

Supporting Information
For

**Chemical Constituents from a Marine Medicinal Brown Alga-
Derived *Xylaria acuta* SC1019**

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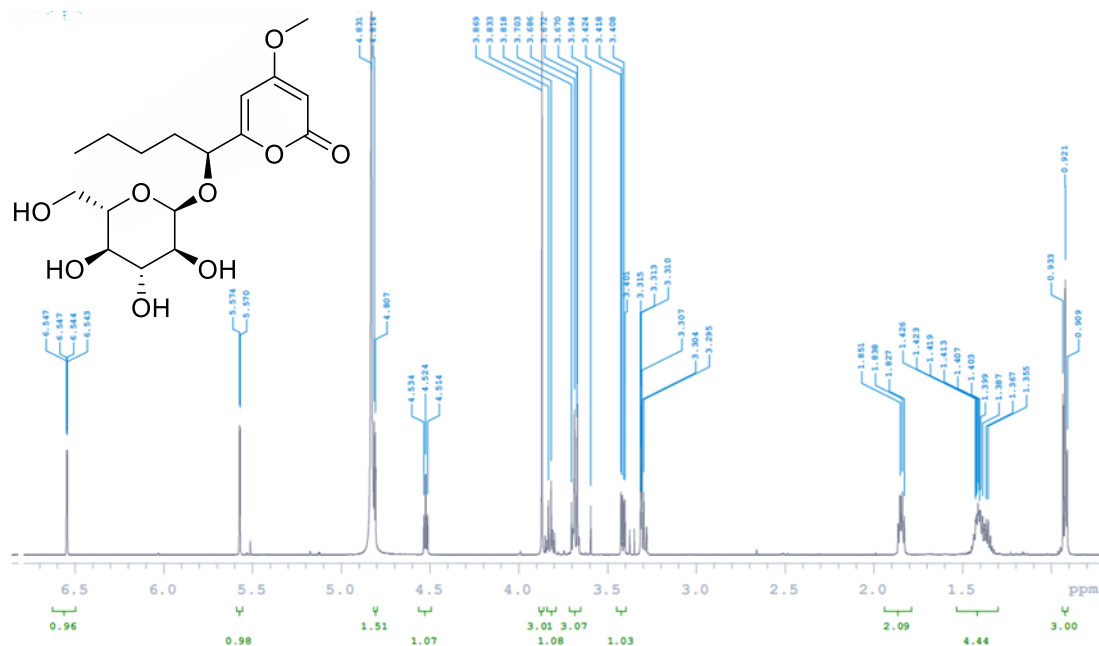


Figure S1. The ^1H NMR (600 MHz, CD_3OD) spectrum of compound 1

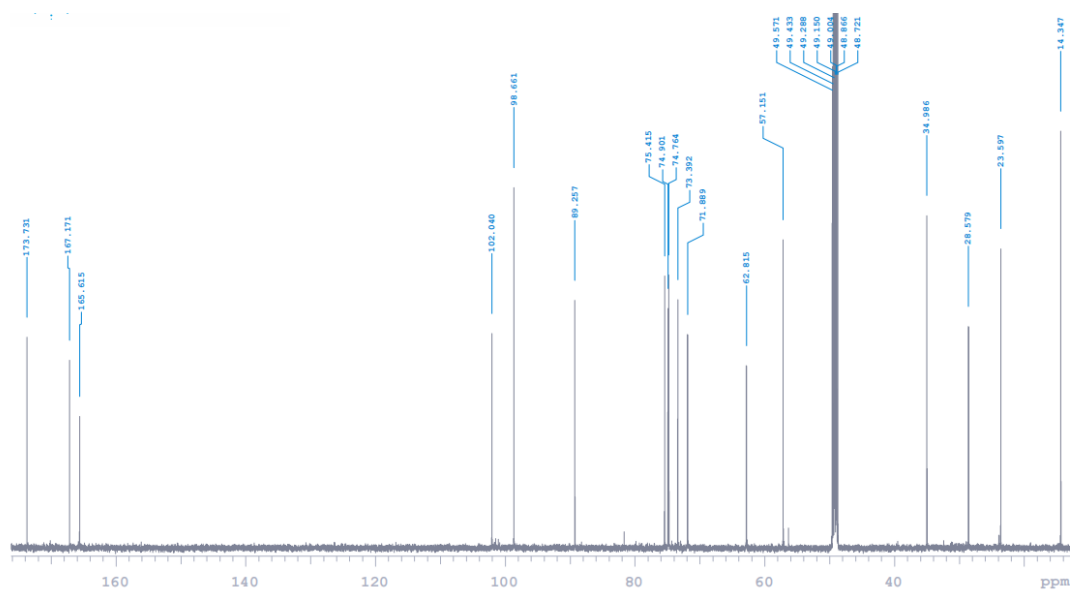


Figure S2. The ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 1

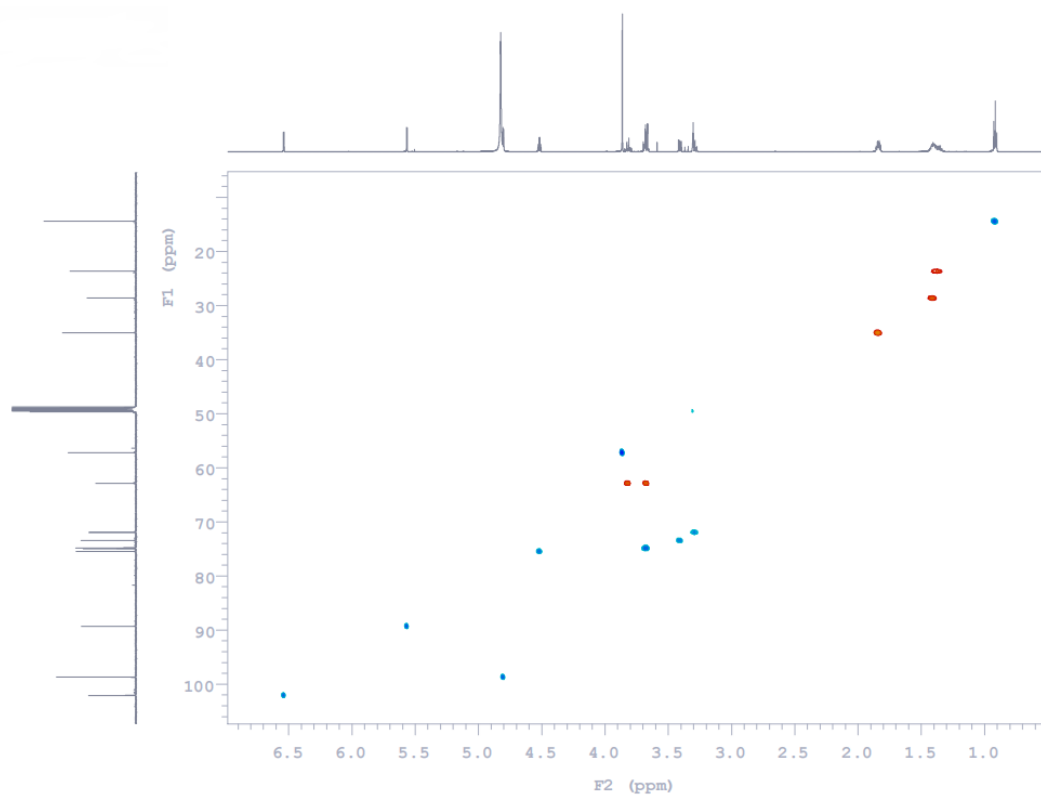


Figure S3. The HSQC (600 MHz, CD₃OD) spectrum of compound **1**

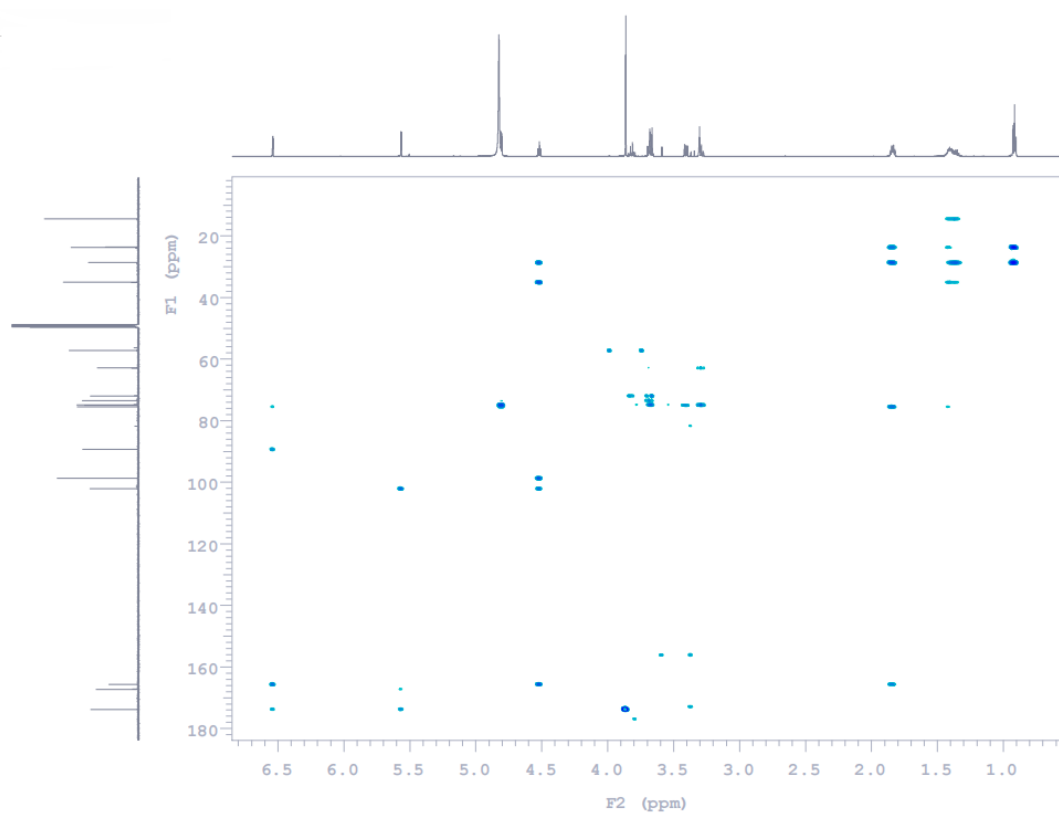


Figure S4. The HMBC (600 MHz, CD₃OD) spectrum of compound **1**

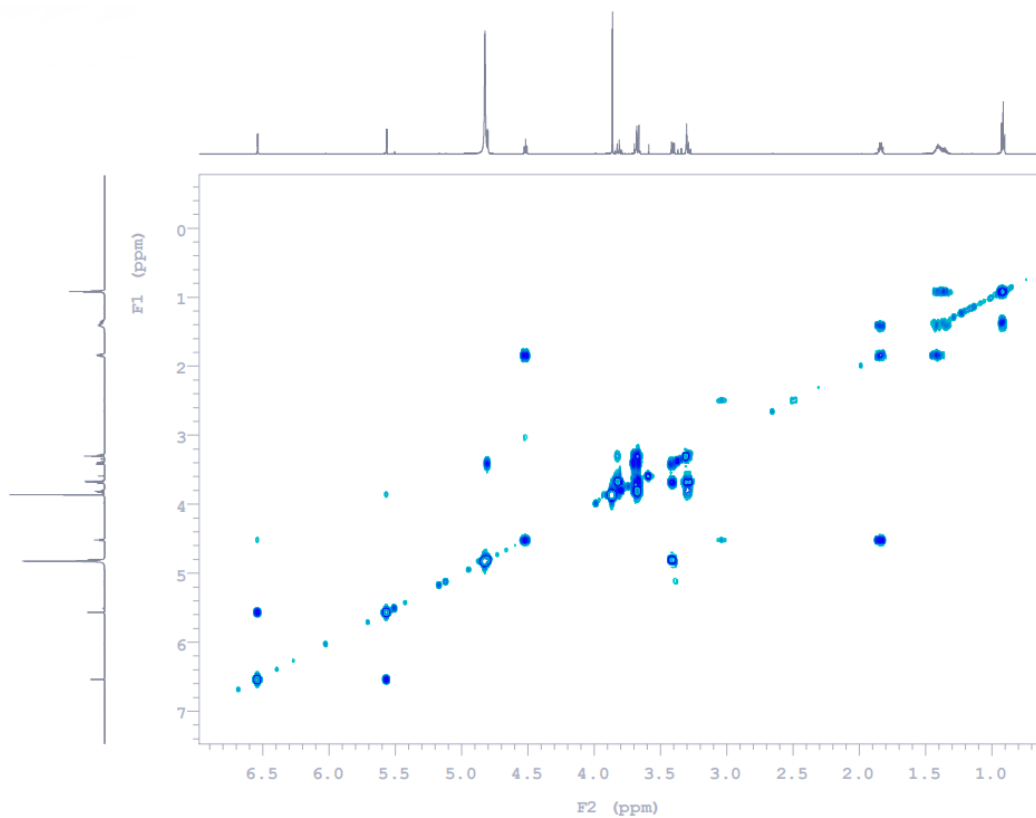


Figure S5. The COSY (600 MHz, CD₃OD) spectrum of compound **1**

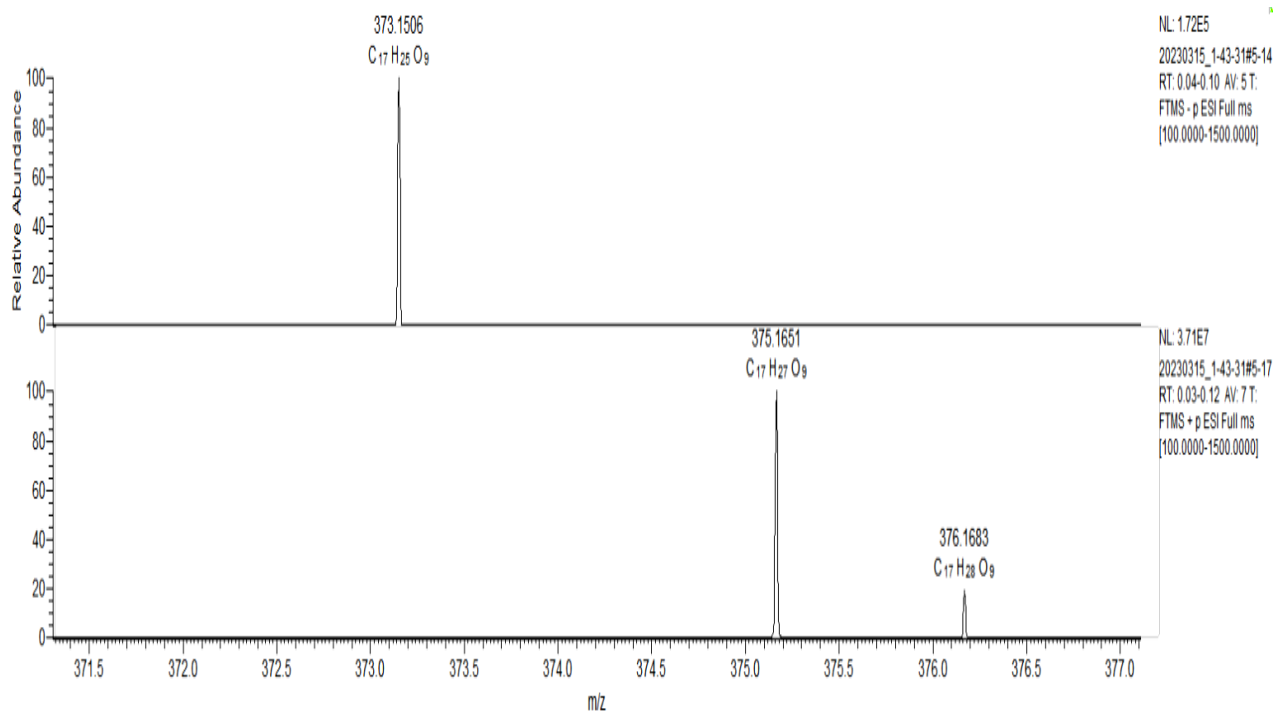


Figure S6. The HRESIMS spectrum of compound **1**

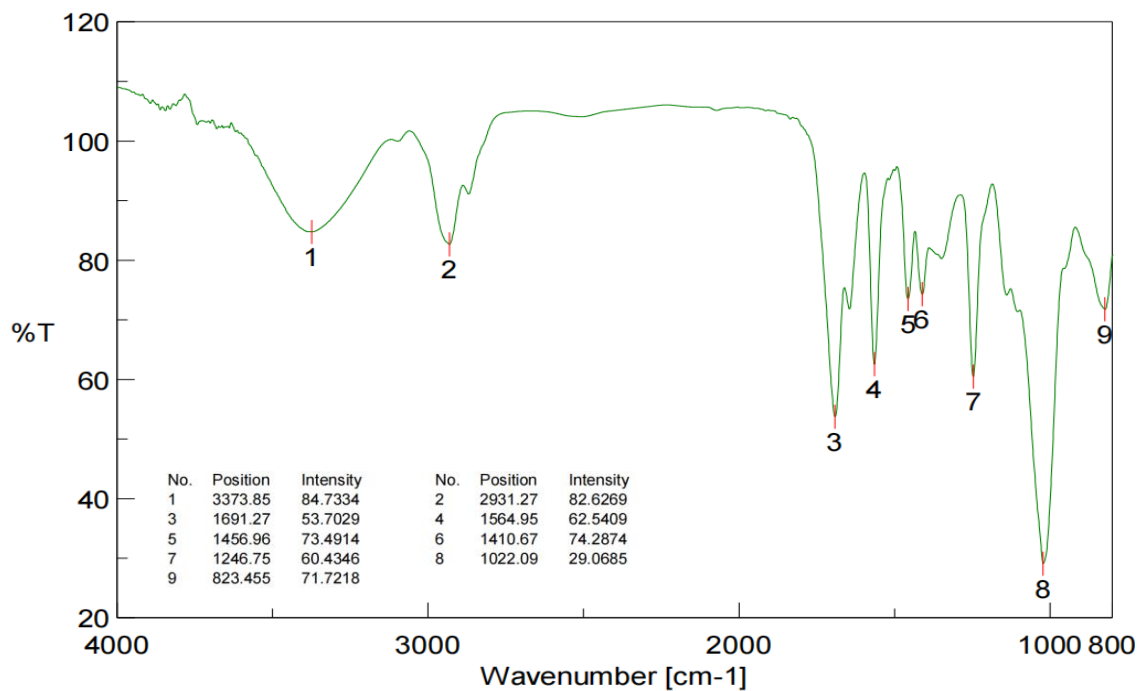


Figure S7. The IR spectrum of compound 1

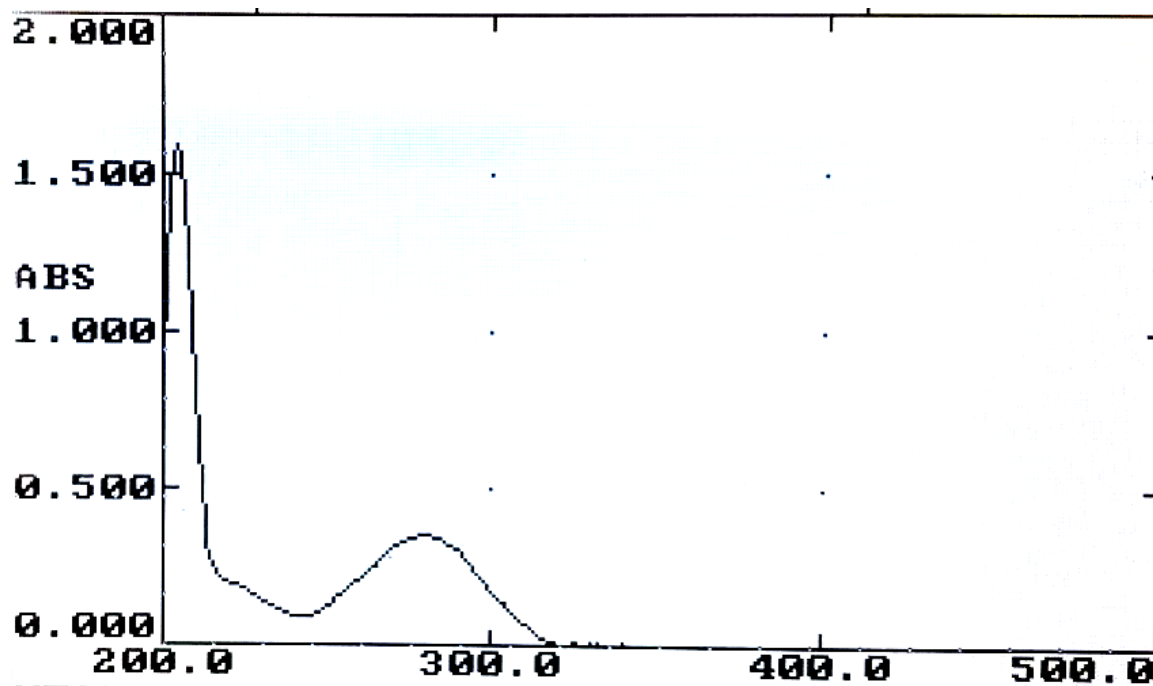


Figure S8. The UV spectrum of compound 1

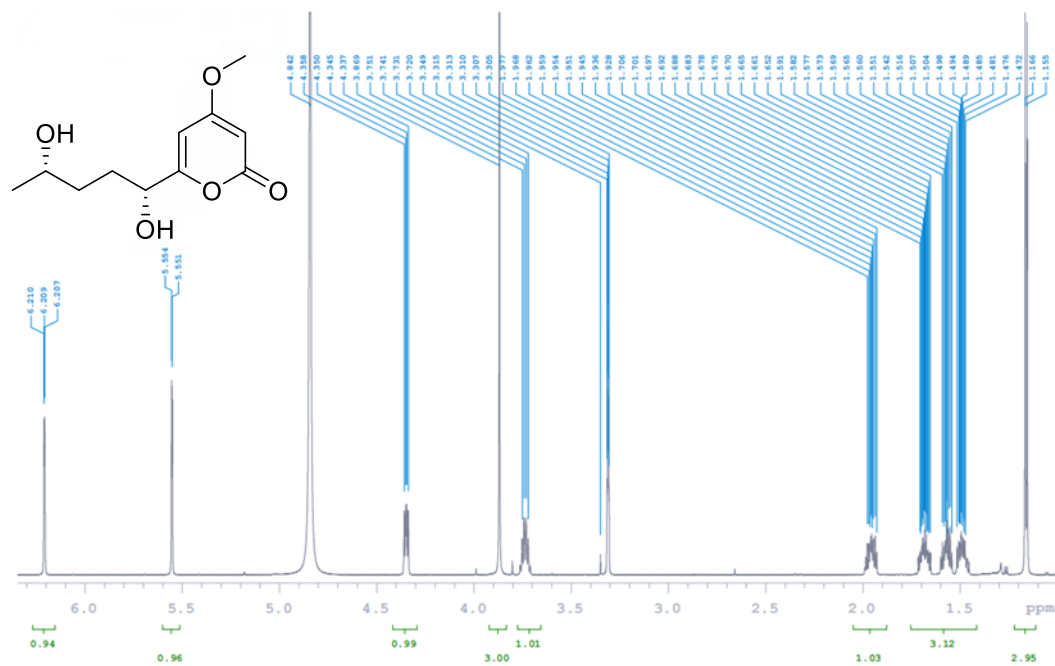


Figure S9. The ^1H NMR (600 MHz, CD_3OD) spectrum of compound 2

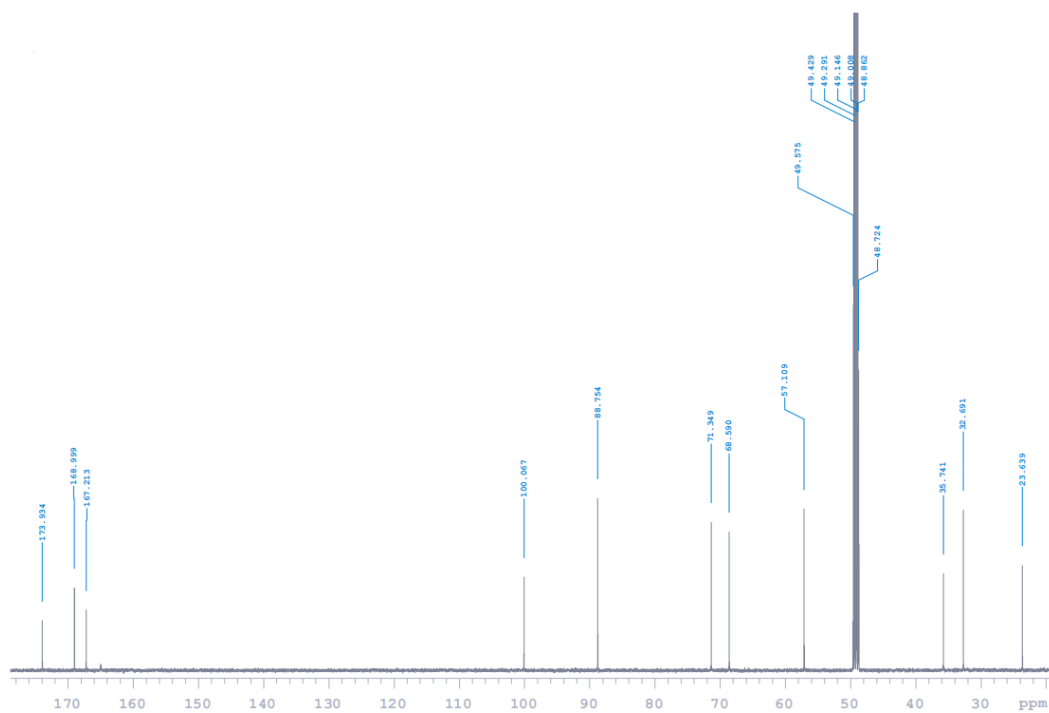


Figure S10. The ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 2

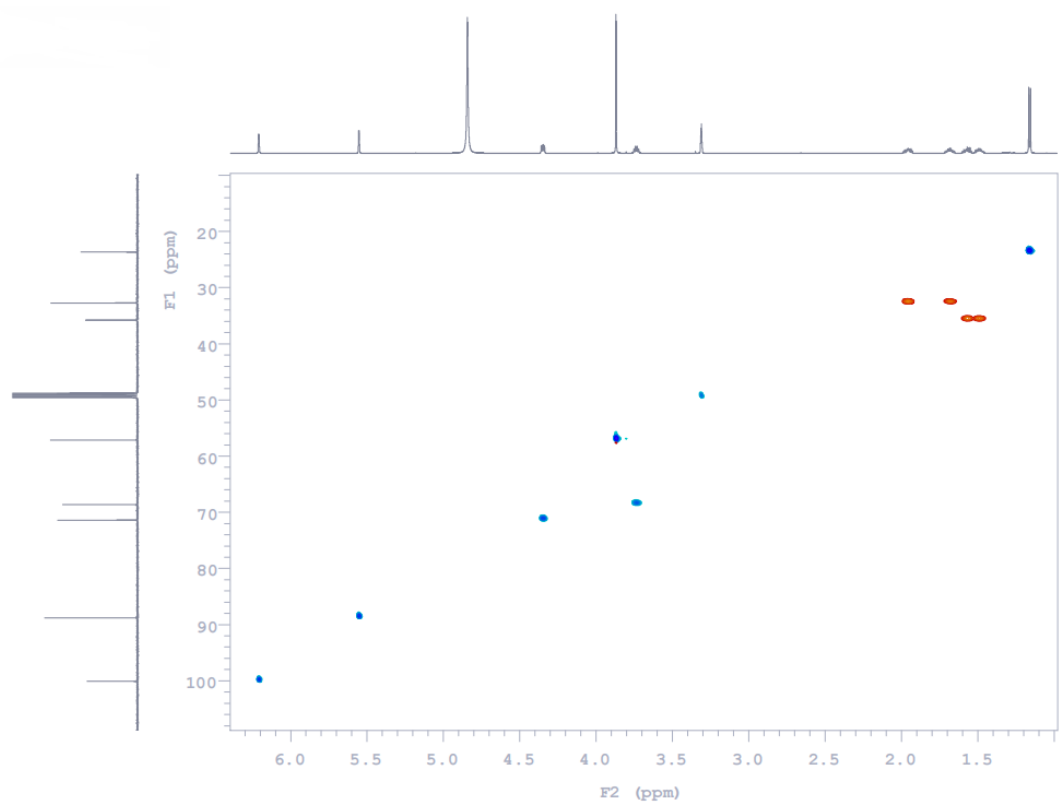


Figure S11. The HSQC (600 MHz, CD₃OD) spectrum of compound **2**

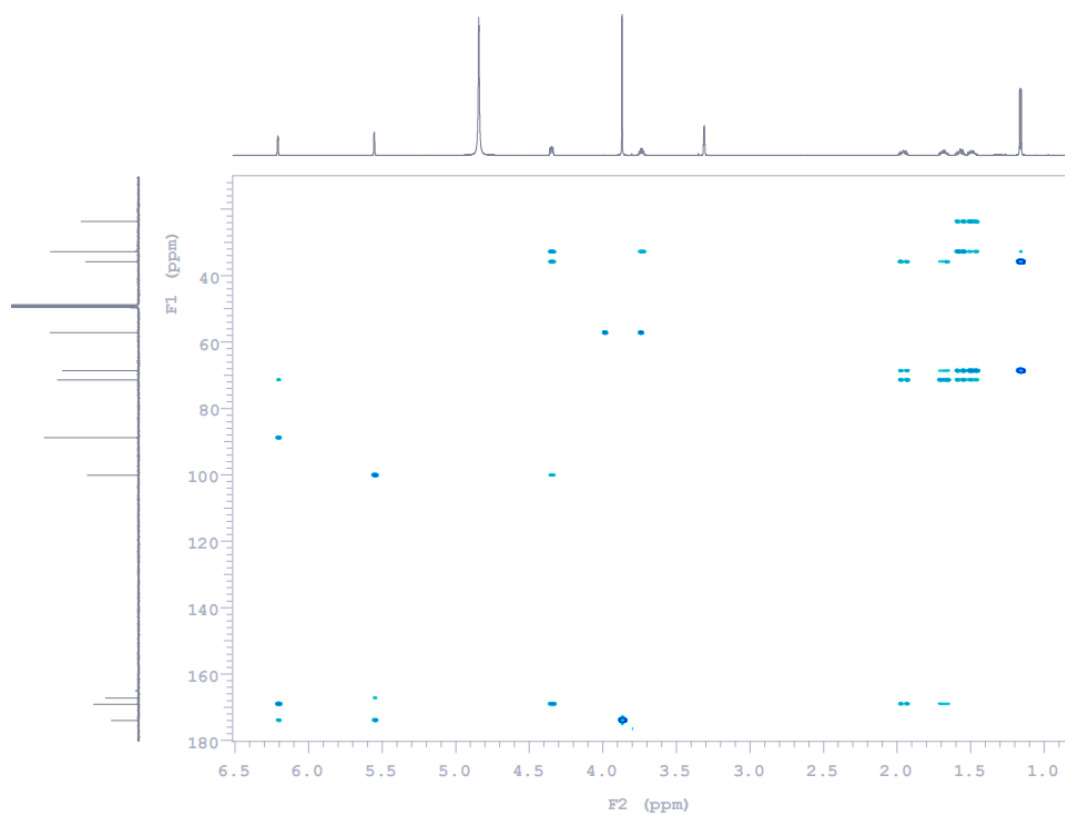


Figure S12. The HMBC (600 MHz, CD₃OD) spectrum of compound **2**

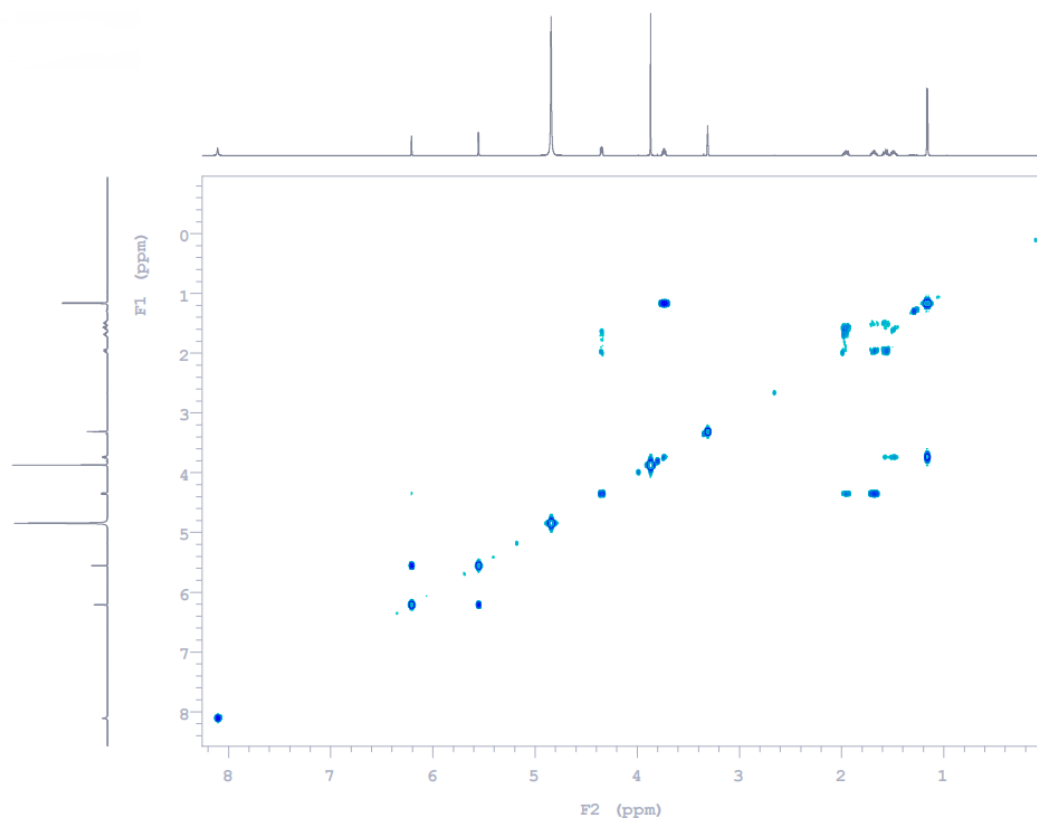


Figure S13. The COSY (600 MHz, CD₃OD) spectrum of compound **2**

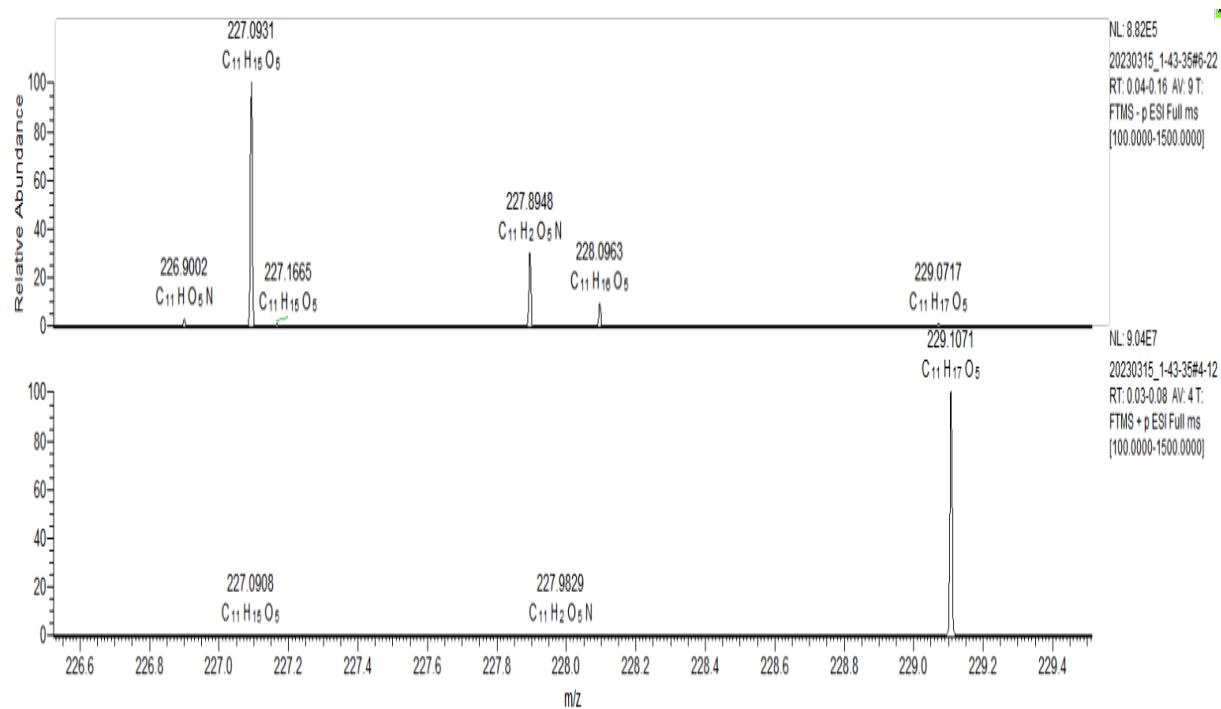


Figure S14. The HRESIMS spectrum of compound **2**

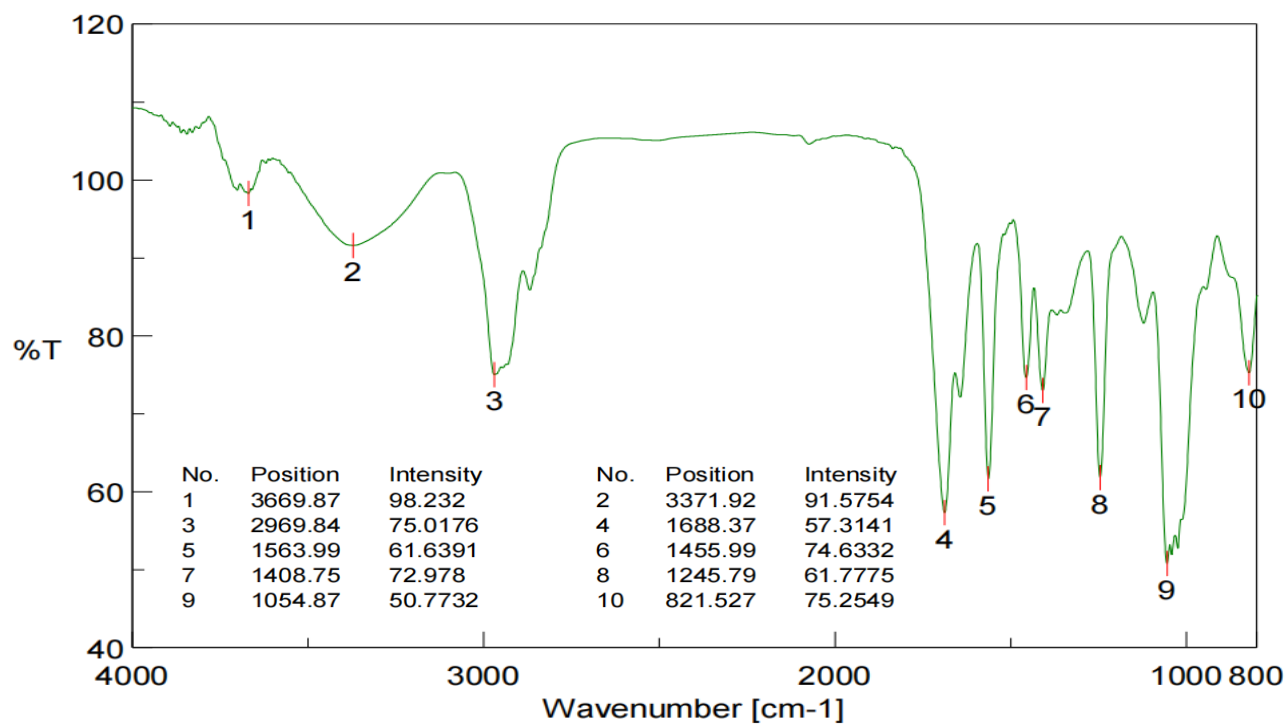


Figure S15. The IR spectrum of compound 2

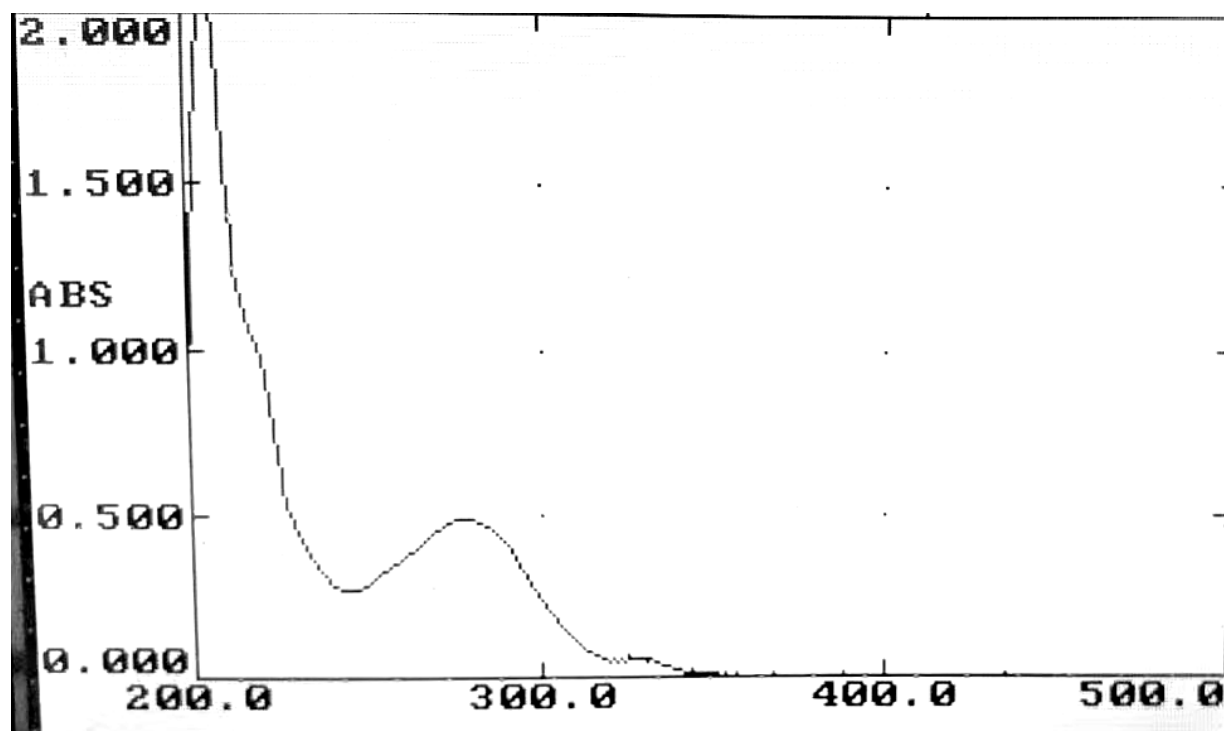


Figure S16. The UV spectrum of compound 2

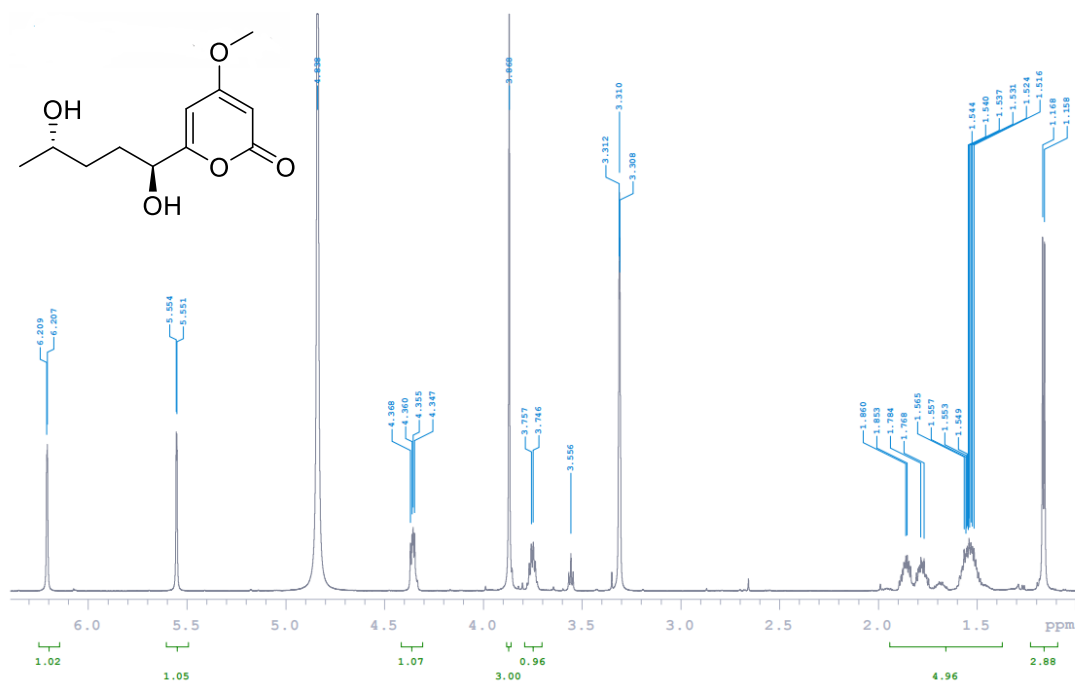


Figure S17. The ¹H NMR (600 MHz, CD₃OD) spectrum of compound **3**

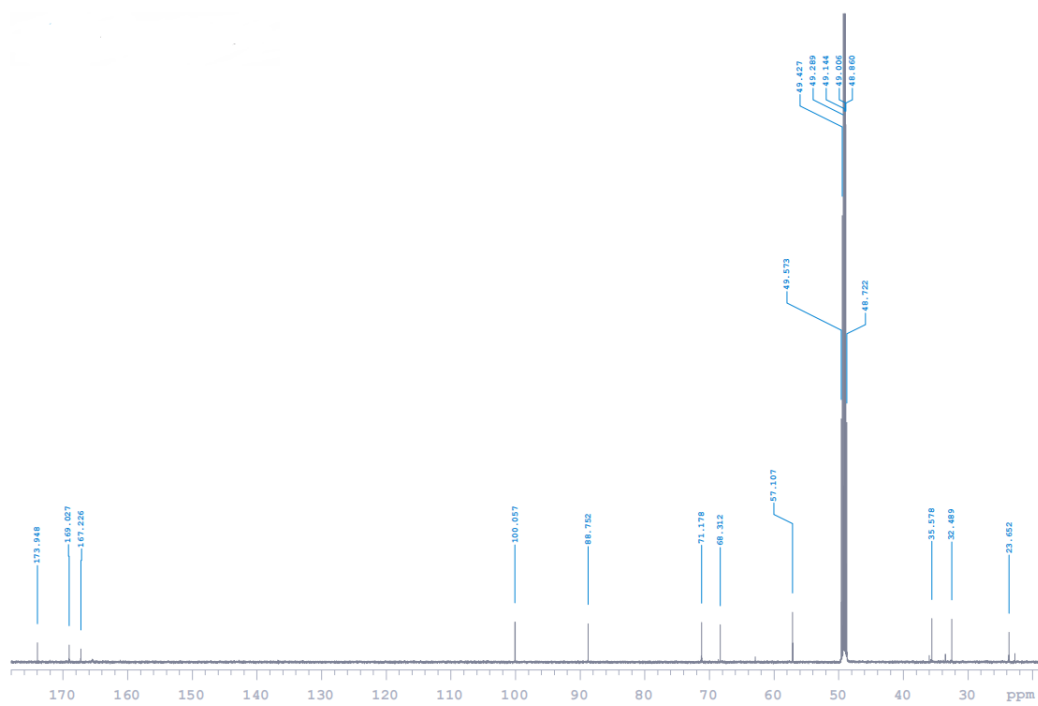


Figure S18. The ¹³C NMR (150 MHz, CD₃OD) spectrum of compound **3**

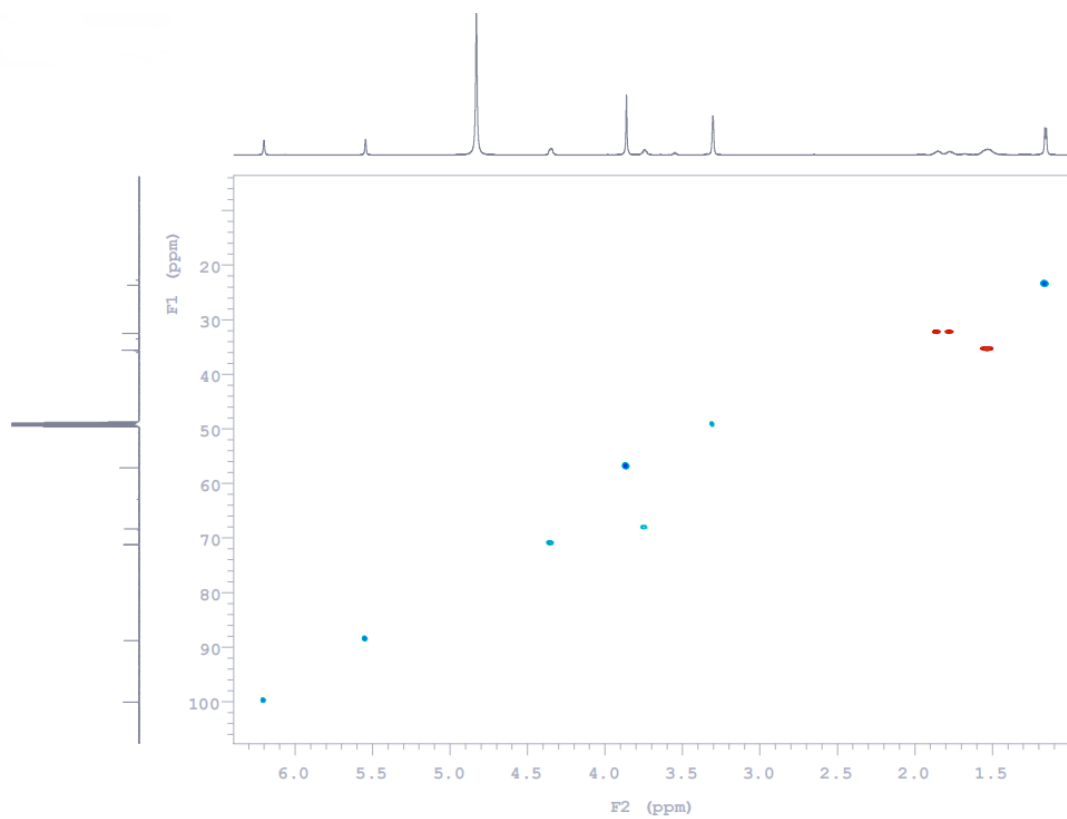


Figure S19. The HSQC (600 MHz, CD₃OD) spectrum of compound **3**

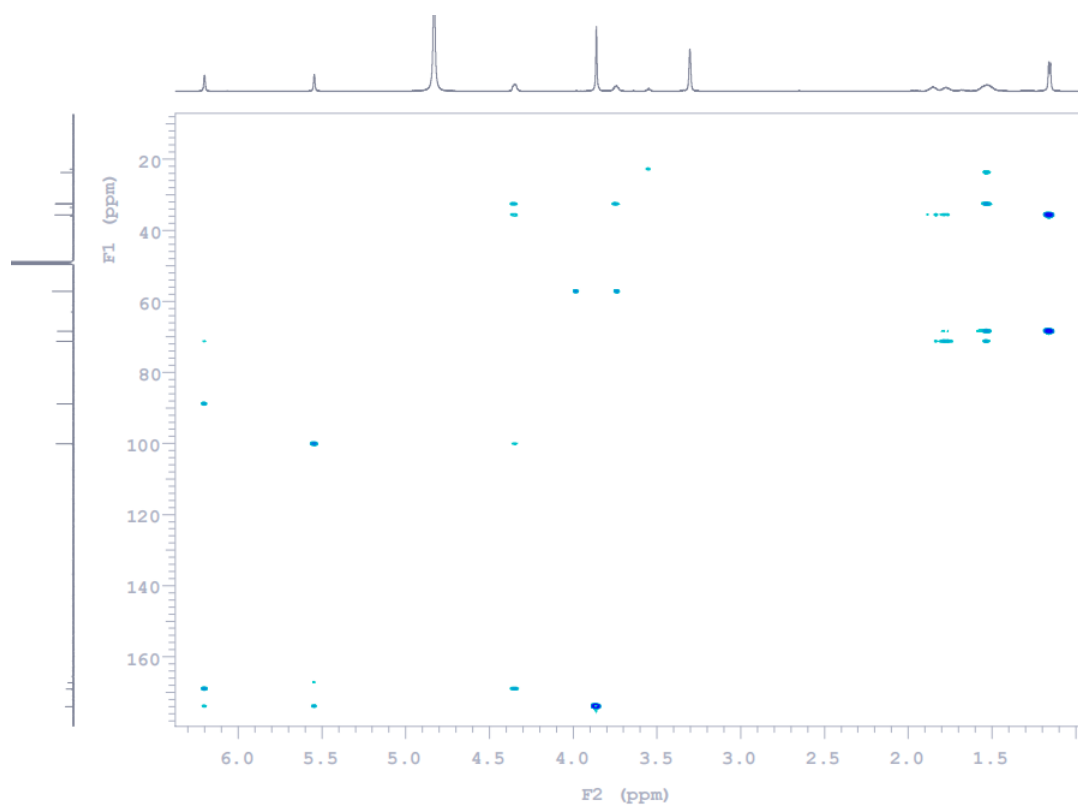


Figure S20. The HMBC (600 MHz, CD₃OD) spectrum of compound **3**

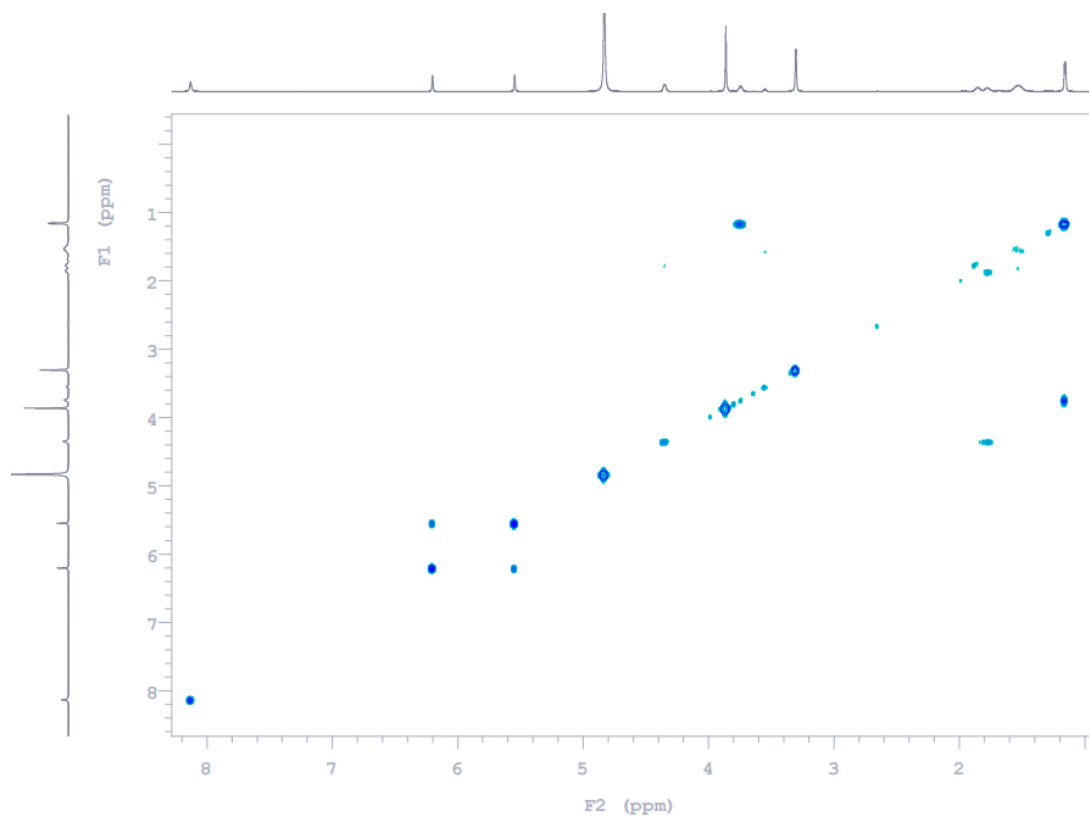


Figure S21. The COSY (600 MHz, CD₃OD) spectrum of compound **3**

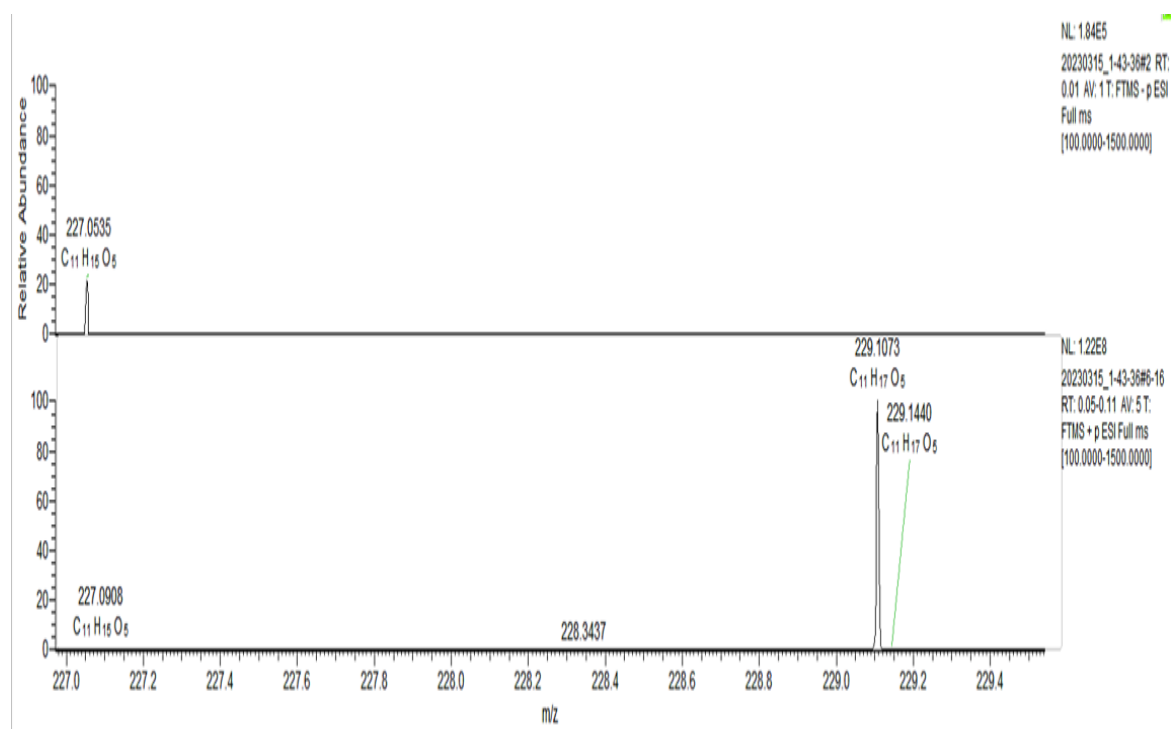


Figure S22. The HRESIMS spectrum of compound **3**

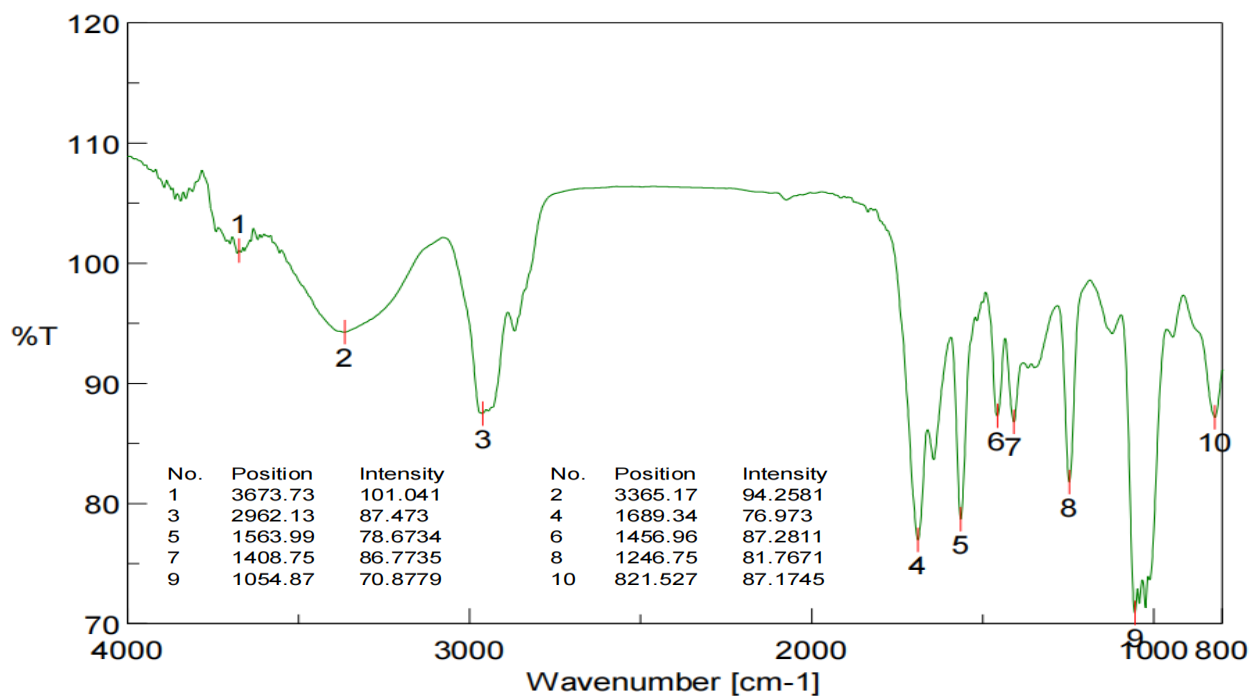


Figure S23. The UV spectrum of compound 3

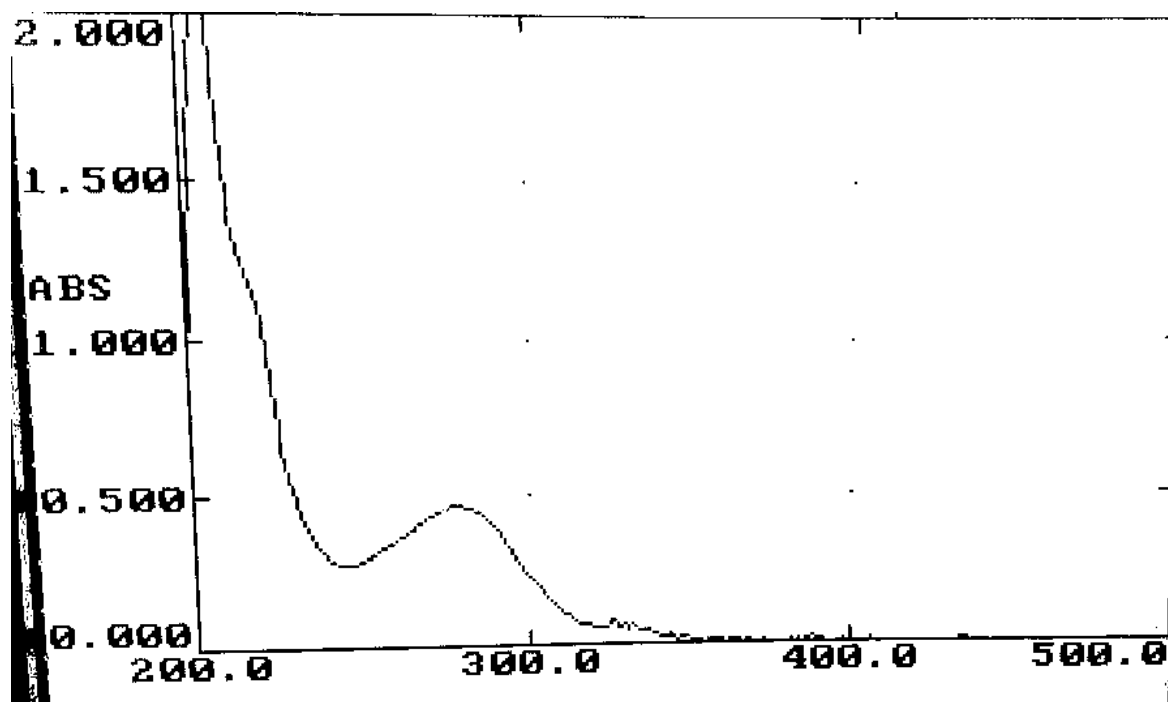


Figure S24. The UV spectrum of compound 3

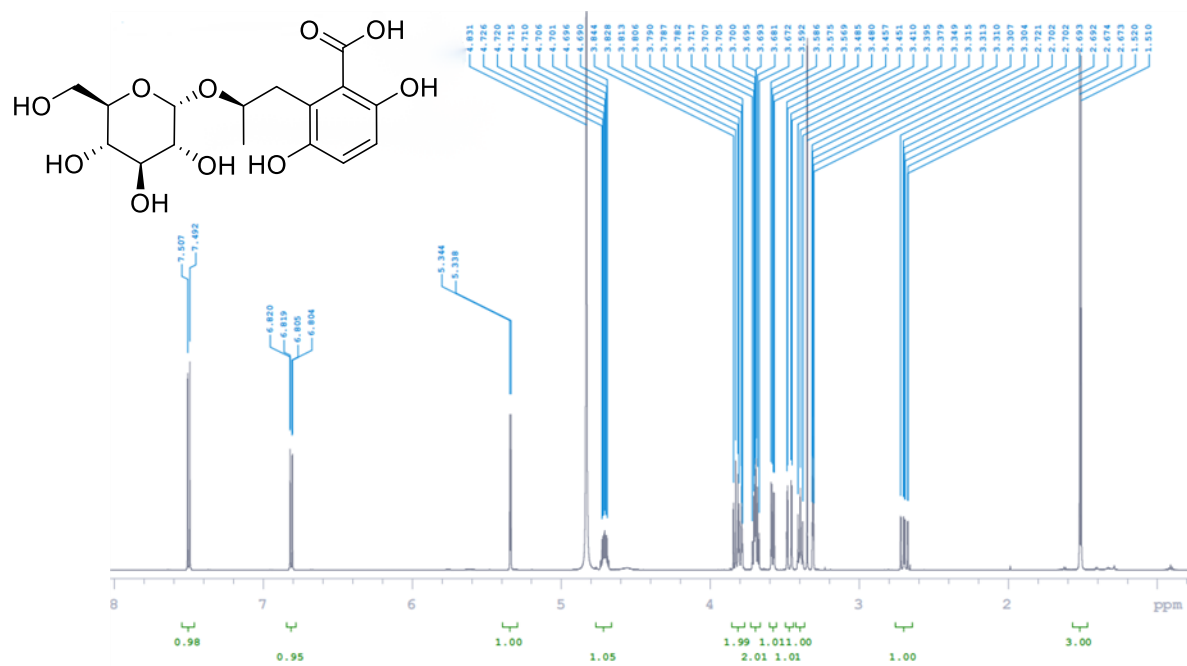


Figure S25. The ¹H NMR (600 MHz, CD₃OD) spectrum of compound 4

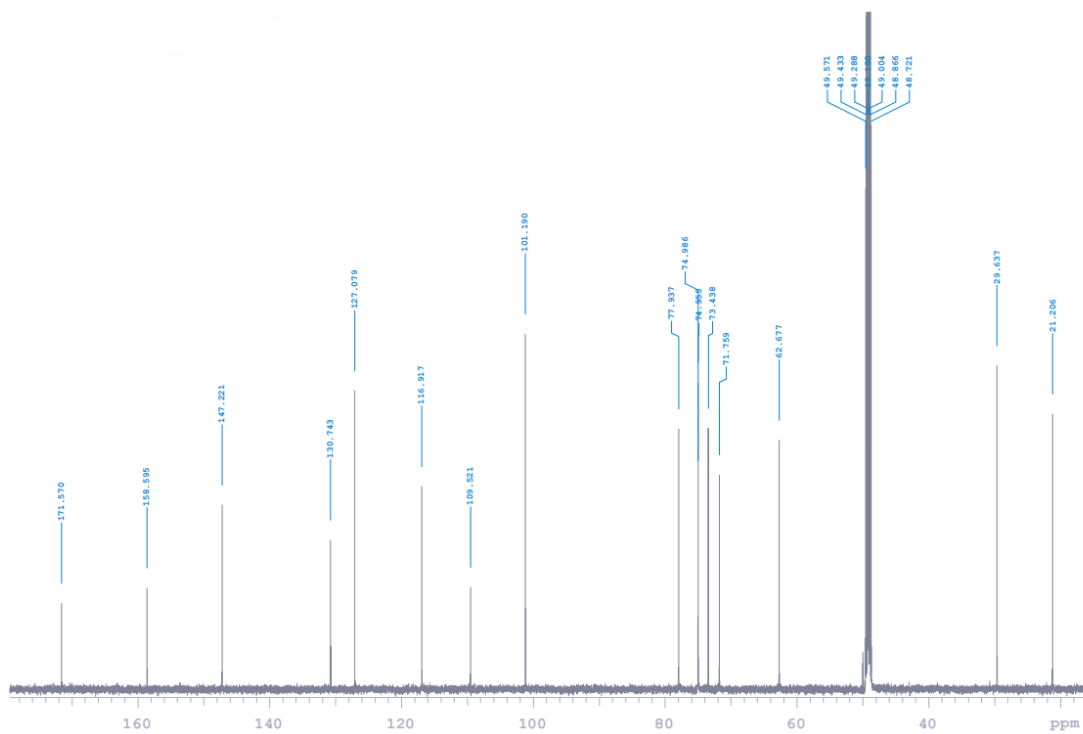


Figure S26. The ¹³C NMR (150 MHz, CD₃OD) spectrum of compound 4

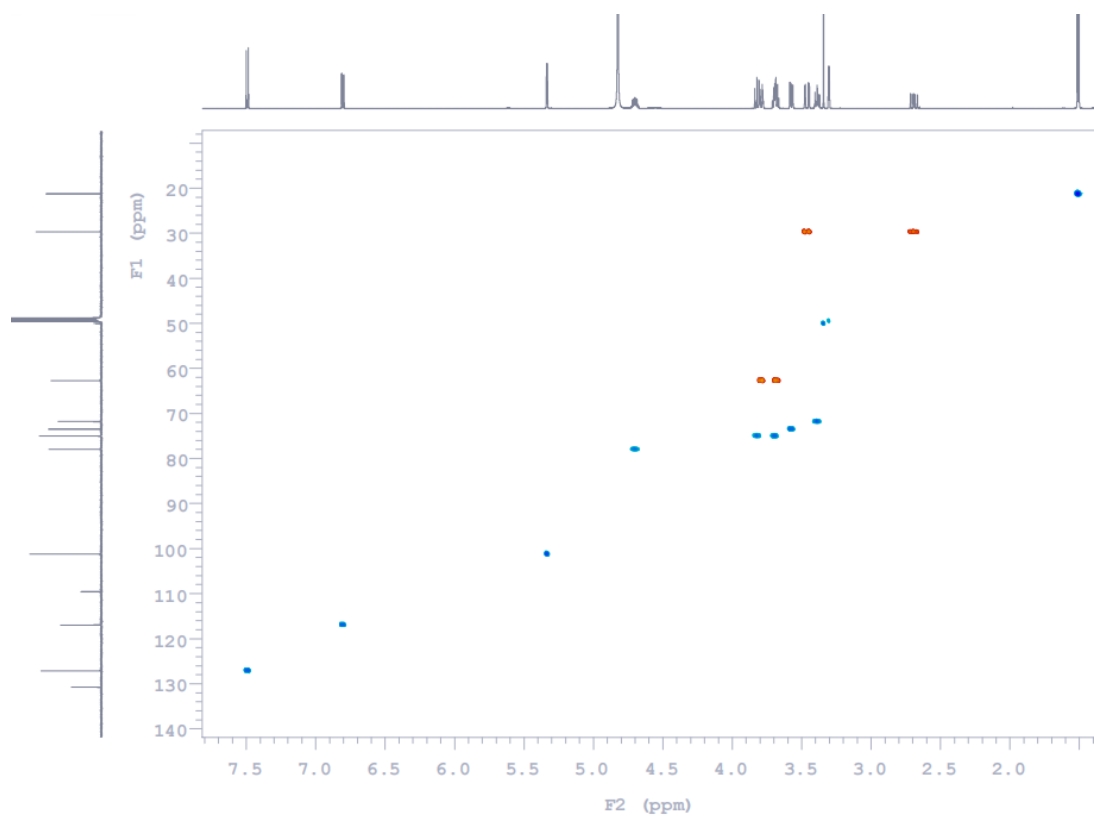


Figure S27. The HSQC (600 MHz, CD₃OD) spectrum of compound **4**

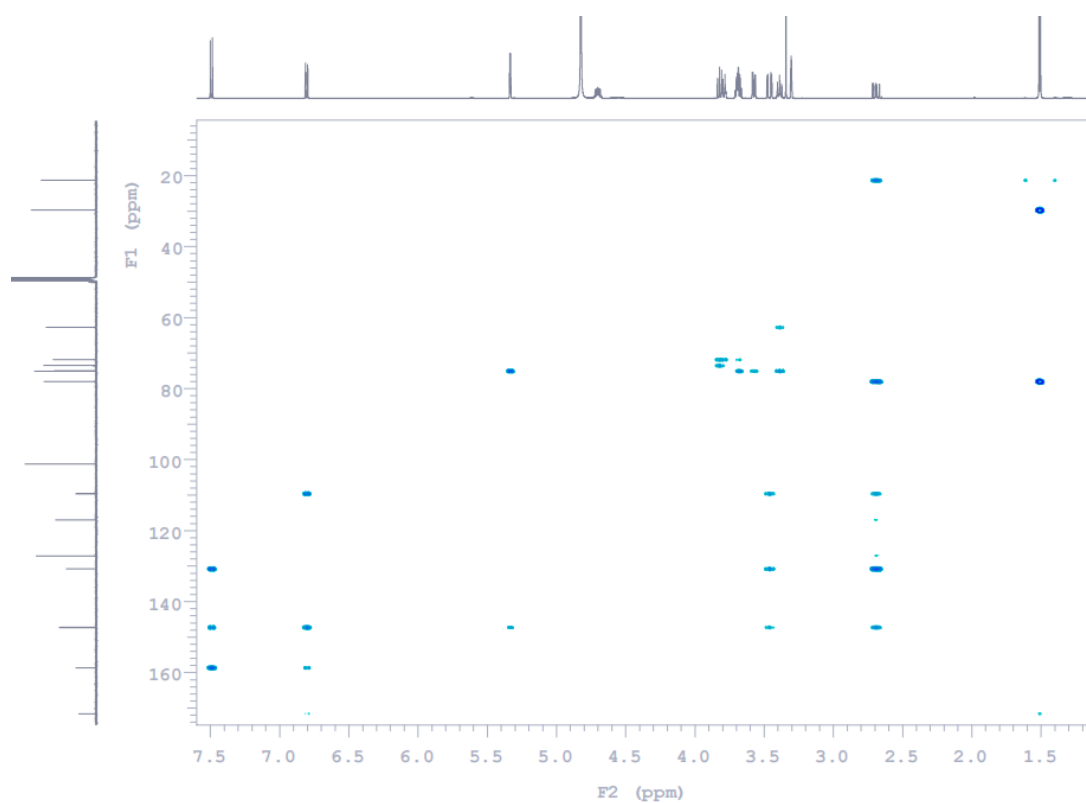


Figure S28. The HMBC (600 MHz, CD₃OD) spectrum of compound **4**

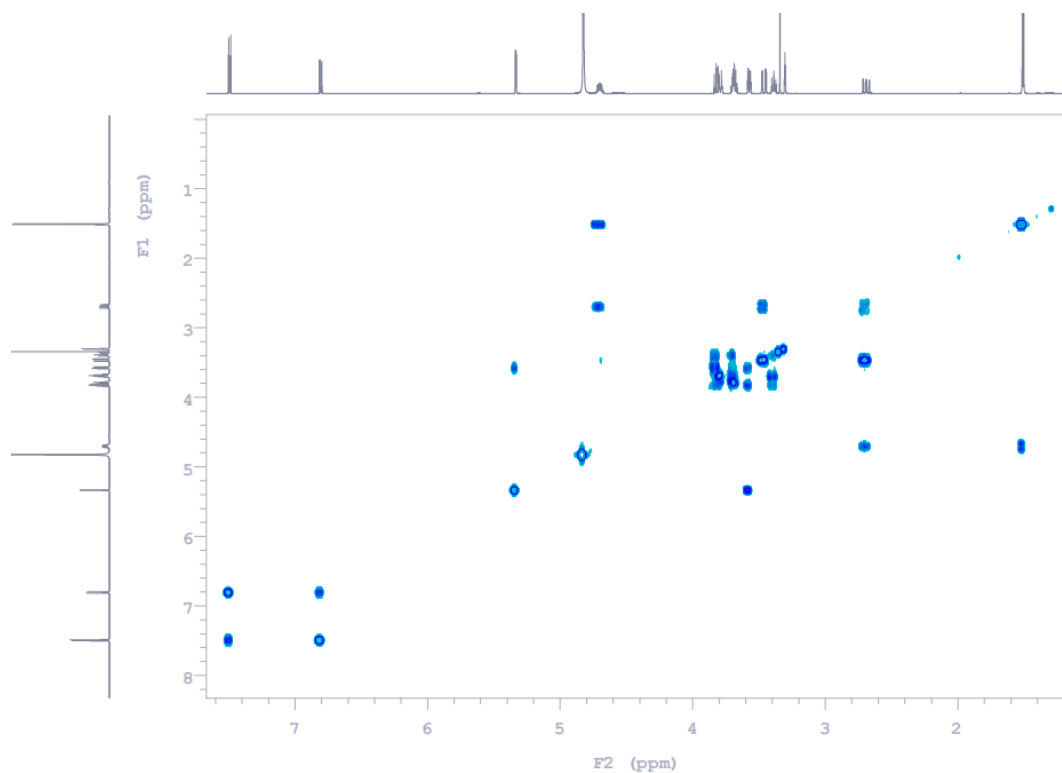


Figure S29. The COSY (600 MHz, CD₃OD) spectrum of compound **4**

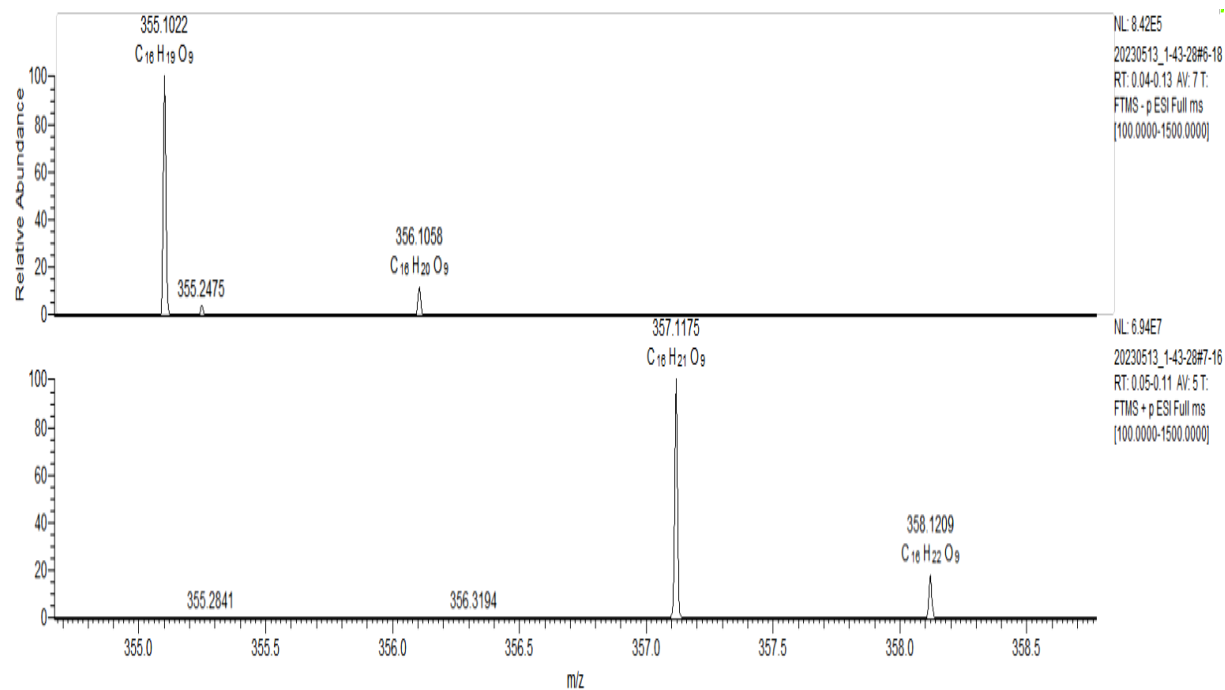


Figure S30. The HRESIMS spectrum of compound **4**

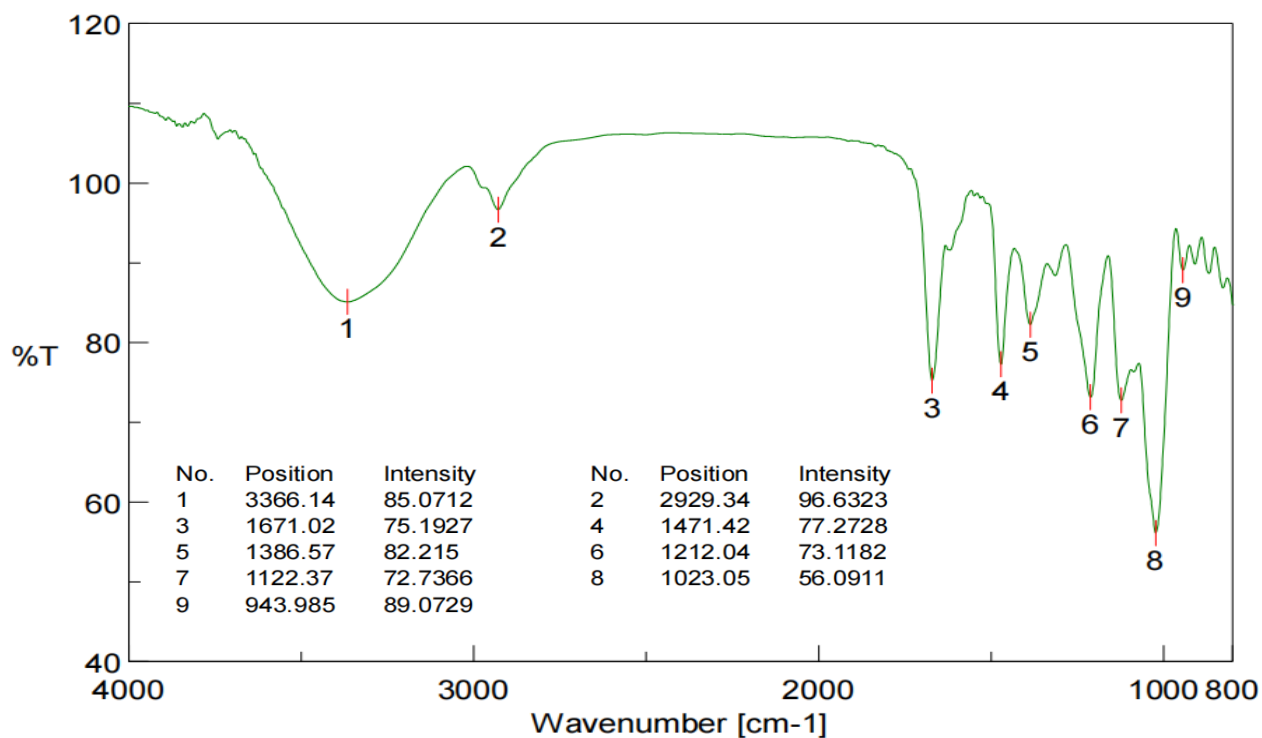


Figure S31. The IR spectrum of compound 4

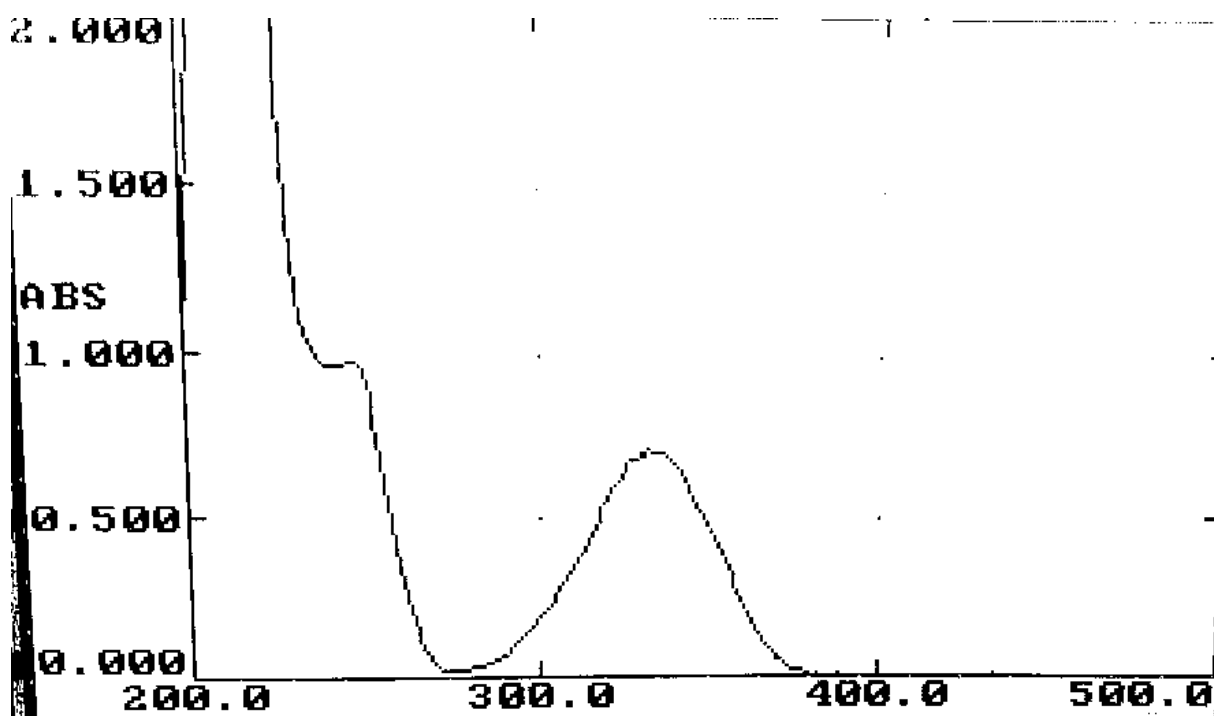


Figure S32. The UV spectrum of compound 4

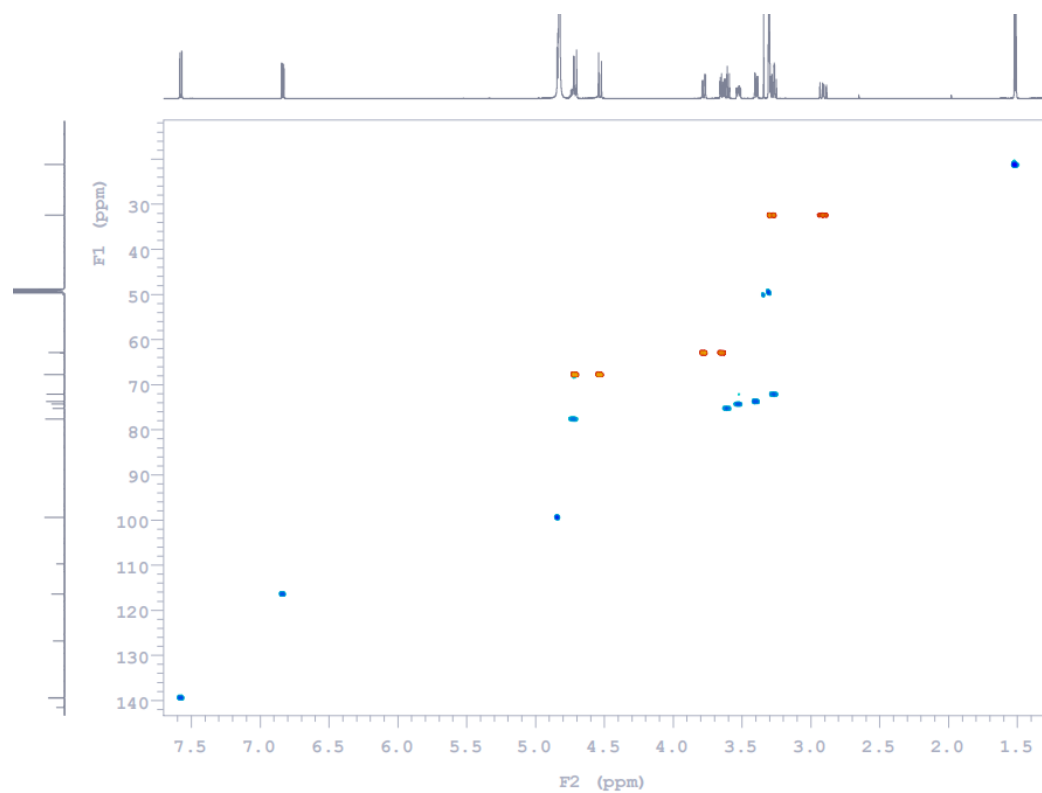


Figure S35. The HSQC (600 MHz, CD₃OD) spectrum of compound **5**

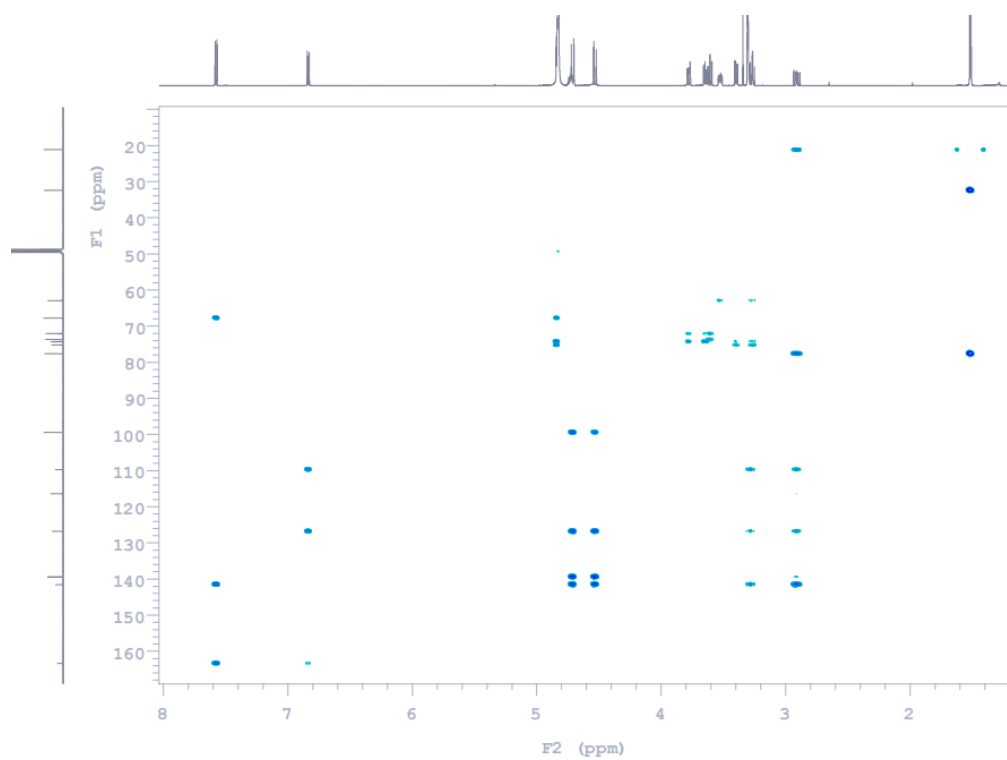


Figure S36. The HMBC (600 MHz, CD₃OD) spectrum of compound **5**

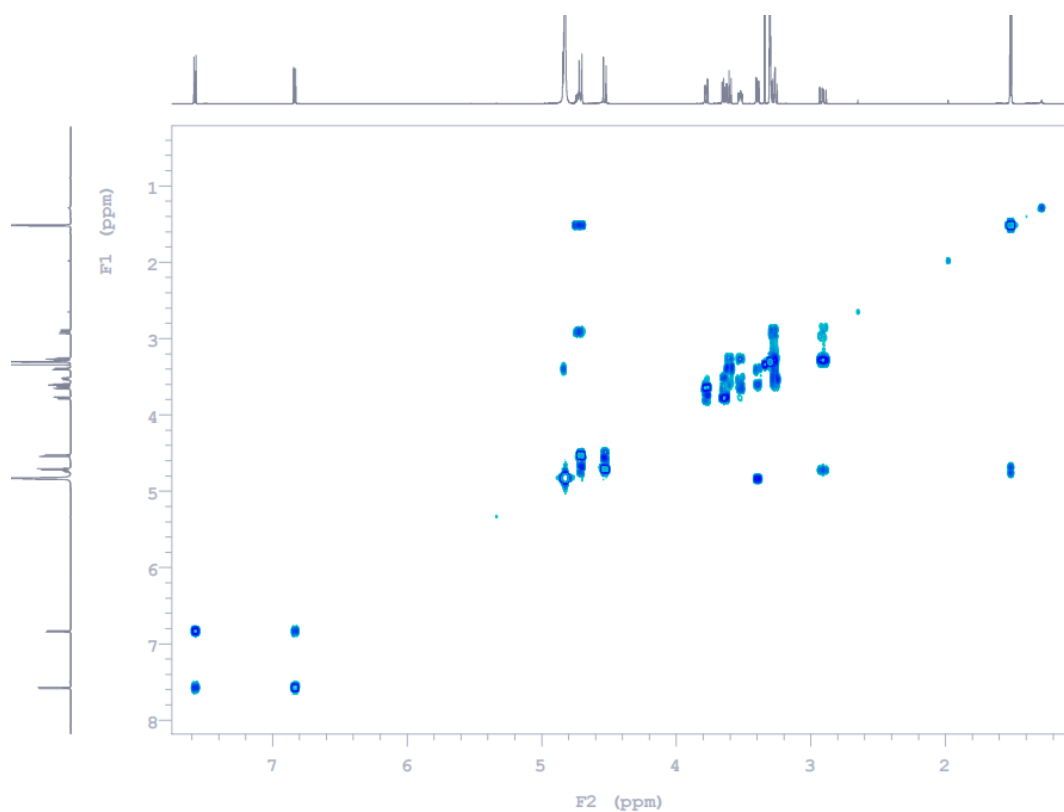


Figure S37. The COSY (600 MHz, CD₃OD) spectrum of compound **5**

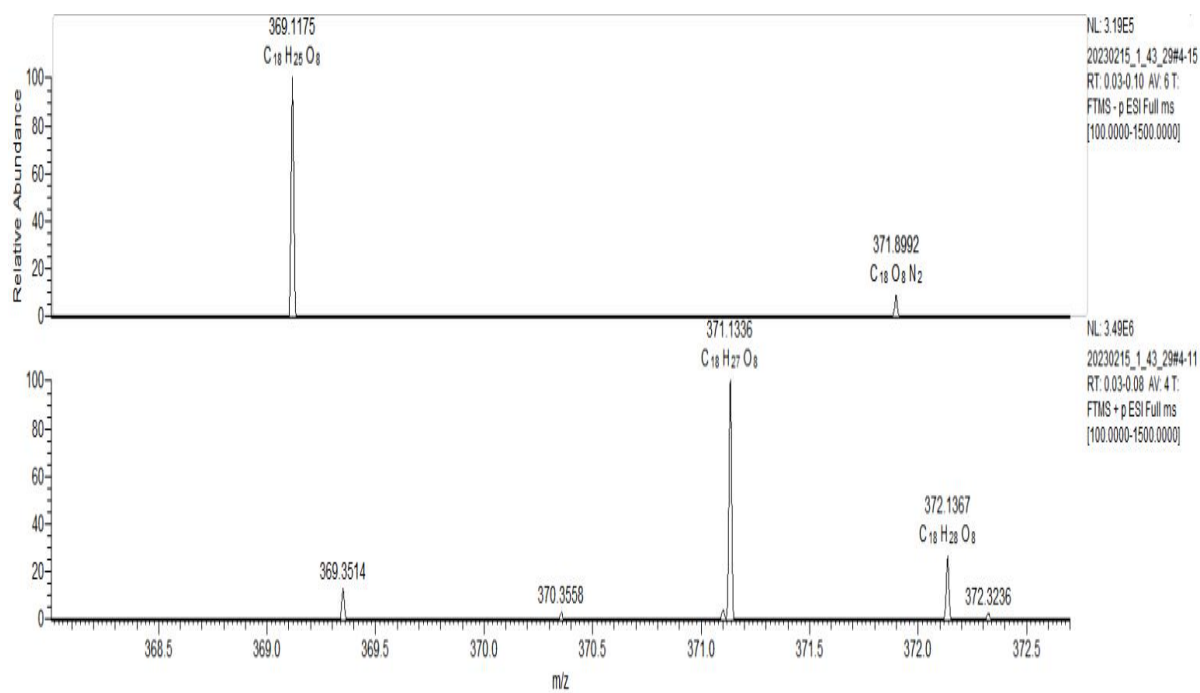


Figure S38. The HRESIMS spectrum of compound **5**

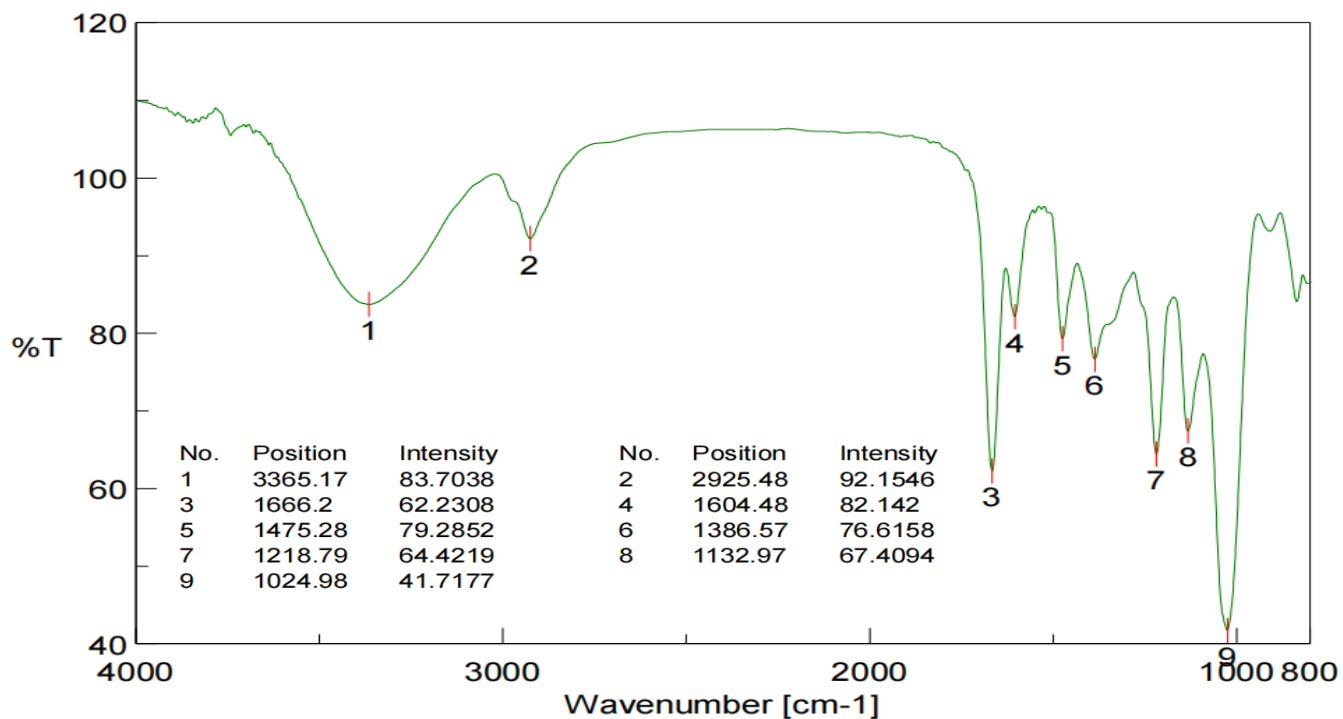


Figure S39. The UV spectrum of compound 5

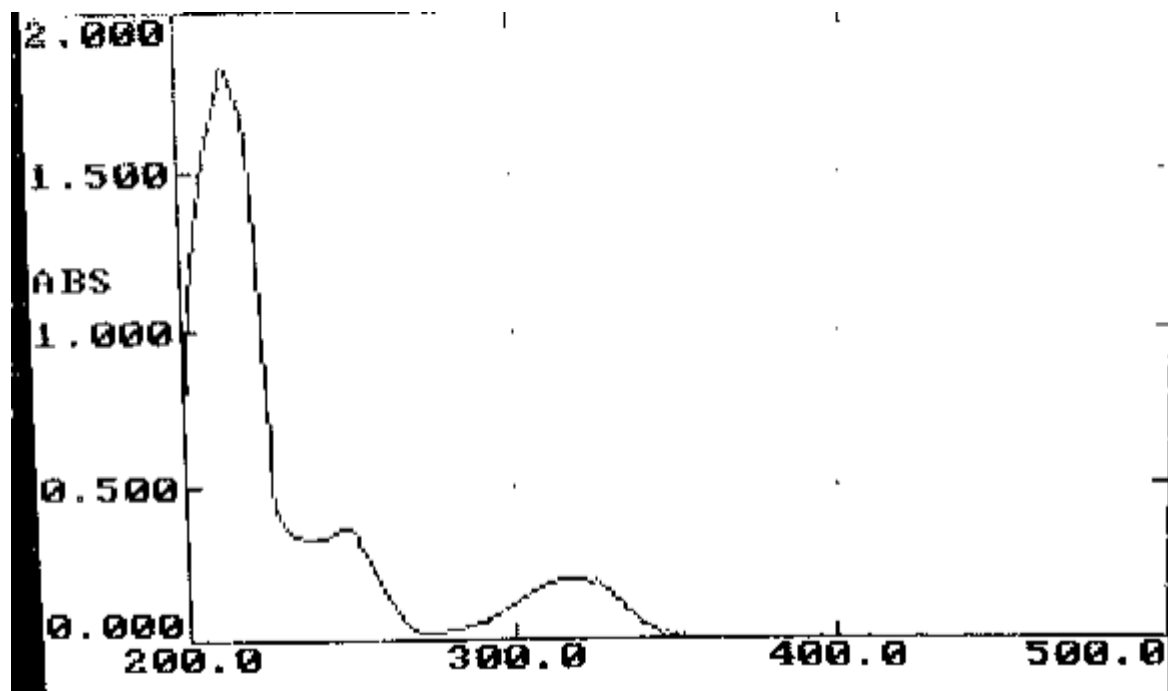


Figure S40. The UV spectrum of compound 5

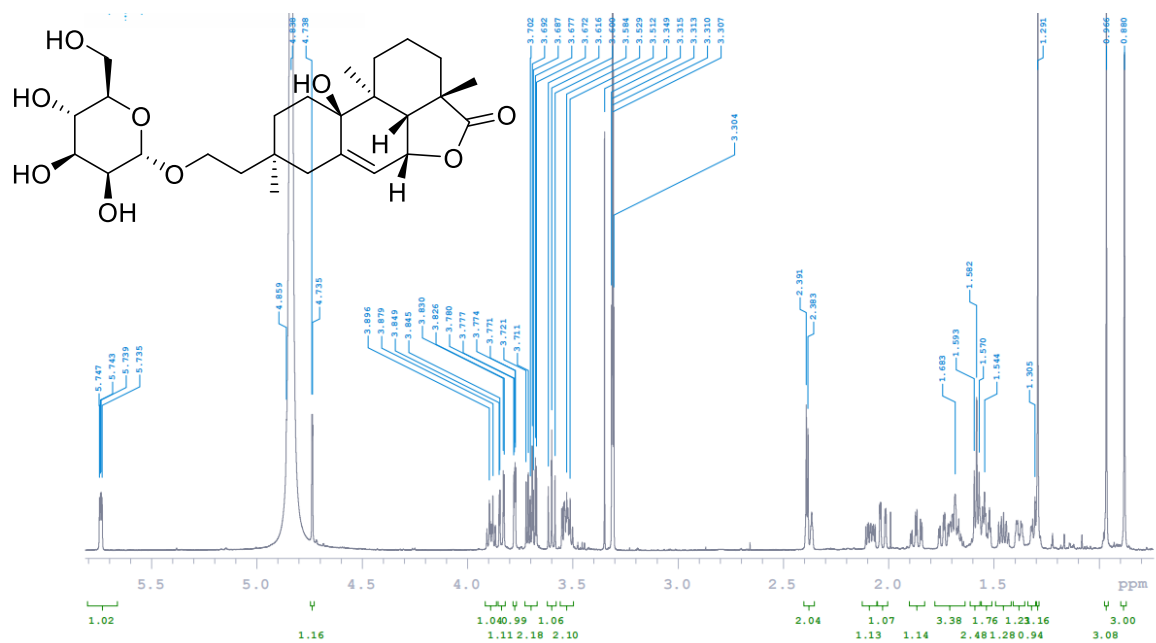


Figure S41. The ^1H NMR (600 MHz, CD_3OD) spectrum of compound **6**

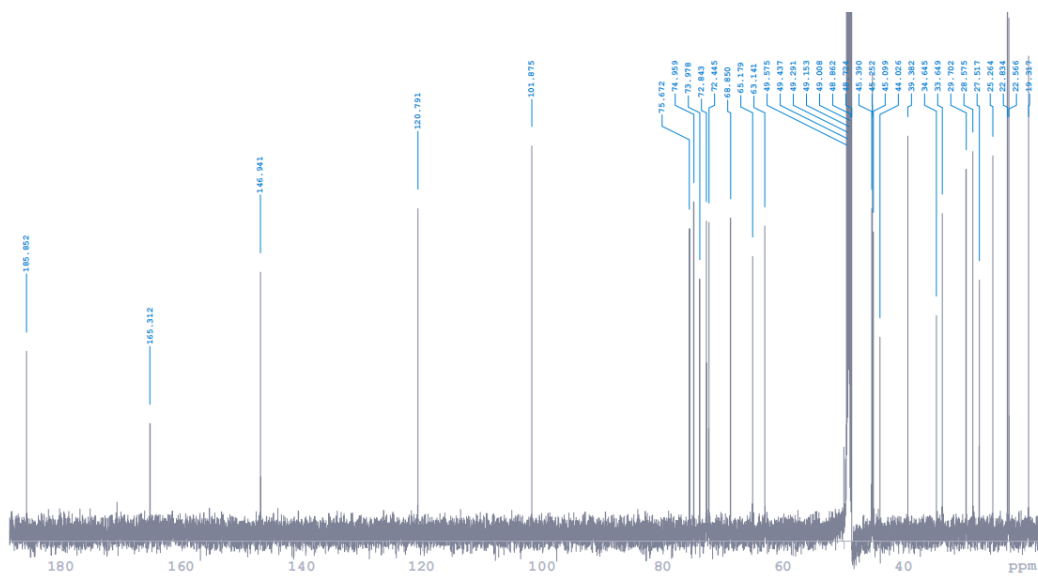


Figure S42. The ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **6**

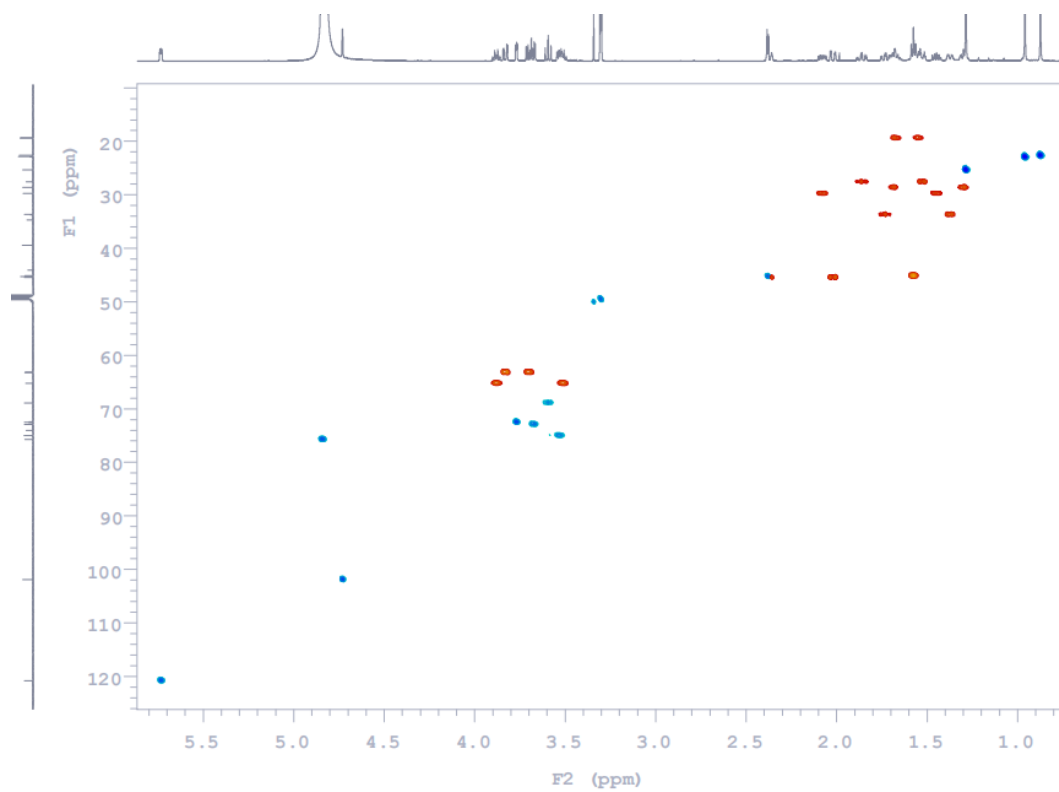


Figure S43. The HSQC (600 MHz, CD_3OD) spectrum of compound **6**

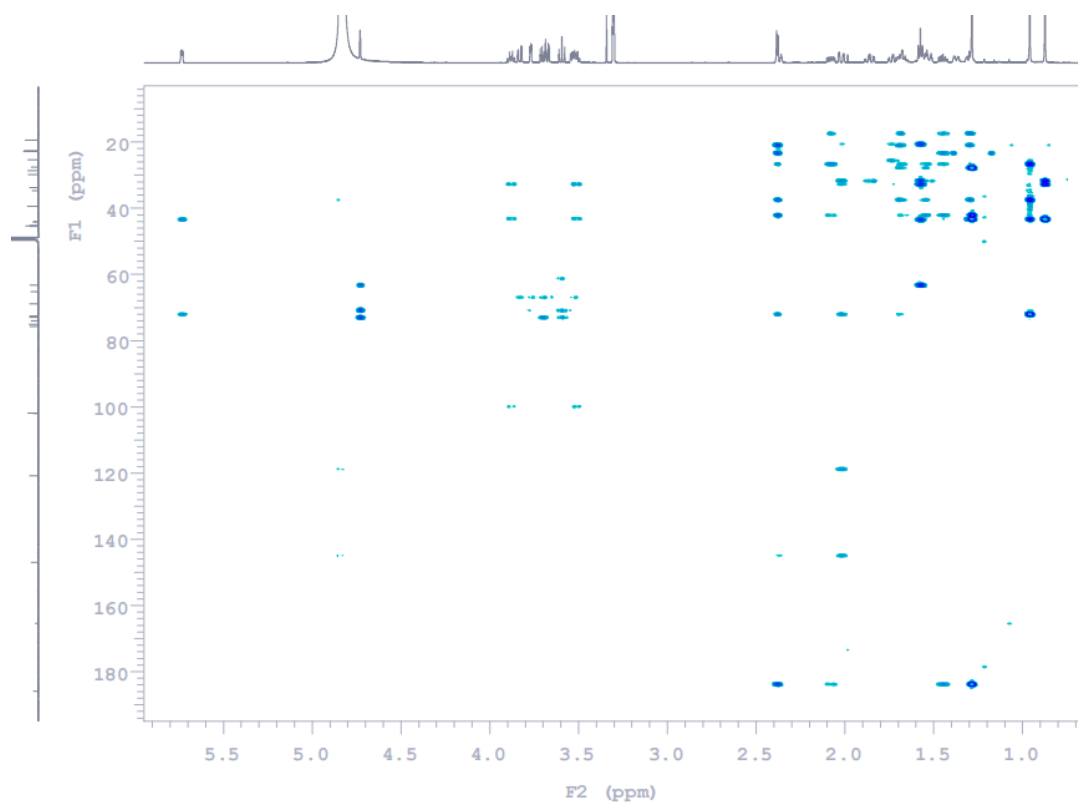


Figure S44. The HMBC (600 MHz, CD_3OD) spectrum of compound **6**

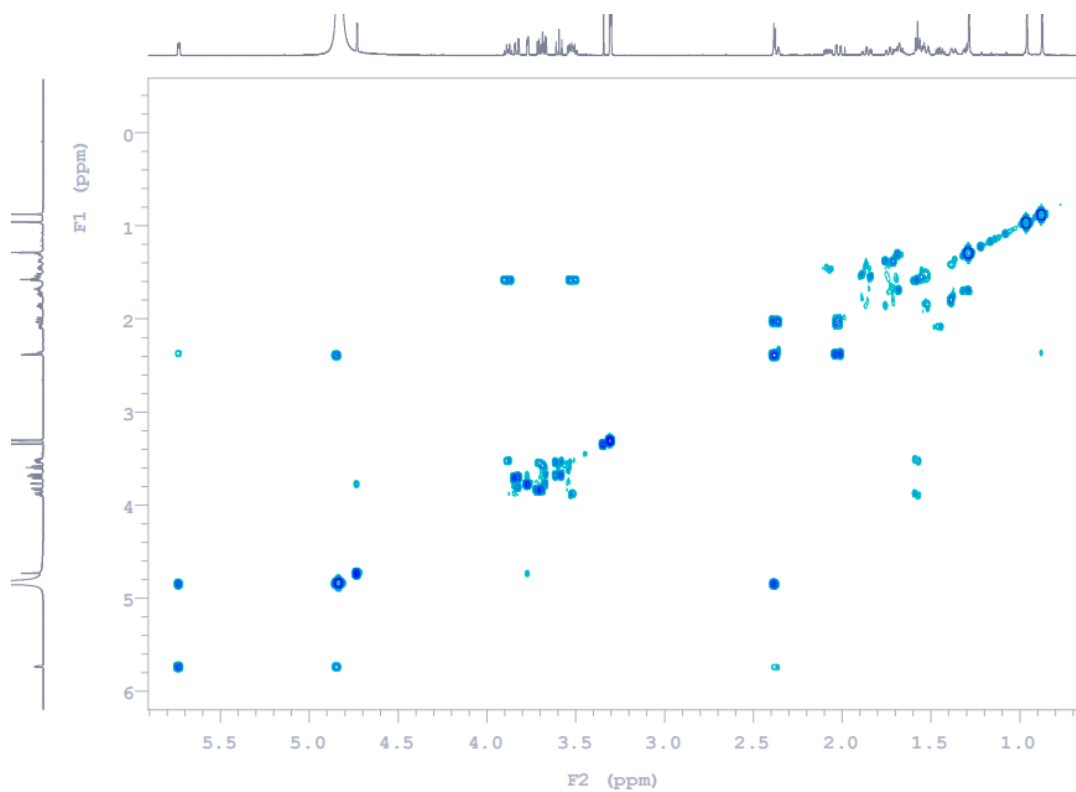


Figure S45. The COSY (600 MHz, CD₃OD) spectrum of compound **6**

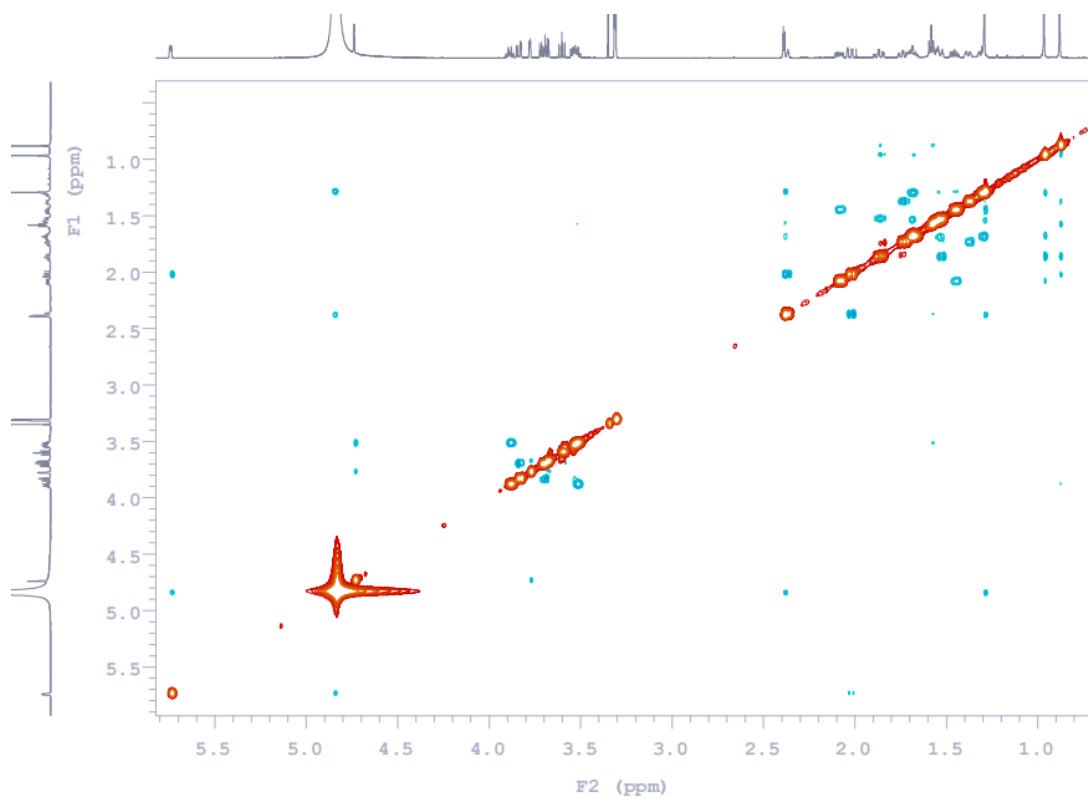


Figure S46. The NOESY (600 MHz, CD₃OD) spectrum of compound **6**

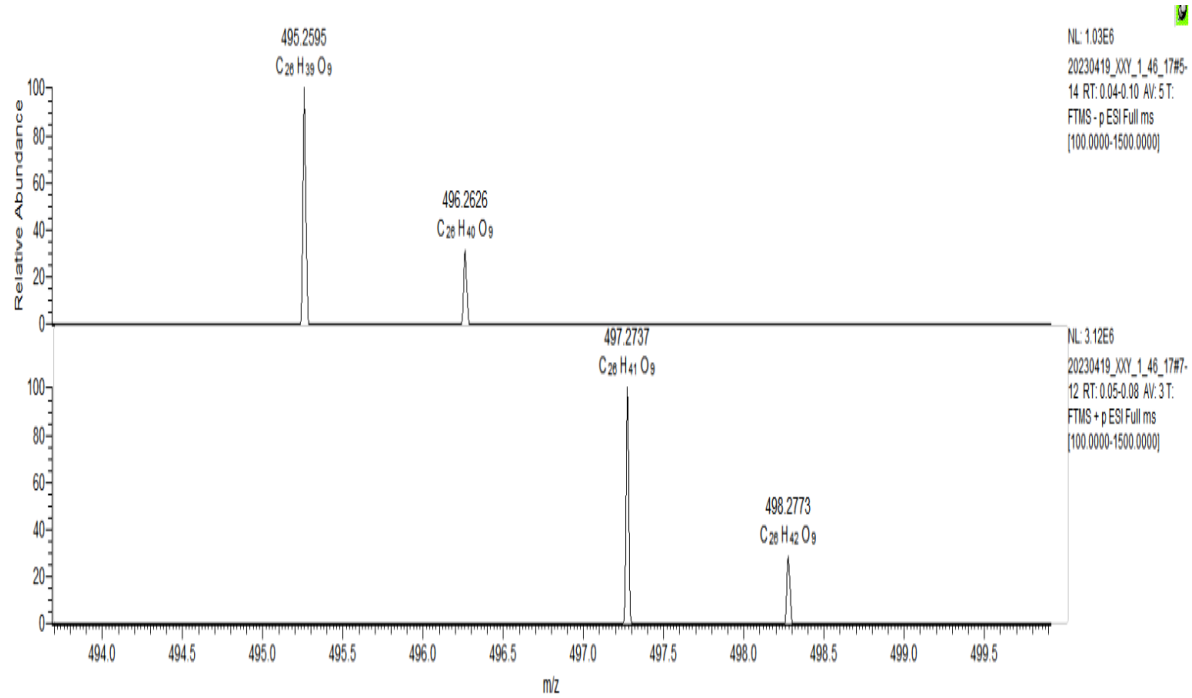


Figure S47. The HRESIMS spectrum of compound **6**

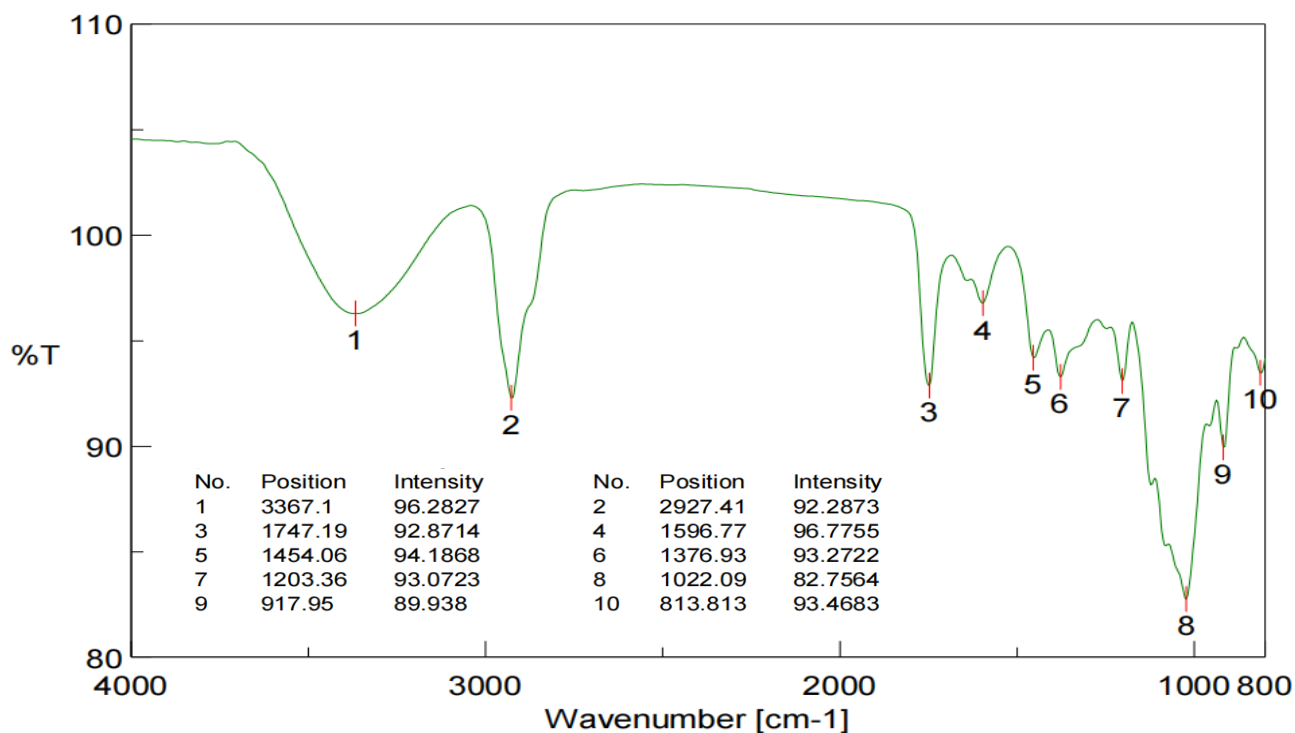


Figure S48. The IR spectrum of compound **6**

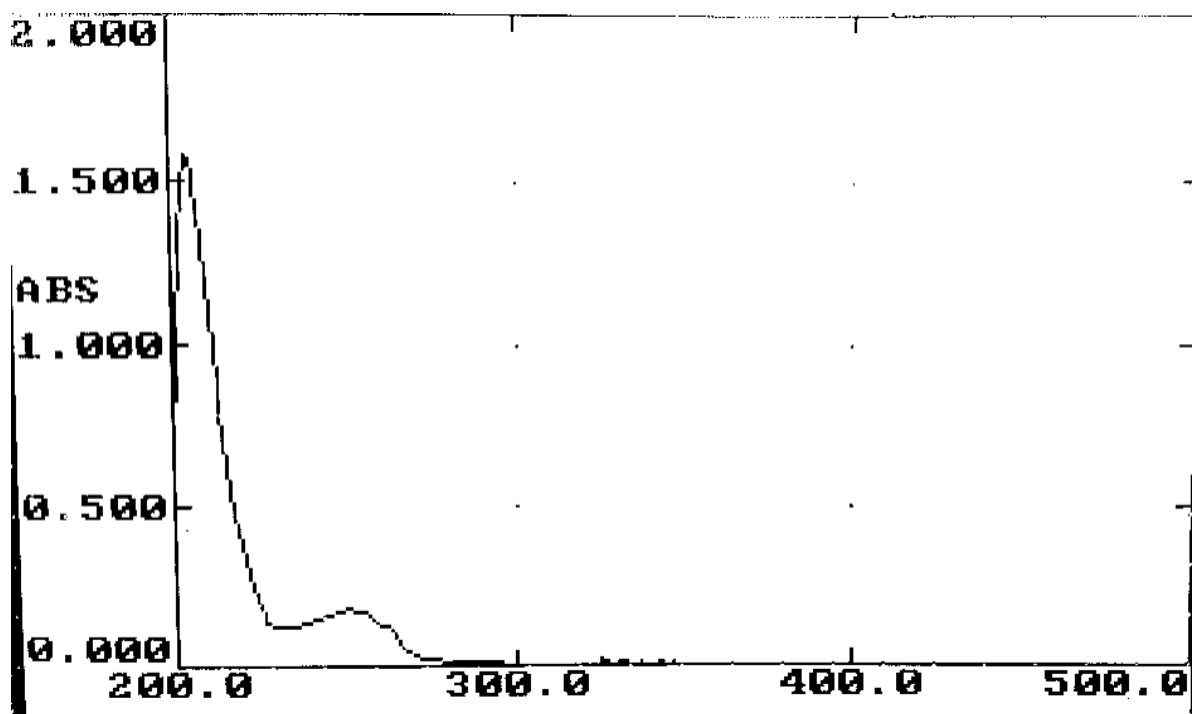


Figure S49. The UV spectrum of compound 6

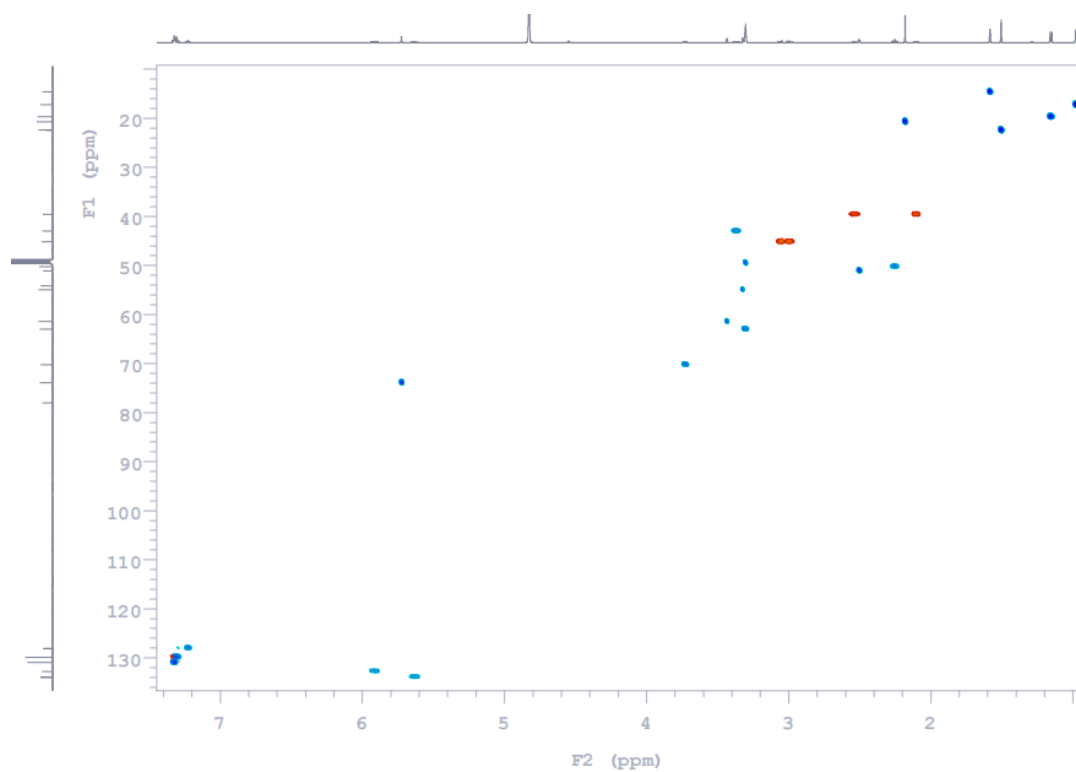


Figure S52. The HSQC (600 MHz, CD₃OD) spectrum of compound **7**

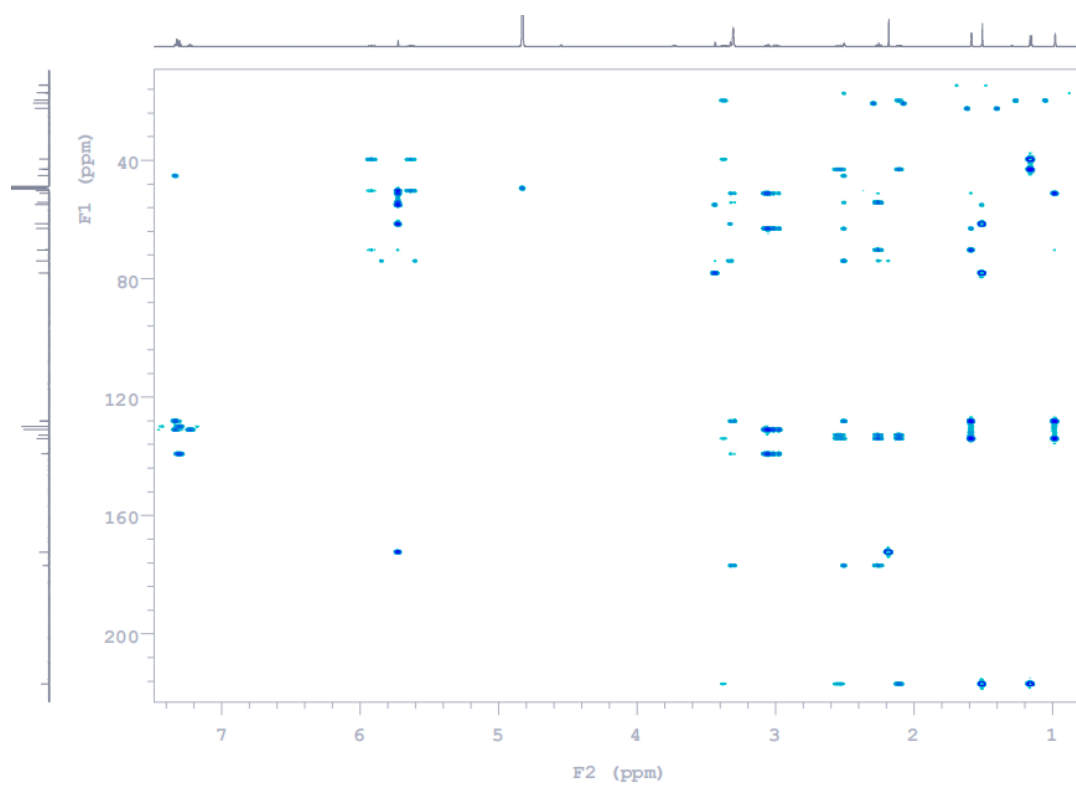


Figure S53. The HMBC (600 MHz, CD₃OD) spectrum of compound **7**

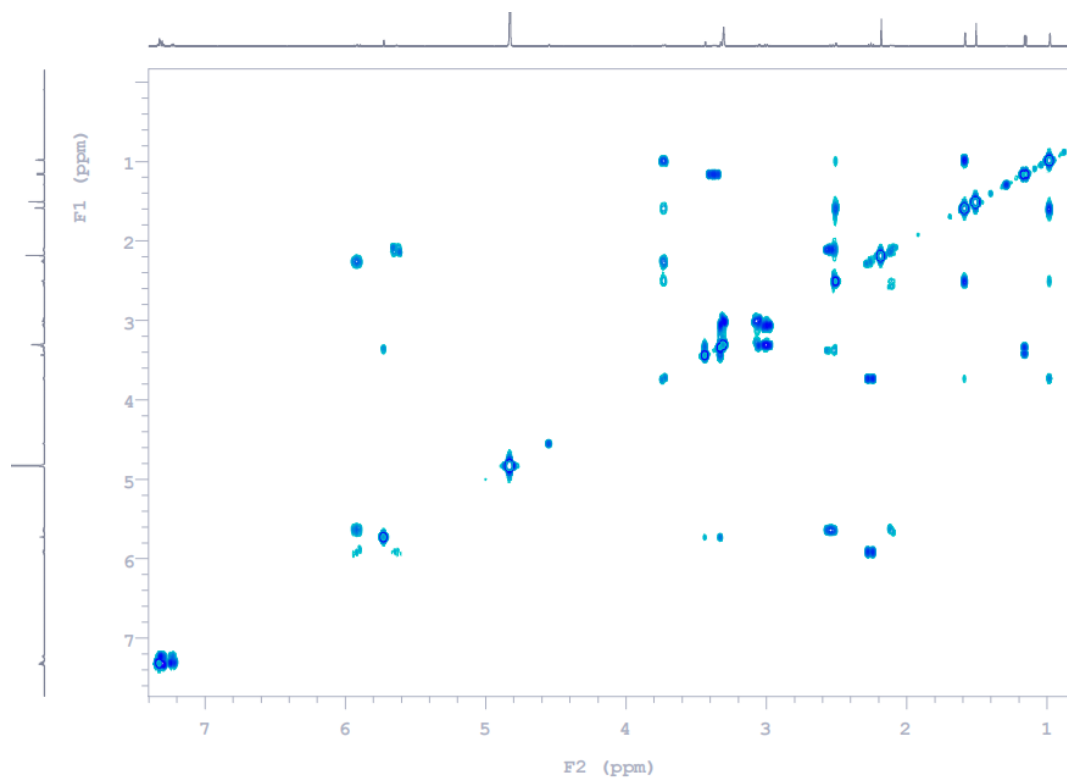


Figure S54. The COSY (600 MHz, CD₃OD) spectrum of compound 7

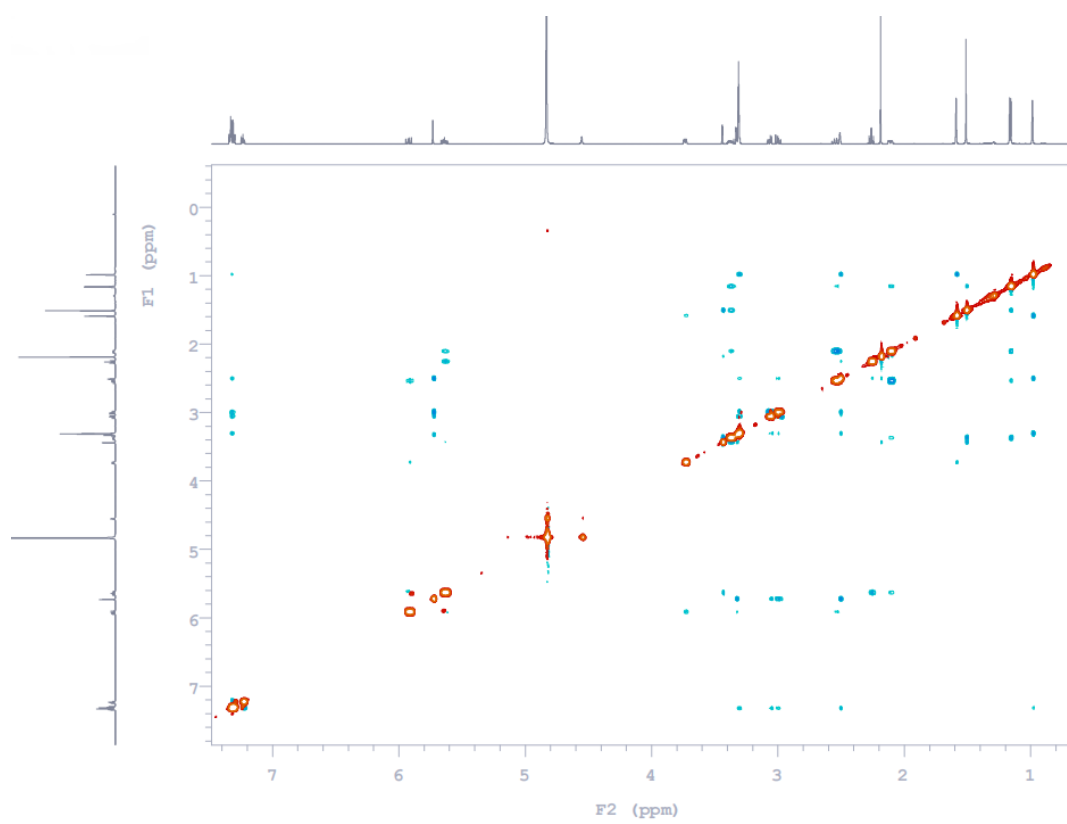


Figure S55. The NOESY (600 MHz, CD₃OD) spectrum of compound 7

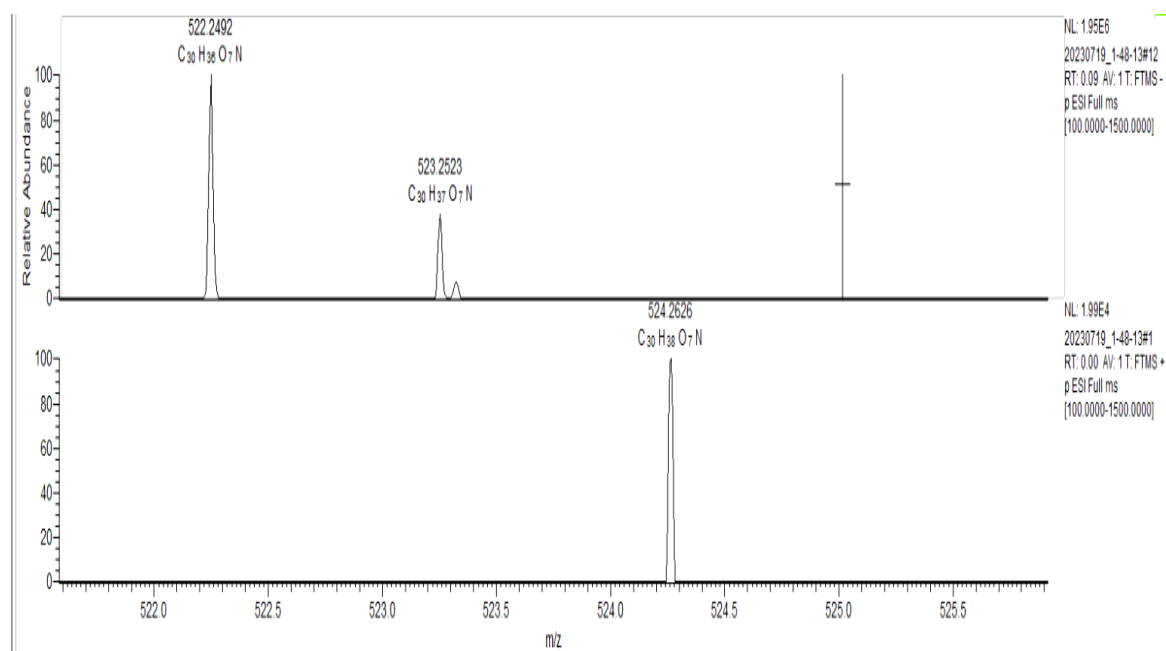


Figure S56. The HRESIMS spectrum of compound 7

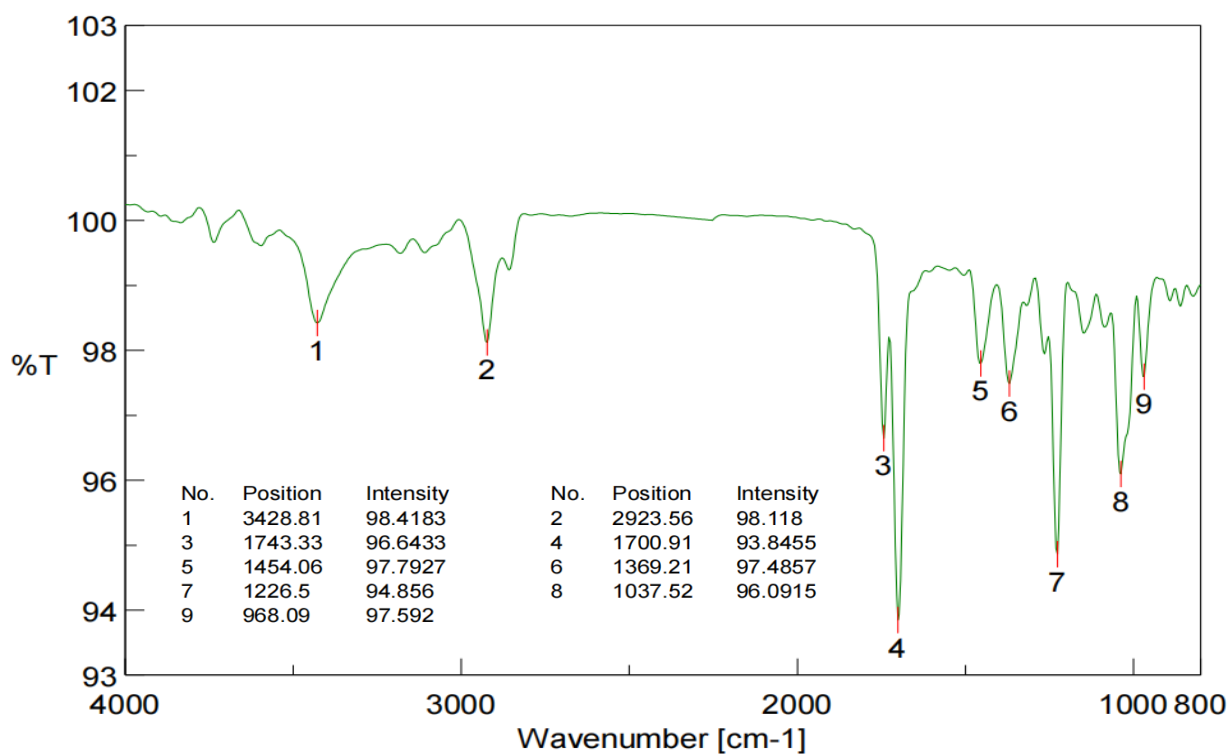


Figure S57. The IR spectrum of compound 7

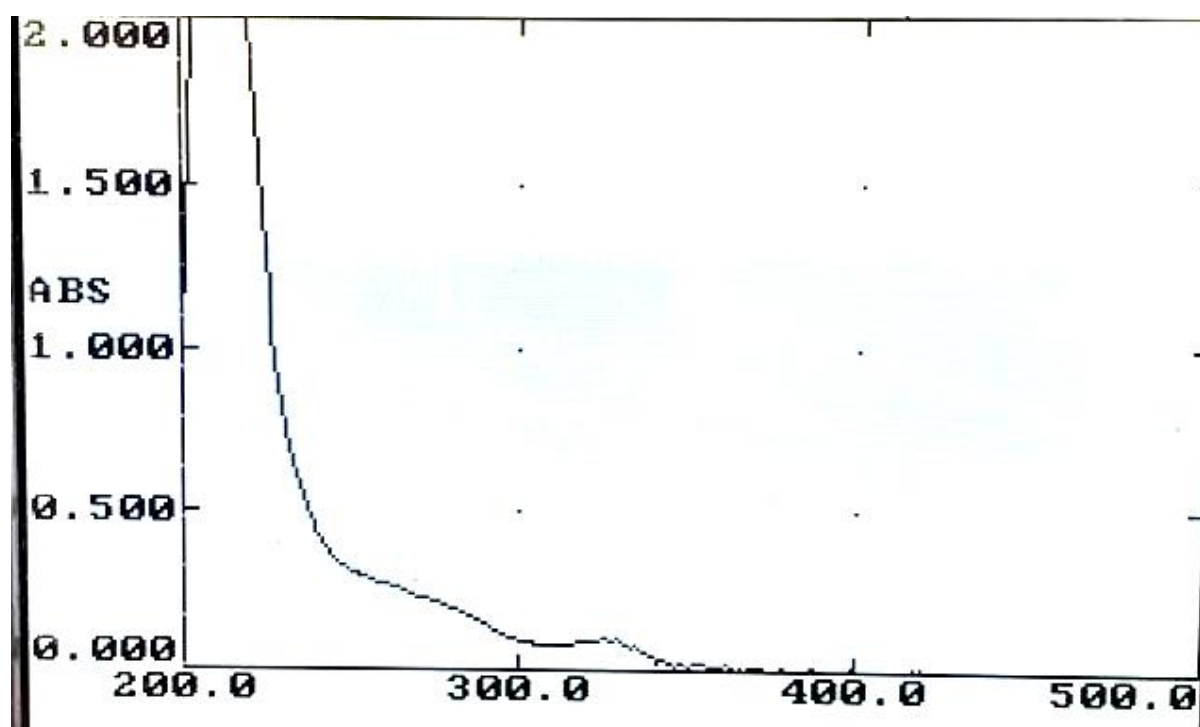


Figure S58. The UV spectrum of compound 7

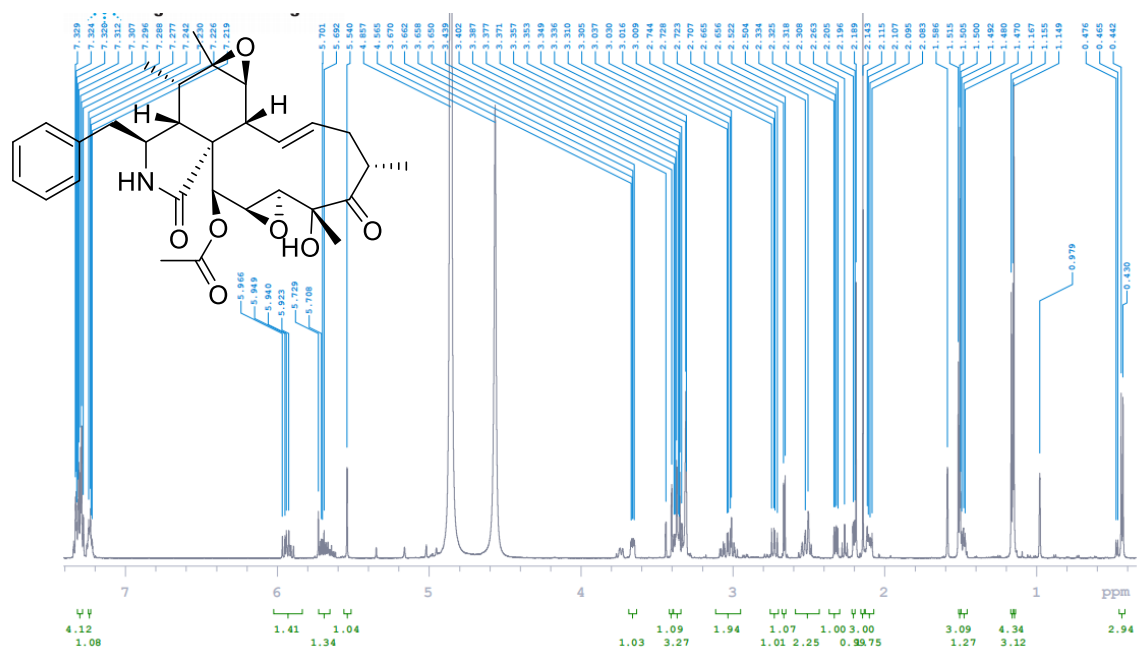


Figure S59. The ^1H NMR (600 MHz, CD_3OD) spectrum of compound **8**

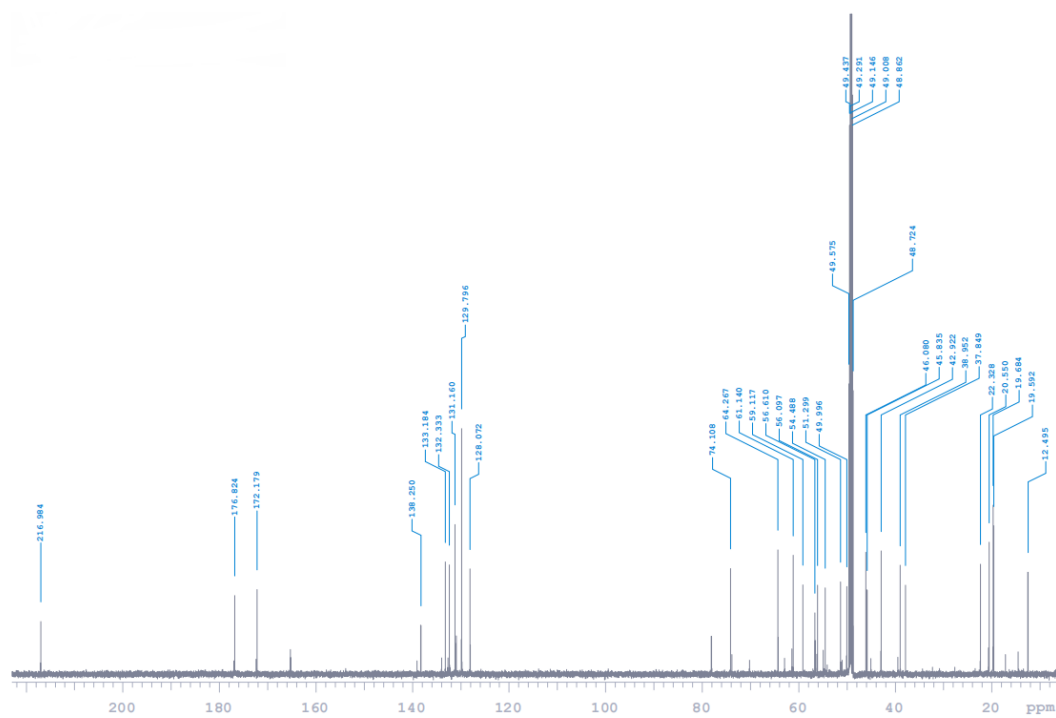


Figure S60. The ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **8**

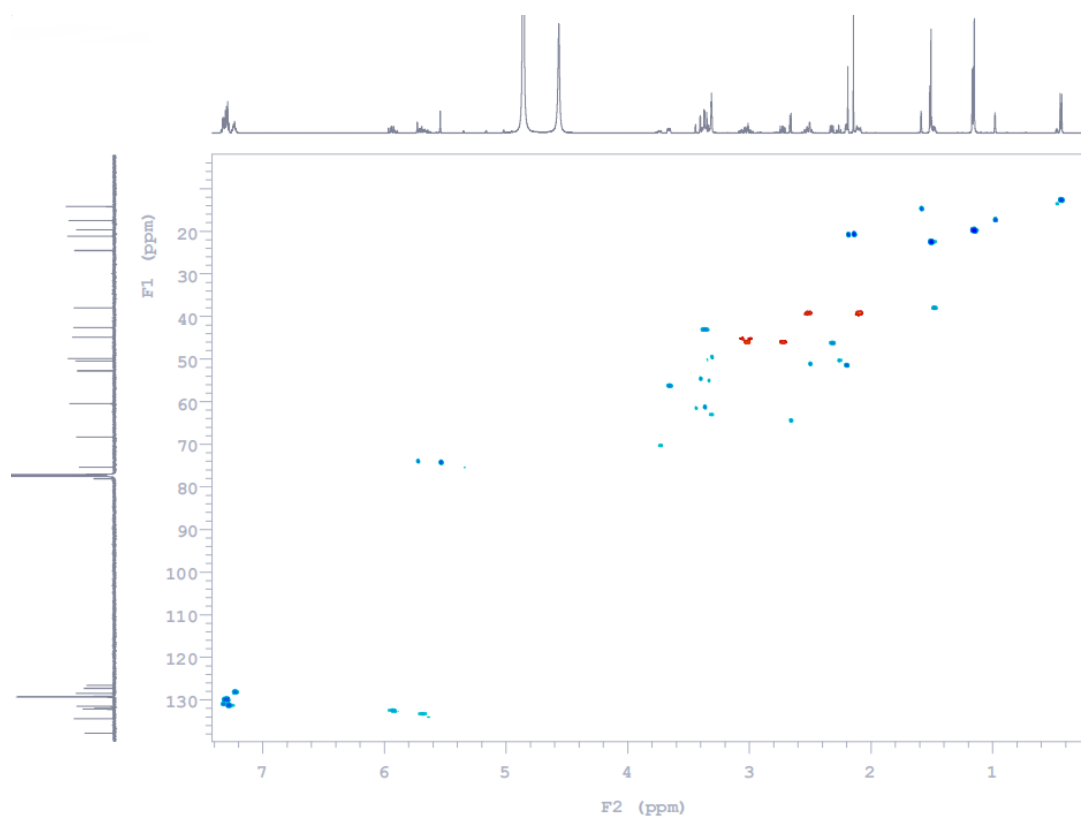


Figure S61. The HSQC (600 MHz, CD₃OD) spectrum of compound **8**

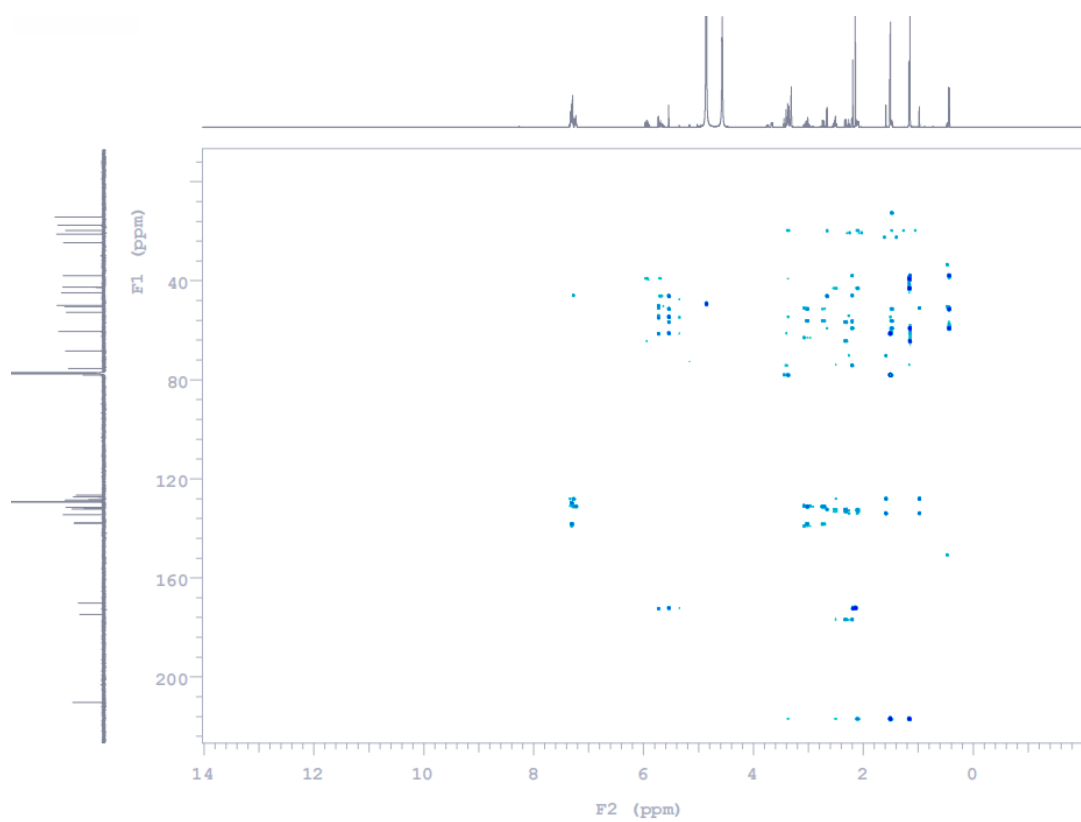


Figure S62. The HMBC (600 MHz, CD₃OD) spectrum of compound **8**

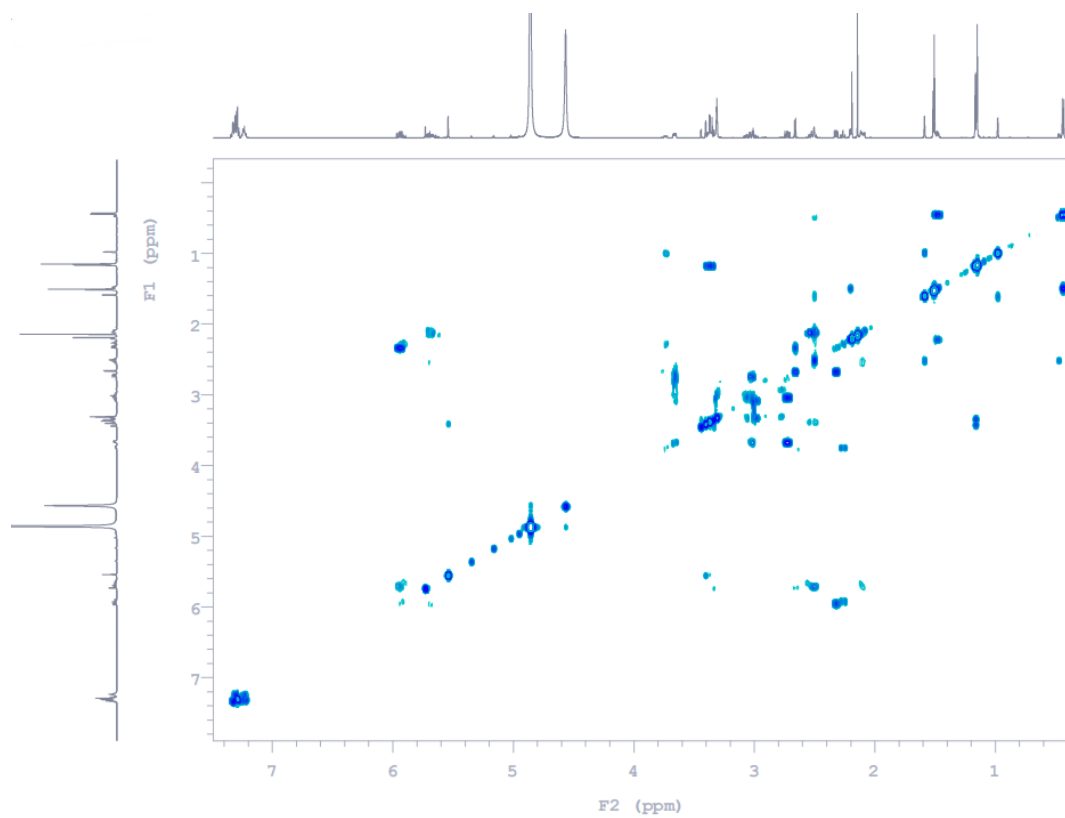


Figure S63. The COSY (600 MHz, CD₃OD) spectrum of compound **8**

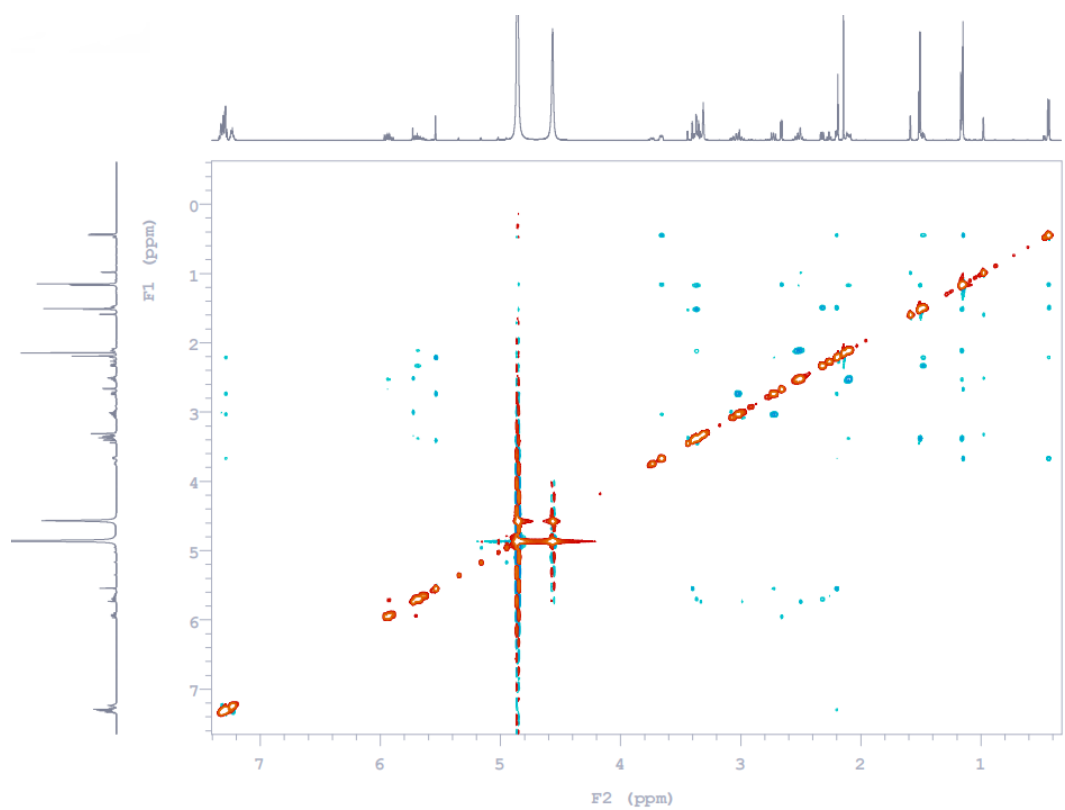


Figure S64. The NOESY (600 MHz, CD₃OD) spectrum of compound **8**

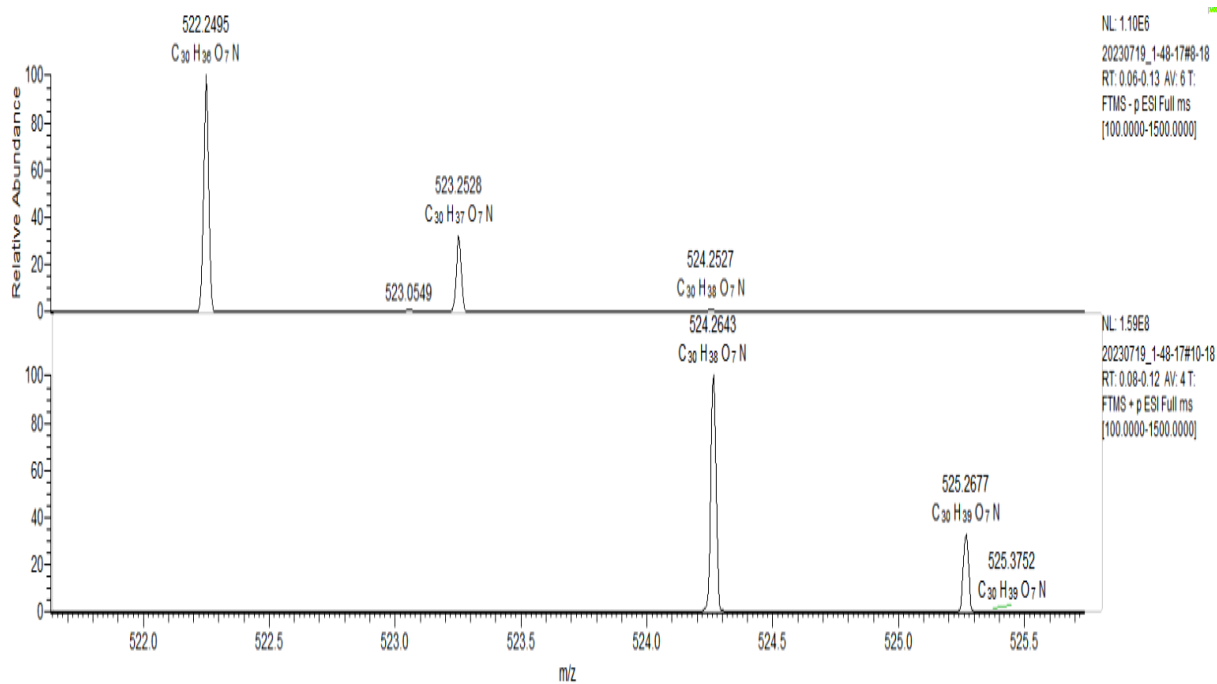


Figure S65. The HRESIMS spectrum of compound 8

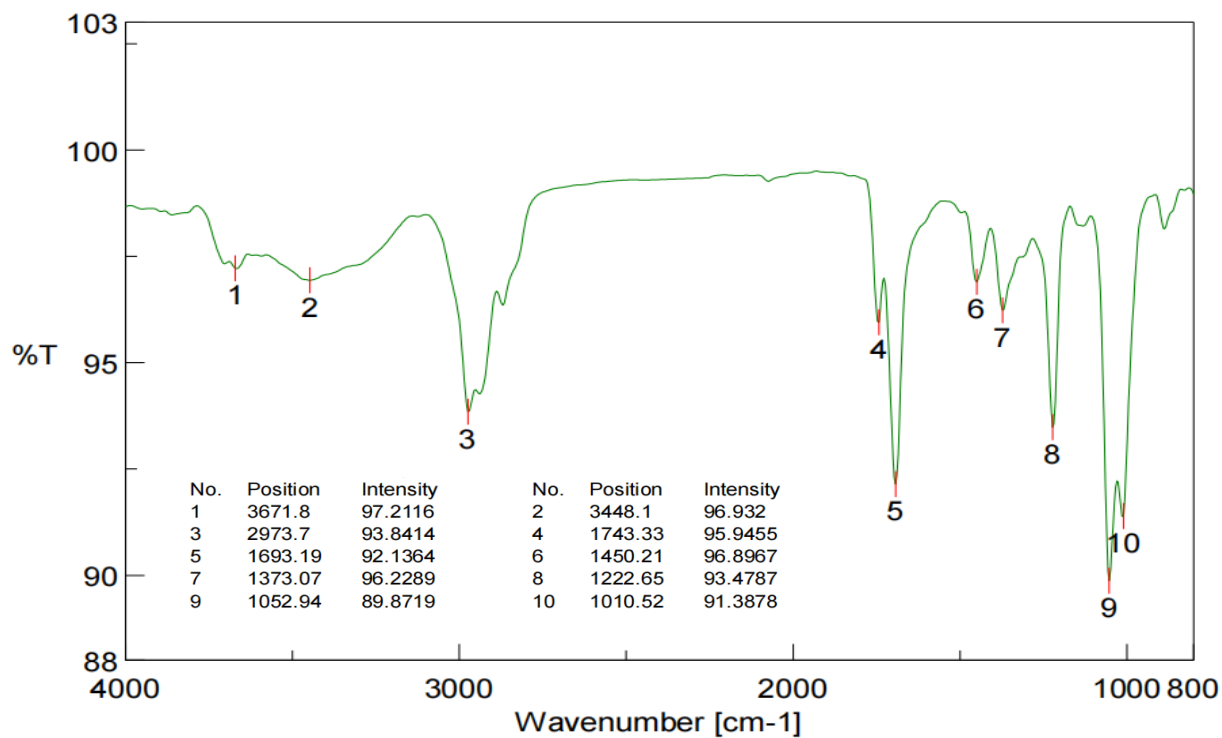


Figure S66. The IR spectrum of compound 8

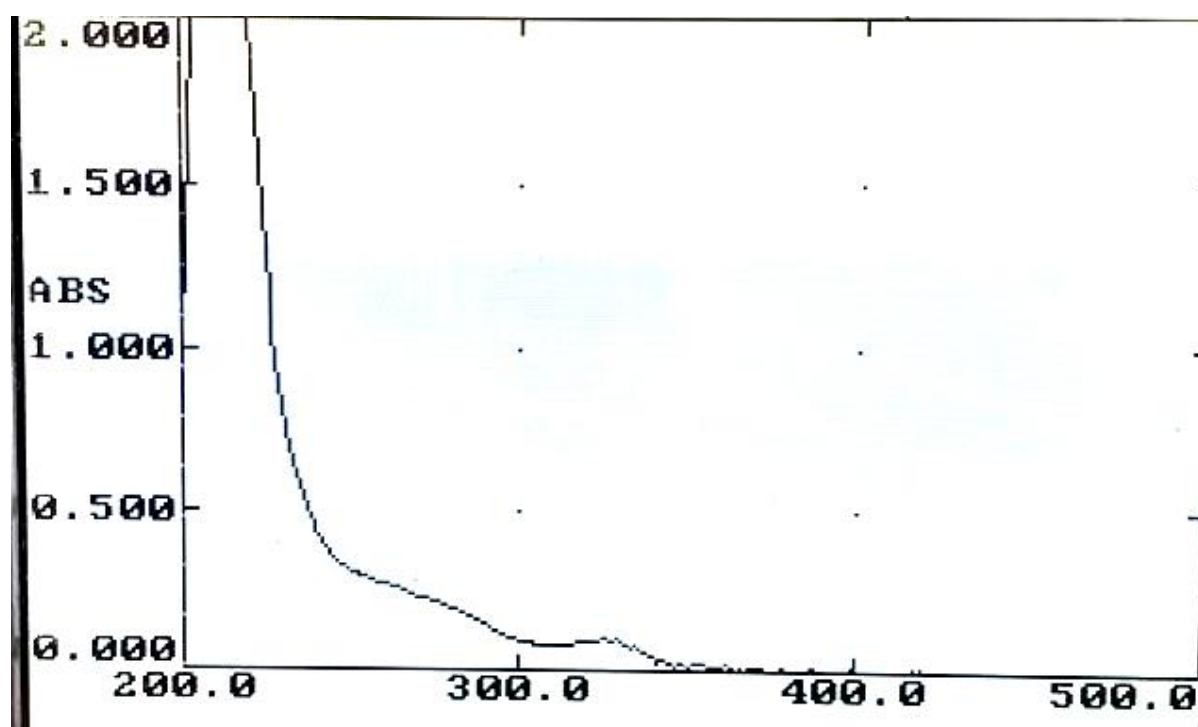


Figure S67. The UV spectrum of compound 8

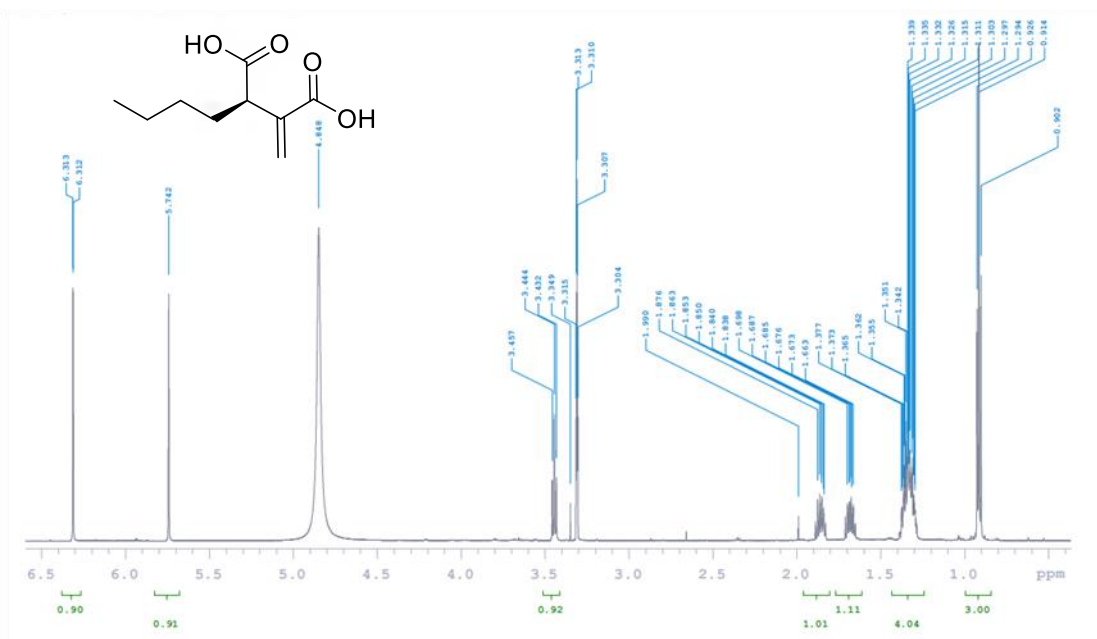


Figure S68. The ¹H NMR (600 MHz, CD₃OD) spectrum of compound 9

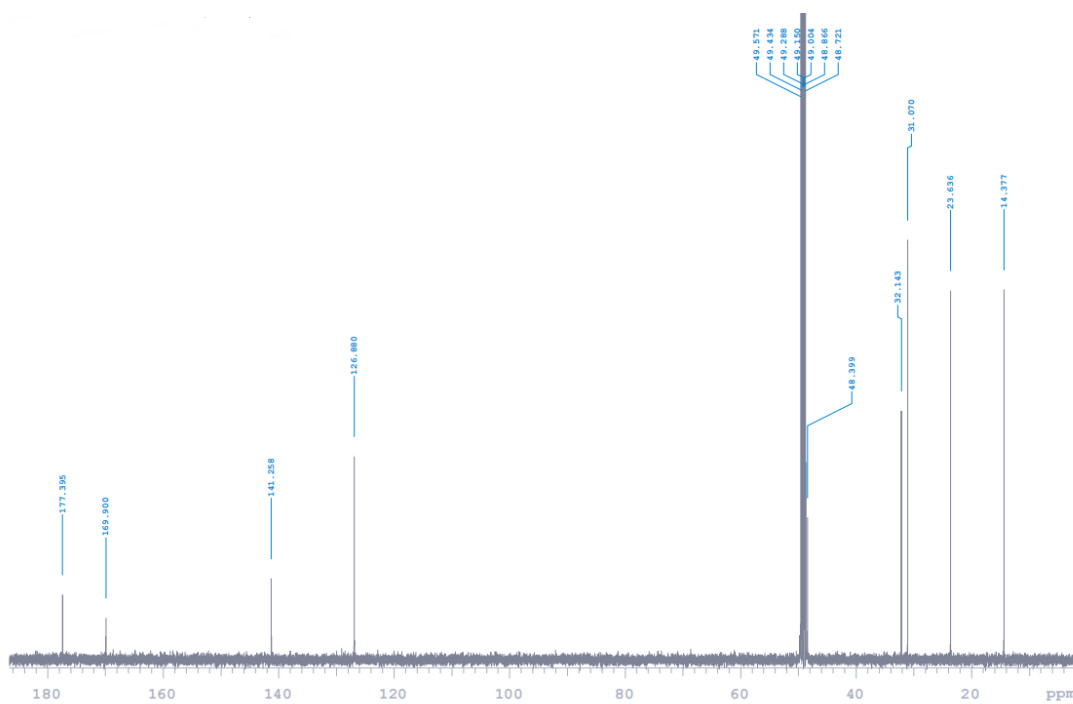


Figure S69. The ¹³C NMR (150 MHz, CD₃OD) spectrum of compound 9

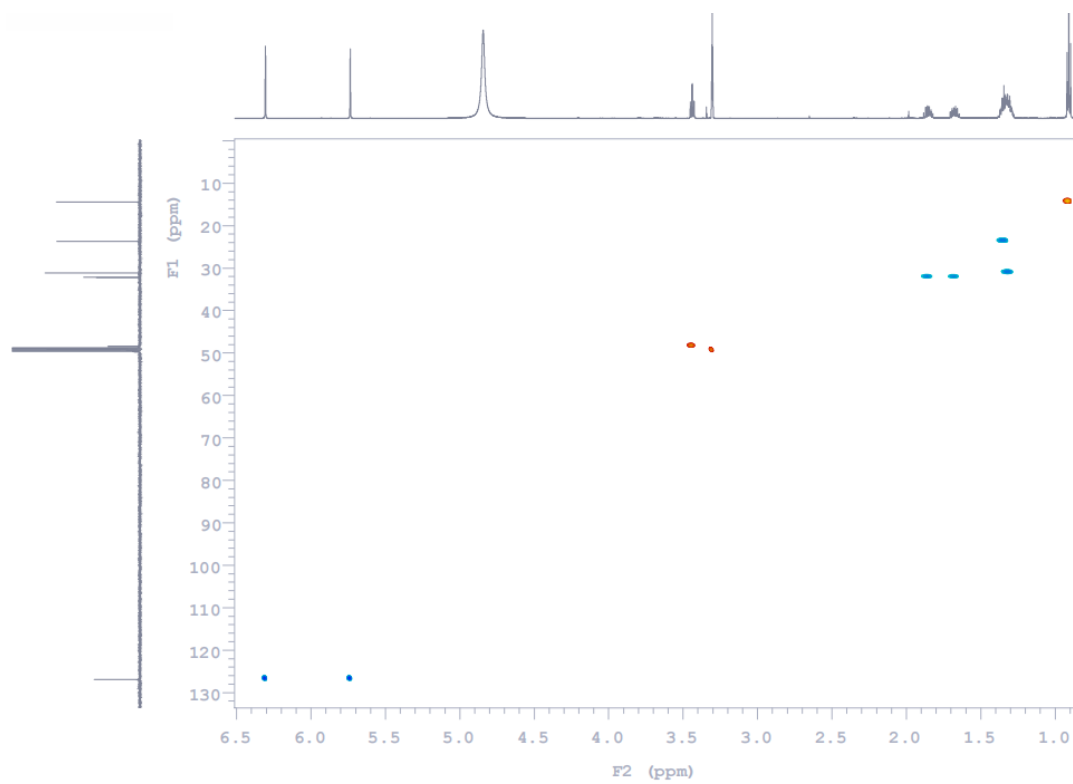


Figure S70. The HSQC (600 MHz, CD_3OD) spectrum of compound **9**

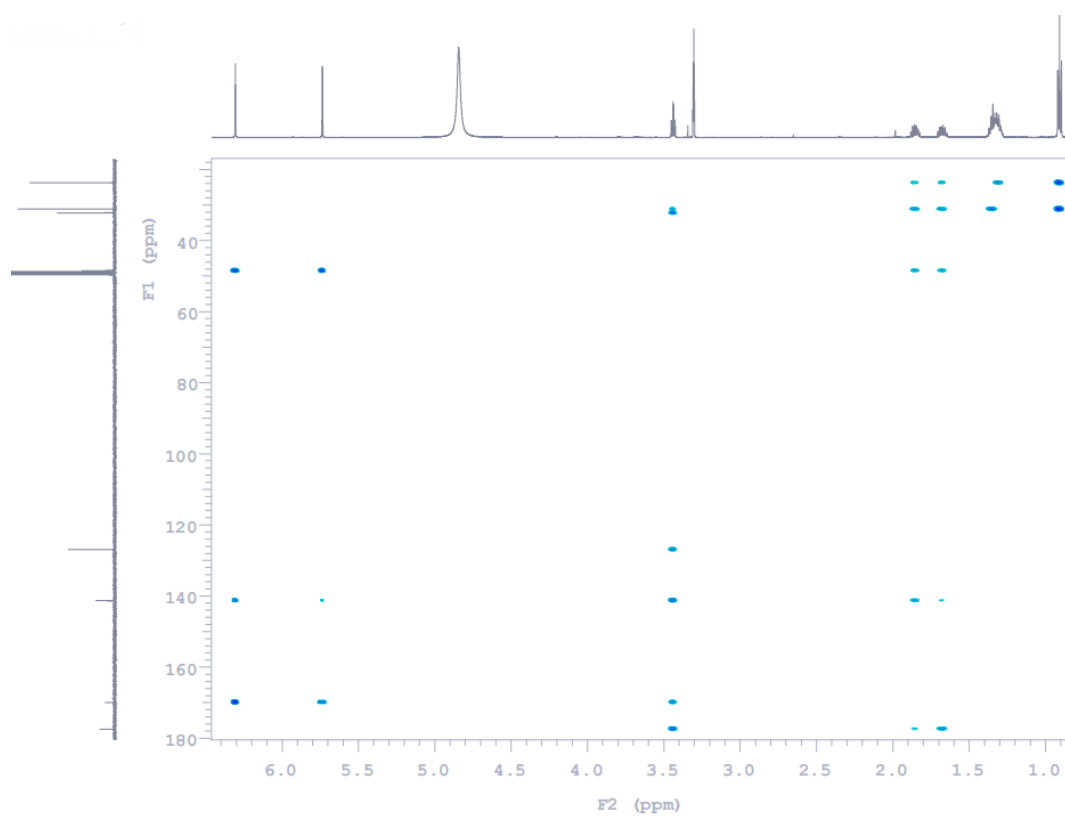


Figure S71. The HMBC (600 MHz, CD_3OD) spectrum of compound **9**

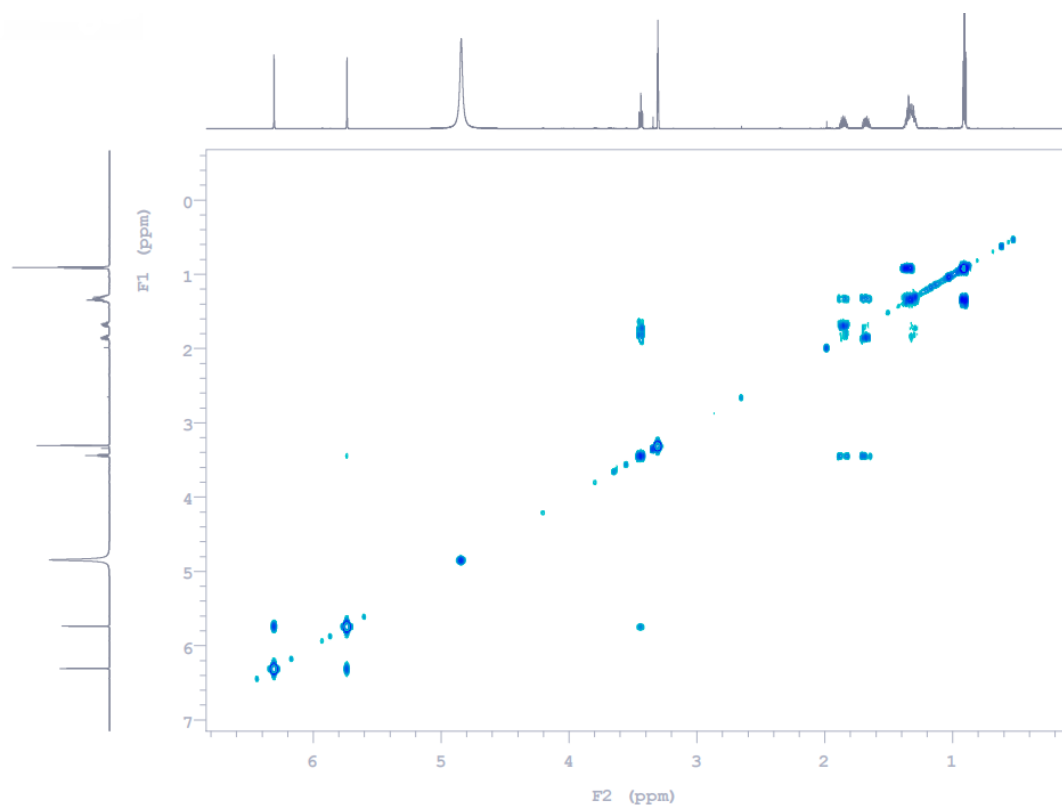


Figure S72. The COSY (600 MHz, CD₃OD) spectrum of compound **9**

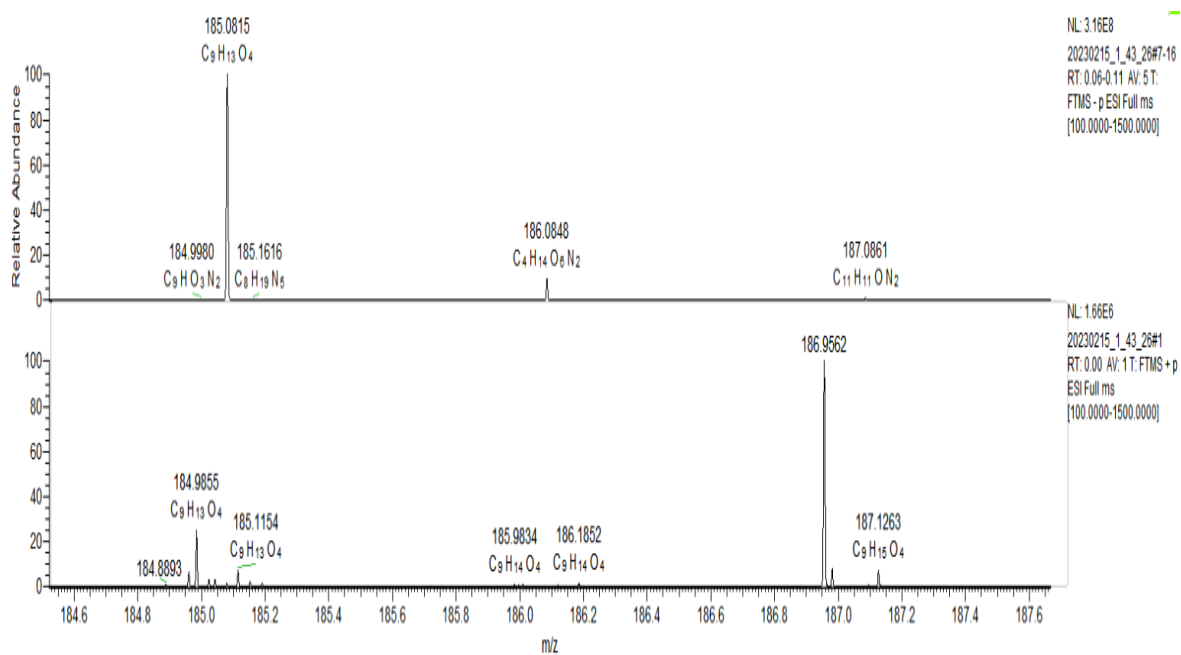


Figure S73. The HRESIMS spectrum of compound **9**

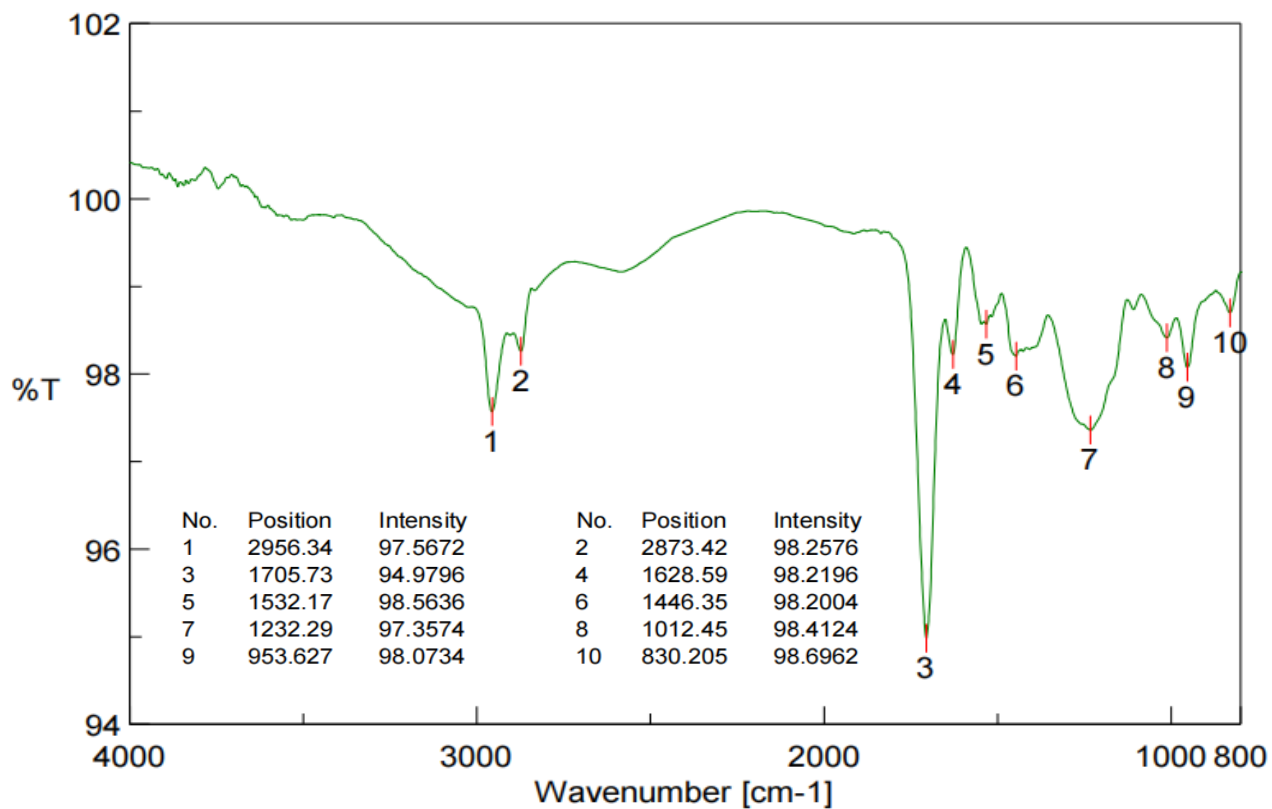


Figure S74. The IR spectrum of compound 9

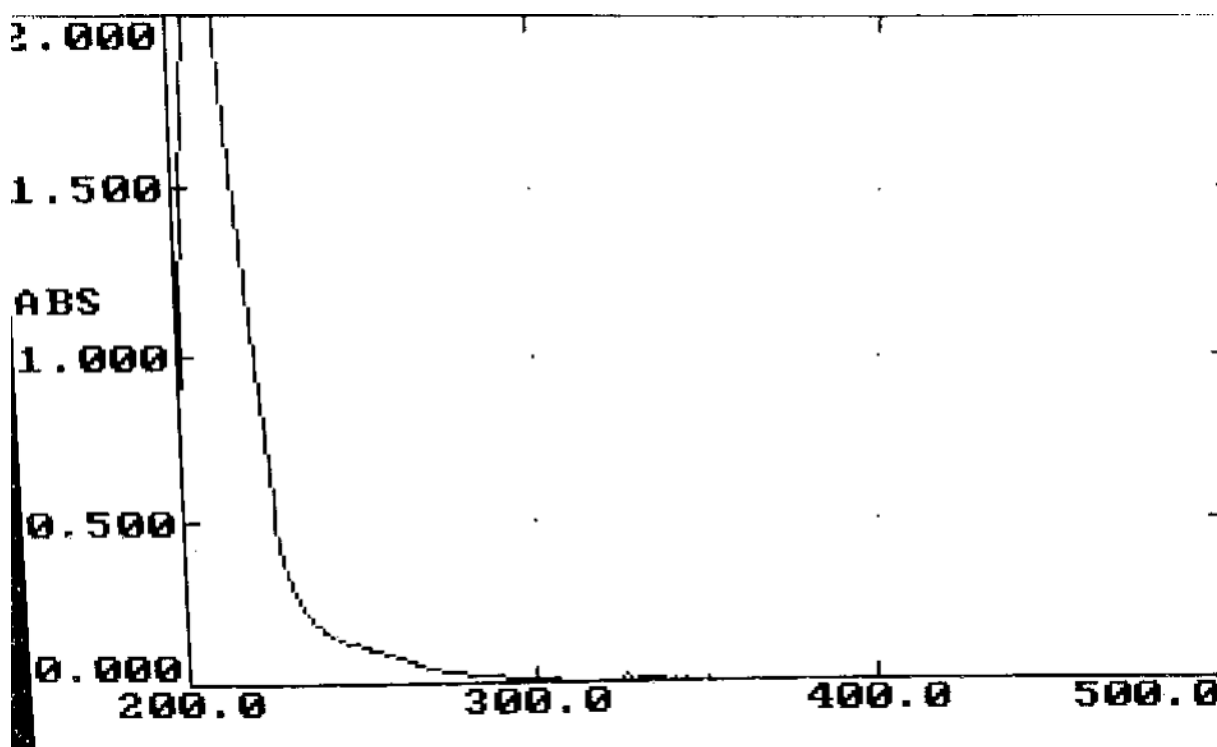


Figure S75. The UV spectrum of compound 9

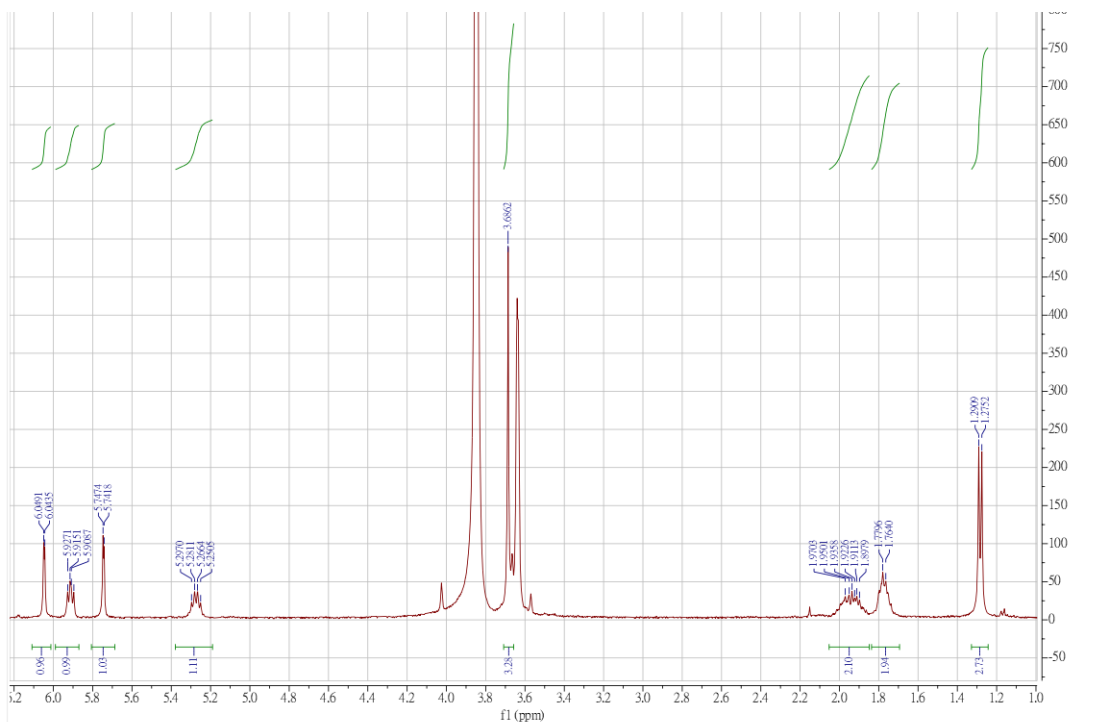


Figure S76. The ^1H NMR (400 MHz, $\text{C}_5\text{D}_5\text{N}$) spectrum of compound 7R, 10R-MTPA ester of **2** (**2S**)

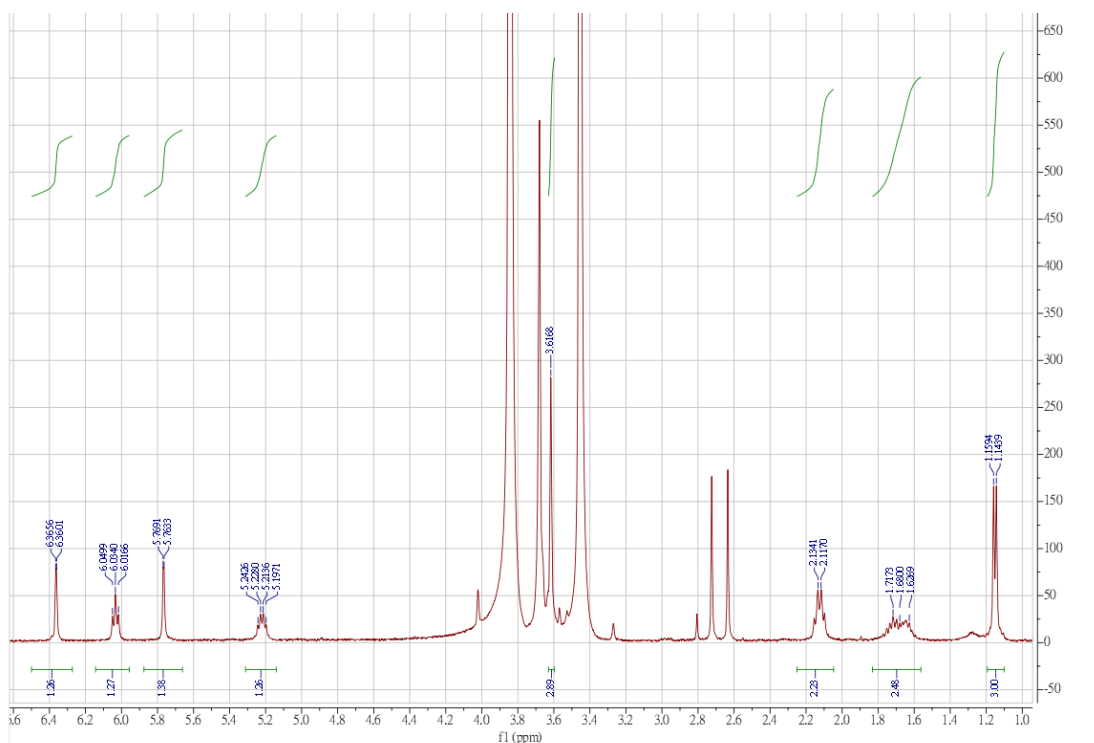


Figure S77. The ^1H NMR (400 MHz, $\text{C}_5\text{D}_5\text{N}$) spectrum of compound 7R, 10R-MTPA ester of **2** (**2R**)

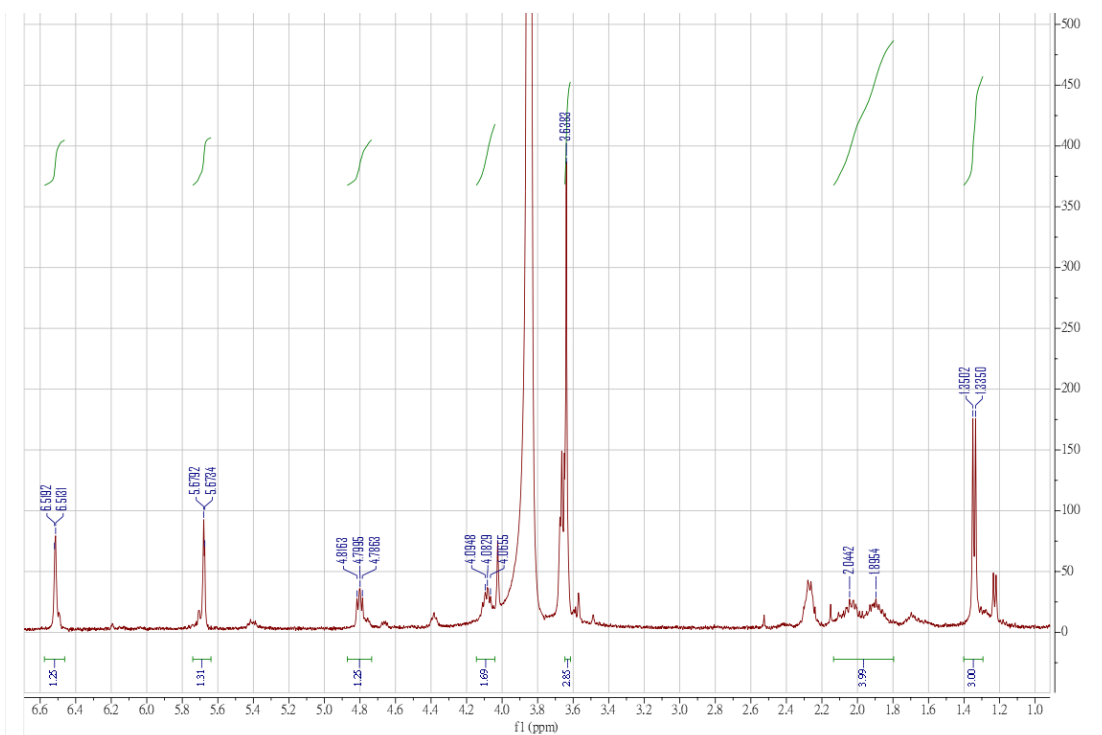


Figure S78. The ^1H NMR (400 MHz, $\text{C}_5\text{D}_5\text{N}$) spectrum of compound 7S, 10R -MTPA ester of 3 (3S)

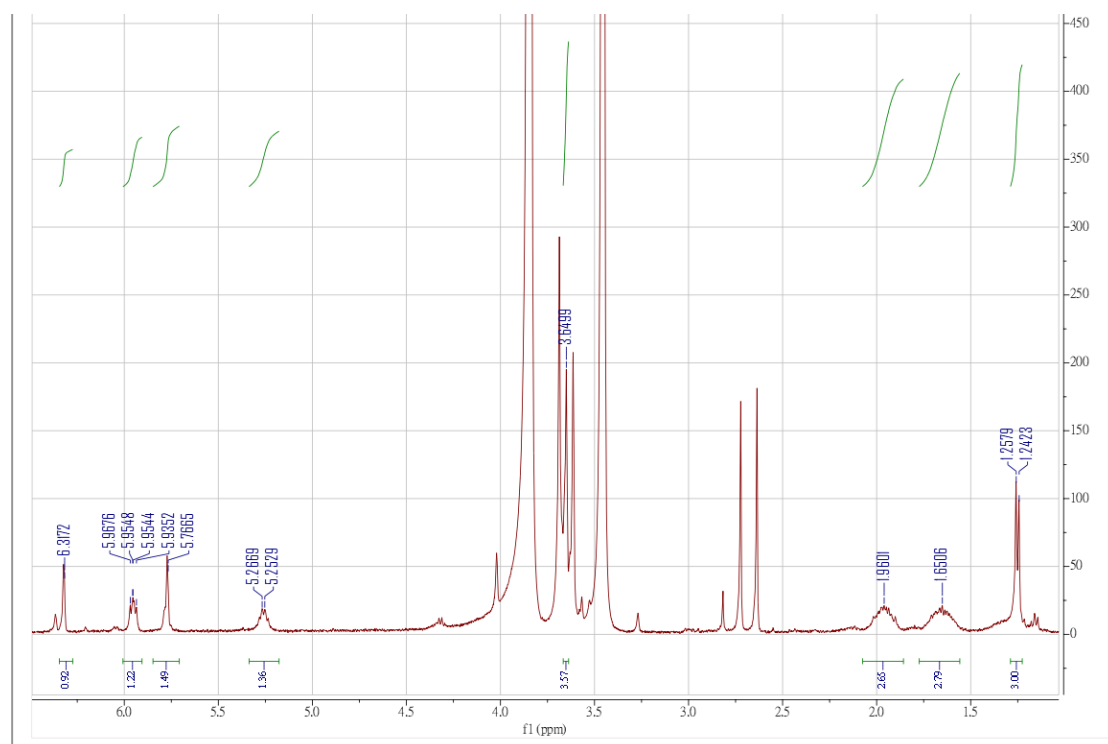


Figure S79. The ^1H NMR (400 MHz, $\text{C}_5\text{D}_5\text{N}$) spectrum of compound 7S, 10R -MTPA ester of 3 (3R)

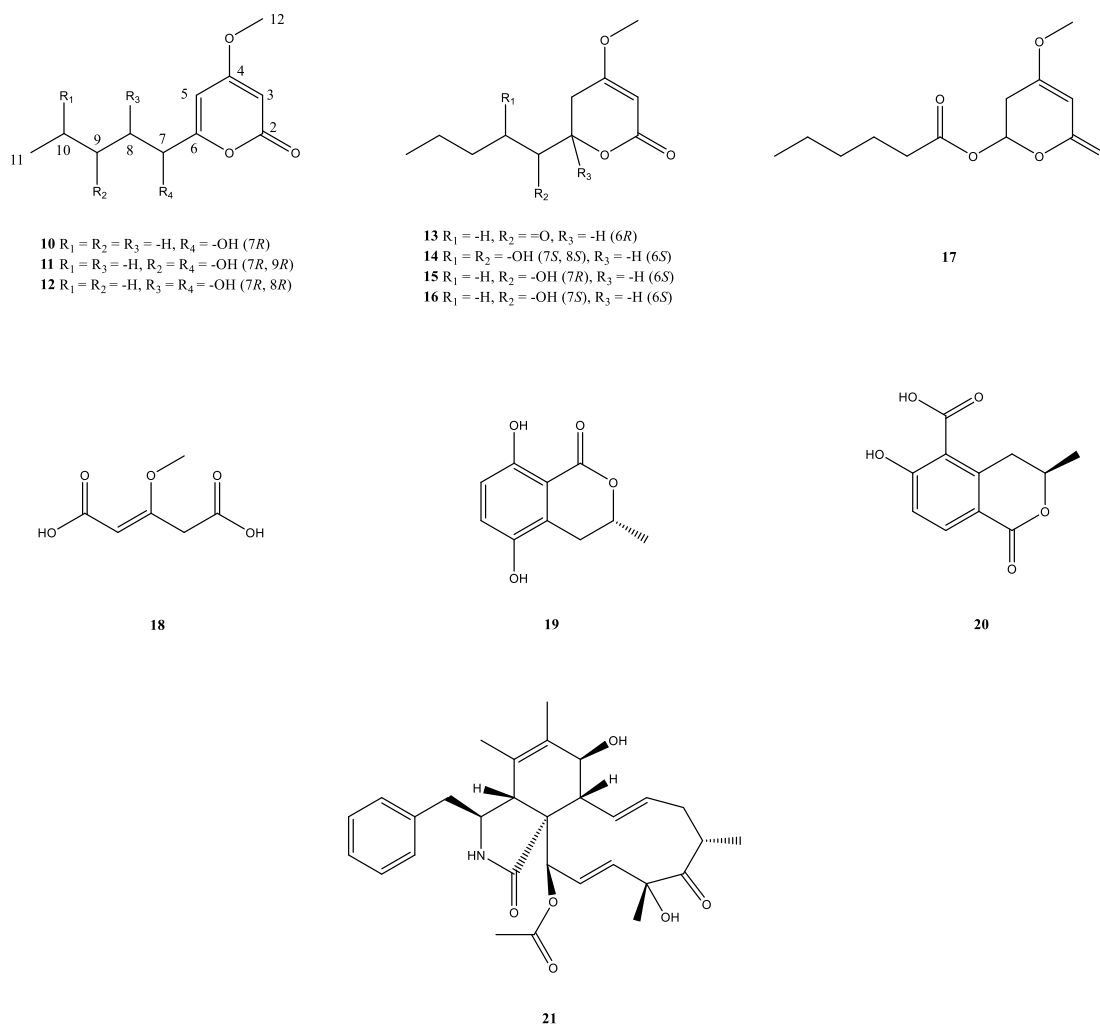


Figure S80. Structures of known compounds isolated in this study

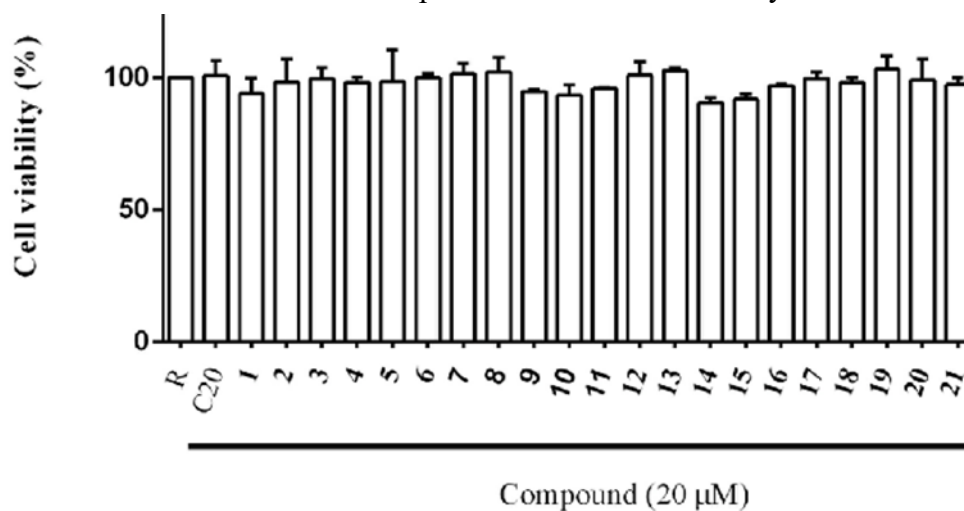


Figure S81. All compounds had no cytotoxicity on the BV-2 cells at a concentration of 20 μ M

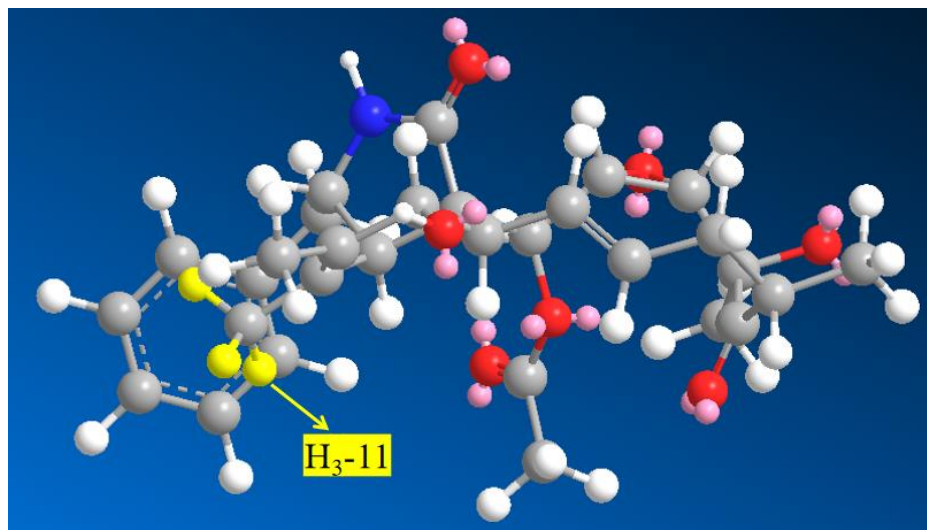


Figure S82. ChemBio 3D Ultra 12.0 Molecular modelling of 7.

Table S1. Crystal data and experimental details for **6**

Crystal data		
Empirical formula	C ₂₆ H ₄₂ O ₁₀	
Formula weight	514.59	
Crystal system	Monoclinic	
Space group	P2 ₁	
Unit cell dimensions	a = 12.9573(4) Å	α = 90°.
	b = 6.4656(2) Å	β = 91.0625(13)°.
	c = 15.2654(5) Å	γ = 90°.
Volume	1278.67(7) Å ³	
Z	2	
F(000)	556	
Density (calculated)	1.337 Mg/m ³	
Wavelength	1.54178 Å	
Cell parameters reflections used	9834	
Theta range for Cell parameters	2.90 to 78.03°.	
Absorption coefficient	0.845 mm ⁻¹	
Temperature	100(2) K	
Crystal size	0.200 x 0.100 x 0.050 mm ³	
Data collection		
Diffractometer	Bruker AXS D8 VENTURE, PhotonIII_C28	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8992	
No. of measured reflections	21066	
No. of independent reflections	5233 [R(int) = 0.0306]	
No. of observed [I > 2σ(I)]	5142	
Completeness to theta = 67.679°	100.0 %	
Theta range for data collection	2.895 to 78.235°.	
Refinement		
Final R indices [I > 2σ(I)]	R1 = 0.0295, wR2 = 0.0773	
R indices (all data)	R1 = 0.0301, wR2 = 0.0779	
Goodness-of-fit on F ²	1.053	
No. of reflections	5233	
No. of parameters	336	
No. of restraints	1	
Absolute structure parameter	0.03(5)	
Largest diff. peak and hole	0.209 and -0.195 e.Å ⁻³	

Table S2. Bond lengths [Å] and angles [°] for **6**

O(1)-C(19)	1.350(2)
O(1)-C(6)	1.4877(19)
O(2)-C(9)	1.445(2)
O(3)-C(19)	1.209(2)
O(4)-C(1')	1.402(2)
O(4)-C(16)	1.440(2)
O(5)-C(2')	1.430(2)
O(6)-C(3')	1.421(2)
O(7)-C(4')	1.426(2)
O(8)-C(1')	1.4267(19)
O(8)-C(5')	1.440(2)
O(9)-C(6')	1.427(2)
C(1)-C(2)	1.536(2)
C(1)-C(10)	1.541(2)
C(2)-C(3)	1.533(2)
C(3)-C(4)	1.535(3)
C(4)-C(19)	1.518(2)
C(4)-C(5)	1.530(2)
C(4)-C(18)	1.550(2)
C(5)-C(6)	1.516(2)
C(5)-C(10)	1.549(2)
C(6)-C(7)	1.494(2)
C(1')-C(2')	1.526(2)
C(2')-C(3')	1.527(2)
C(3')-C(4')	1.524(2)
C(4')-C(5')	1.531(2)
C(5')-C(6')	1.512(2)
C(7)-C(8)	1.335(2)
C(8)-C(14)	1.512(2)
C(8)-C(9)	1.534(2)
C(9)-C(11)	1.534(2)
C(9)-C(10)	1.563(2)
C(10)-C(20)	1.549(2)
C(11)-C(12)	1.529(2)
C(12)-C(13)	1.537(2)
C(13)-C(17)	1.528(3)

C(13)-C(14)	1.543(2)
C(13)-C(15)	1.544(2)
C(15)-C(16)	1.520(2)
C(19)-O(1)-C(6)	109.07(13)
C(1')-O(4)-C(16)	112.41(14)
C(1')-O(8)-C(5')	113.52(13)
C(2)-C(1)-C(10)	110.55(15)
C(3)-C(2)-C(1)	113.27(15)
C(2)-C(3)-C(4)	116.46(15)
C(19)-C(4)-C(5)	100.50(14)
C(19)-C(4)-C(3)	117.08(15)
C(5)-C(4)-C(3)	114.90(14)
C(19)-C(4)-C(18)	104.62(14)
C(5)-C(4)-C(18)	111.37(14)
C(3)-C(4)-C(18)	107.86(14)
C(6)-C(5)-C(4)	102.04(14)
C(6)-C(5)-C(10)	110.88(14)
C(4)-C(5)-C(10)	114.49(14)
O(1)-C(6)-C(7)	114.26(14)
O(1)-C(6)-C(5)	103.57(13)
C(7)-C(6)-C(5)	114.14(14)
O(4)-C(1')-O(8)	111.73(14)
O(4)-C(1')-C(2')	108.18(14)
O(8)-C(1')-C(2')	110.94(14)
O(5)-C(2')-C(1')	107.01(14)
O(5)-C(2')-C(3')	110.24(14)
C(1')-C(2')-C(3')	111.37(14)
O(6)-C(3')-C(4')	111.95(15)
O(6)-C(3')-C(2')	107.81(14)
C(4')-C(3')-C(2')	111.08(14)
O(7)-C(4')-C(3')	107.29(14)
O(7)-C(4')-C(5')	110.98(14)
C(3')-C(4')-C(5')	108.55(14)
O(8)-C(5')-C(6')	106.22(14)
O(8)-C(5')-C(4')	108.38(13)
C(6')-C(5')-C(4')	114.87(14)
O(9)-C(6')-C(5')	109.85(14)

C(8)-C(7)-C(6)	122.16(16)
C(7)-C(8)-C(14)	120.80(16)
C(7)-C(8)-C(9)	122.51(15)
C(14)-C(8)-C(9)	116.49(14)
O(2)-C(9)-C(11)	104.88(14)
O(2)-C(9)-C(8)	108.42(13)
C(11)-C(9)-C(8)	110.58(14)
O(2)-C(9)-C(10)	111.03(14)
C(11)-C(9)-C(10)	112.04(13)
C(8)-C(9)-C(10)	109.76(14)
C(1)-C(10)-C(5)	106.28(14)
C(1)-C(10)-C(20)	108.17(14)
C(5)-C(10)-C(20)	114.25(14)
C(1)-C(10)-C(9)	113.43(14)
C(5)-C(10)-C(9)	105.44(13)
C(20)-C(10)-C(9)	109.36(14)
C(12)-C(11)-C(9)	113.53(14)
C(11)-C(12)-C(13)	112.15(15)
C(17)-C(13)-C(12)	112.22(15)
C(17)-C(13)-C(14)	108.38(14)
C(12)-C(13)-C(14)	108.02(15)
C(17)-C(13)-C(15)	109.98(15)
C(12)-C(13)-C(15)	110.84(15)
C(14)-C(13)-C(15)	107.22(13)
C(8)-C(14)-C(13)	114.67(14)
C(16)-C(15)-C(13)	118.16(15)
O(4)-C(16)-C(15)	109.84(15)
O(3)-C(19)-O(1)	121.82(17)
O(3)-C(19)-C(4)	127.69(17)
O(1)-C(19)-C(4)	110.43(14)

Symmetry transformations used to generate equivalent atoms:

Table S3. Crystal data and experimental details for **7**

Crystal data	
Empirical formula	C ₃₀ H ₃₉ N O ₈
Formula weight	541.62
Crystal system	Monoclinic
Space group	P2 ₁
Unit cell dimensions	a = 13.1017(11) Å α = 90°. b = 7.0595(6) Å β = 93.773(4)°. c = 15.8773(14) Å γ = 90°.
Volume	1465.3(2) Å ³
Z	2
F(000)	580
Density (calculated)	1.228 Mg/m ³
Wavelength	1.54178 Å
Cell parameters reflections used	9934
Theta range for Cell parameters	2.79 to 78.20°.
Absorption coefficient	0.727 mm ⁻¹
Temperature	100(2) K
Crystal size	0.400 x 0.030 x 0.020 mm ³
Data collection	
Diffractometer	Bruker AXS D8 VENTURE, PhotonIII_C28
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8878
No. of measured reflections	27723
No. of independent reflections	5863 [R(int) = 0.0505]
No. of observed [I > 2σ(I)]	5512
Completeness to theta = 67.679°	99.8 %
Theta range for data collection	2.789 to 78.765°.
Refinement	
Final R indices [I > 2σ(I)]	R1 = 0.0364, wR2 = 0.0911
R indices (all data)	R1 = 0.0406, wR2 = 0.0940
Goodness-of-fit on F ²	1.066
No. of reflections	5863
No. of parameters	362
No. of restraints	1
Absolute structure parameter	-0.04(9)
Largest diff. peak and hole	0.196 and -0.224 e.Å ⁻³

Table S4. Bond lengths [Å] and angles [°] for **7**

O(1)-C(1)	1.237(3)
O(2)-C(7)	1.428(2)
O(3)-C(17)	1.217(3)
O(4)-C(18)	1.415(3)
O(5)-C(19)	1.450(3)
O(5)-C(20)	1.459(2)
O(6)-C(24)	1.350(3)
O(6)-C(21)	1.447(2)
O(7)-C(24)	1.204(3)
N(1)-C(1)	1.334(3)
N(1)-C(3)	1.457(3)
C(1)-C(9)	1.533(3)
C(3)-C(10)	1.539(3)
C(3)-C(4)	1.567(3)
C(4)-C(5)	1.511(3)
C(4)-C(9)	1.563(3)
C(5)-C(6)	1.336(3)
C(5)-C(11)	1.513(3)
C(6)-C(12)	1.509(3)
C(6)-C(7)	1.519(3)
C(7)-C(8)	1.543(3)
C(8)-C(13)	1.509(3)
C(8)-C(9)	1.549(3)
C(9)-C(21)	1.554(3)
C(10)-C(1')	1.512(3)
C(13)-C(14)	1.326(3)
C(14)-C(15)	1.508(3)
C(15)-C(16)	1.540(3)
C(16)-C(17)	1.515(3)
C(16)-C(22)	1.538(3)
C(17)-C(18)	1.540(3)
C(18)-C(19)	1.526(3)
C(18)-C(23)	1.529(3)
C(19)-C(20)	1.463(3)
C(20)-C(21)	1.510(3)
C(24)-C(25)	1.495(3)

C(1')-C(2')	1.393(3)
C(1')-C(6')	1.399(3)
C(2')-C(3')	1.393(4)
C(3')-C(4')	1.385(4)
C(4')-C(5')	1.380(5)
C(5')-C(6')	1.392(4)

C(19)-O(5)-C(20)	60.38(13)
C(24)-O(6)-C(21)	118.84(17)
C(1)-N(1)-C(3)	115.55(17)
O(1)-C(1)-N(1)	124.90(19)
O(1)-C(1)-C(9)	125.56(18)
N(1)-C(1)-C(9)	109.54(17)
N(1)-C(3)-C(10)	111.07(17)
N(1)-C(3)-C(4)	103.01(16)
C(10)-C(3)-C(4)	115.65(18)
C(5)-C(4)-C(9)	116.29(17)
C(5)-C(4)-C(3)	108.70(17)
C(9)-C(4)-C(3)	104.80(16)
C(6)-C(5)-C(4)	123.08(19)
C(6)-C(5)-C(11)	123.3(2)
C(4)-C(5)-C(11)	113.57(18)
C(5)-C(6)-C(12)	123.93(19)
C(5)-C(6)-C(7)	120.12(18)
C(12)-C(6)-C(7)	115.95(18)
O(2)-C(7)-C(6)	107.74(16)
O(2)-C(7)-C(8)	109.50(16)
C(6)-C(7)-C(8)	111.36(17)
C(13)-C(8)-C(7)	109.82(17)
C(13)-C(8)-C(9)	116.39(17)
C(7)-C(8)-C(9)	109.29(16)
C(1)-C(9)-C(8)	111.13(16)
C(1)-C(9)-C(21)	109.75(16)
C(8)-C(9)-C(21)	112.47(16)
C(1)-C(9)-C(4)	103.48(16)
C(8)-C(9)-C(4)	112.03(16)
C(21)-C(9)-C(4)	107.56(16)
C(1')-C(10)-C(3)	112.26(17)

C(14)-C(13)-C(8)	123.9(2)
C(13)-C(14)-C(15)	124.4(2)
C(14)-C(15)-C(16)	113.89(18)
C(17)-C(16)-C(22)	108.03(19)
C(17)-C(16)-C(15)	109.36(18)
C(22)-C(16)-C(15)	110.67(19)
O(3)-C(17)-C(16)	121.2(2)
O(3)-C(17)-C(18)	117.7(2)
C(16)-C(17)-C(18)	121.1(2)
O(4)-C(18)-C(19)	109.36(18)
O(4)-C(18)-C(23)	109.49(19)
C(19)-C(18)-C(23)	109.06(19)
O(4)-C(18)-C(17)	108.34(19)
C(19)-C(18)-C(17)	109.25(17)
C(23)-C(18)-C(17)	111.32(19)
O(5)-C(19)-C(20)	60.10(13)
O(5)-C(19)-C(18)	112.88(17)
C(20)-C(19)-C(18)	121.05(19)
O(5)-C(20)-C(19)	59.52(13)
O(5)-C(20)-C(21)	112.15(17)
C(19)-C(20)-C(21)	124.21(19)
O(6)-C(21)-C(20)	108.81(17)
O(6)-C(21)-C(9)	107.31(15)
C(20)-C(21)-C(9)	118.09(17)
O(7)-C(24)-O(6)	123.7(2)
O(7)-C(24)-C(25)	125.7(2)
O(6)-C(24)-C(25)	110.6(2)
C(2')-C(1')-C(6')	118.8(2)
C(2')-C(1')-C(10)	121.3(2)
C(6')-C(1')-C(10)	119.8(2)
C(3')-C(2')-C(1')	120.2(2)
C(4')-C(3')-C(2')	120.3(3)
C(5')-C(4')-C(3')	120.2(2)
C(4')-C(5')-C(6')	119.8(3)
C(5')-C(6')-C(1')	120.7(2)

Symmetry transformations used to generate equivalent atoms: