

Supporting Information

Anti-adipogenic Cyathane Diterpenoids from *Onychium japonicum*

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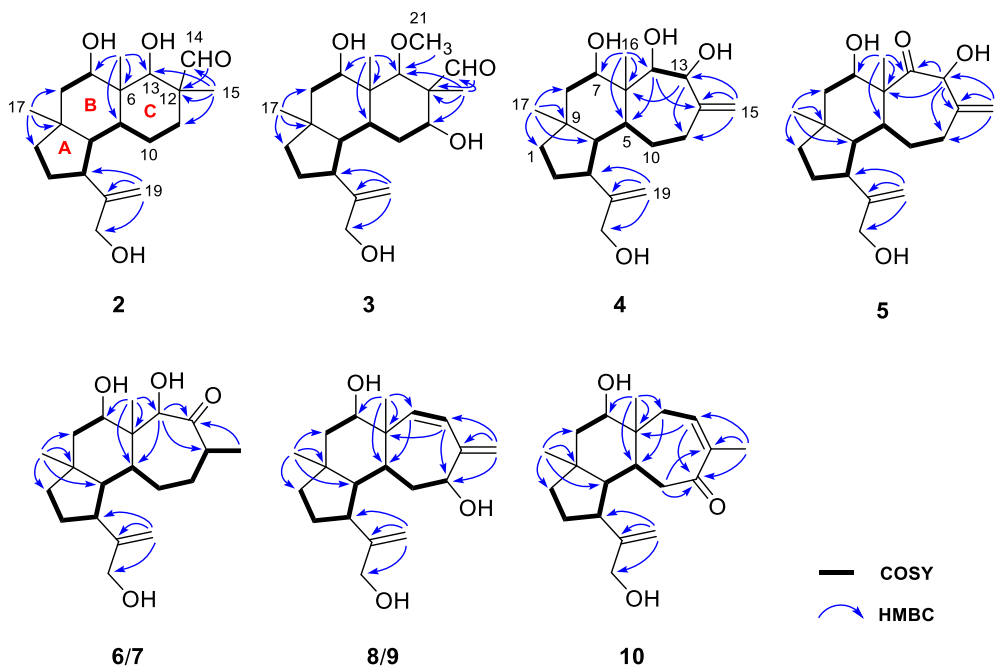


Figure S1. Key ^1H - ^1H COSY and HMBC correlations for compounds 2–10.

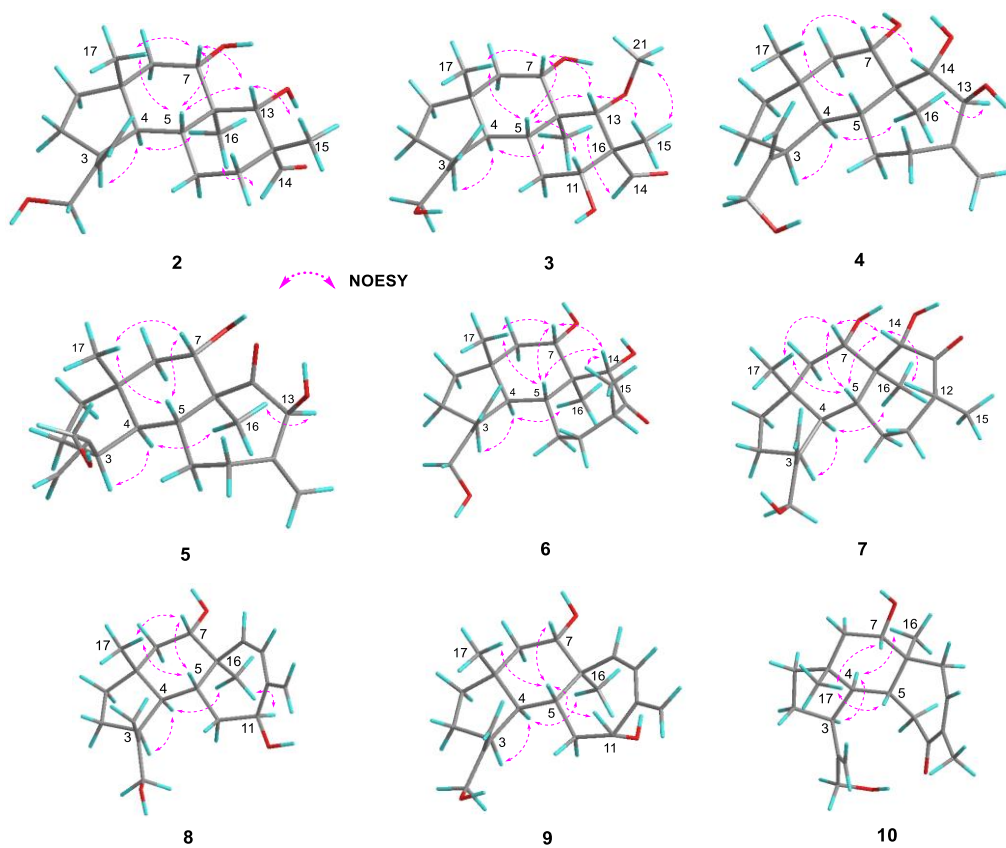


Figure S2. Key NOESY correlations for compounds 2–10.

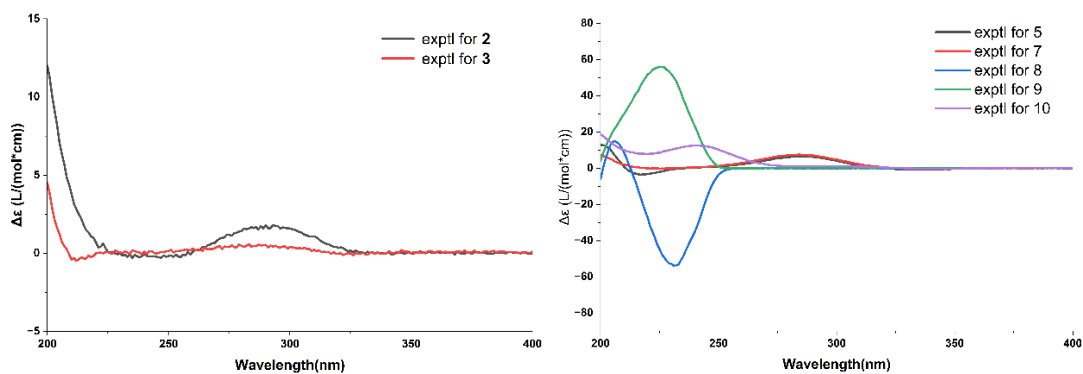


Figure S3. Experimental ECD spectra of compounds **2**, **3**, **5** and **7–10**.

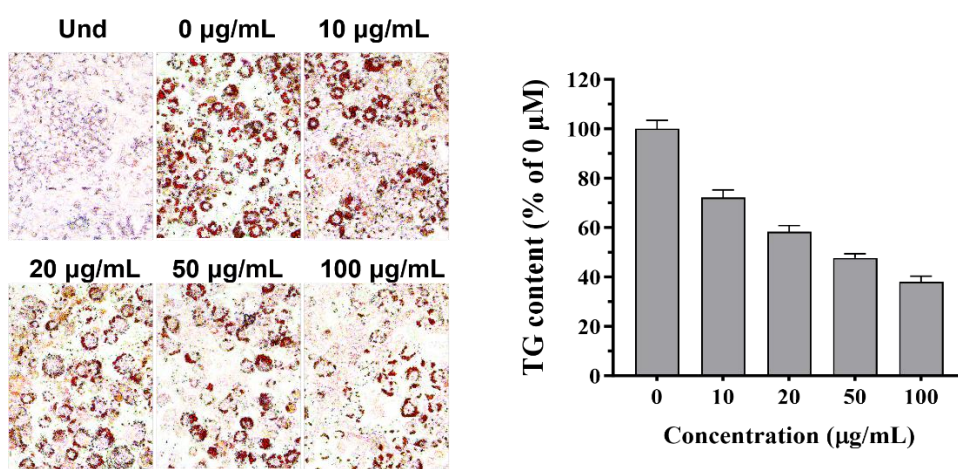
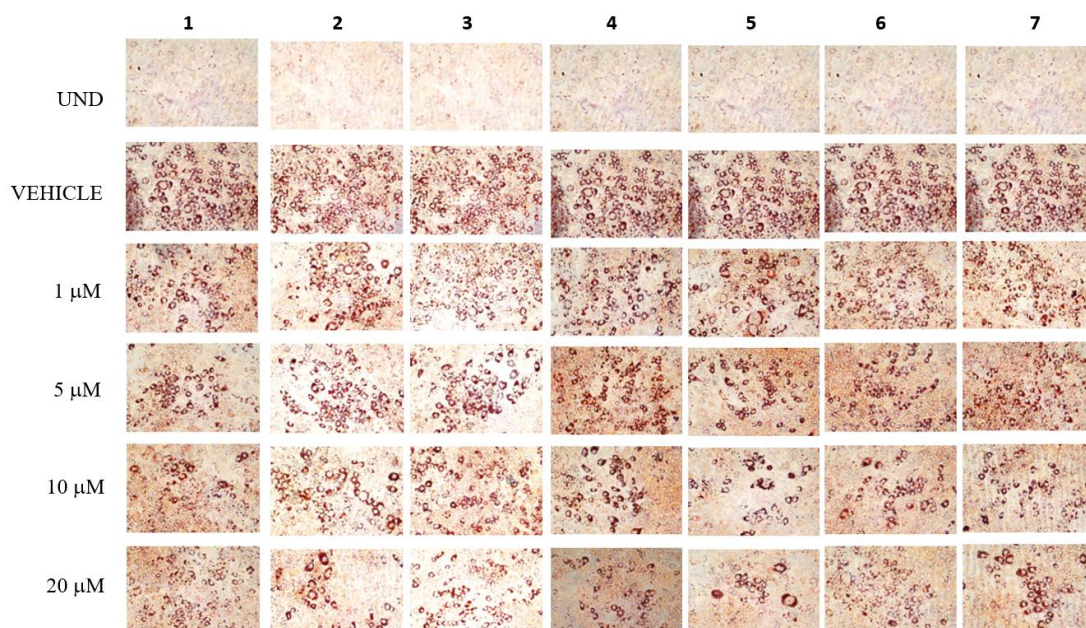


Figure S4. Anti-adipogenic effect of crude extract of *Onychium japonicum* on 3T3-L1 adipocytes.



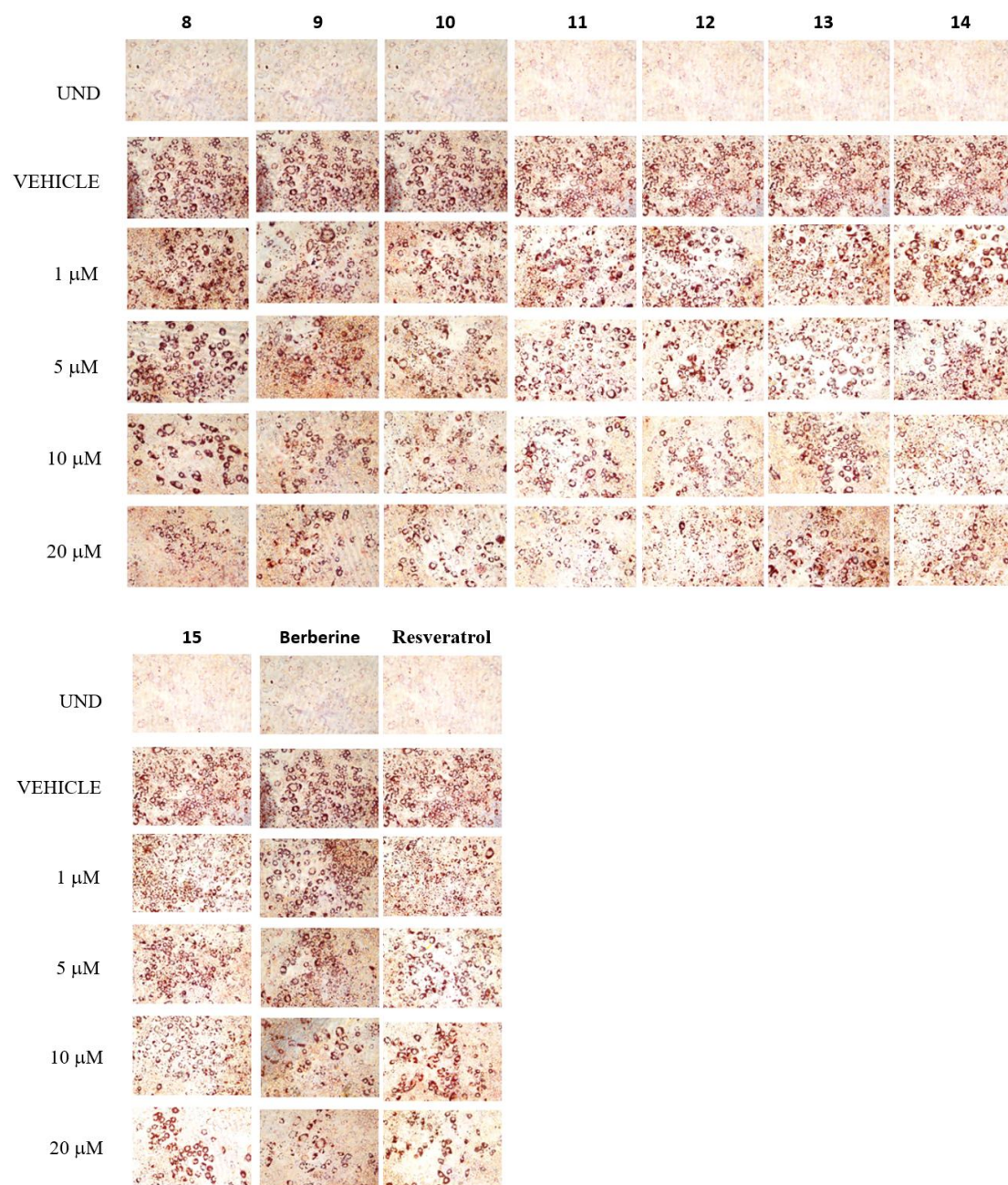


Figure S5. Anti-adipogenic effect of compounds **1–15** on 3T3-L1 adipocytes.

Figure S8. The ^1H - ^1H COSY spectrum of **1** in CD_3OD .

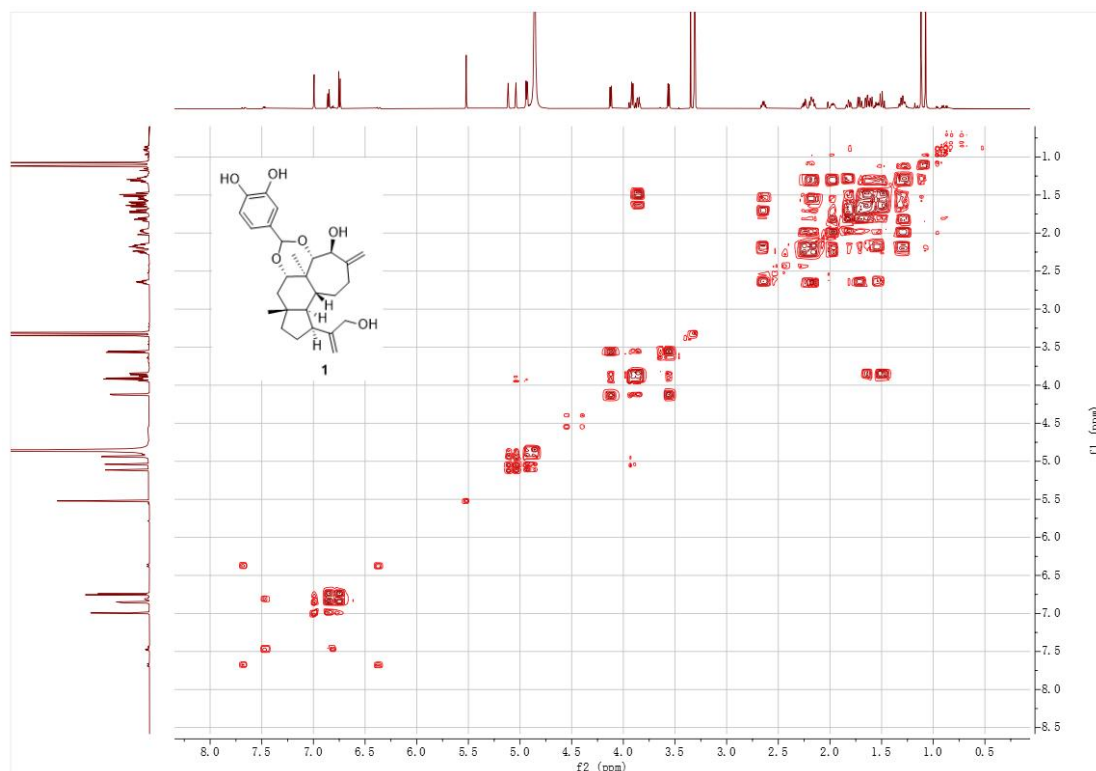


Figure S9. The HSQC spectrum of **1** in CD_3OD .

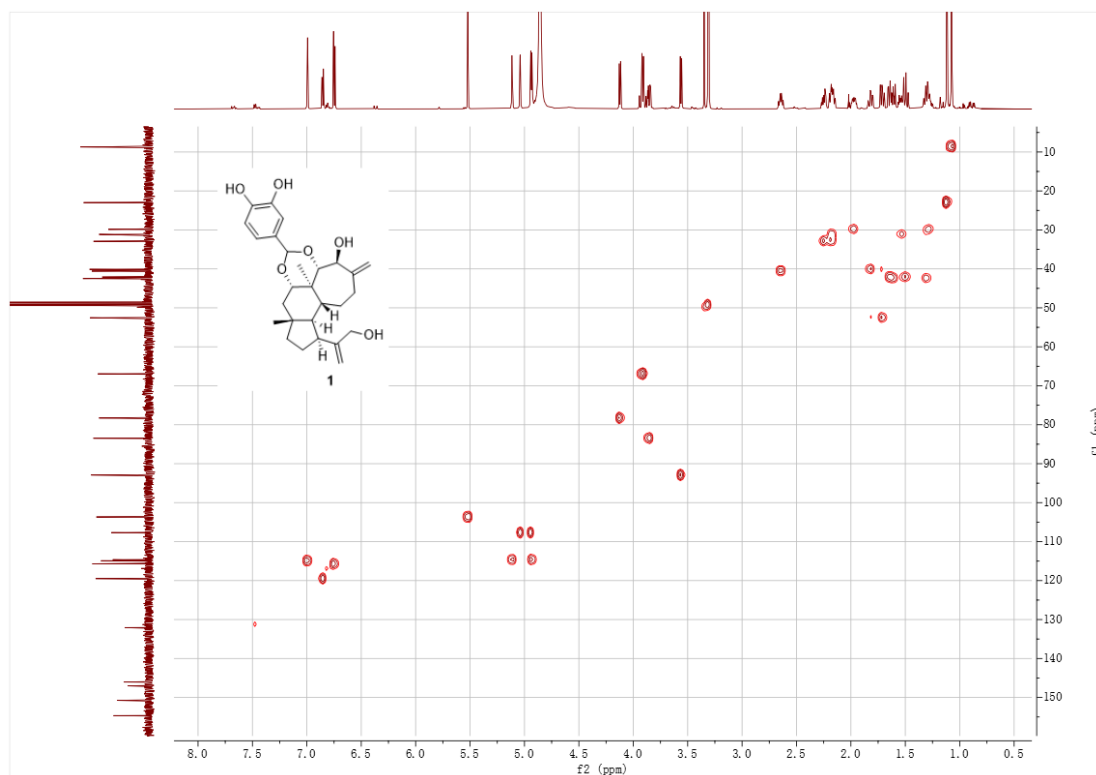


Figure S10. The HMBC spectrum of **1** in CD₃OD.

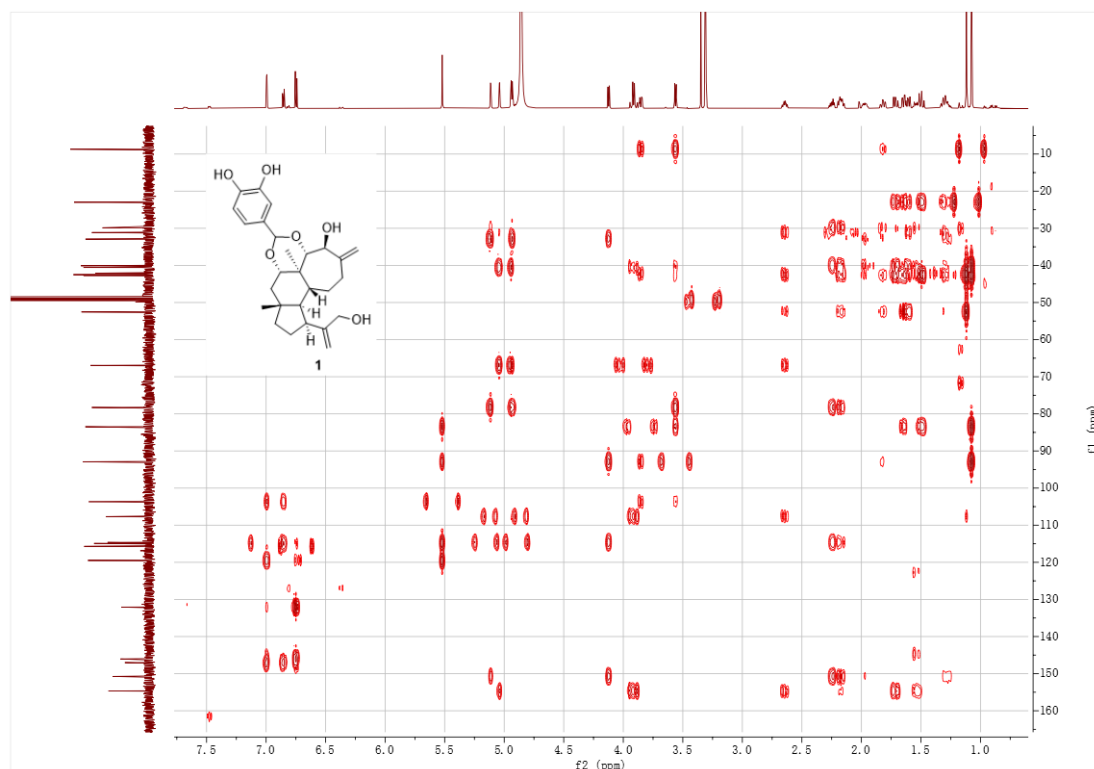


Figure S11. The NOESY spectrum of **1** in CD₃OD.

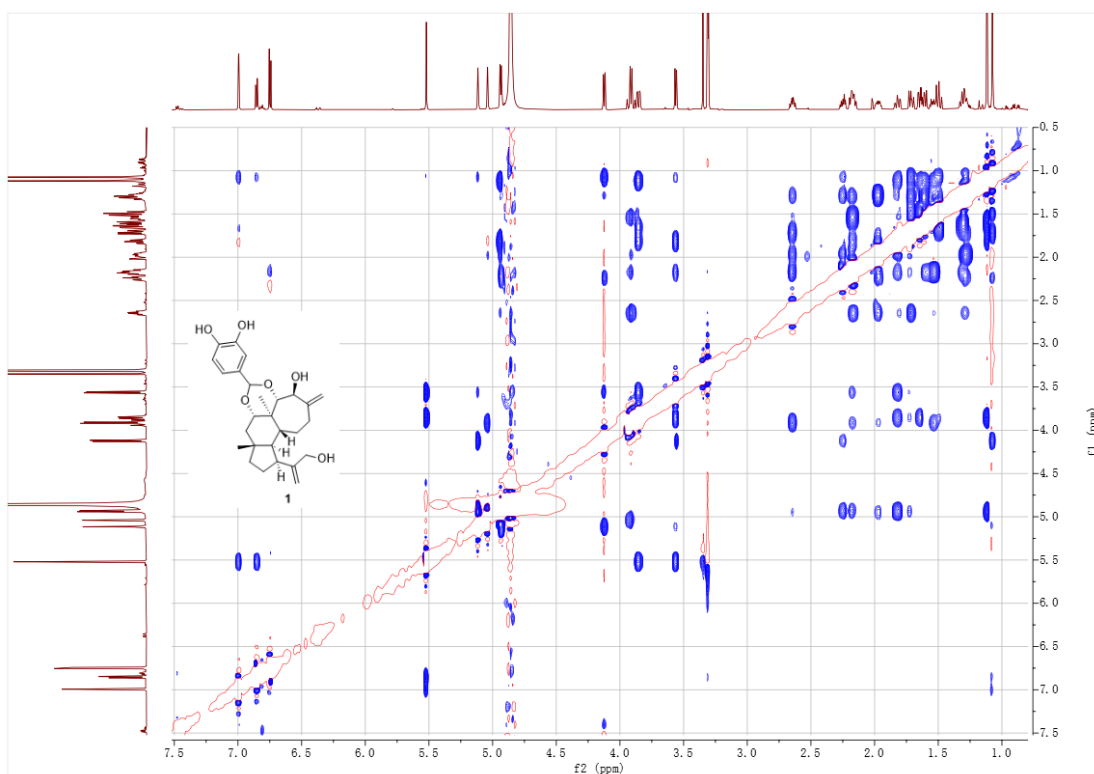
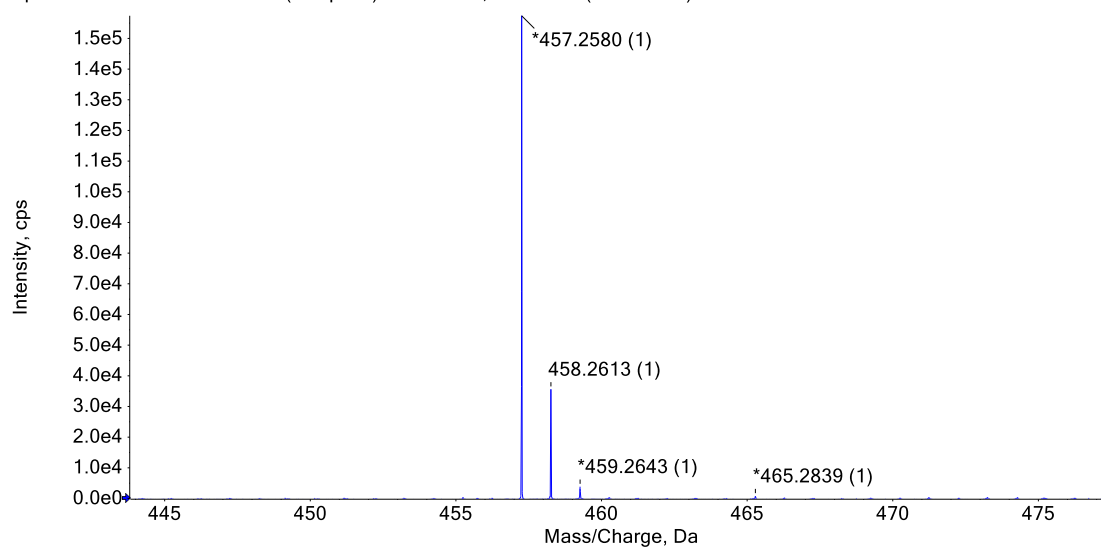


Figure S12. The (+)-HRESIMS spectrum of **1**.

Spectrum from XYZW-40.wiff2 (sample 1) - XYZW-40, +TOF MS (100 - 1000) from 1.382 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
457.2580	457.2580	-0.5	-1.1	C ₂₇ H ₃₇ O ₆	[M+H] ⁺

Figure S13. The IR spectrum of **1**.

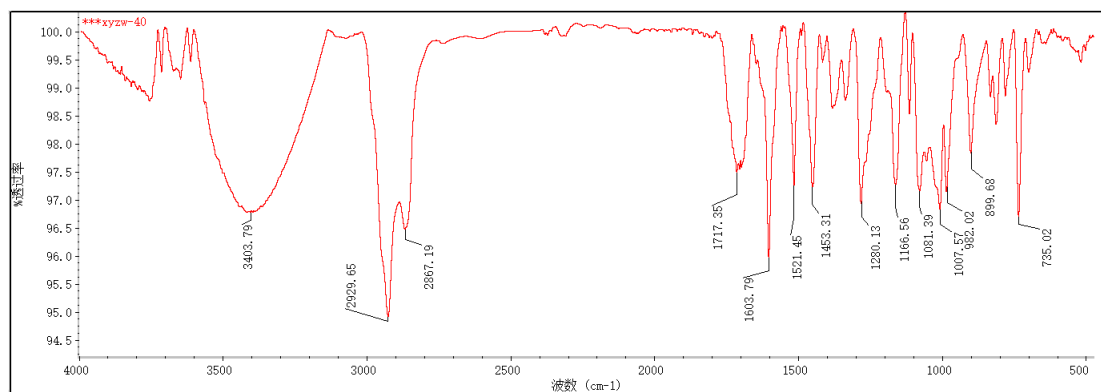


Figure S16. The ^1H - ^1H COSY spectrum of **2** in CD_3OD .

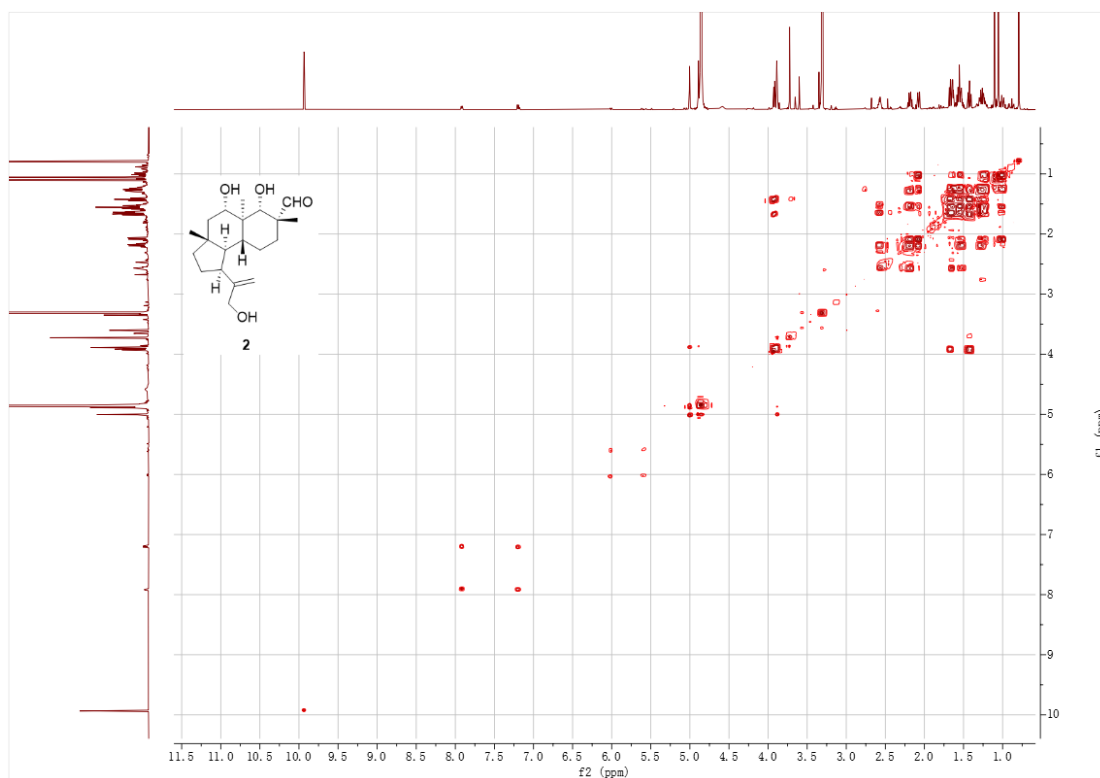


Figure S17. The HSQC spectrum of **2** in CD_3OD .

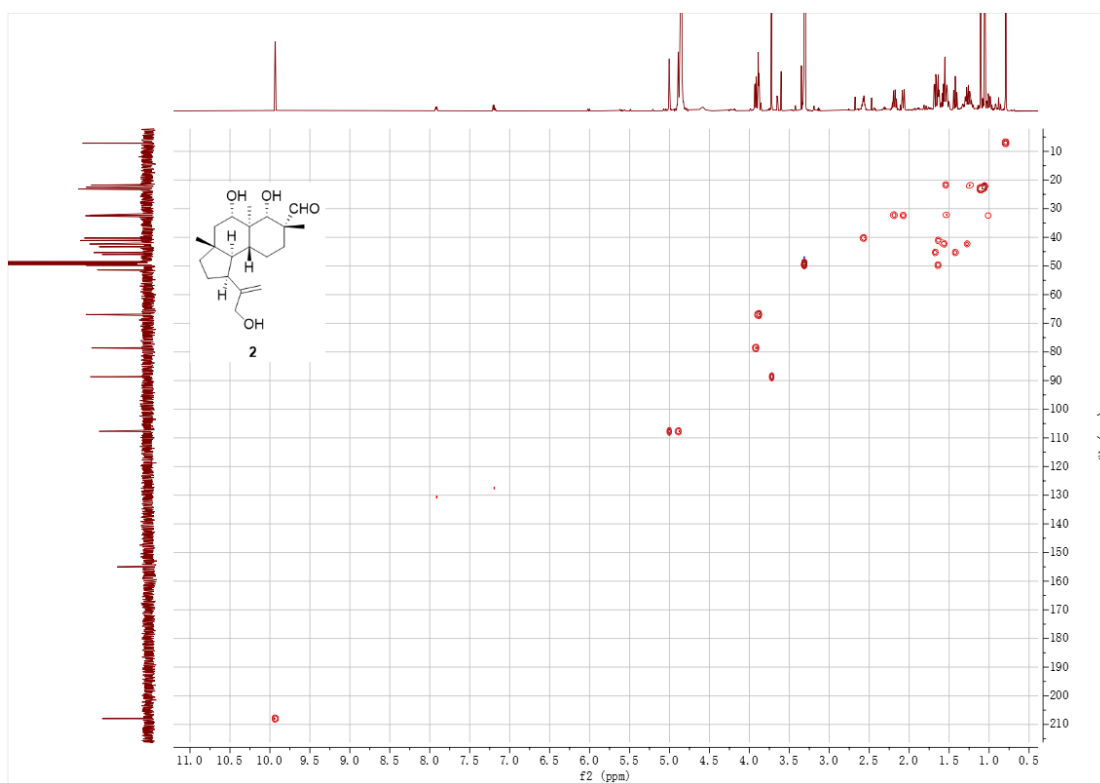


Figure S18. The HMBC spectrum of **2** in CD₃OD.

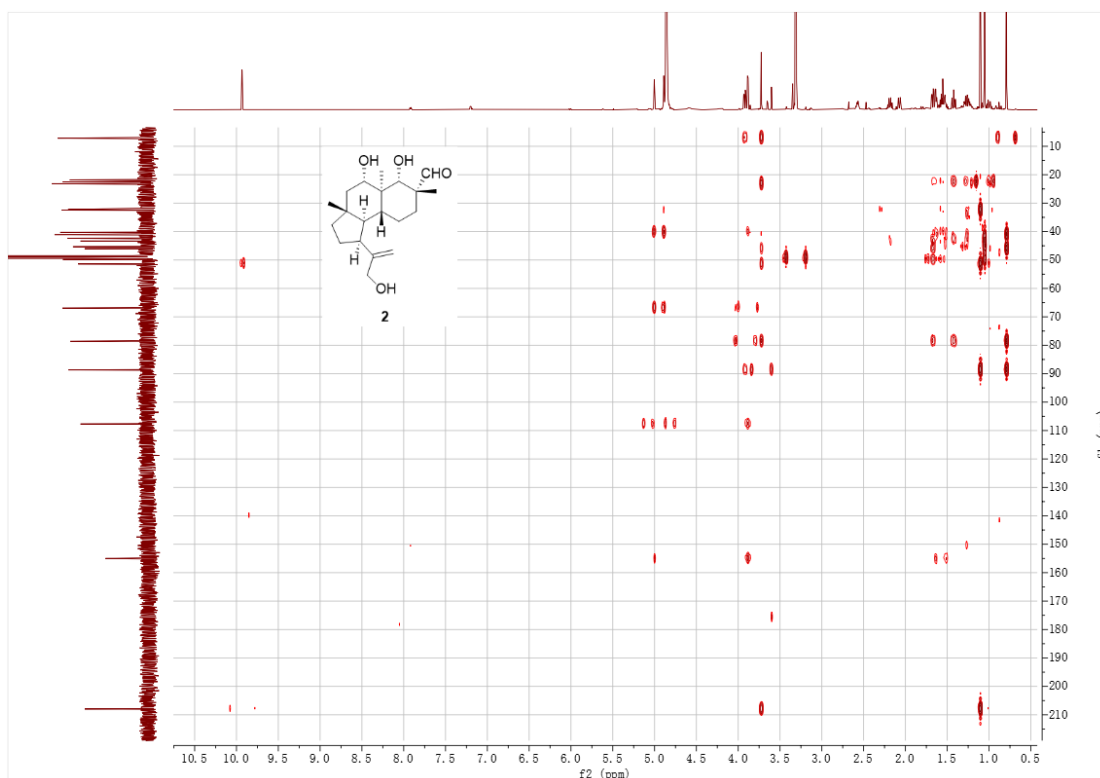


Figure S19. The NOESY spectrum of **2** in CD₃OD.

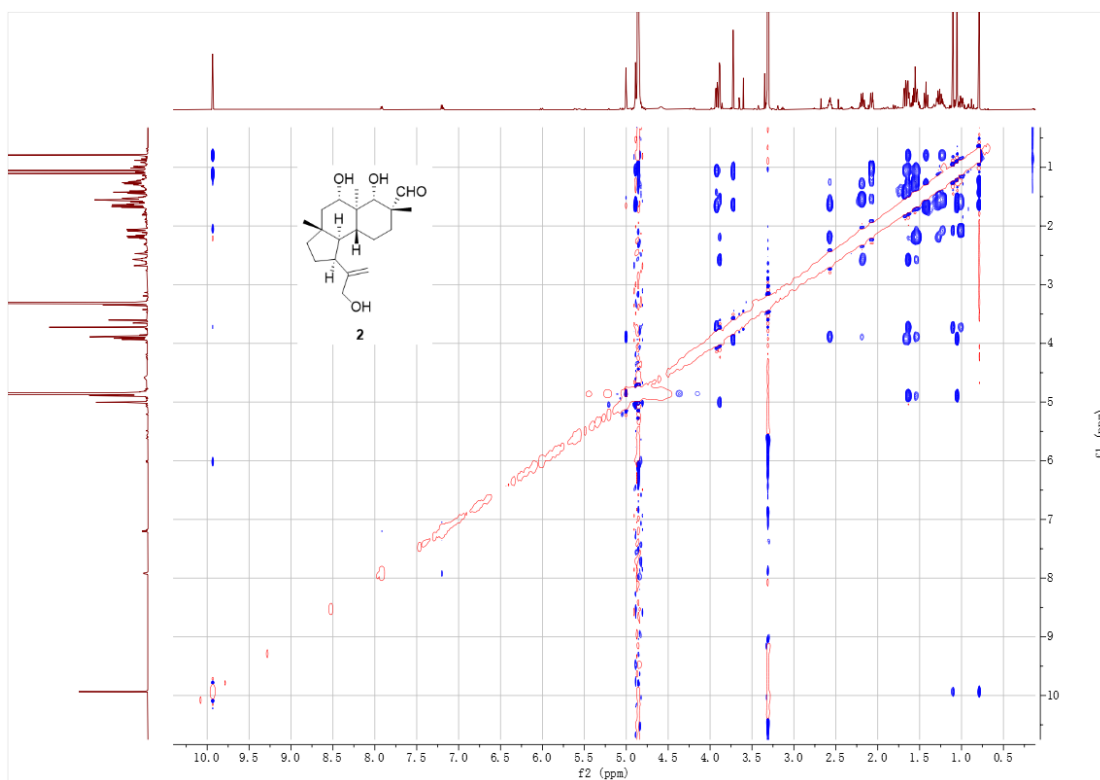
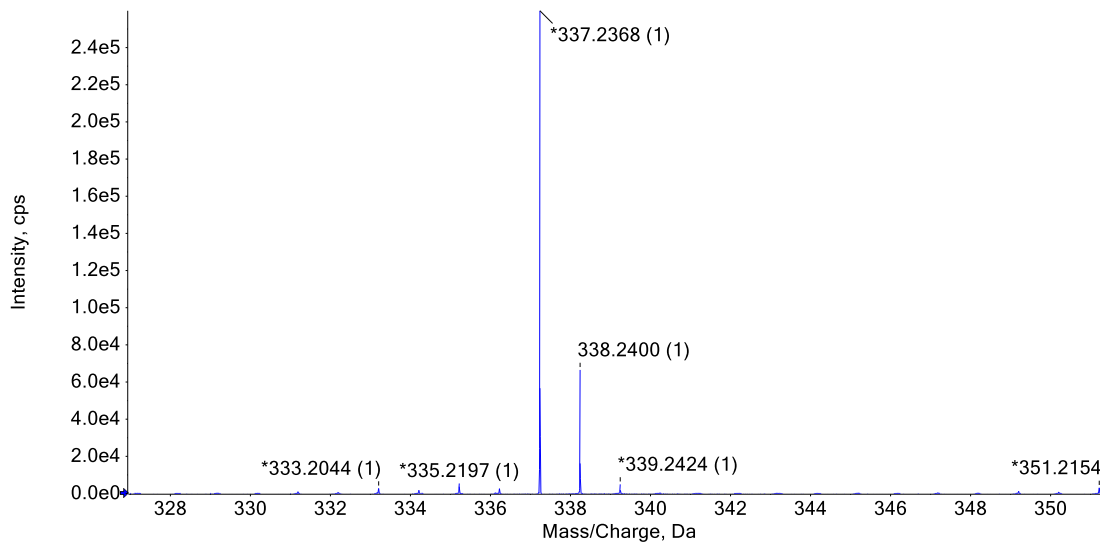


Figure S20. The (+)-HRESIMS spectrum of **2**.

Spectrum from XYZW-25.wiff2 (sample 1) - XYZW-25, +TOF MS (100 - 1000) from 1.346 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
337.2368	337.2373	-0.5	-1.5	C ₂₀ H ₃₃ O ₄	[M+H] ⁺

Figure S21. The IR spectrum of **2**.

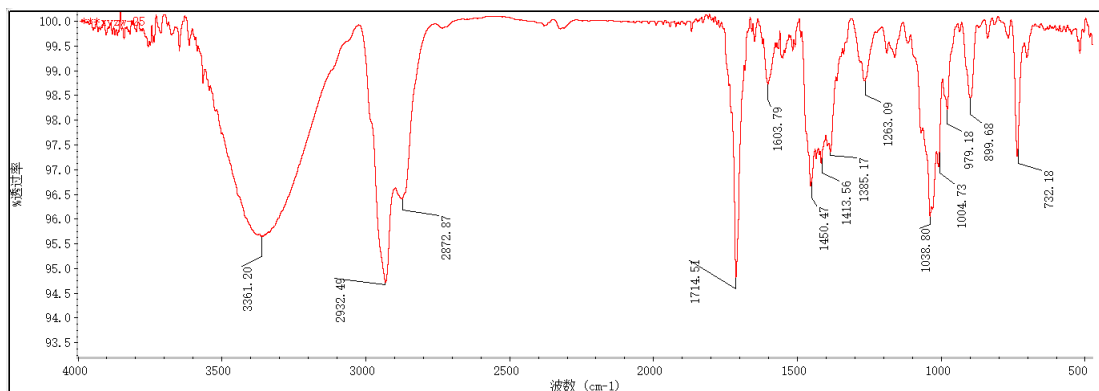


Figure S22. The ^1H NMR spectrum of **3** in CD_3OD .

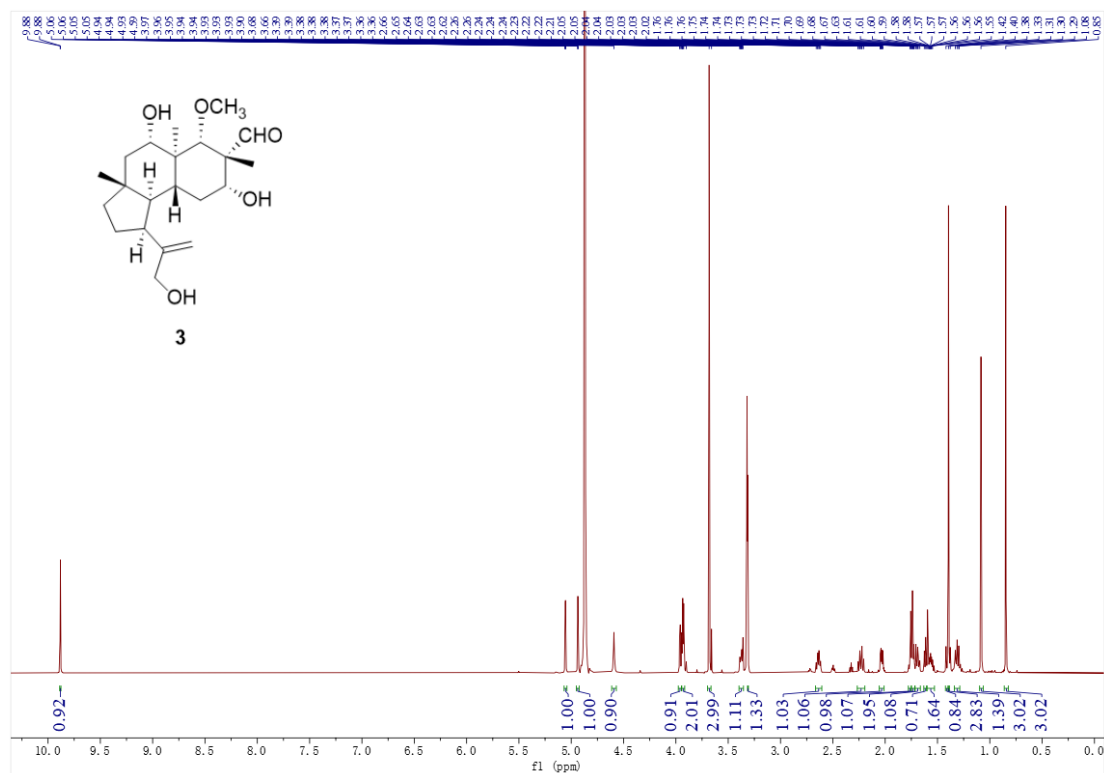


Figure S23. The ^{13}C NMR and DEPT spectrum of **3** in CD_3OD .

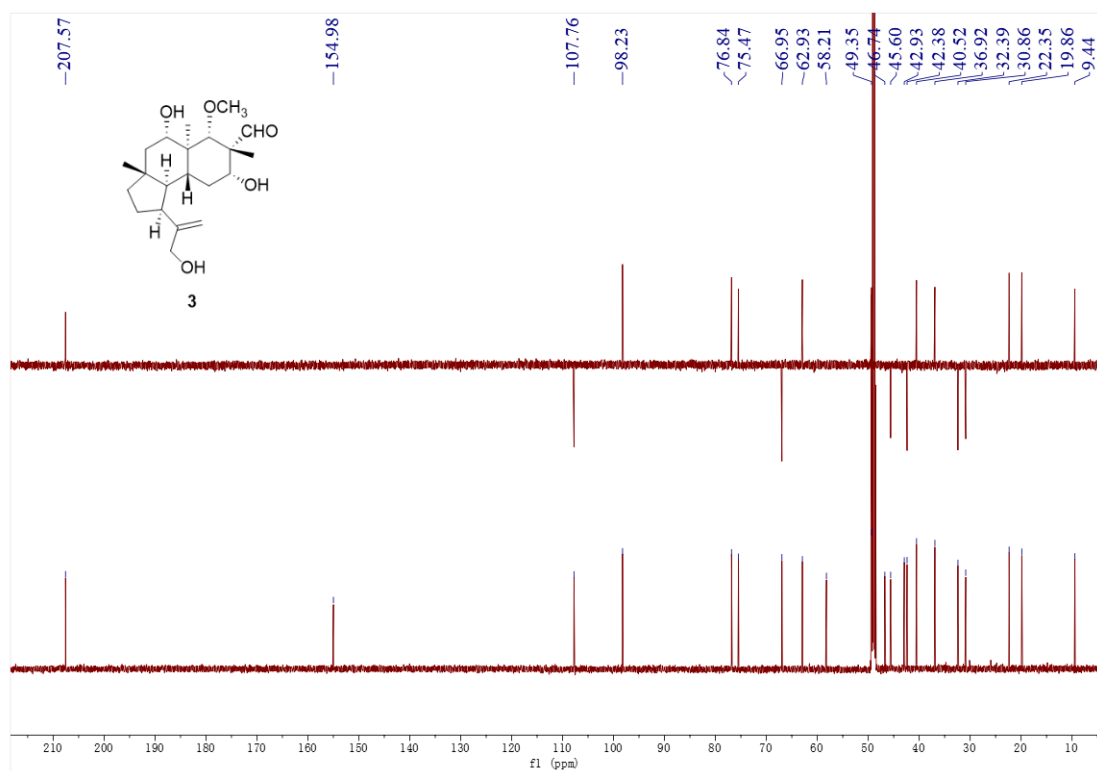


Figure S24. The ^1H - ^1H COSY spectrum of **3** in CD_3OD .

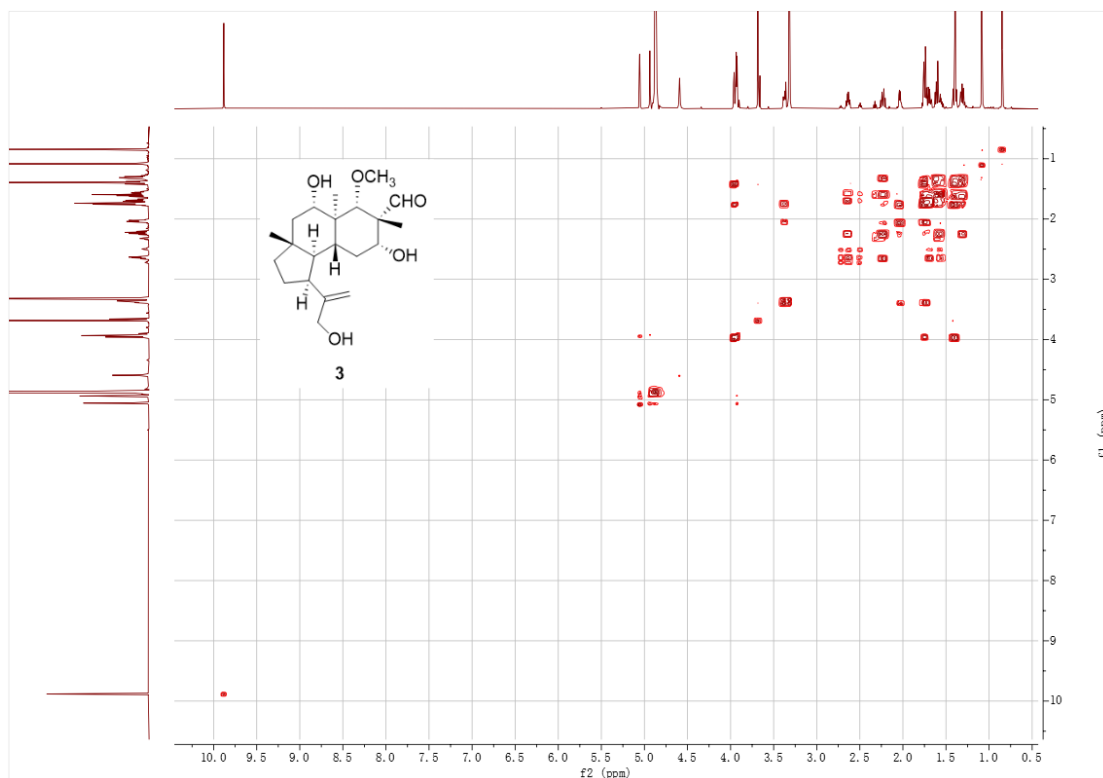


Figure S25. The HSQC spectrum of **3** in CD_3OD .

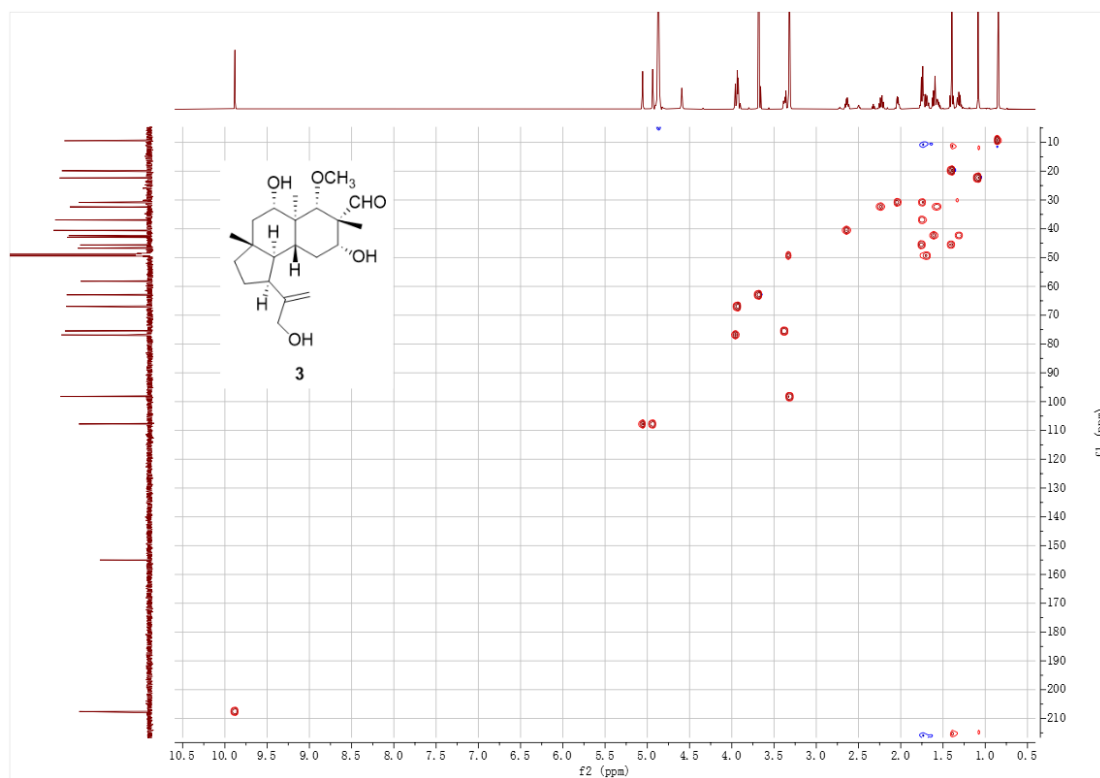


Figure S26. The HMBC spectrum of **3** in CD₃OD.



Figure S27. The NOESY spectrum of **3** in CD₃OD.

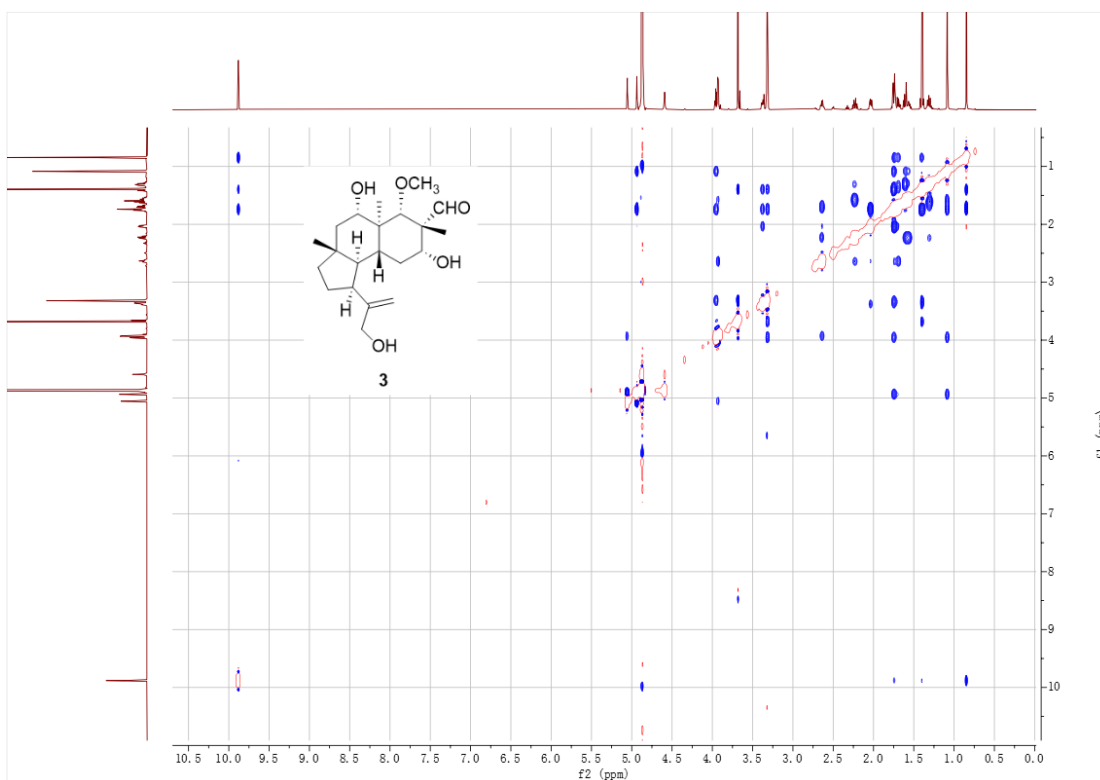
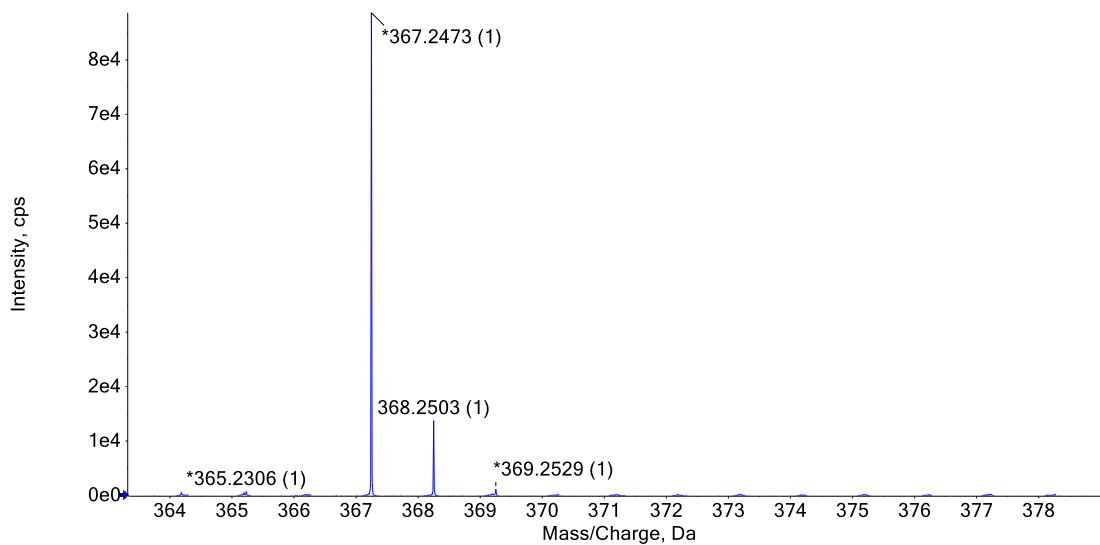


Figure S28. The (+)-HRESIMS spectrum of **3**.

Spectrum from XYZW-2.wiff2 (sample 1) - XYZW-2, +TOF MS (100 - 1000) from 1.346 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
367.2473	367.2479	-0.6	-1.5	C ₂₁ H ₃₅ O ₅	[M+H] ⁺

Figure S29. The IR spectrum of **3**.

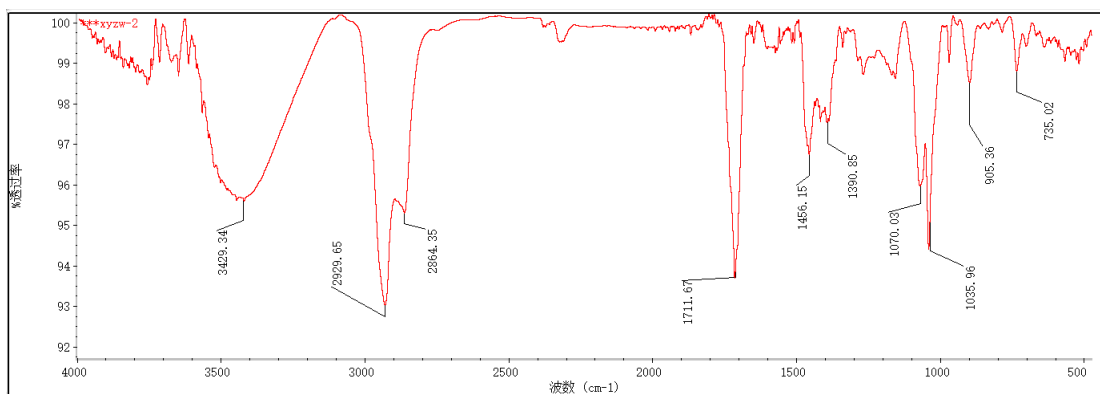


Figure S30. The ^1H NMR spectrum of **4** in CD_3OD .

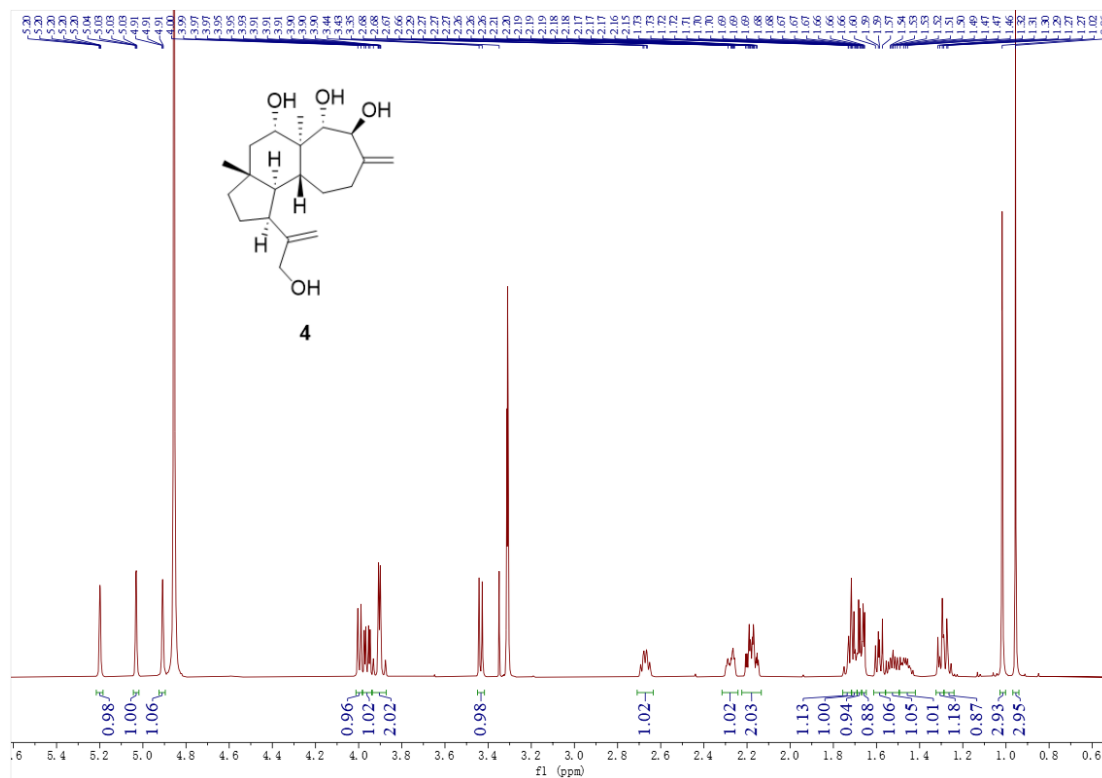


Figure S31. The ^{13}C NMR and DEPT spectrum of **4** in CD_3OD .

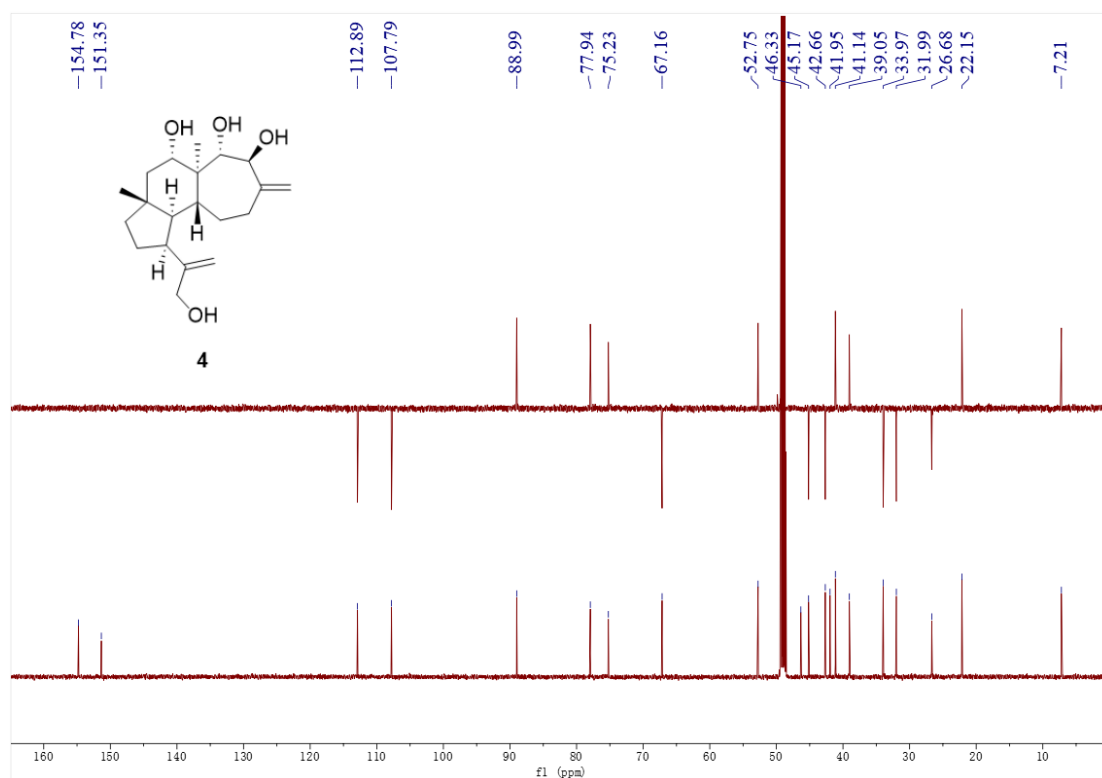


Figure S32. The ^1H - ^1H COSY spectrum of **4** in CD_3OD .

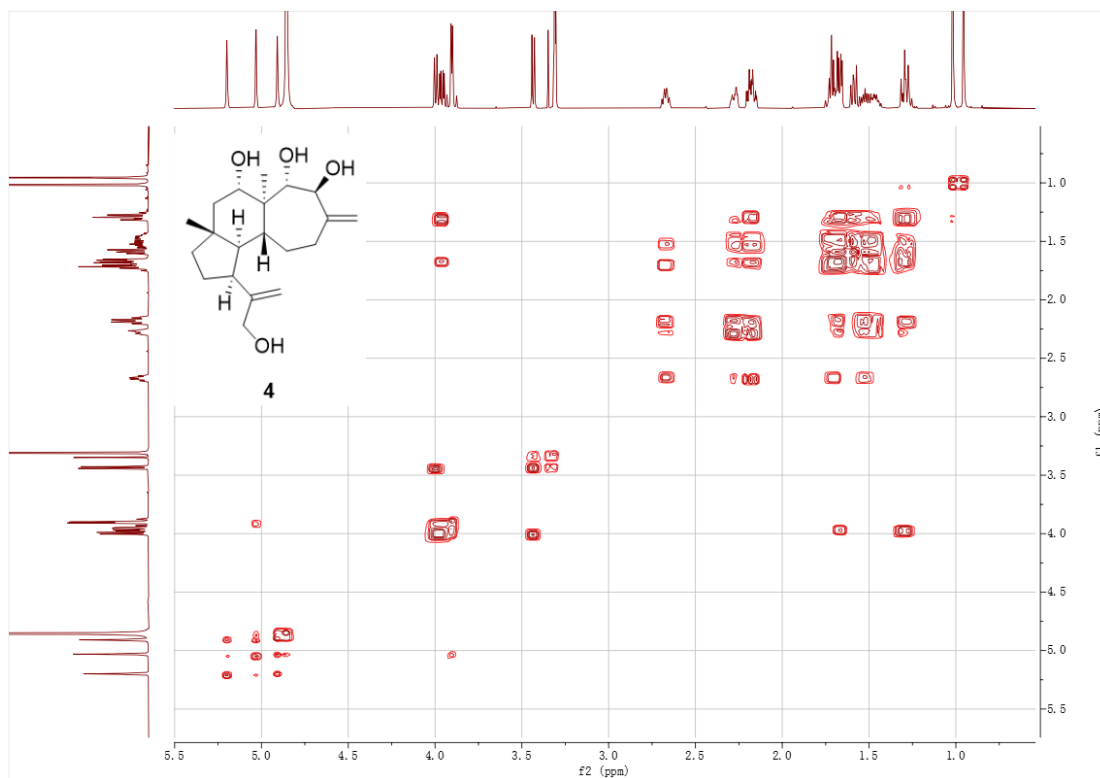


Figure S33. The HSQC spectrum of **4** in CD_3OD .

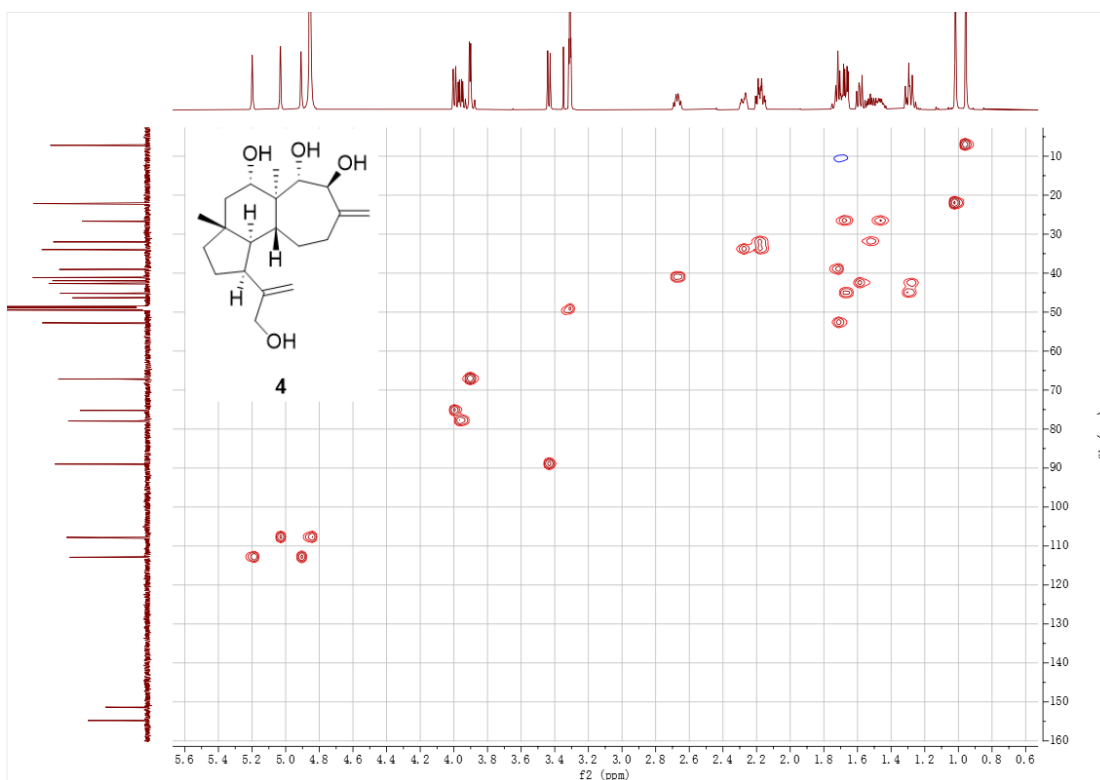


Figure S34. The HMBC spectrum of **4** in CD₃OD.

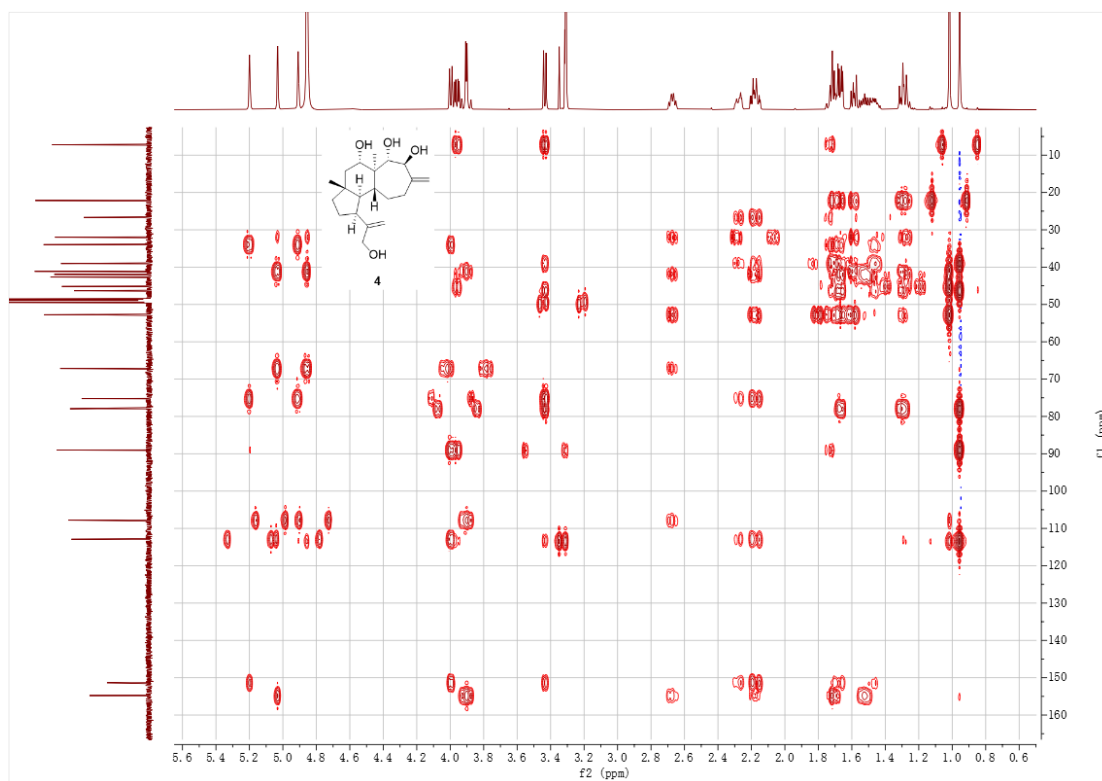


Figure S35. The NOESY spectrum of **4** in CD₃OD.

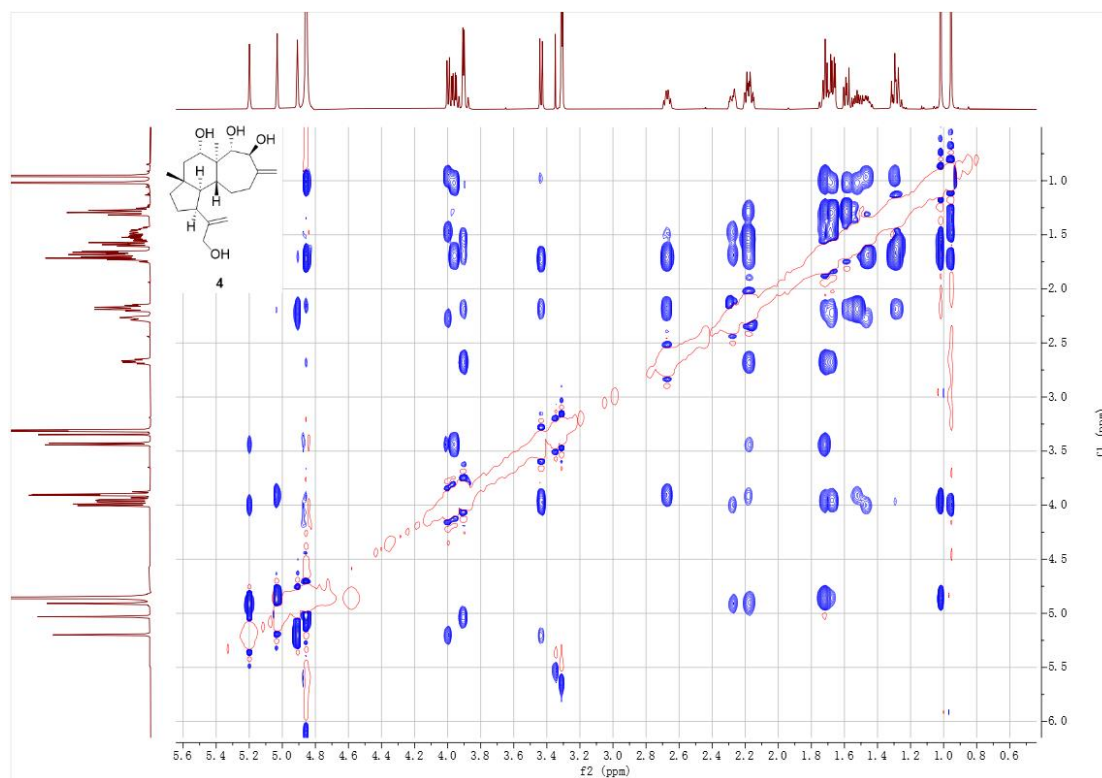
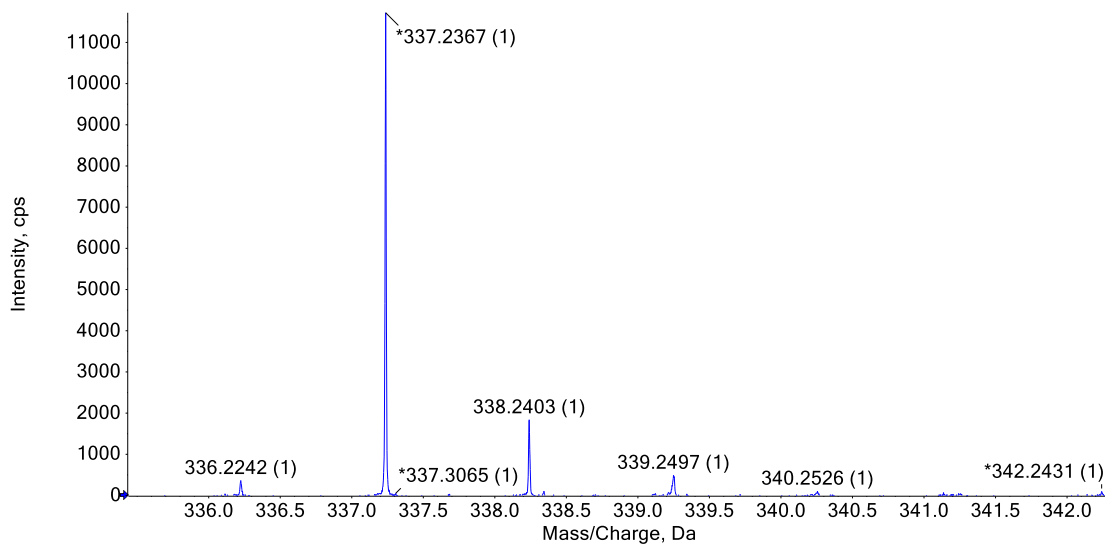


Figure S36. The (+)-HRESIMS spectrum of **4**.

Spectrum from XYZW-17.wiff2 (sample 1) - XYZW-17, +TOF MS (100 - 1000) from 1.370 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
337.2367	337.2373	-0.6	-2.0	C ₂₀ H ₃₃ O ₄	[M+H] ⁺

Figure S37. The IR spectrum of **4**.

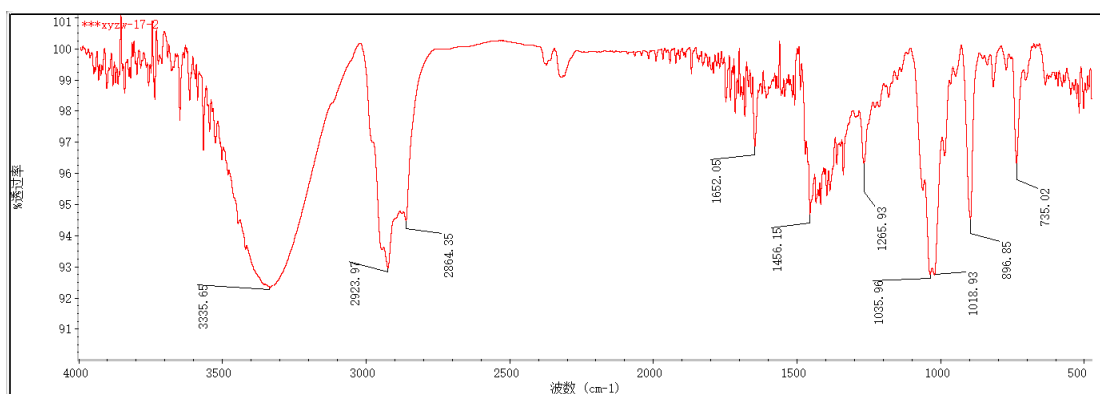


Figure S38. The ^1H NMR spectrum of **5** in CD_3OD .

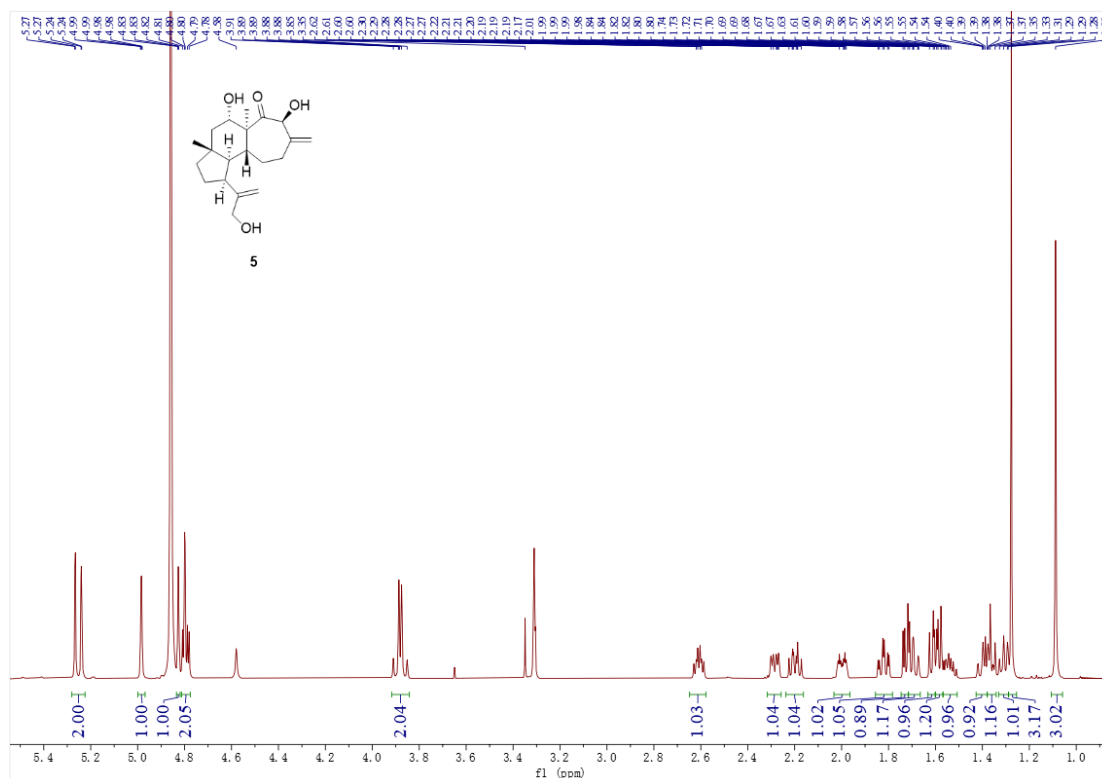


Figure S39. The ^{13}C NMR and DEPT spectrum of **5** in CD_3OD .

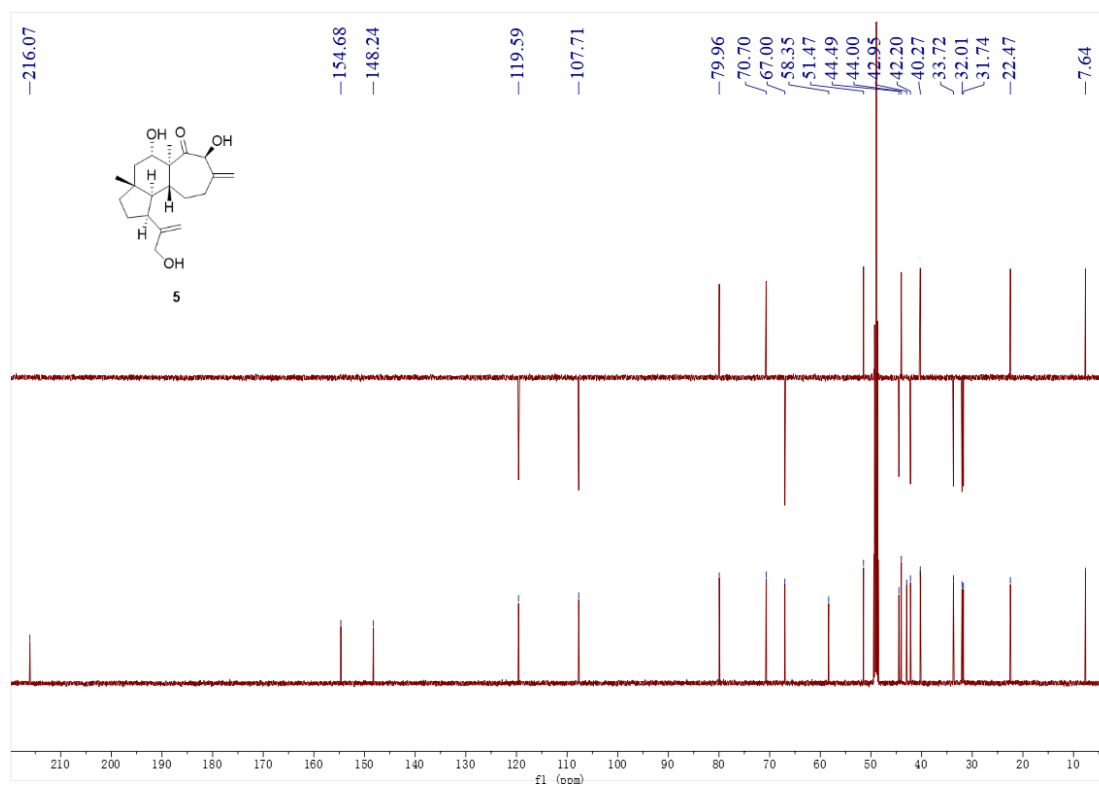


Figure S40. The ^1H - ^1H COSY spectrum of **5** in CD_3OD .

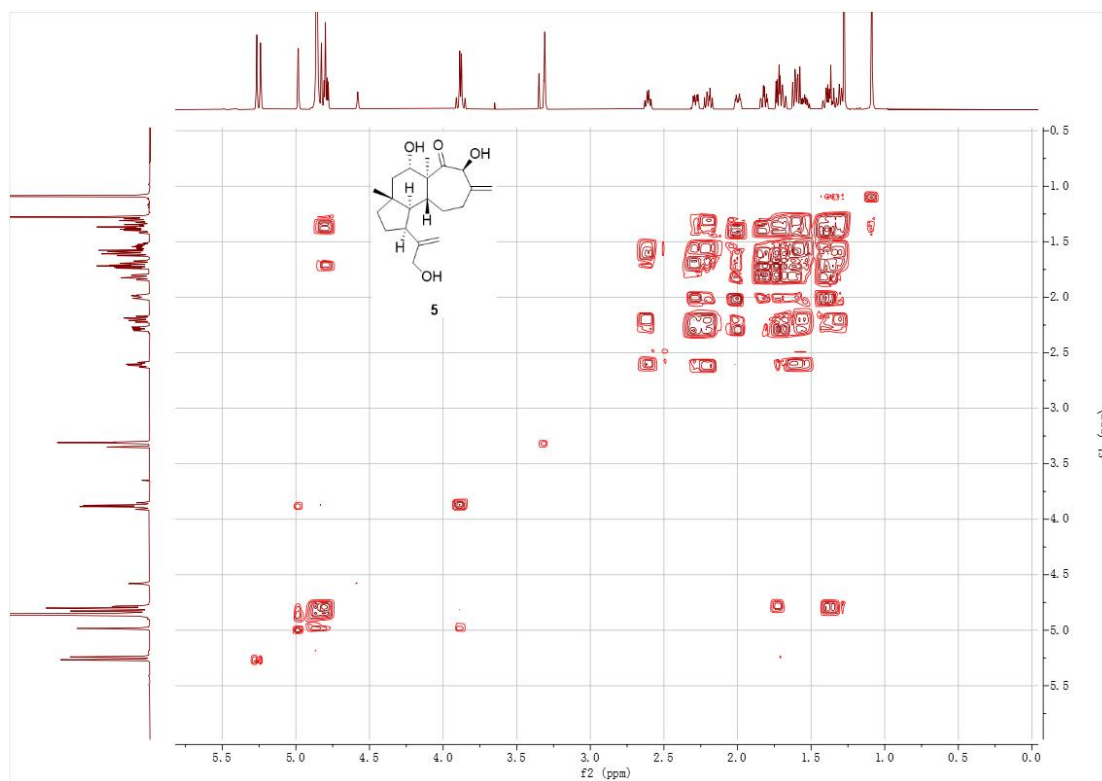


Figure S41. The HSQC spectrum of **5** in CD_3OD .

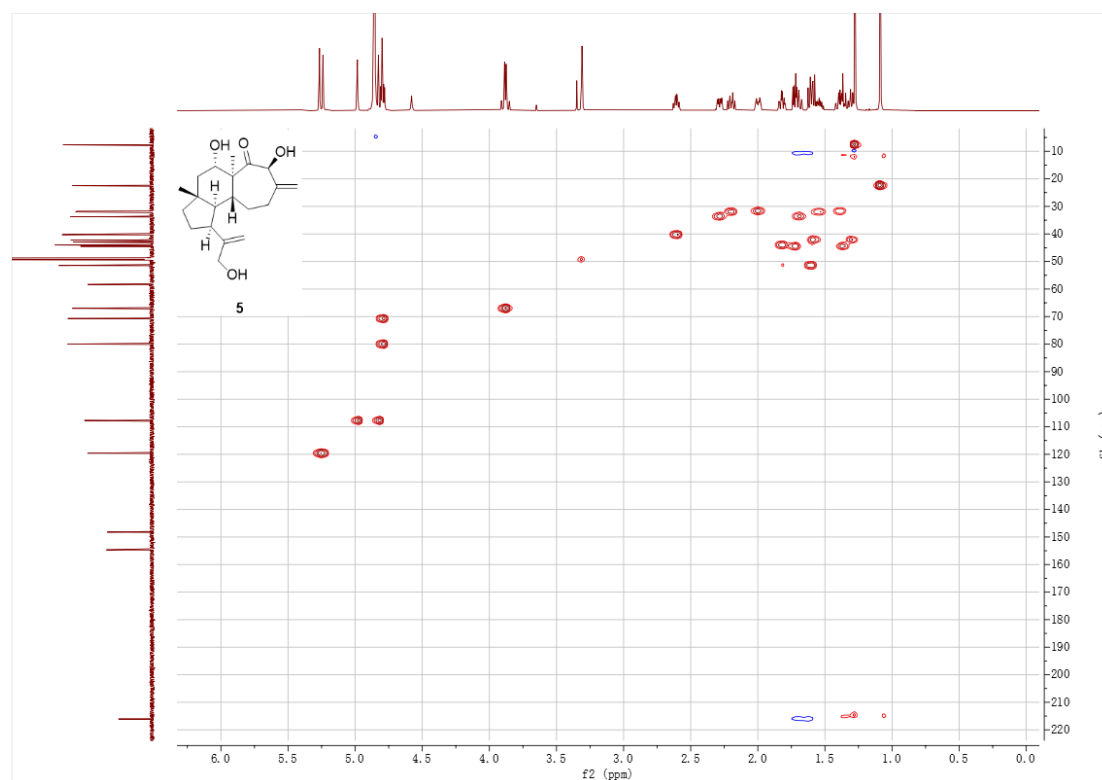


Figure S42. The HMBC spectrum of **5** in CD₃OD.

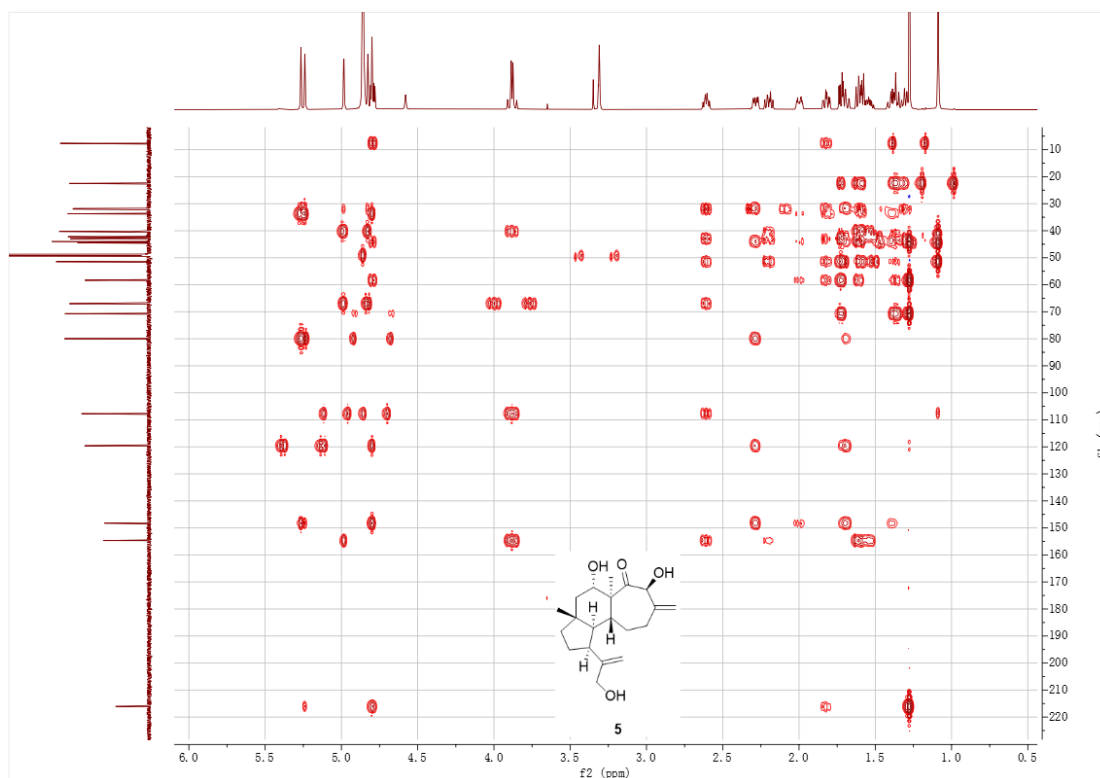


Figure S43. The NOESY spectrum of **5** in CD₃OD.

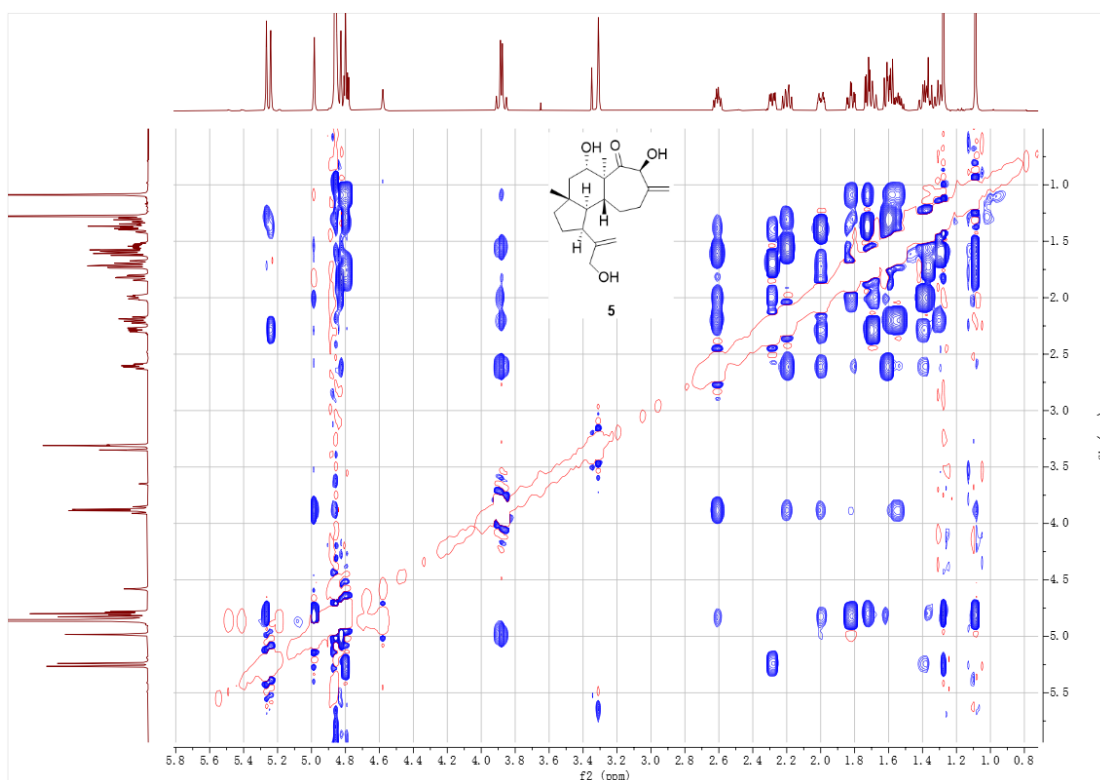
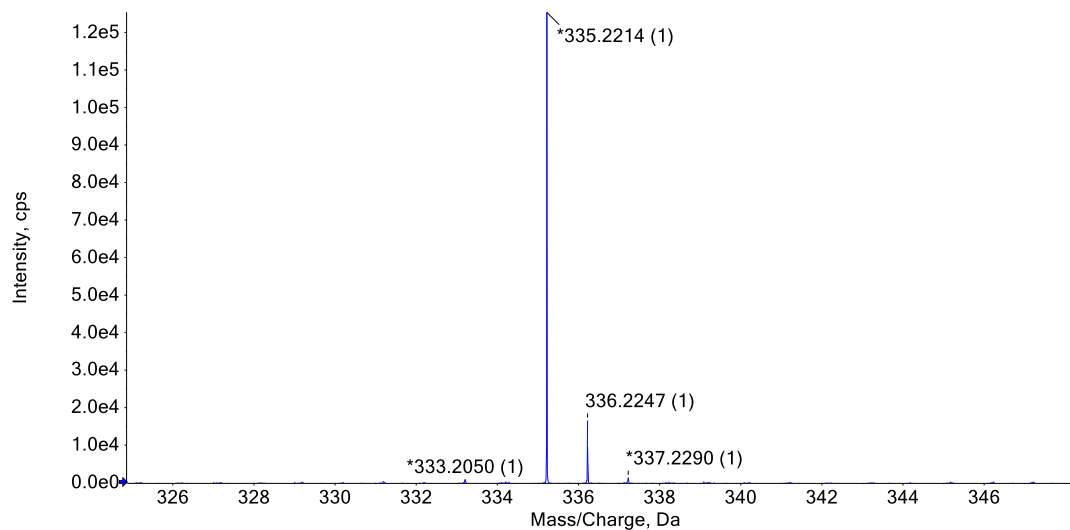


Figure S44. The (+)-HRESIMS spectrum of **5**.

Spectrum from XYZW-1.wiff2 (sample 1) - XYZW-1, +TOF MS (100 - 1000) from 1.358 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
335.2214	335.2217	-0.3	-1.0	C ₂₀ H ₃₁ O ₄	[M+H] ⁺

Figure S45. The IR spectrum of **5**.

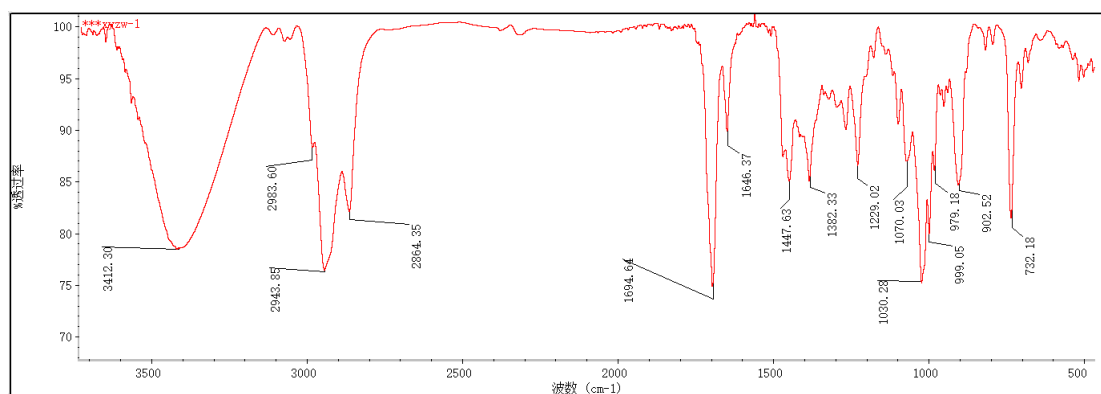


Figure S46. The ^1H NMR spectrum of **6** in CD_3OD .

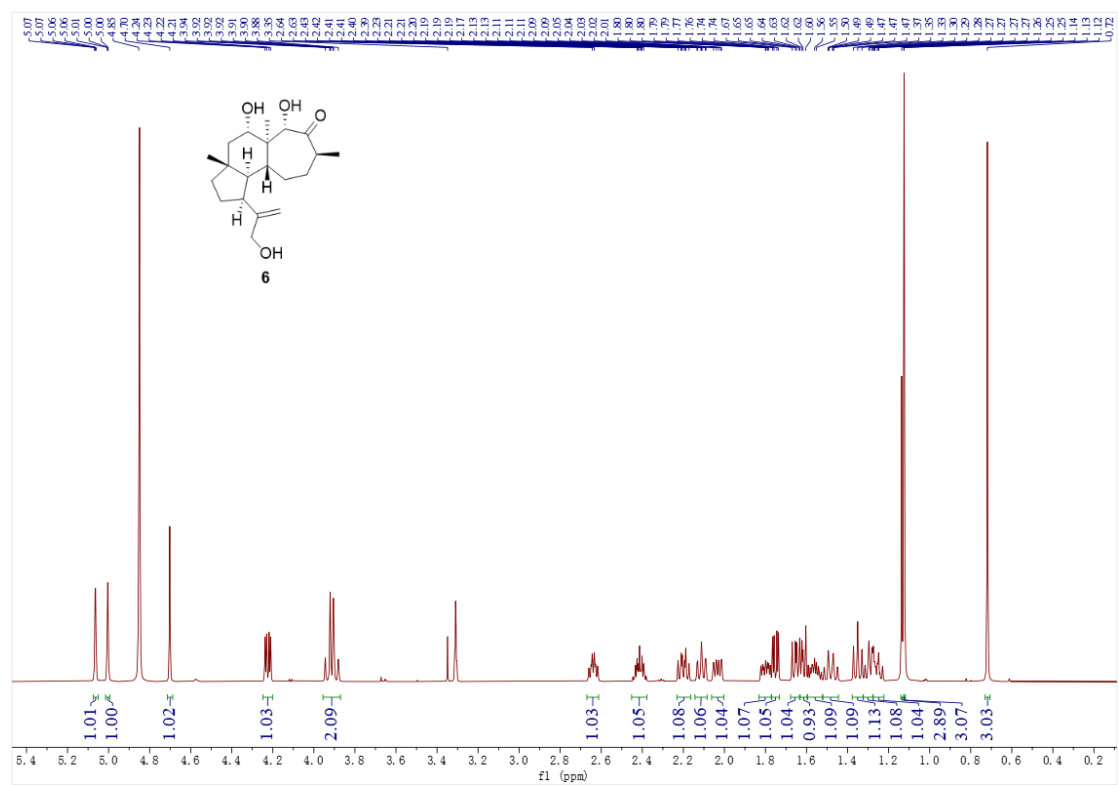


Figure S47. The ^{13}C NMR and DEPT spectrum of **6** in CD_3OD .

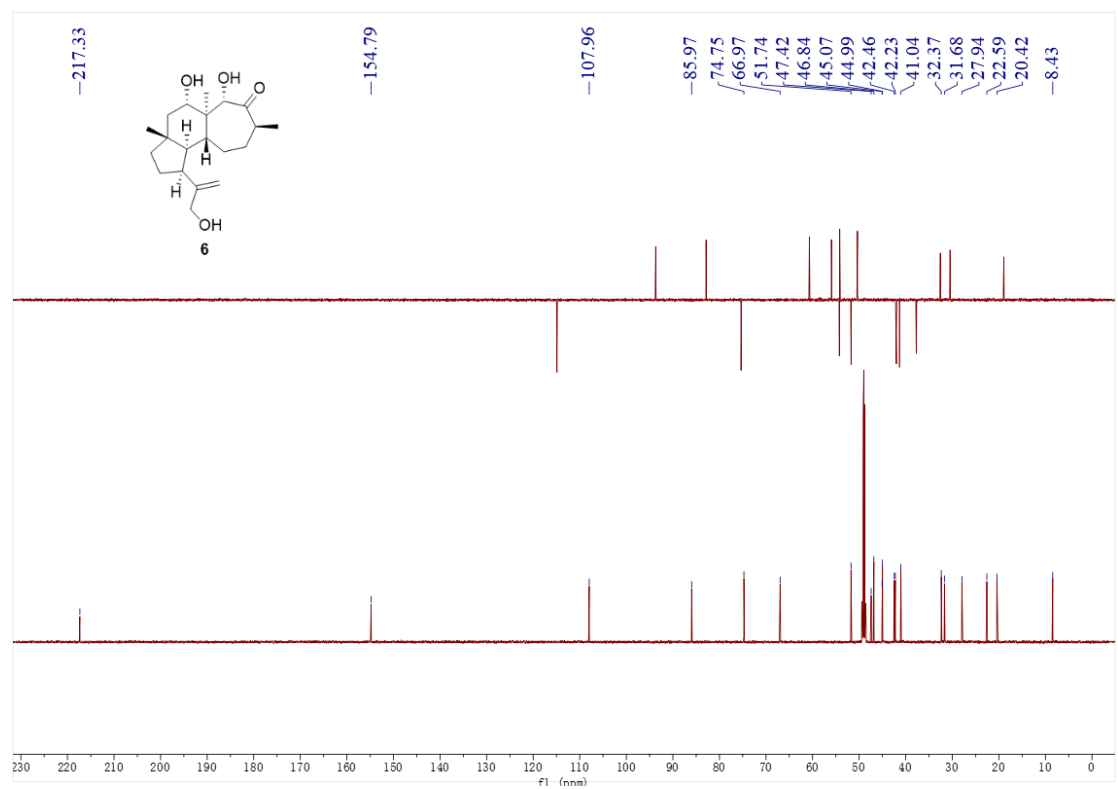


Figure S48. The ^1H - ^1H COSY spectrum of **6** in CD_3OD .

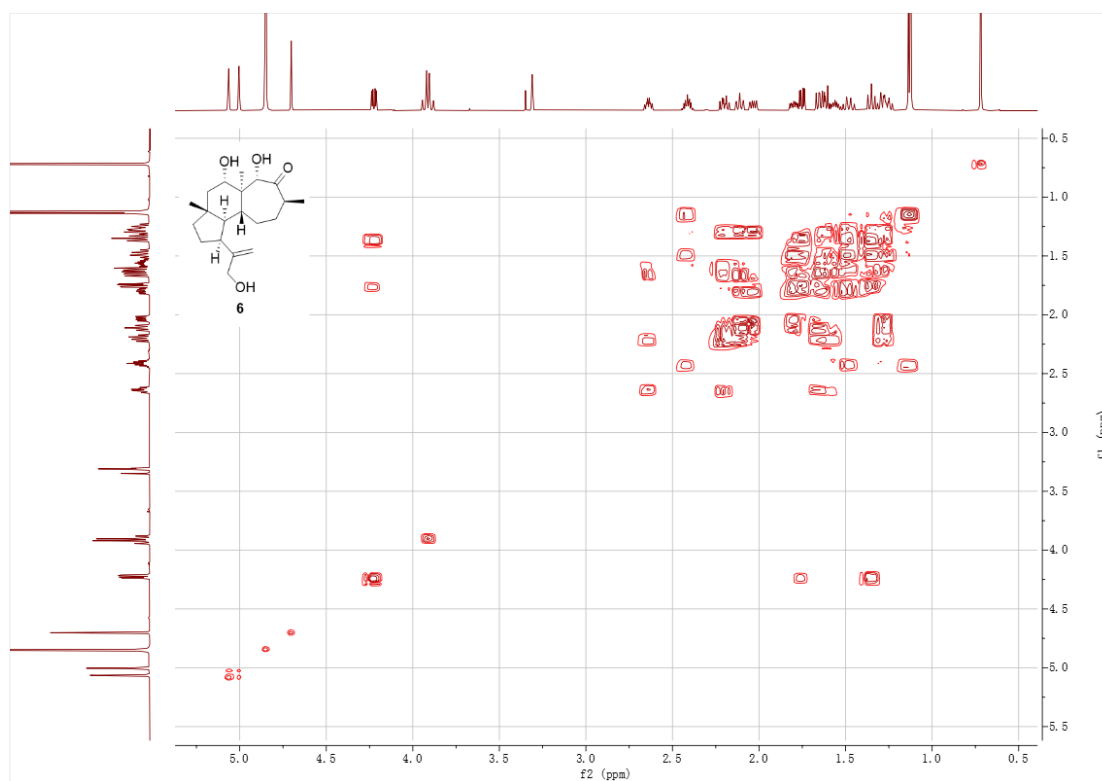


Figure S49. The HSQC spectrum of **6** in CD_3OD .

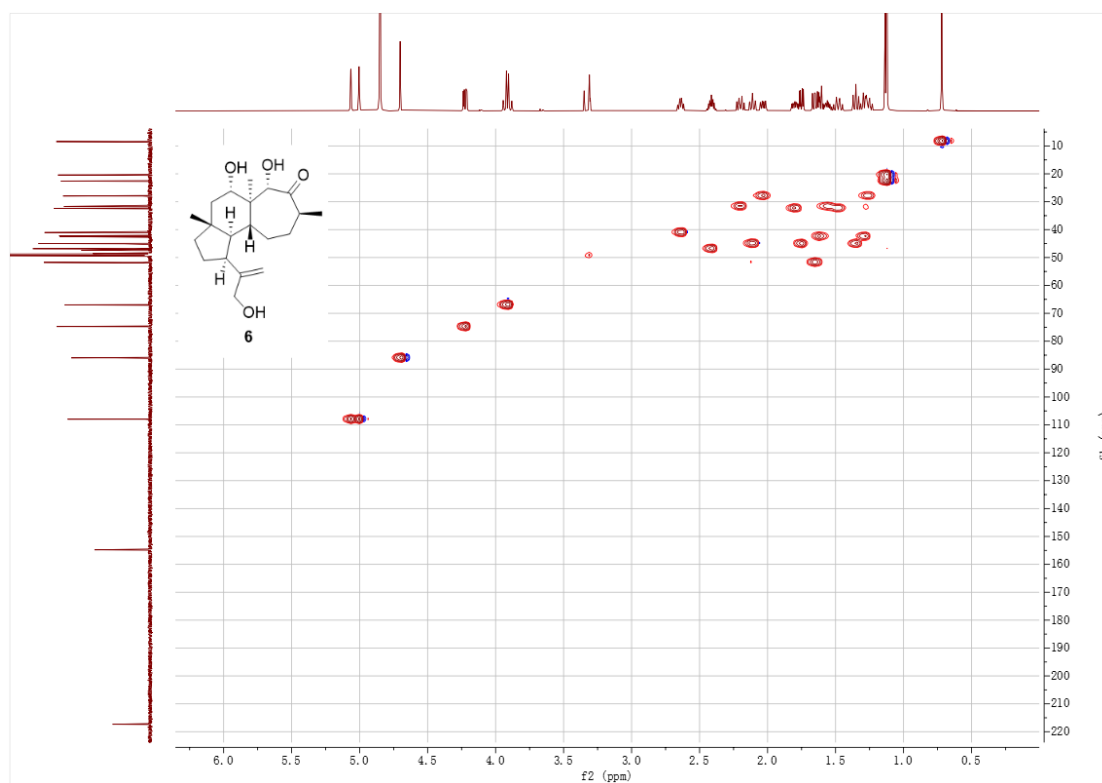


Figure S50. The HMBC spectrum of **6** in CD₃OD.

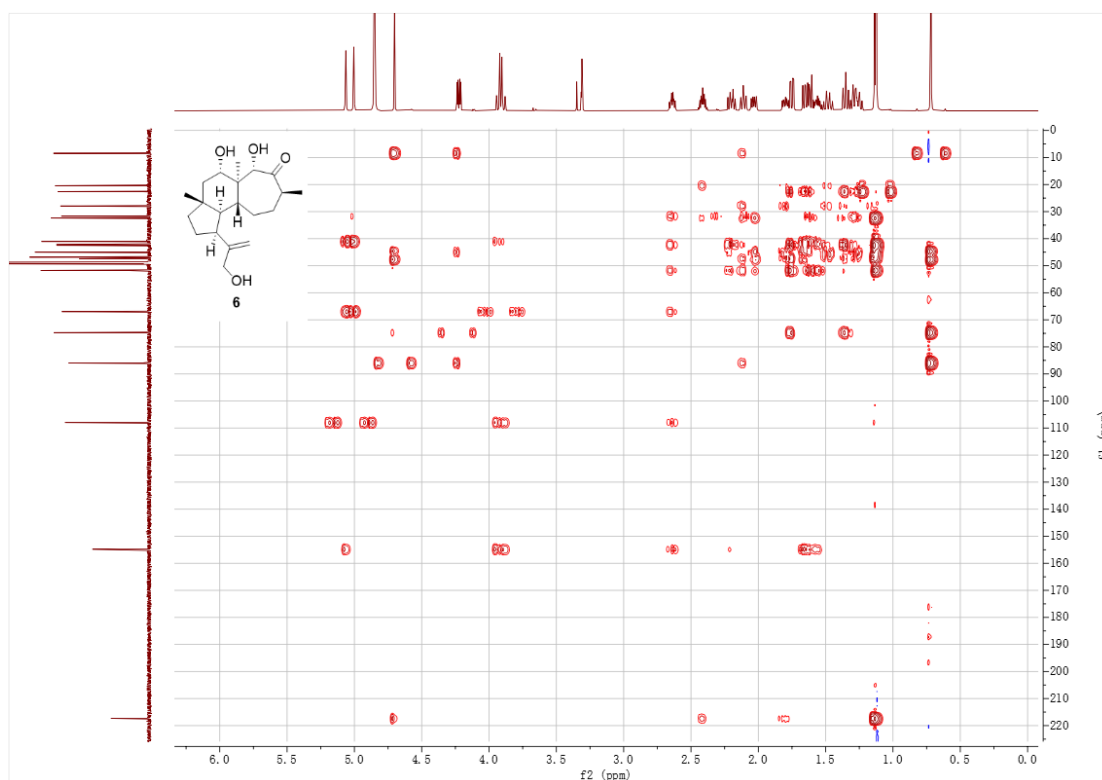


Figure S51. The NOESY spectrum of **6** in CD₃OD.

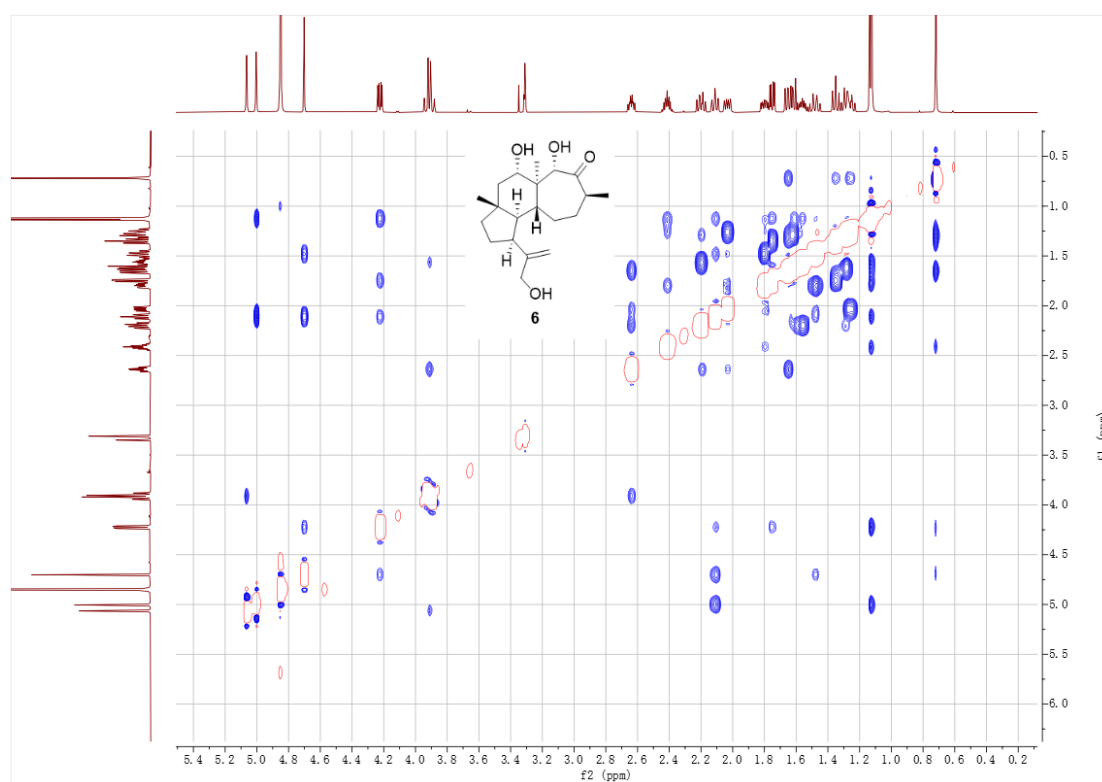
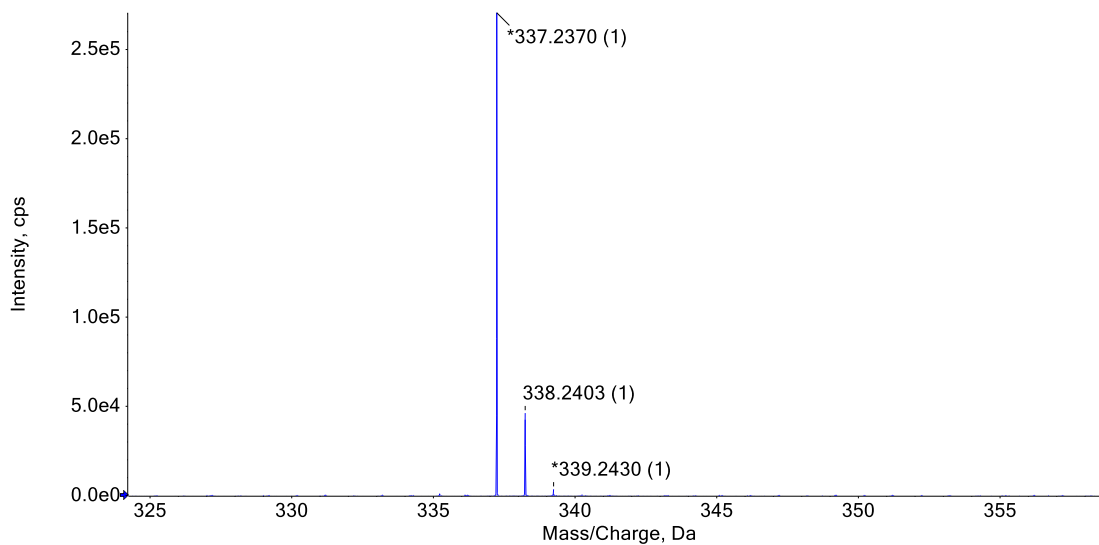


Figure S52. The (+)-HRESIMS spectrum of **6**.

Spectrum from XYZW-43.wiff2 (sample 1) - XYZW-43, +TOF MS (100 - 1000) from 1.406 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
337.2370	337.2373	-0.3	-0.9	C ₂₀ H ₃₃ O ₄	[M+H] ⁺

Figure S53. The IR spectrum of **6**.

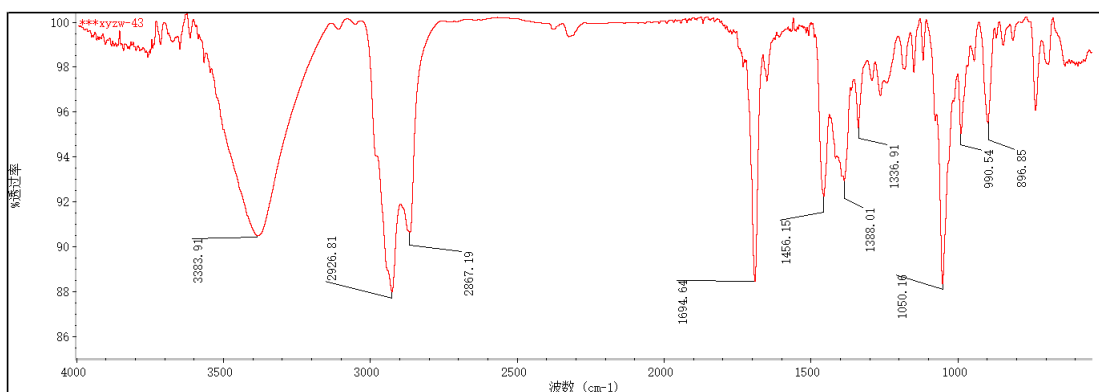


Figure S56. The ^1H - ^1H COSY spectrum of **7** in CD_3OD .

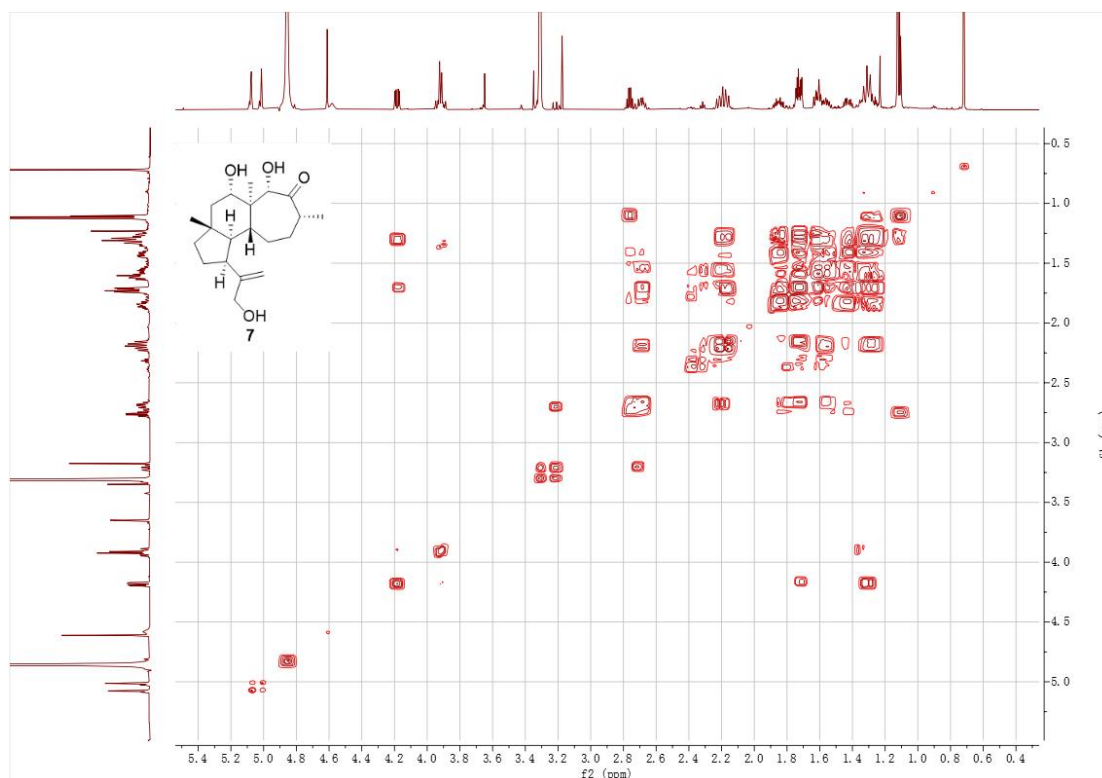


Figure S57. The HSQC spectrum of **7** in CD_3OD .

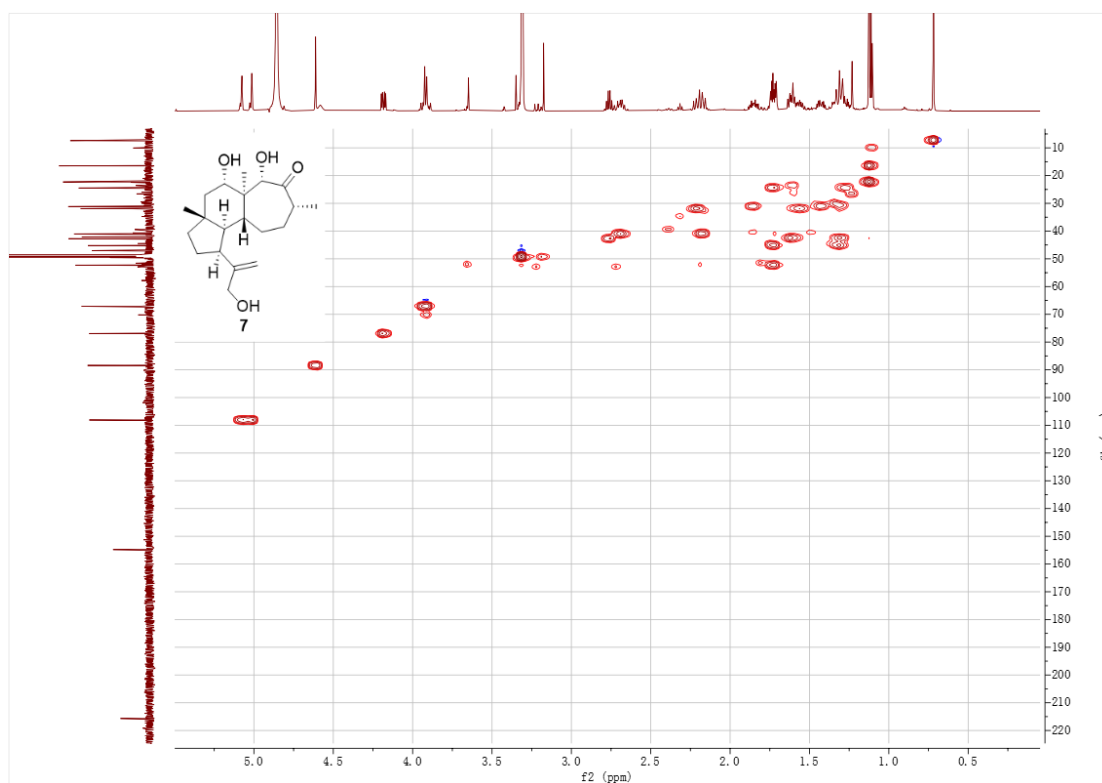


Figure S58. The HMBC spectrum of **7** in CD₃OD.

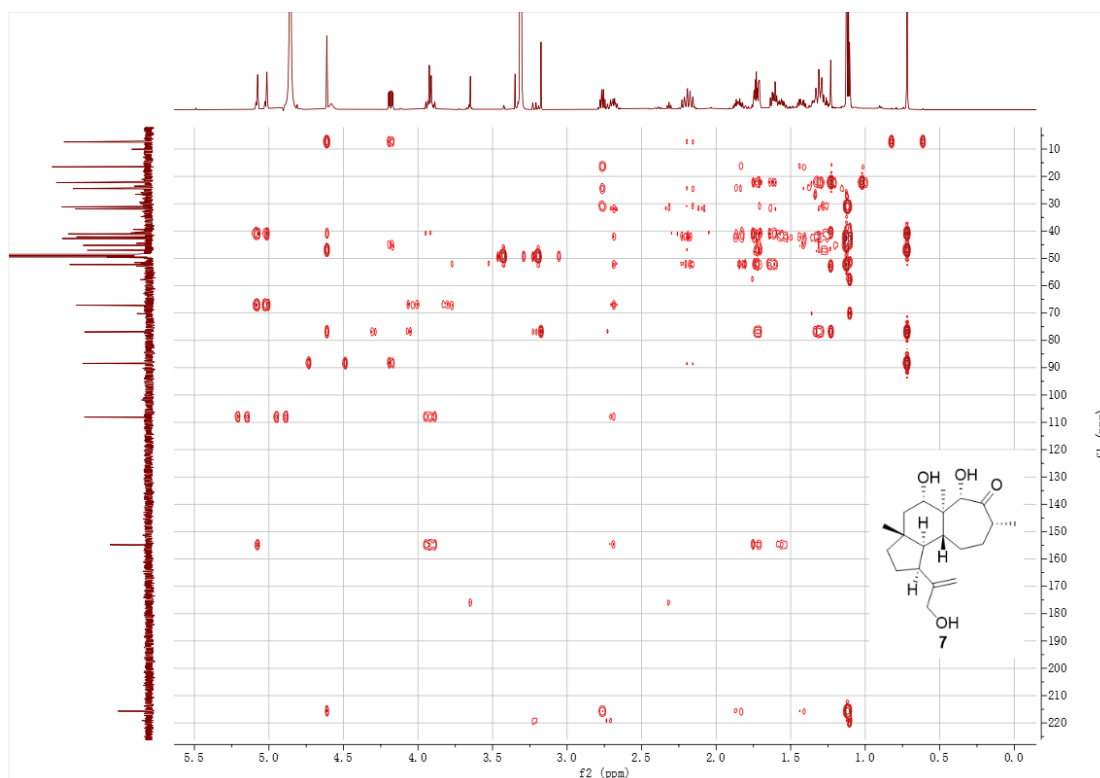


Figure S59. The NOESY spectrum of **7** in CD₃OD.

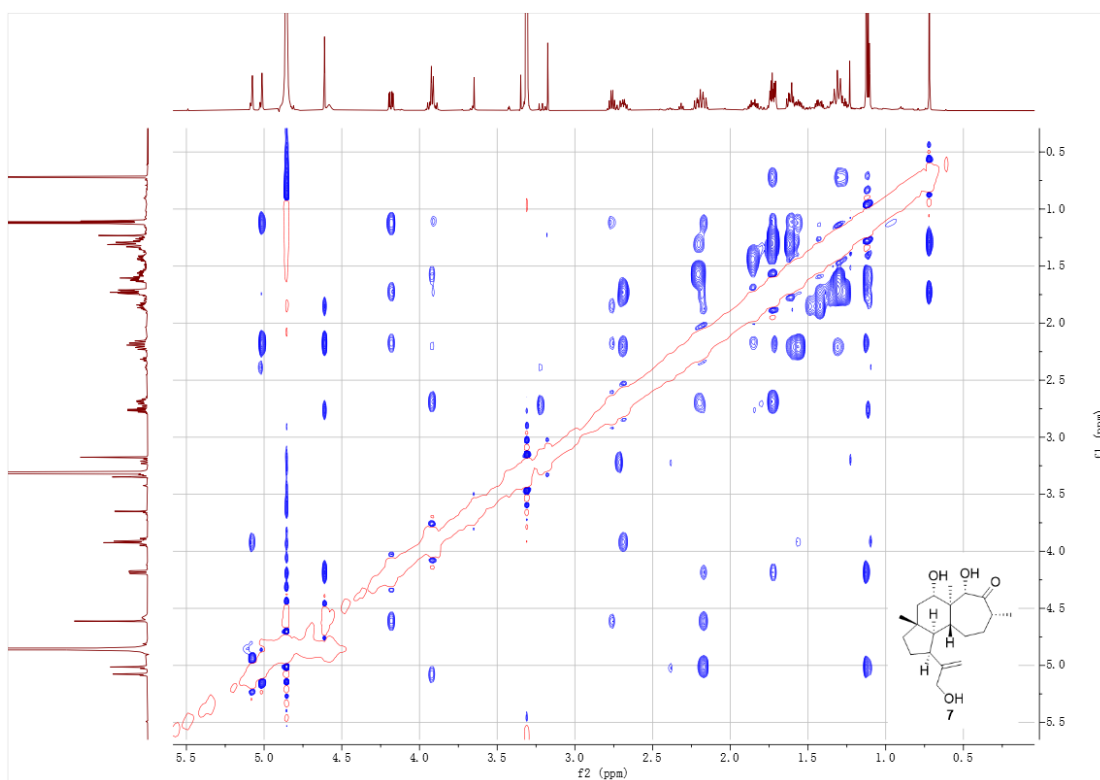
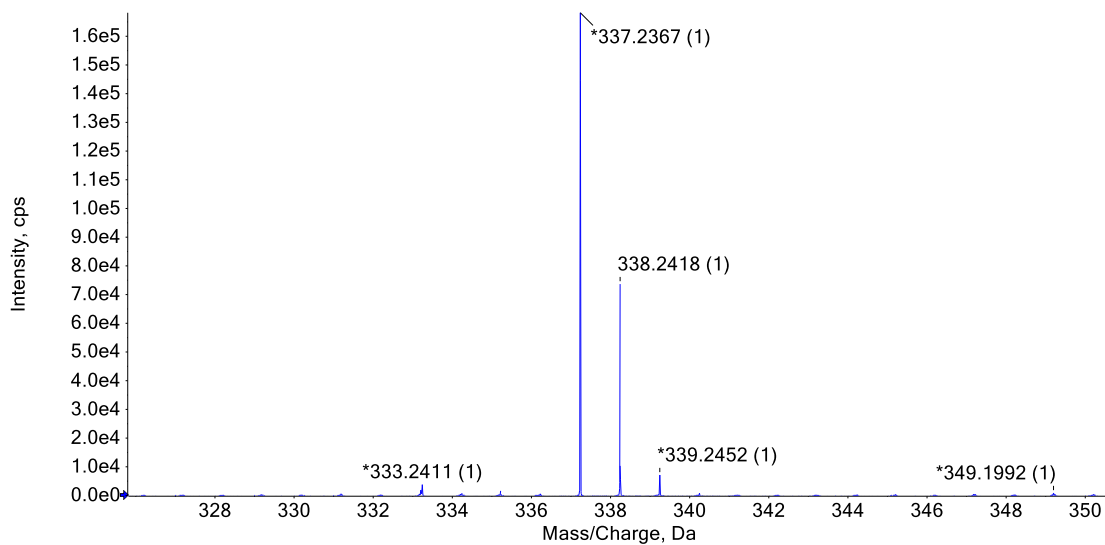


Figure S60. The (+)-HRESIMS spectrum of **7**.

Spectrum from XYZW-42.wiff2 (sample 1) - XYZW-42, +TOF MS (100 - 1000) from 1.394 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
337.2367	337.2373	-0.6	-1.8	C ₂₀ H ₃₃ O ₄	[M+H] ⁺

Figure S61. The IR spectrum of **7**.

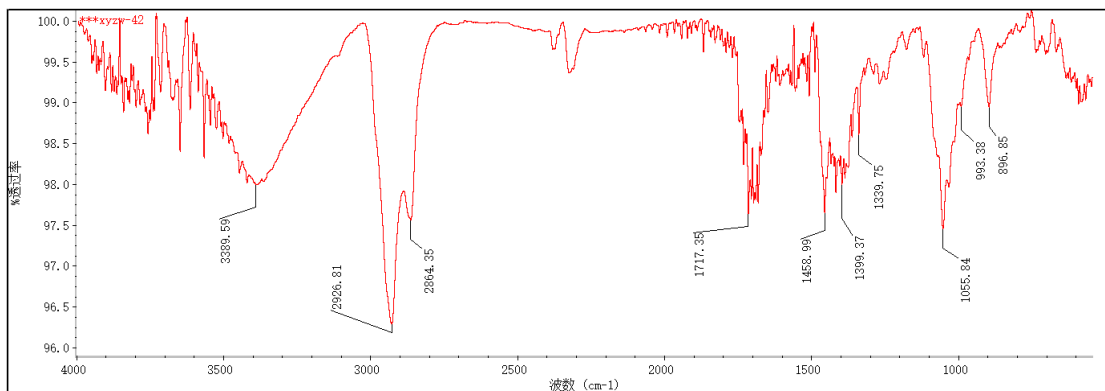


Figure S64. The ^1H - ^1H COSY spectrum of **8** in CD_3OD .

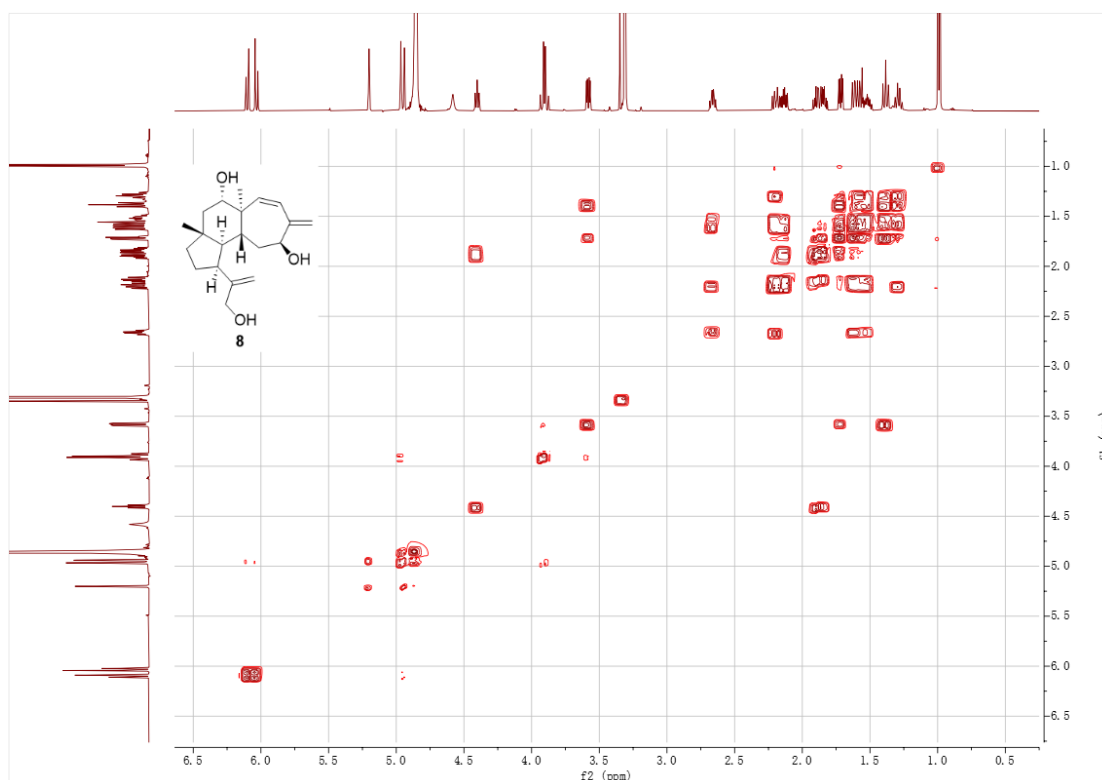


Figure S65. The HSQC spectrum of **8** in CD_3OD .

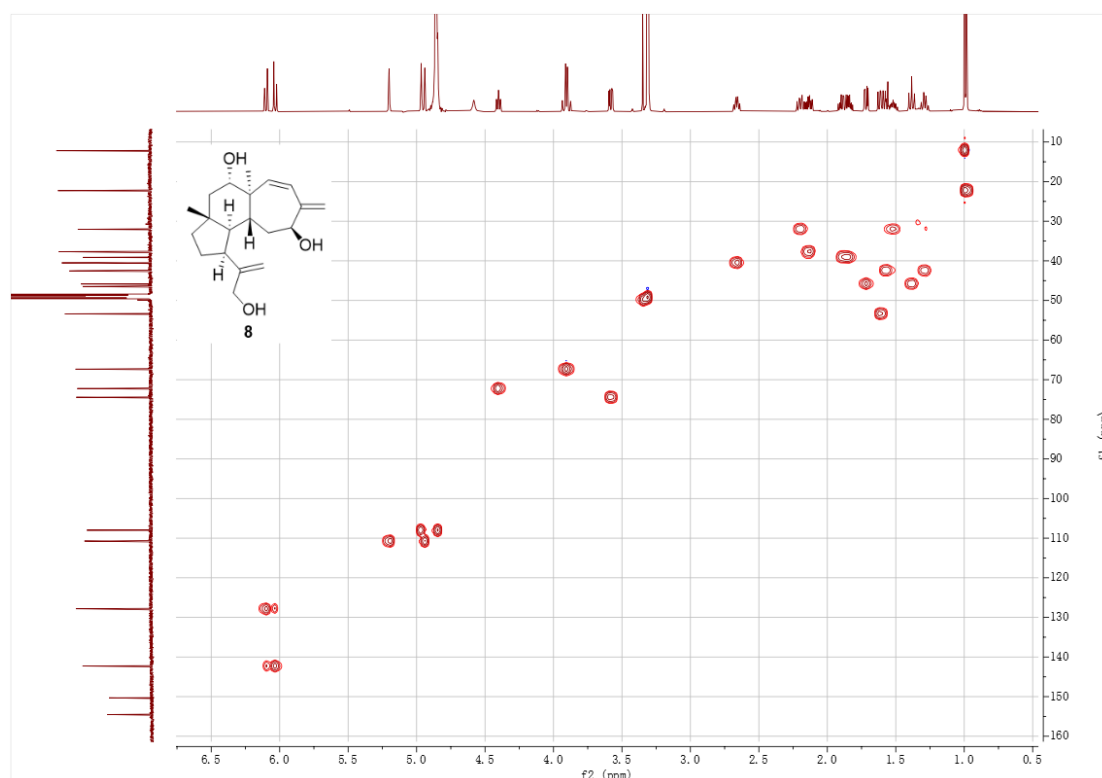


Figure S66. The HMBC spectrum of **8** in CD₃OD.

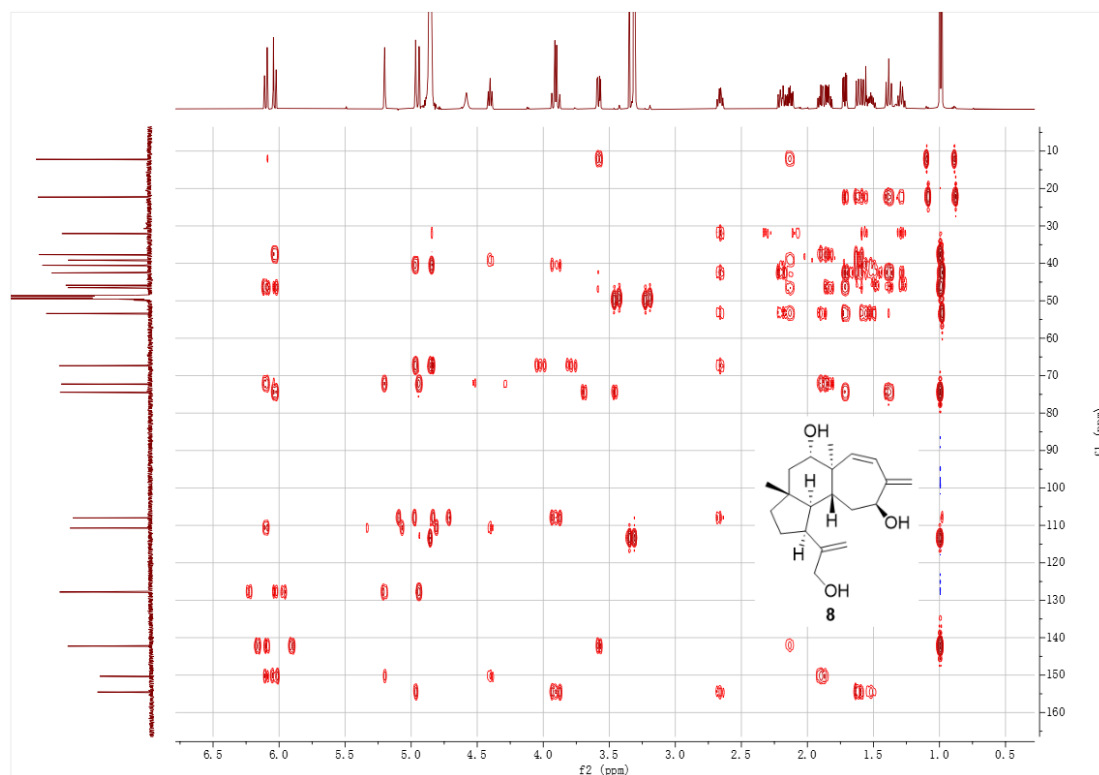


Figure S67. The NOESY spectrum of **8** in CD₃OD.

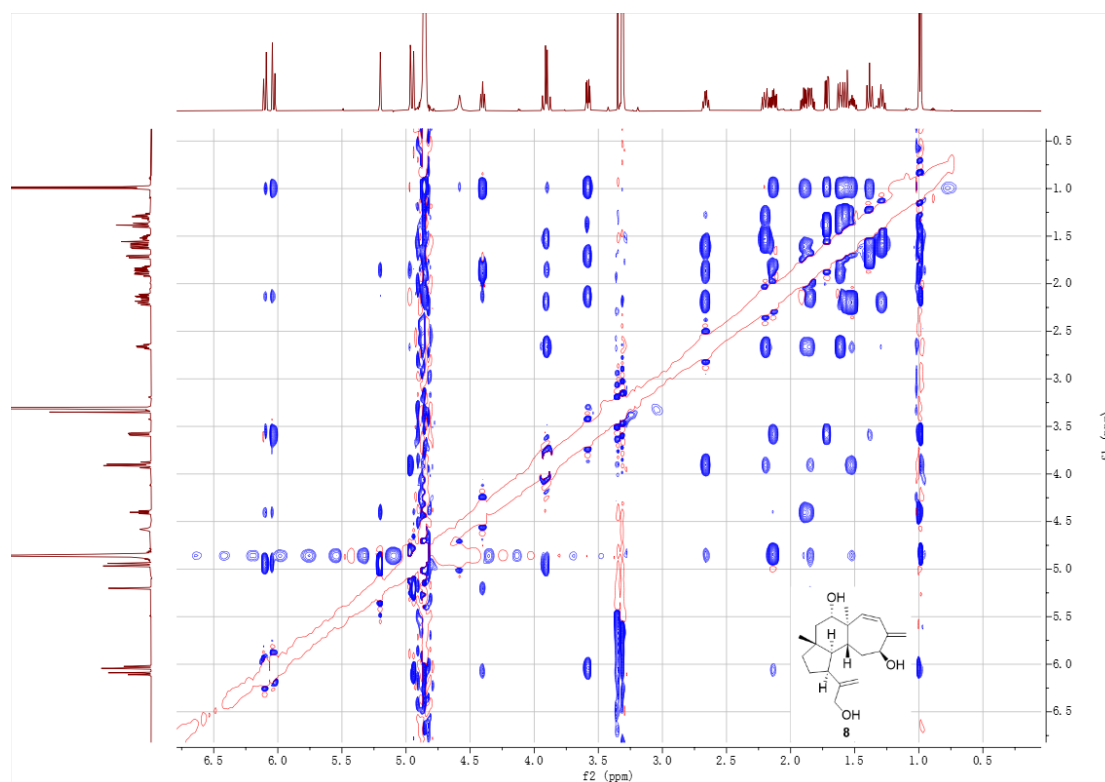
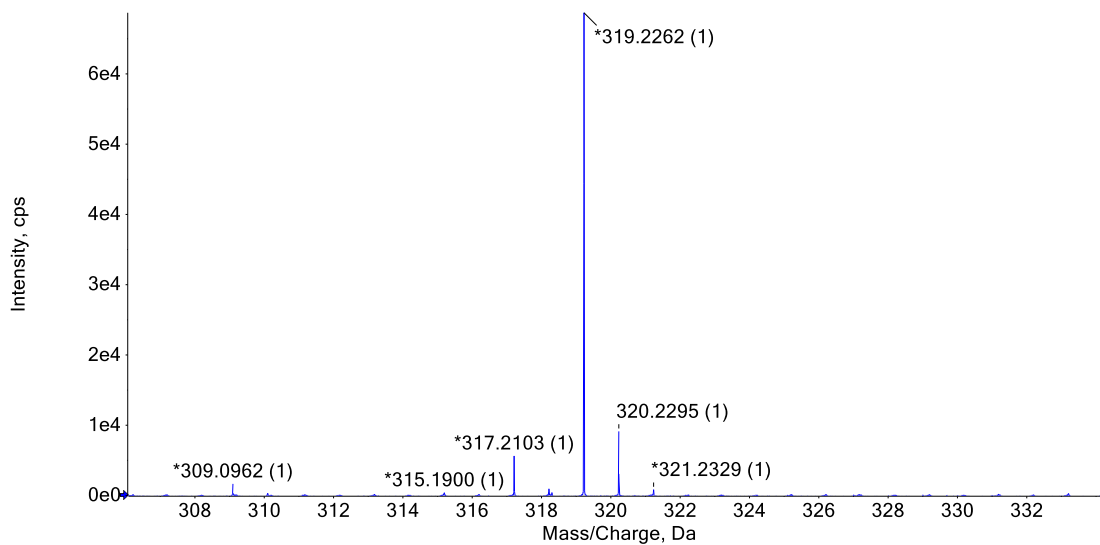


Figure S68. The (+)-HRESIMS spectrum of **8**.

Spectrum from XYZW-19.wiff2 (sample 1) - XYZW-19, +TOF MS (100 - 1000) from 1.370 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
319.2262	319.2267	-0.5	-1.7	C ₂₀ H ₃₁ O ₃	[M+H] ⁺

Figure S69. The IR spectrum of **8**.

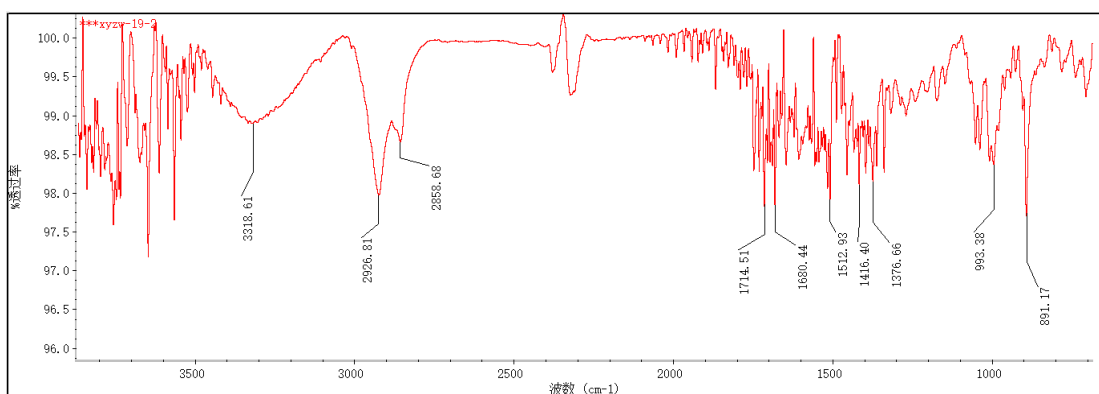


Figure S70. The ^1H NMR spectrum of **9** in CD_3OD .

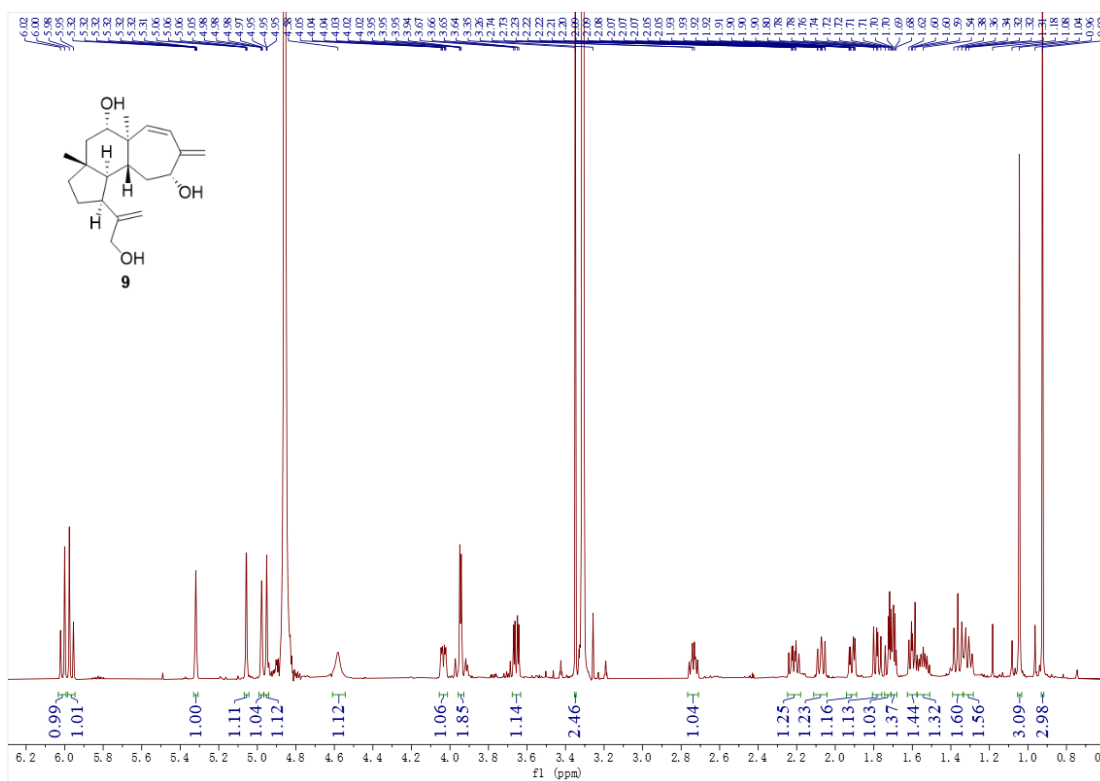


Figure S71. The ^{13}C NMR and DEPT spectrum of **9** in CD_3OD .

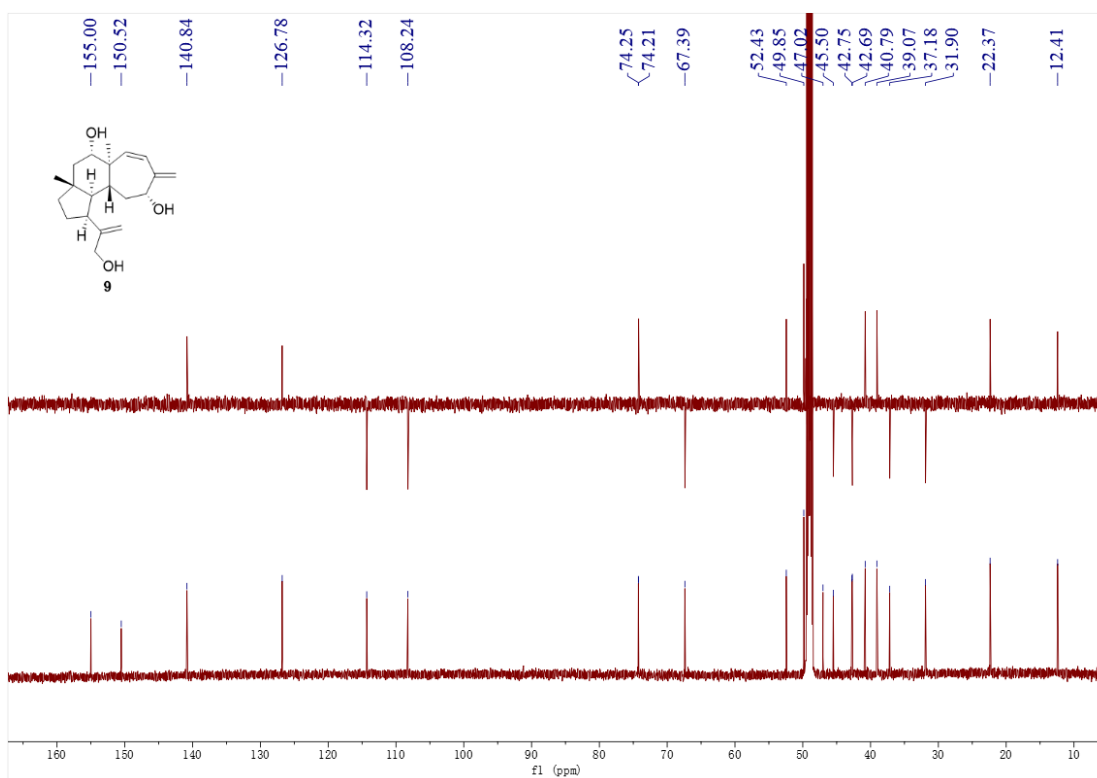


Figure S72. The ^1H - ^1H COSY spectrum of **9** in CD_3OD .

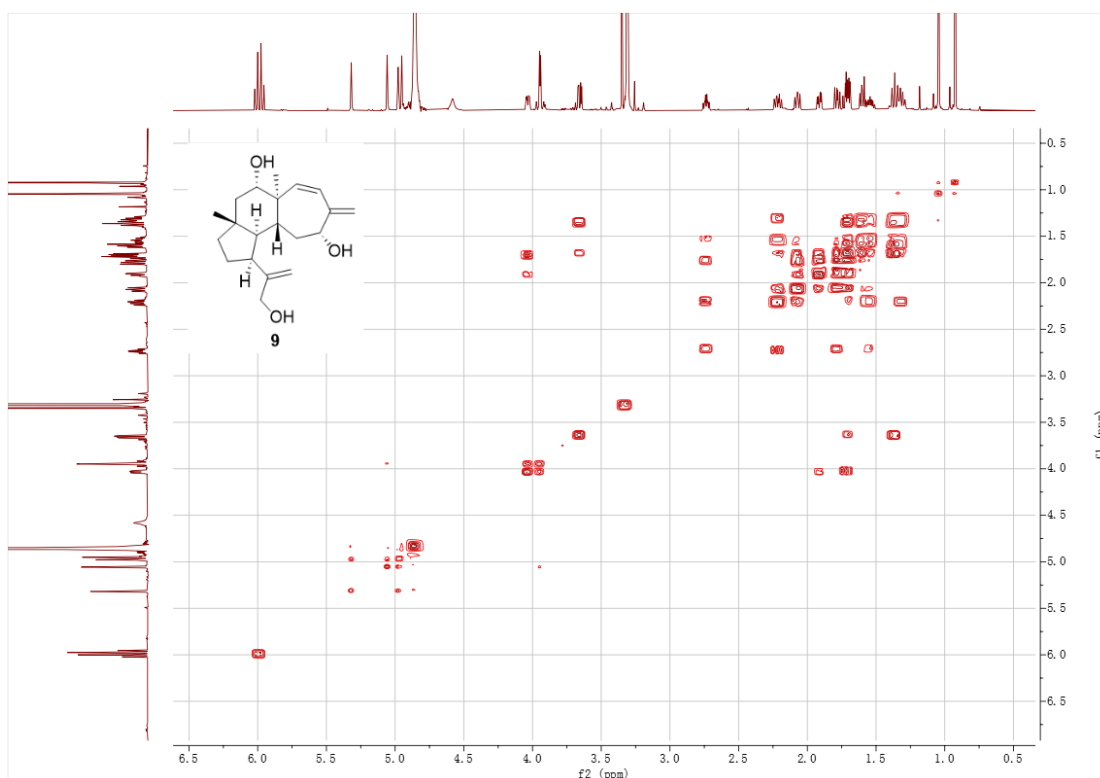


Figure S73. The HSQC spectrum of **9** in CD_3OD .

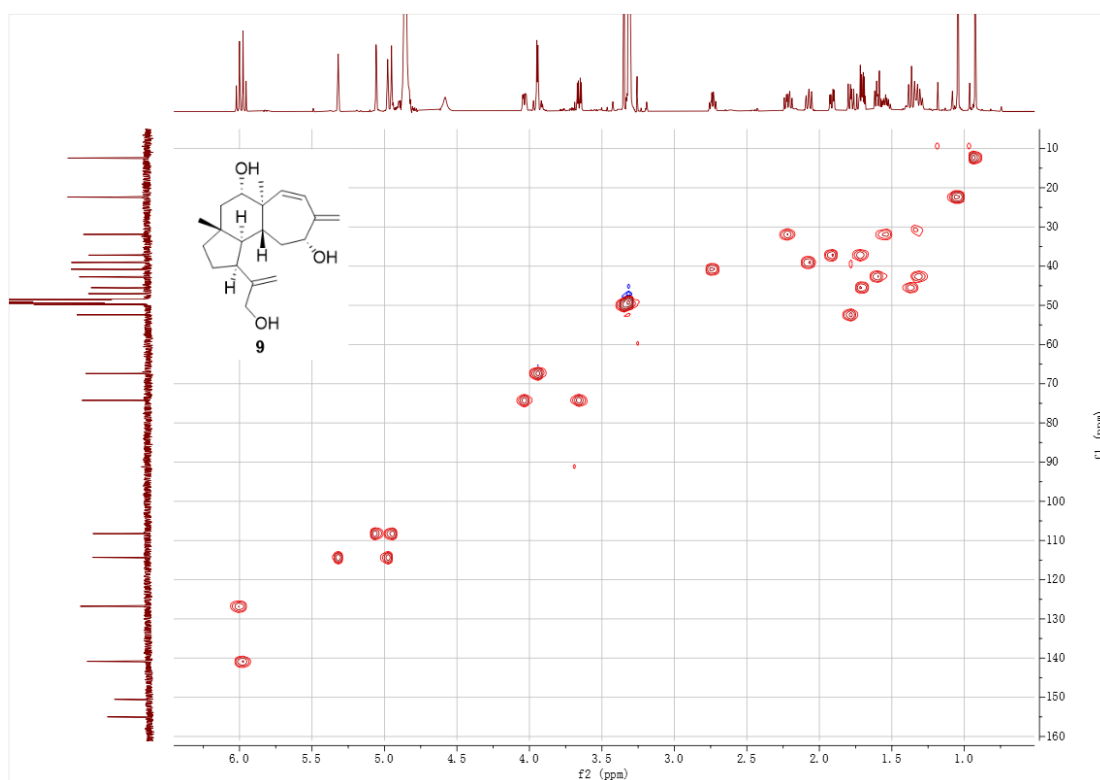


Figure S74. The HMBC spectrum of **9** in CD₃OD.

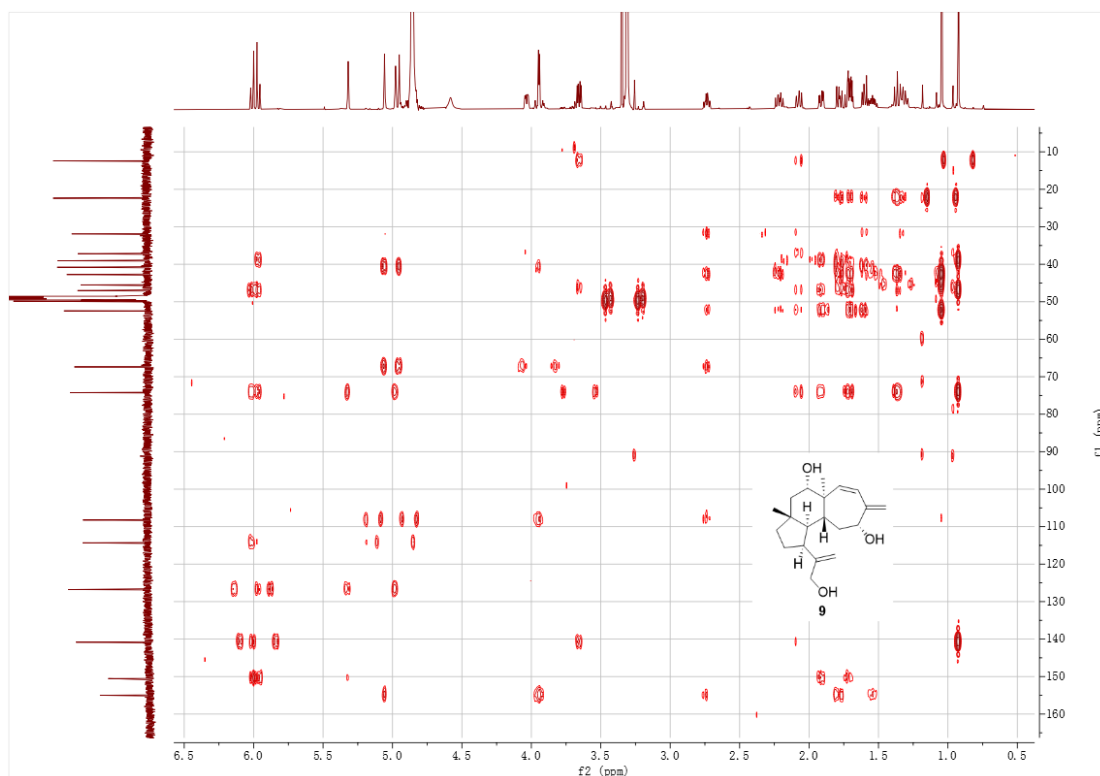


Figure S75. The NOESY spectrum of **9** in CD₃OD.

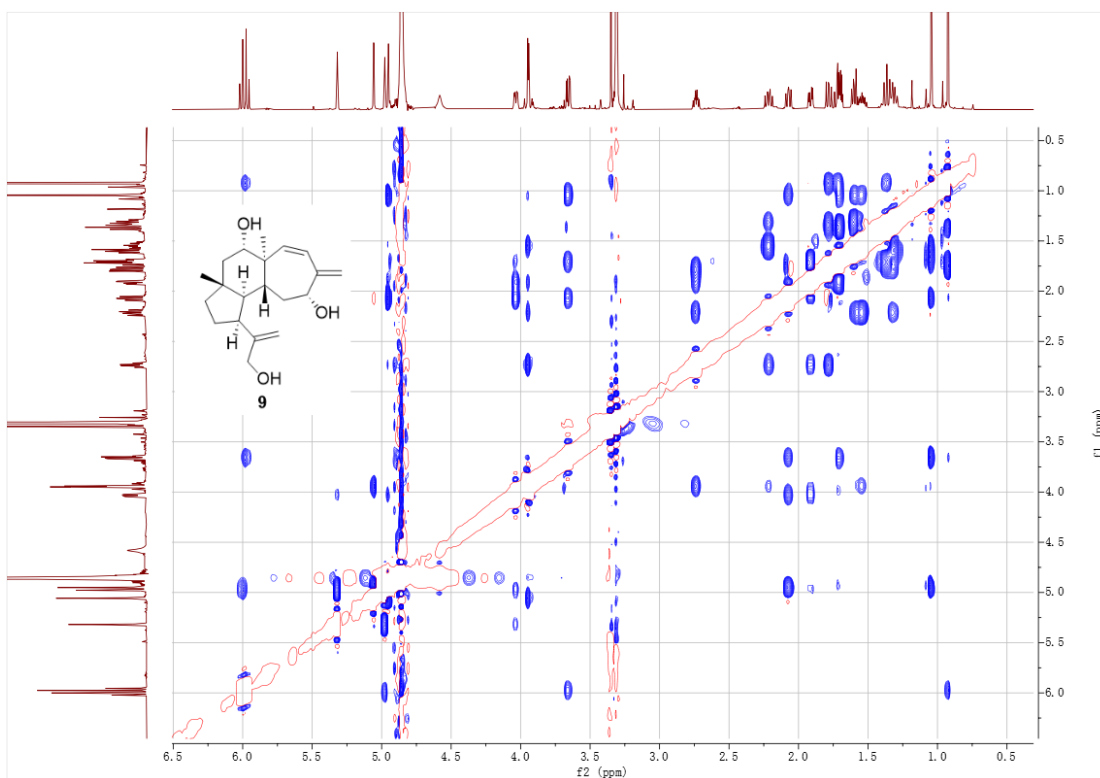
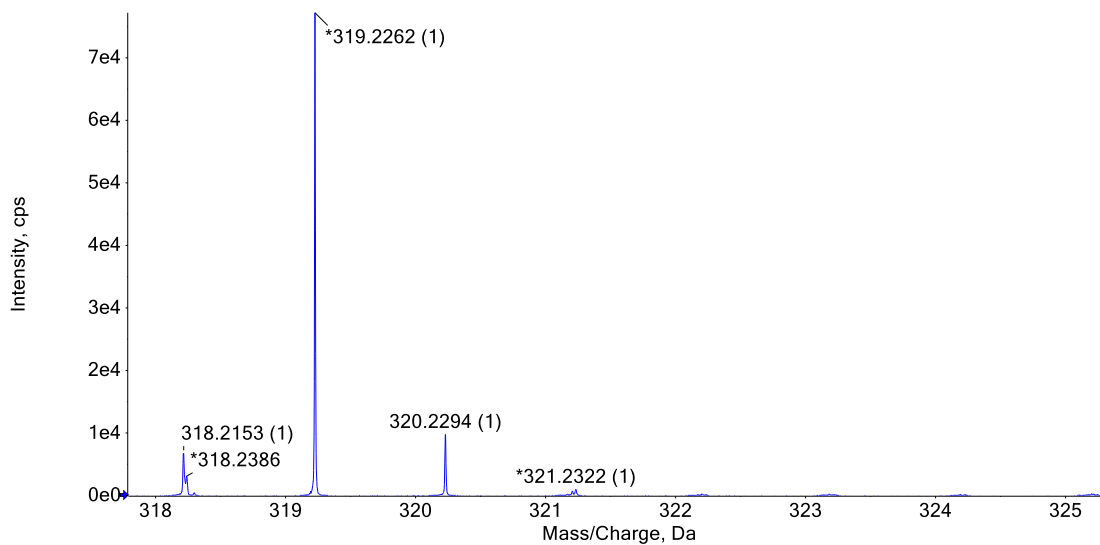


Figure S76. The (+)-HRESIMS spectrum of **9**.

Spectrum from XYZW-18.wiff2 (sample 1) - XYZW-18, +TOF MS (100 - 1000) from 1.358 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
319.2262	319.2267	-0.5	-1.6	C ₂₀ H ₃₁ O ₃	[M+H] ⁺

Figure S77. The IR spectrum of **9**.

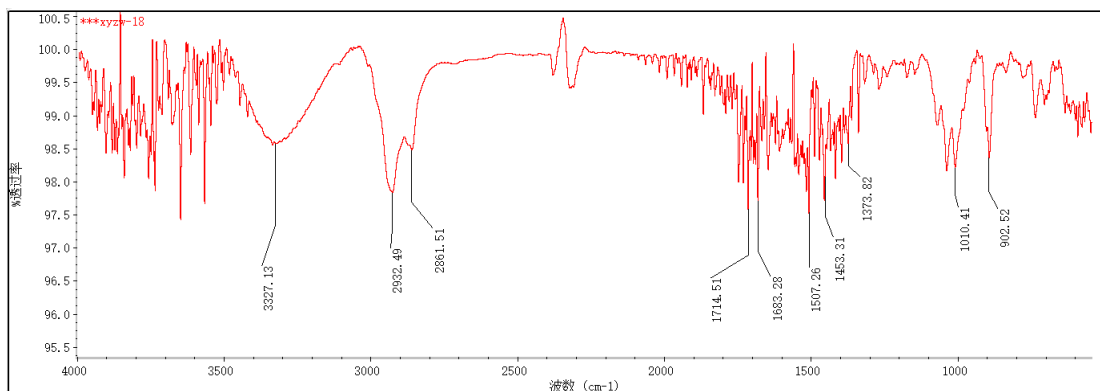


Figure S78. The ^1H NMR spectrum of **10** in CD_3OD .

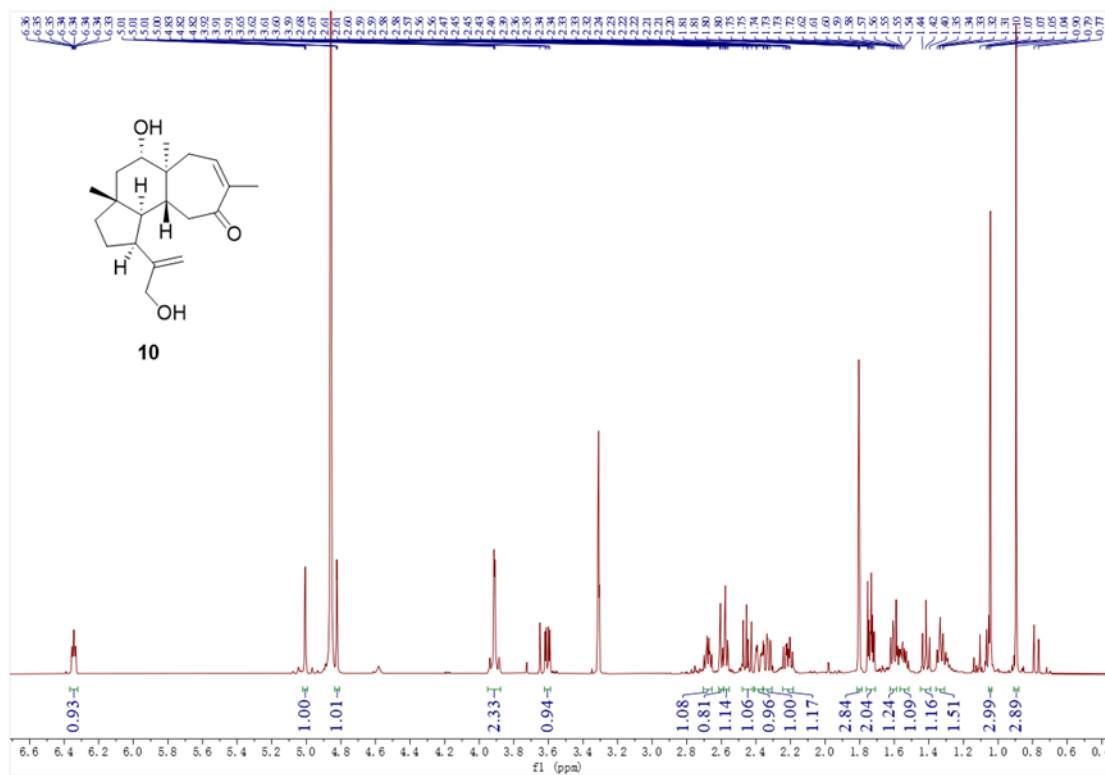


Figure S79. The ^{13}C NMR and DEPT spectrum of **10** in CD_3OD .

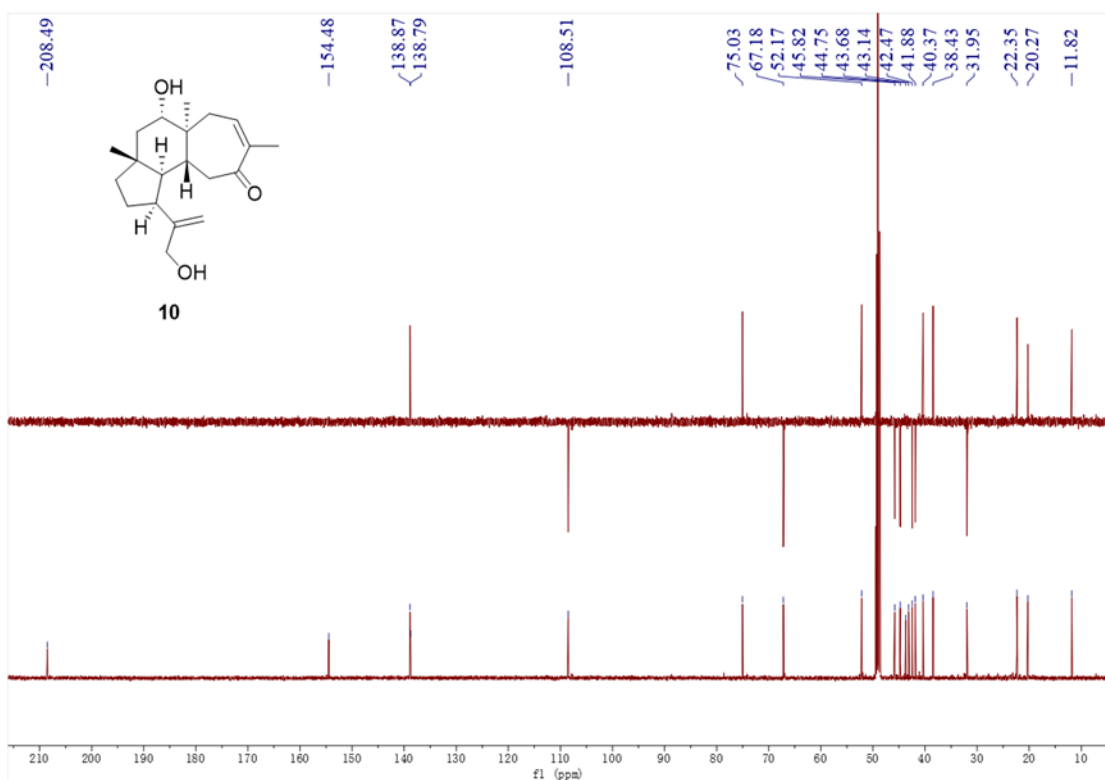


Figure S80. The ^1H - ^1H COSY spectrum of **10** in CD_3OD .

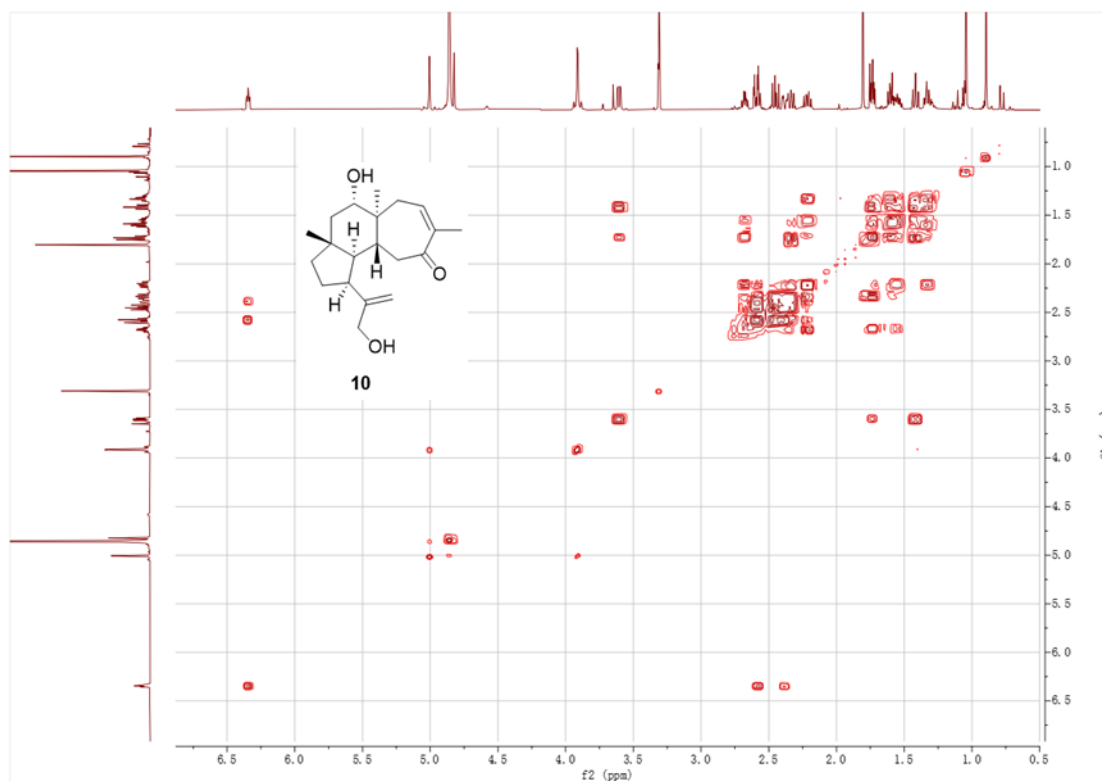


Figure S81. The HSQC spectrum of **10** in CD_3OD .

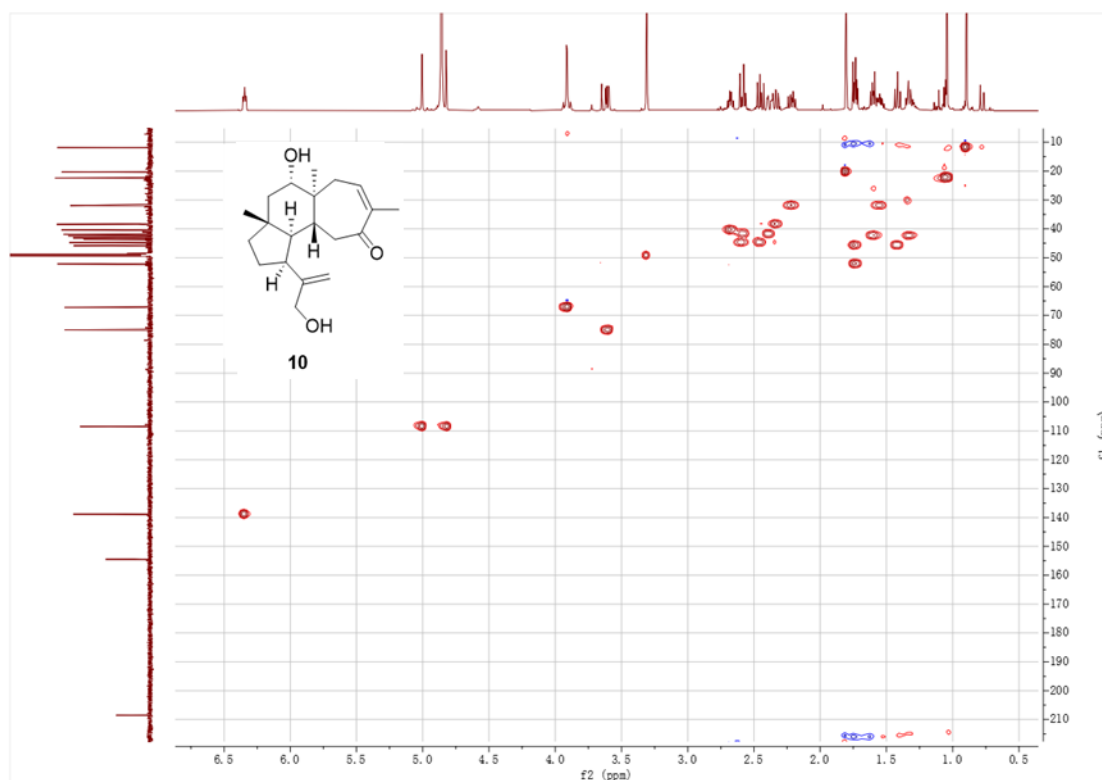


Figure S82. The HMBC spectrum of **10** in CD₃OD.

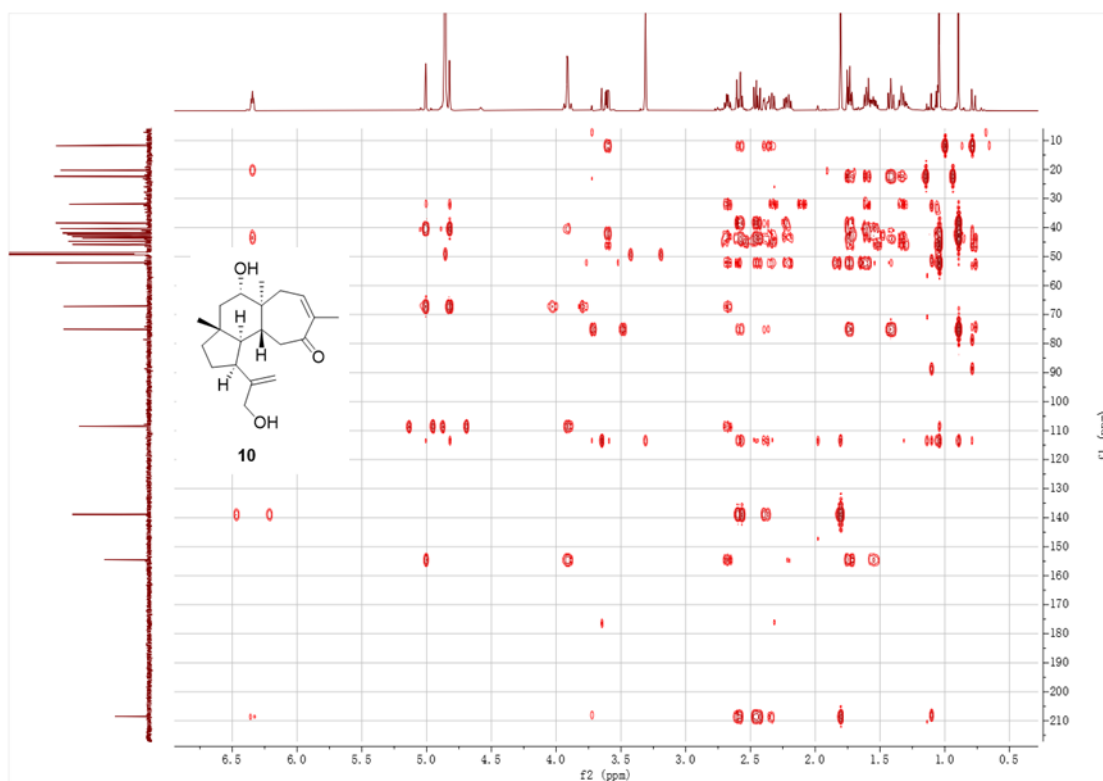


Figure S83. The NOESY spectrum of **10** in CD₃OD.

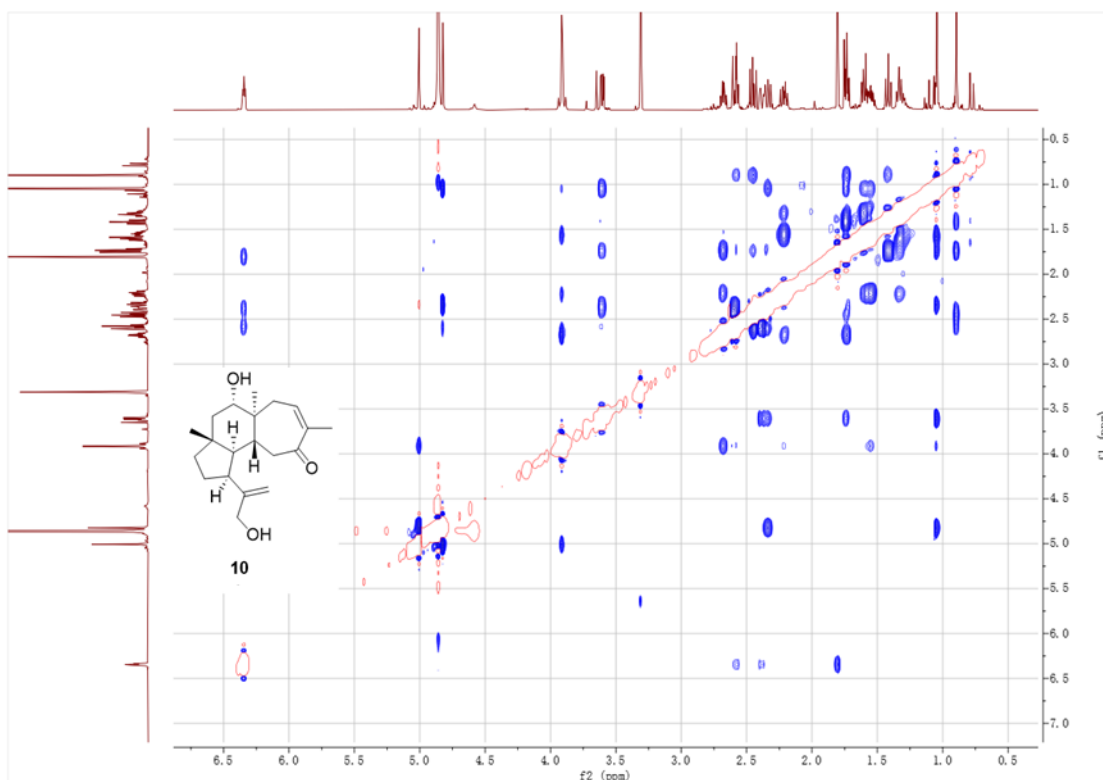
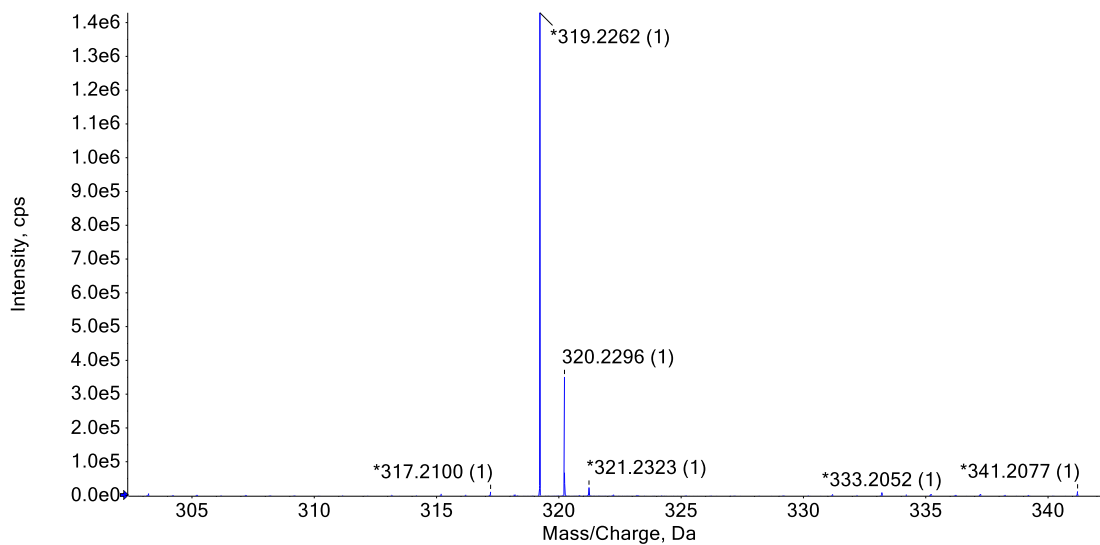


Figure S84. The (+)-HRESIMS spectrum of **10**.

Spectrum from XYZW-30.wiff2 (sample 1) - XYZW-30, +TOF MS (100 - 1000) from 1.358 min



Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
319.2262	319.2267	-0.5	-1.8	C ₂₀ H ₃₁ O ₃	[M+H] ⁺

Figure S85. The IR spectrum of **10**.

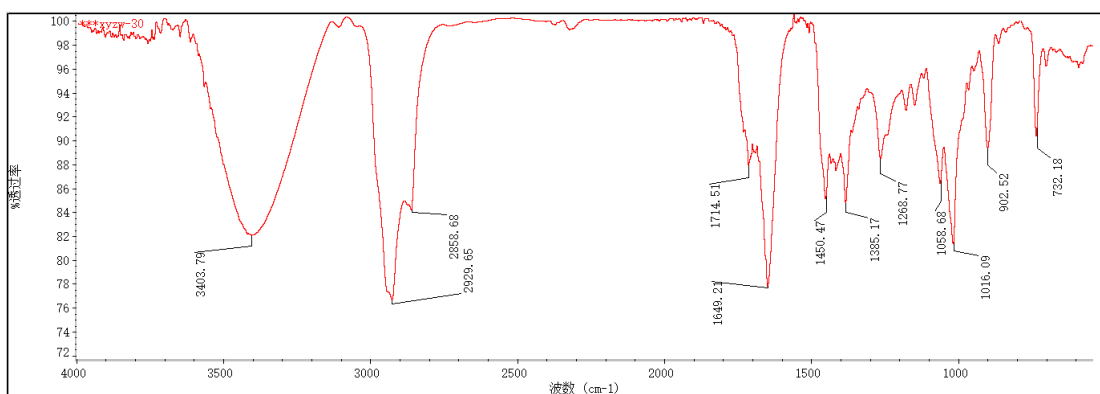
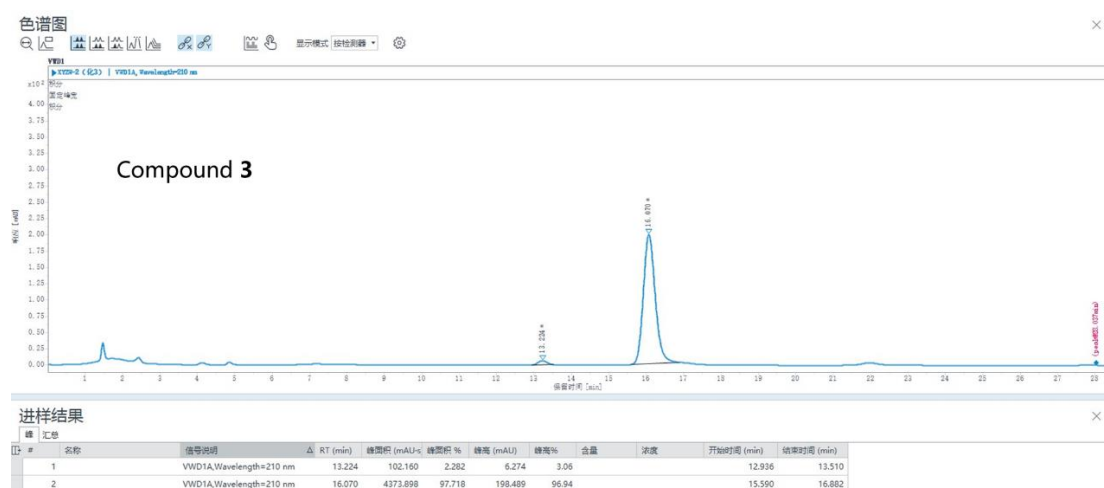
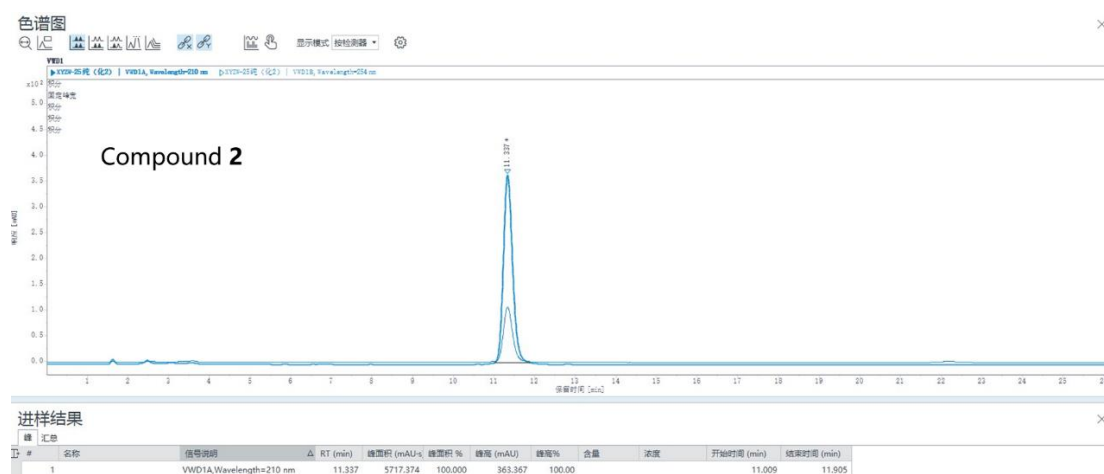
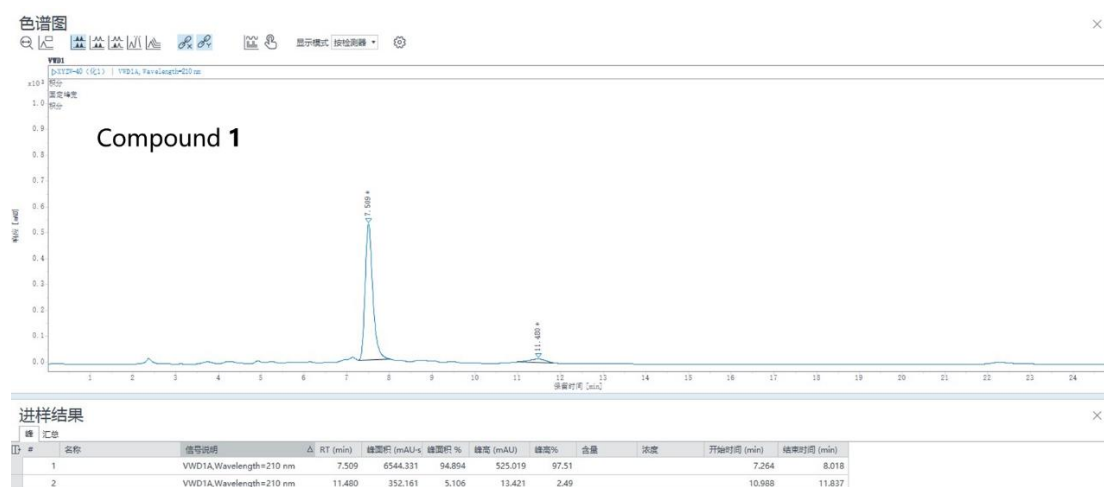
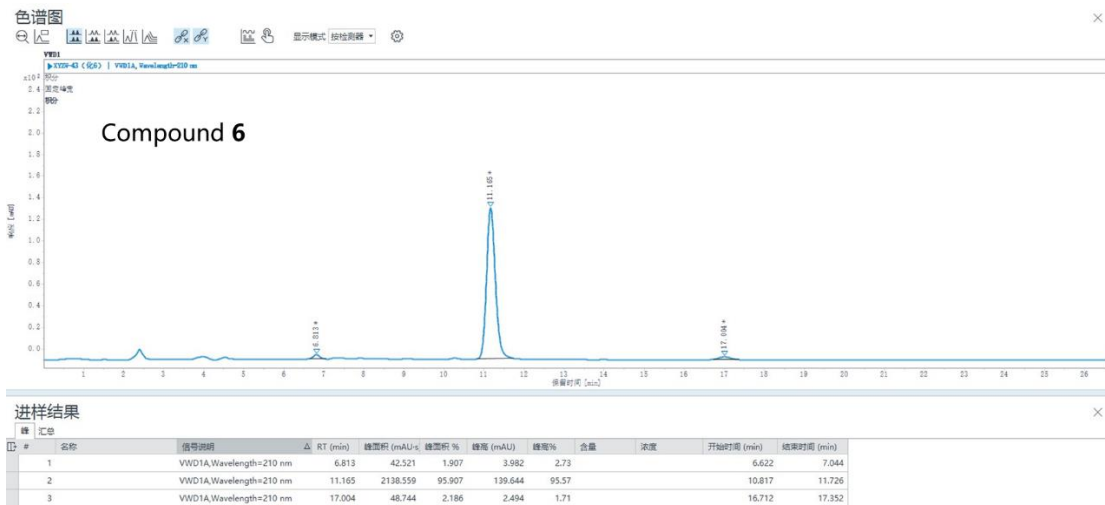
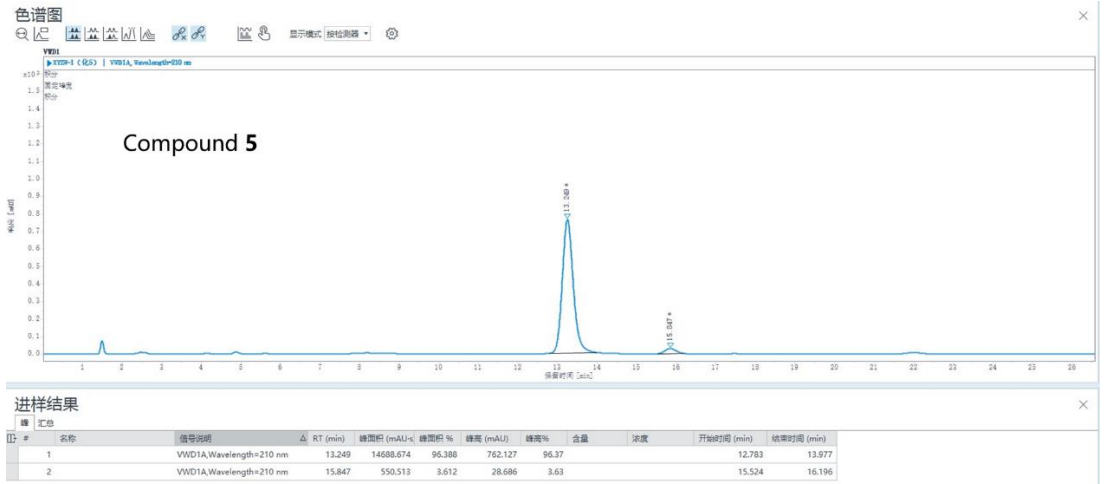
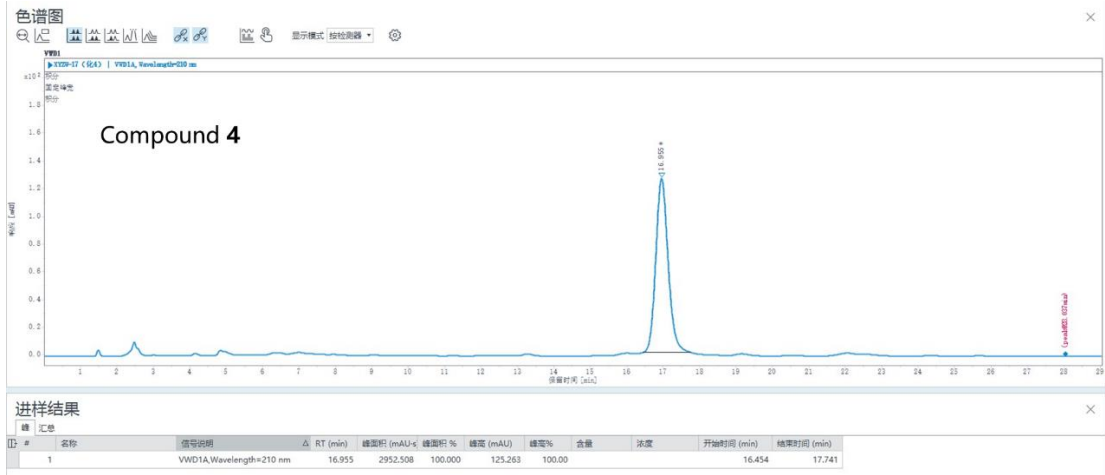


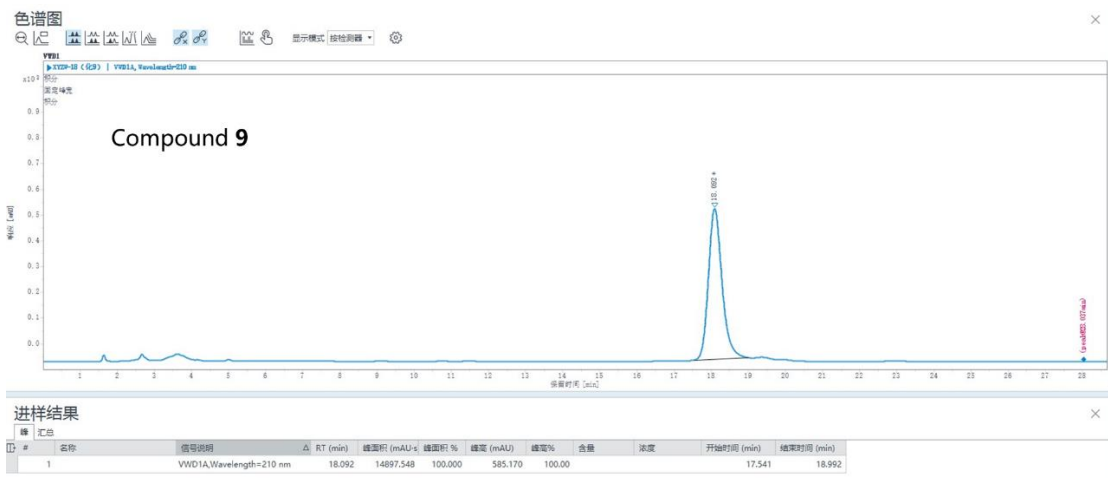
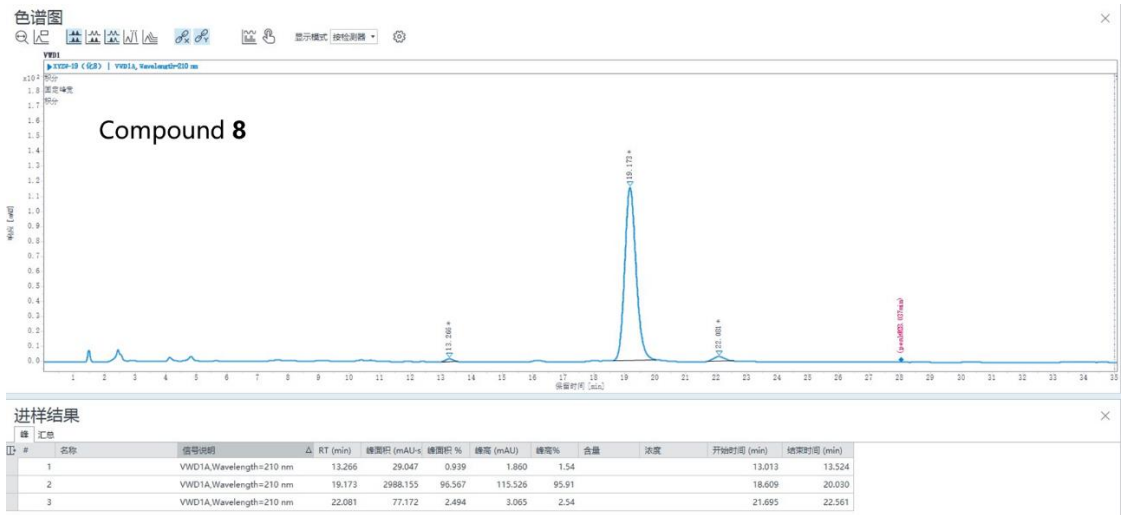
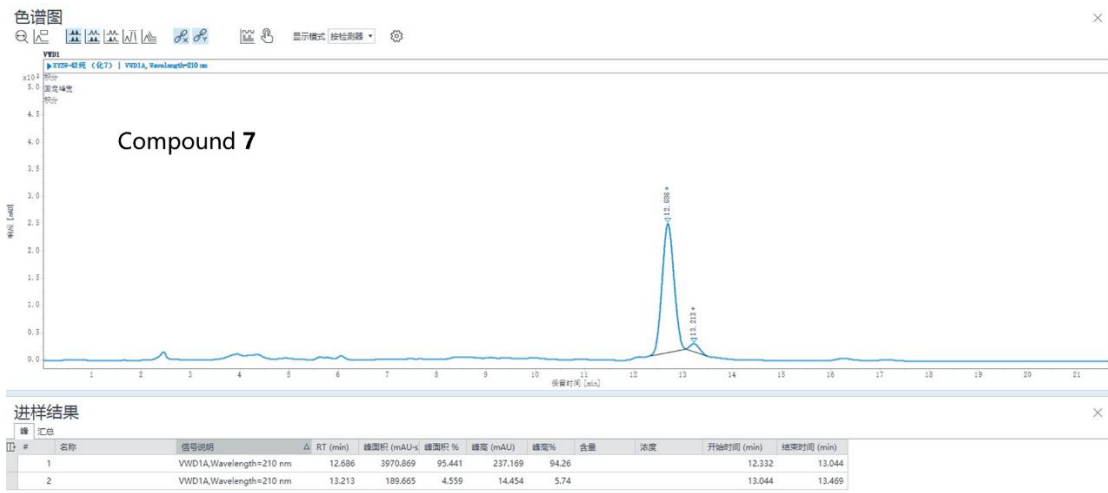
Figure S86. DP4+ detailed results of 7.

Functional mPW1PW91		Solvent? PCM		Basis Set 6-31+G(d,p)	
		DP4+	0.00%	100.00%	-
Nuclei	sp2?	Experiments	Isomer 1	Isomer 2	Isomer 3
C		45.2	45.8	45.5	
C		42.1	45.0	44.9	
C		52.3	55.7	54.3	
C		41	38.7	37.5	
C		47	50.4	49.8	
C		76.9	76.1	79.4	
C		24.5	30.5	27.4	
C		31.2	29.6	34.4	
C		42.7	50.9	45.8	
C	x	215.7	218.0	218.7	
C		88.4	88.4	91.3	
C		42.6	43.88	44.08	
C		31.9	34.08	36.25	
C		41.1	41.39	43.39	
C		7.4	9.41	7.57	
C		22.3	24.24	23.80	
C	x	154.8	158.78	159.45	
C		67.1	71.85	69.14	
C	x	108.1	109.08	103.23	
C		16.5	18.85	18.18	
H		1.73	1.71	1.65	
H		1.33	1.25	1.11	
H		1.73	1.52	1.76	
H		2.17	2.37	2.18	
H		4.18	4.33802462	4.23284495	
H		1.26	2.01930891	1.04988099	
H		1.73	1.25777024	1.15341173	
H		1.43	1.59865451	1.05175728	
H		1.85	1.71093915	1.68011971	
H		2.76	2.75502117	3.02265443	
H		4.61	4.59197747	4.42877673	
H		1.63	1.57126245	1.58519638	
H		1.31	1.25202199	1.28539516	
H		2.21	2.21900762	2.140571	
H		1.56	1.43111004	1.48869761	
H		2.69	3.26571894	2.31422671	
H		0.72	0.69	0.69834428	
H		1.12	1.06	1.10898156	
H		3.92	3.97586356	4.16119126	
H		3.92	4.09252068	3.92943446	
H		5.08	5.24528967	5.49520245	
H		5.01	5.36363782	5.31704247	
H		1.12	1.23	1.00917787	

Figure S87. HPLC spectra and purities of compounds 1–15.







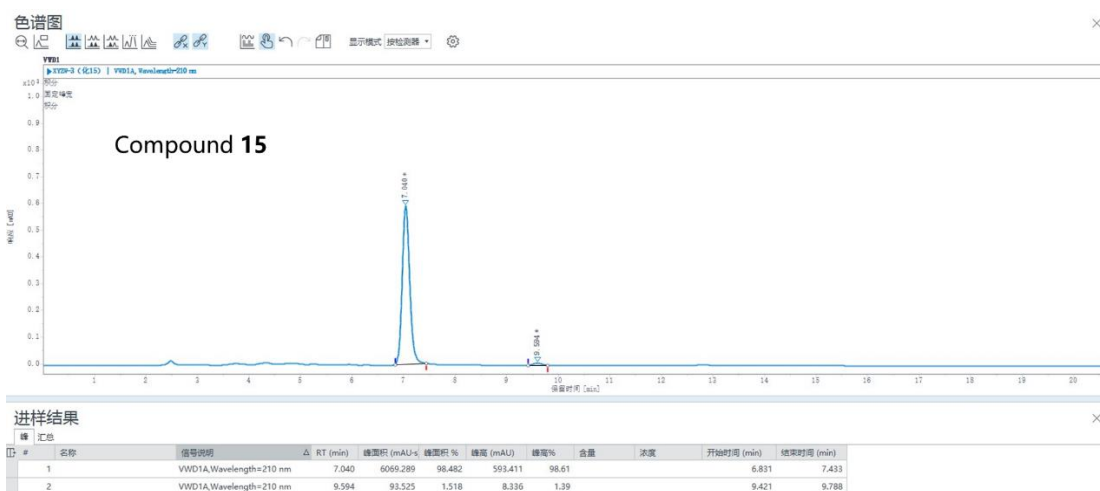
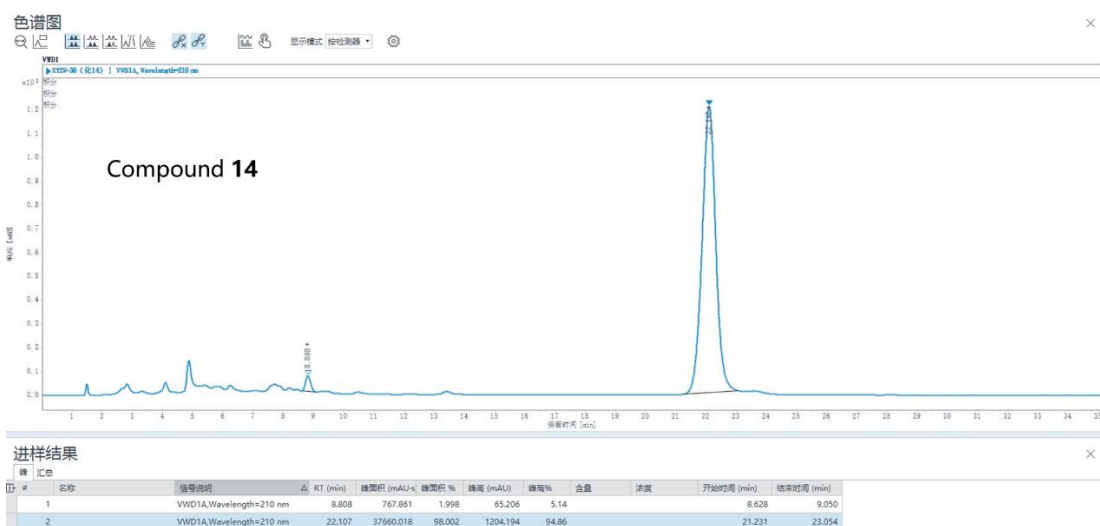
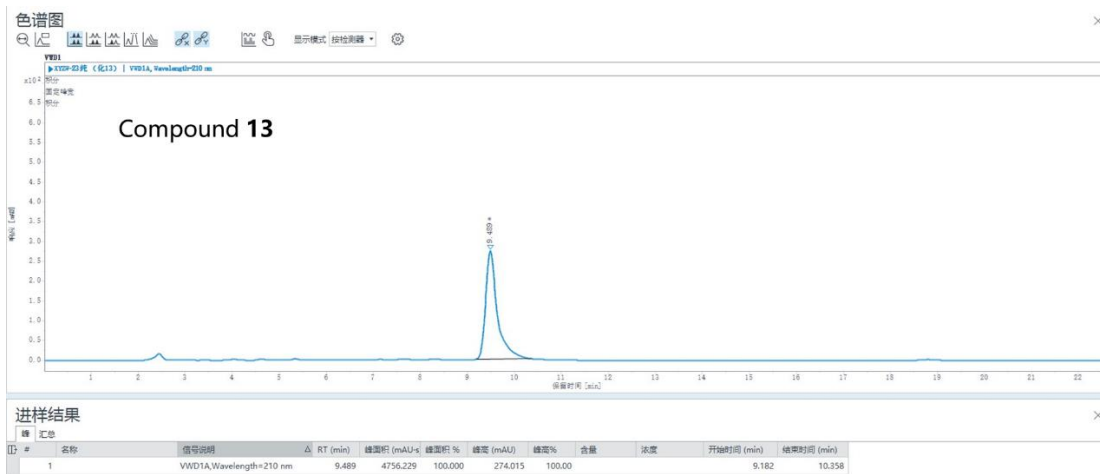


Table S1. Re-optimized conformers, energies and proportions for **1**.

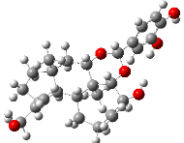
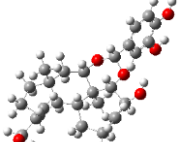
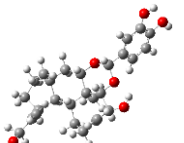
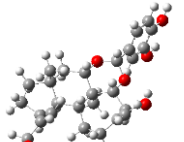
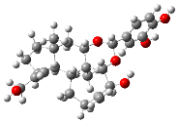
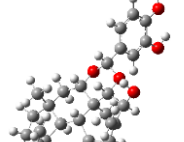
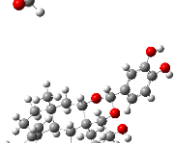
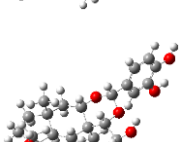
Number	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1501.448498	-942173.0326	35.29
2		-1501.448104	-942172.7854	23.24
3		-1501.448087	-942172.7747	22.83
4		-1501.447525	-942172.422	12.58
5		-1501.44649	-942171.7726	4.20
6		-1501.445022	-942170.8514	0.89
7		-1501.444654	-942170.6205	0.60
8		-1501.4442	-942170.3356	0.37

Table S2. Re-optimized conformers, energies and proportions for **2**.


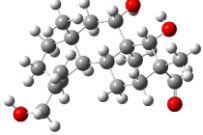
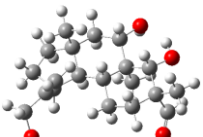
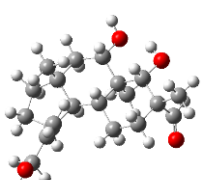

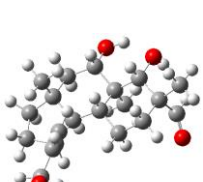
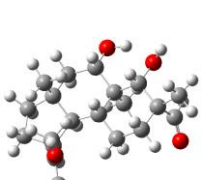
Number	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1081.927937	-678919.9409	45.11
2		-1081.927326	-678919.5574	23.61
3		-1081.927025	-678919.3686	17.16
4		-1081.926398	-678918.9751	8.83
5		-1081.925745	-678918.5654	4.42
6		-1081.924041	-678917.4961	0.73
7		-1081.922596	-678916.5893	0.16

Table S3. Re-optimized conformers, energies and proportions for **4**.

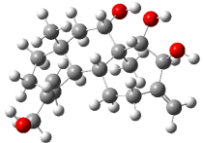
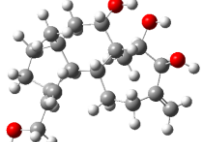

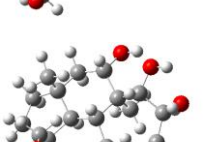
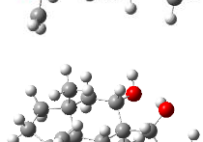
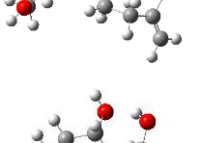
Number	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1081.895141	-678899.3611	86.57
2		-1081.892482	-678897.6925	5.17
3		-1081.89228	-678897.5658	4.17
4		-1081.892116	-678897.4628	3.50
5		-1081.890423	-678896.4005	0.58
6		-1081.886496	-678893.9362	0.01

Table S4. Re-optimized conformers, energies and proportions for **6**.

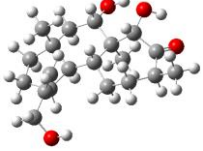
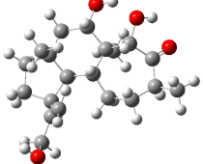
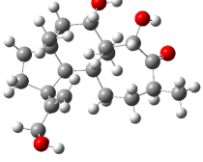
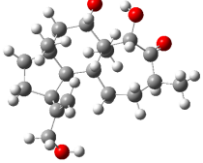

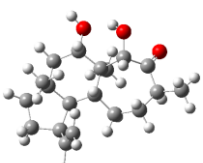
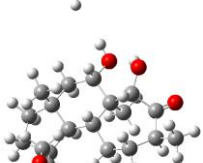
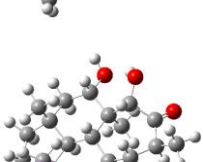
Number	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1081.931903	-678922.4296	53.29
2		-1081.931269	-678922.0317	27.21
3		-1081.930953	-678921.8334	19.47
4		-1081.924342	-678917.685	0.02
5		-1081.923976	-678917.4553	0.01
6		-1081.922774	-678916.701	0
7		-1081.921756	-678916.0622	0
8		-1081.921615	-678915.9737	0

Table S5. mPW1PW91/6-31+G** reoptimized of **12R*-7**.

	<i>G</i> (kcal/mol)	ΔG (kcal/mol)	Boltzmann factor	Equilibrium mole fraction	Imaginary frequency
12R*-7-c1	-678917.6686	0	1	0.997549748	0
12R*-7-c2	-678913.8076	3.861065283	0.001467837	0.001464241	0
12R*-7-c3	-678913.5195	4.149092093	0.000902232	0.000900022	0
12R*-7-c4	-678911.8918	5.776851454	0.000057655	0.000057514	0
12R*-7-c5	-678911.4758	6.192890180	0.000028546	0.000028476	0

Table S6. mPW1PW91/6-31+G** reoptimized of **12S*-7**.

	<i>G</i> (kcal/mol)	ΔG (kcal/mol)	Boltzmann factor	Equilibrium mole fraction	Imaginary frequency
12S*-7-c1	-678915.7579	0	1	0.934814500	0
12S*-7-c2	-678913.6739	2.083958687	0.029563241	0.027636146	0
12S*-7-c3	-678913.5628	2.195027850	0.024504588	0.022907245	0
12S*-7-c4	-678913.1738	2.584083672	0.012698457	0.011870702	0
12S*-7-c5	-678912.3128	3.445026557	0.002964660	0.002771407	0