

Supplementary Information

Ent*-abietane diterpenoids and their probable biogenetic precursors from the roots of *Euphorbia fischeriana

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Table 1. The 3D conformers of (5*R*,7*R*,9*S*,10*R*)-1 with Boltzmann distribution over 1%.

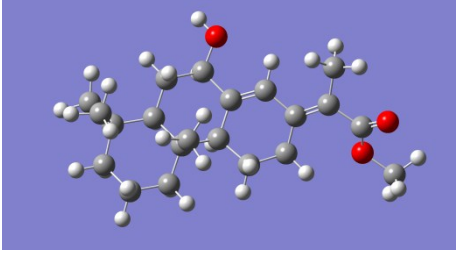
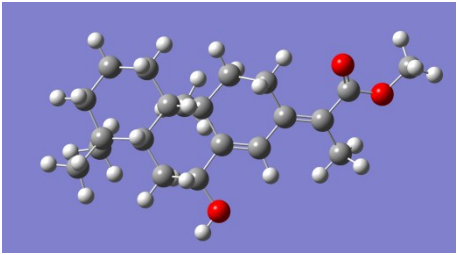
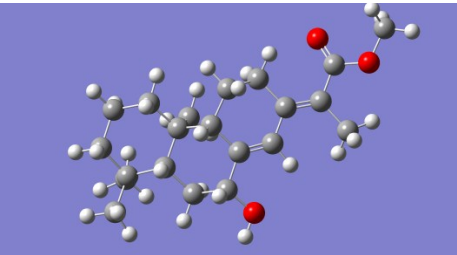
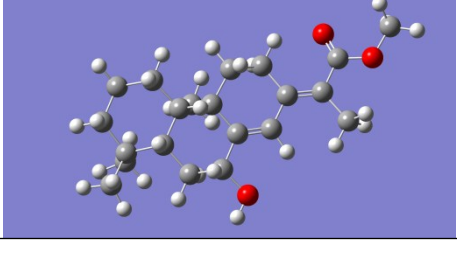
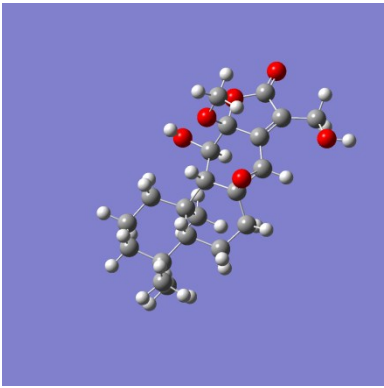
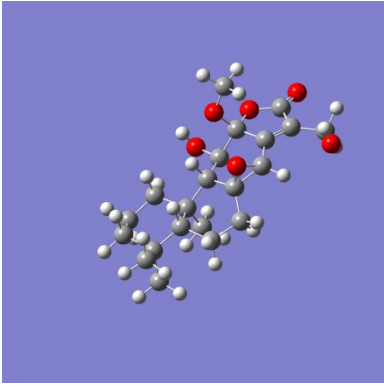
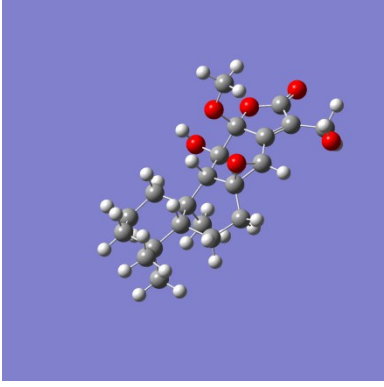
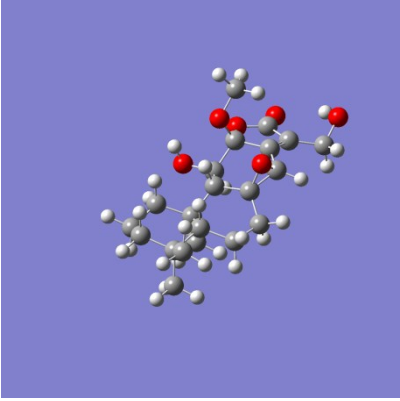
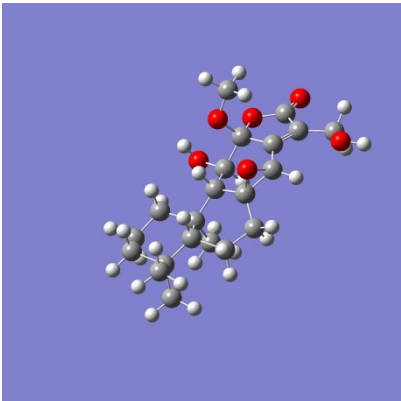
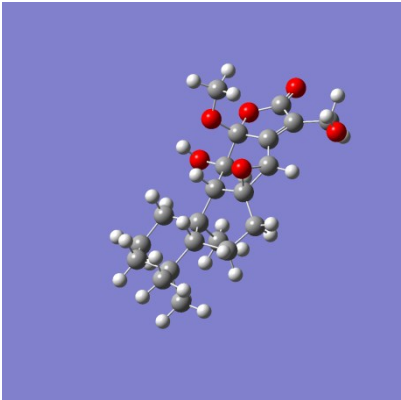
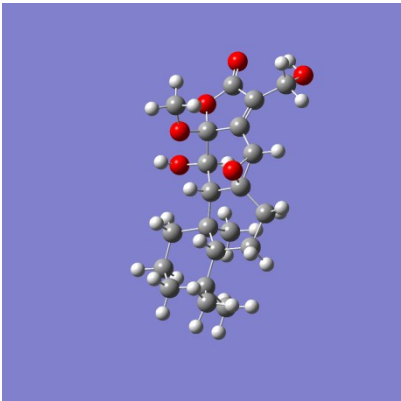
No.	Conformer	Population (%)
1		49.3
2		41.4
3		5.3
4		3.7

Table 2. The 3D conformers of (5*R*,8*S*,9*R*,12*R*,14*R*)-**5** with Boltzmann distribution over 1%.

No.	Conformer	Population (%)
1		10.63
3		9.58
4		18.98
5		21.23

6		10.62
8		9.59
9		18.99

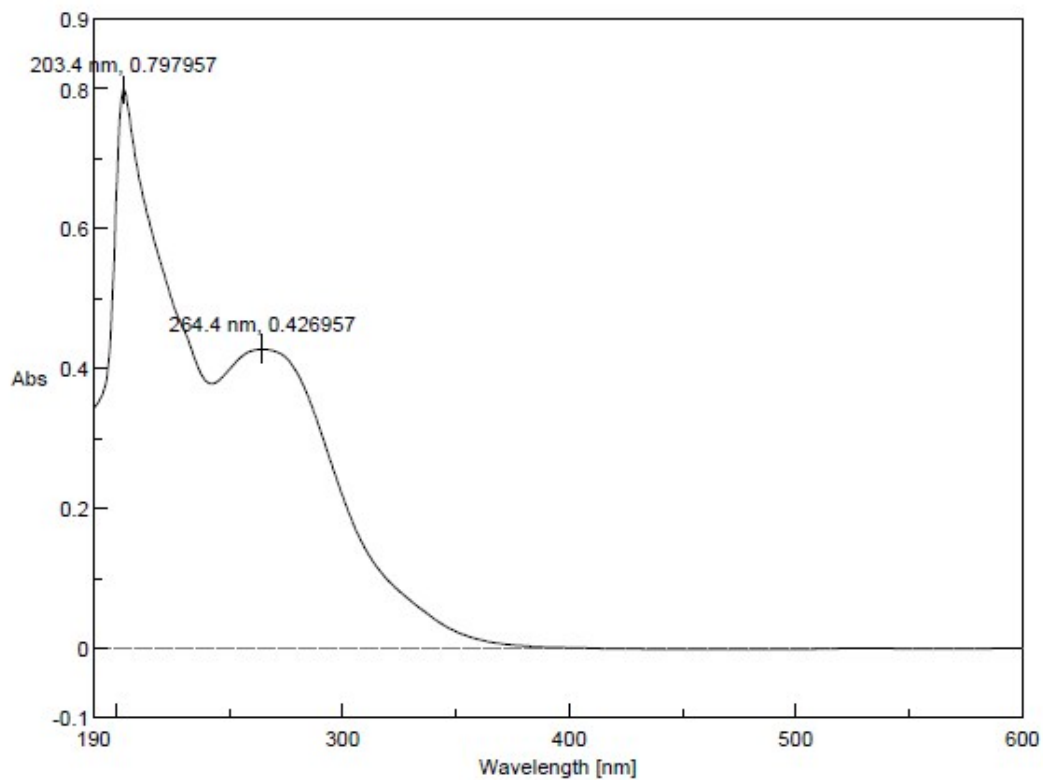


Figure S1. The UV spectrum of compound 1 in MeOH

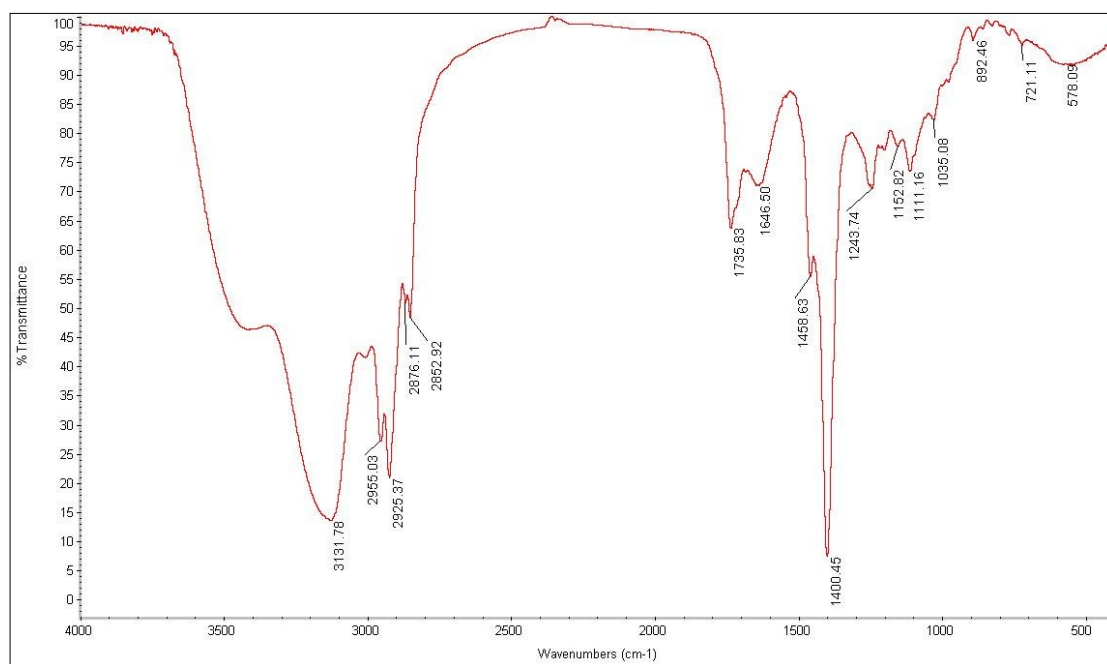


Figure S2. The IR spectrum of compound 1

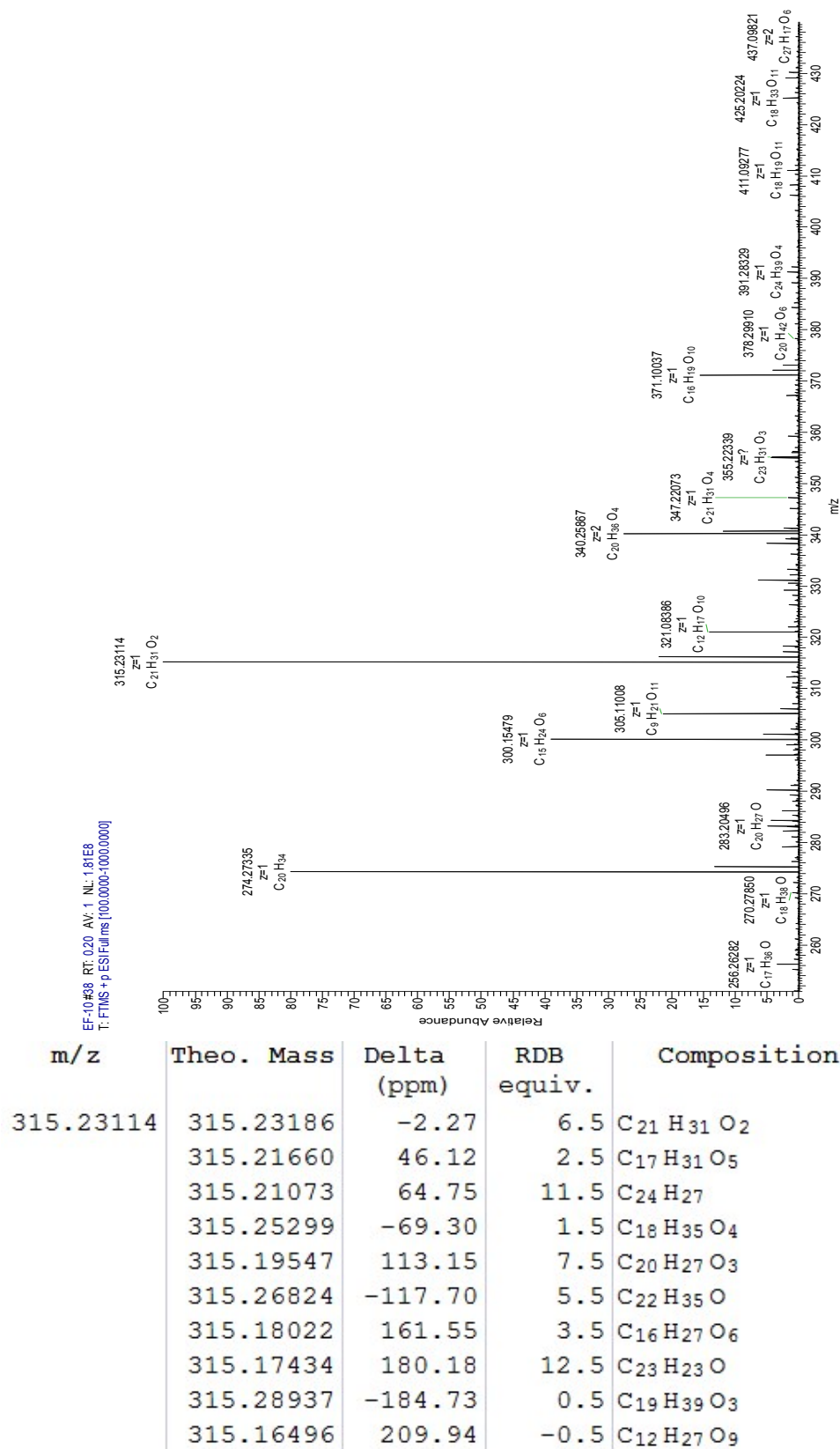


Figure S3. The HRESIMS spectrum of compound 1

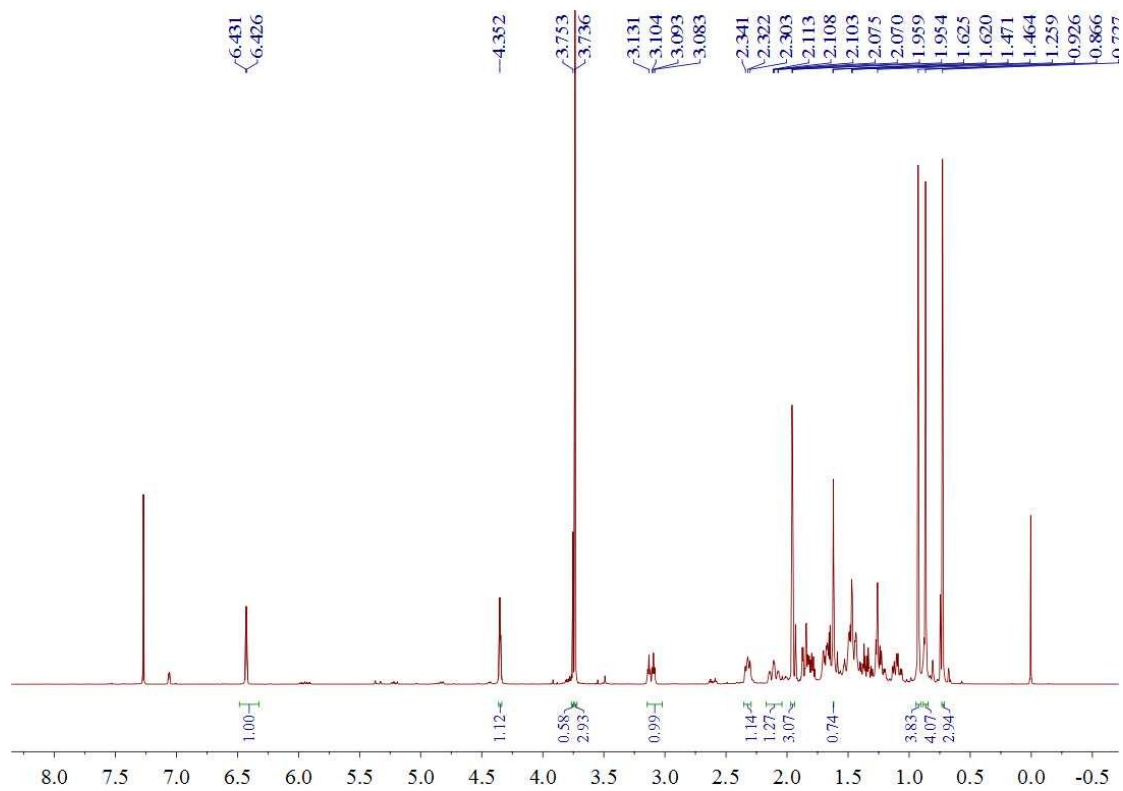


Figure S4. The ^1H NMR spectrum of compound **1** (CDCl_3 , 400 MHz)

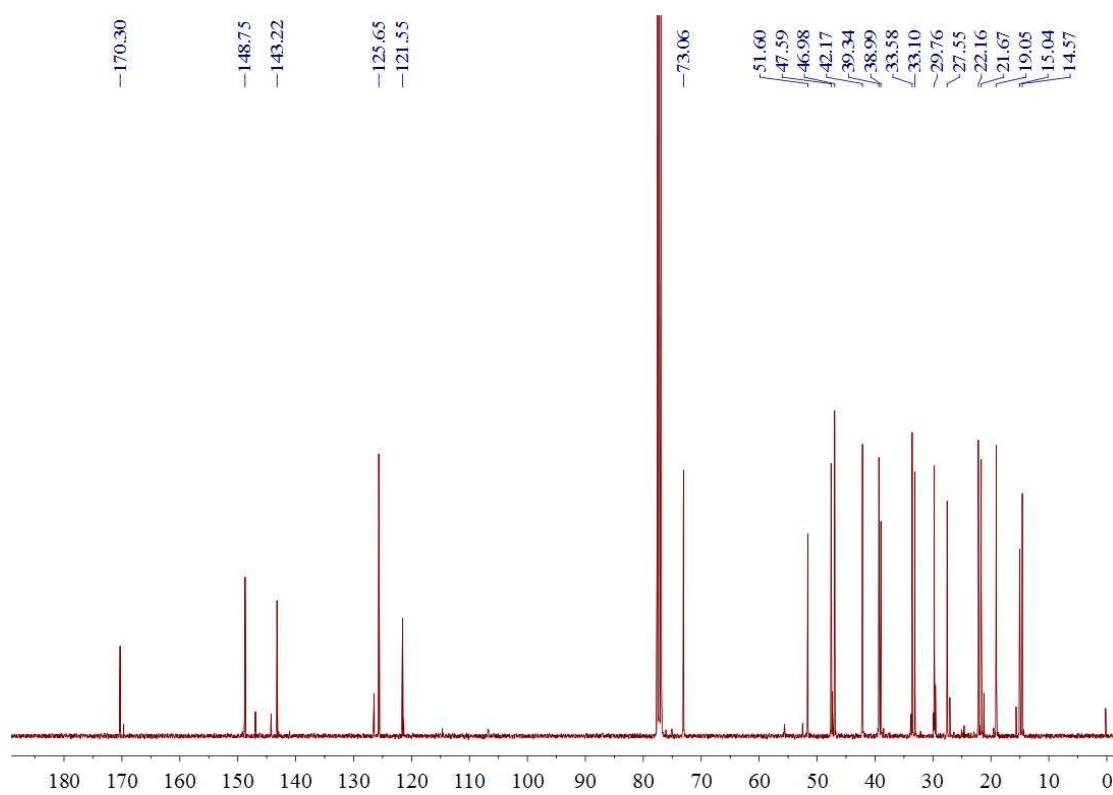


Figure S5. The ^{13}C NMR spectrum of compound **1** (CDCl_3 , 100 MHz)

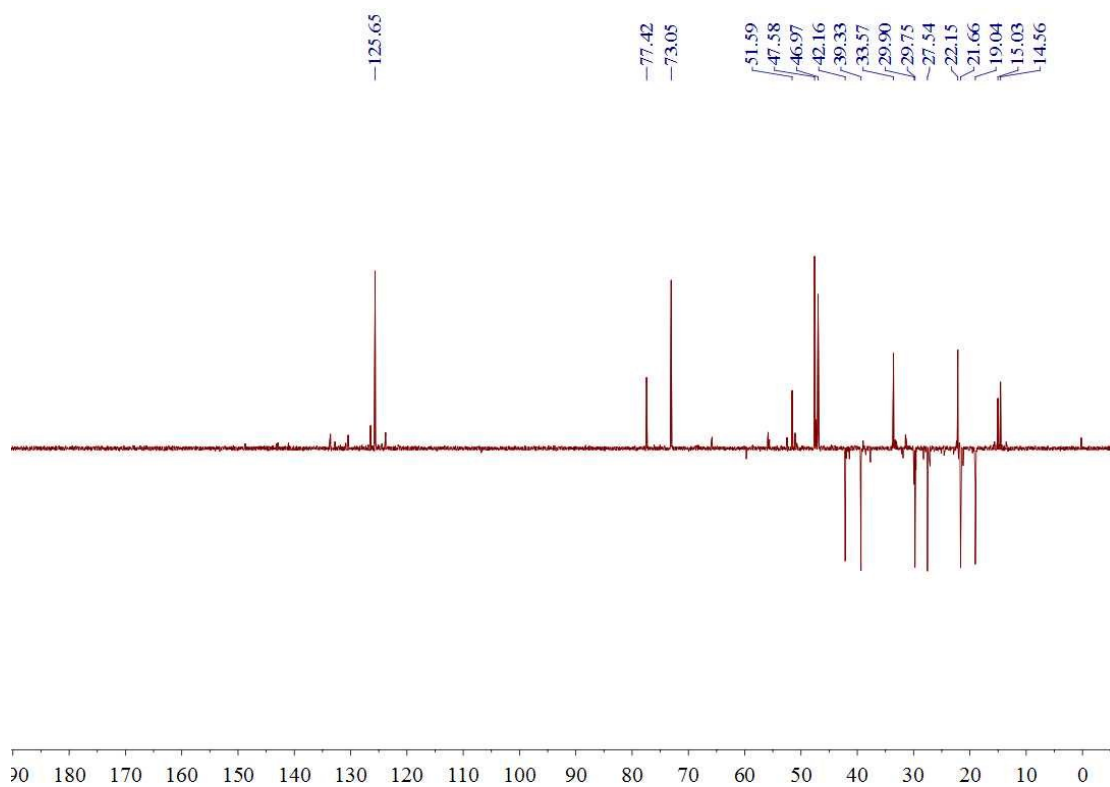


Figure S6. The DEPT-135 spectrum of compound **1** (CDCl_3 , 100 MHz)

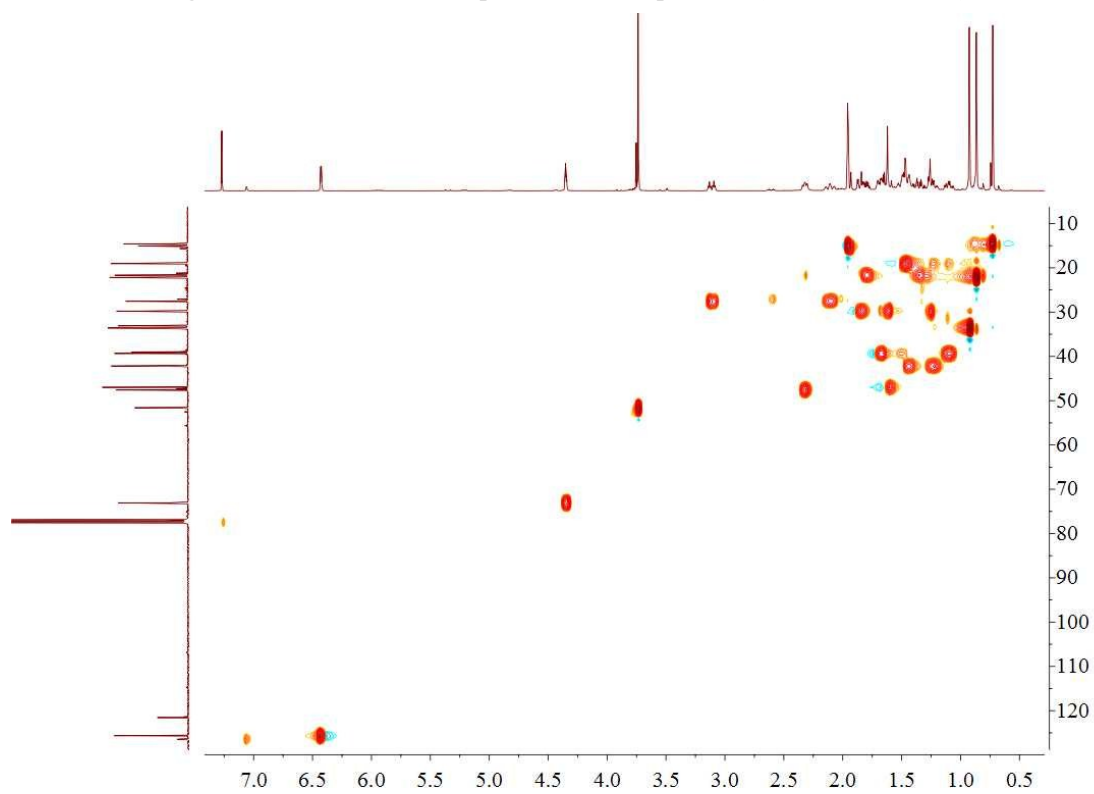


Figure S7. The HSQC spectrum of compound **1**

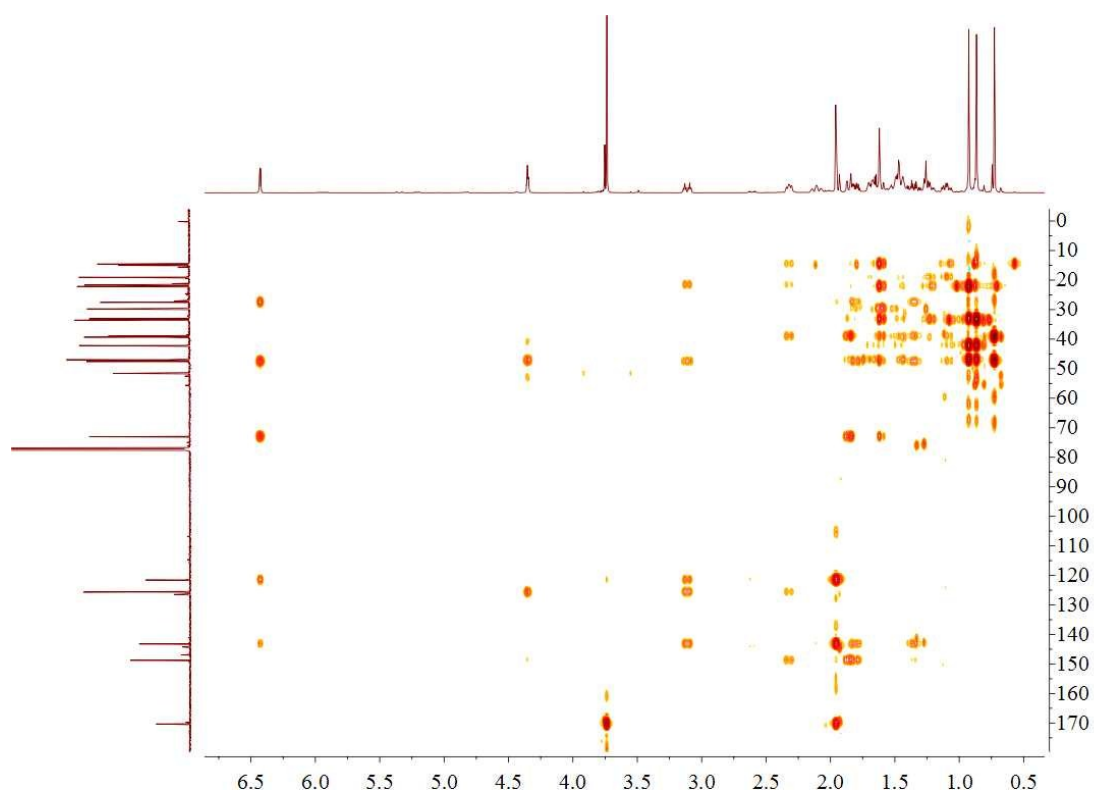


Figure S8. The HMBC spectrum of compound **1**

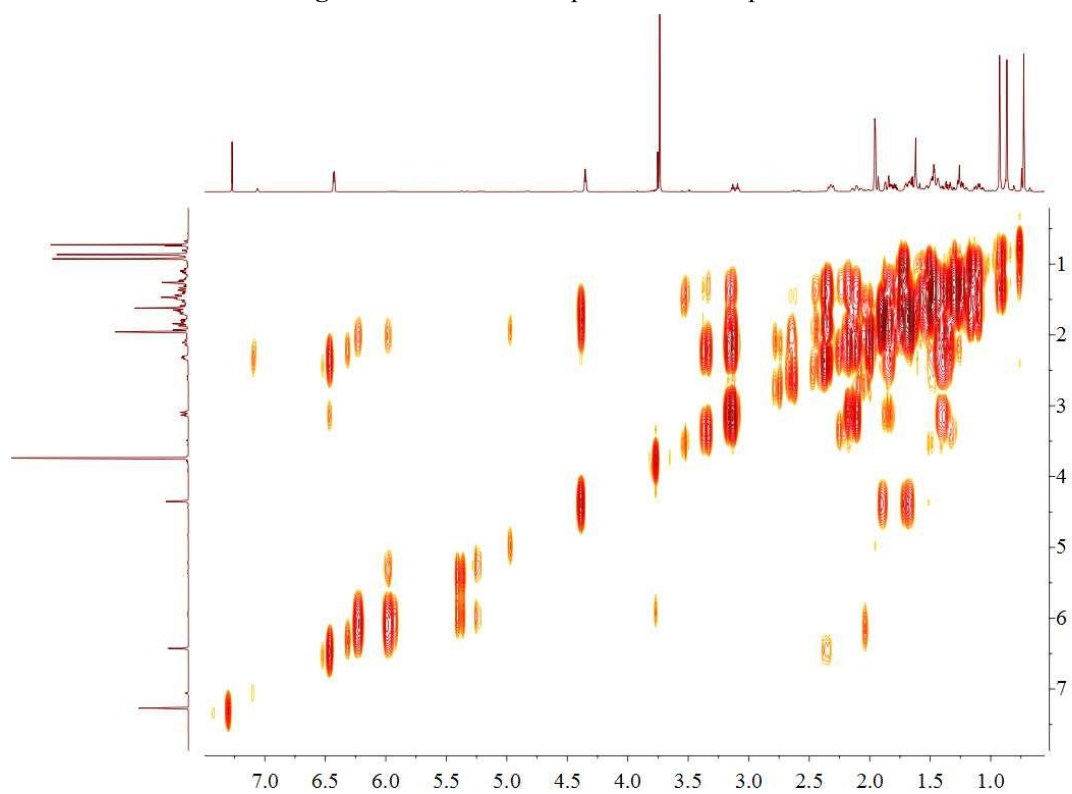


Figure S9. The COSY spectrum of compound **1** (CDCl₃, 400 MHz)

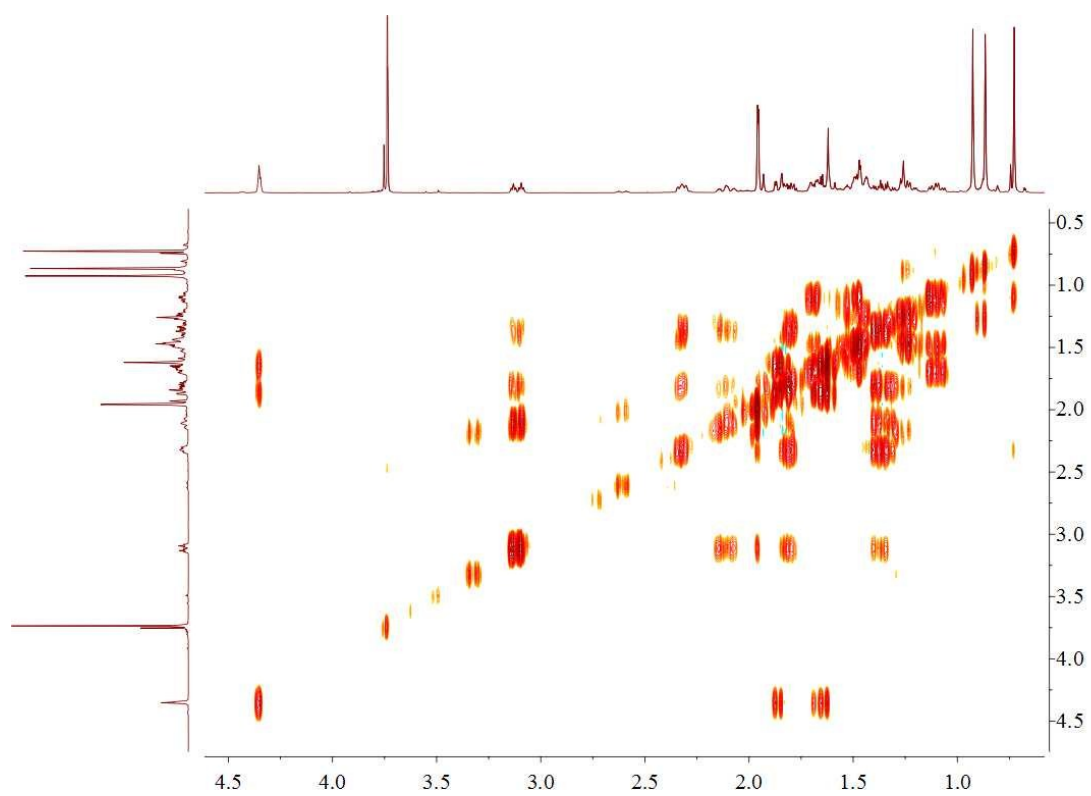


Figure S10. The expanded COSY spectrum of compound **1** (CDCl₃, 400 MHz)

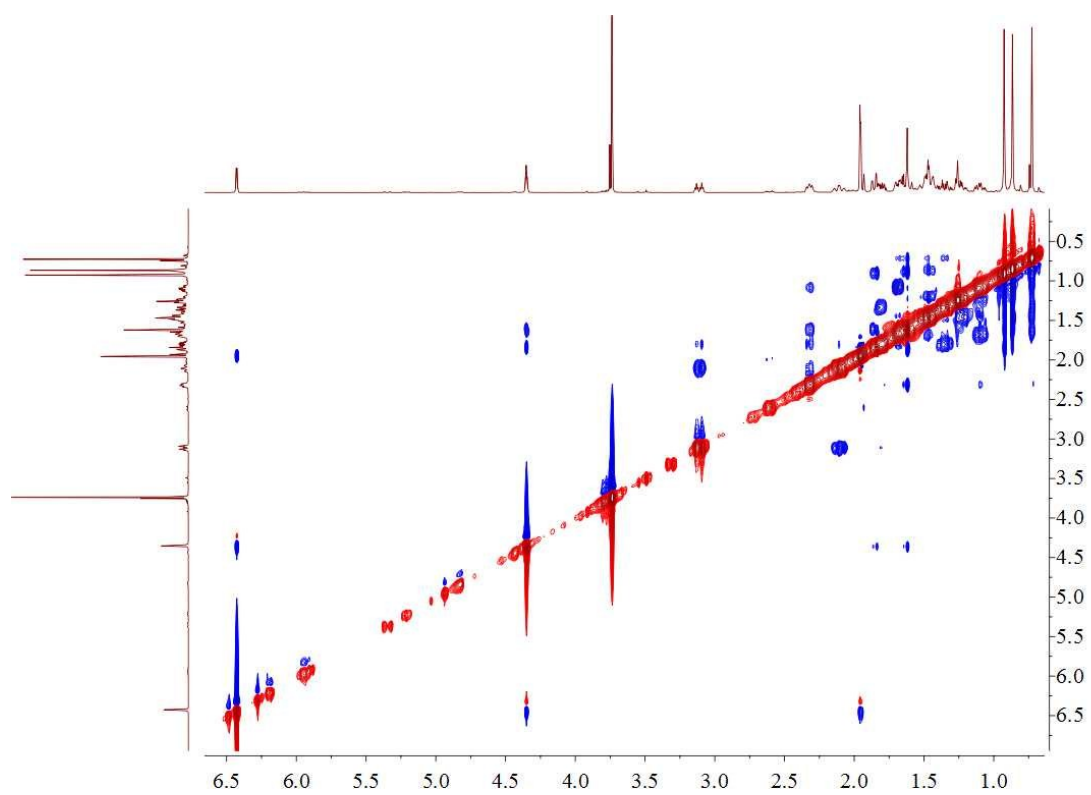


Figure S11. The NOESY spectrum of compound **1** (CDCl₃, 400 MHz)

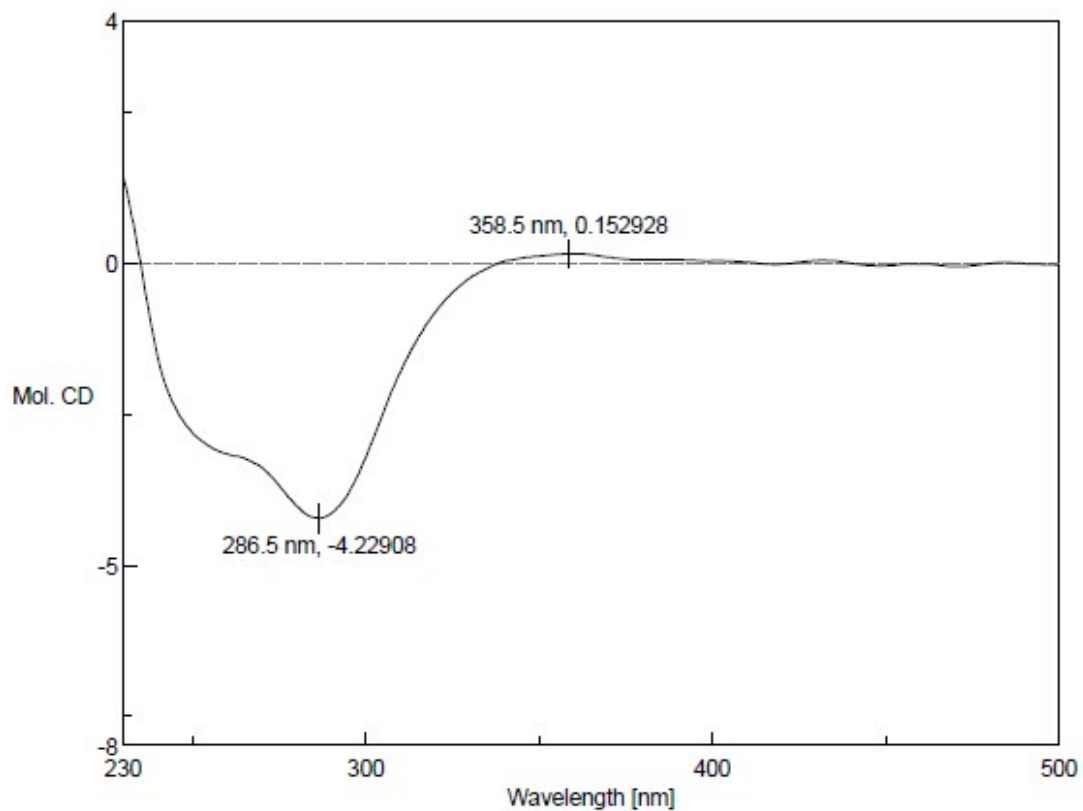


Figure S12. The ECD spectrum of compound **1** in MeOH

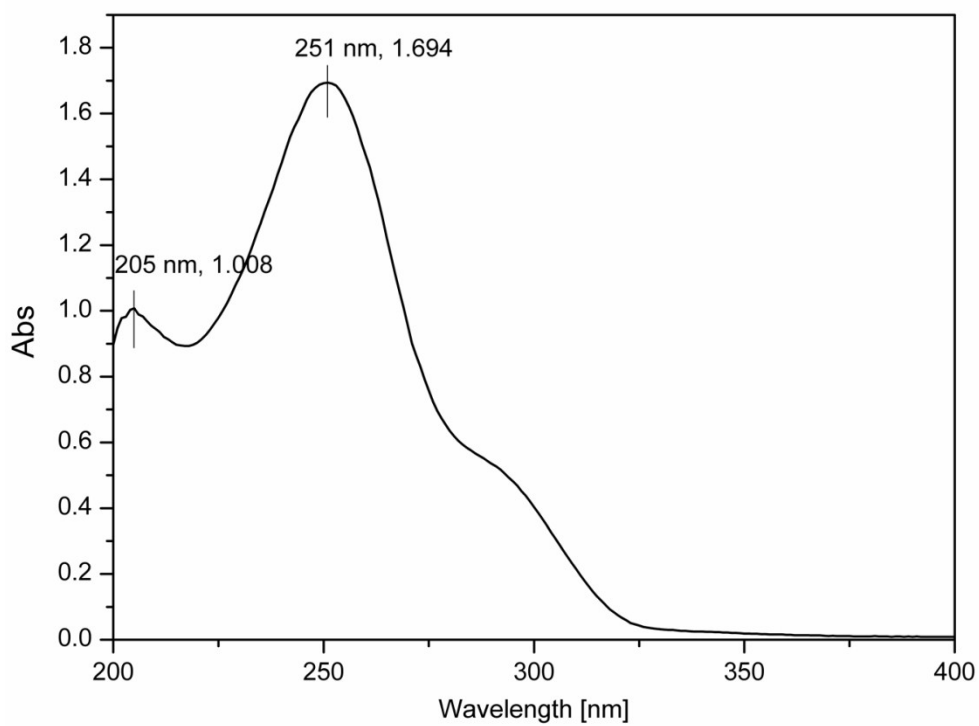


Figure S13. The UV spectrum of compound **2** in MeOH

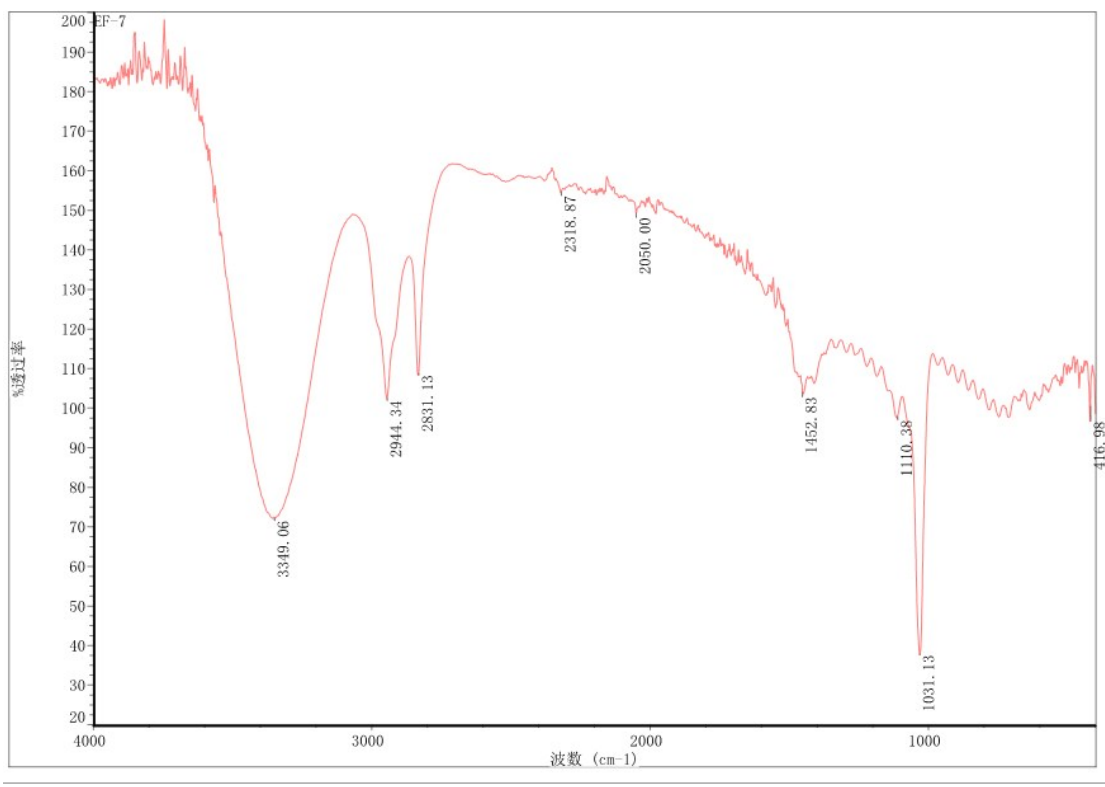


Figure S14. The IR spectrum of compound **2**

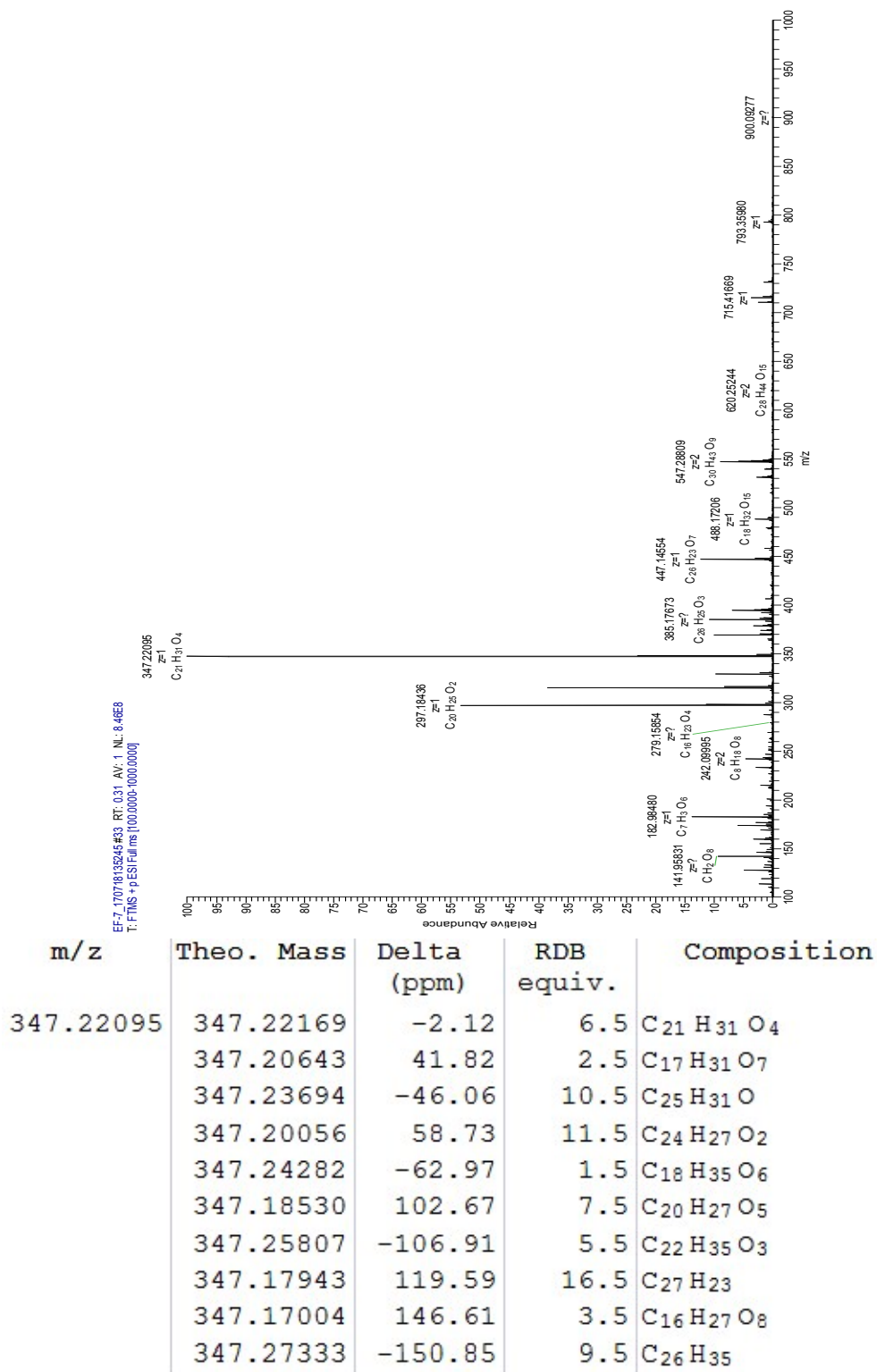


Figure S15. The HRESIMS spectrum of compound 2

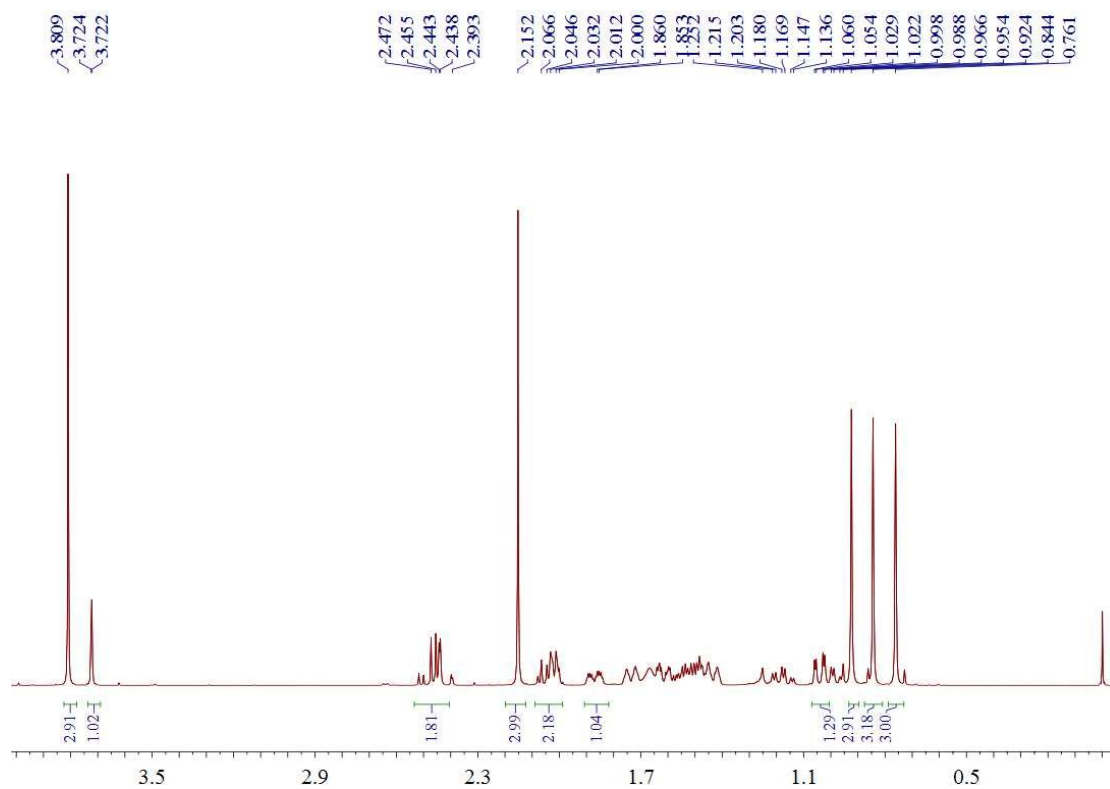


Figure S16. The ^1H NMR spectrum of compound **2** (CDCl_3 , 400 MHz)

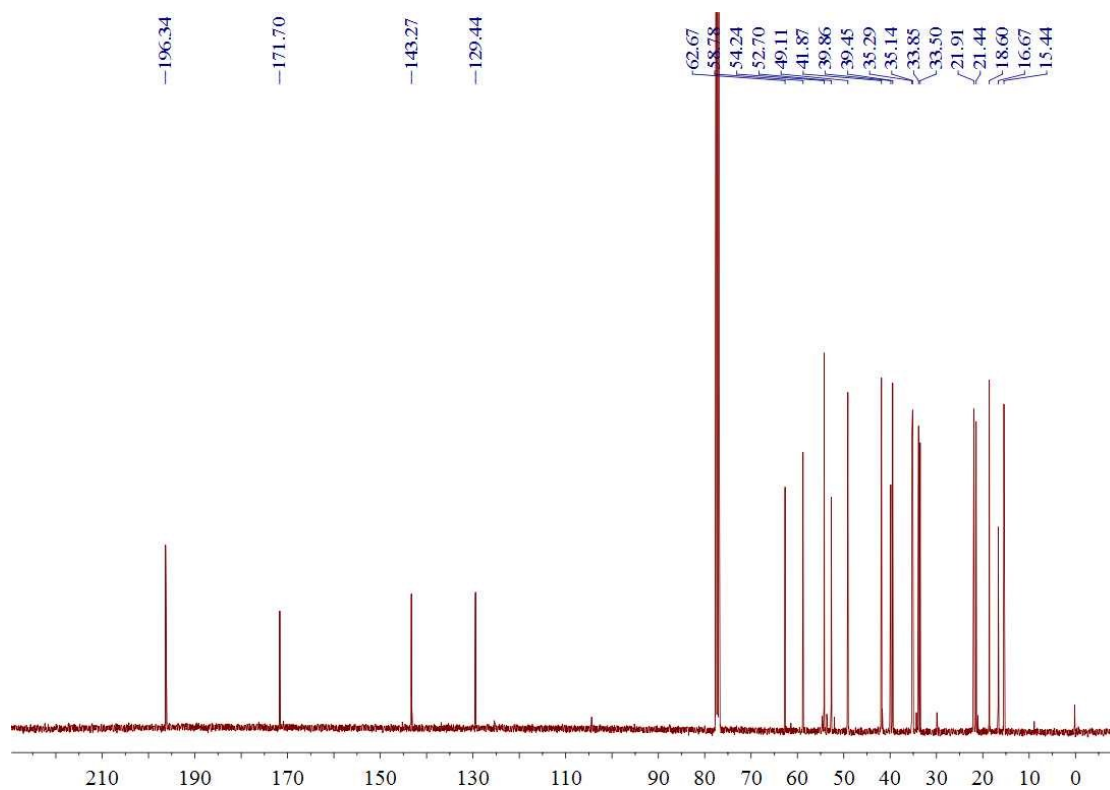


Figure S17. The ^{13}C NMR spectrum of compound **2** (CDCl_3 , 100 MHz)

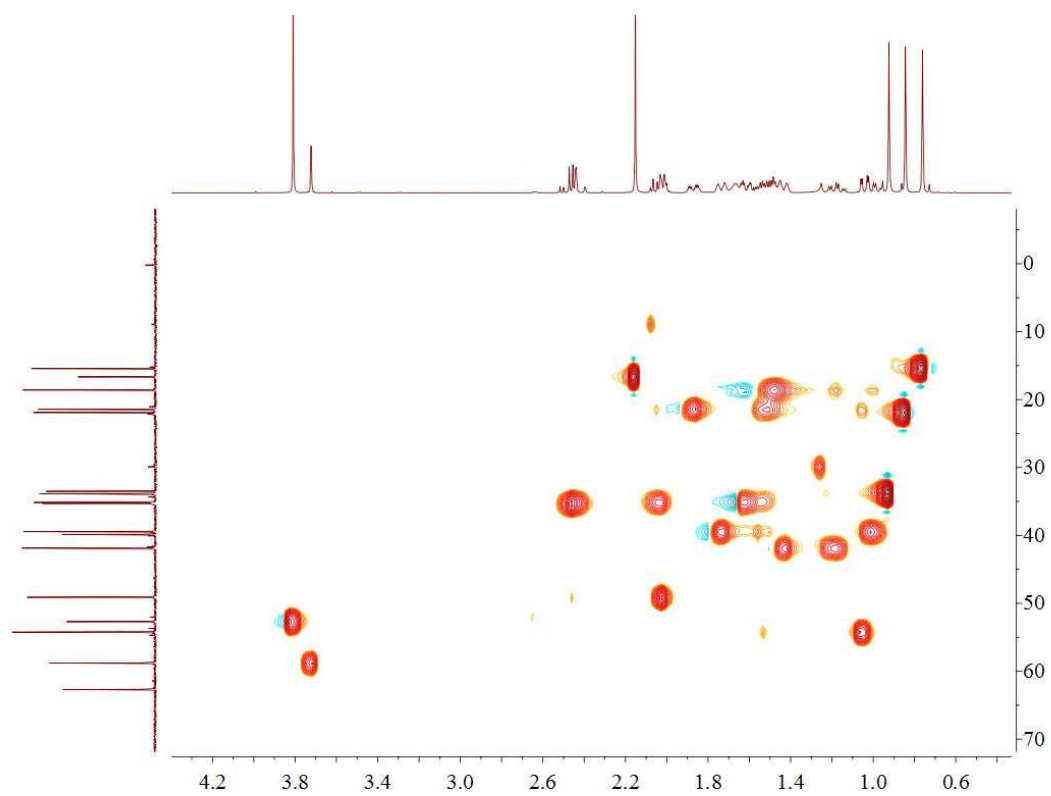


Figure S18. The HSQC spectrum of compound 2

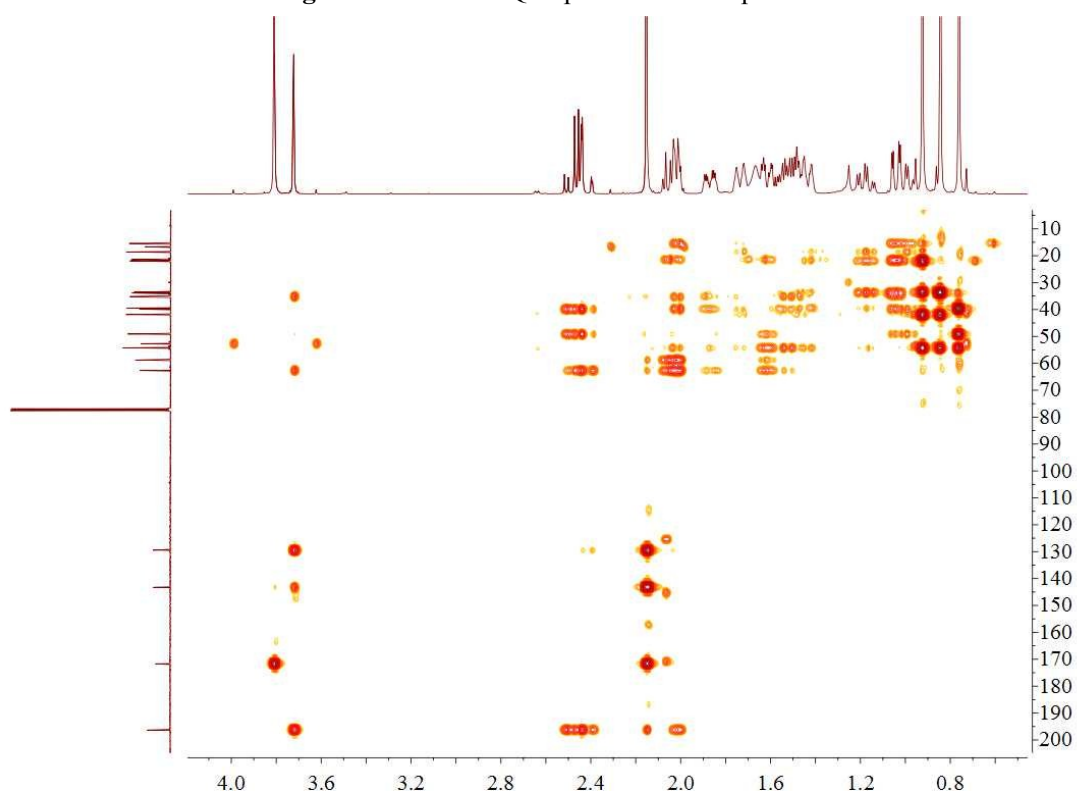


Figure S19. The HMBC spectrum of compound 2

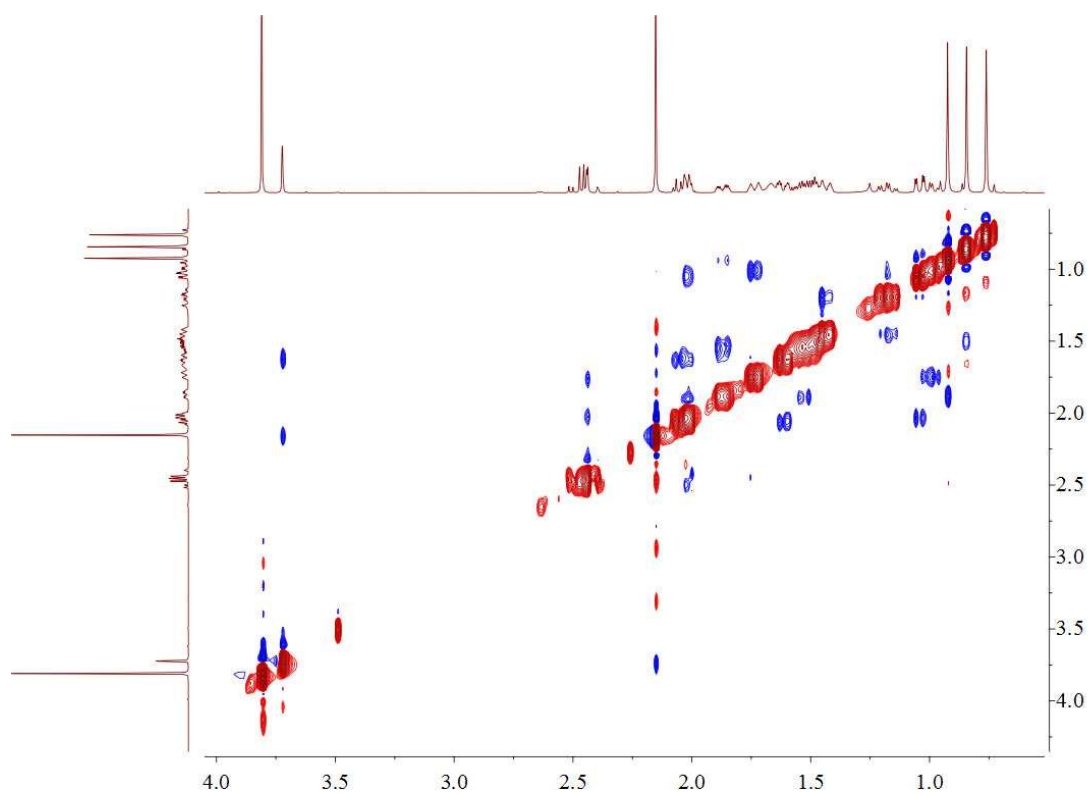


Figure S20. The NOESY spectrum of compound **2** (CDCl₃, 400 MHz)

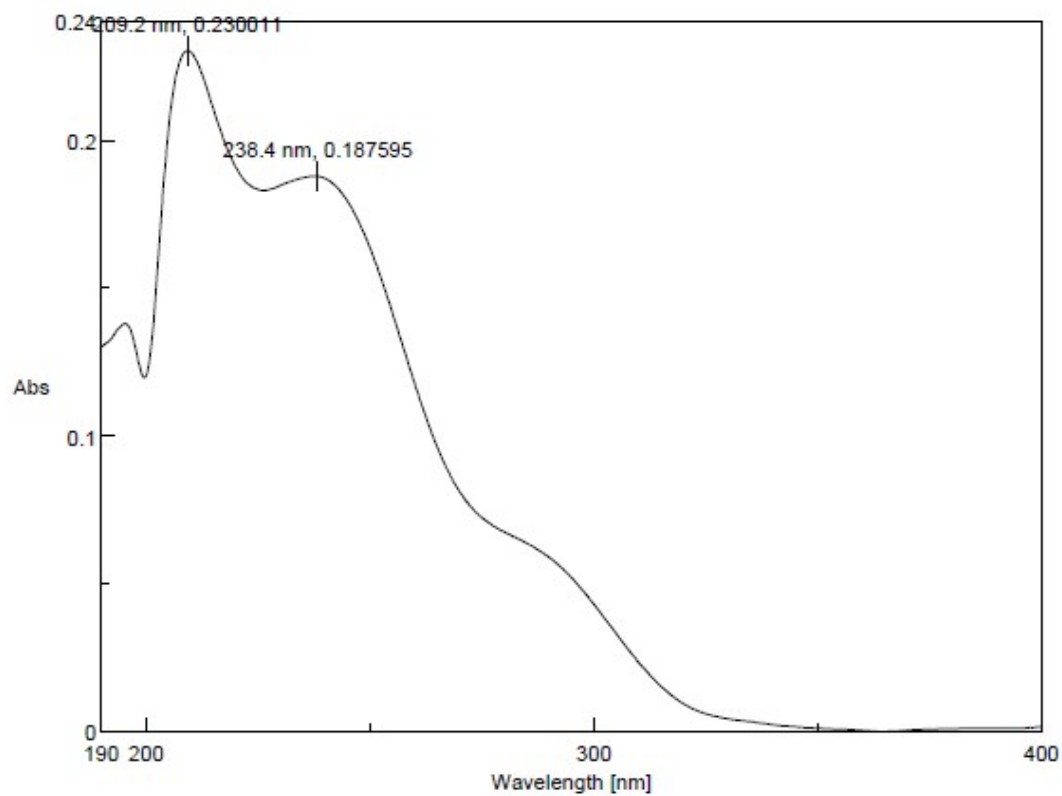


Figure S21. The UV spectrum of compound 3 in MeOH

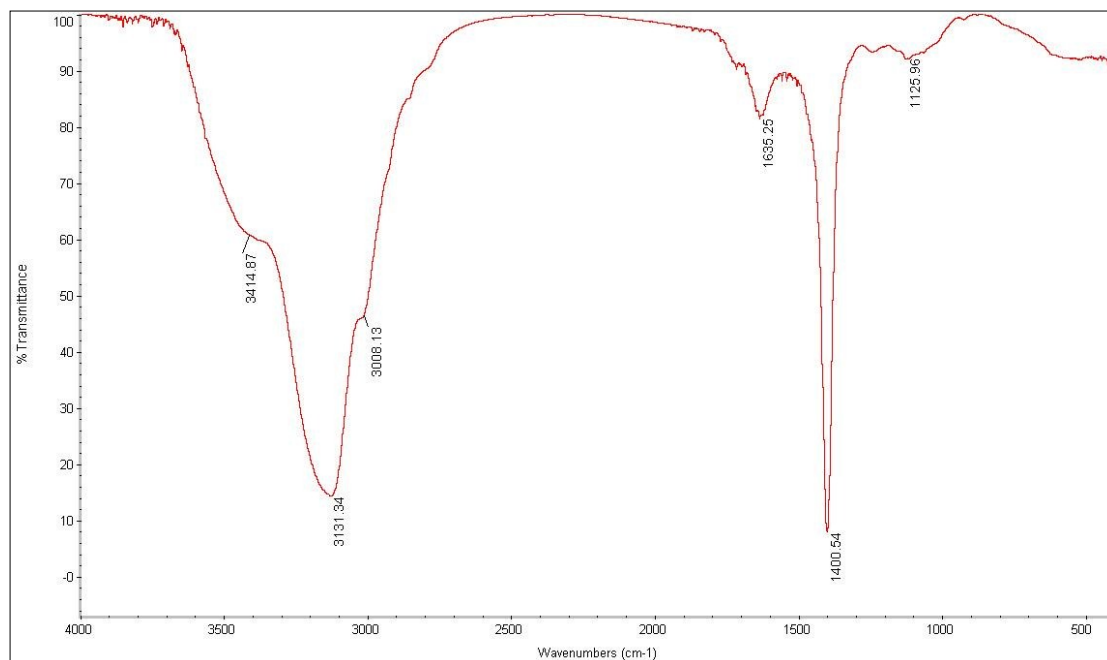
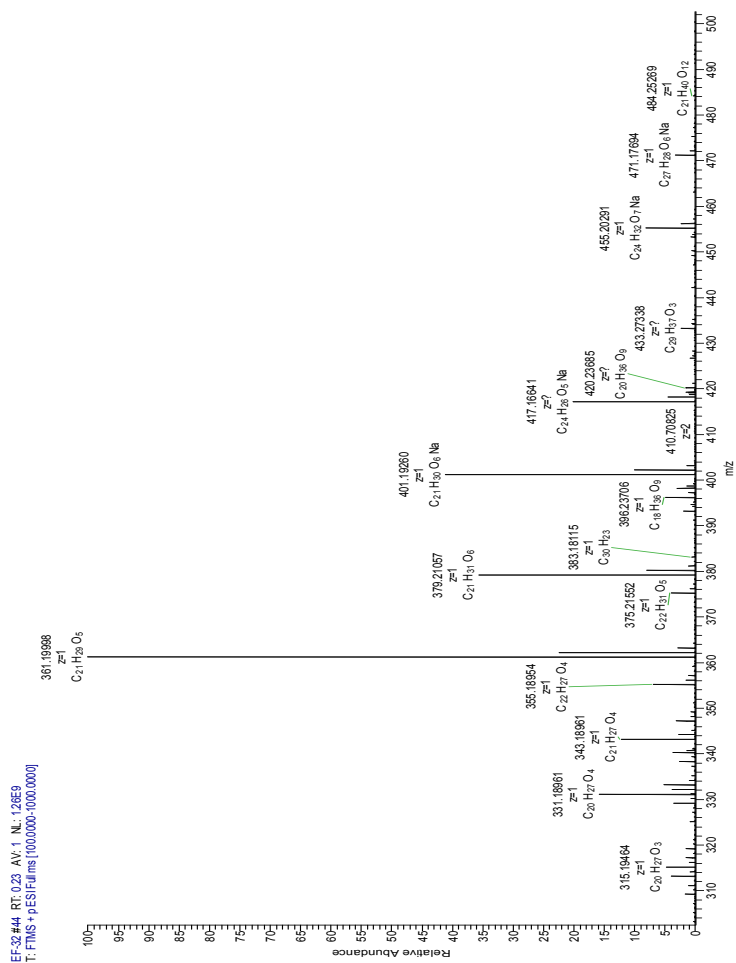


Figure S22. The IR spectrum of compound 3



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
379.21057	379.21152	-2.49	6.5	C ₂₁ H ₃₁ O ₆
	379.20564	13.00	15.5	C ₂₈ H ₂₇ O
	379.19626	37.74	2.5	C ₁₇ H ₃₁ O ₉
	379.22677	-42.72	10.5	C ₂₅ H ₃₁ O ₃
	379.19039	53.23	11.5	C ₂₄ H ₂₇ O ₄
	379.23264	-58.21	1.5	C ₁₈ H ₃₅ O ₈
	379.24203	-82.96	14.5	C ₂₉ H ₃₁
	379.17513	93.46	7.5	C ₂₀ H ₂₇ O ₇
	379.24790	-98.44	5.5	C ₂₂ H ₃₅ O ₅
	379.16926	108.95	16.5	C ₂₇ H ₂₃ O ₂

Figure S23. The HRESIMS spectrum of compound 3

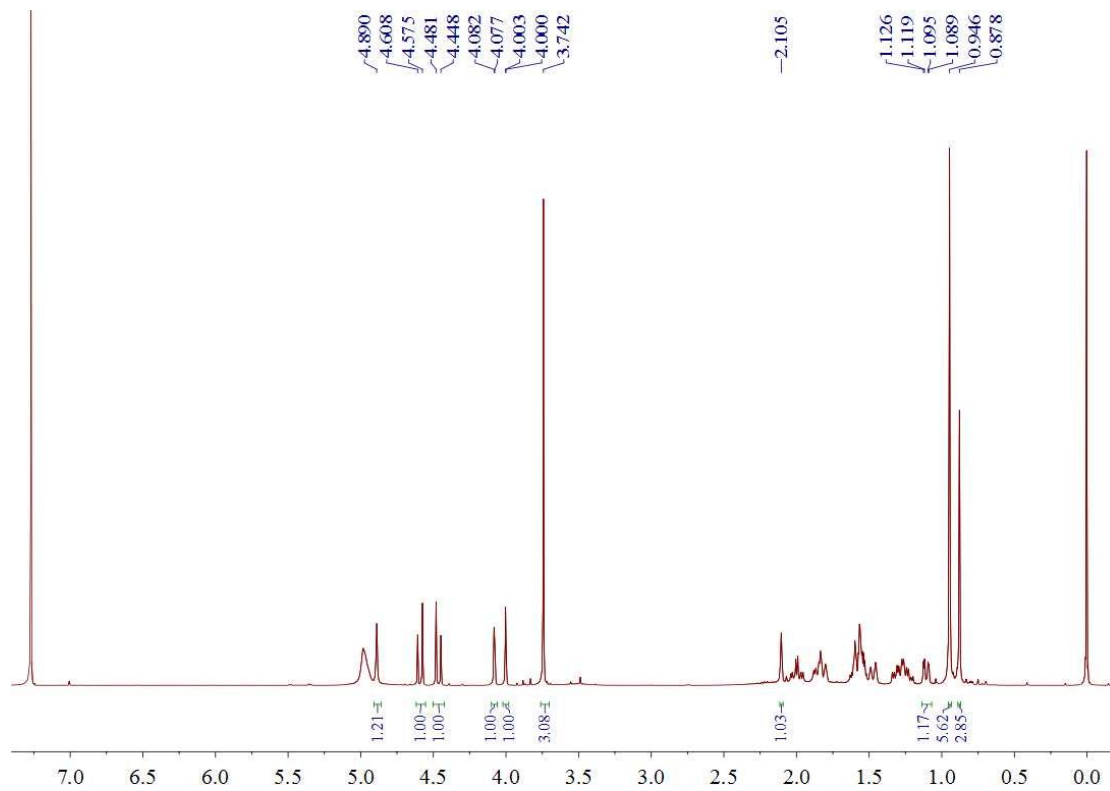


Figure S24. The ^1H NMR spectrum of compound **3** (CDCl_3 , 400 MHz)

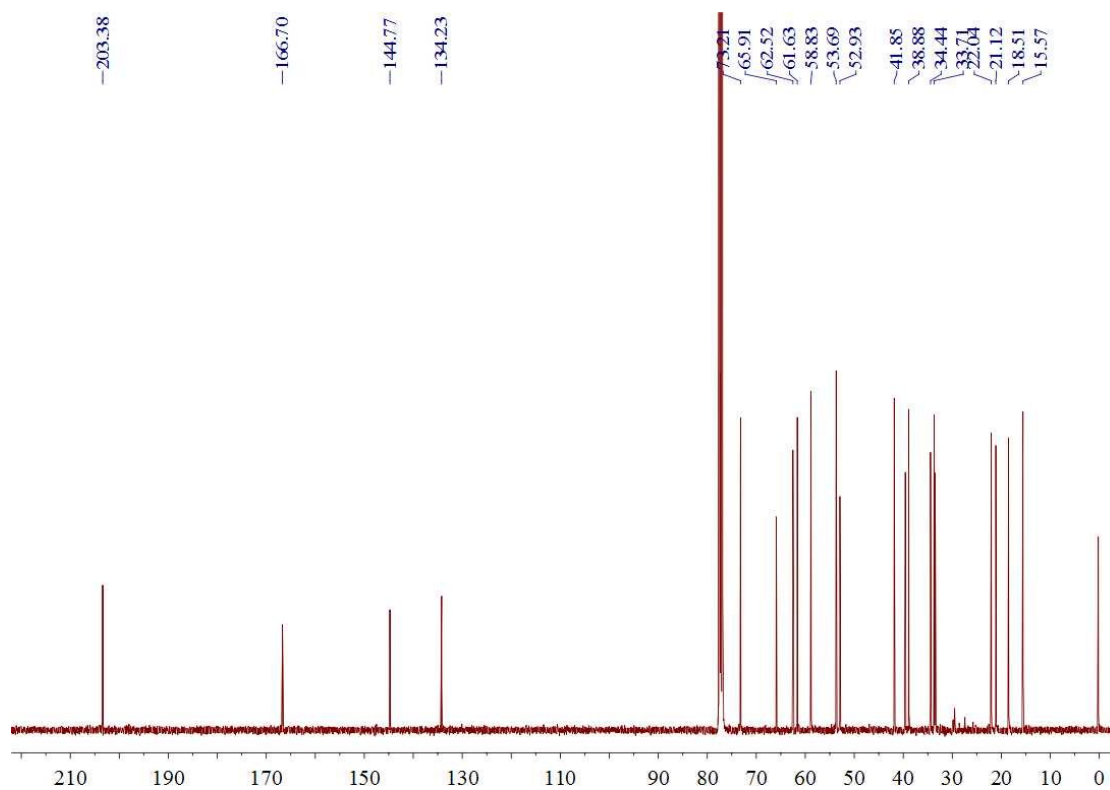


Figure S25. The ^{13}C NMR spectrum of compound **3** (CDCl_3 , 100 MHz)

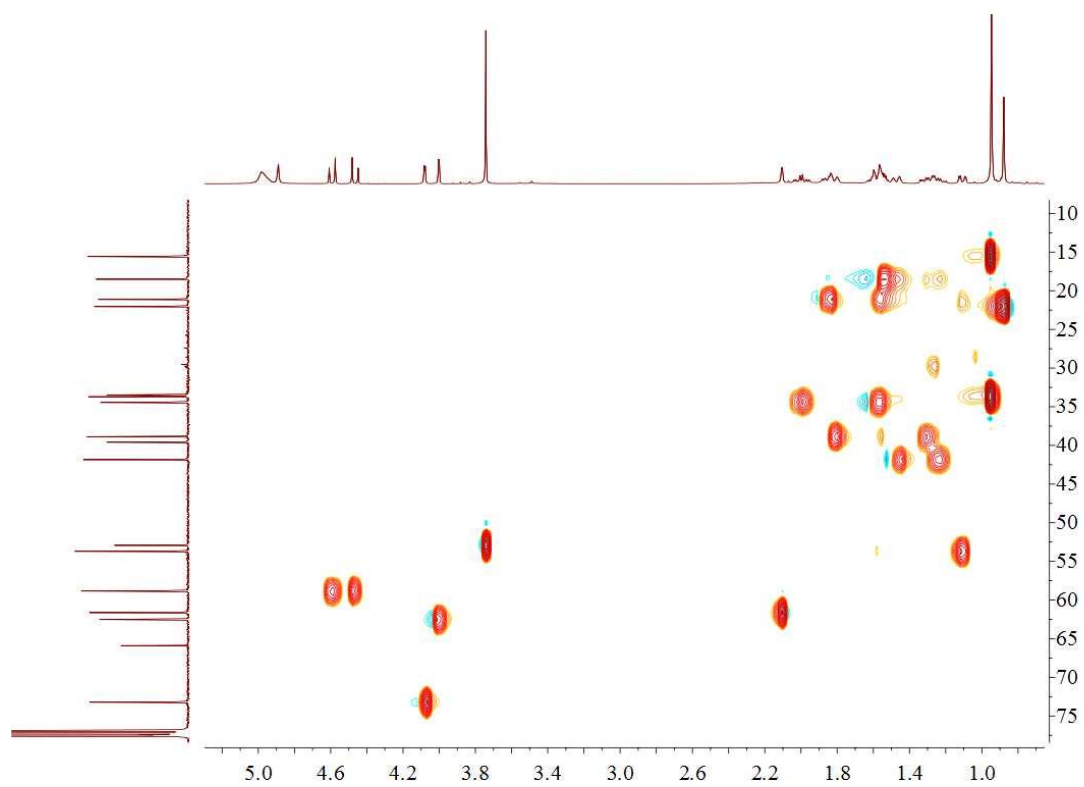


Figure S26. The HSQC spectrum of compound **3**

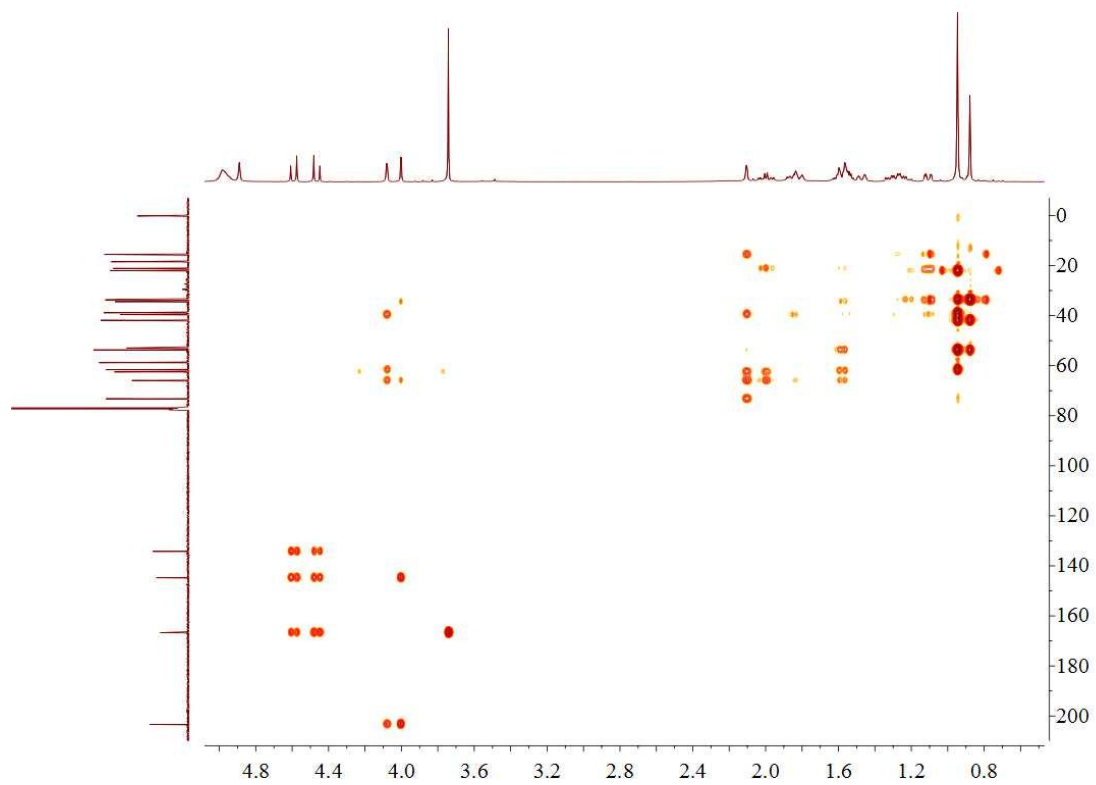


Figure S27. The HMBC spectrum of compound **3**

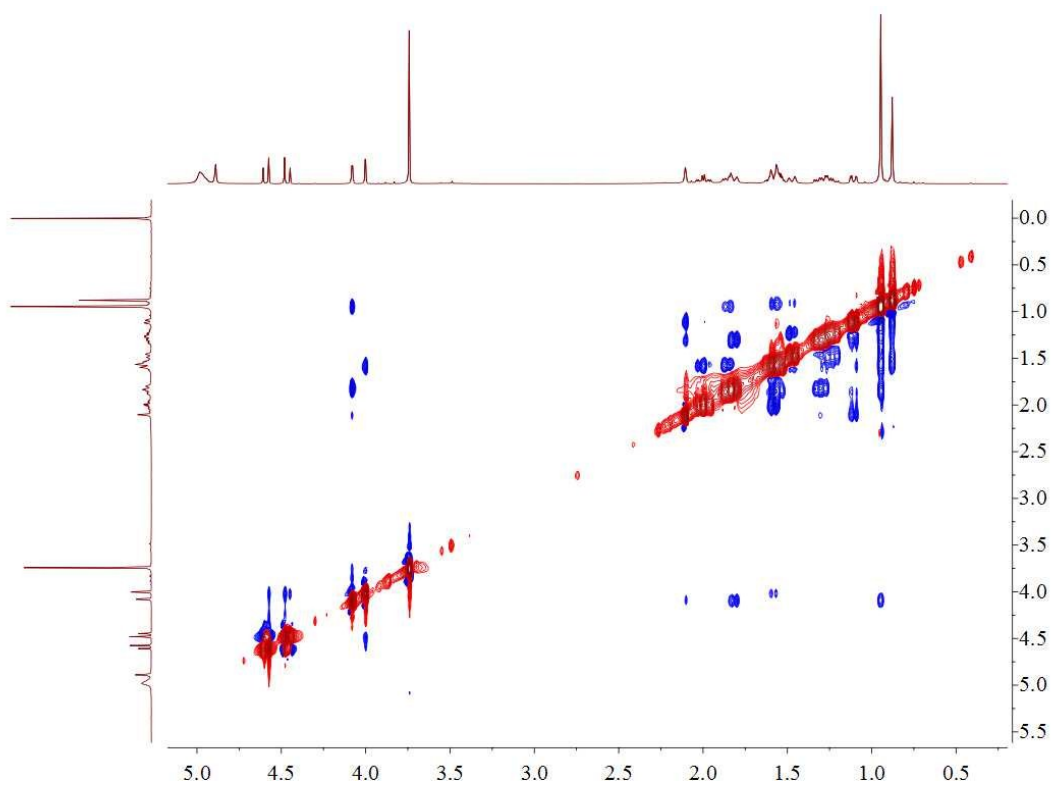


Figure S28. The NOESY spectrum of compound **3** (CDCl_3 , 400 MHz)

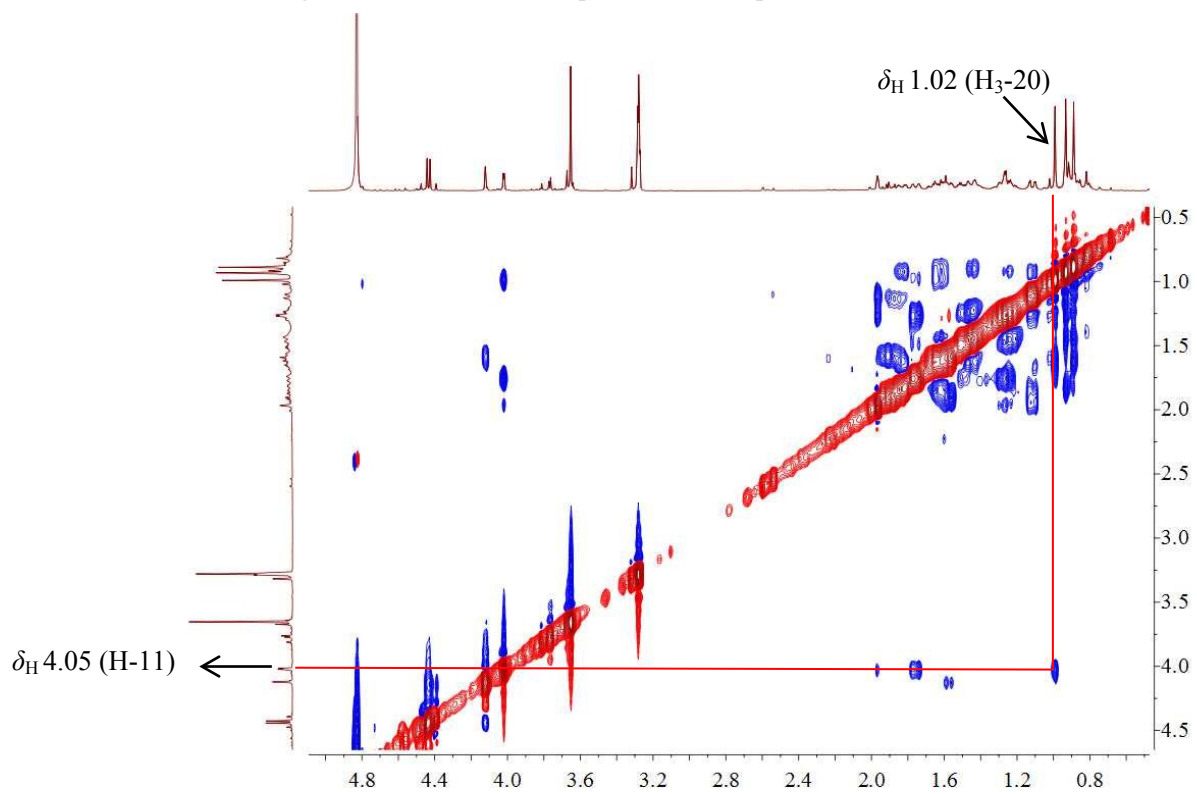


Figure S29. The NOESY spectrum of compound **3** (CD_3OD , 400 MHz)

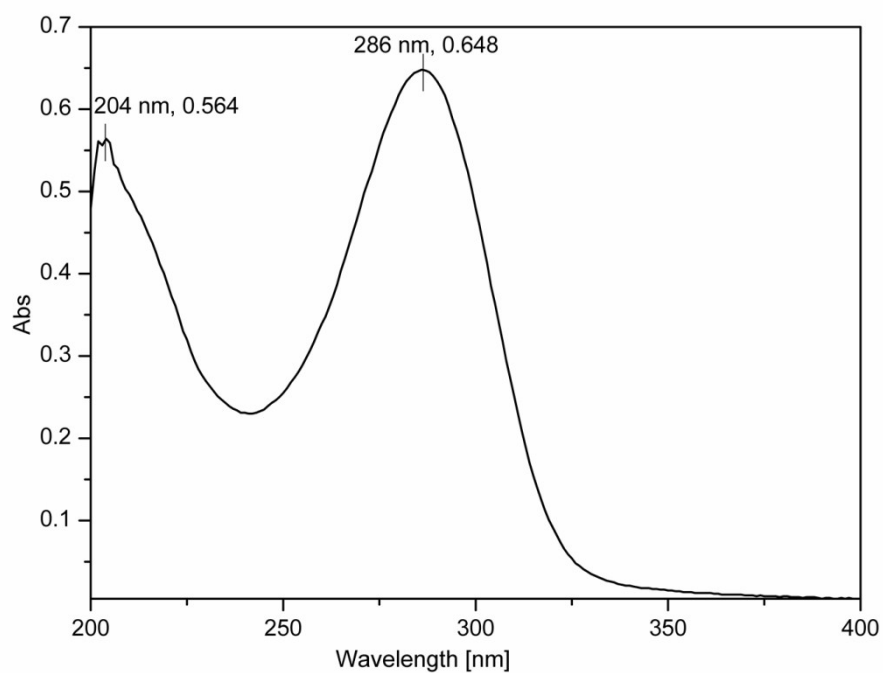


Figure S30. The UV spectrum of compound 4 in MeOH

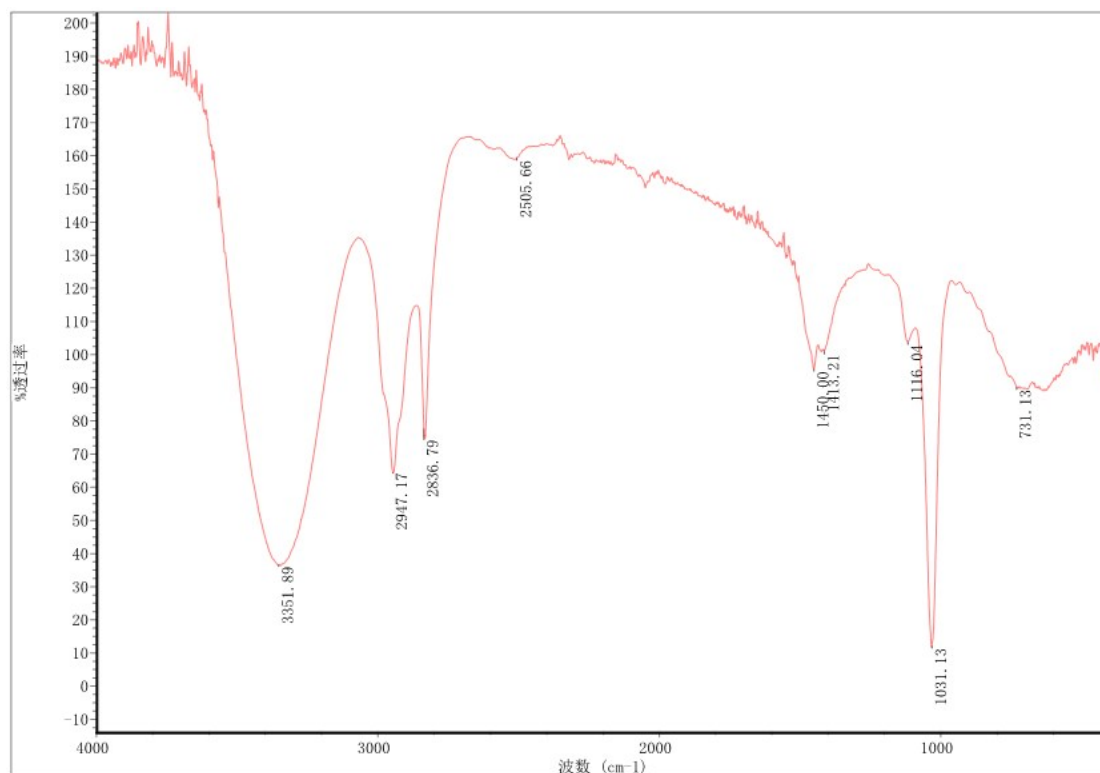
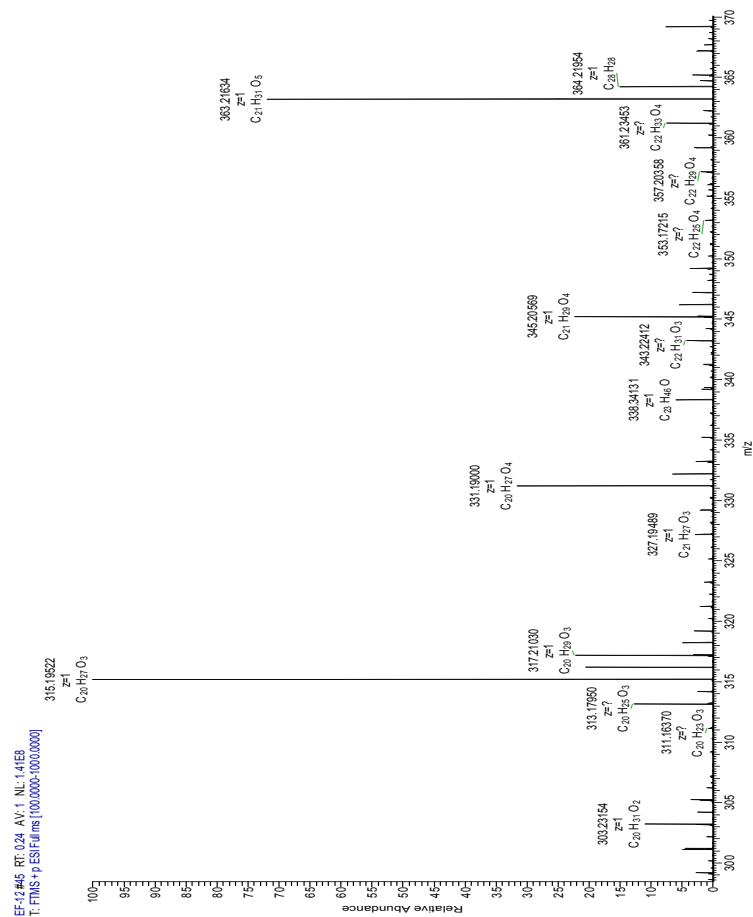


Figure S31. The IR spectrum of compound 4



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
331.19000	331.19039	-1.16	7.5	C ₂₀ H ₂₇ O ₄
	331.17513	44.90	3.5	C ₁₆ H ₂₇ O ₇
	331.20564	-47.23	11.5	C ₂₄ H ₂₇ O
	331.16926	62.63	12.5	C ₂₃ H ₂₃ O ₂
	331.21152	-64.96	2.5	C ₁₇ H ₃₁ O ₆
	331.15987	90.96	-0.5	C ₁₂ H ₂₇ O ₁₀
	331.15400	108.70	8.5	C ₁₉ H ₂₃ O ₅
	331.22677	-111.03	6.5	C ₂₁ H ₃₁ O ₃
	331.14813	126.43	17.5	C ₂₆ H ₁₉
	331.13874	154.76	4.5	C ₁₅ H ₂₃ O ₈

Figure S32. The HRESIMS spectrum of compound **4**

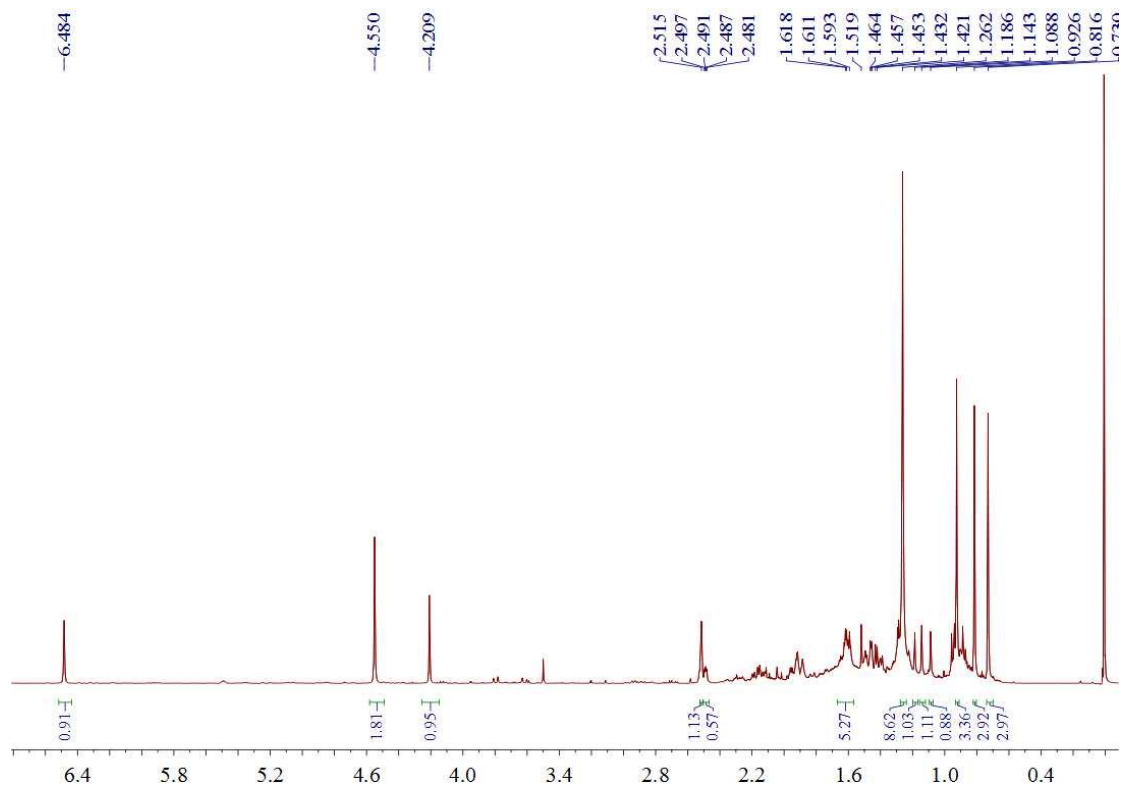


Figure S33. The ^1H NMR spectrum of compound **4** (CDCl_3 , 400 MHz)

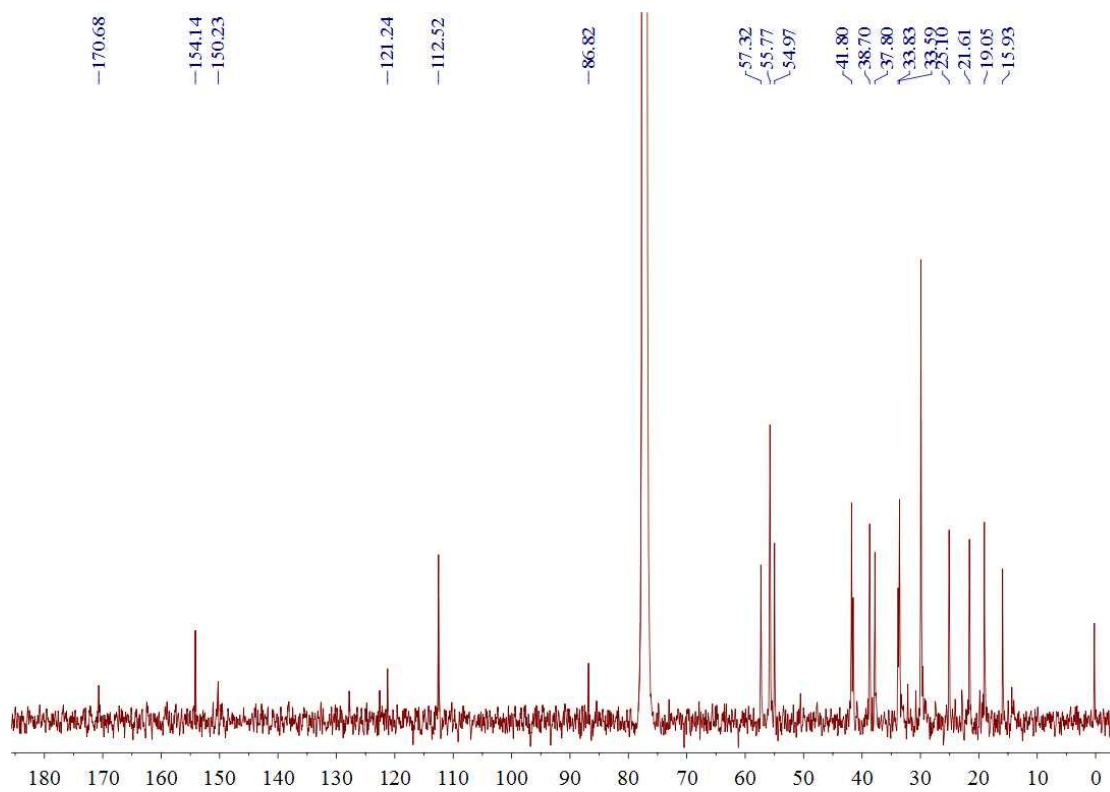


Figure S34. The ^{13}C NMR spectrum of compound **4** (CDCl_3 , 100 MHz)

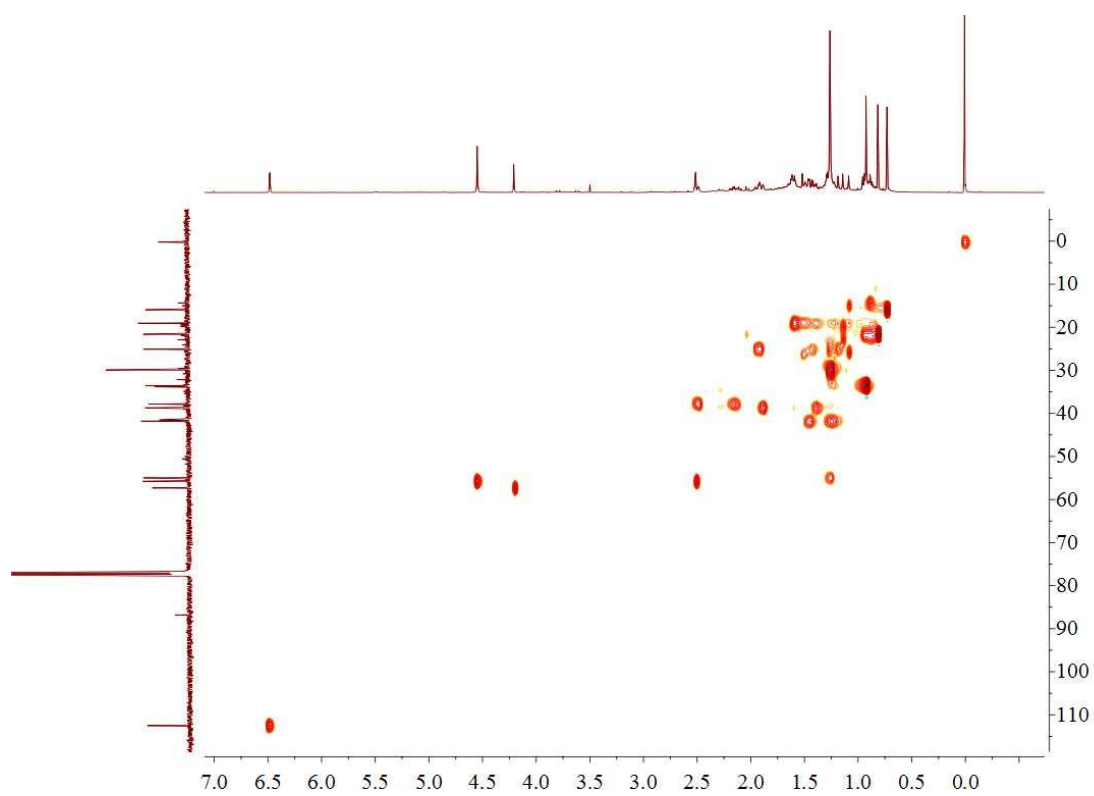


Figure S35. The HSQC spectrum of compound **4**

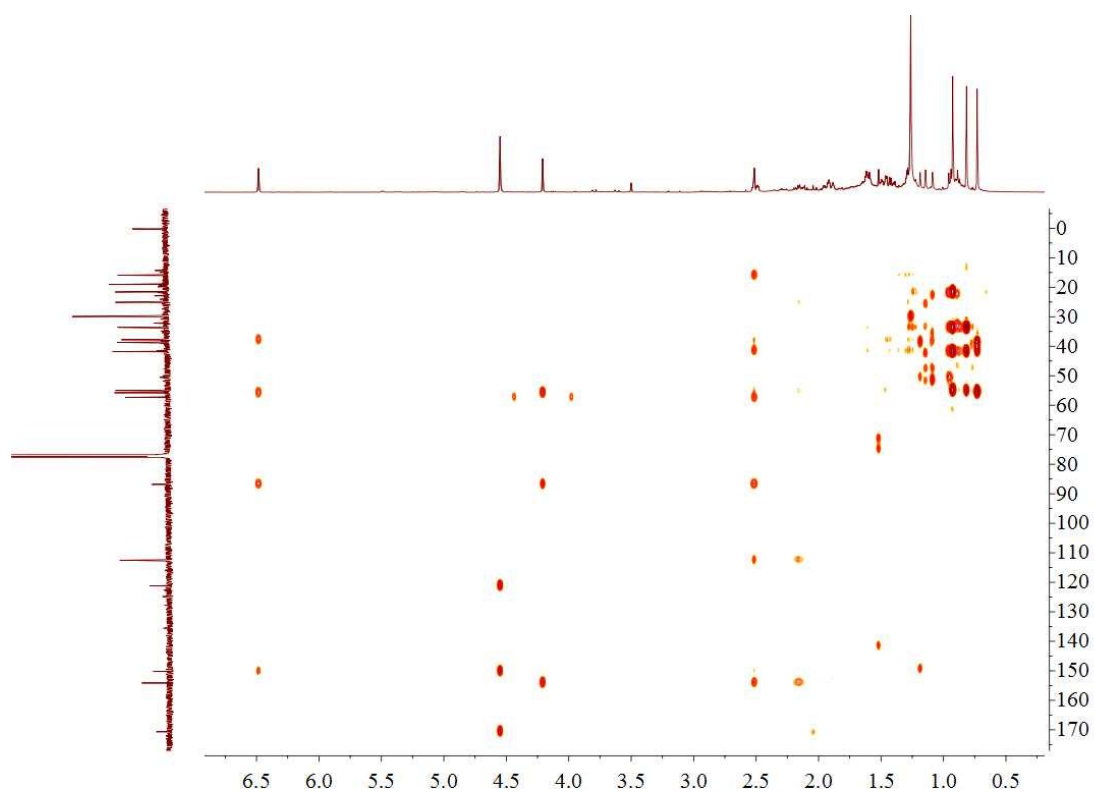


Figure S36. The HMBC spectrum of compound **4** (CDCl₃, 400 MHz)

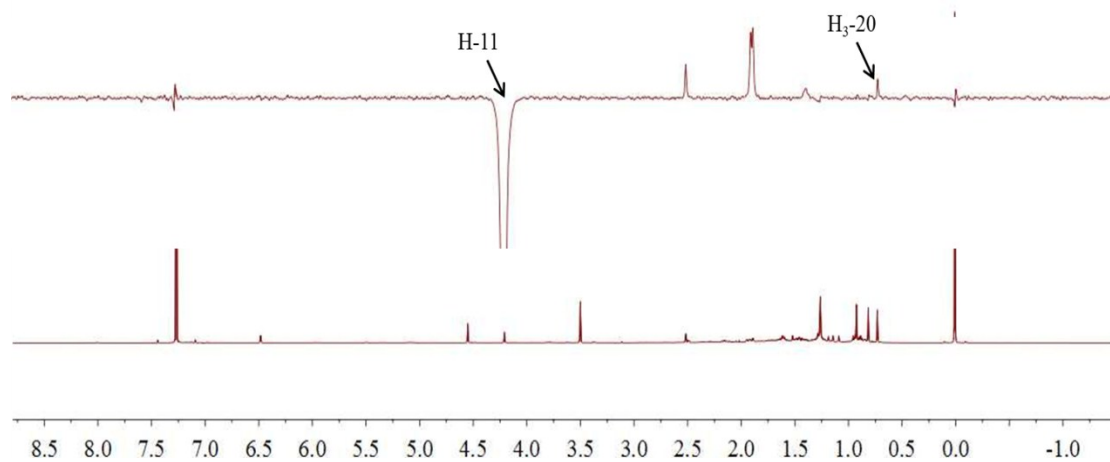


Figure S37. The NOE spectrum of compound **4** (CDCl₃, 600 MHz)

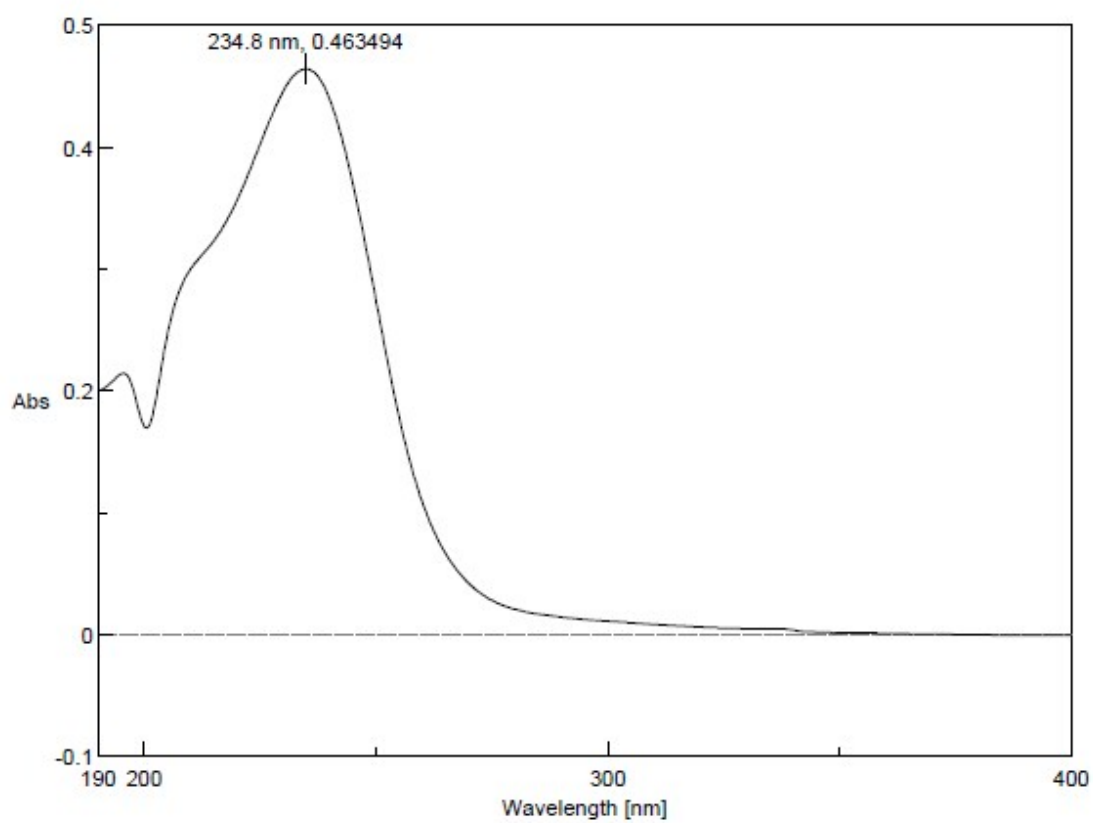


Figure S38. The UV spectrum of compound **5** in MeOH

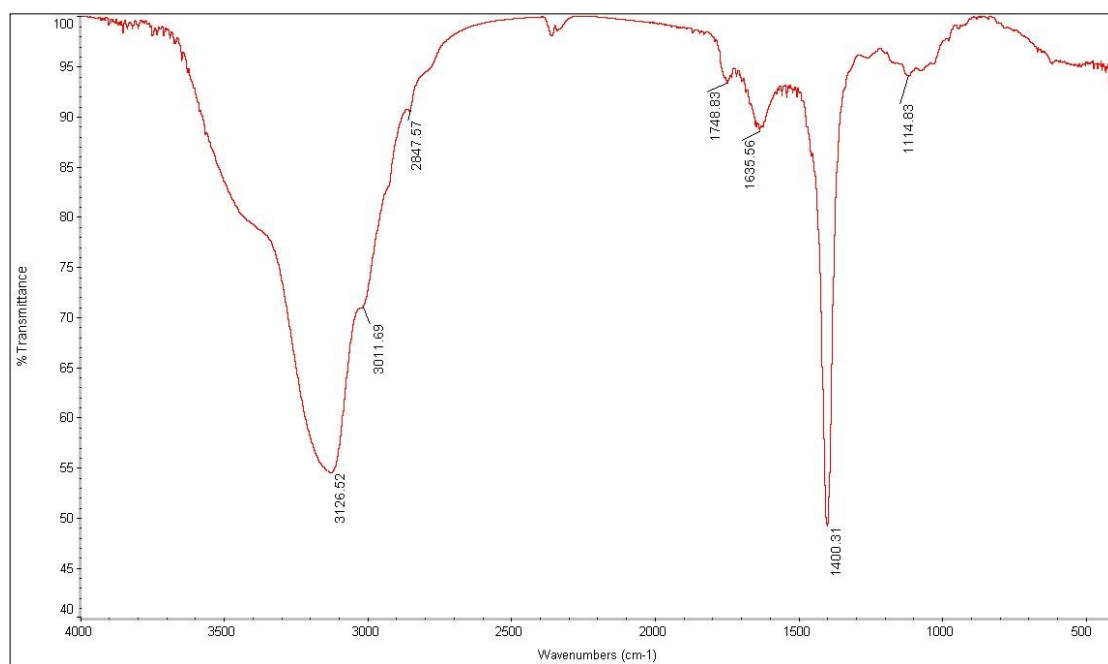


Figure S39. The IR spectrum of compound **5**

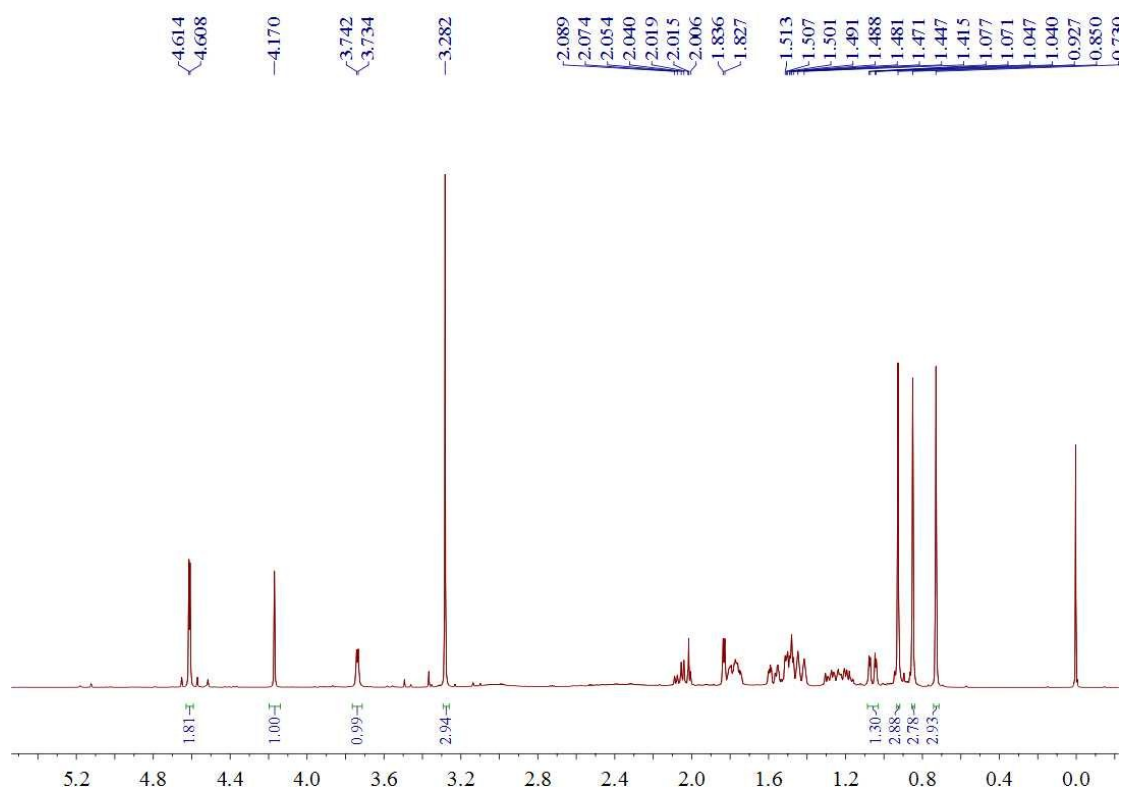


Figure S41. The ^1H NMR spectrum of compound **5** (CDCl_3 , 400 MHz)

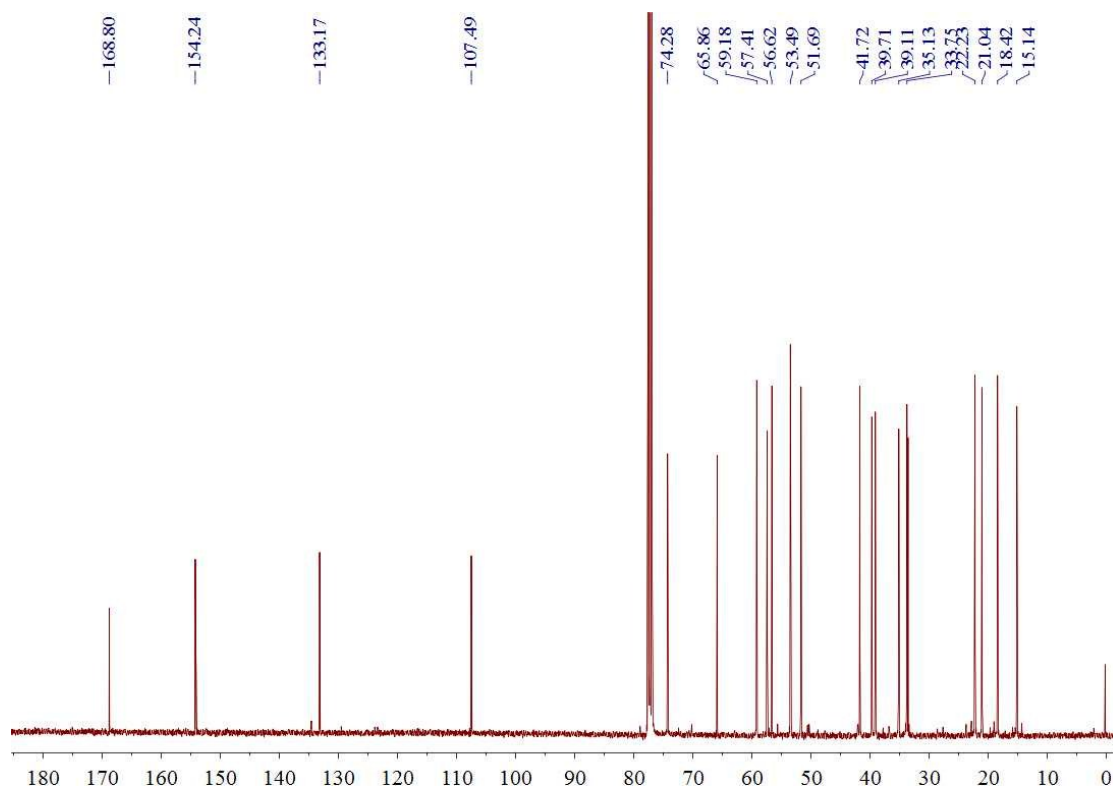


Figure S42. The ^{13}C NMR spectrum of compound **5** (CDCl_3 , 100 MHz)

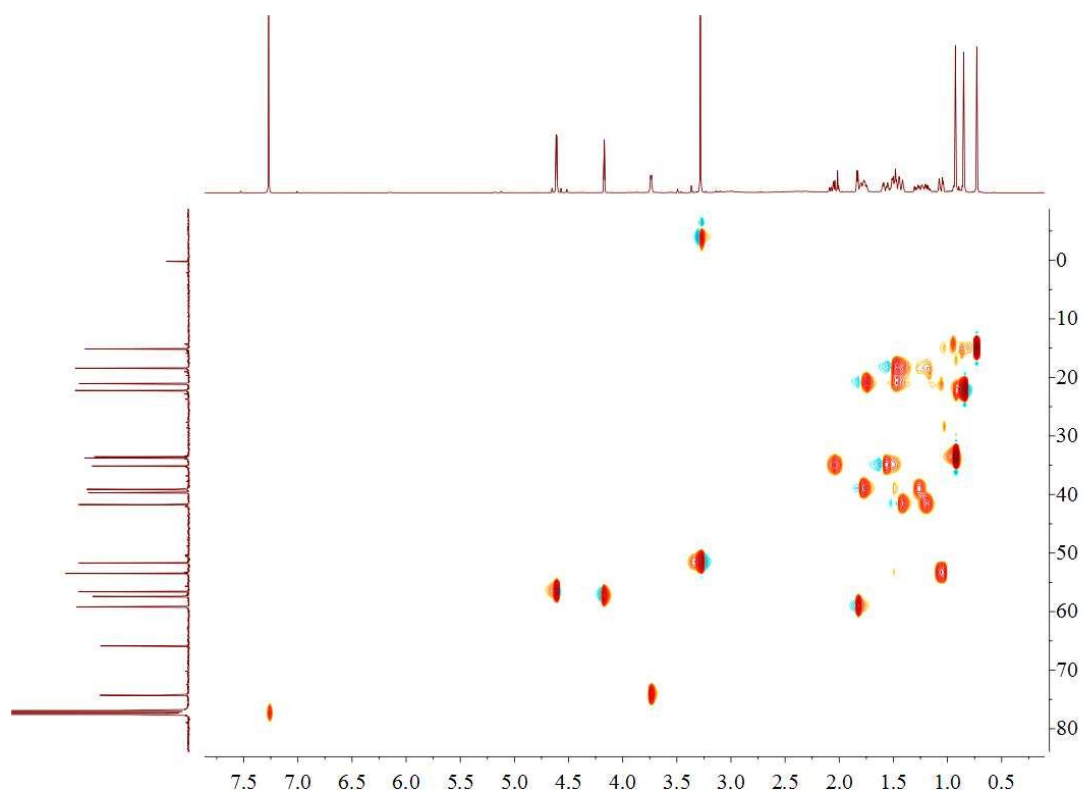


Figure S43. The HSQC spectrum of compound **5**

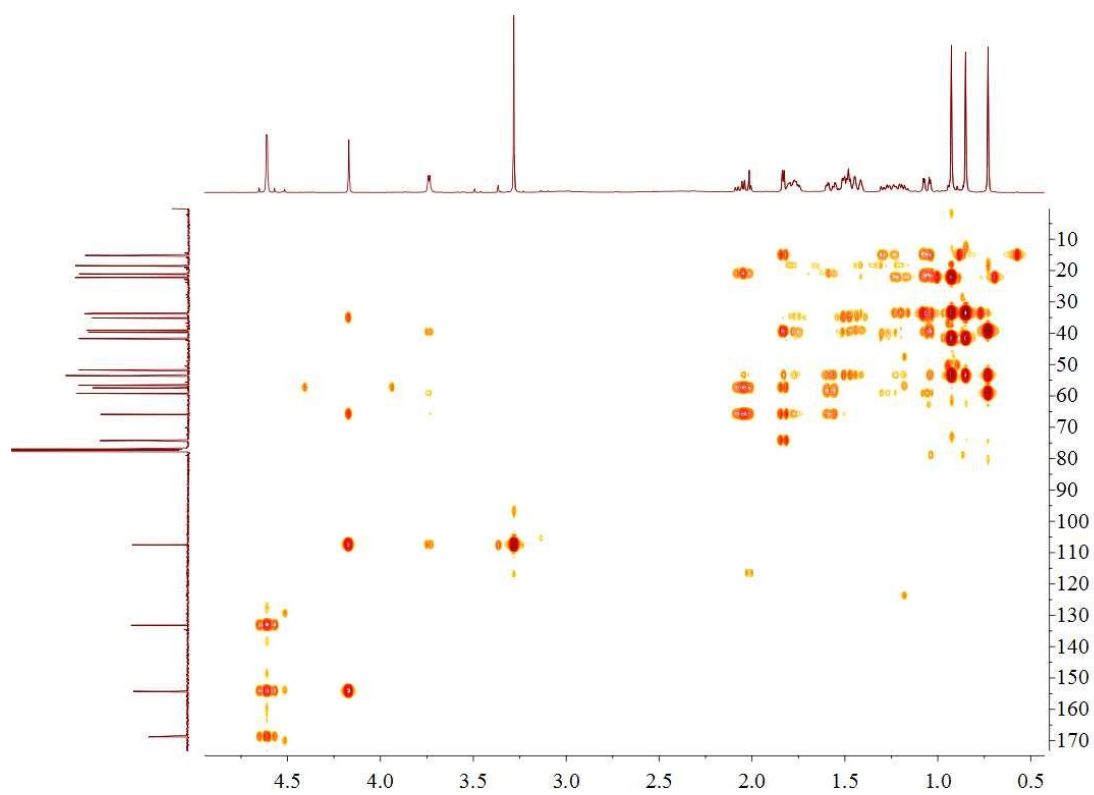


Figure S44. The HMBC spectrum of compound **5**

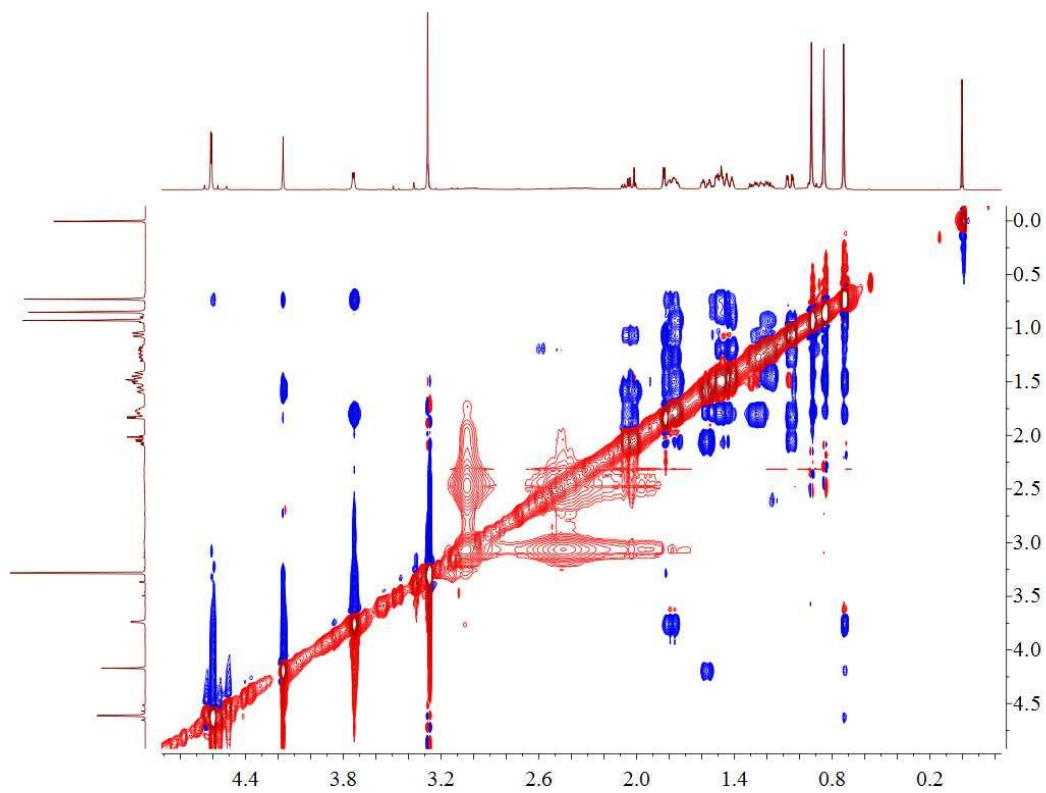


Figure S45. The NOESY spectrum of compound **5** (CDCl_3 , 400 MHz)

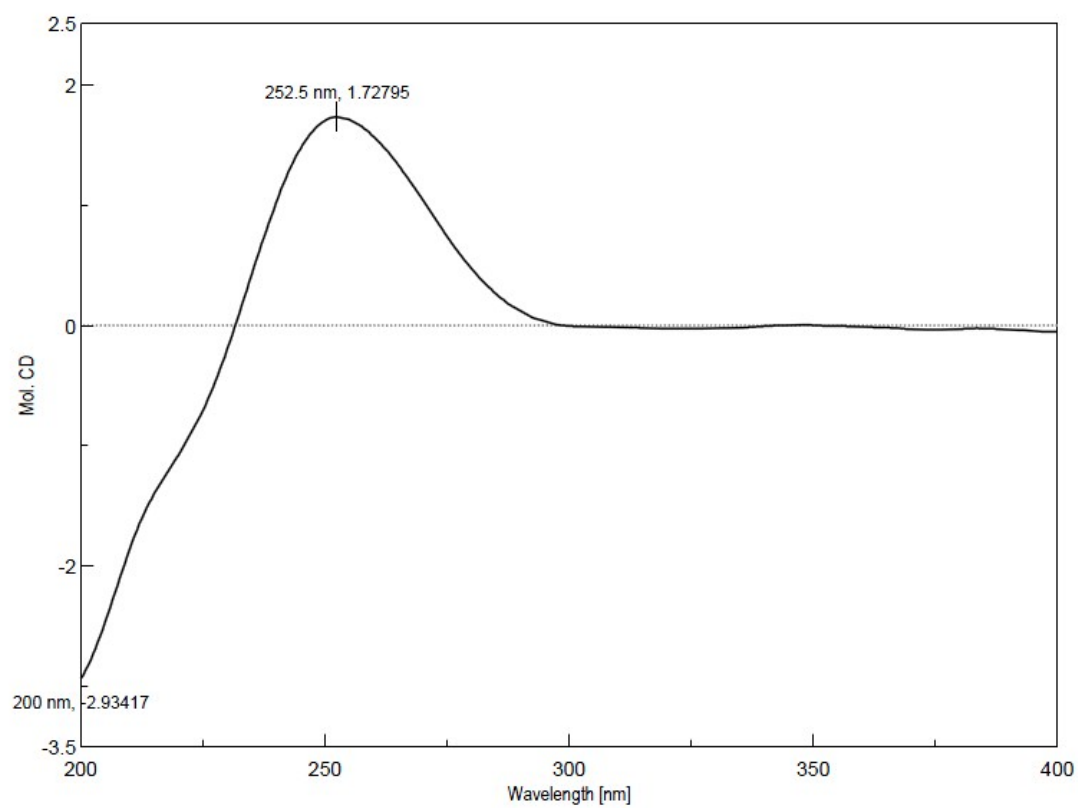


Figure S46. The ECD spectrum of compound **5** in MeOH