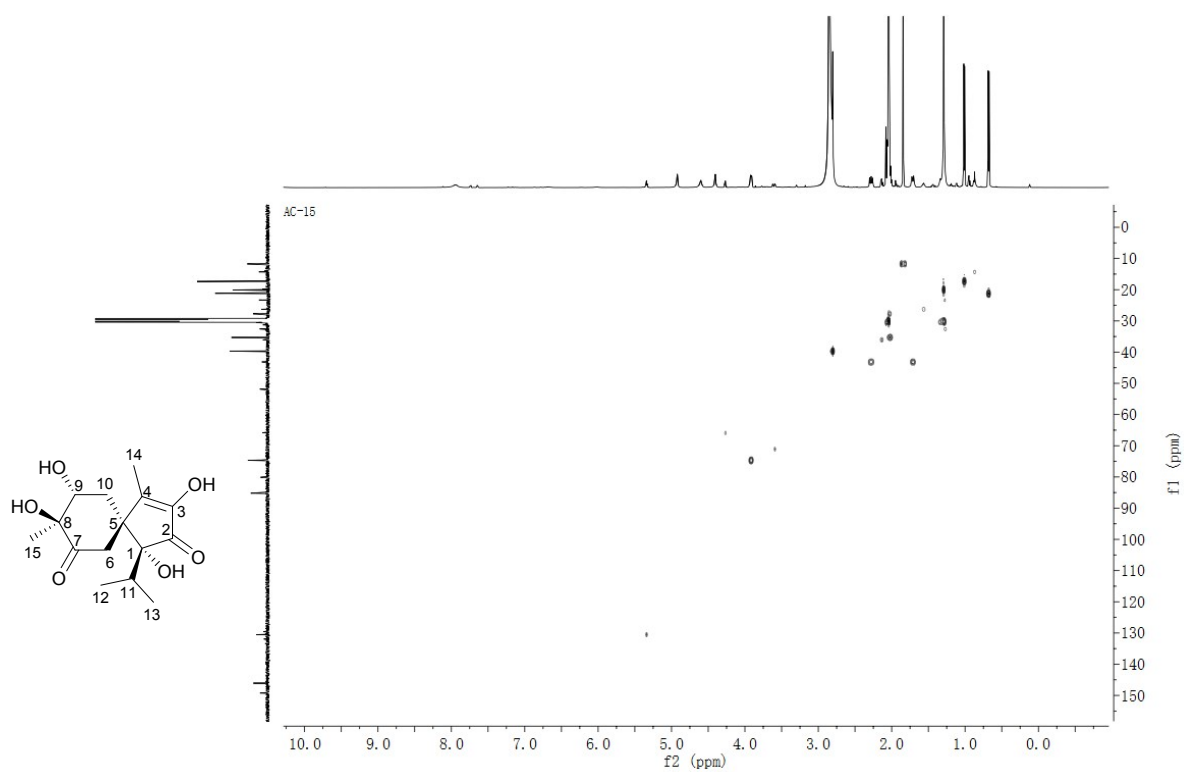


Figure S5. HSQC spectrum of compound **1**

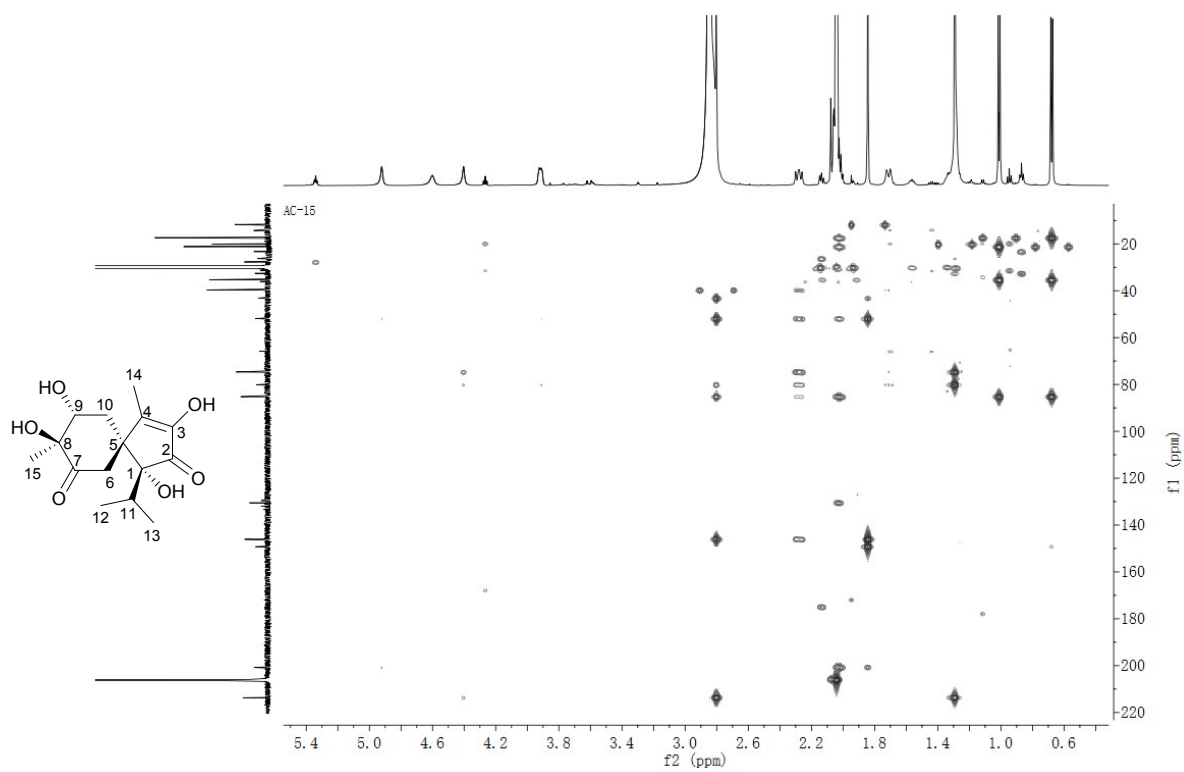


Figure S6. HMBC spectrum of compound **1**

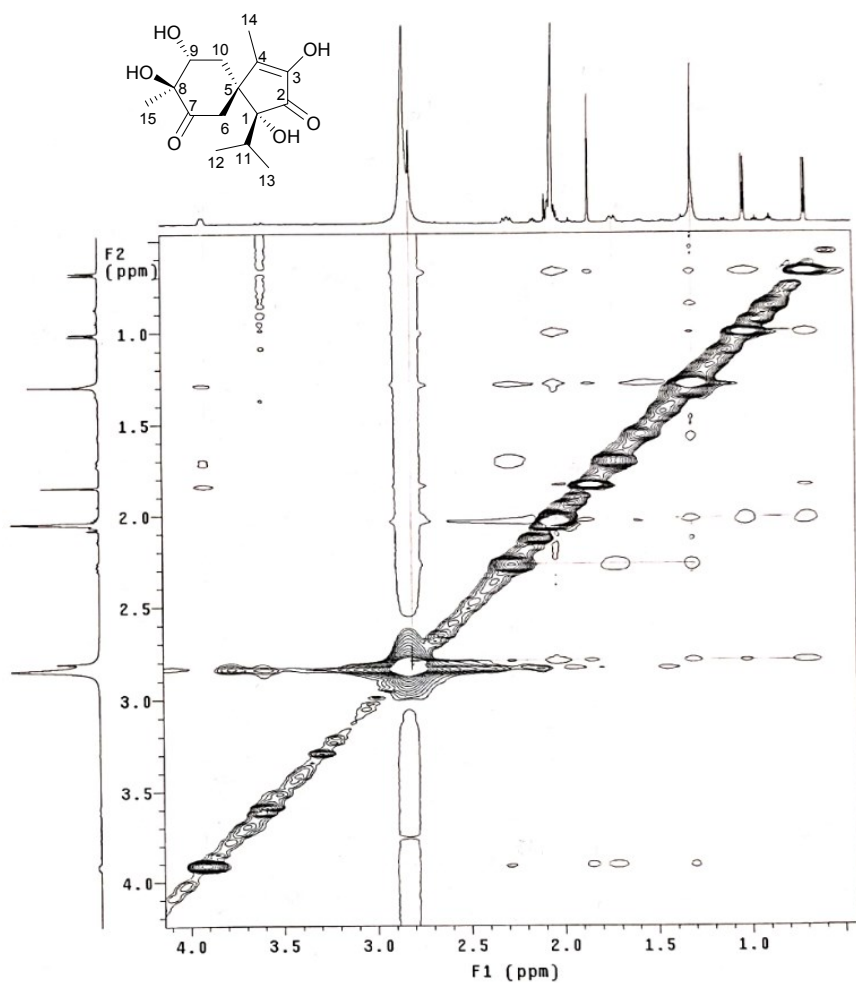


Figure S7. NOESY spectrum of compound **1**

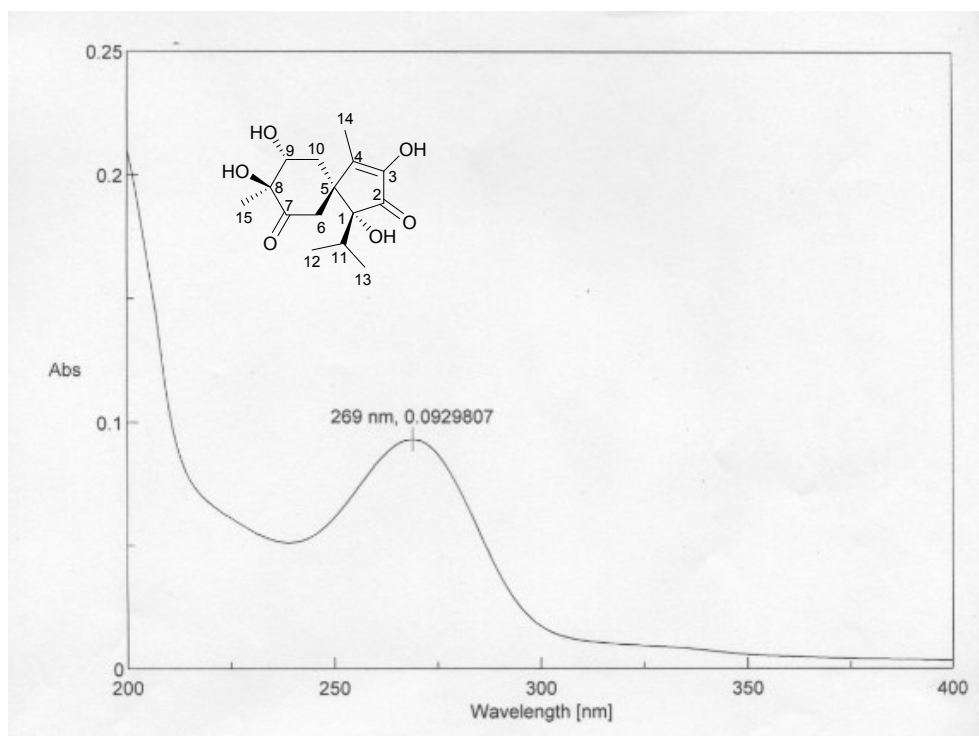


Figure S8. UV spectrum of compound **1**

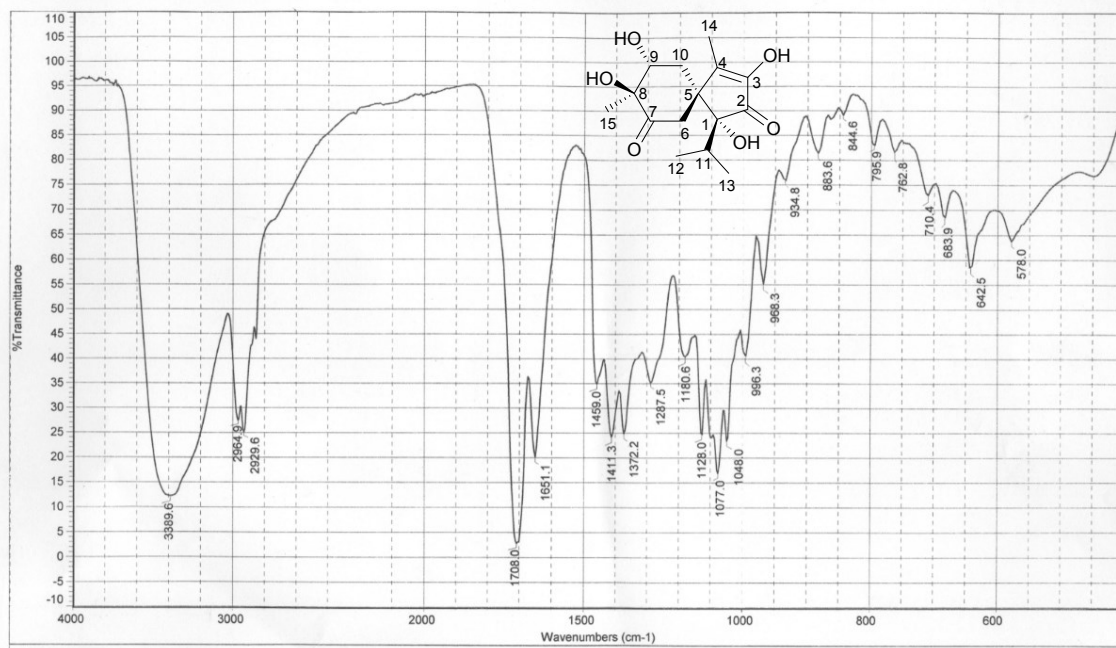


Figure S9. IR spectrum of compound 1

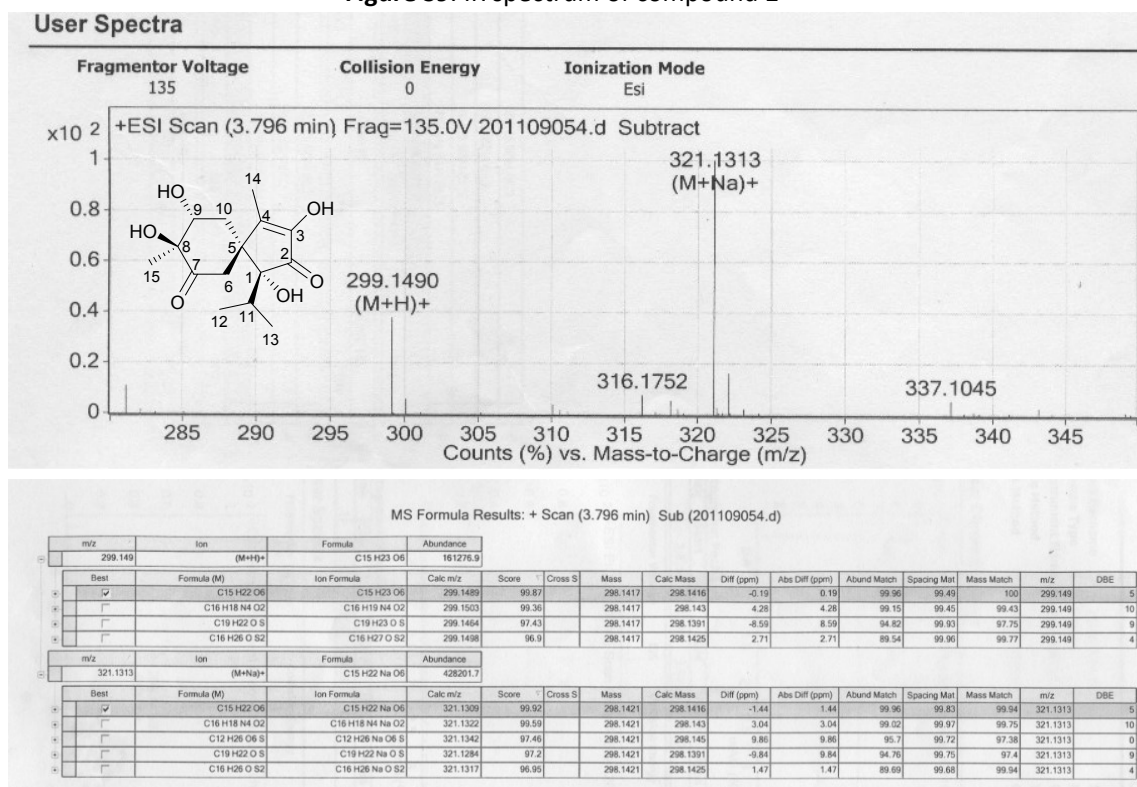


Figure S10. HRESIMS spectrum of compound 1

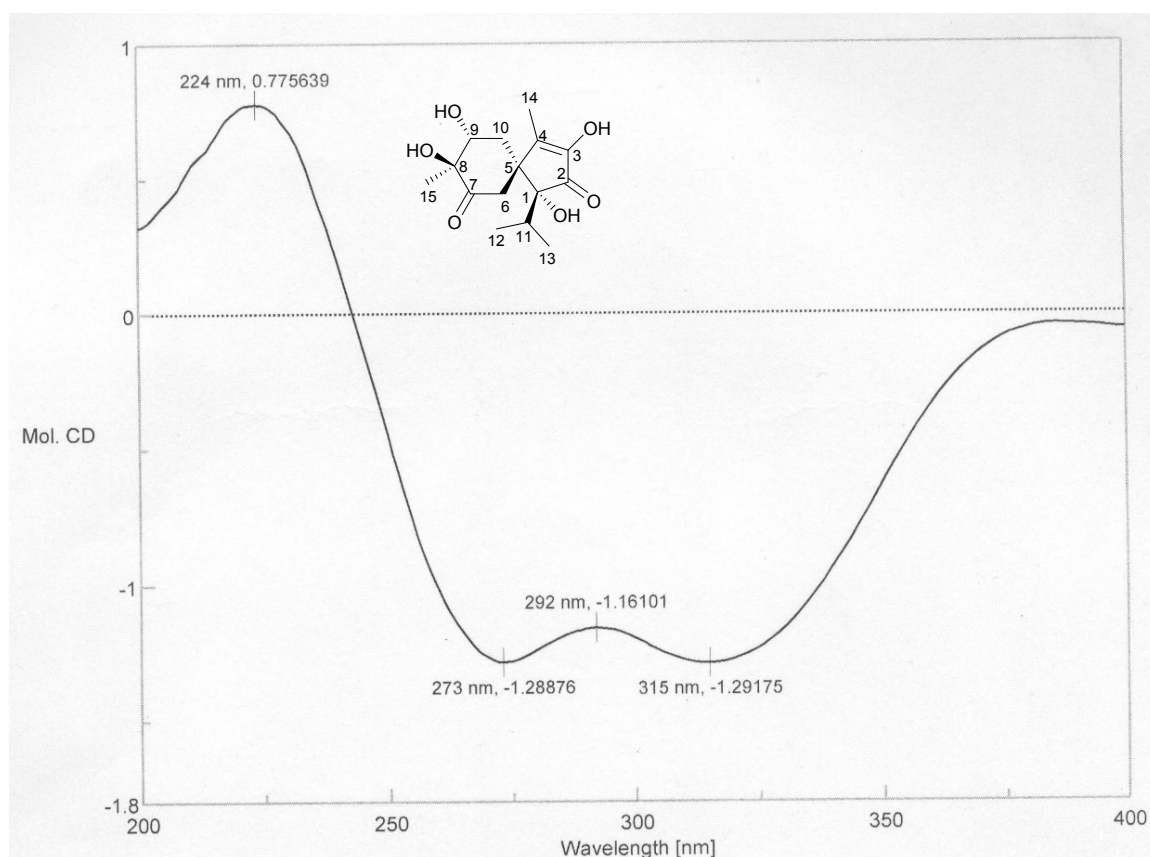


Figure S11. CD spectrum of compound **1**

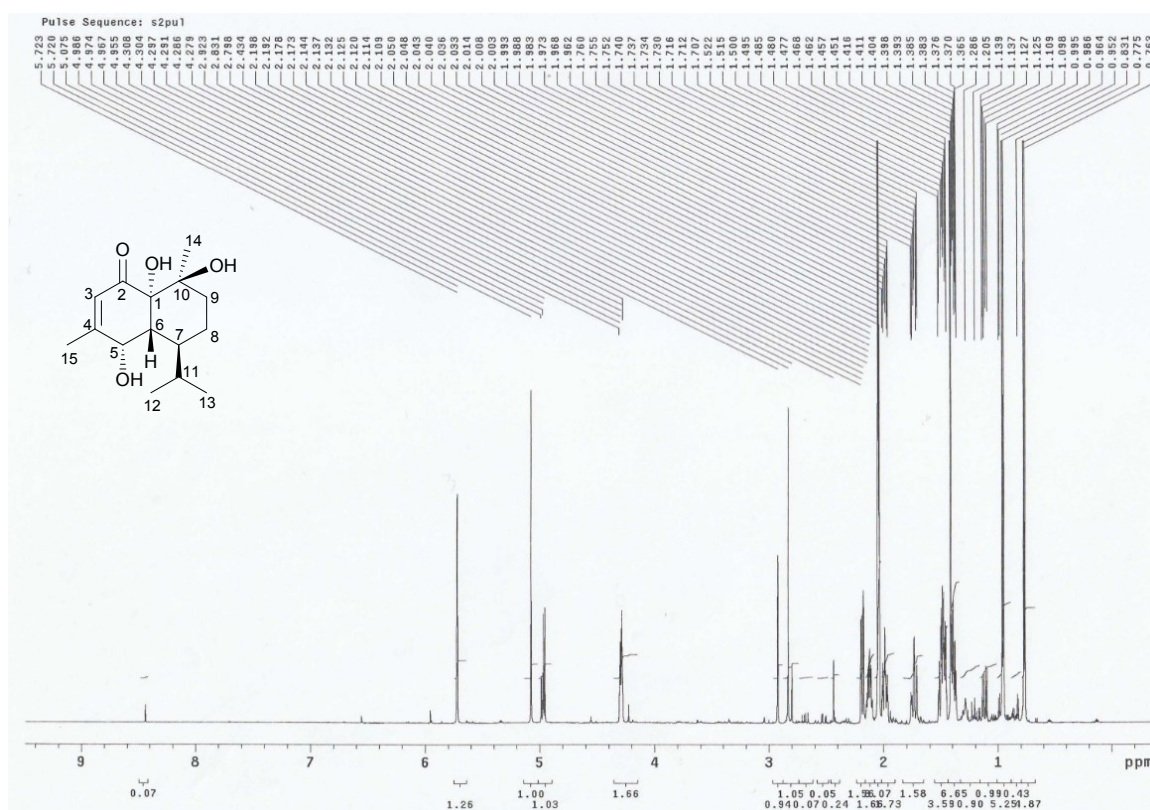


Figure S12. ^1H NMR spectrum of compound **2** (600 MHz, CD_3COCD_3)

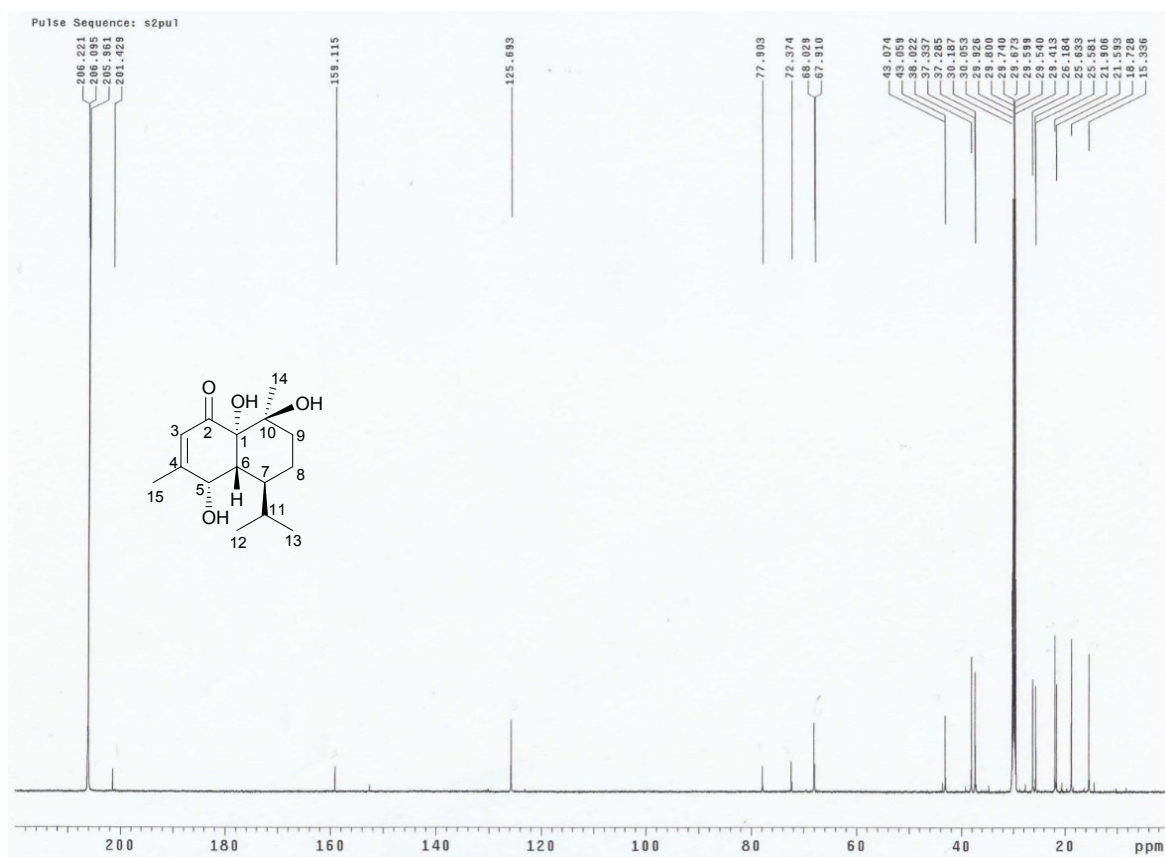


Figure S13. ^{13}C NMR spectrum of compound **2** (150 MHz, CD_3COCD_3)

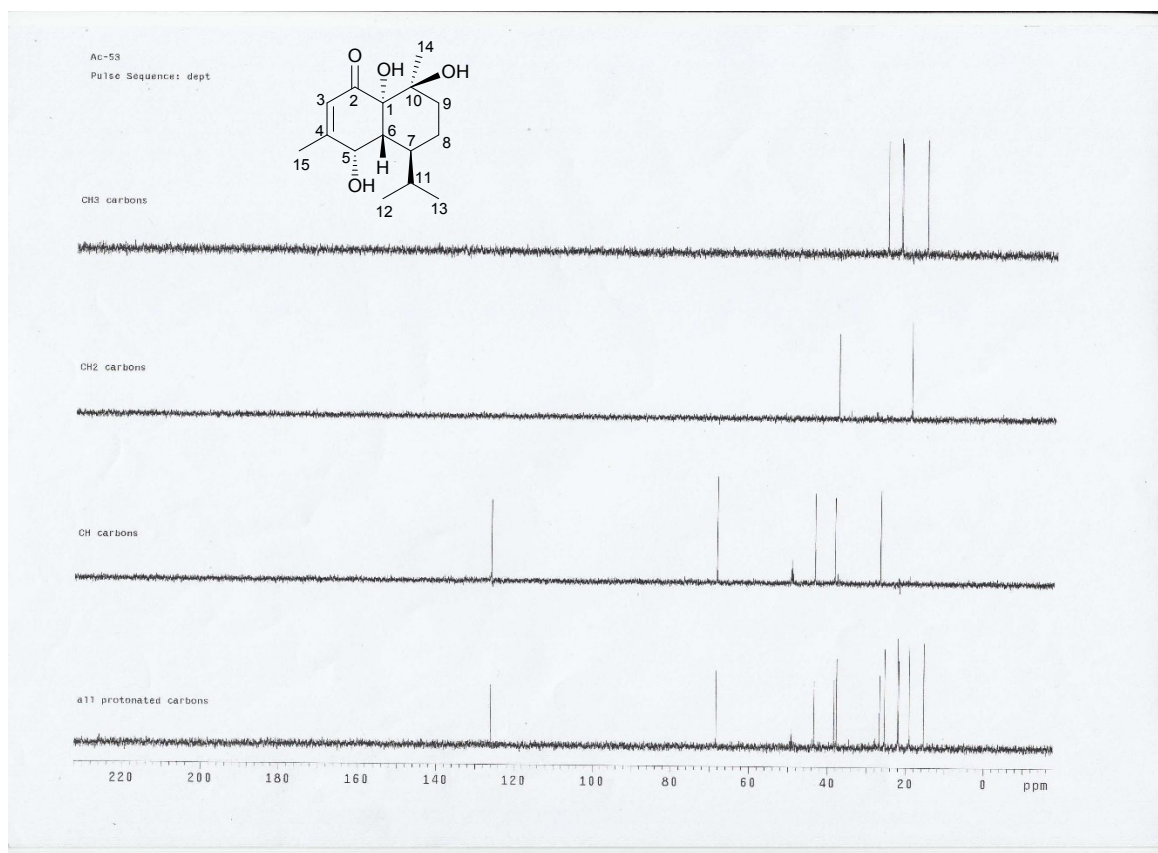


Figure S14. DEPT spectrum of compound **2**

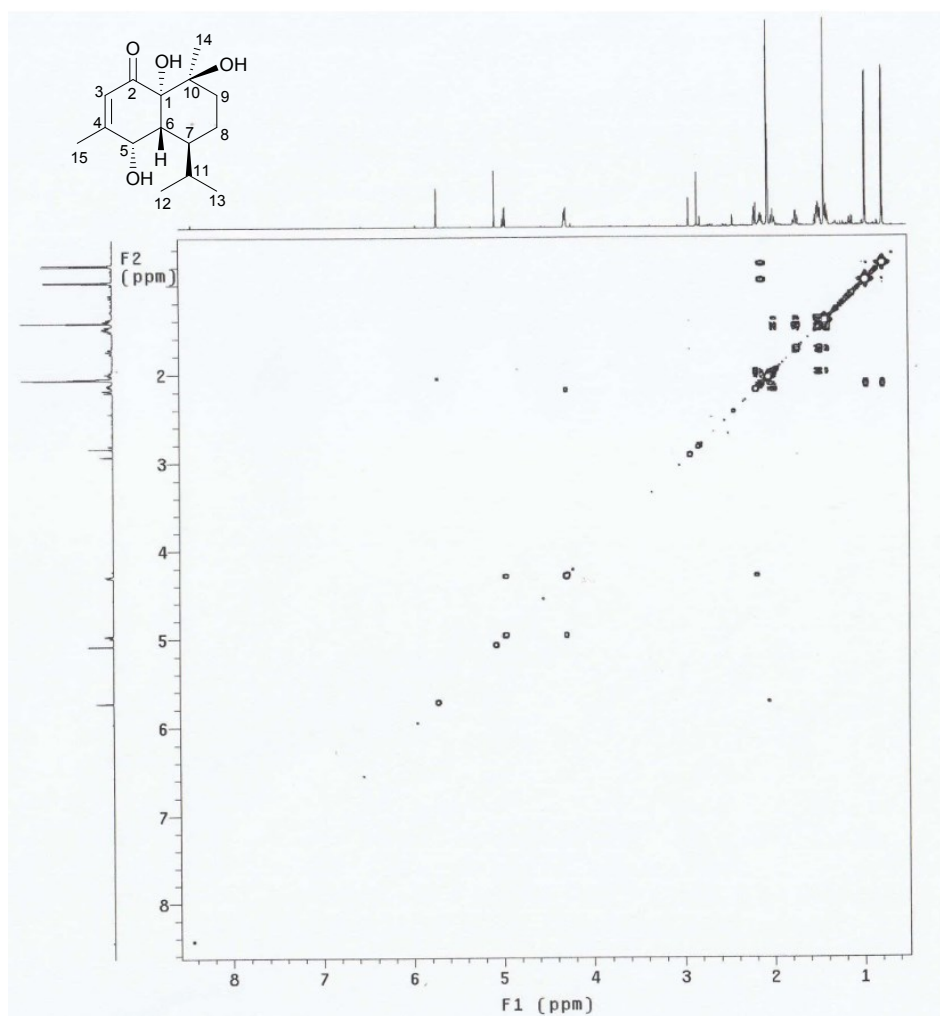


Figure S15. ^1H - ^1H COSY spectrum of compound **2**

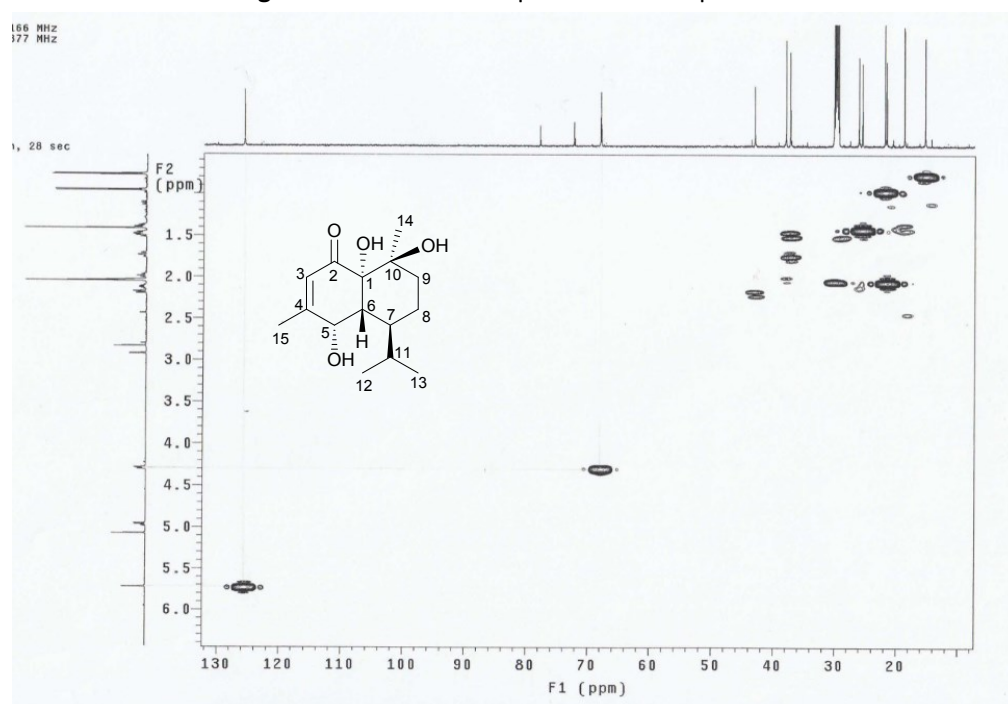


Figure S16. HMQC spectrum of compound **2**

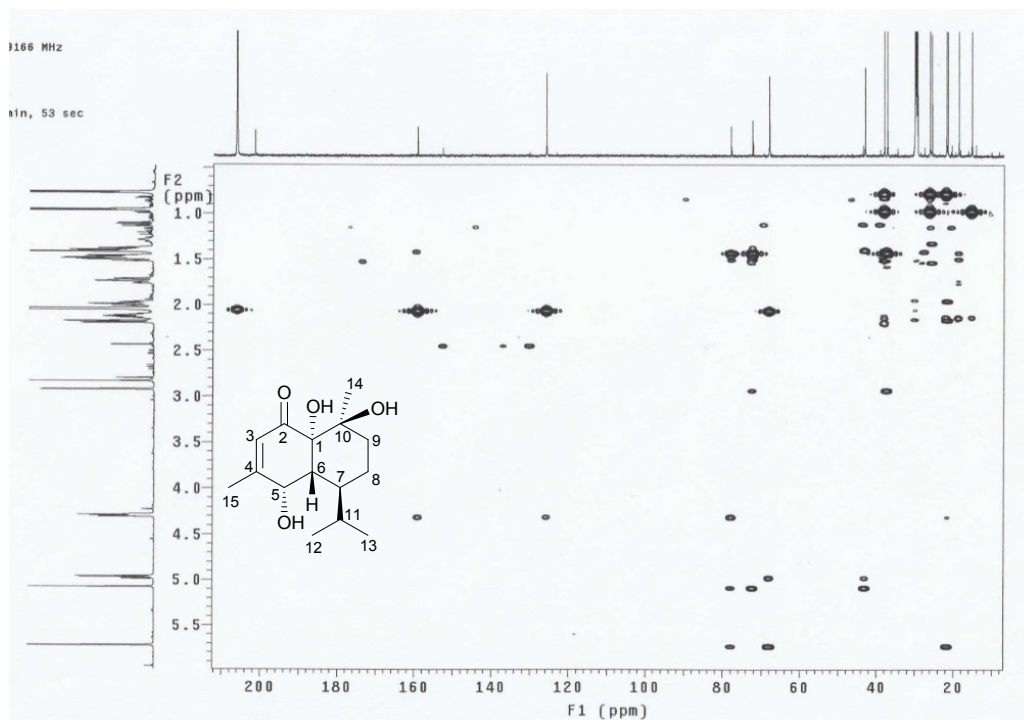


Figure S17. HMBC spectrum of compound **2**

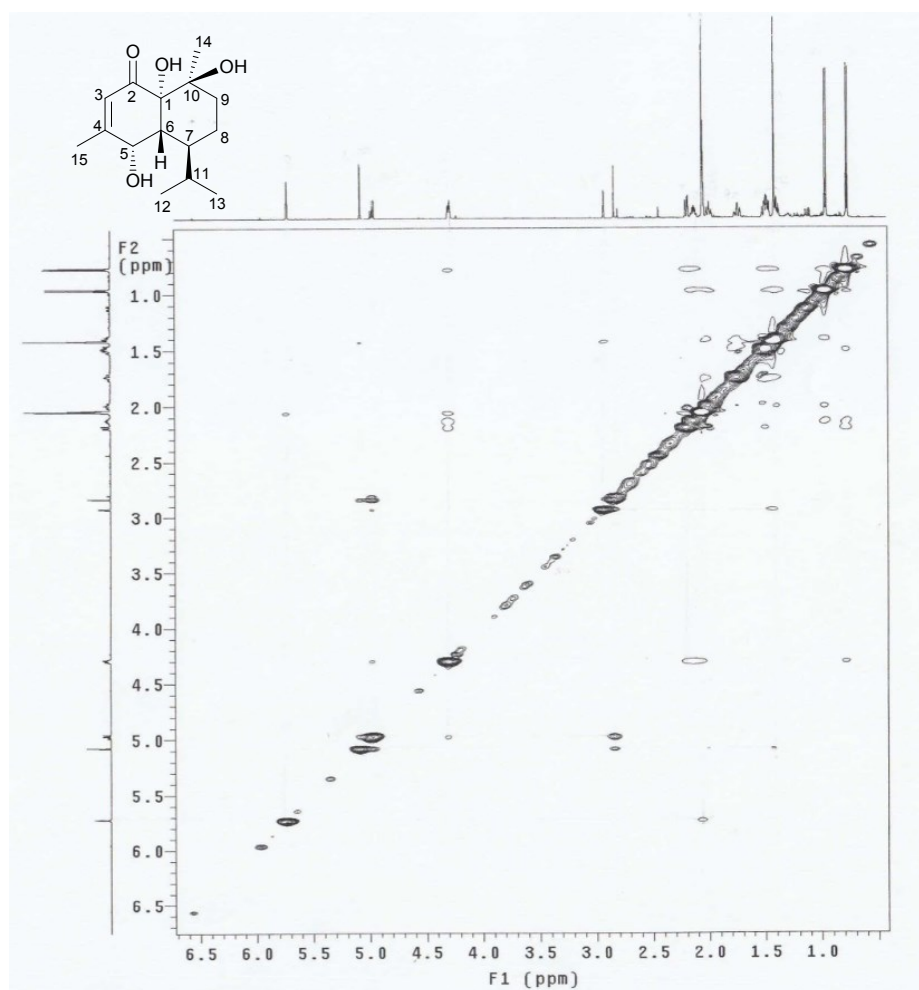


Figure S18. NOESY spectrum of compound **2**

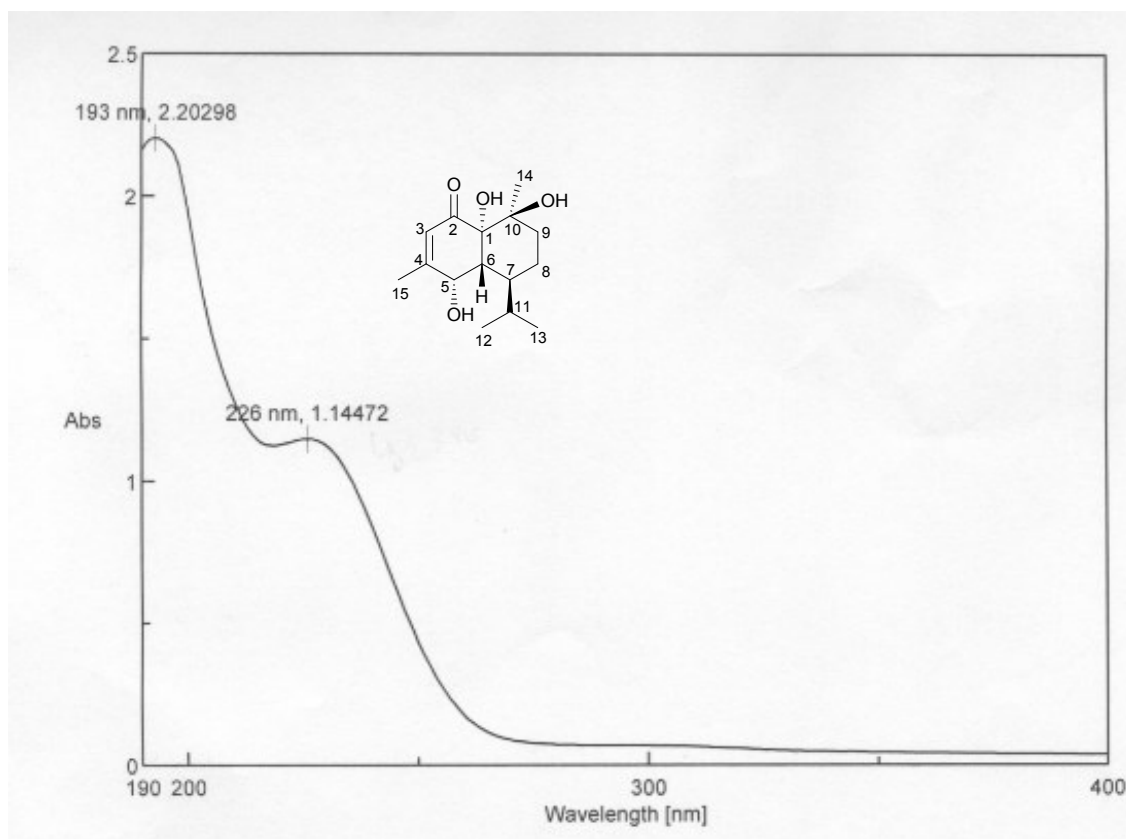


Figure S19. UV spectrum of compound **2**

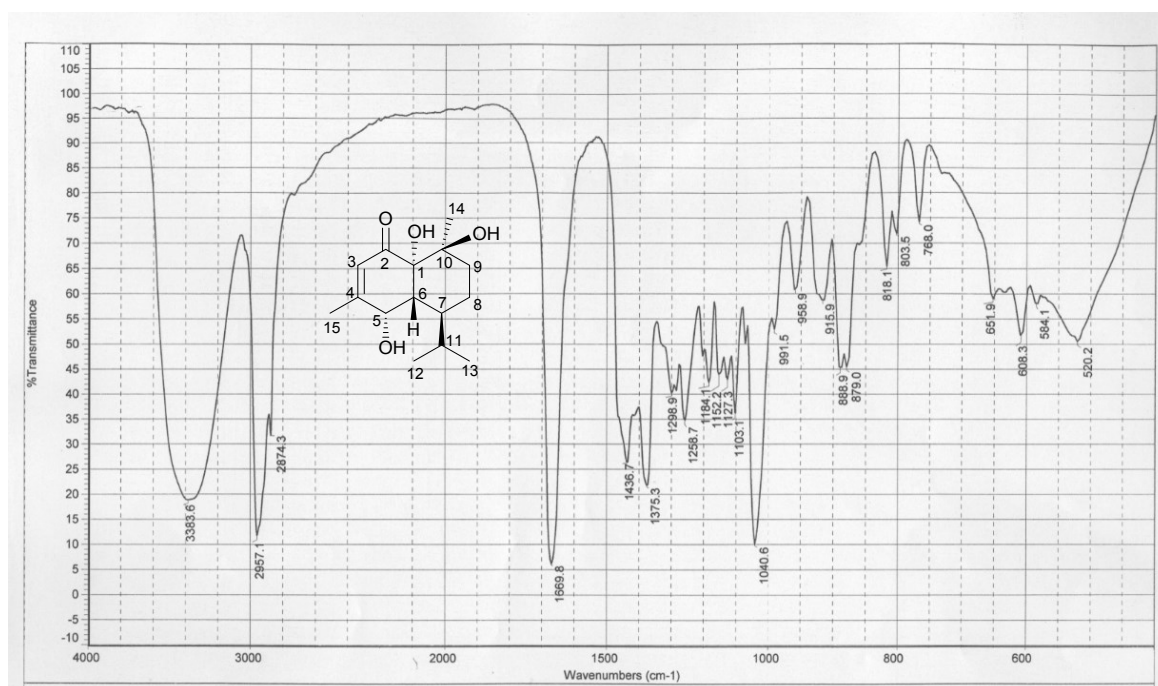


Figure S20. IR spectrum of compound **2**

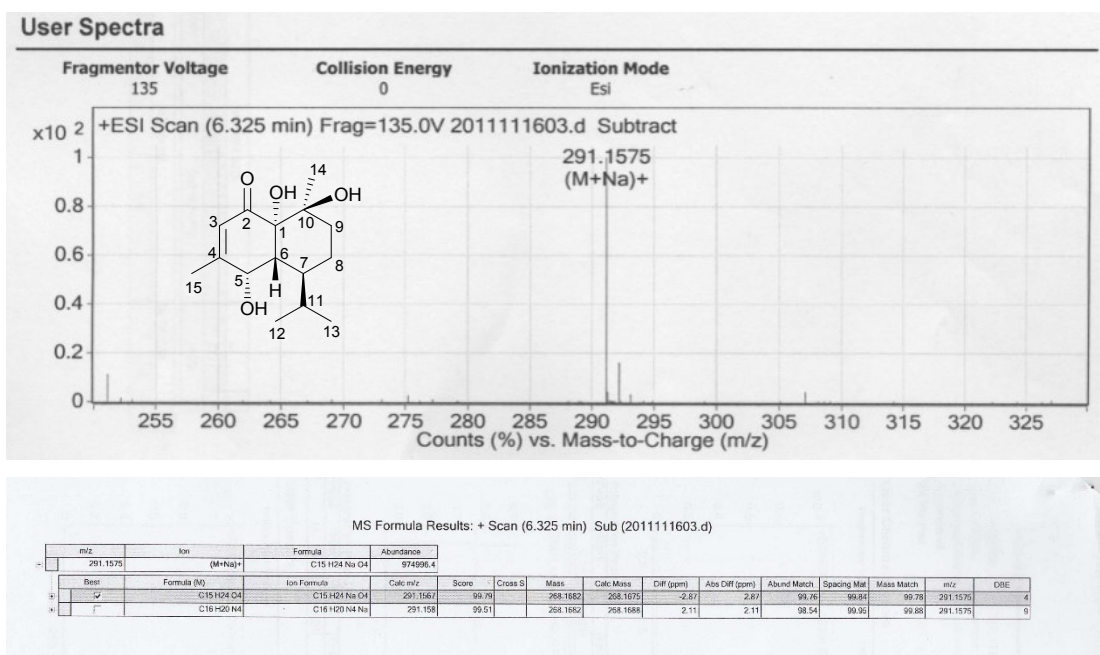


Figure S21. HRESIMS spectrum of compound **2**

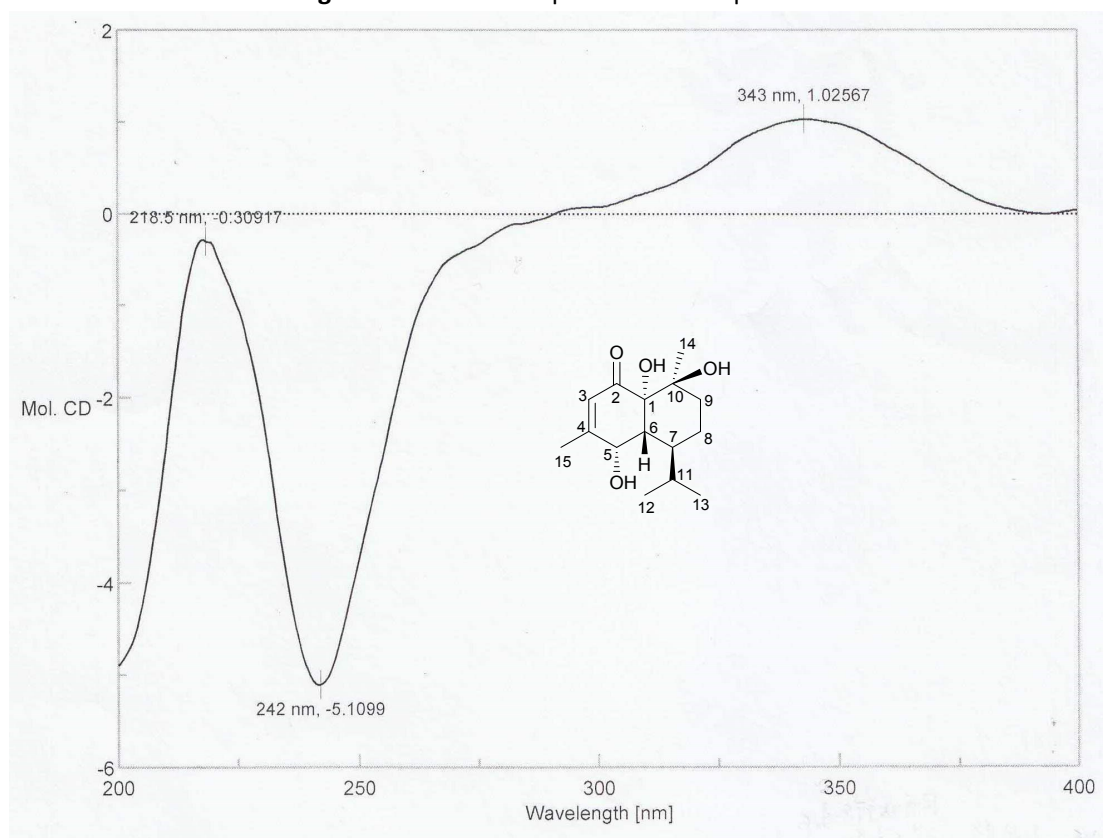


Figure S22. CD spectrum of compound **2**

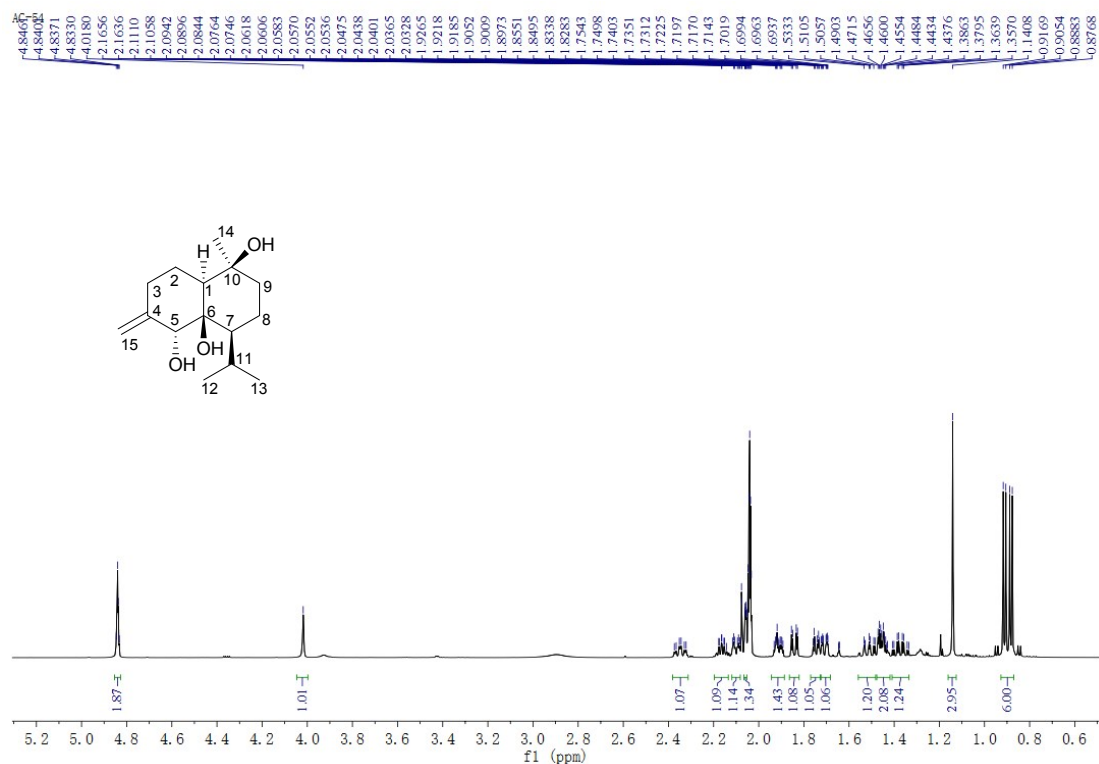


Figure S23. ¹H NMR spectrum of compound **3** (600 MHz, CD₃COCD₃)

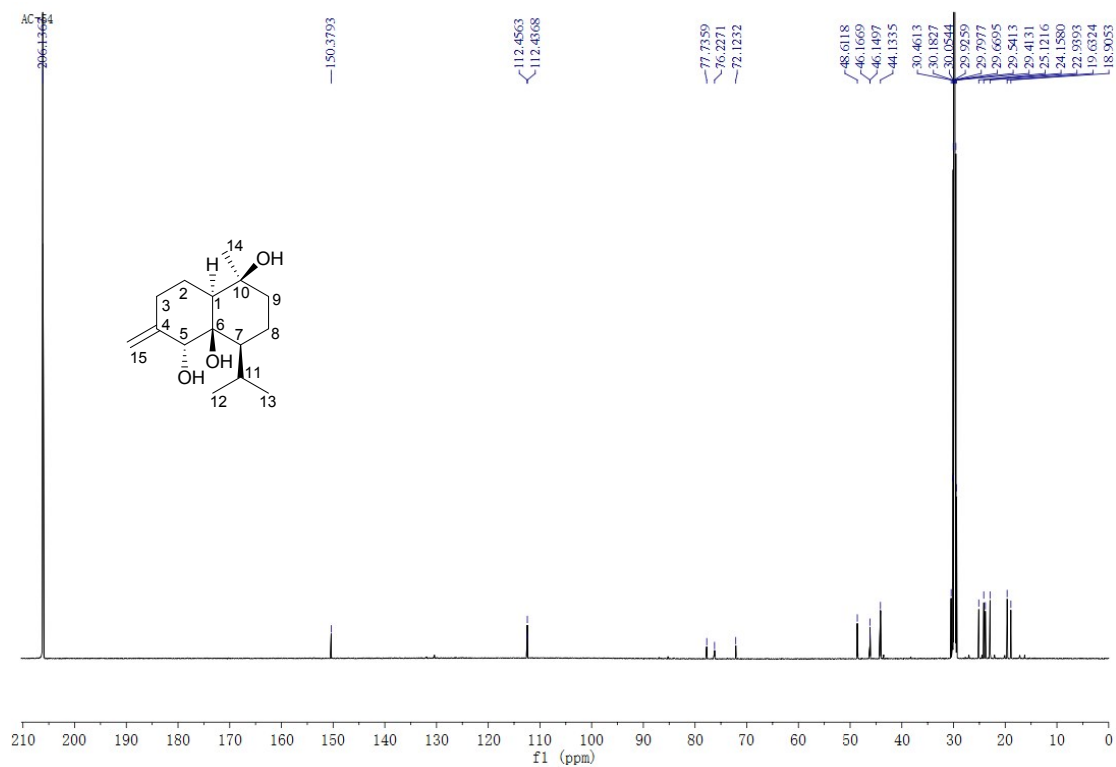
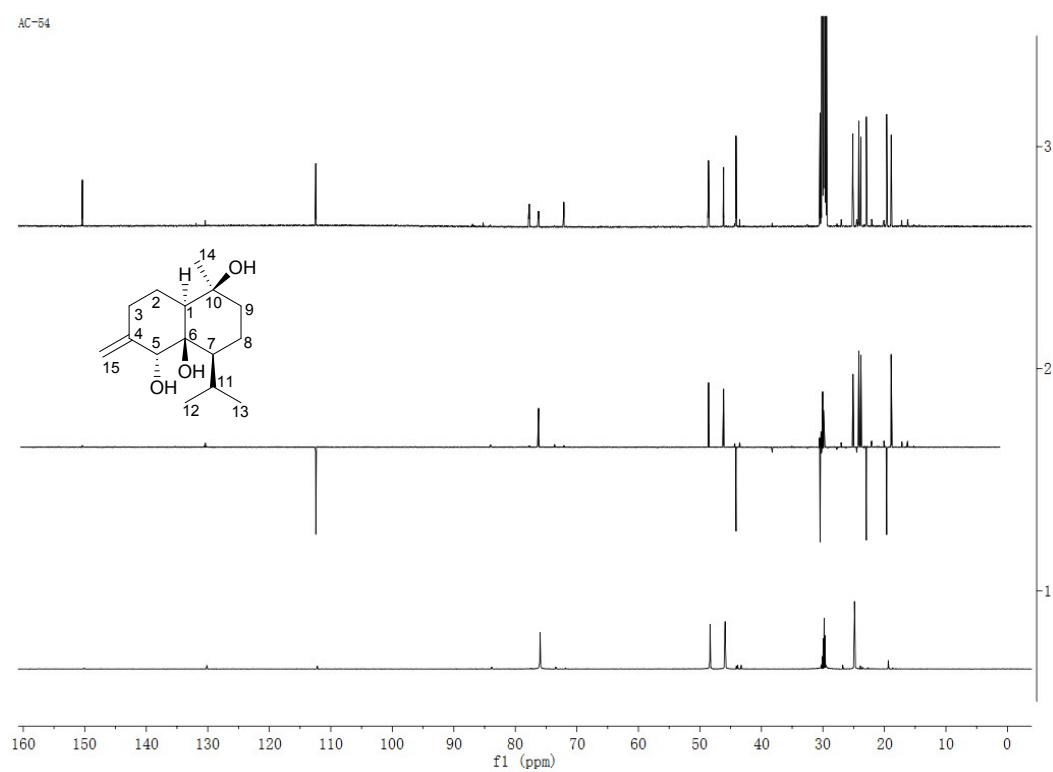
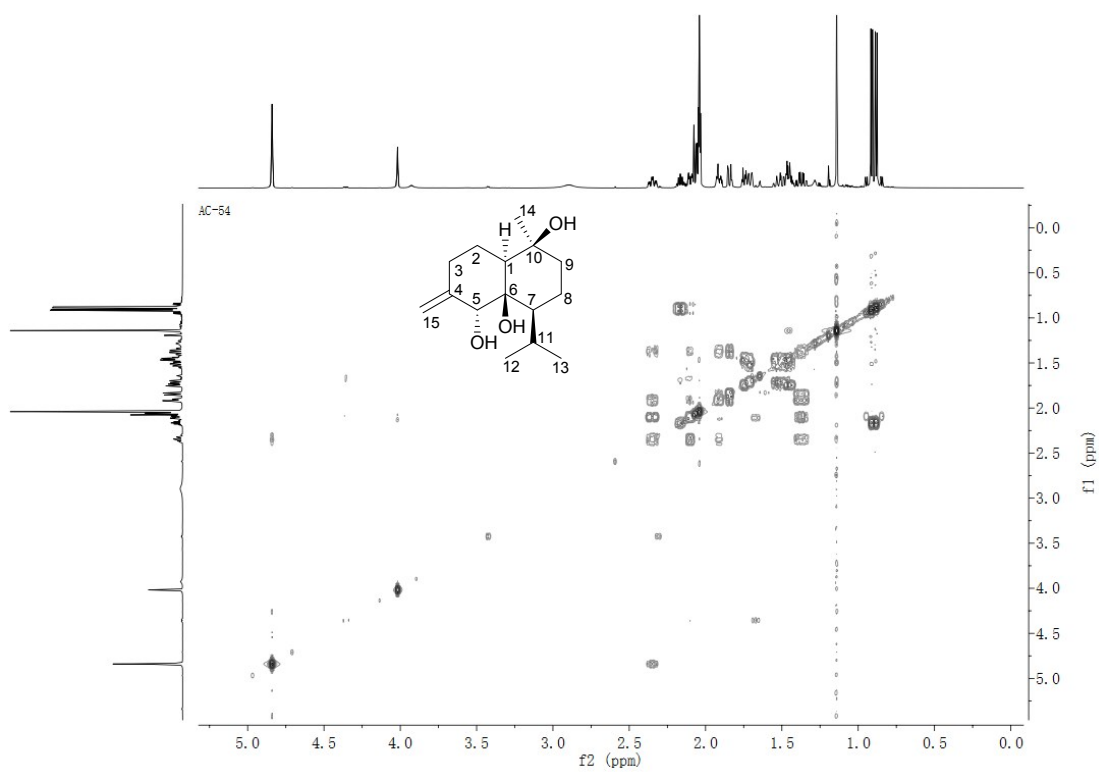


Figure S24. ¹³C NMR spectrum of compound **3** (150 MHz, CD₃COCD₃)

**Figure S25. DEPT spectrum of compound 3****Figure S26. ^1H - ^1H COSY spectrum of compound 3**

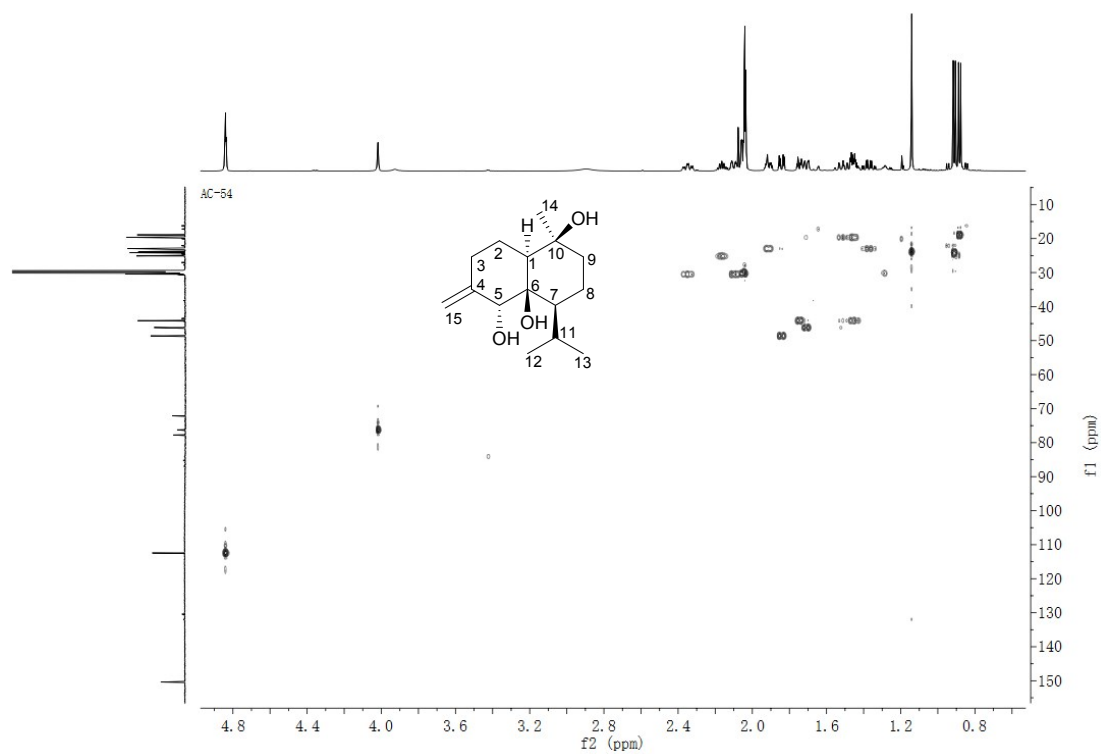


Figure S27. HSQC spectrum of compound 3

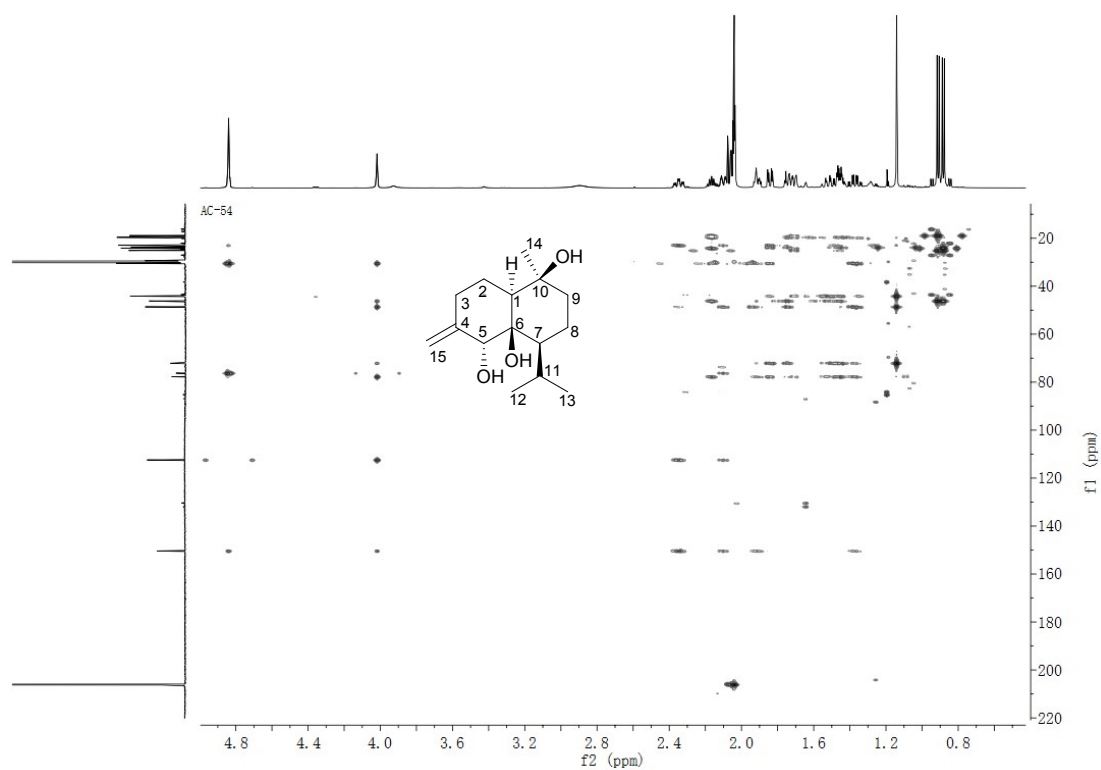


Figure S28. HMBC spectrum of compound 3

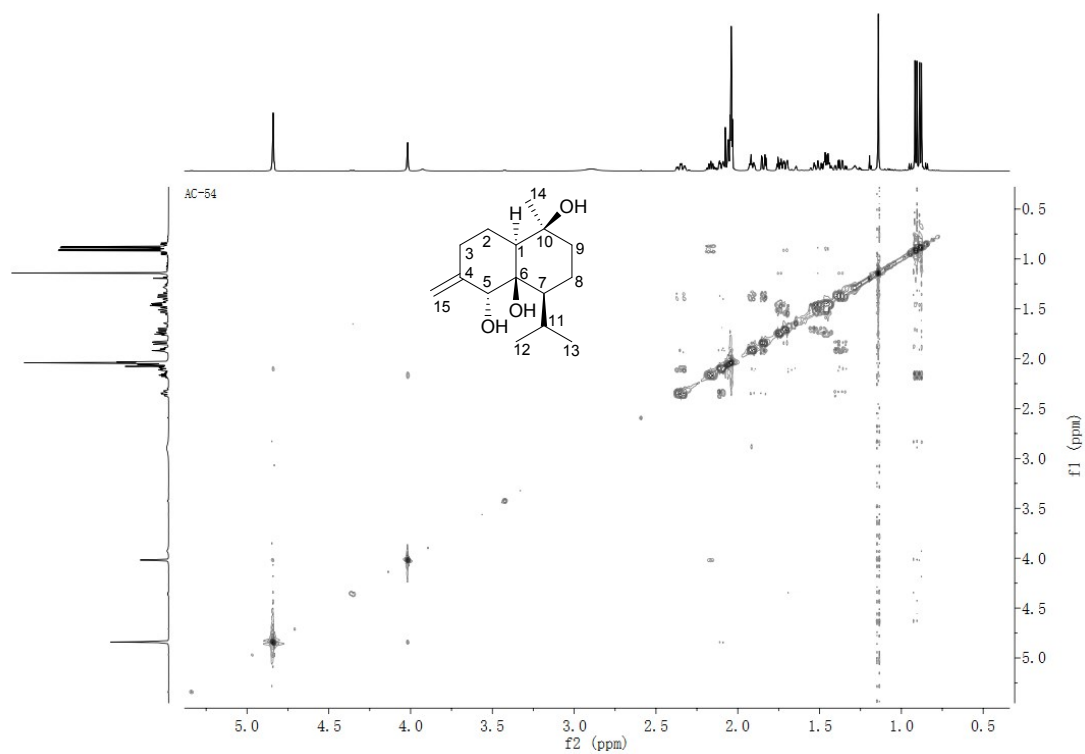


Figure S29. NOESY spectrum of compound **3**

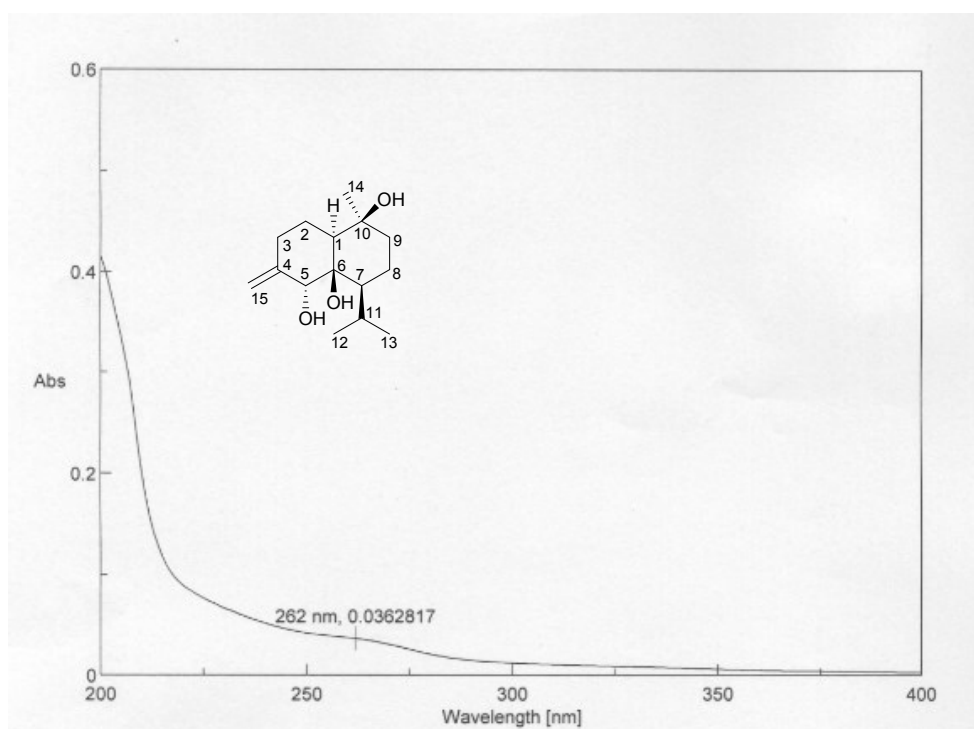


Figure S30. UV spectrum of compound **3**

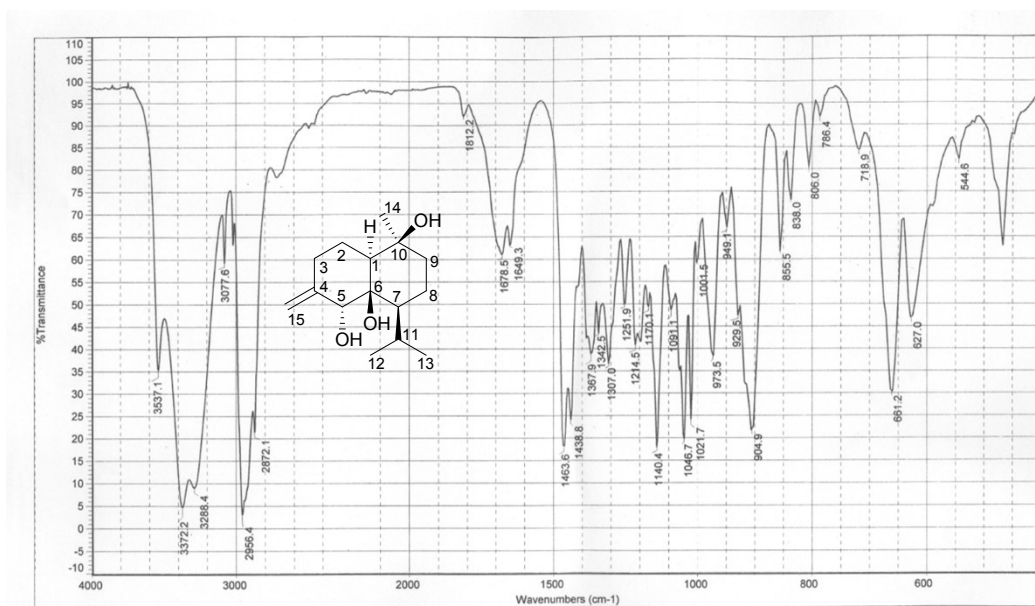


Figure S31. IR spectrum of compound 3

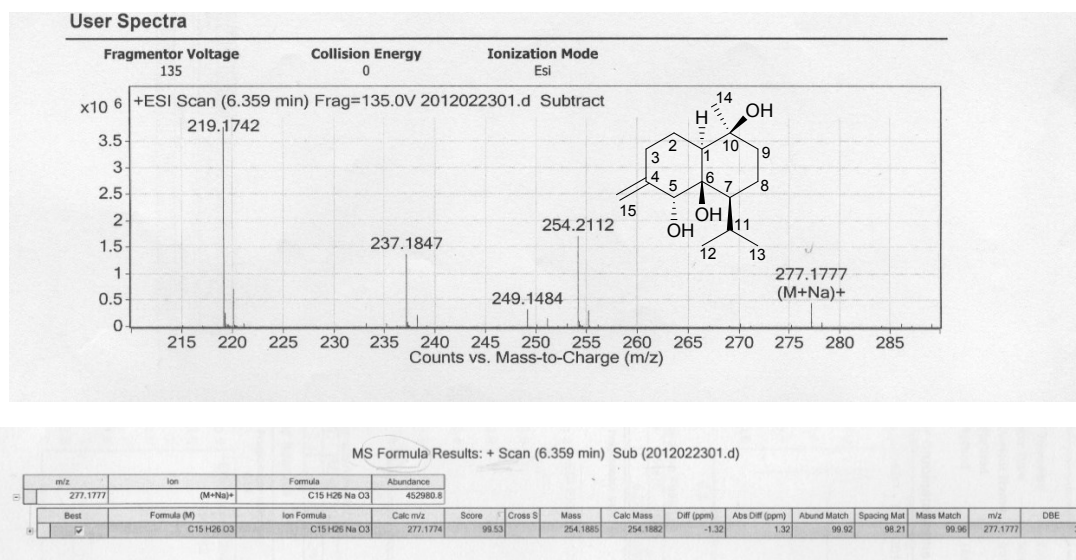


Figure S32. HRESIMS spectrum of compound 3

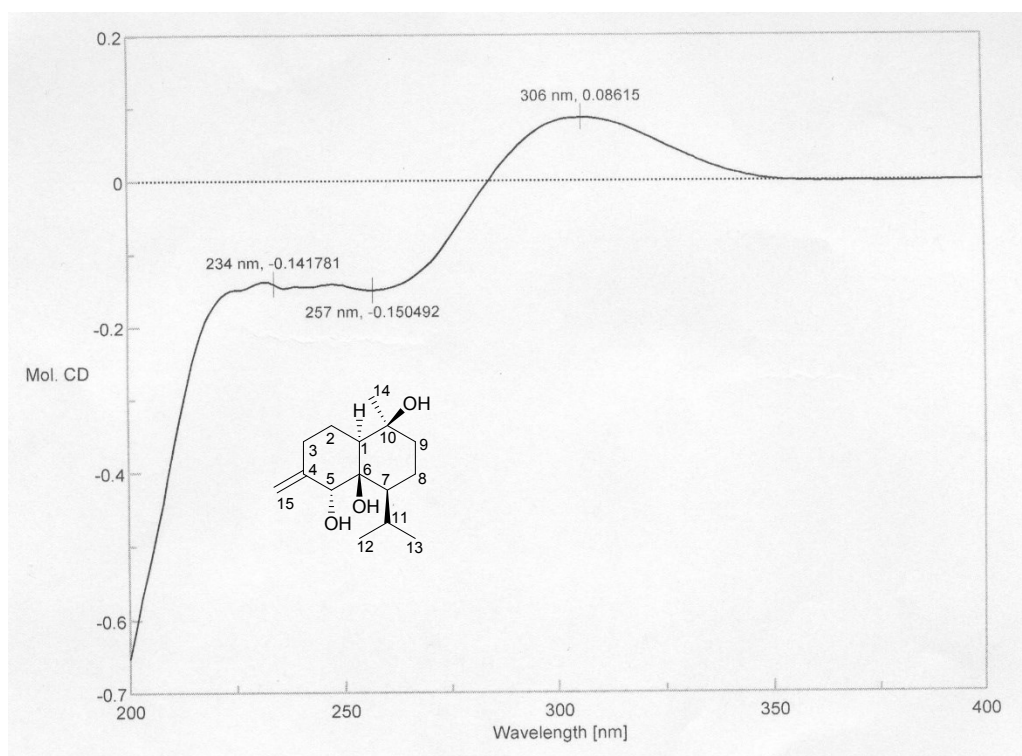


Figure S33. CD spectrum of compound **3**

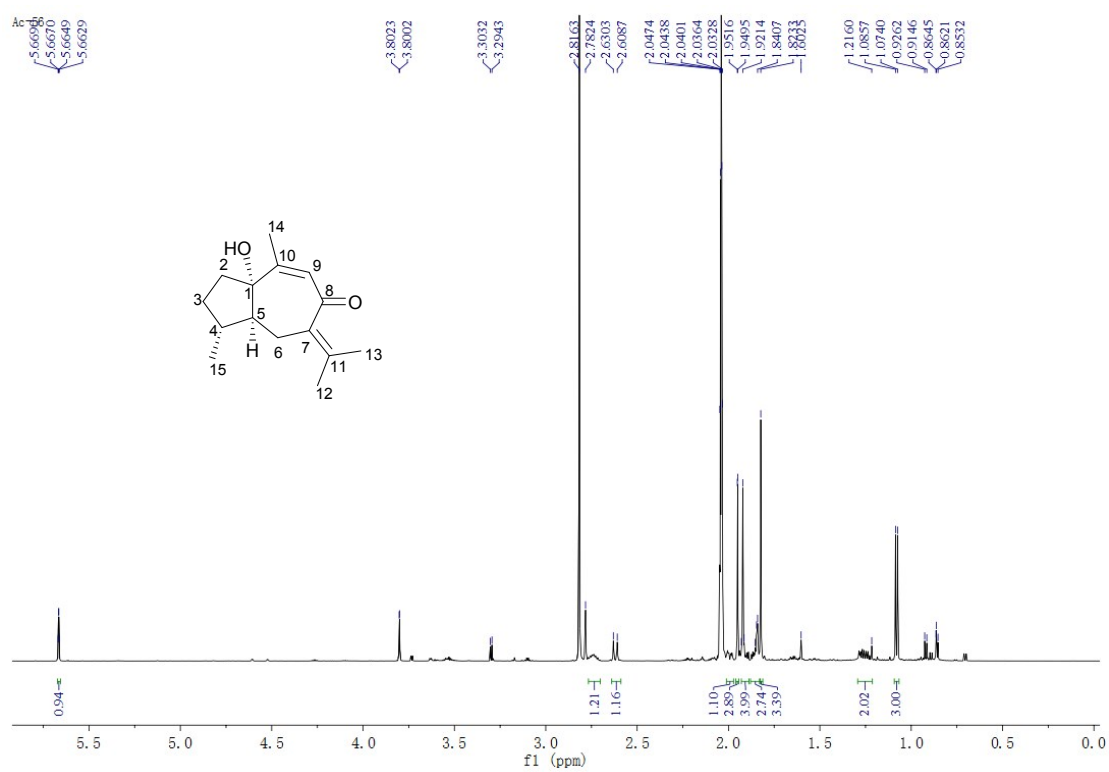


Figure S34. ^1H NMR spectrum of compound **4** (600 MHz, CD_3COCD_3)

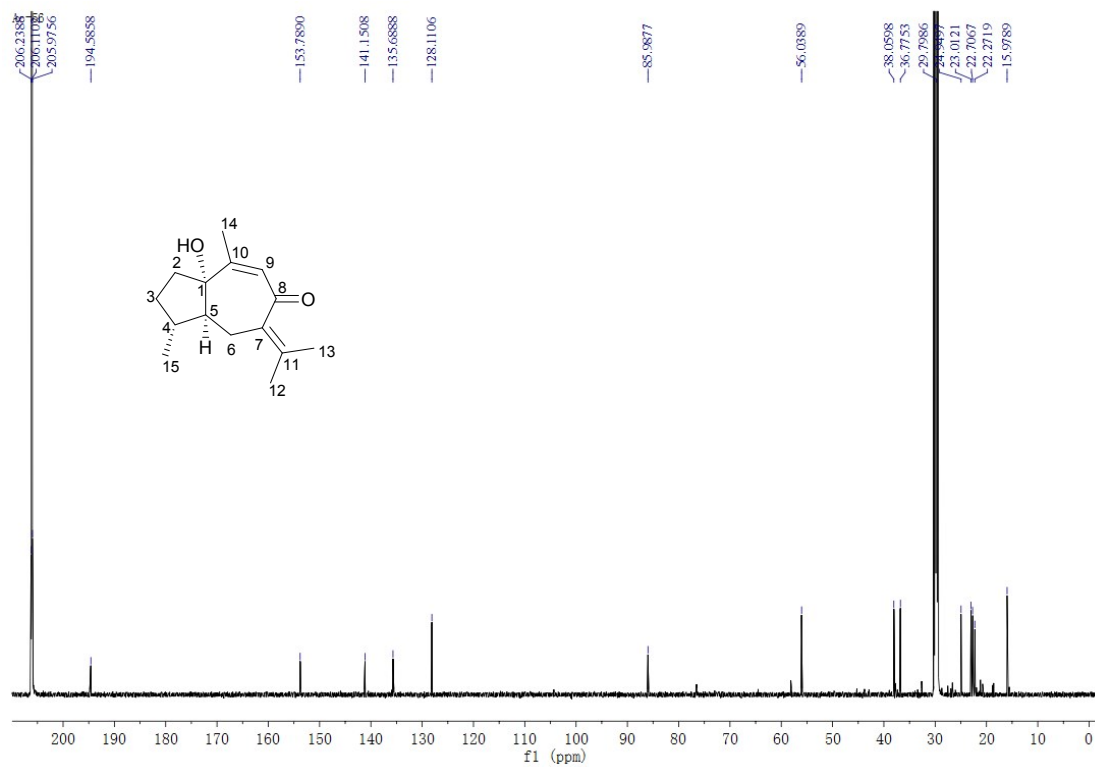


Figure S35. ¹³C NMR spectrum of compound **4** (150 MHz, CD₃COCD₃)

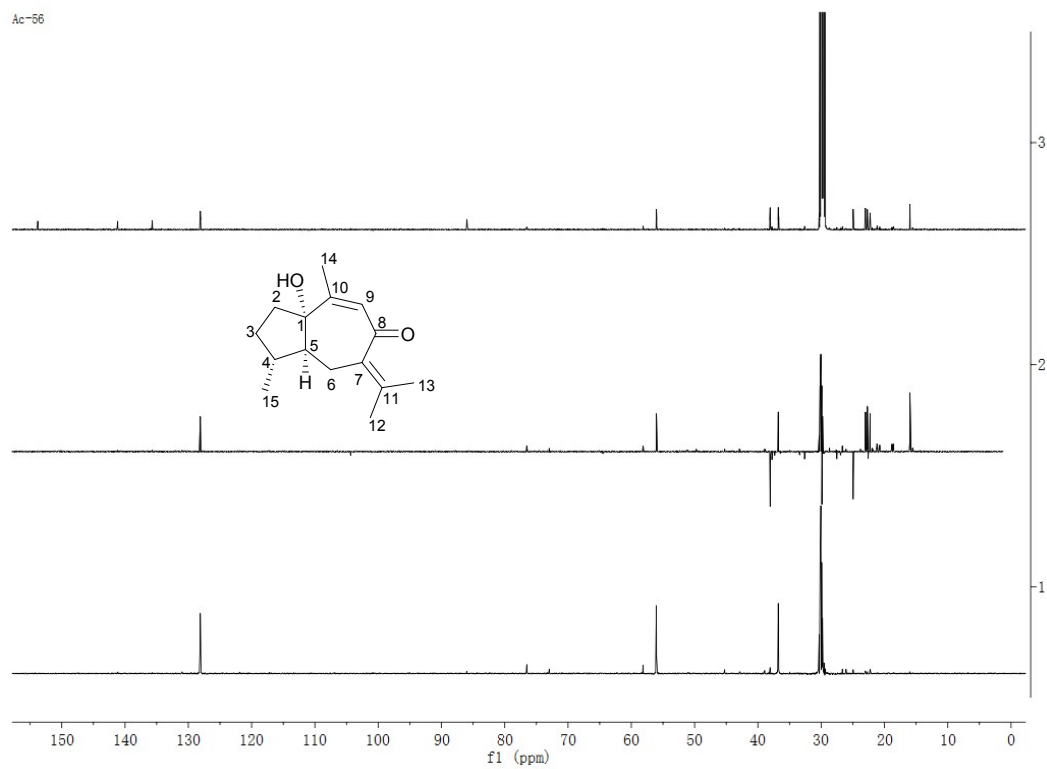


Figure S36. DEPT spectrum of compound **4**

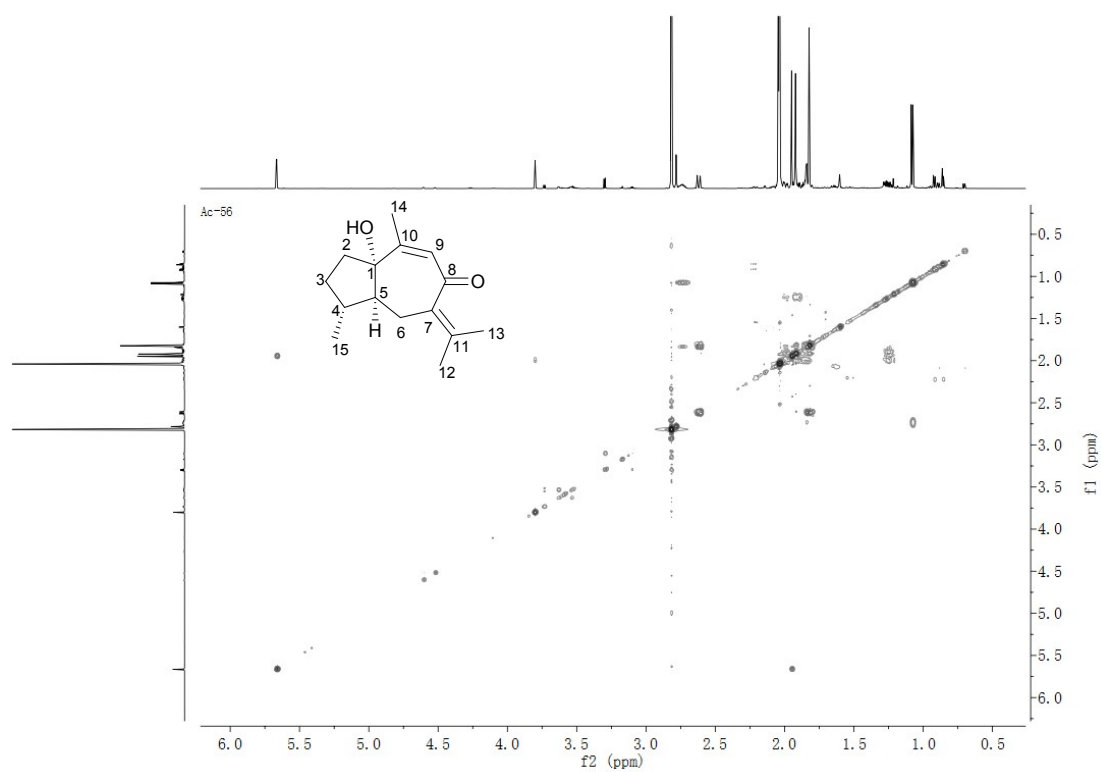


Figure S37. ^1H - ^1H COSY spectrum of compound **4**

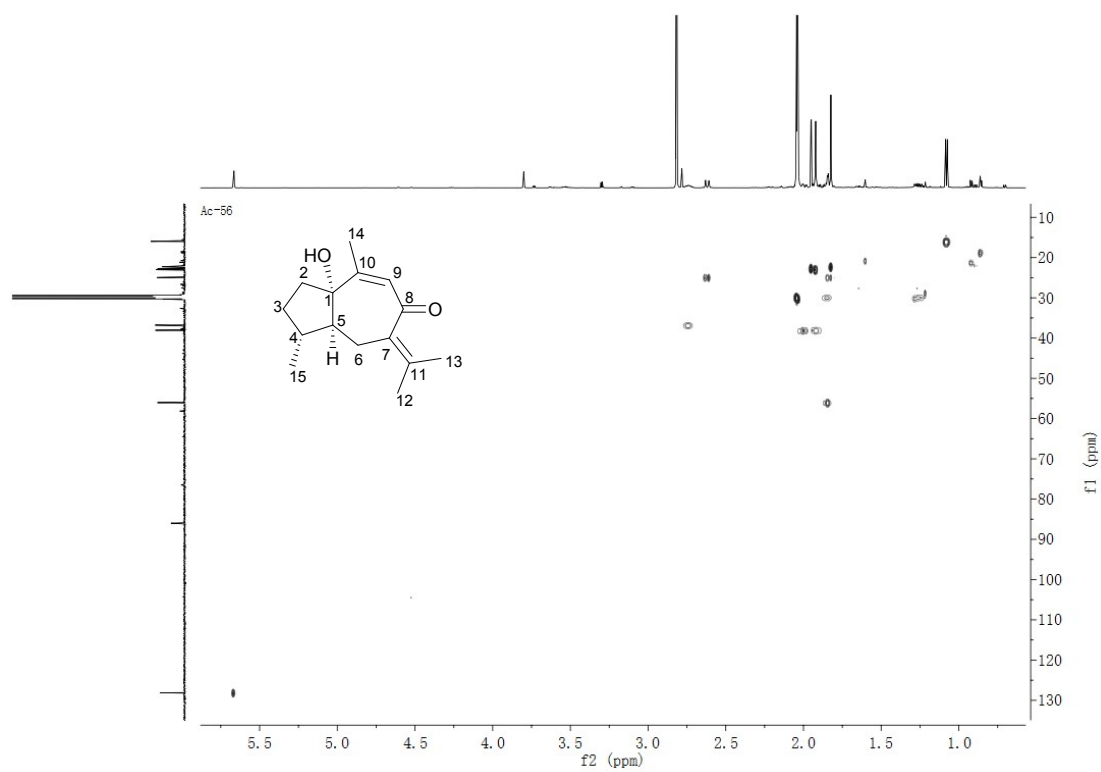


Figure S38. HSQC spectrum of compound **4**

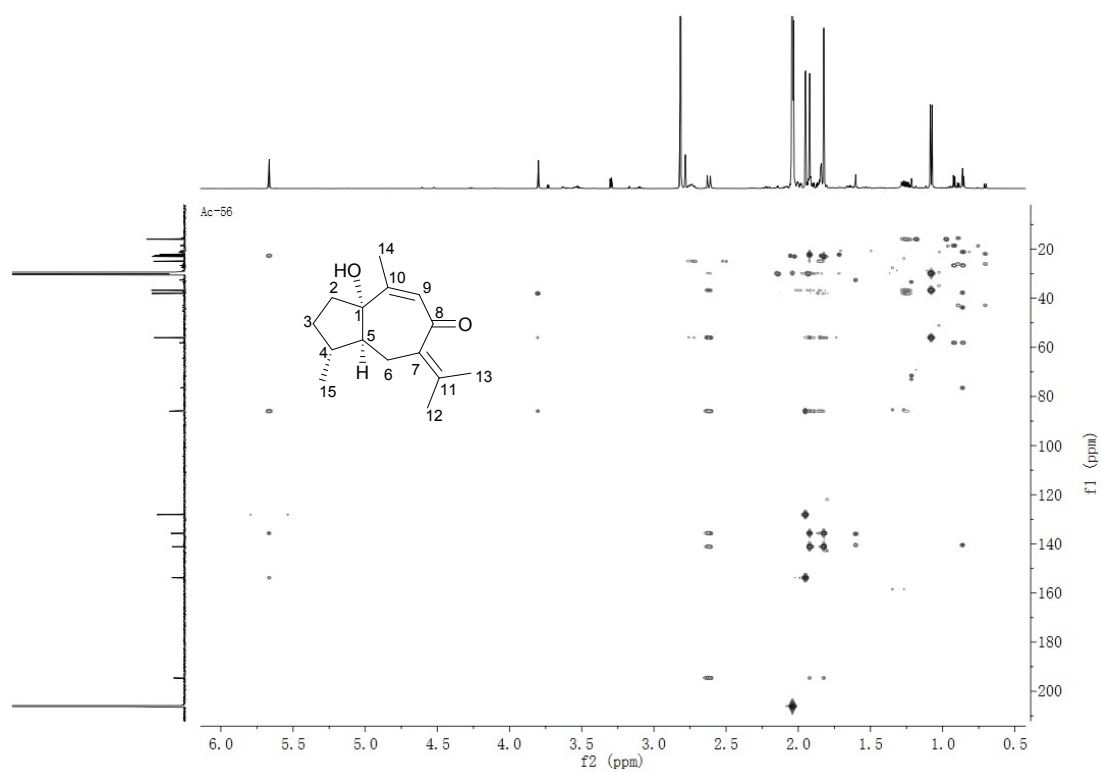


Figure S39. HMBC spectrum of compound **4**

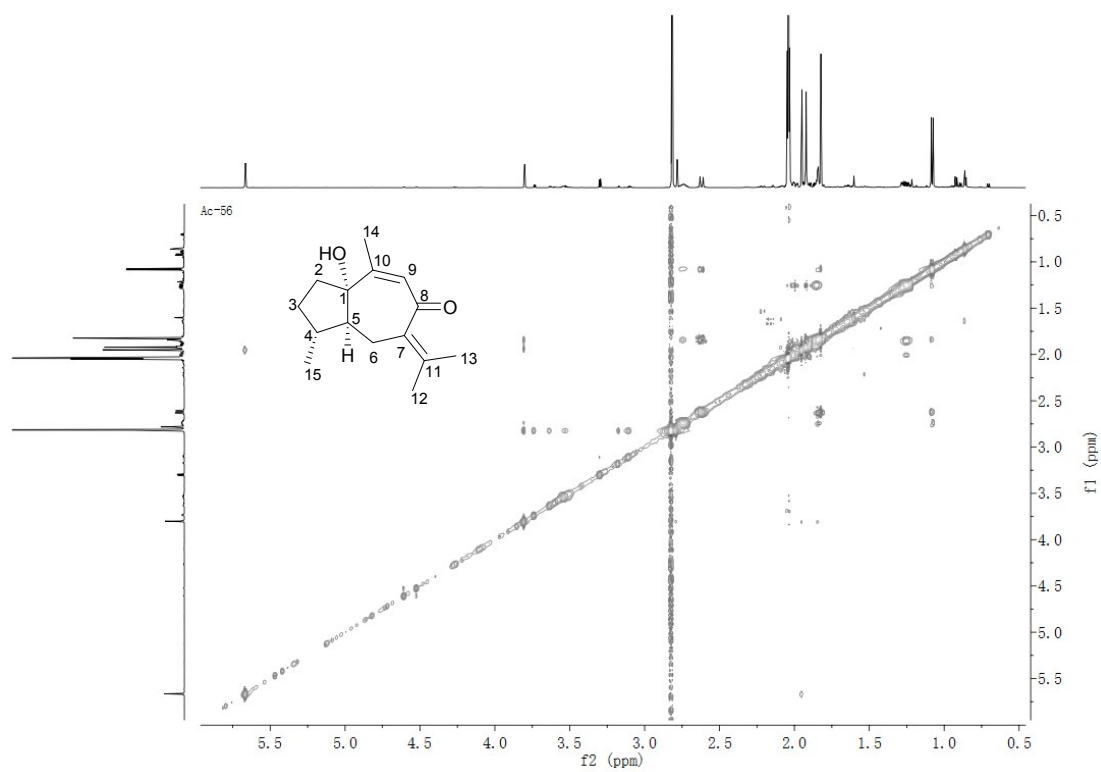


Figure S40. NOESY spectrum of compound **4**

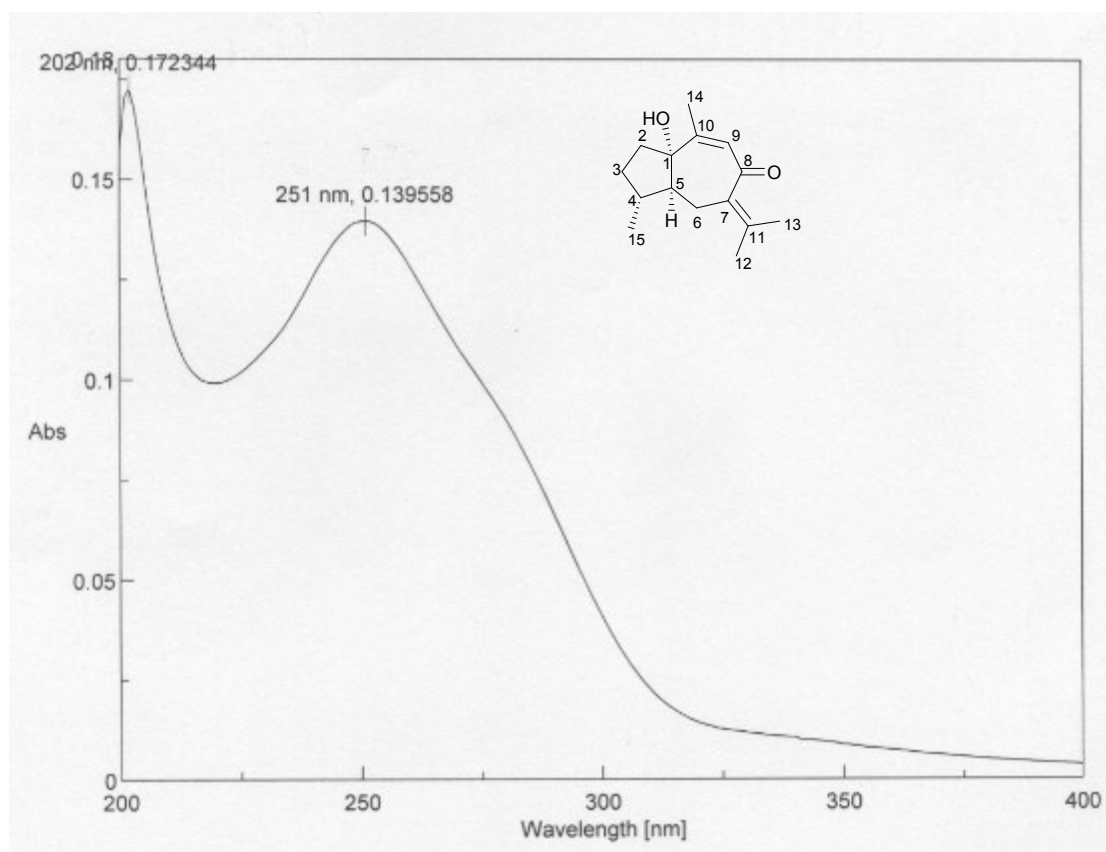


Figure S41. UV spectrum of compound **4**

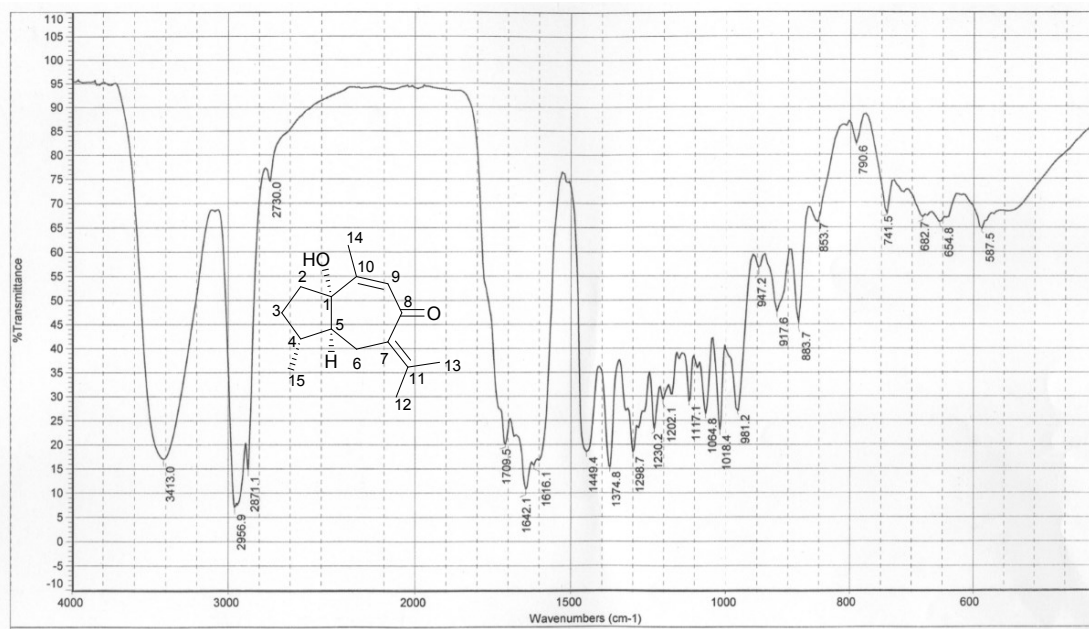


Figure S42. IR spectrum of compound **4**

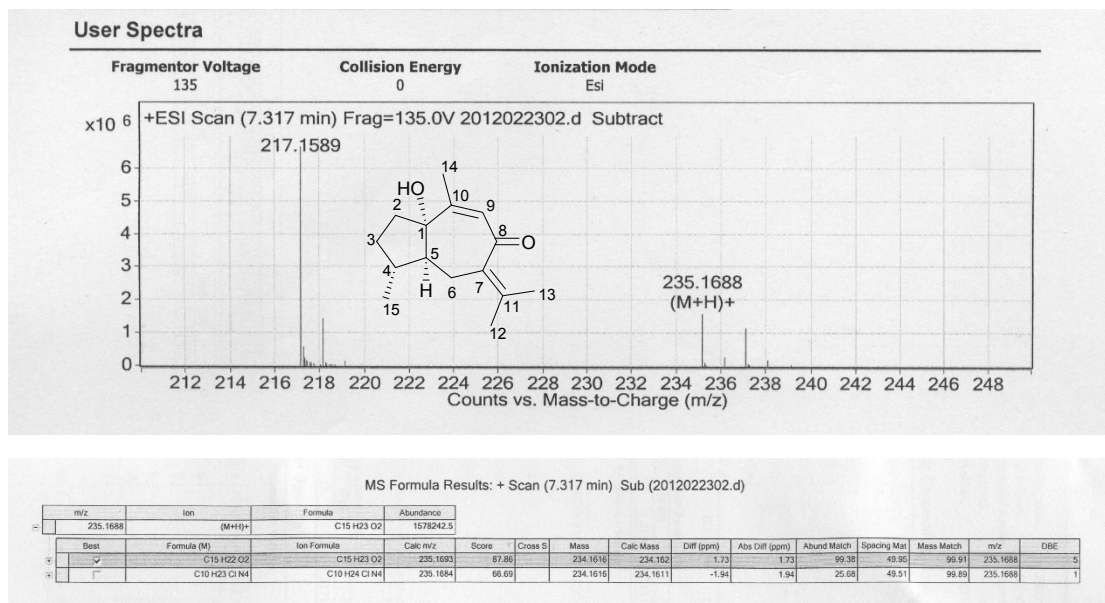


Figure S43. HRESIMS spectrum of compound **4**

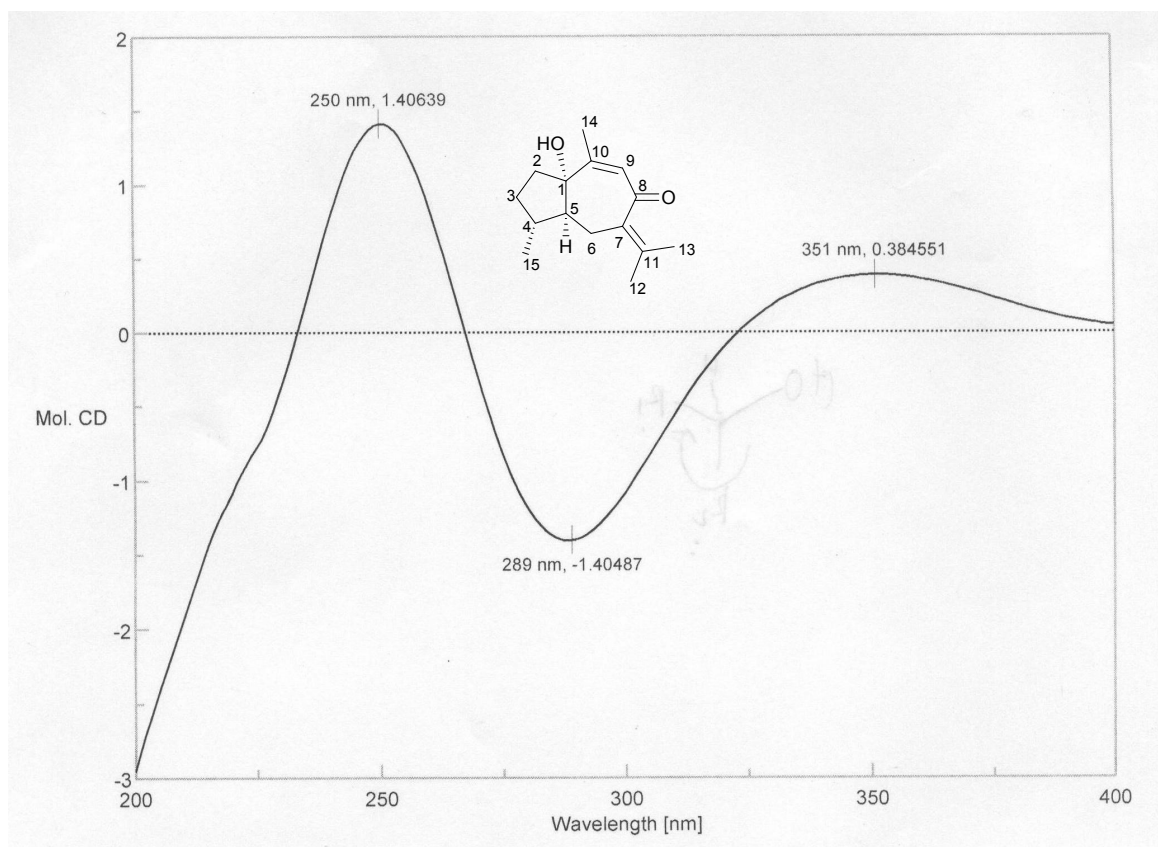


Figure S44. CD spectrum of compound **4**

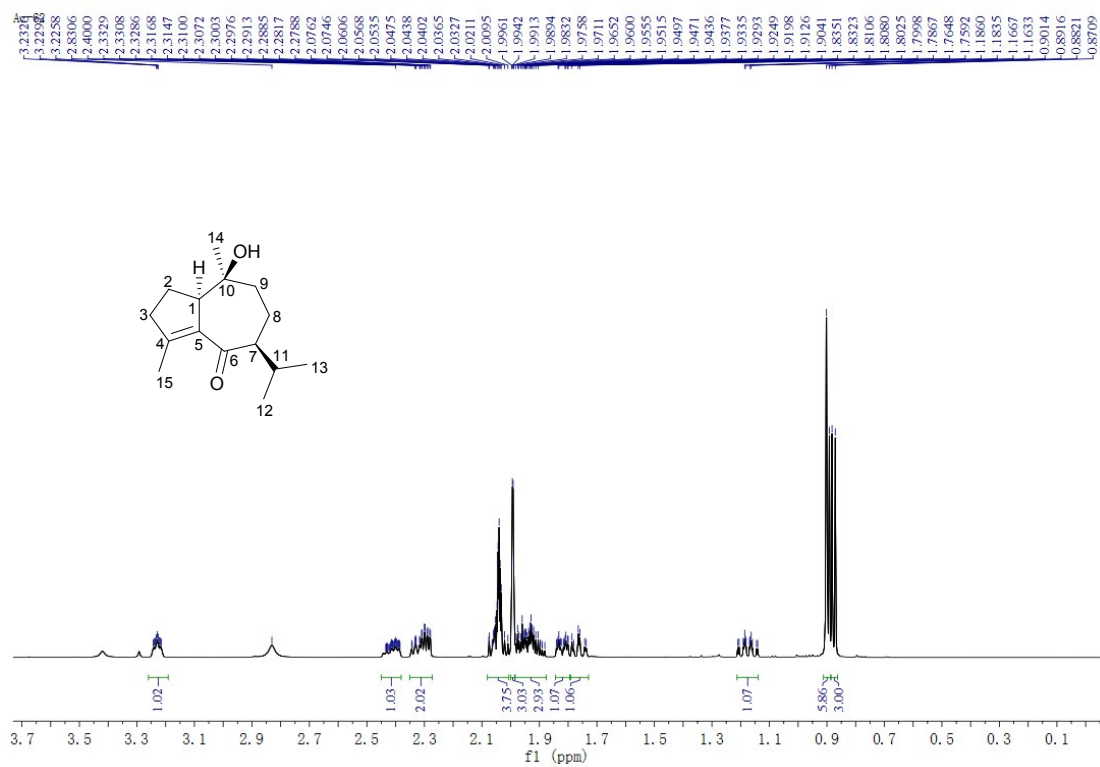


Figure S45. ¹H NMR spectrum of compound **5** (600 MHz, CD₃COCD₃)

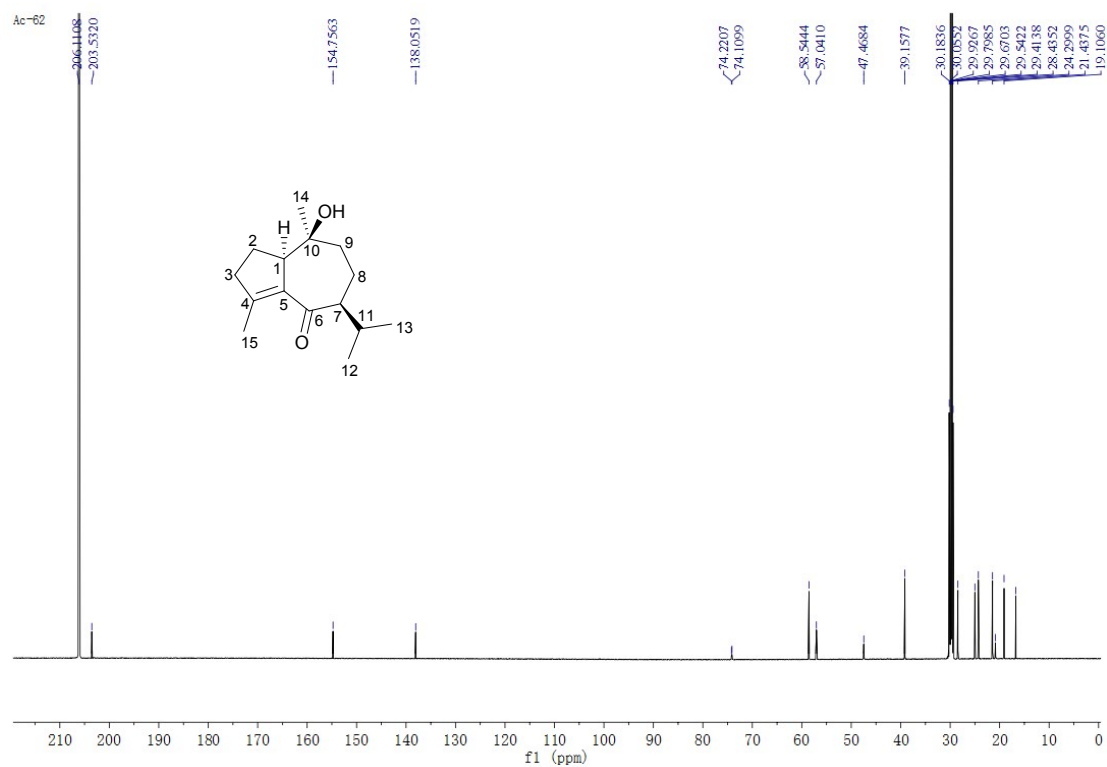


Figure S46. ¹³C NMR spectrum of compound **5** (150 MHz, CD₃COCD₃)

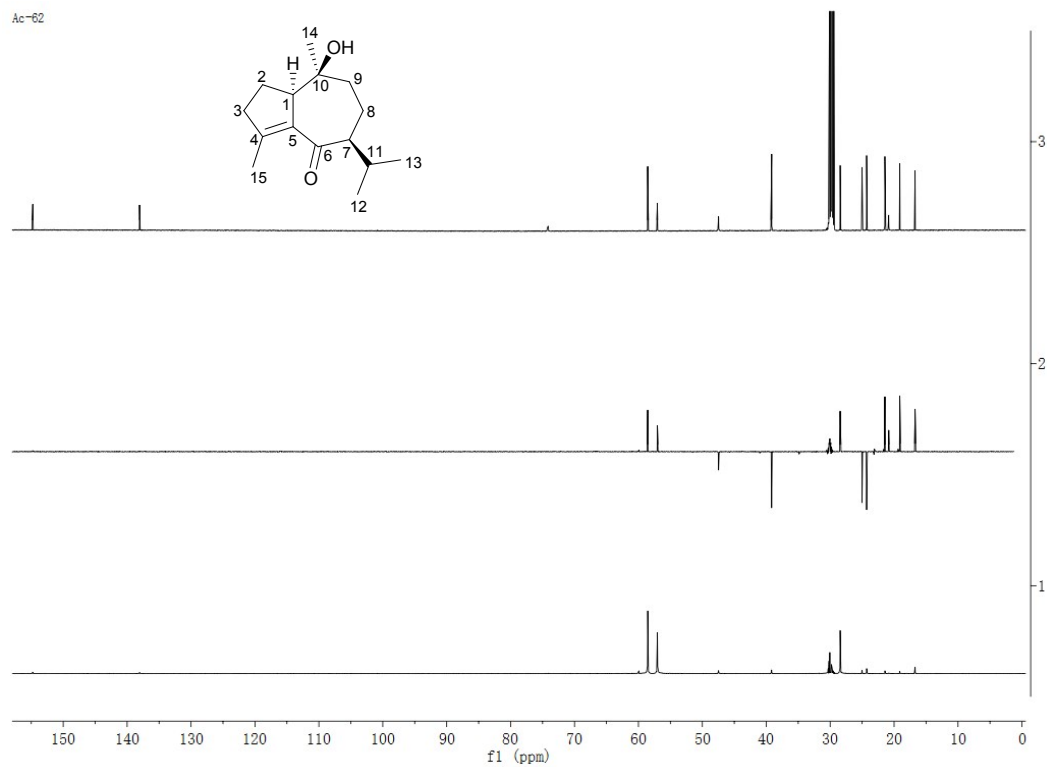


Figure S47. DEPT spectrum of compound 5

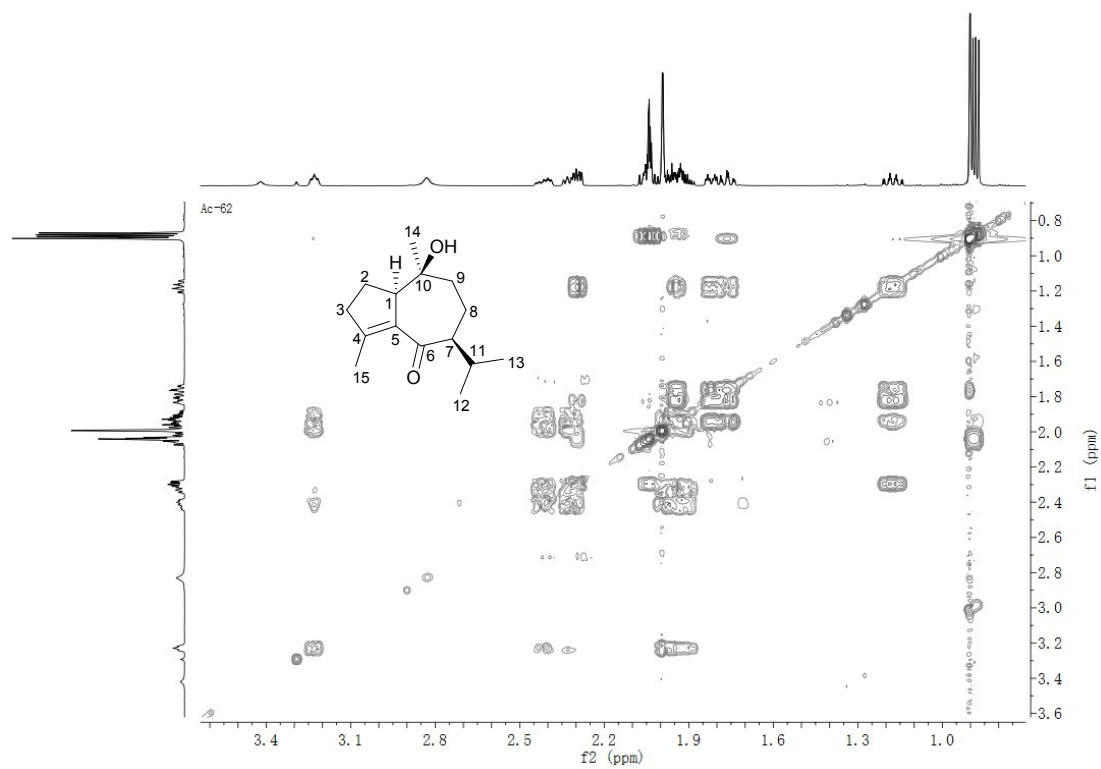


Figure S48. ^1H - ^1H COSY spectrum of compound 5

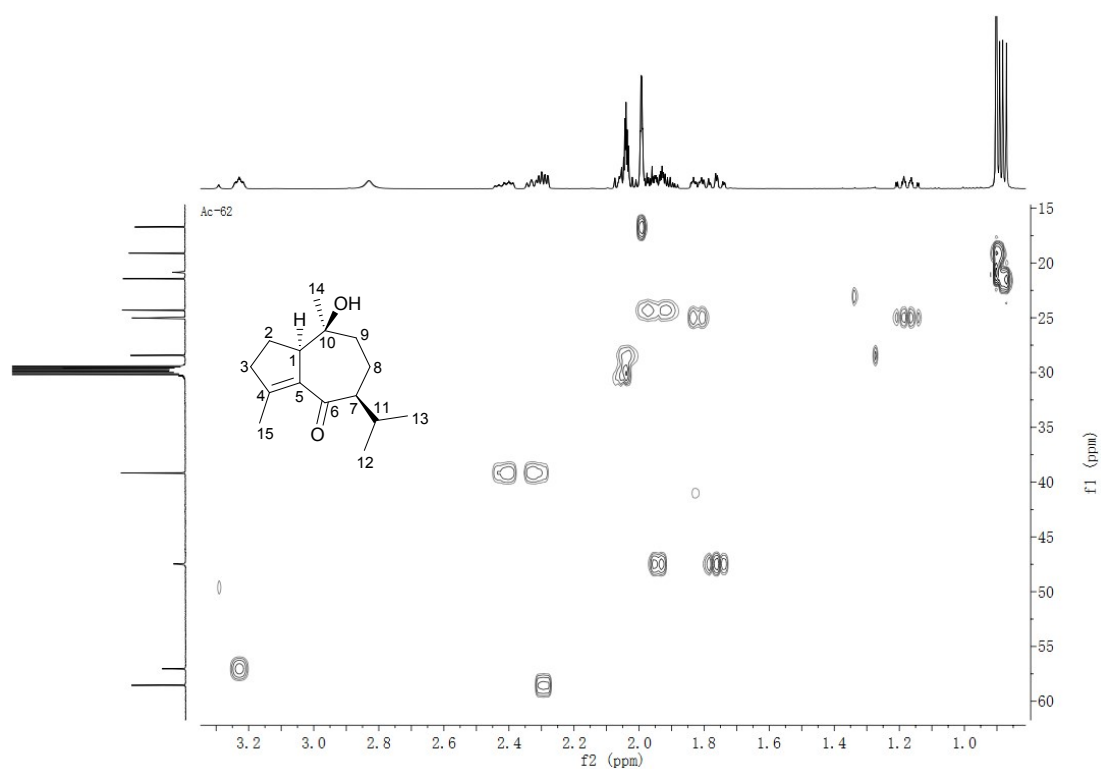


Figure S49. HSQC spectrum of compound 5

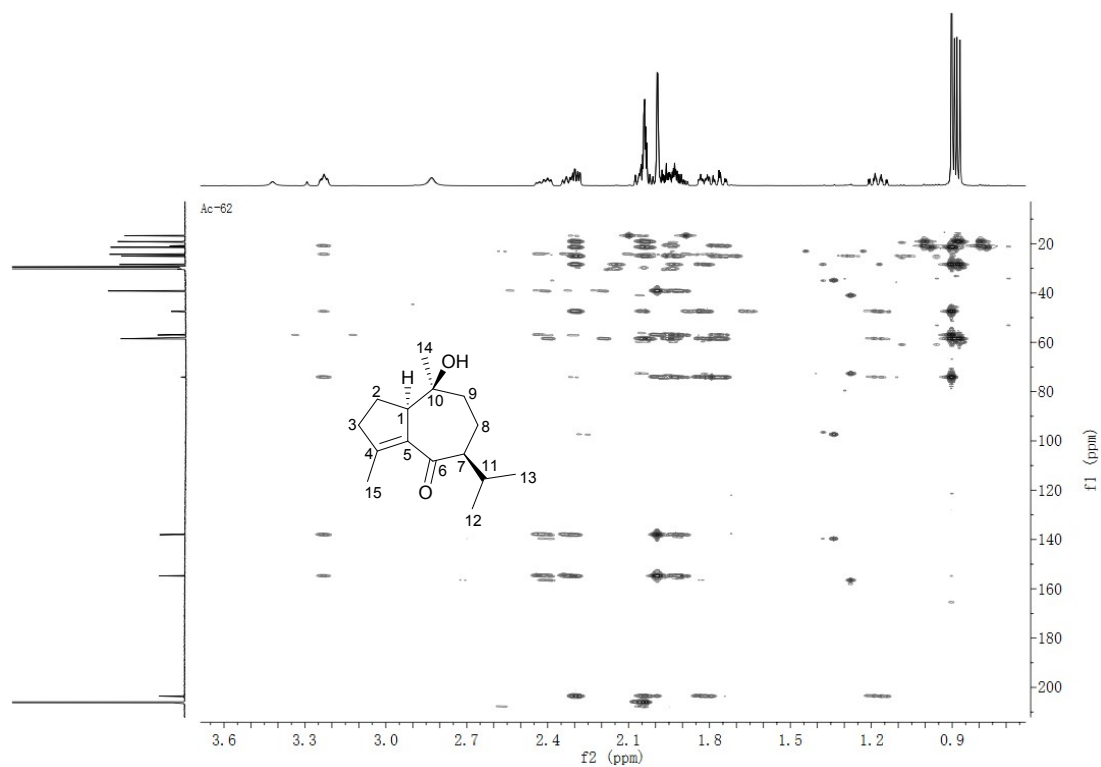


Figure S50. HMBC spectrum of compound 5

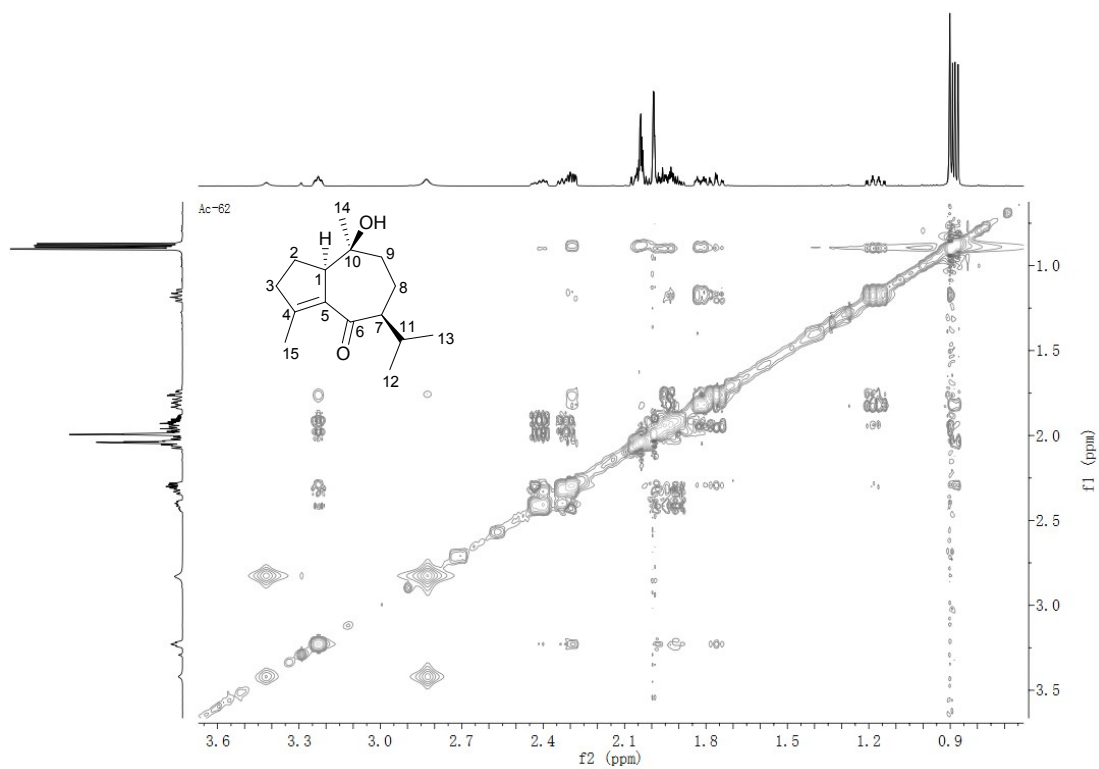


Figure S51. NOESY spectrum of compound **5**

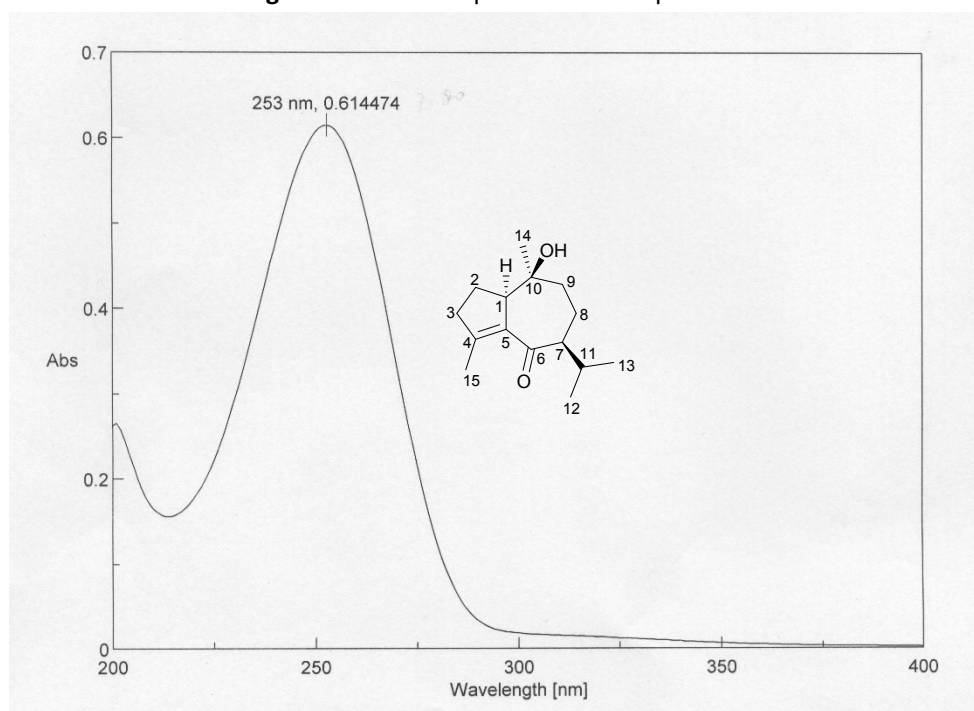


Figure S52. UV spectrum of compound **5**

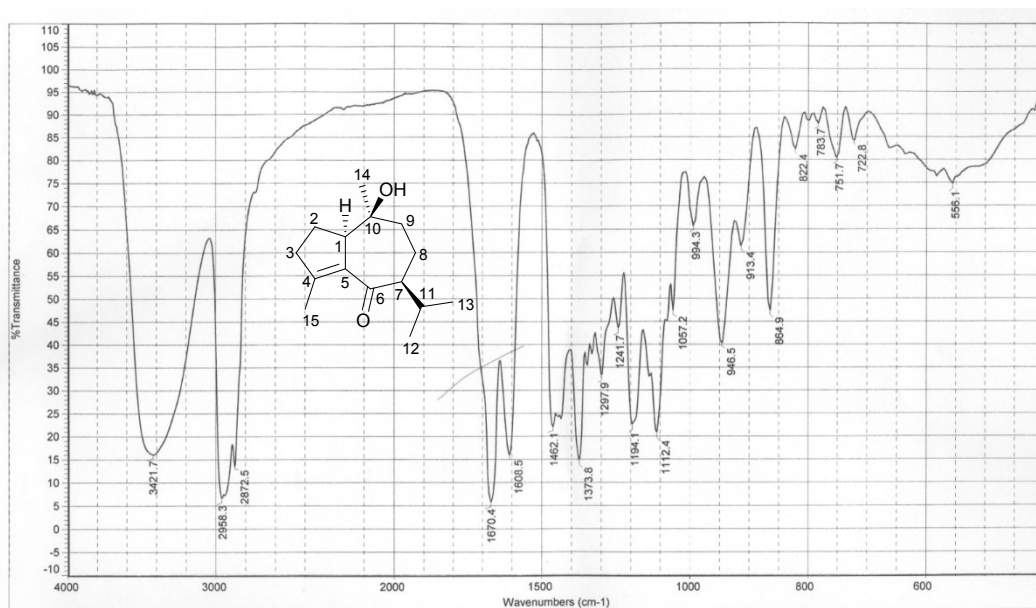


Figure S53. IR spectrum of compound 5

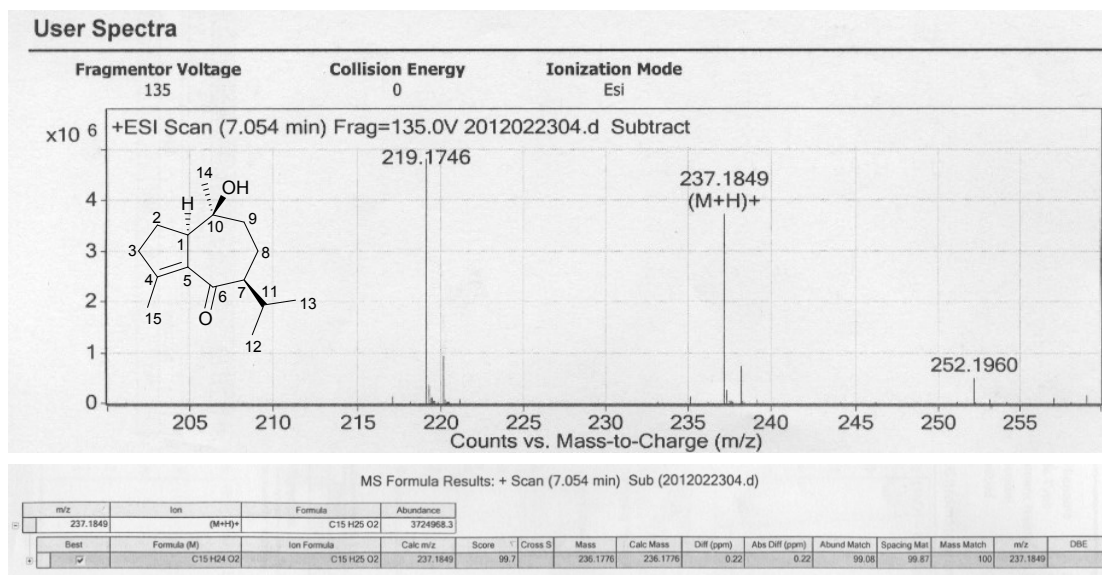


Figure S54. HRESIMS spectrum of compound 5

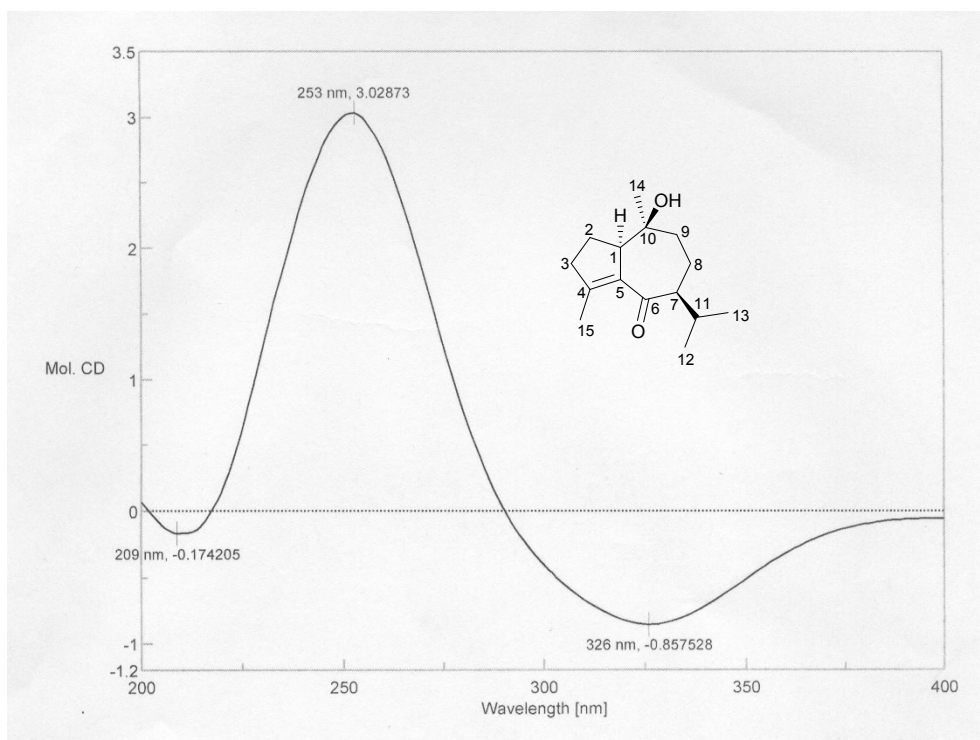


Figure S55. CD spectrum of compound **5**

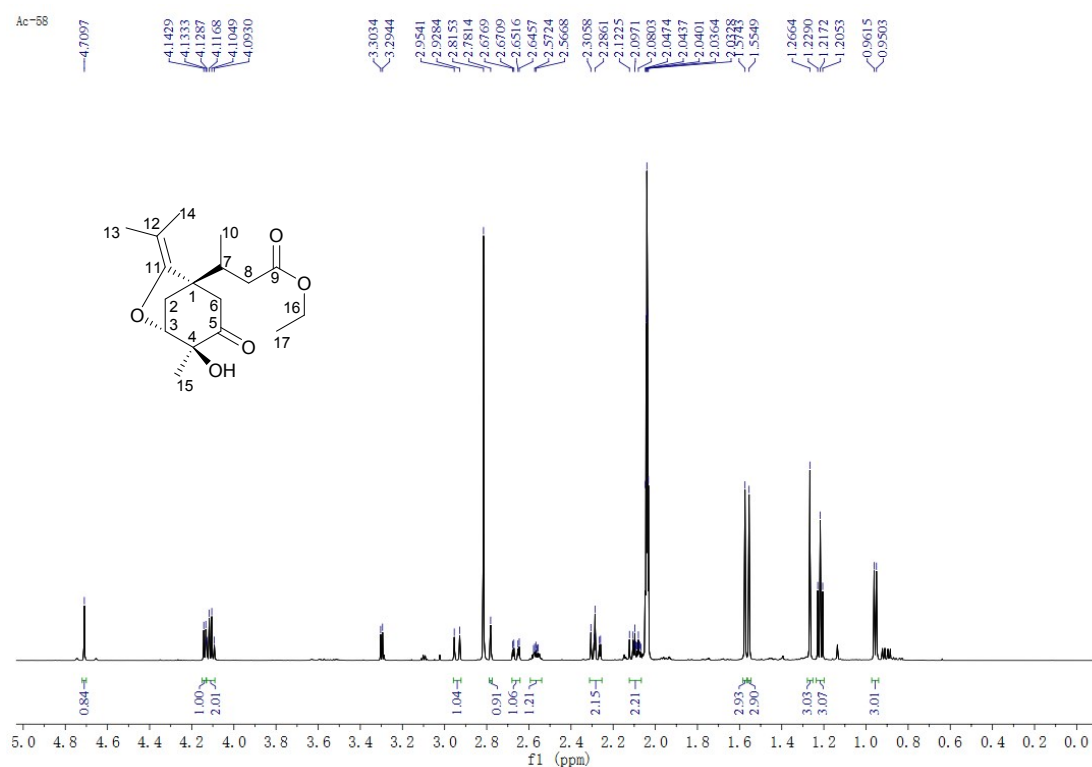


Figure S56. ^1H NMR spectrum of compound **6** (600 MHz, CD_3COCD_3)

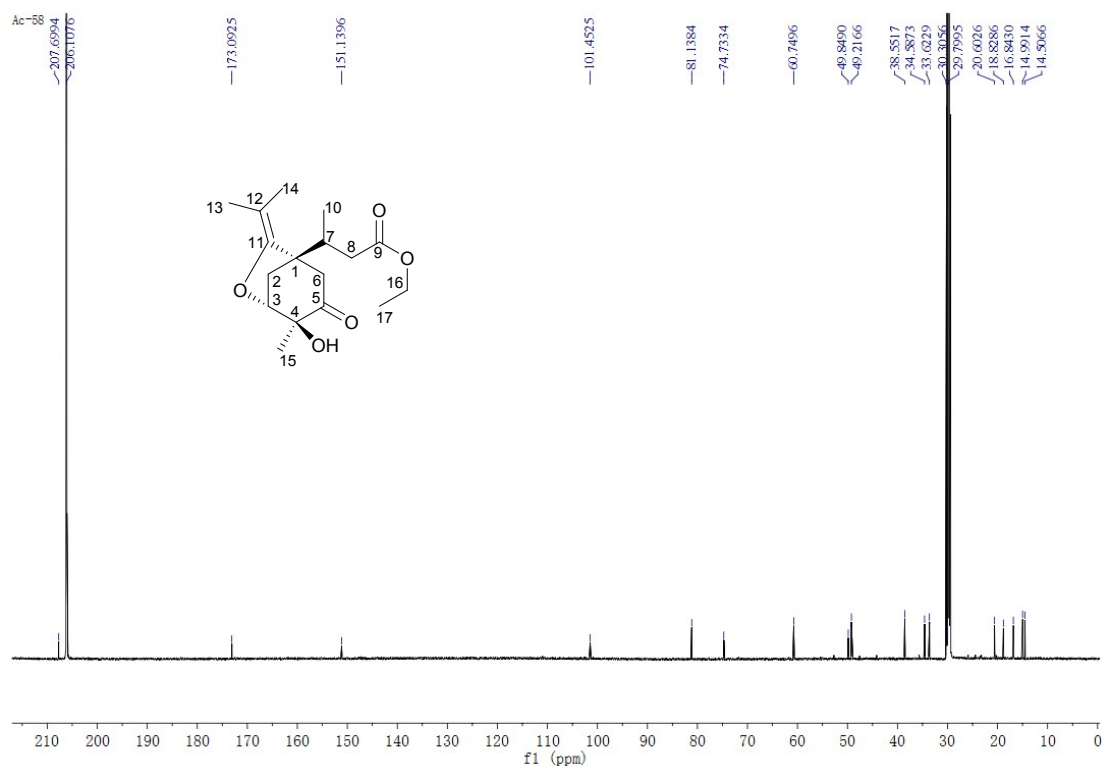


Figure S57. ^{13}C NMR spectrum of compound **6** (150 MHz, CD_3COCD_3)

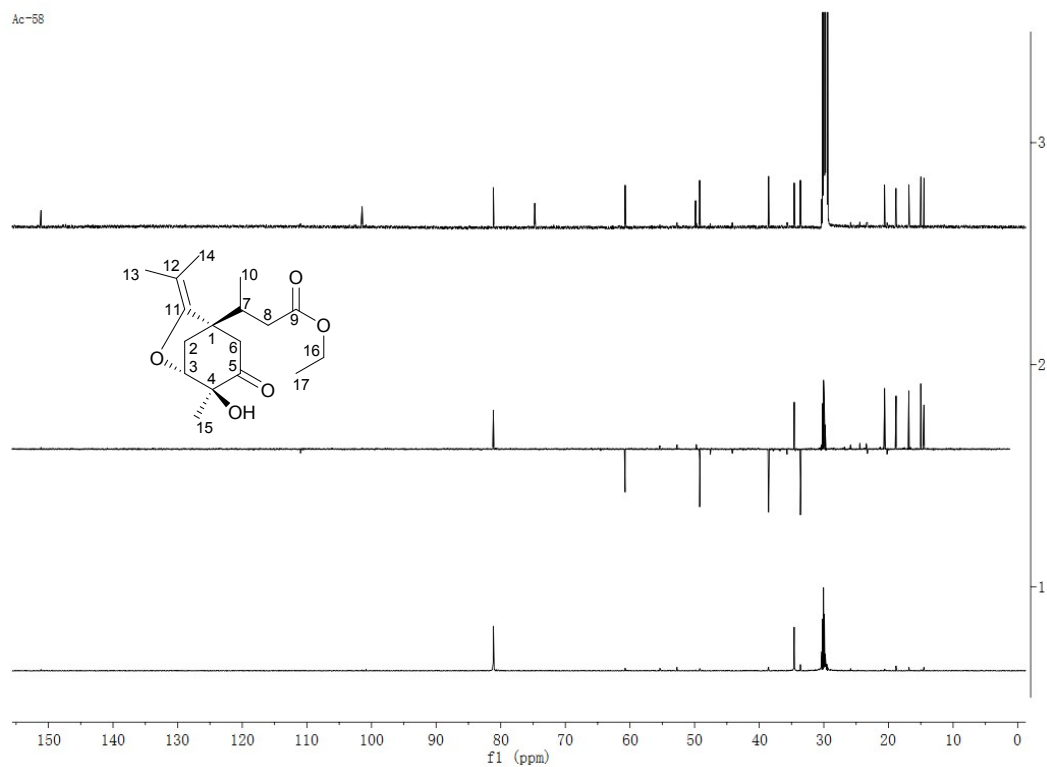


Figure S58. DEPT spectrum of compound **6**

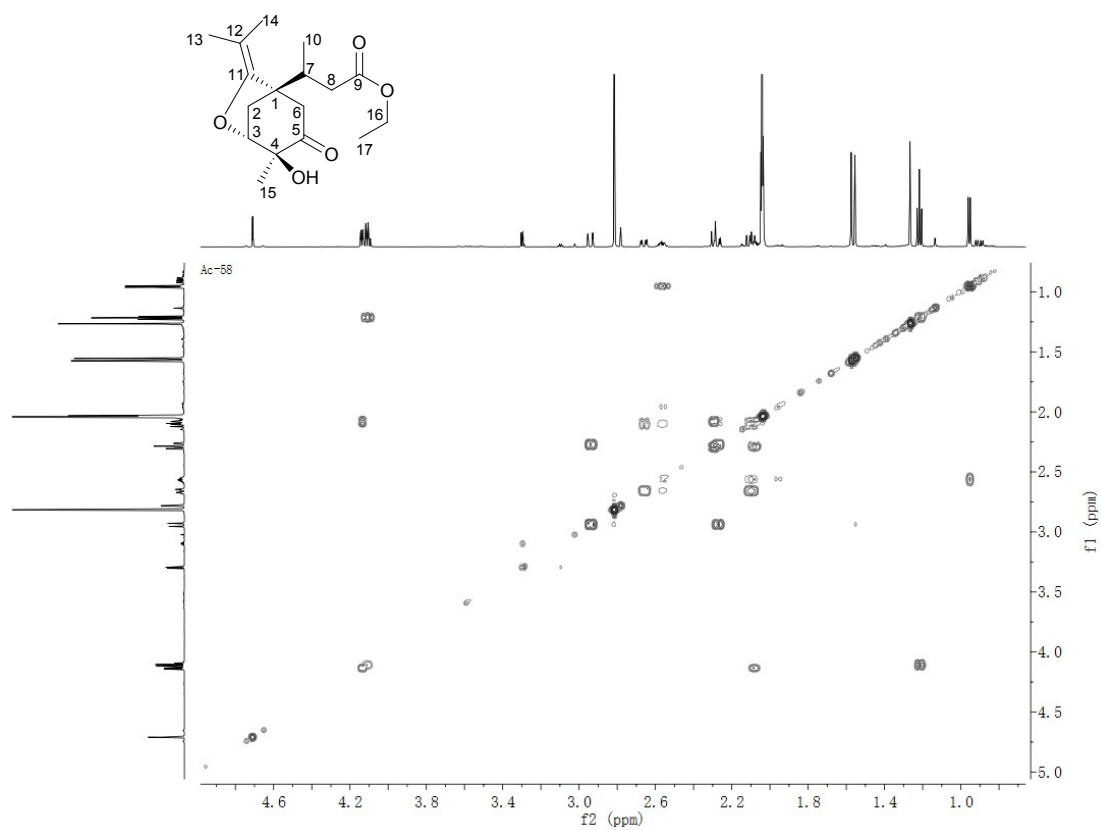


Figure S59. ^1H - ^1H COSY spectrum of compound **6**

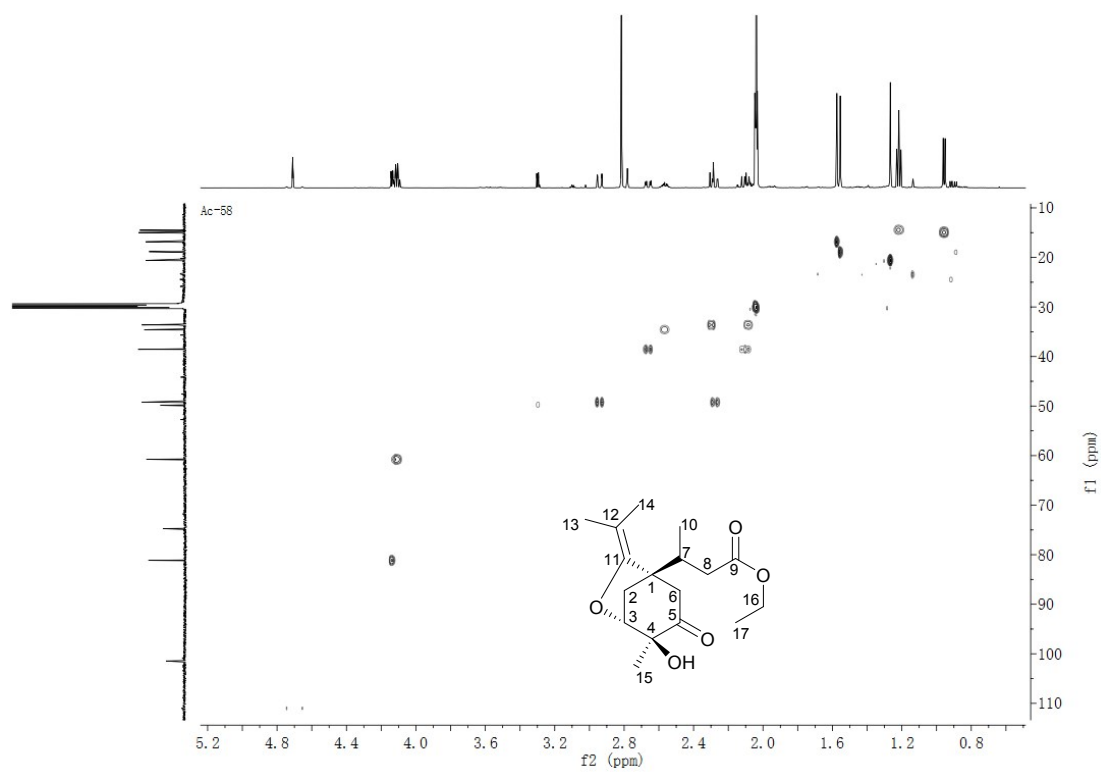


Figure S60. HSQC spectrum of compound **6**

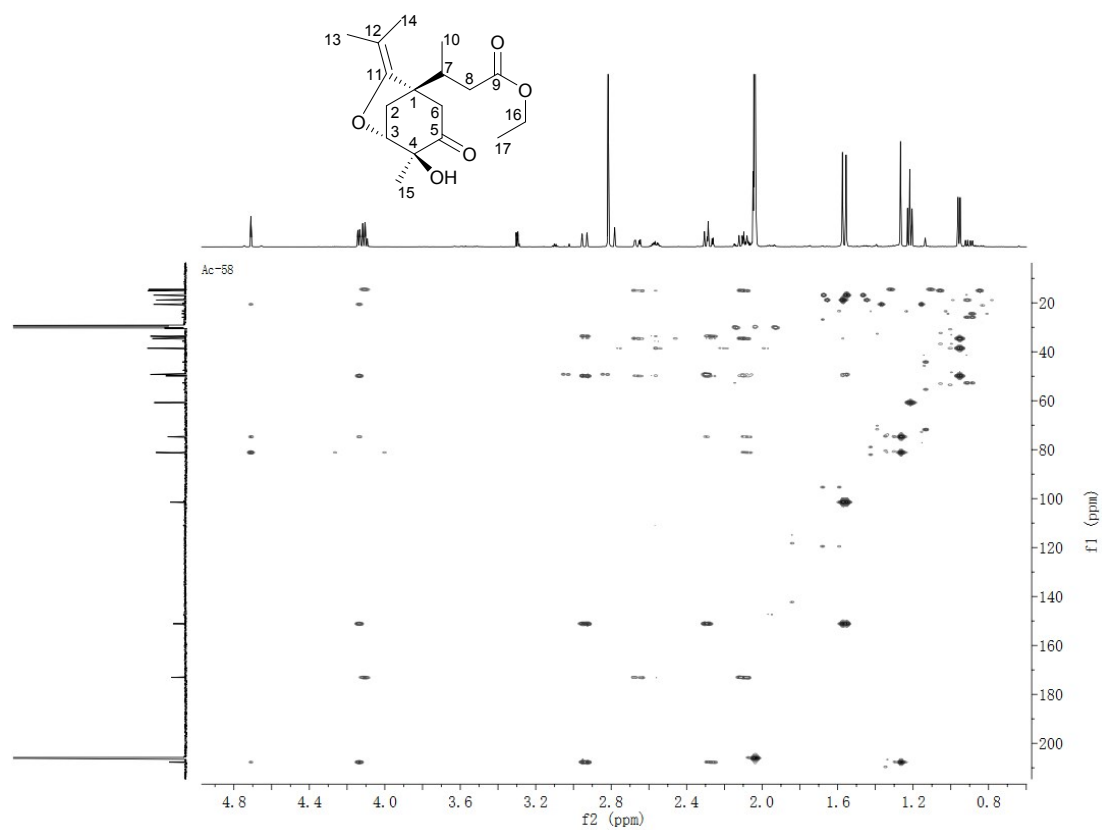


Figure S61. HMBC spectrum of compound 6

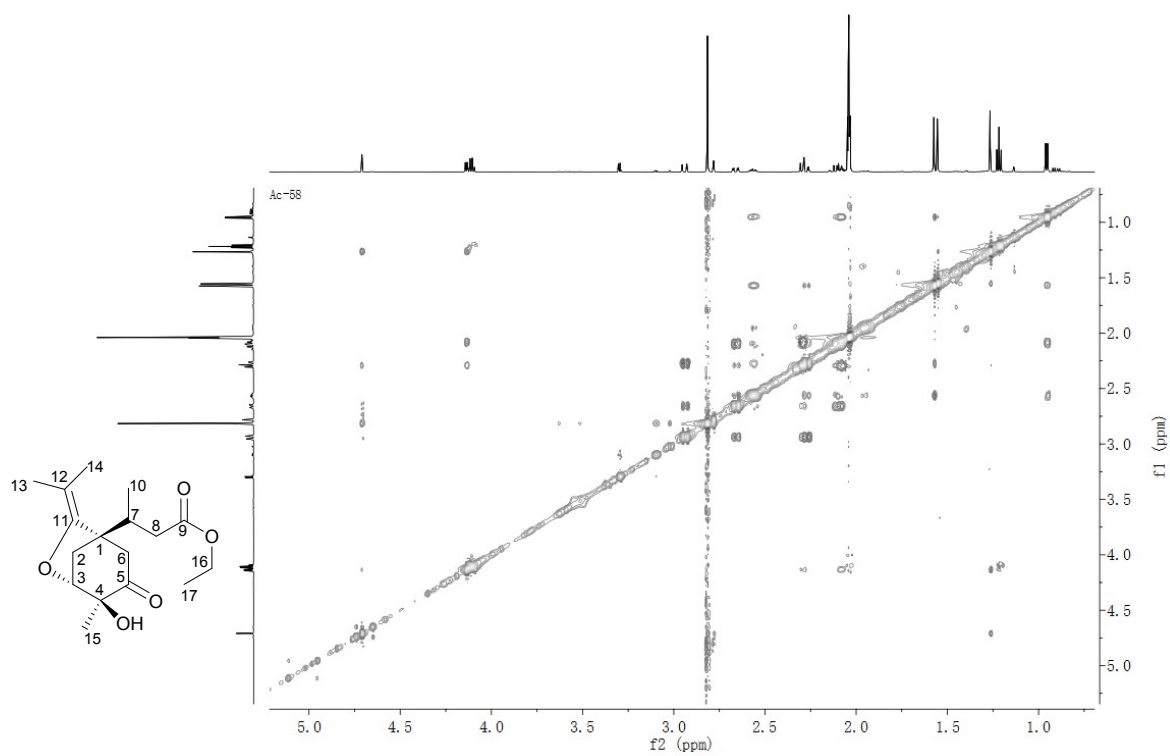


Figure S62. NOESY spectrum of compound 6

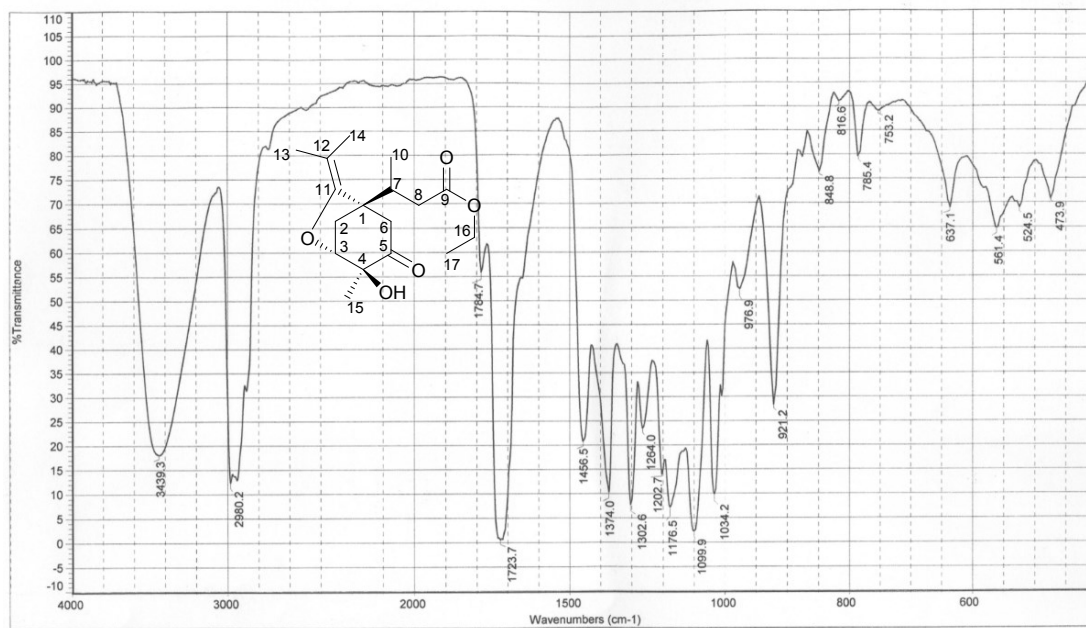


Figure S63. IR spectrum of compound 6

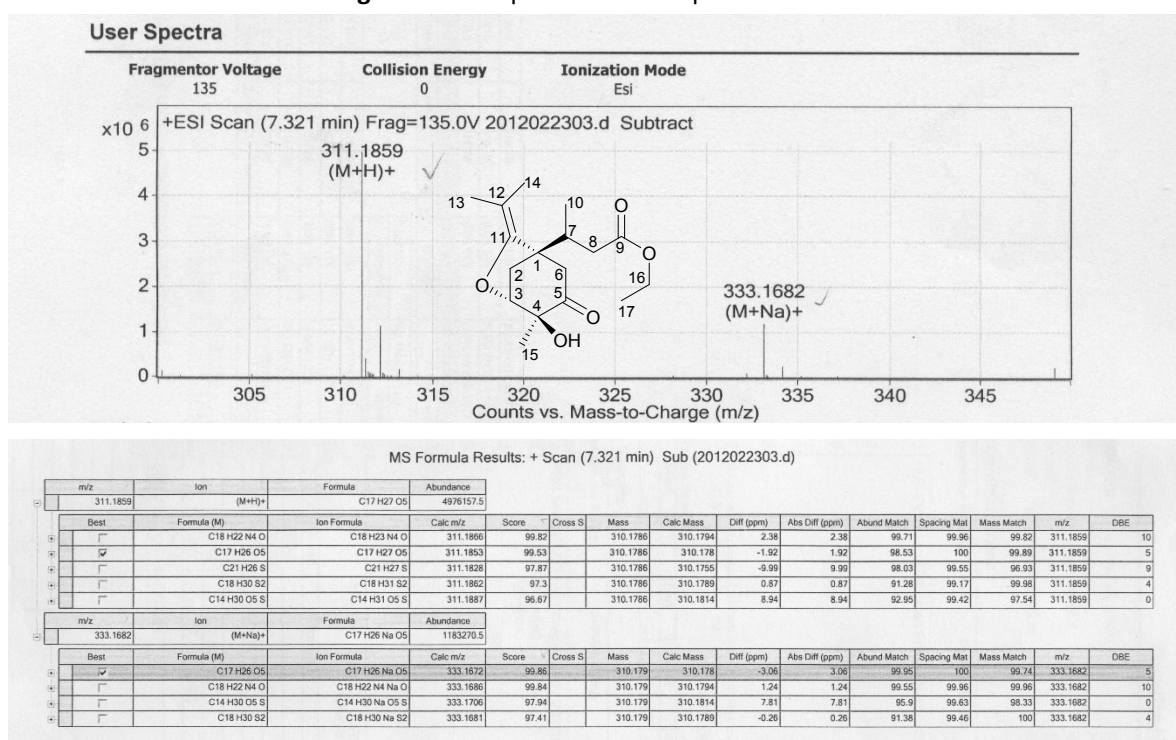


Figure S64. HRESIMS spectrum of compound 6

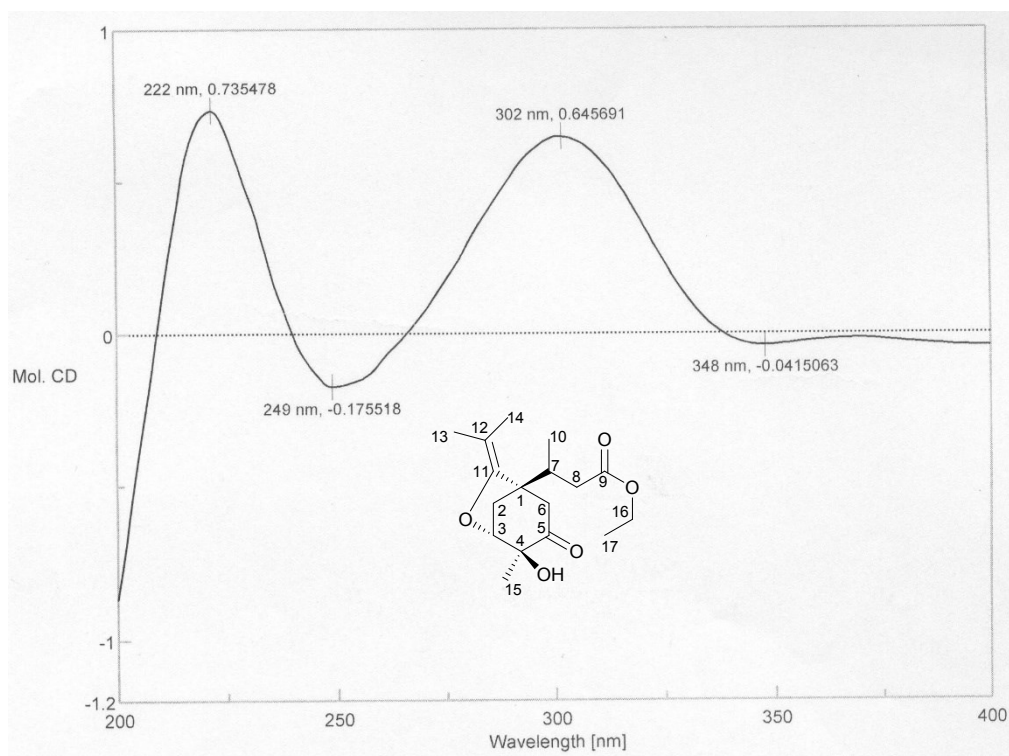


Figure S65. CD spectrum of compound **6**

Table S1. DP4+ probability analysis of compound **6a** (Isomer 1) and **6b** (Isomer 2)

Functional mPW1PW91		Solvent? PCM	Basis Set 6-311G(d,p)		Type of Data Unscaled Shifts		
		DP4+	100.00%	0.00%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
c		49.8	53.0	53.6			
c		33.6	36.4	37.1			
c		81.1	83.6	83.7			
c		74.7	76.6	76.6			
c	x	207.7	216.8	217.1			
c		49.2	52.5	52.3			
c		34.6	38.0	37.6			
c		38.6	40.7	38.8			
c	x	173.1	180.1	180.6			
c		15	15.7	17.3			
c	x	151.1	158.3	158.6			
c	x	101.5	111.00	111.07			
c		18.8	18.42	18.27			
c		16.8	20.24	20.35			
c		20.6	21.18	21.10			
c		60.7	64.44	64.38			
c		14.5	15.87	15.84			
h		2.08	2.17	2.08			
h		2.29	2.20	2.28			
h		4.14	4.22	4.21			
h		2.28	2.82	3.26			
h		2.94	2.68	2.38			
h		2.57	2.60	2.59			
h		2.1	2.11	2.75			
h		2.66	2.64	2.13			
h		0.96	0.87	0.62			
h		0.96	0.82	1.2			
h		0.96	1.04	1.1			
h		1.56	2.06	1.84			
h		1.56	1.44	1.5			
h		1.56	1.5	1.41			
h		1.57	1.3	1.64			
h		1.57	1.87	2.02			
h		1.57	1.83	1.3			
h		1.27	1.65	1.67			
h		1.27	0.94	0.9			
h		1.27	1.36	1.37			
h		4.12	4.22	4.03			
h		4.12	4.13	4.22			
h		1.22	1.29	1.26			
h		1.22	1.36	1.26			
h		1.22	1.23	1.34			
DP4+ (H data)		100.00%	0.00%				
DP4+ (C data)		93.42%	6.58%				
DP4+ (all data)		100.00%	0.00%				