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**Biological and Chemical Guided Isolation of
3,4-Secograyanane Diterpenoids from the Roots of
*Pieris formosa***

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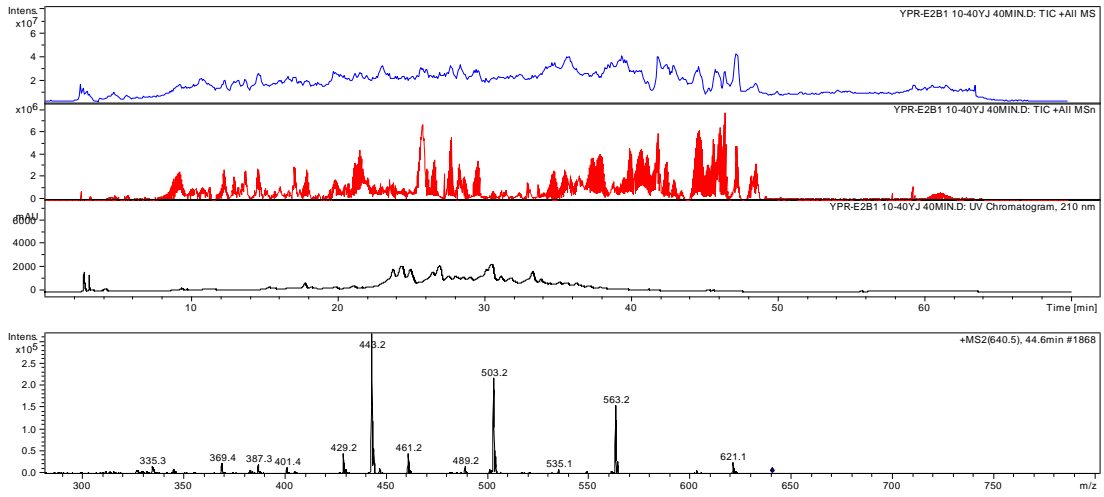


Figure S1. Online HPLC/UV/ESI-MS² analyses of fraction D1a

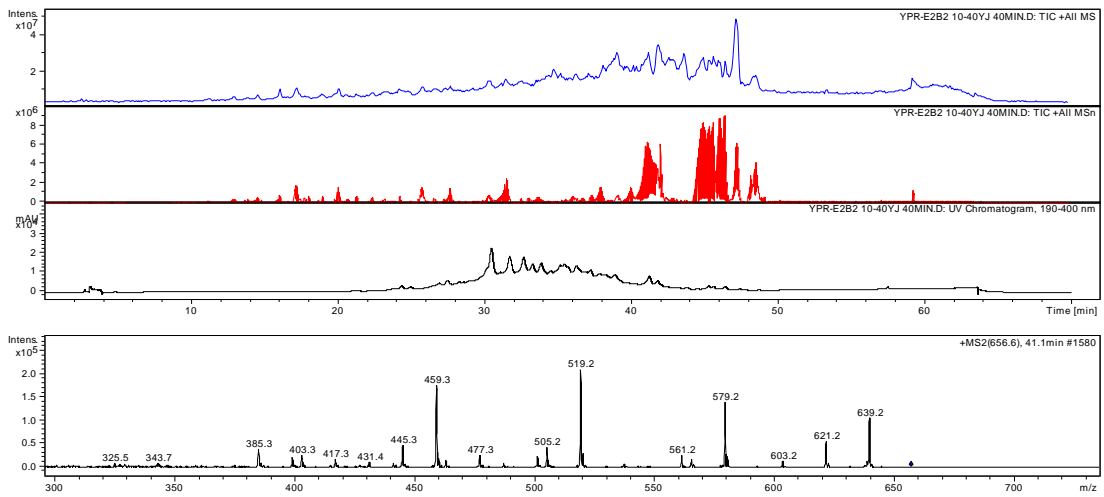


Figure S2. Online HPLC/UV/ESI-MS² analyses of fraction D2a

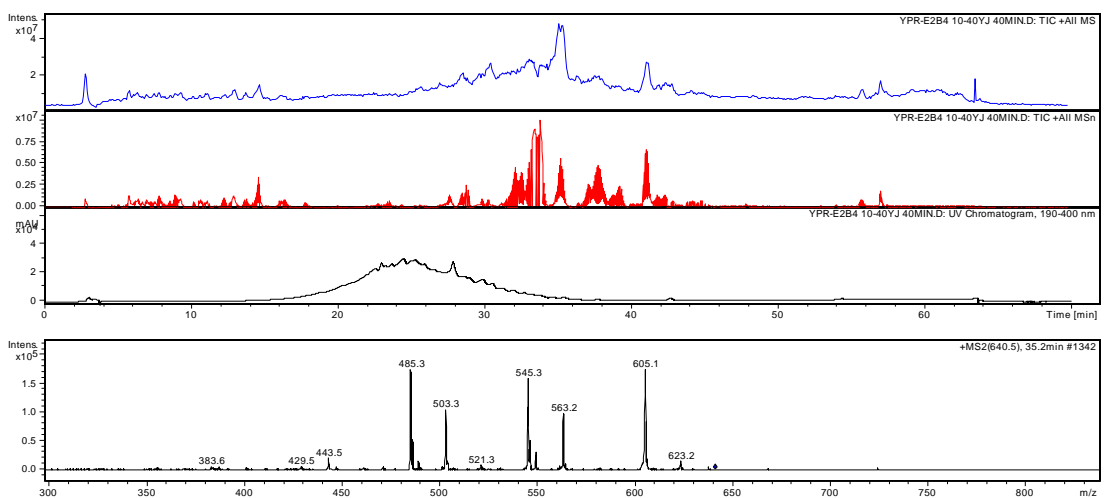


Figure S3. Online HPLC/UV/ESI-MS² analyses of fraction D2b

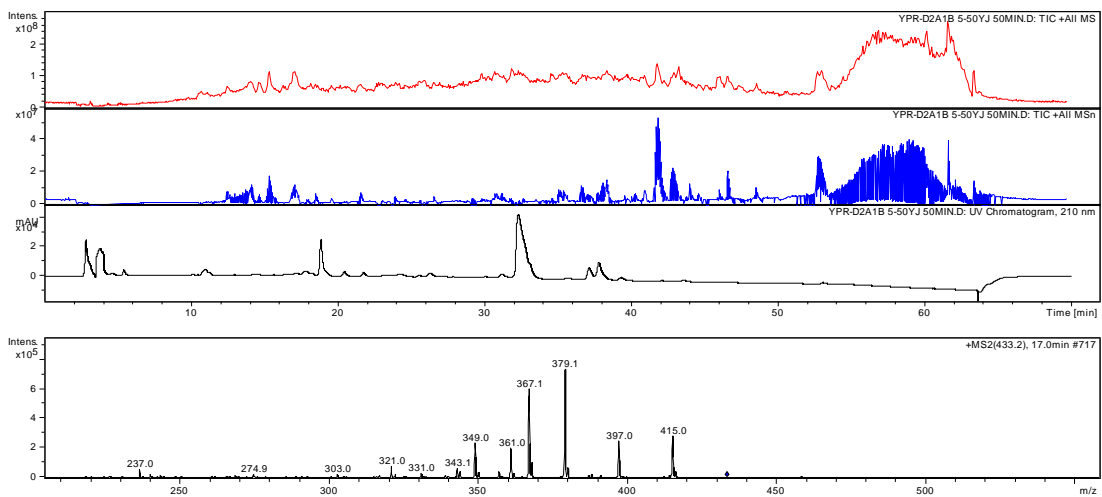


Figure S4. Online HPLC/UV/ESIMS² analyses of fraction E1a

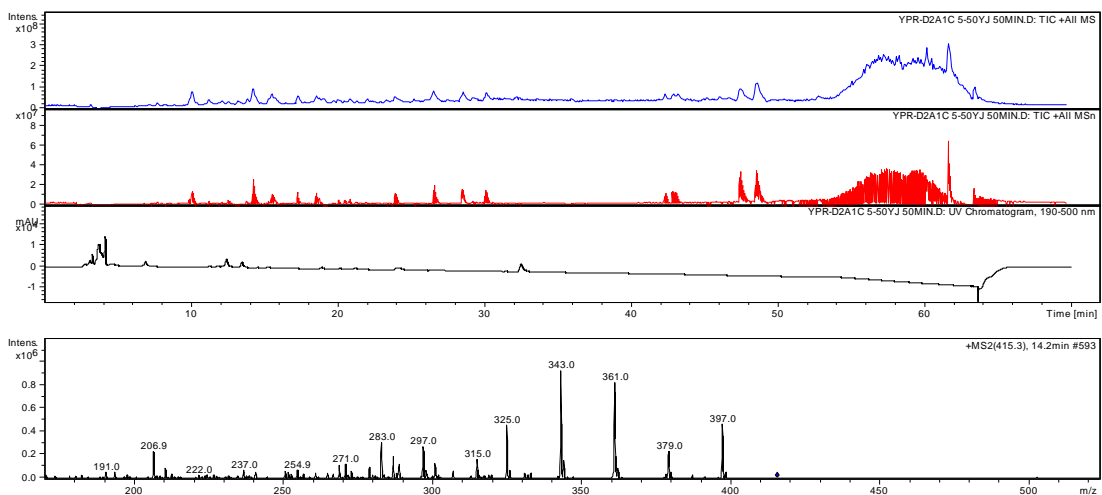


Figure S5. Online HPLC/UV/ESIMS² analyses of fraction E1b

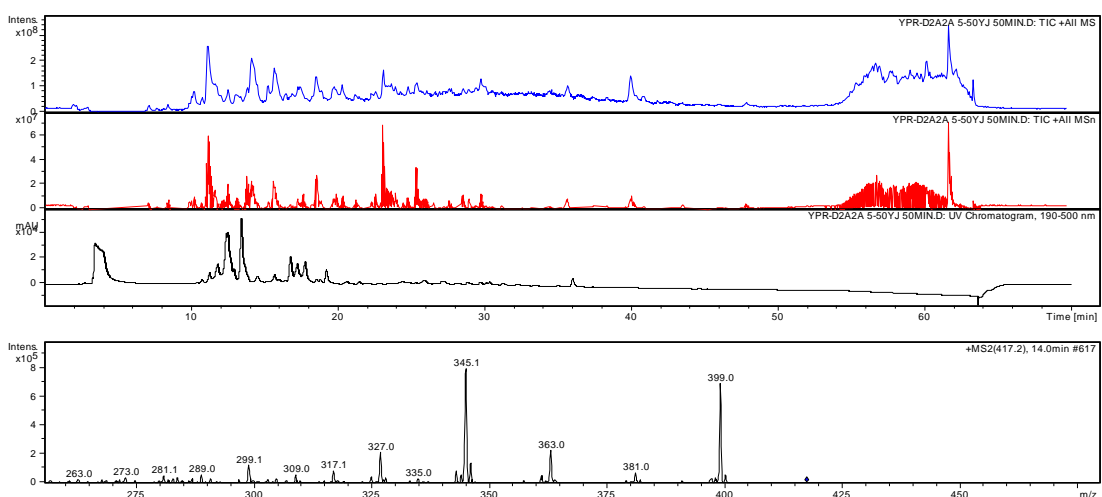


Figure S6. Online HPLC/UV/ESIMS² analyses of fraction E2a

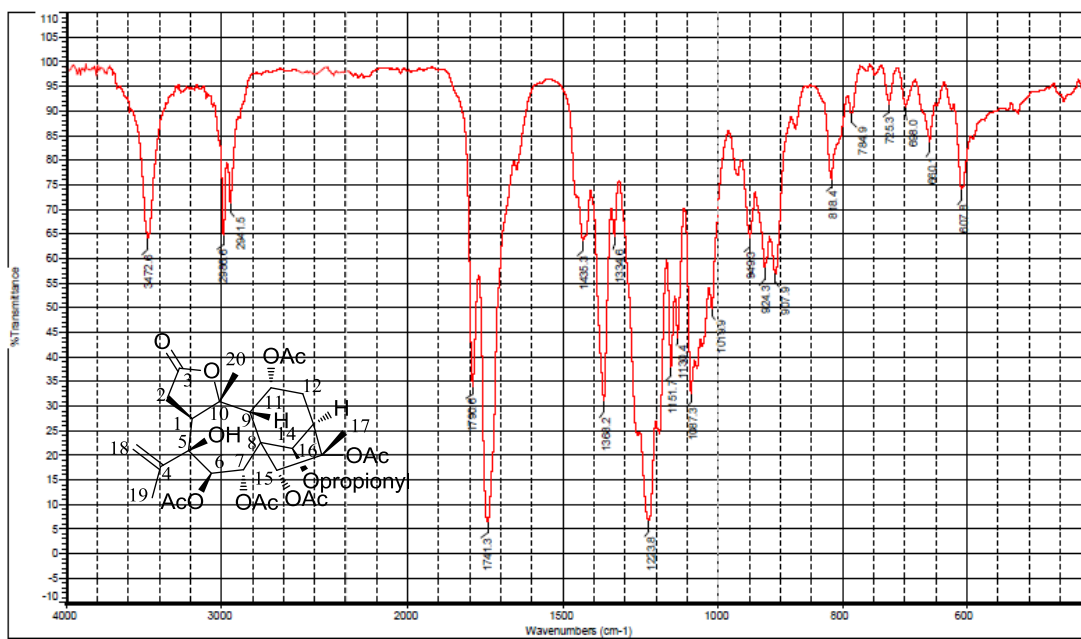


Figure S7. IR spectrum of **1**

MS Formula Results: + Scan (7.193 min) Sub (2015050501.d)

m/z	Ion	Formula	Abundance
703.2568	(M+Na) ⁺	C33 H44 Na O15	82303.1

Best	Formula (M)	Ion Formula	Score	Cross Sec	Mass	Calc Mass	Calc m/z	Diff (ppm)	Ads Diff (ppm)	Mass Match	Abund Match	Spacing Match	List
<input checked="" type="checkbox"/>	C33 H44 O15	C33 H44 Na O15	99.72		680.2676	680.2688	703.2572	0.64	0.64	99.99	99.24	99.75	12
<input type="checkbox"/>	C46 H36 N2 O4	C46 H36 N2 Na O4	98.52		680.2676	680.2675	703.2567	-0.13	0.13	100	95.1	99.67	30
<input type="checkbox"/>	C28 H44 N2 O17	C28 H44 N2 Na O17	98.45		680.2676	680.2684	703.2532	-5.29	5.29	99.07	96.28	99.8	8
<input type="checkbox"/>	C51 H36 O2	C51 H36 Na O2	96.87		680.2676	680.2715	703.2608	5.8	5.8	96.88	91.24	99.63	34

Figure S8. (+)-HRESIMS data of **1**

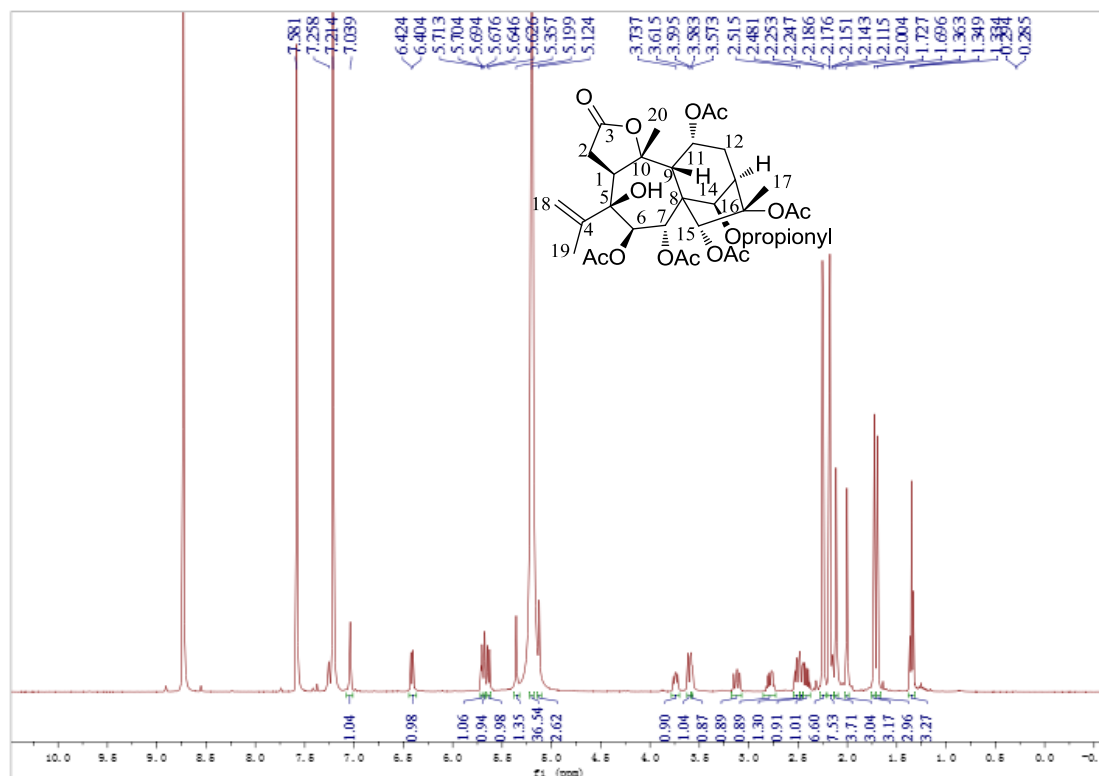


Figure S9. ¹H NMR spectrum of **1** (500 MHz, in C₅D₅N)

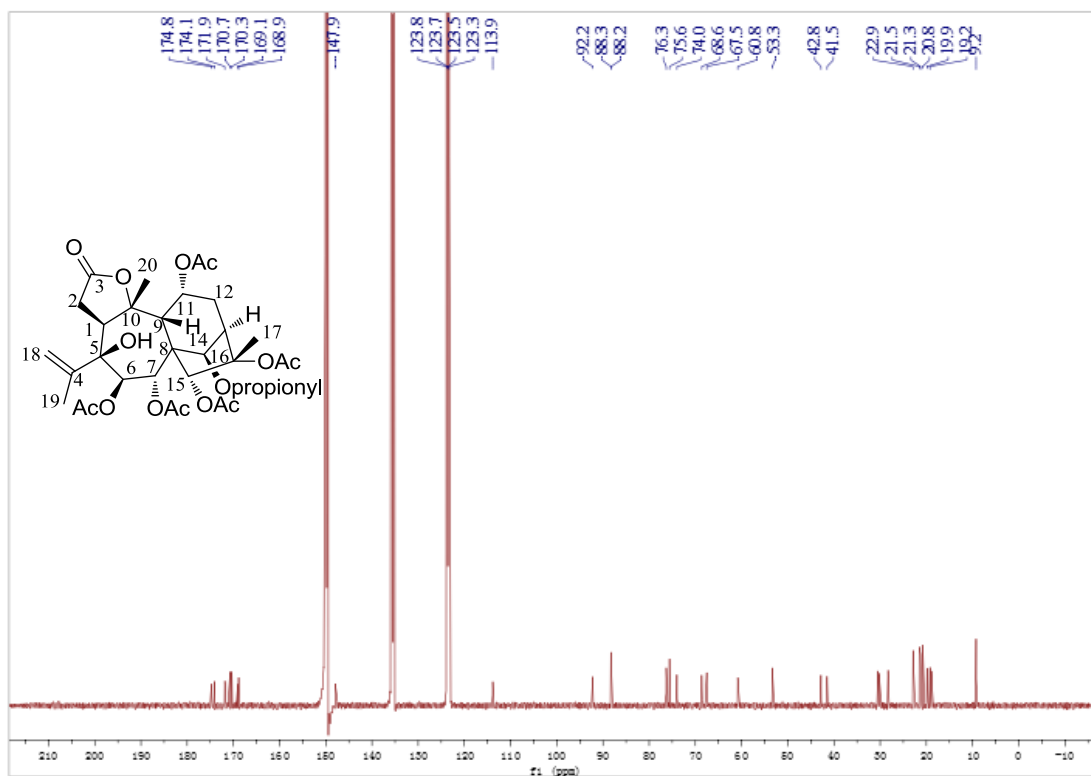


Figure S10. ^{13}C NMR spectrum of **1** (125 MHz, in $\text{C}_5\text{D}_5\text{N}$)

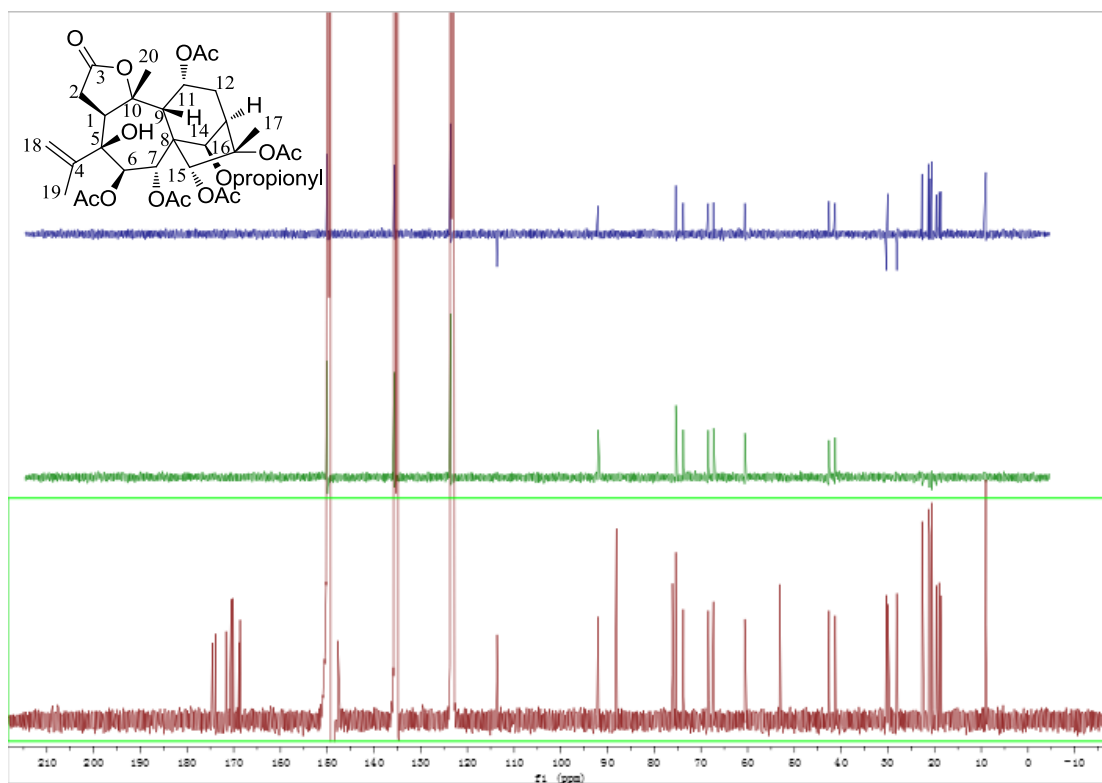


Figure S11. DEPT spectrum of **1** (125 MHz, in $\text{C}_5\text{D}_5\text{N}$)

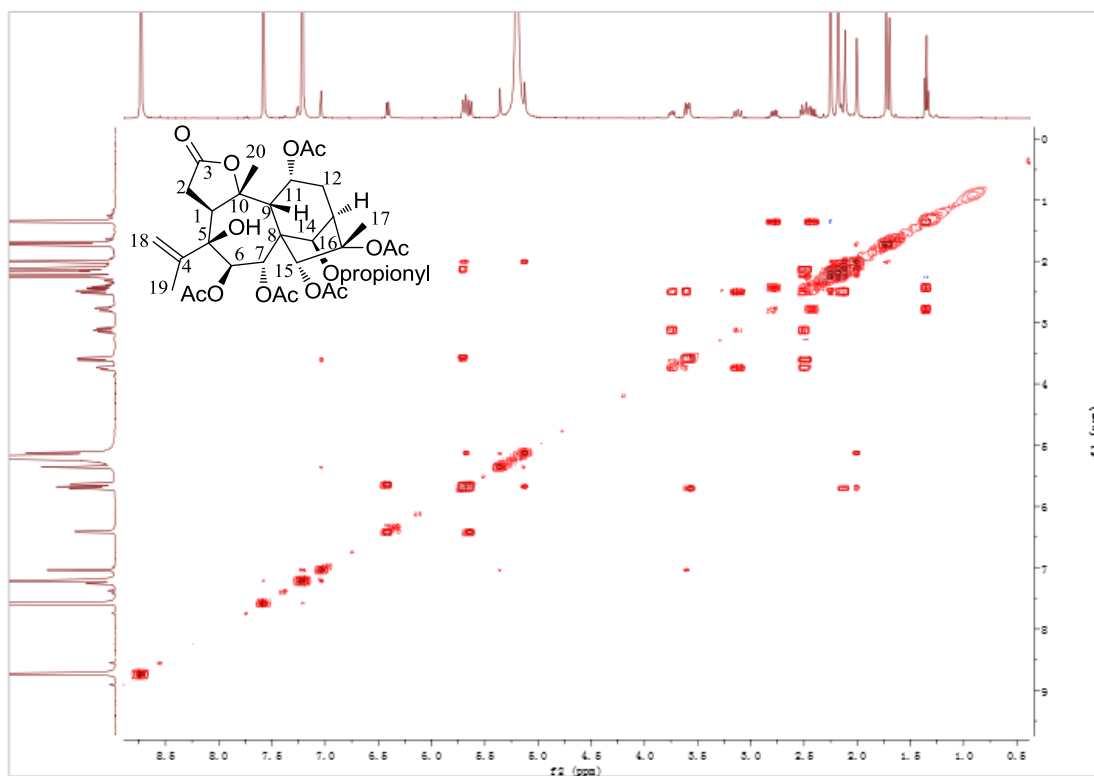


Figure S12. ^1H - ^1H COSY spectrum of **1** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

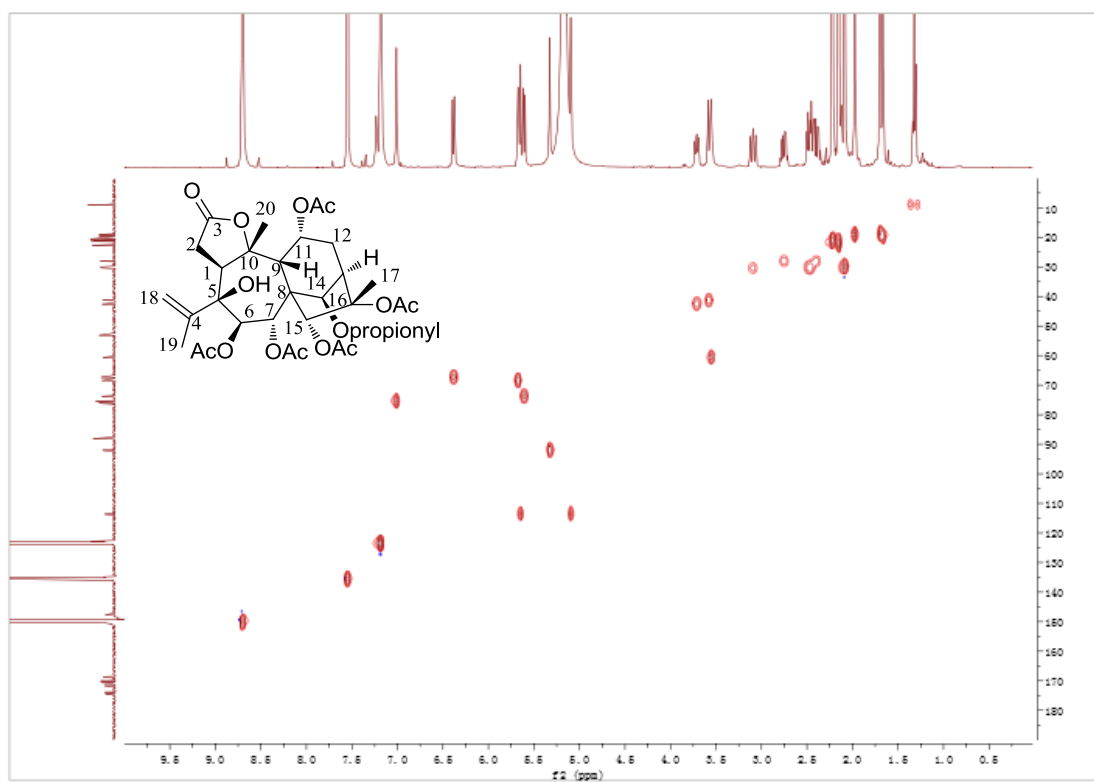


Figure S13. HSQC spectrum of **1** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

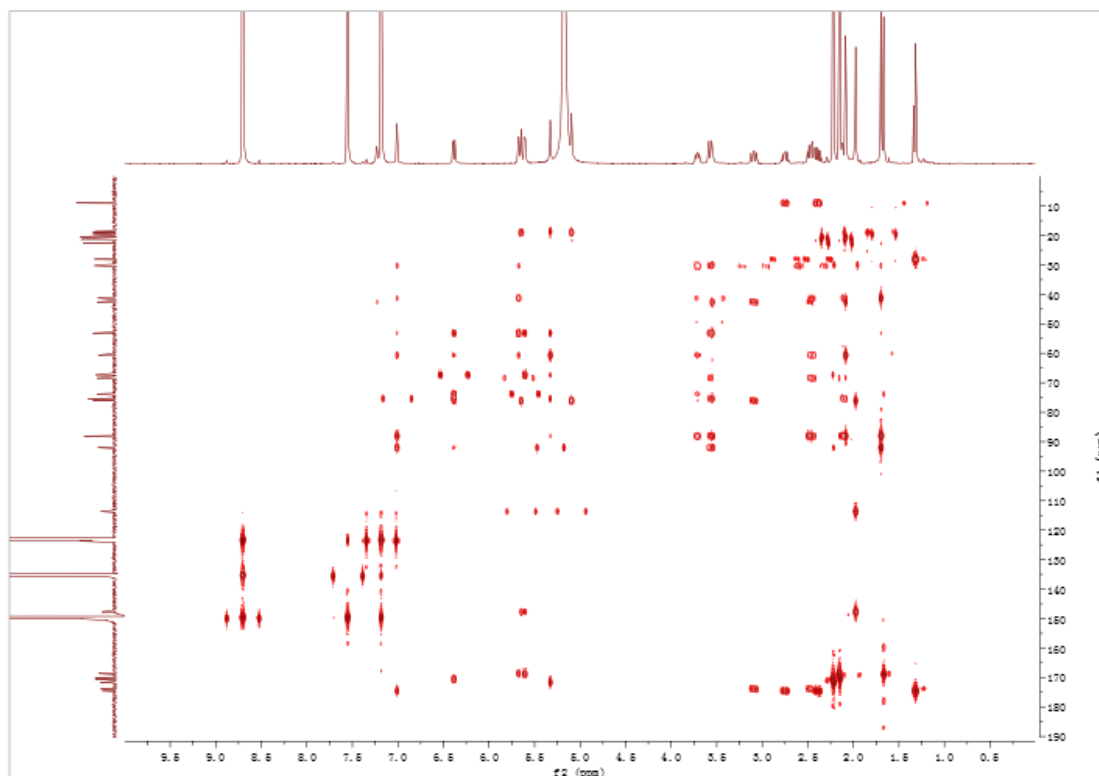


Figure S14. HMBC spectrum of **1** (500 MHz, in C_5D_5N)

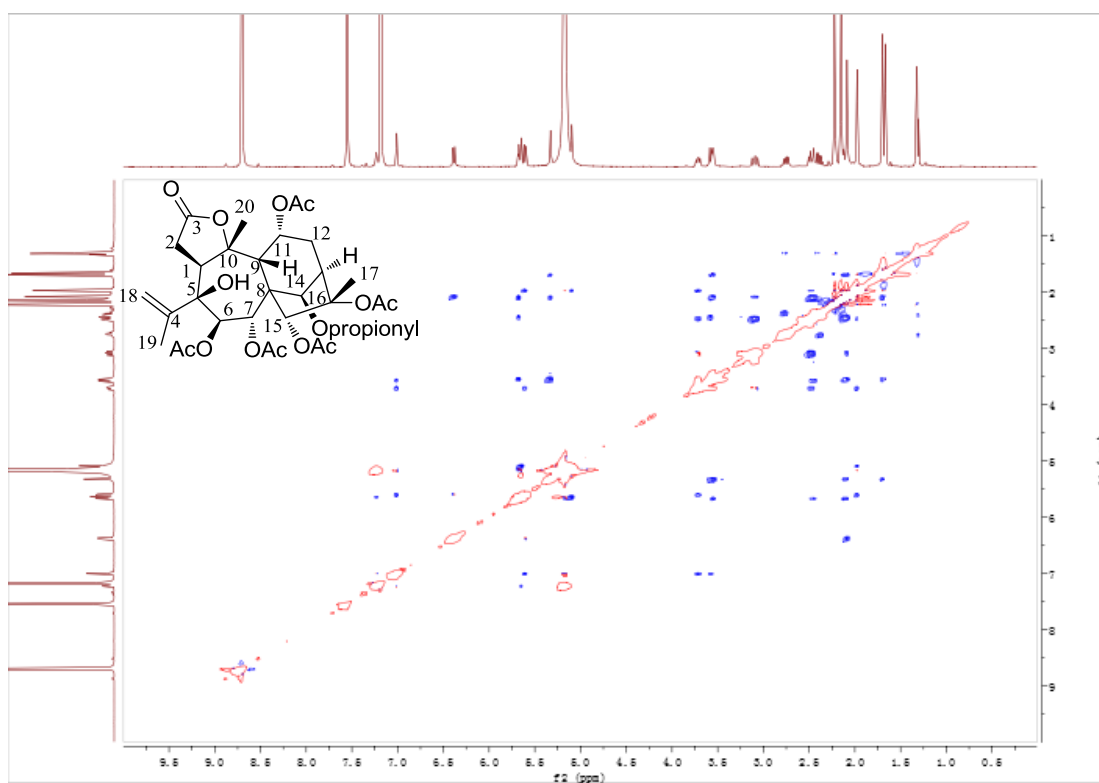
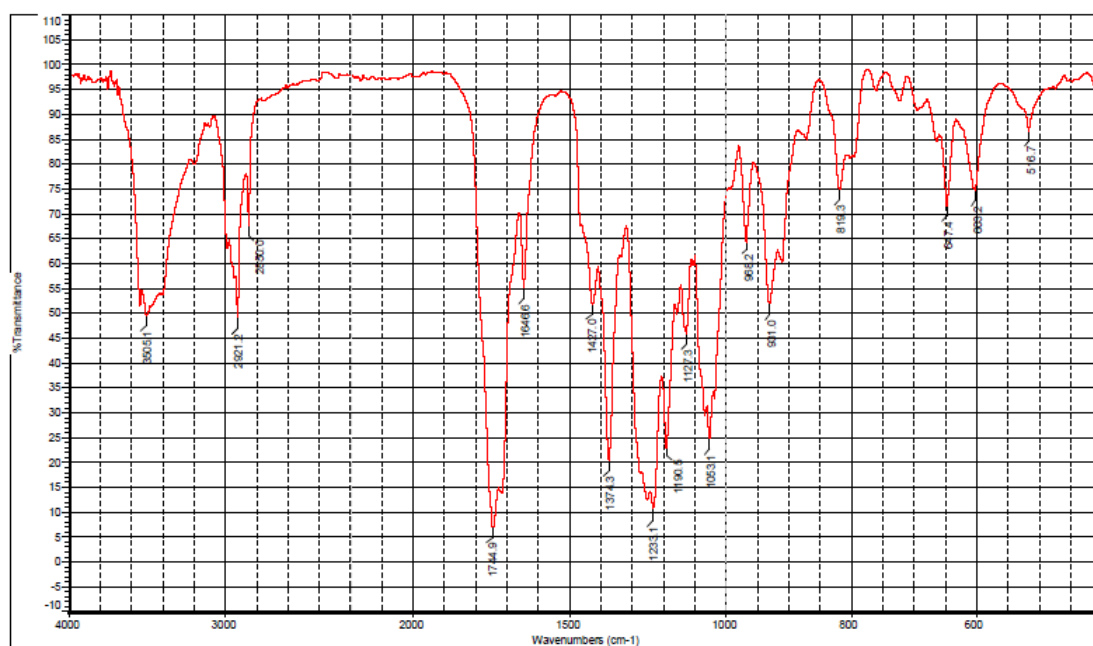


Figure S15. NOESY spectrum of **1** (500 MHz, in C_5D_5N)

Table S1. Crystal data and structure refinement for **1**

Identification code	exp_3806
Empirical formula	C33H44O16
Formula weight	696.68
Temperature/K	104.3
Crystal system	triclinic
Space group	P1
a / Å, b / Å, c / Å	8.6705(4), 17.6150(9), 17.7494(7)
$\alpha/^\circ, \beta/^\circ, \gamma/^\circ$	64.166(4), 89.173(3), 76.713(4)
Volume/Å ³	2638.3(2)
Z	3
$\rho_{\text{calc}}/\text{mg mm}^{-3}$	1.315
μ/mm^{-1}	0.894
F(000)	1110
Crystal size/mm ³	0.40 × 0.26 × 0.04
2 θ range for data collection	9.1 to 142.46°
Index ranges	-10 ≤ h ≤ 10, -22 ≤ k ≤ 22, -21 ≤ l ≤ 22
Reflections collected	38245
Independent reflections	16761[R(int) = 0.0353 (inf-0.9Å)]
Data/restraints/parameters	16761/5/1364
Goodness-of-fit on F ²	1.020
Final R indexes [I > 2 σ (I) i.e. F _o > 4 σ (F _o)]	R ₁ = 0.0444, wR ₂ = 0.1138
Final R indexes [all data]	R ₁ = 0.0467 wR ₂ = 0.1165
Largest diff. peak/hole/e Å ⁻³	0.464/-0.446
Flack Parameters	0.00(8)
Completeness	0.983

**Figure S16.** IR spectrum of **2**

MS Formula Results: + Scan (6.290 min) Sub (2015091701.d)

m/z	Ion	Formula	Abundance										
661.2477	(M+Na) ⁺	C31 H42 Na O14	344442.6										
Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DGE
✓	C31 H42 O14	C31 H42 Na O14	99.86		638.2584	638.2575	661.2467	-1.47	1.47	99.93	99.73	99.89	11
✓	C32 H38 Na O10	C32 H38 Na O10	96.62		638.2584	638.2588	661.246	0.81	0.81	96.99	96.76	99.83	16
✓	C27 H38 Na O12	C27 H38 Na O12	96.47		638.2584	638.2543	661.244	-5.7	5.7	98.93	99.86	99.96	12
✓	C20 H42 Na O17	C20 H42 Na O17	96.62		638.2584	638.2606	661.2499	3.49	3.49	99.4	95.87	99.99	3
✓	C44 H34 Na O3	C44 H34 Na O3	96.34		638.2584	638.2569	661.2462	-2.28	2.28	99.83	87.58	99.86	26
✓	C49 H34 Na O	C49 H34 Na O	94.54		638.2584	638.261	661.2502	4.02	4.02	99.47	81.9	99.84	33

Figure S17. (+)-HRESIMS data of **2**

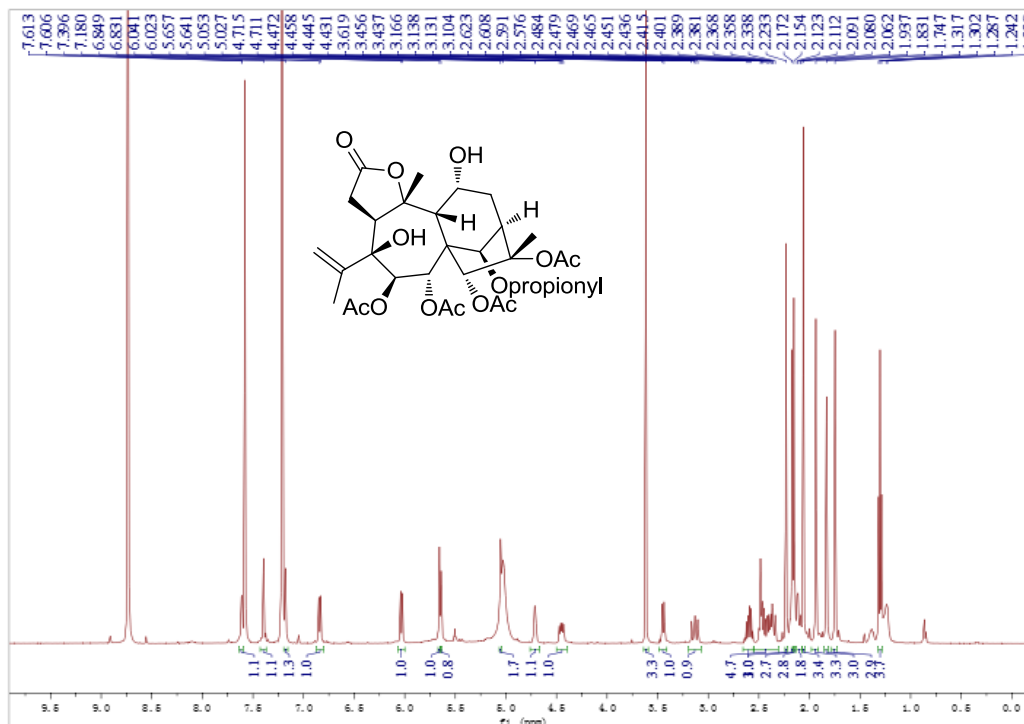


Figure S18. ¹H NMR spectrum of **2** (500 MHz, in C₅D₅N)

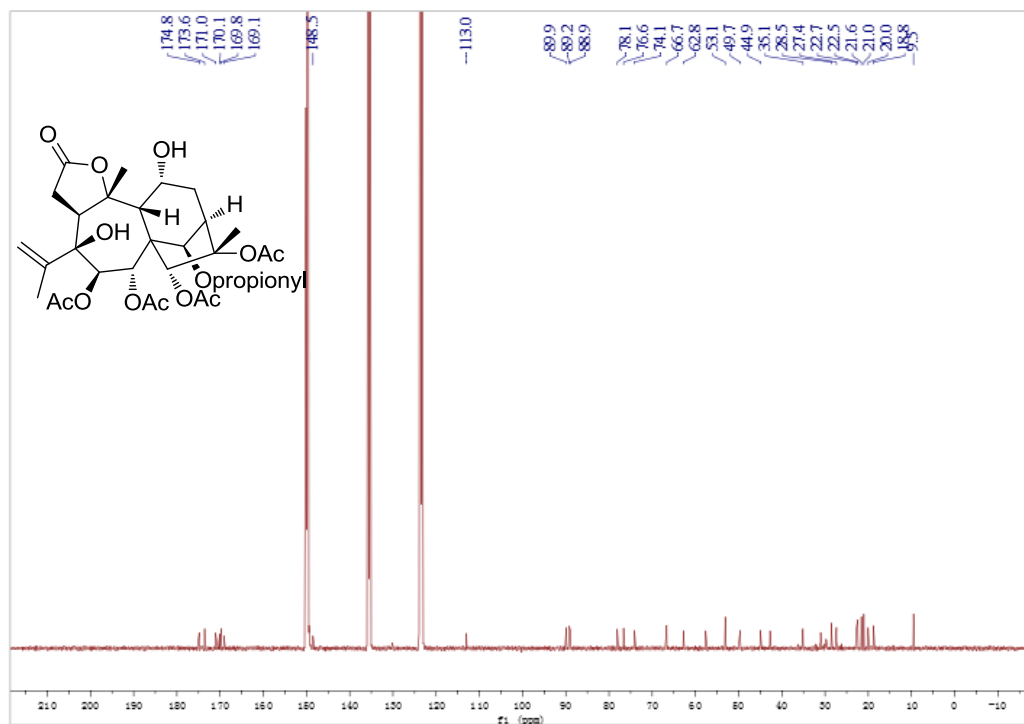


Figure S19. ¹³C NMR spectrum of **2** (125 MHz, in C₅D₅N)

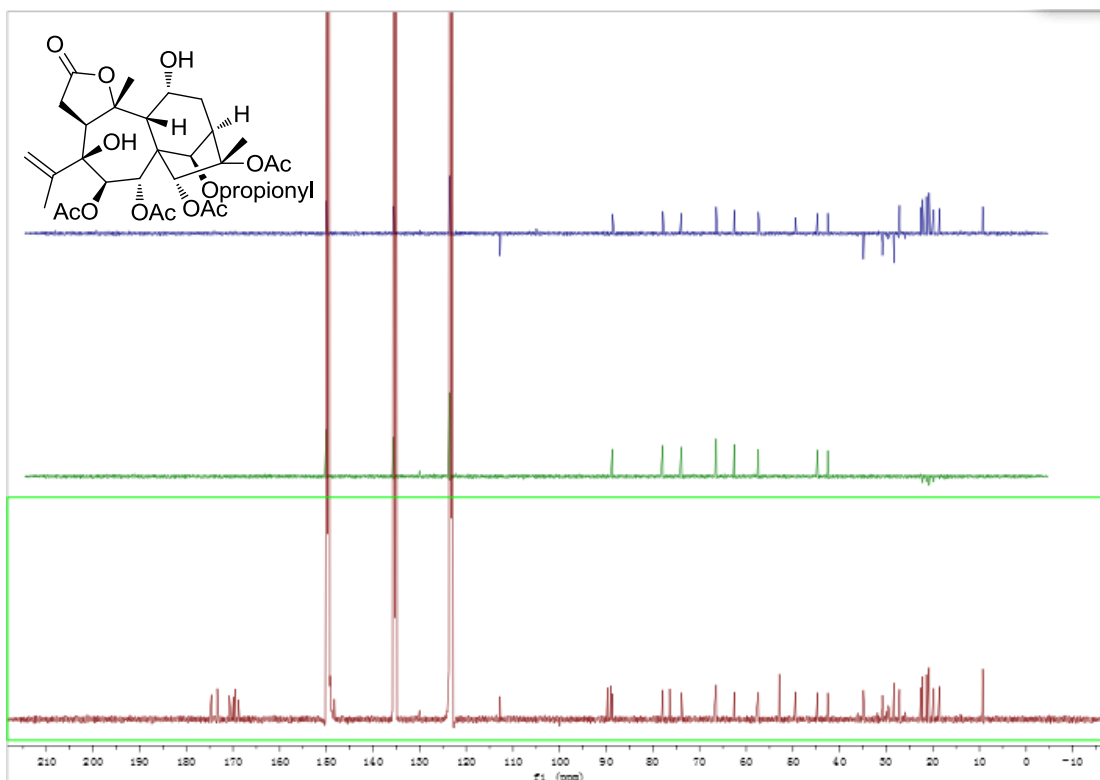


Figure S20. DEPT spectrum of **2** (125 MHz, in $\text{C}_5\text{D}_5\text{N}$)

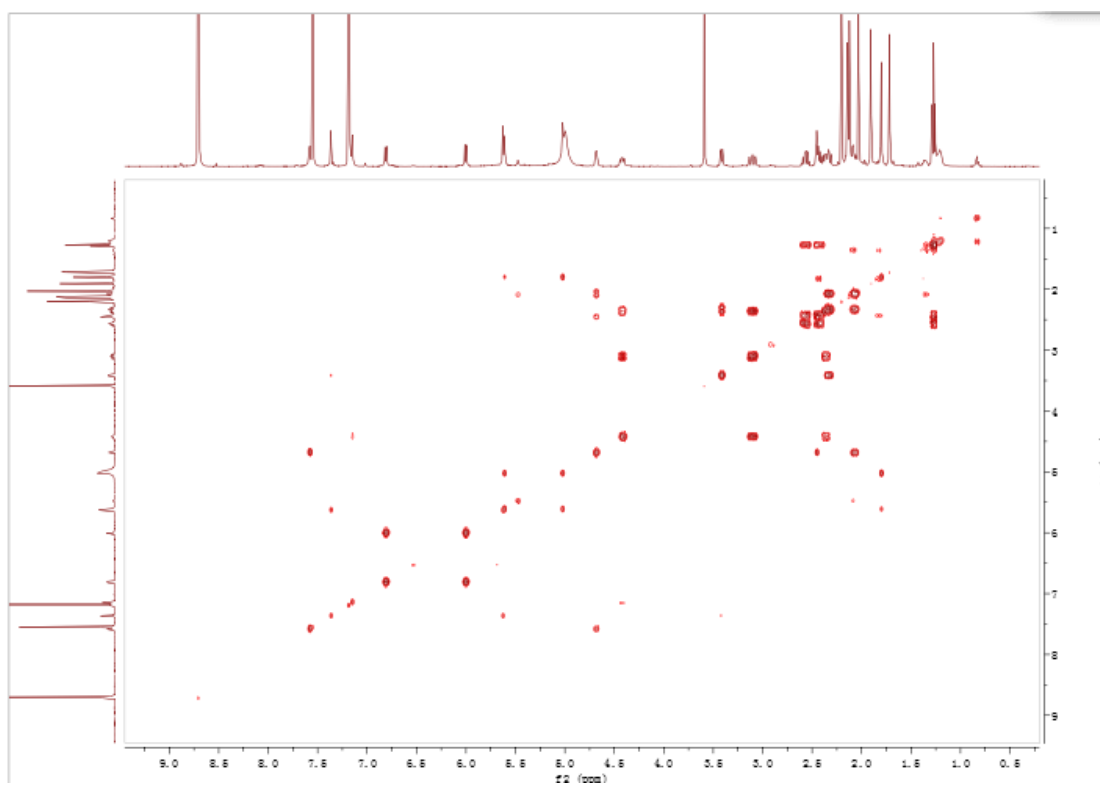


Figure S21. ^1H - ^1H COSY spectrum of **2** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

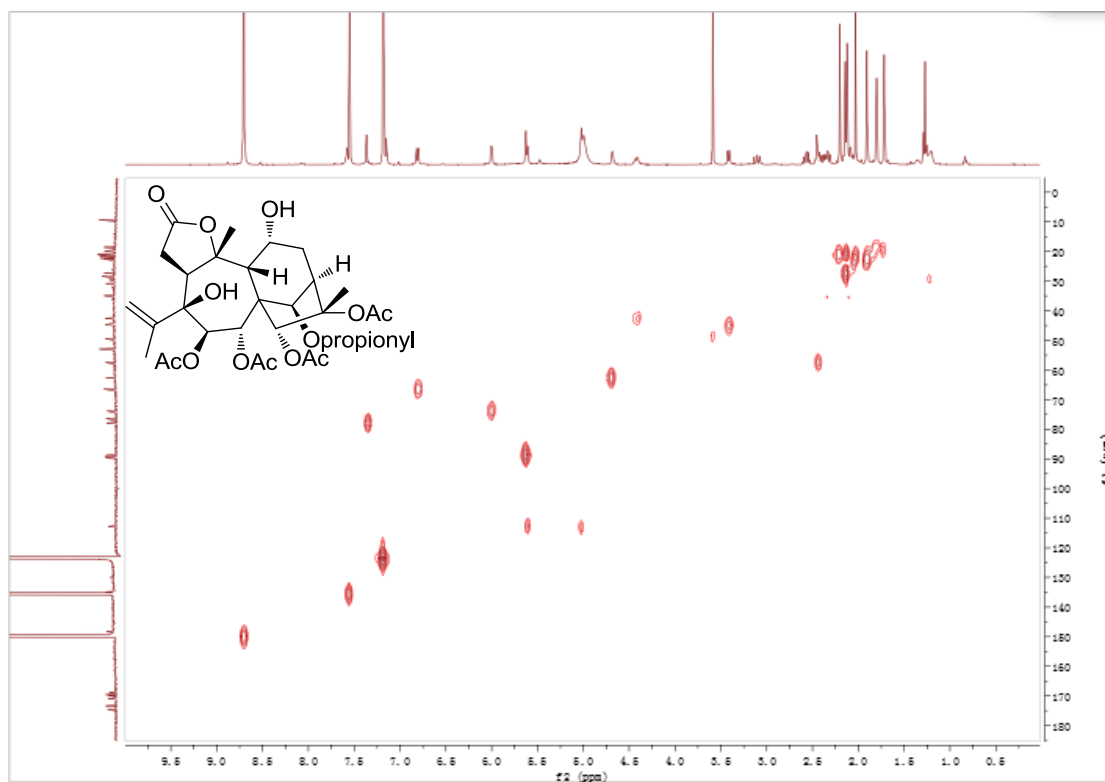


Figure S22. HSQC spectrum of **2** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

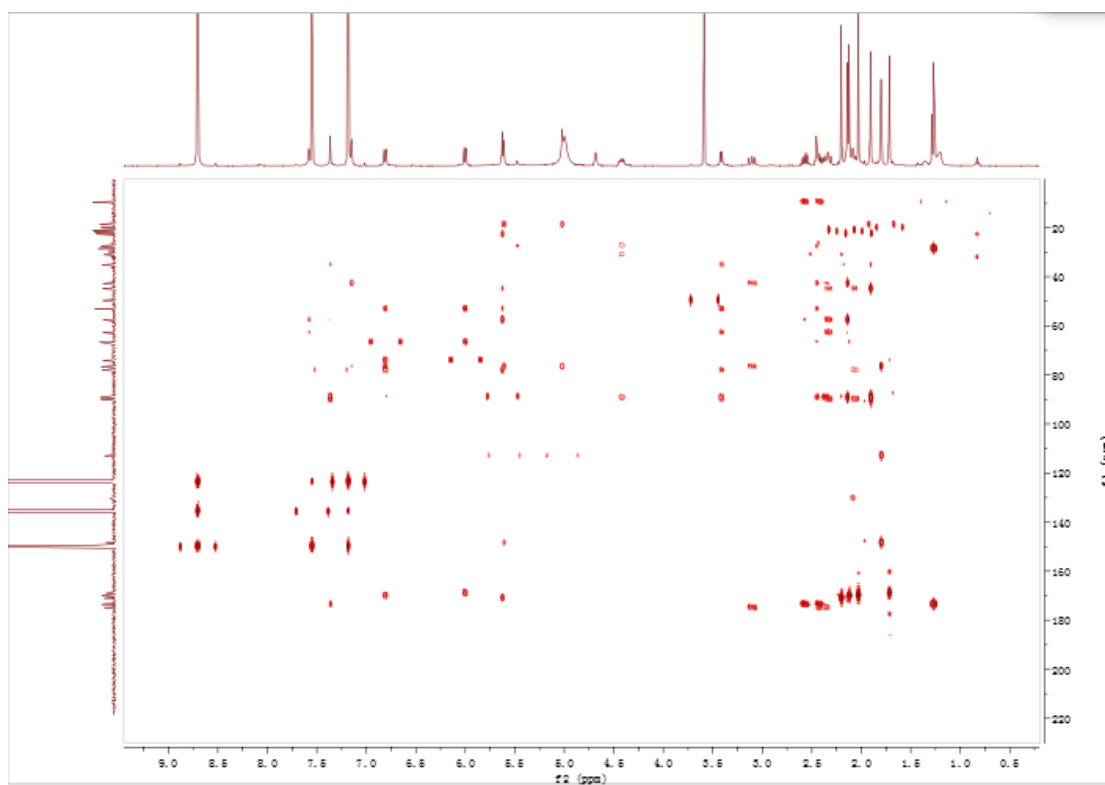


Figure S23. HMBC spectrum of **2** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

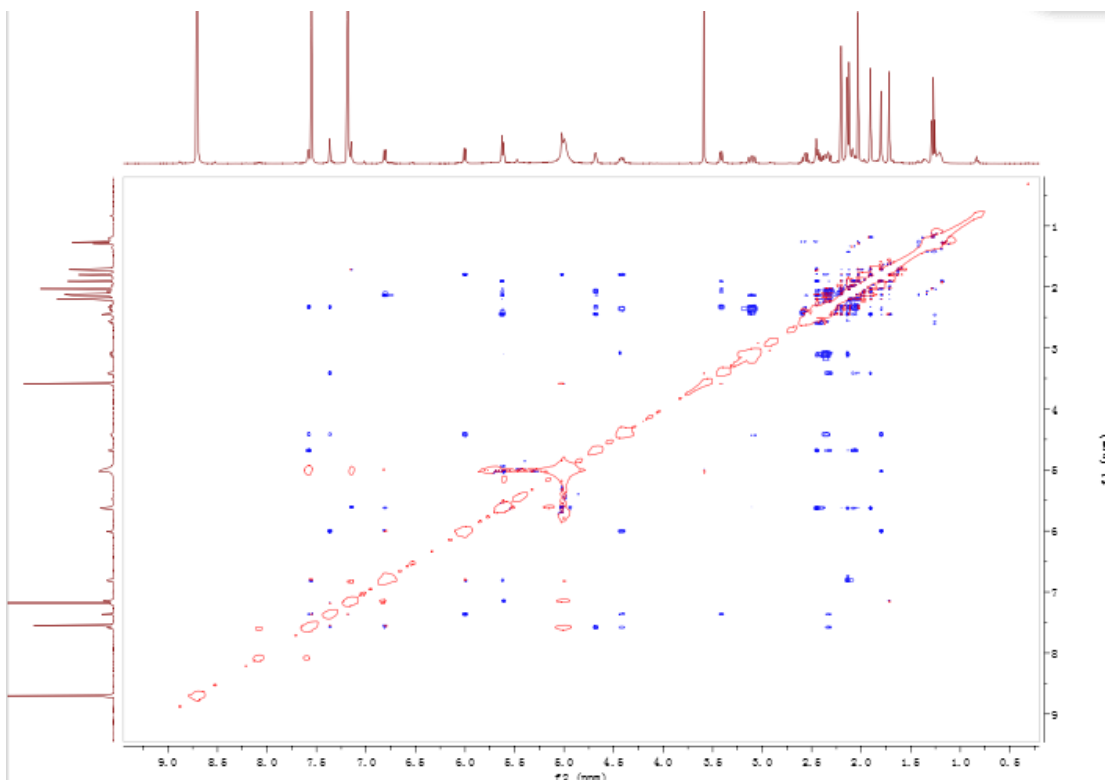


Figure S24. NOESY spectrum of **2** (500 MHz, in C₅D₅N)

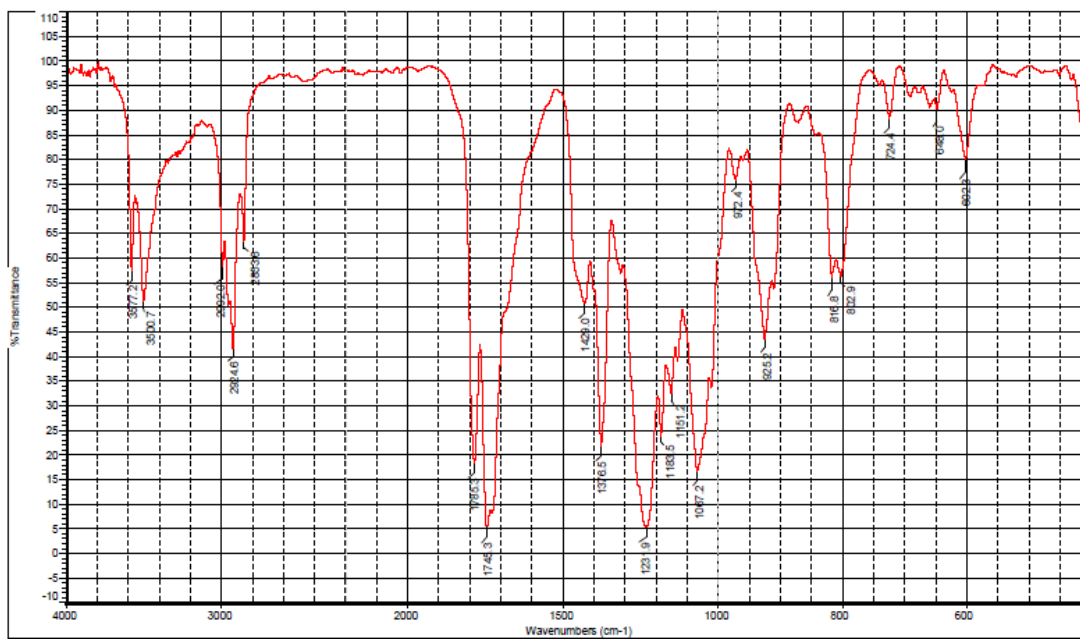


Figure S25. IR spectrum of **3**

MS Formula Results: + Scan (6.357 min) Sub (2015052601.d)

m/z	Ion	Formula	Abundance
861.2467	(M+Na) ⁺	C ₃₁ H ₄₂ NaO ₁₄	57921.8

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spcing Match	DBE
✓	C ₃₁ H ₄₂ O ₁₄	C ₃₁ H ₄₂ NaO ₁₄	99.81		638.2575	638.2575	661.2467	-0.08	0.08	100	99.87	99.37	11
	C ₃₂ H ₃₈ NaO ₁₅	C ₃₂ H ₃₈ NaO ₁₅	99.59		638.2575	638.2568	661.2448	-2	2	99.87	99.3	99.37	15
	C ₂₇ H ₃₈ NaO ₁₂	C ₂₇ H ₃₈ NaO ₁₂	99.42		638.2575	638.2548	661.244	-4.32	4.32	99.38	99.45	99.44	12
	C ₂₀ H ₄₂ NaO ₁₇	C ₂₀ H ₄₂ NaO ₁₇	97.74		638.2575	638.2808	661.3499	4.88	-4.88	99.21	93.8	99.51	3
	C ₄₄ H ₃₄ N ₂ O ₃	C ₄₄ H ₃₄ N ₂ NaO ₃	97.03		638.2575	638.2859	661.3462	-0.89	0.89	99.97	90.28	99.23	29
	C ₄₉ H ₃₄ O	C ₄₉ H ₃₄ NaO	95.11		638.2575	638.281	661.2502	5.42	5.42	99.03	85.2	99.17	33

Figure S26. (+)-HRESIMS data of **3**

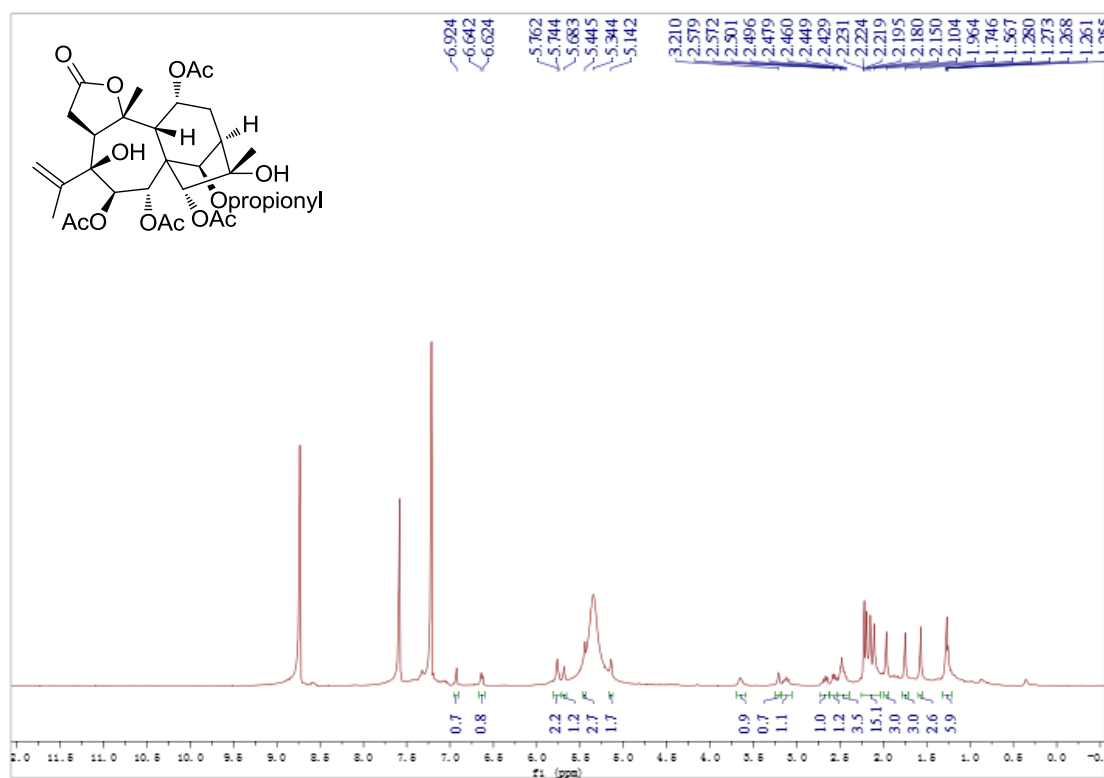


Figure S27. ^1H NMR spectrum of **3** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

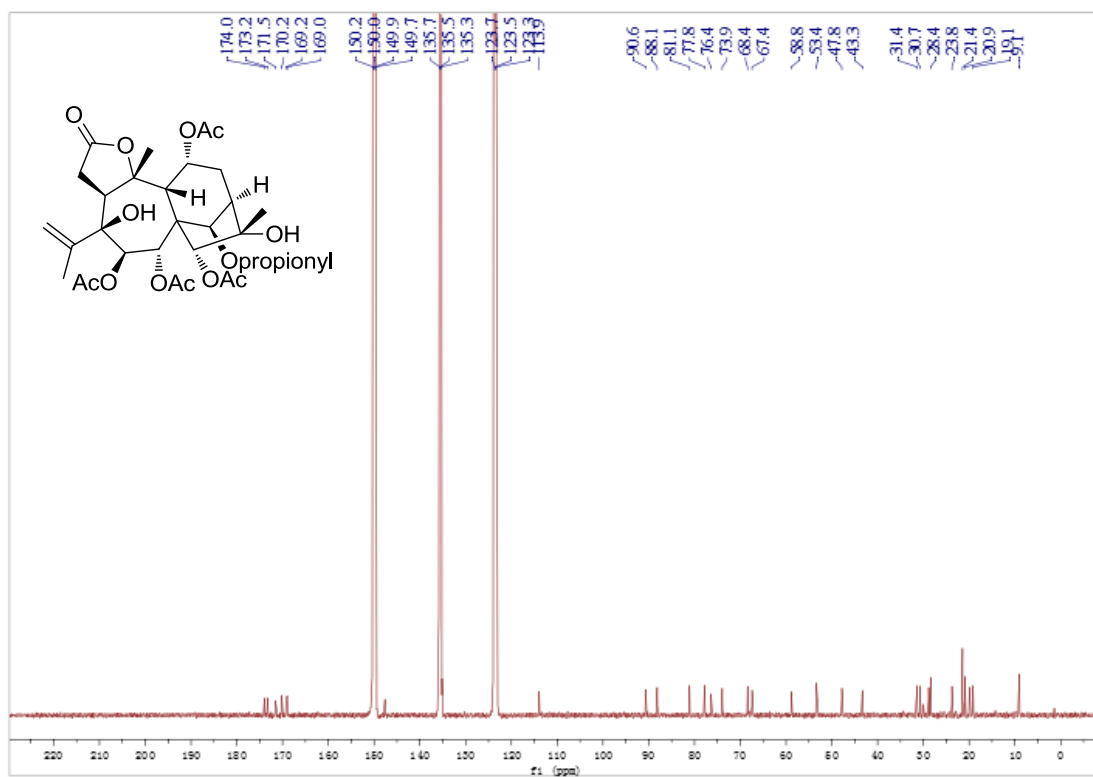


Figure S28. ^{13}C NMR spectrum of **3** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

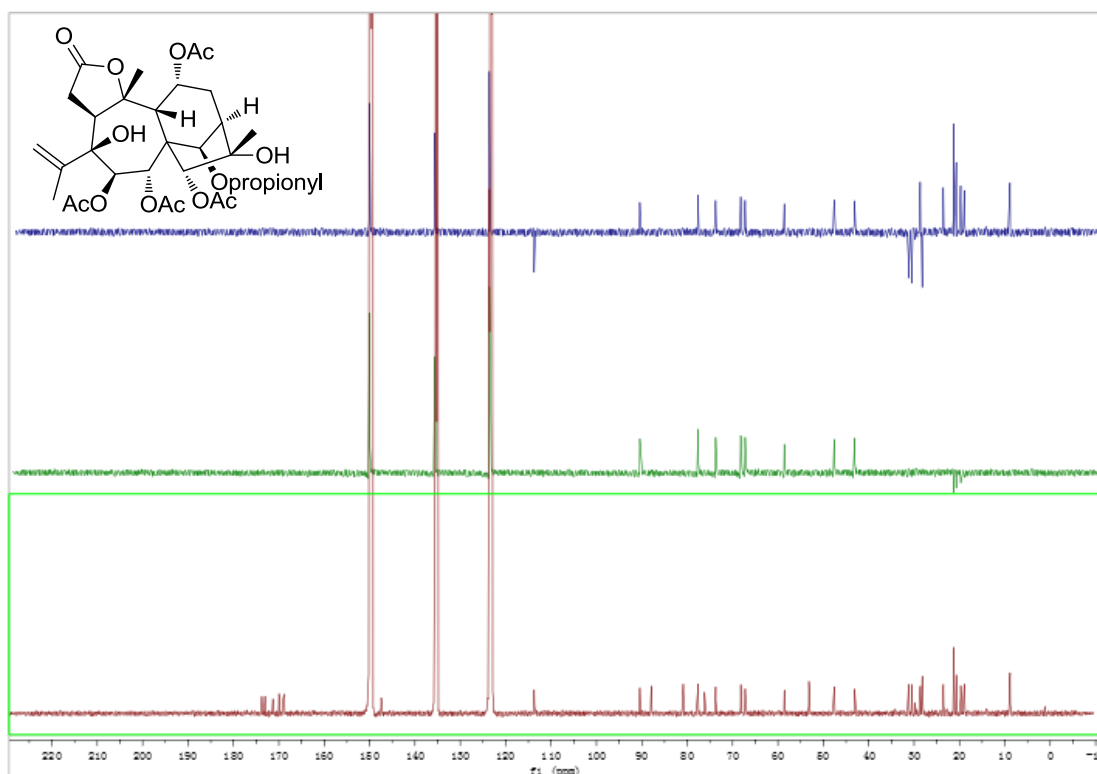


Figure S29. DEPT spectrum of **3** (150 MHz, in C_5D_5N)

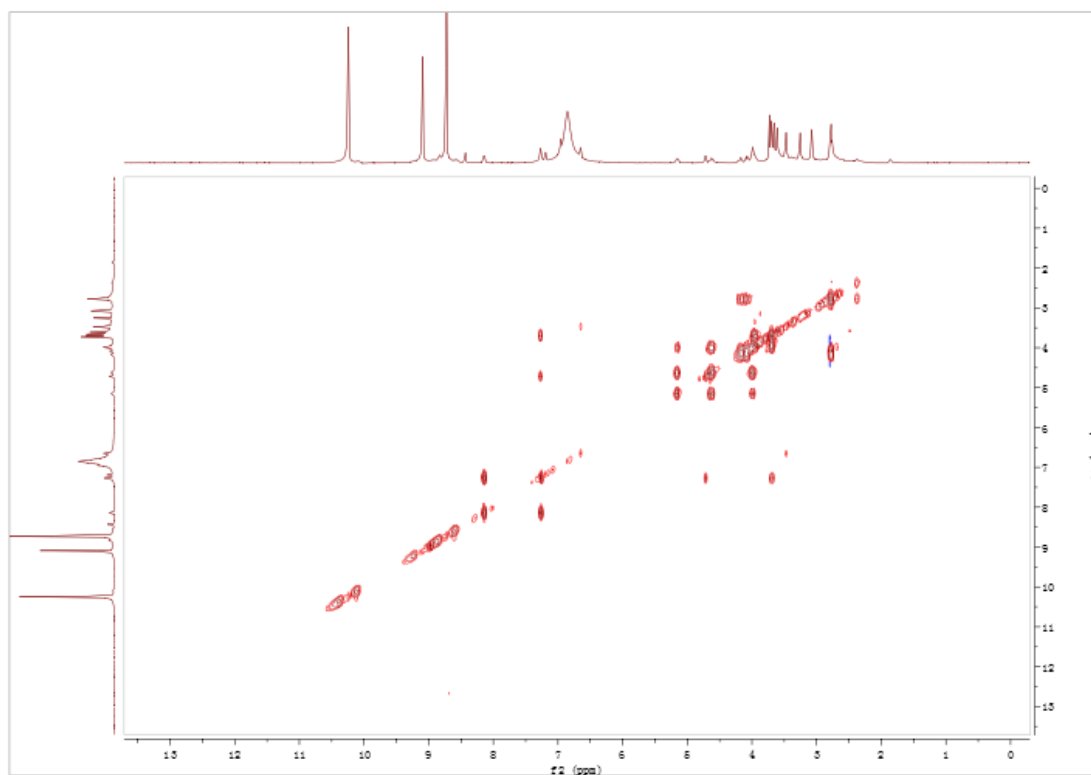


Figure S30. 1H - 1H COSY spectrum of **3** (600 MHz, in C_5D_5N)

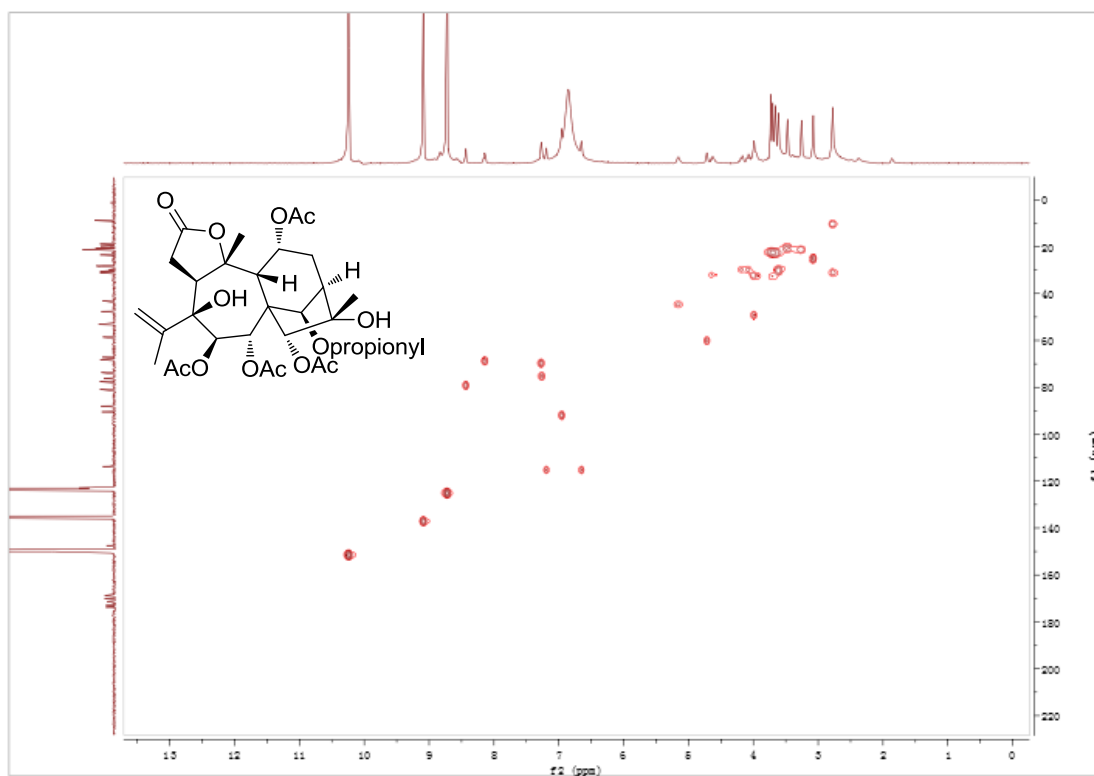


Figure S31. HSQC spectrum of **3** (600 MHz, in C₅D₅N)

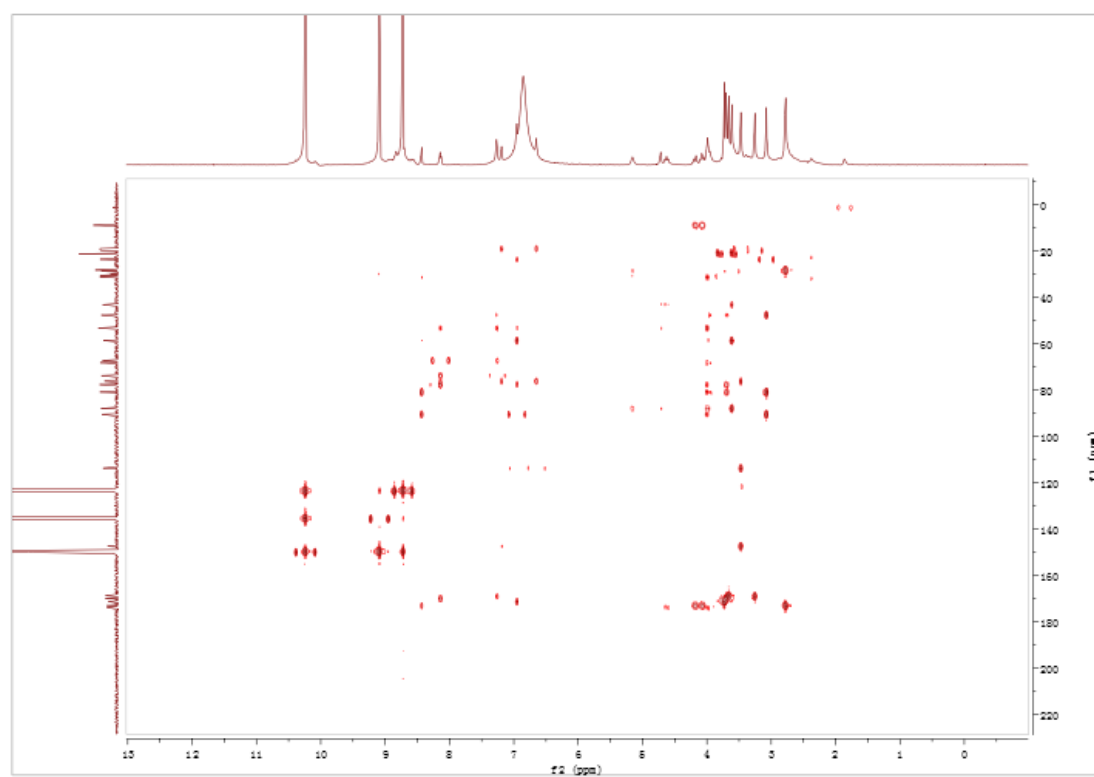


Figure S32. HMBC spectrum of **3** (600 MHz, in C₅D₅N)

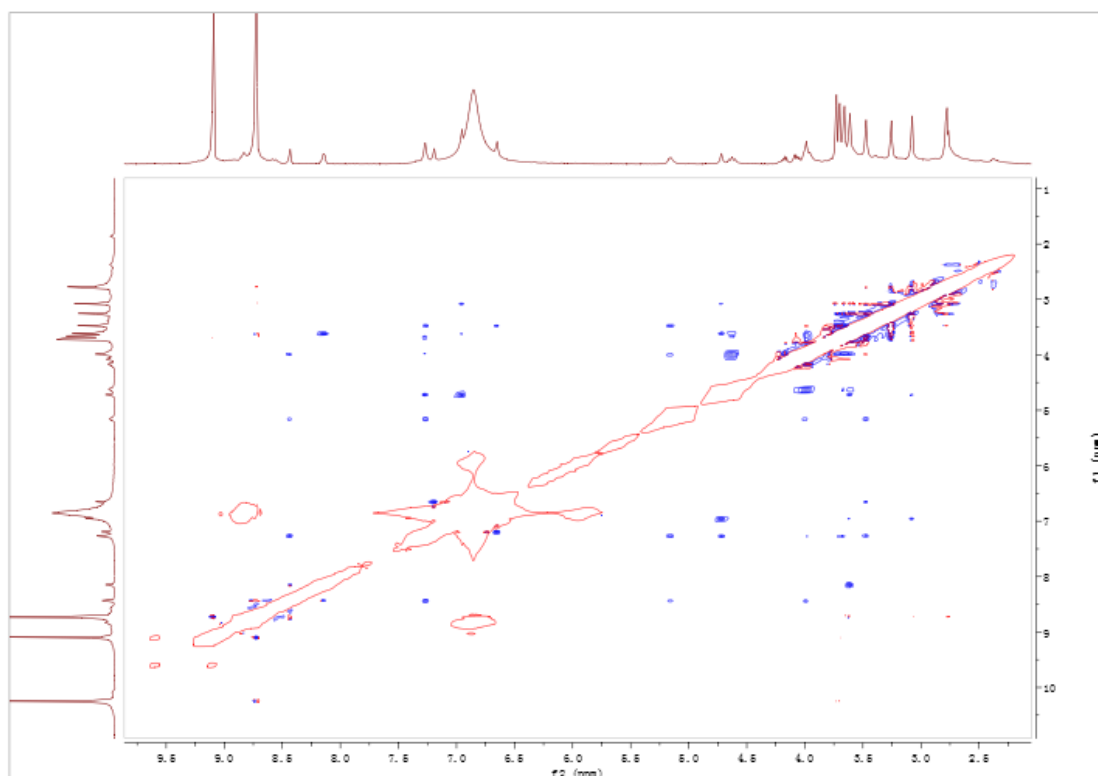


Figure S33. NOESY spectrum of **3** (600 MHz, in C_5D_5N)

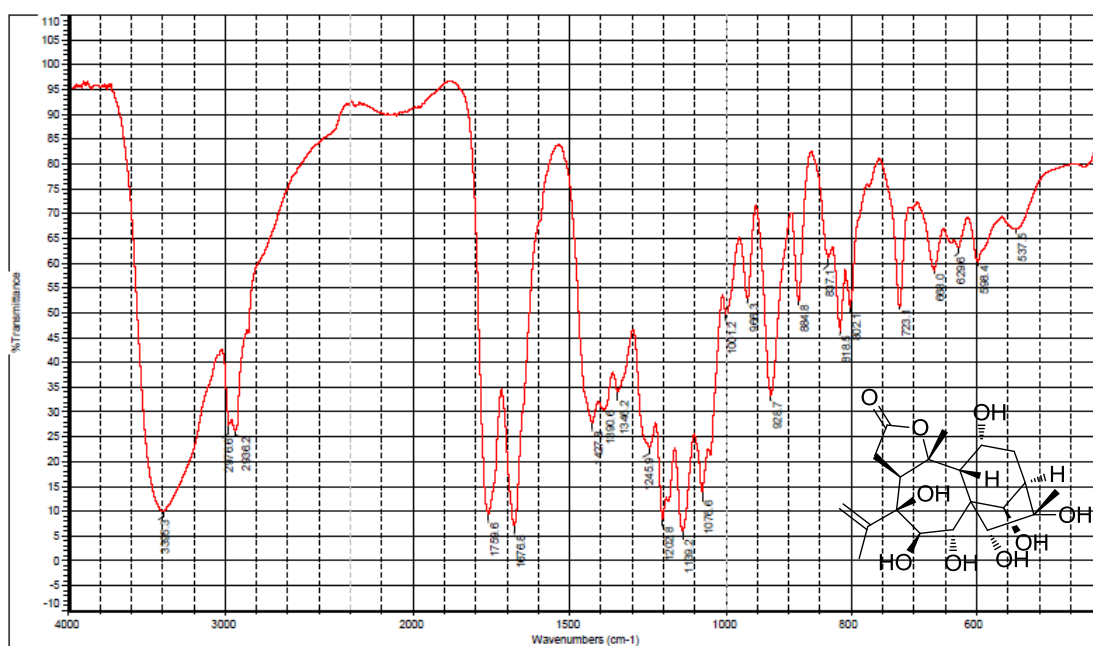


Figure S34. IR spectrum of **4**

MS Formula Results: + Scan (3.630 min) Sub (2016053006.d)

m/z	Ion	Formula	Abundance
415.1984	(M+H) ⁺	C20 H31 O9	49119.2

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C20 H31 O9	C20 H31 O9	99.01		414.1911	414.1989	415.1993	4.98	4.98	99.19	99.46	99.33	6
✓	C17 H34 O9 S	C17 H35 O9 S	97.86		414.1911	414.1924	415.1998	3.15	3.15	99.57	93.88	99.23	1
✓	C21 H34 O4 S2	C21 H35 O4 S2	97.47		414.1911	414.1899	415.1971	-2.9	2.9	99.72	92.42	99.05	5
✓	C18 H39 O4 S3	C18 H39 O4 S3	94.22		414.1911	414.1932	415.2005	5.23	5.23	99.1	82.21	98.88	0

Figure S35. (+)-HRESIMS data of **4**

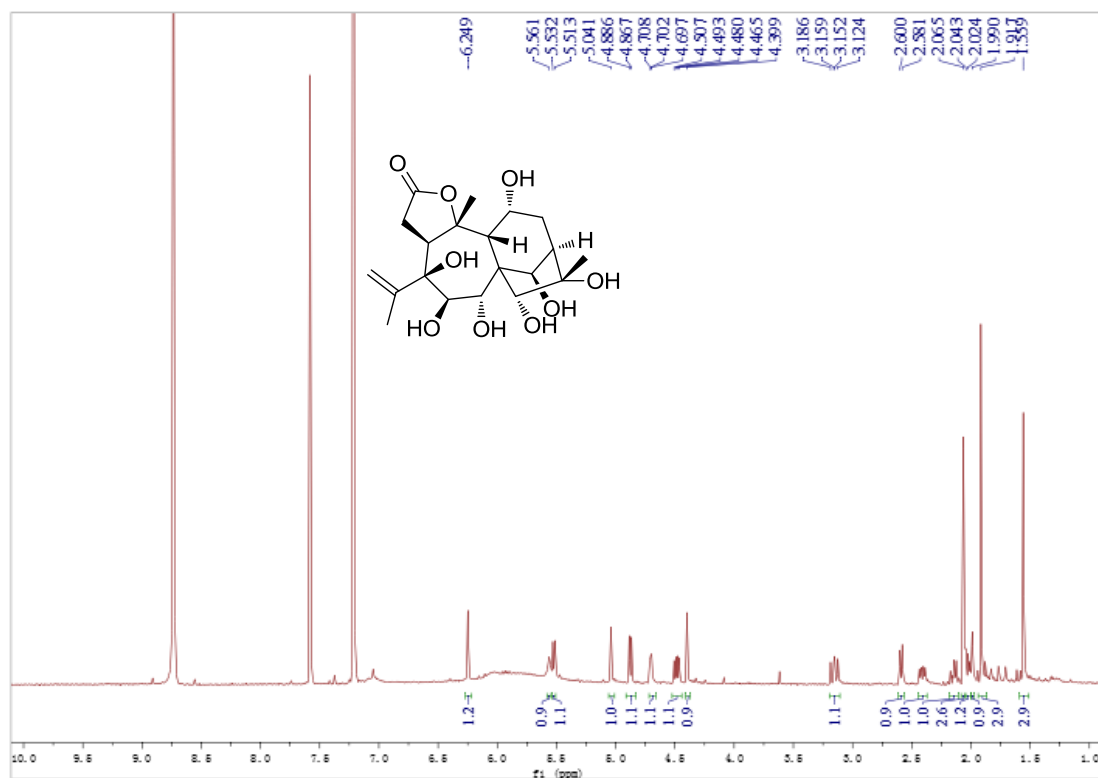


Figure S36. ^1H NMR spectrum of **4** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

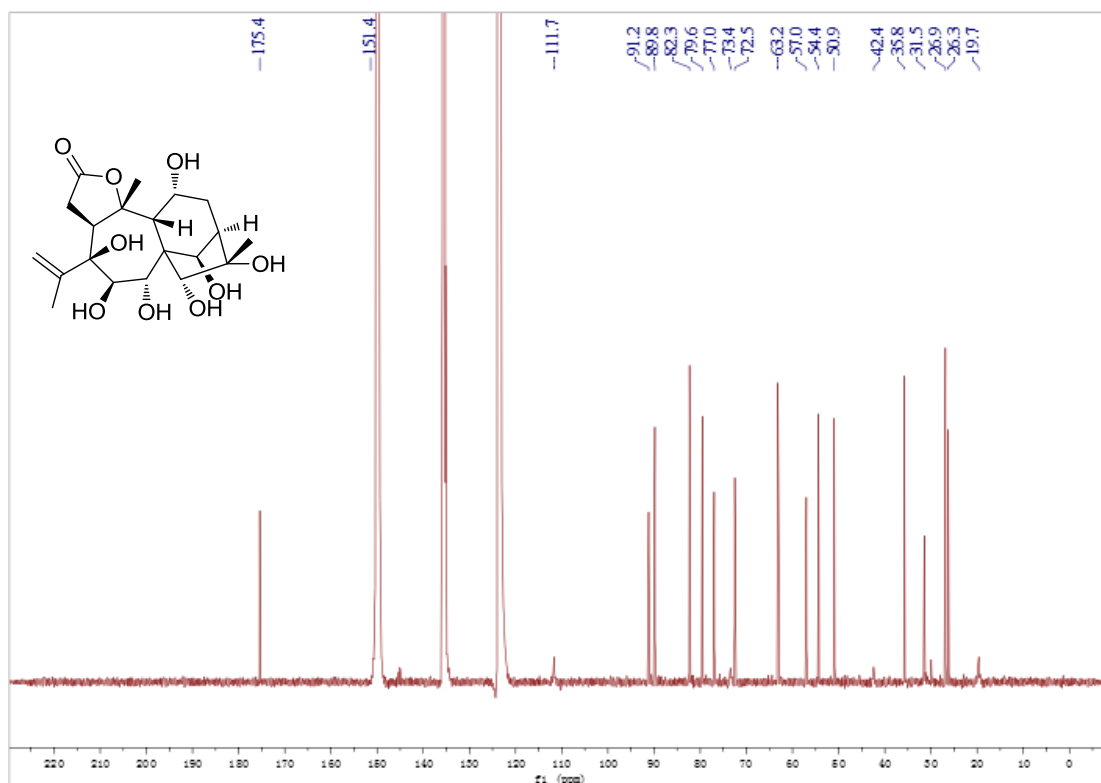


Figure S37. ^{13}C NMR spectrum of **4** (125 MHz, in $\text{C}_5\text{D}_5\text{N}$)

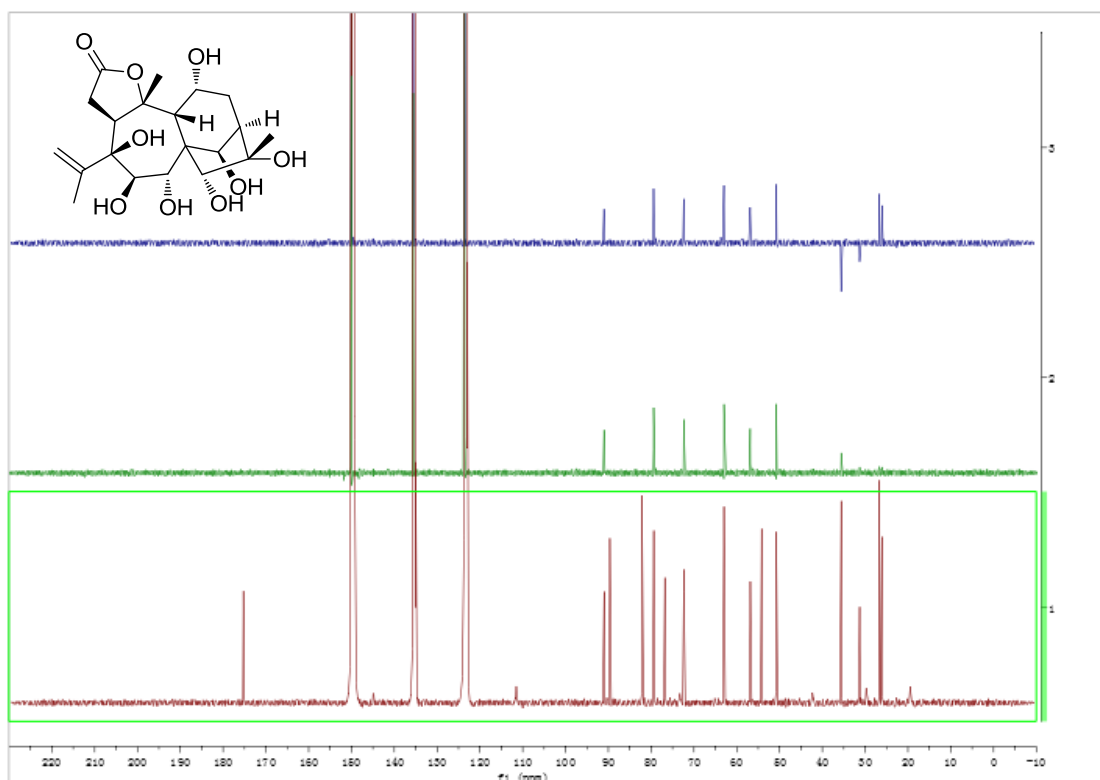


Figure S38. DEPT spectrum of **4** (125 MHz, in C₅D₅N)

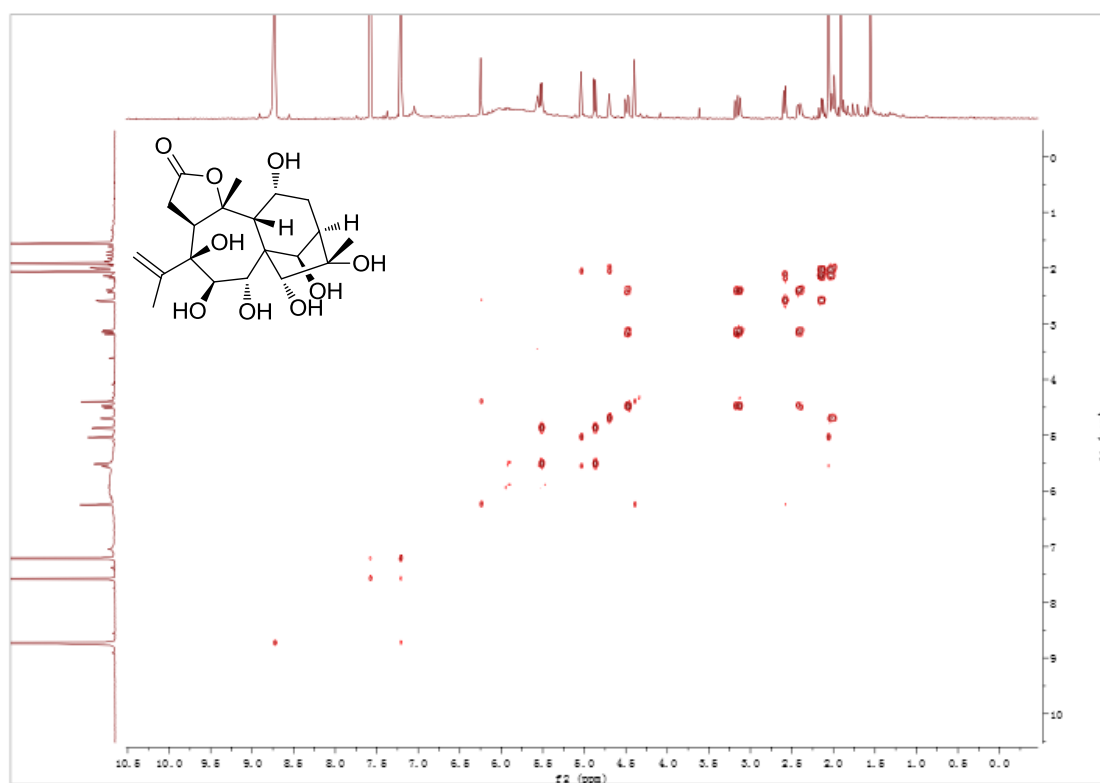


Figure S39. ¹H-¹H COSY spectrum of **4** (500 MHz, in C₅D₅N)

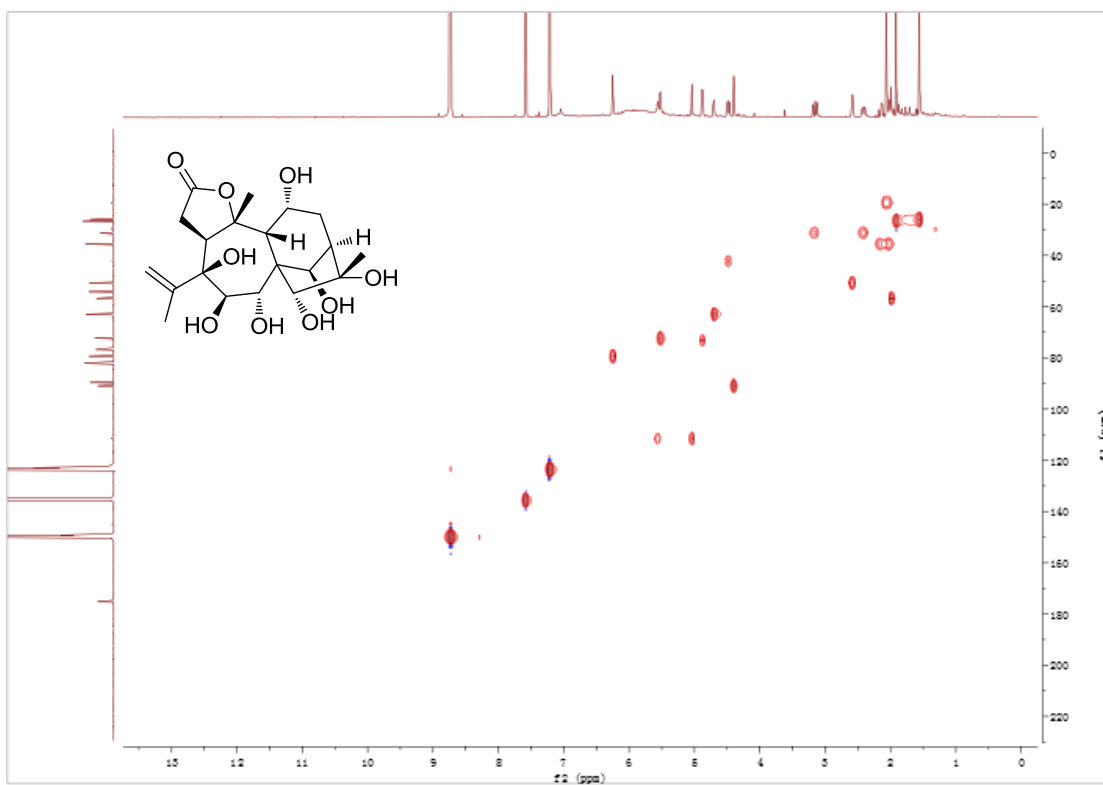


Figure S40. HSQC spectrum of **4** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

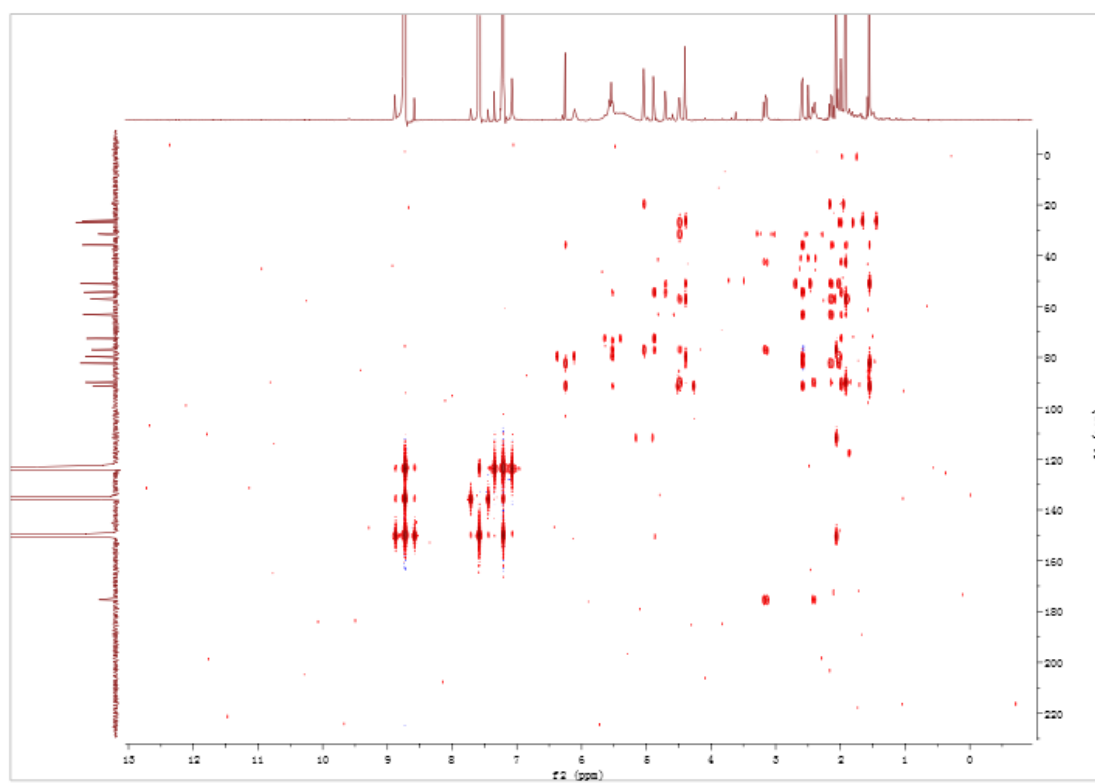


Figure S41. HMBC spectrum of **4** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

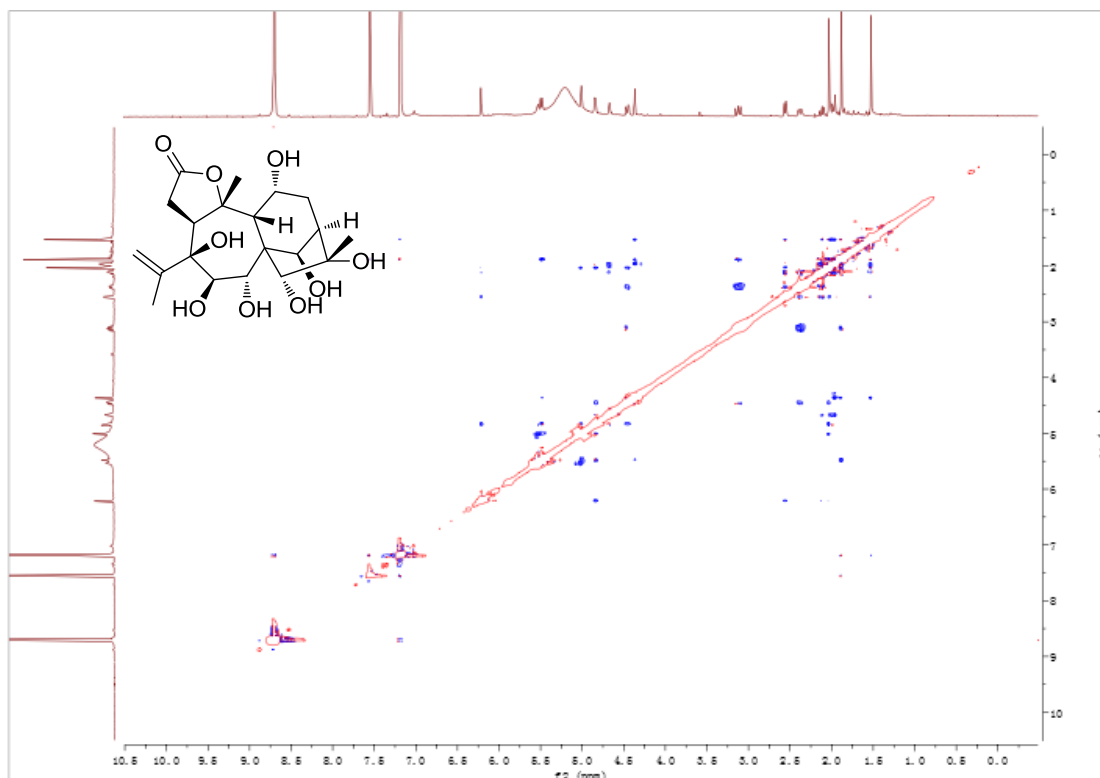


Figure S42. NOESY spectrum of **4** (500 MHz, in C₅D₅N)

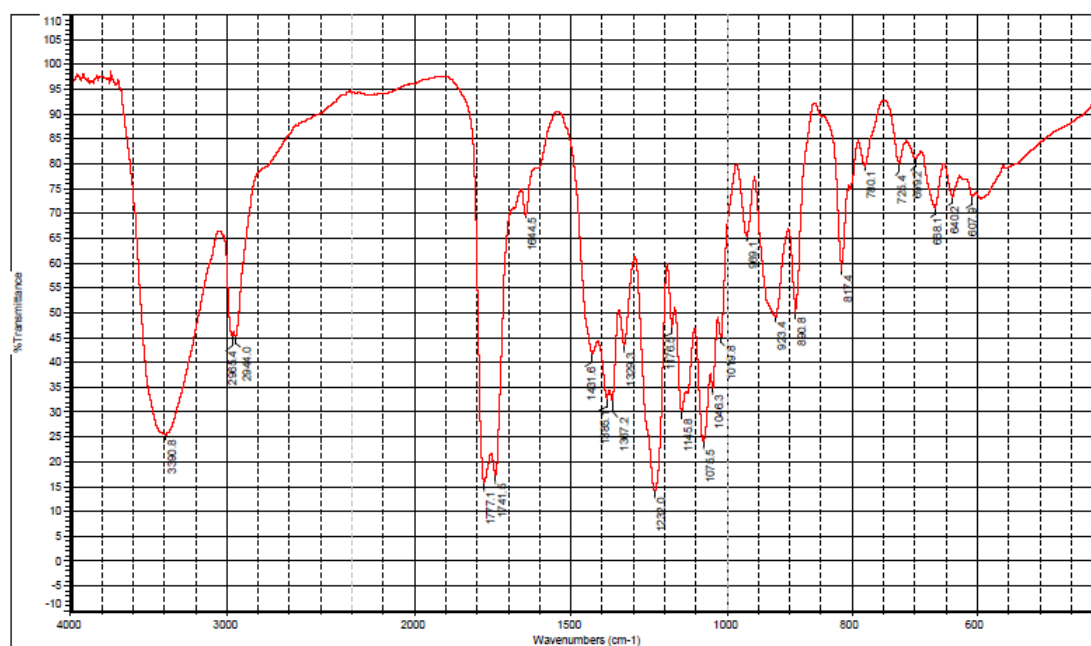


Figure S43. IR spectrum of **5**

MS Formula Results: + Scan (4.539 min) Sub (2016110802.d)

m/z	Ion	Formula	Abundance										
457.2075	(M+H) ⁺	C22 H33 O10	386179.8										
Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DfE
		C22 H32 O10	99.94		456.2002	456.1995	457.2068	-1.37	1.37	99.94	99.95	99.91	7
		C23 H36 O5 S2	97.56		456.2002	456.2004	457.2077	0.53	0.53	99.99	91.9	99.51	6
		C27 H36 S3	94.65		456.2002	456.1979	457.2052	-4.96	4.96	99.17	83.14	98.42	10

Figure S44. (+)-HRESIMS data of **5**

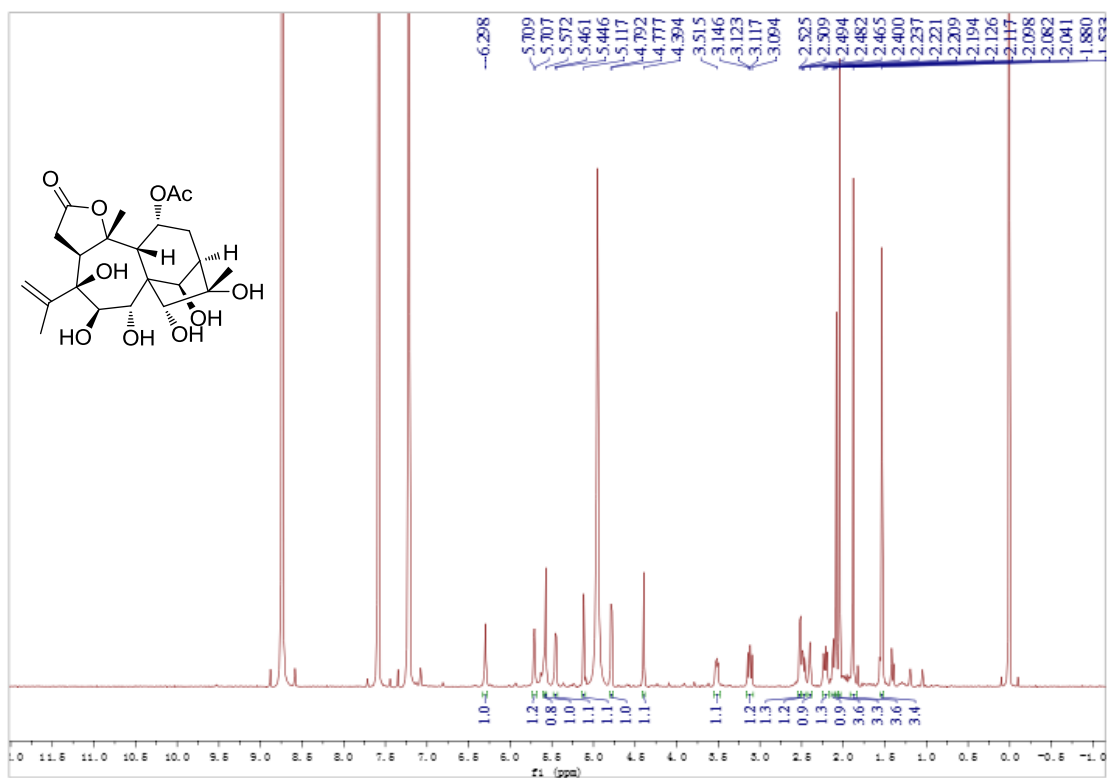


Figure S45. ^1H NMR spectrum of **5** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

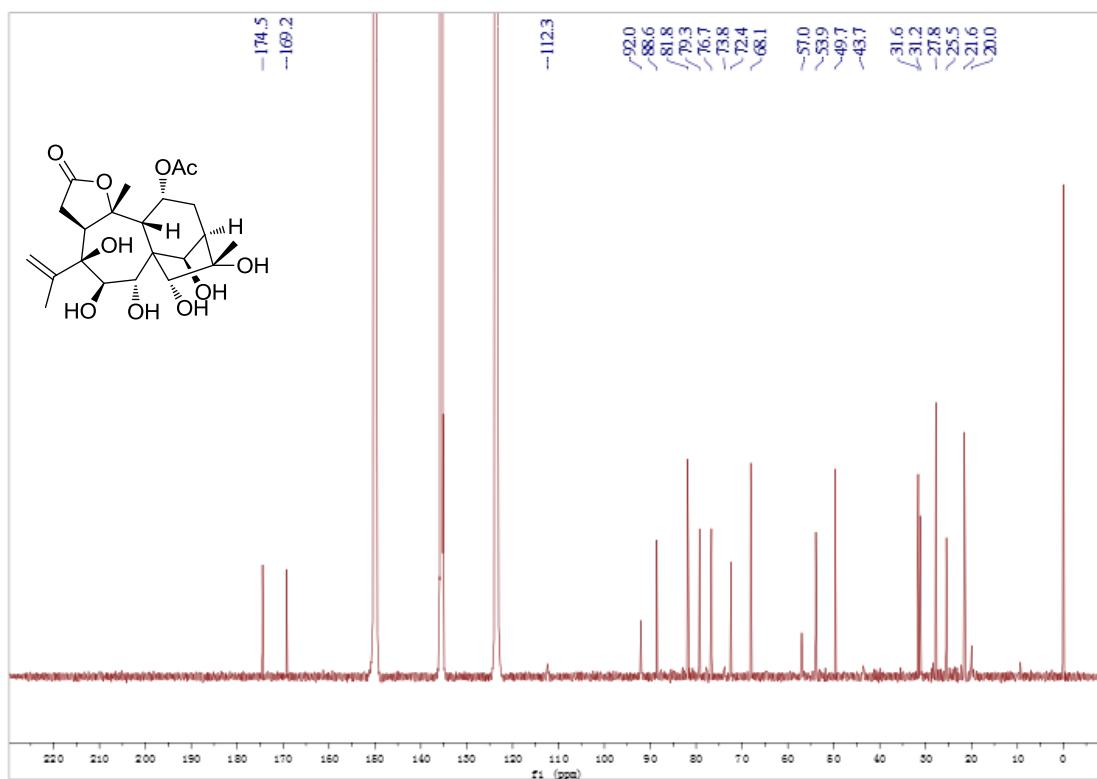


Figure S46. ^{13}C NMR spectrum of **5** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

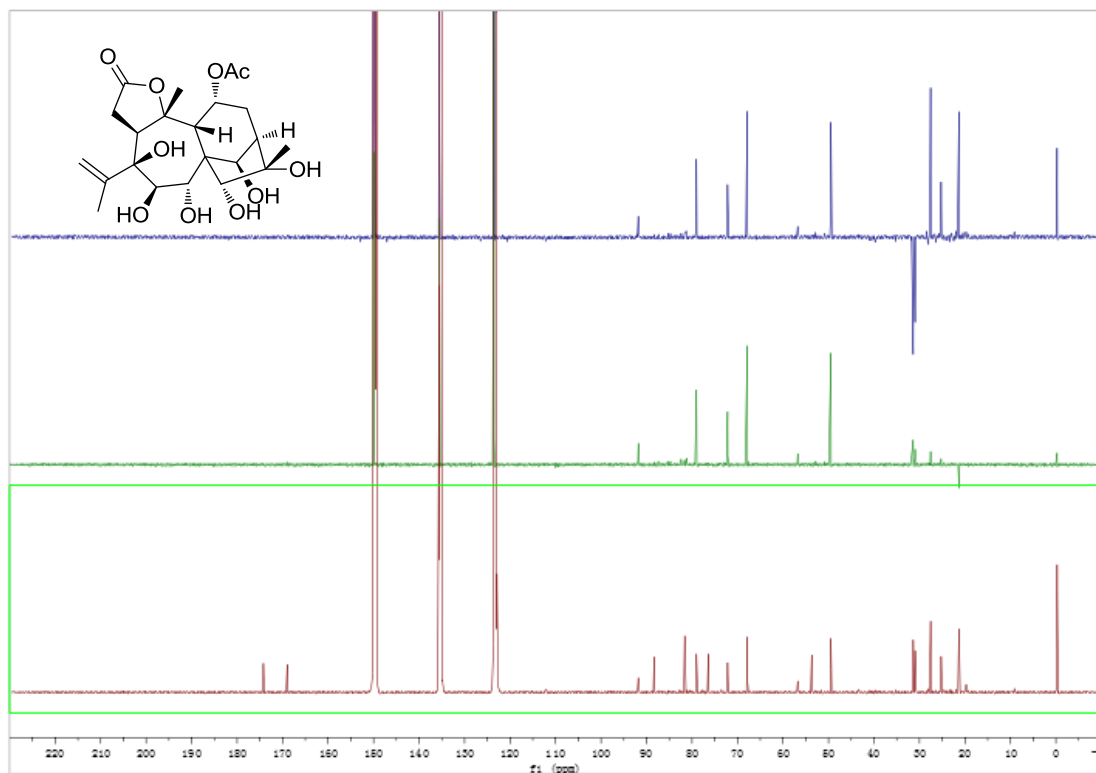


Figure S47. DEPT spectrum of **5** (150 MHz, in C_5D_5N)

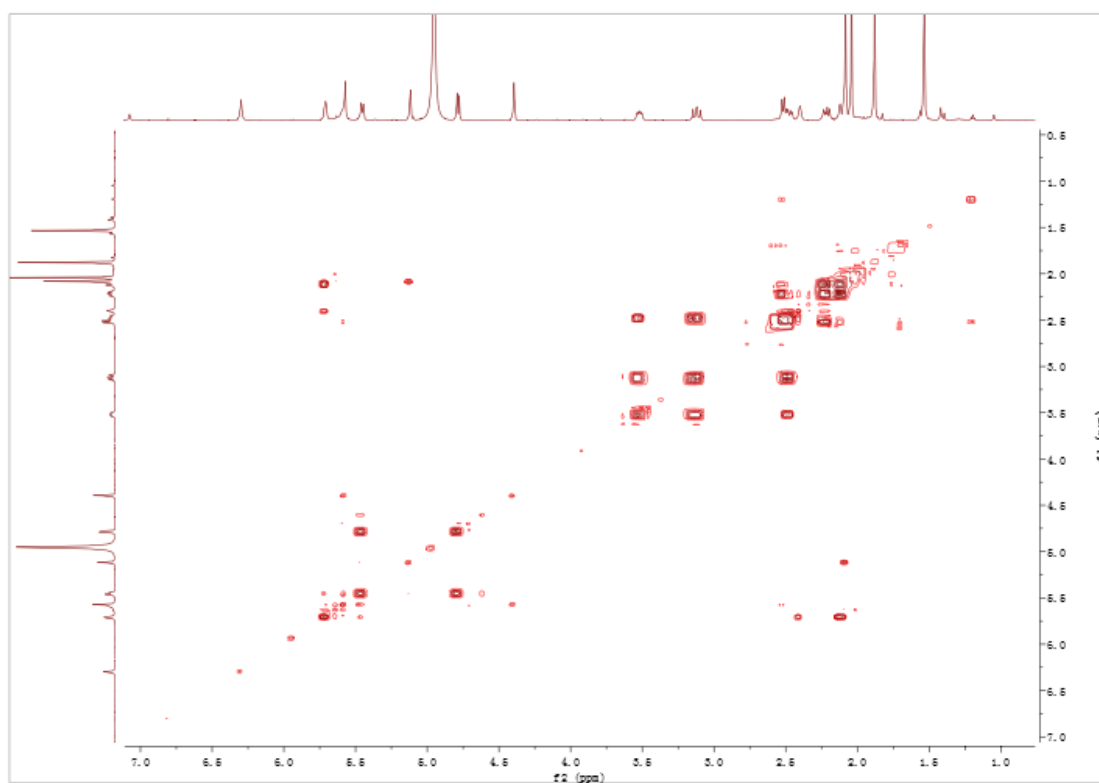


Figure S48. 1H - 1H COSY spectrum of **5** (600 MHz, in C_5D_5N)

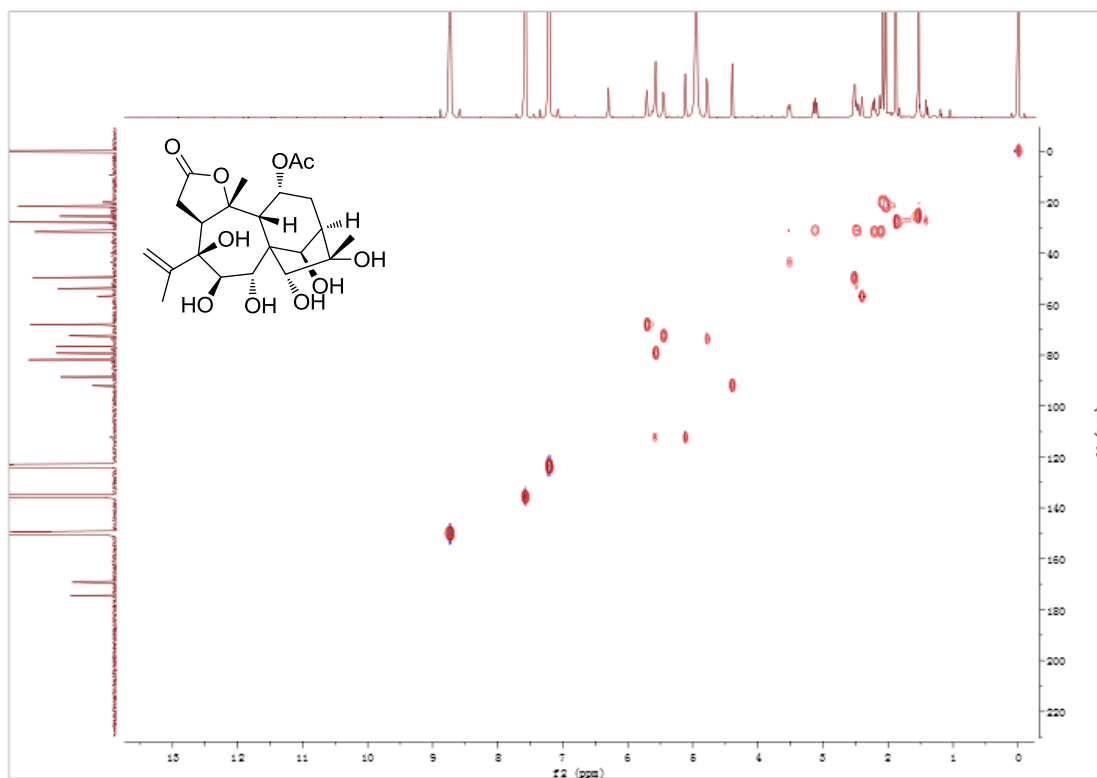


Figure S49. HSQC spectrum of **5** (600 MHz, in C_5D_5N)

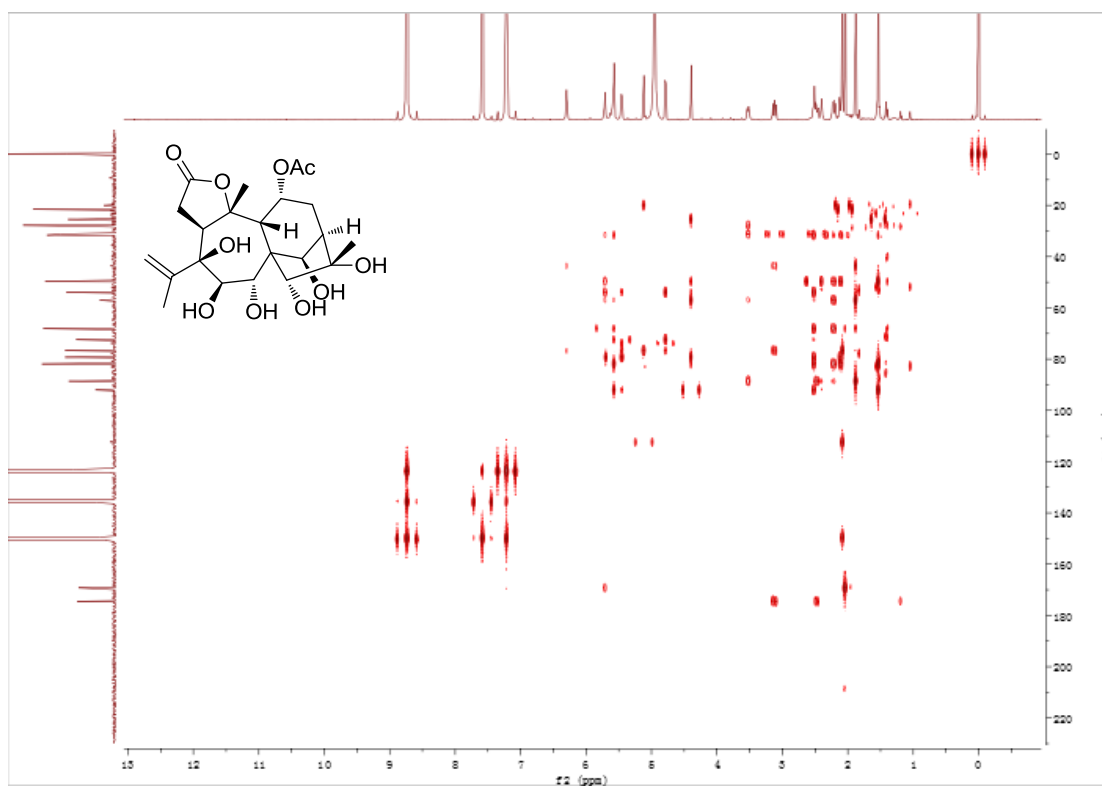


Figure S50. HMBC spectrum of **5** (600 MHz, in C_5D_5N)

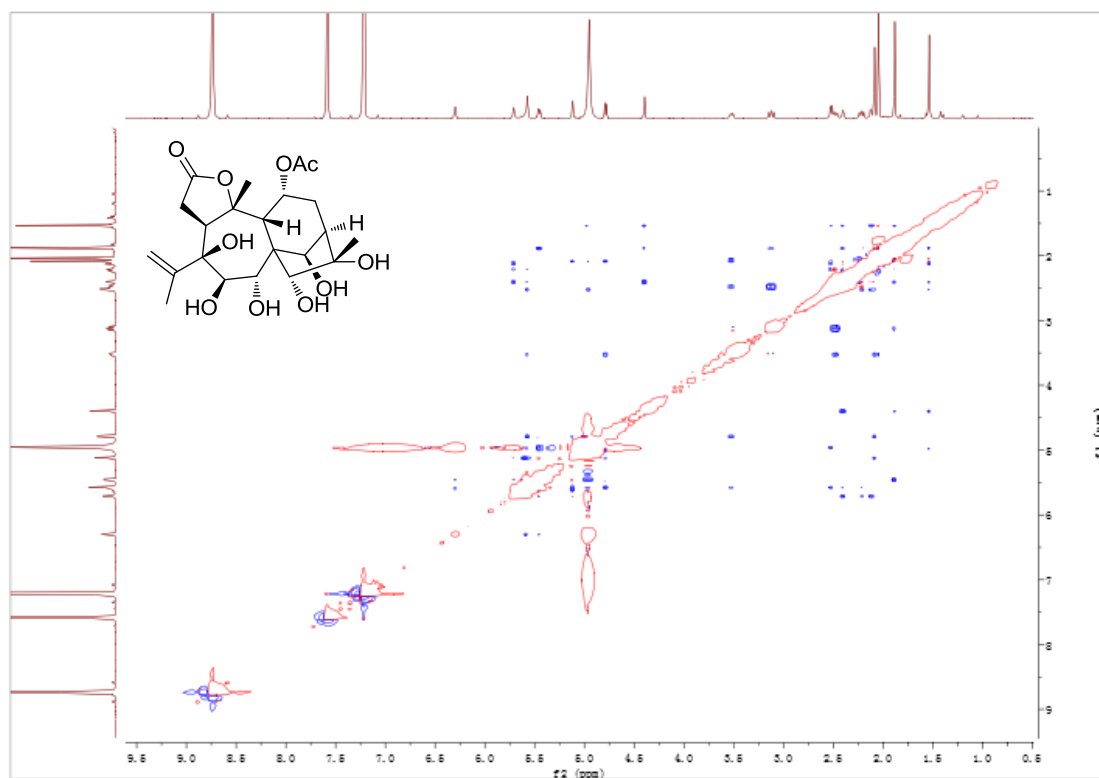


Figure S51. NOESY spectrum of **5** (600 MHz, in C_5D_5N)

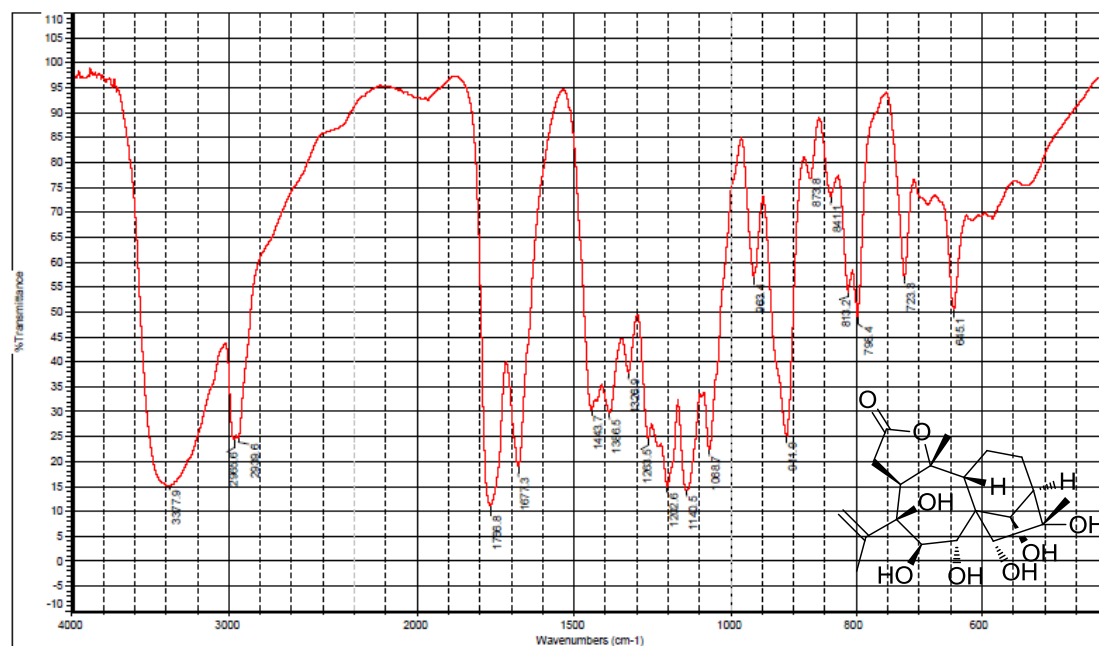


Figure S52. IR spectrum of **6**

MS Formula Results: + Scan (5.098 min) Sub (2016111001.d)

m/z	Ion	Formula	Abundance										
421.1831	(M+Na) ⁺	C20 H30 Na O8	314907.9										
Best	Formula (M)	Ion Formula	Score	Cross Sto	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Alts Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
	C20 H30 O8	C20 H30 Na O8	99.91		396.1939	396.1941	421.1833	0.38	0.36	100	99.84	99.84	6
	C24 H30 O3 S	C24 H30 Na O3 S	96.05		398.1939	398.1916	421.1808	-5.91	5.91	96.96	95.13	99.71	10
	C21 H34 O3 S2	C21 H34 Na O3 S2	97.26		398.1939	398.1949	421.1842	2.55	2.55	99.81	91.11	99.52	5

Figure S53. (+)-HRESIMS data of **6**

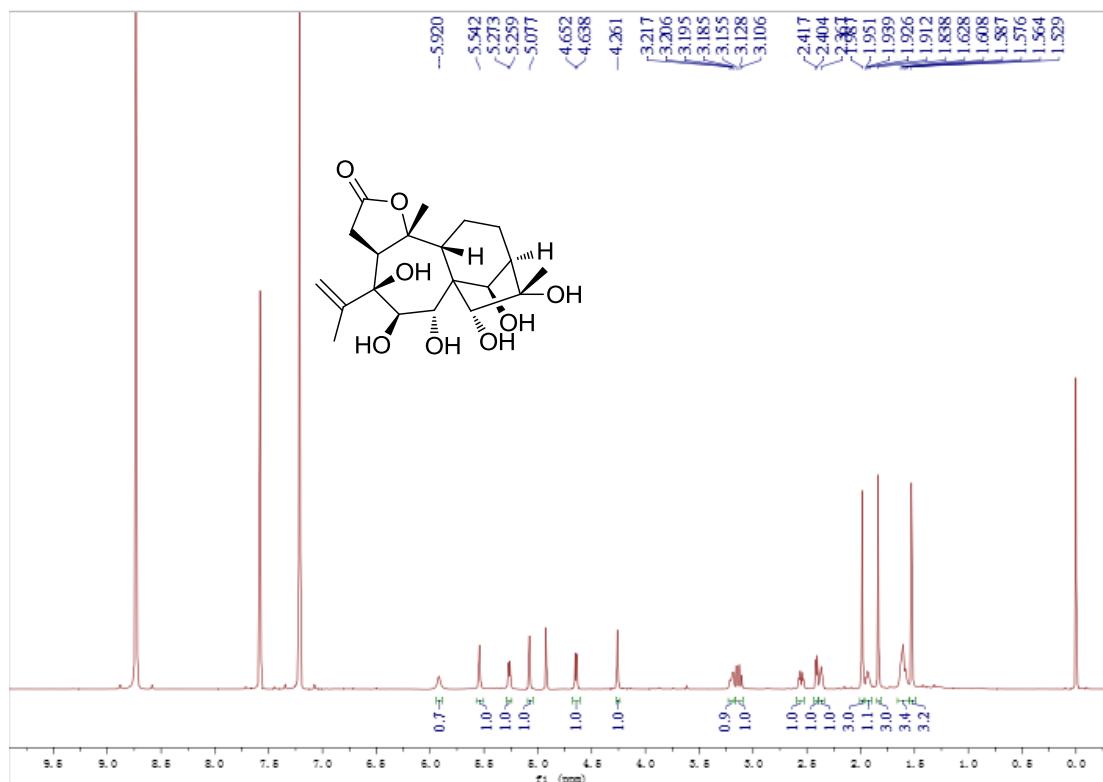


Figure S54. ¹H NMR spectrum of **6** (600 MHz, in C₅D₅N)

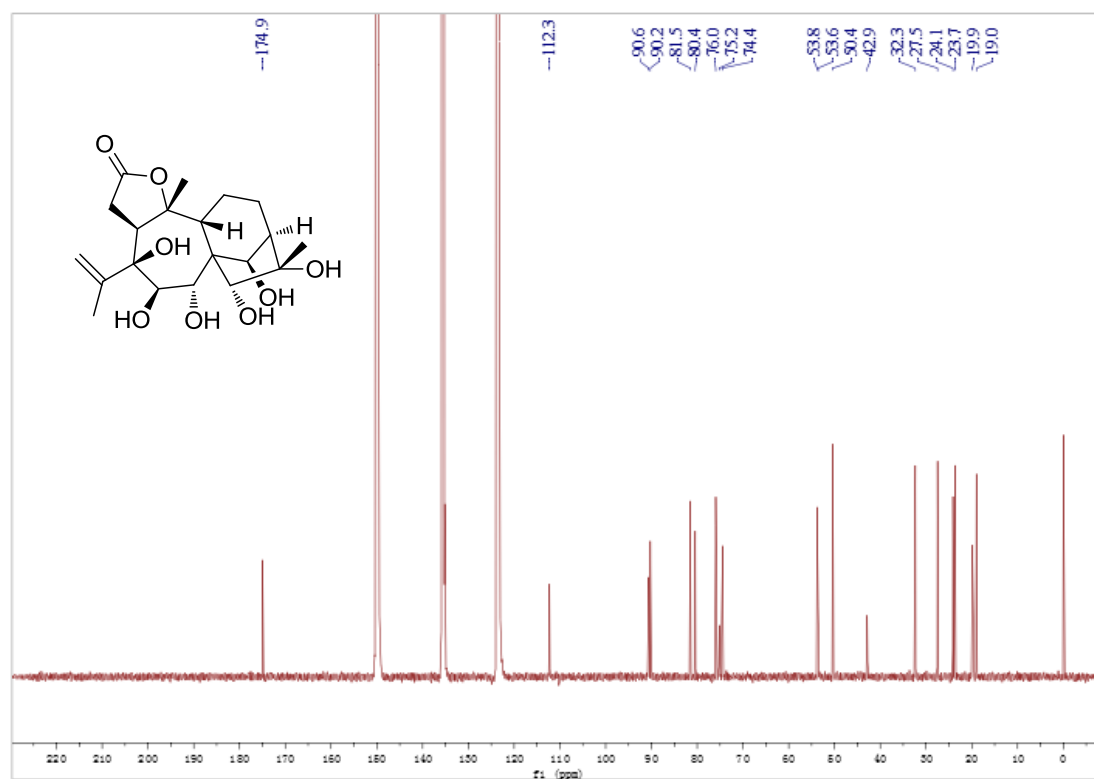


Figure S55. ¹³C NMR spectrum of **6** (150 MHz, in C₅D₅N)

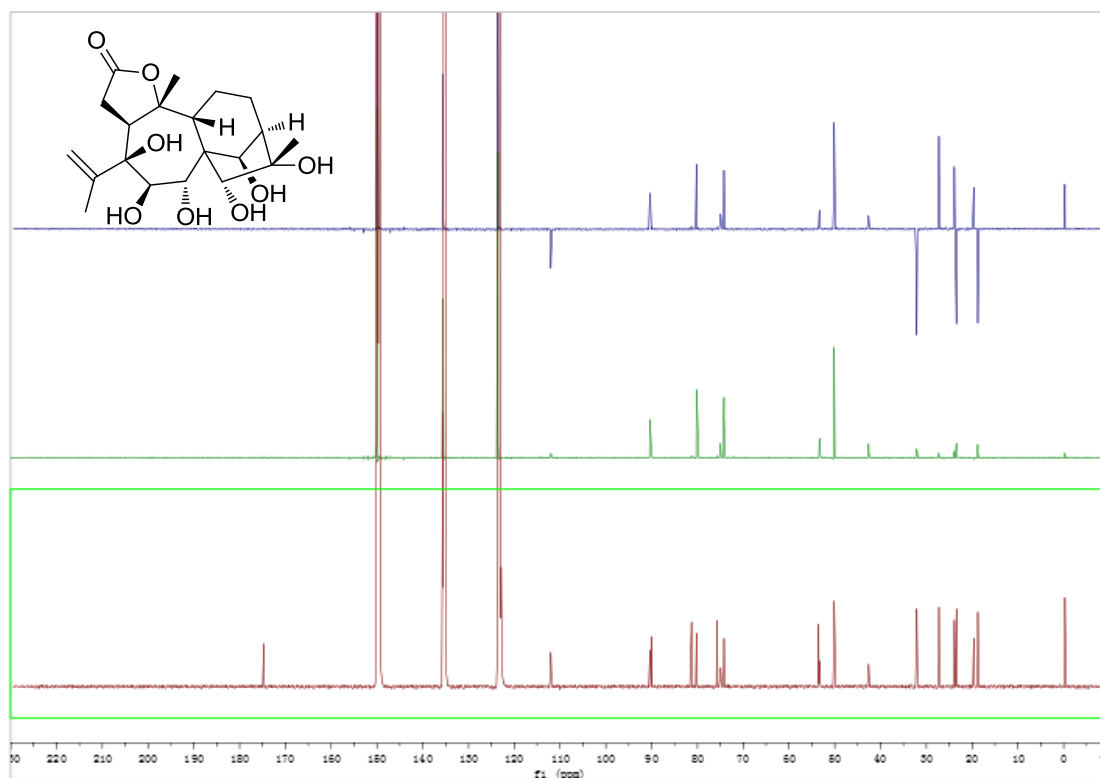


Figure S56. DEPT spectrum of **6** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

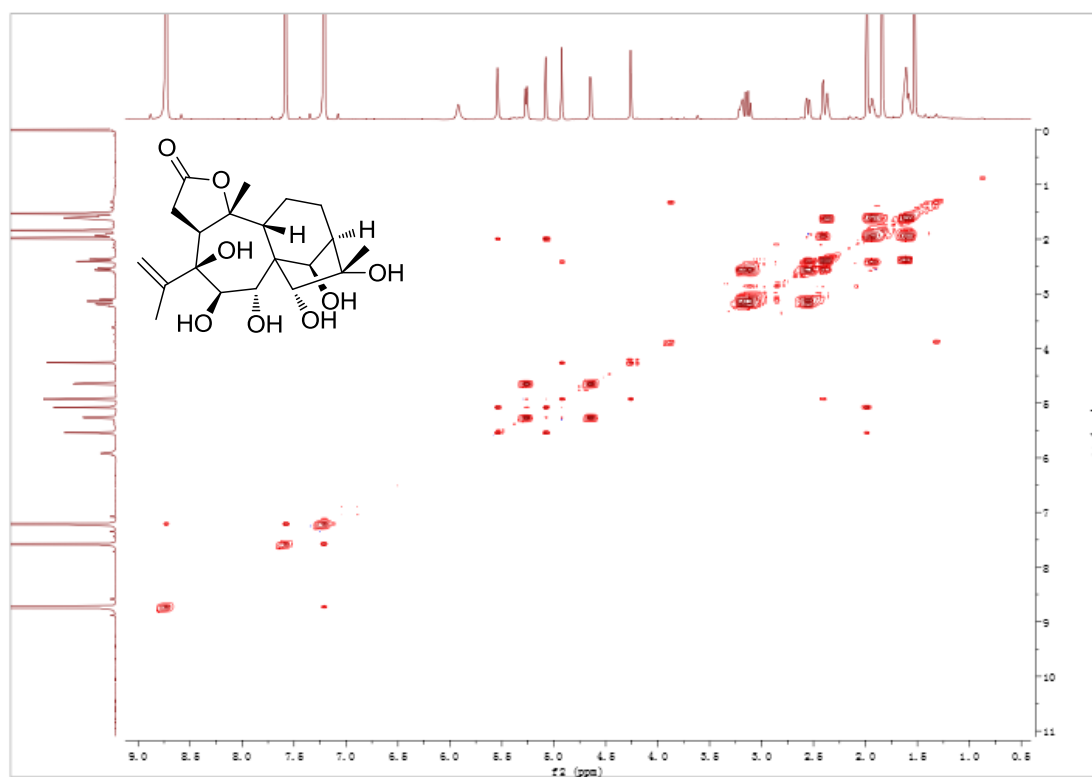


Figure S57. ^1H - ^1H COSY spectrum of **6** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

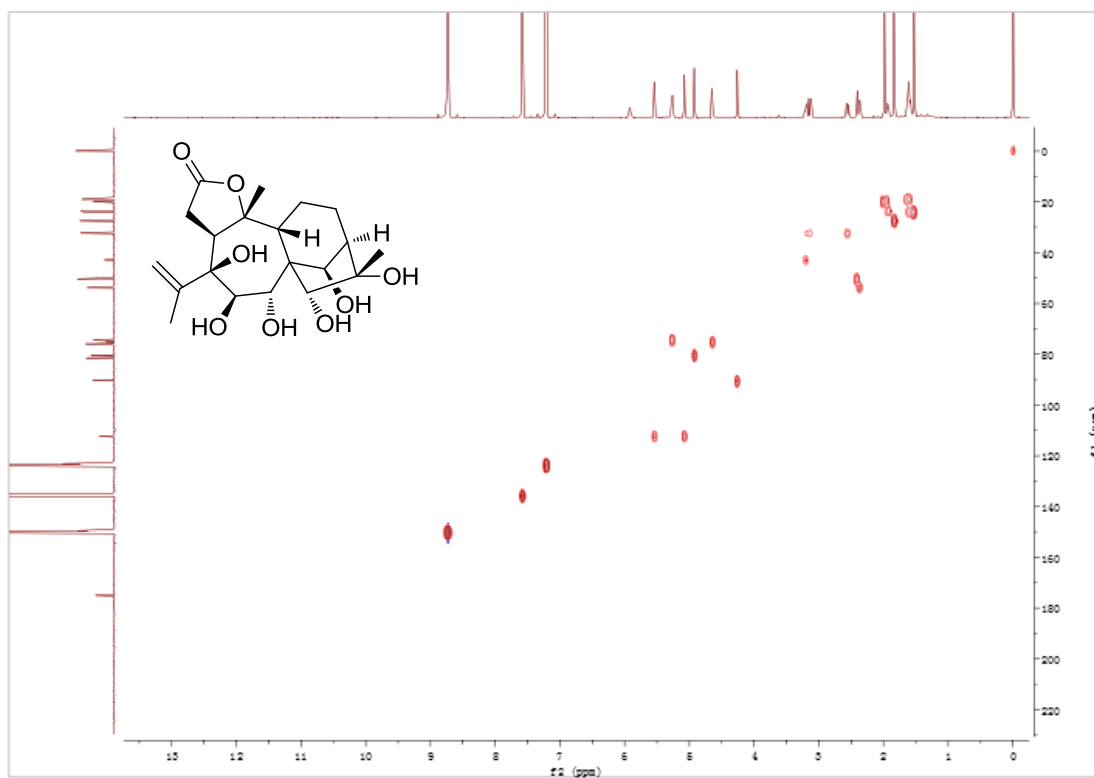


Figure S58. HSQC spectrum of **6** (600 MHz, in C₅D₅N)

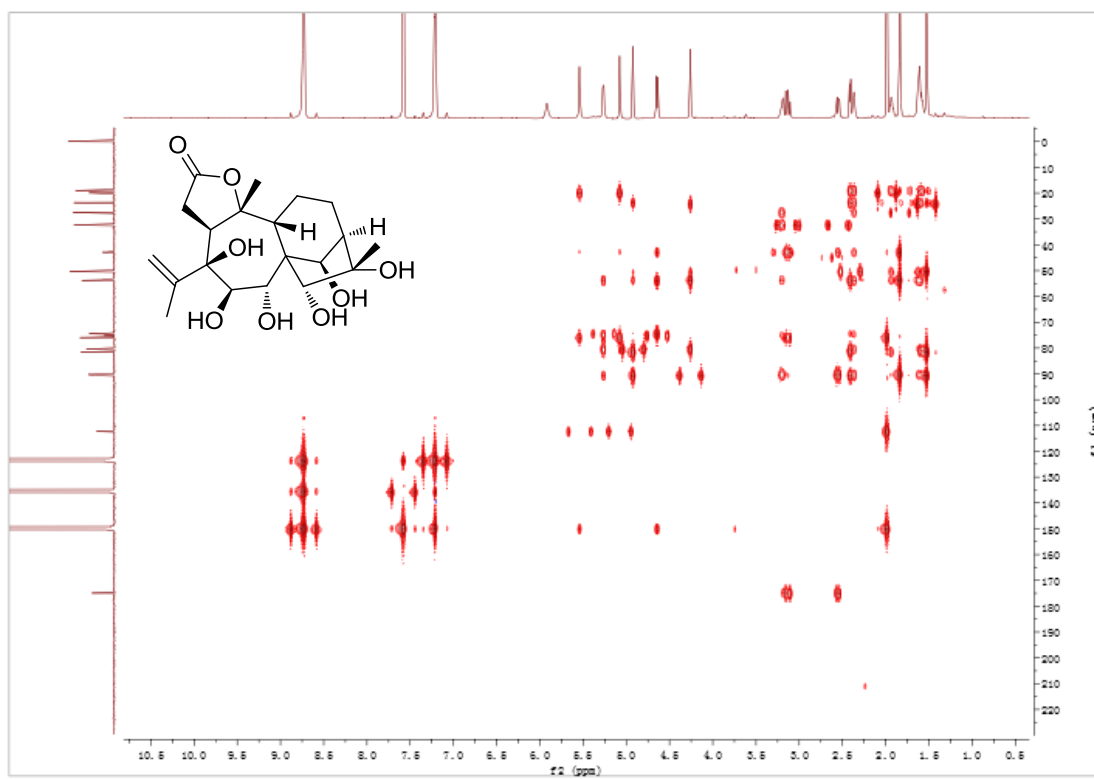


Figure S59. HMBC spectrum of **6** (600 MHz, in C₅D₅N)

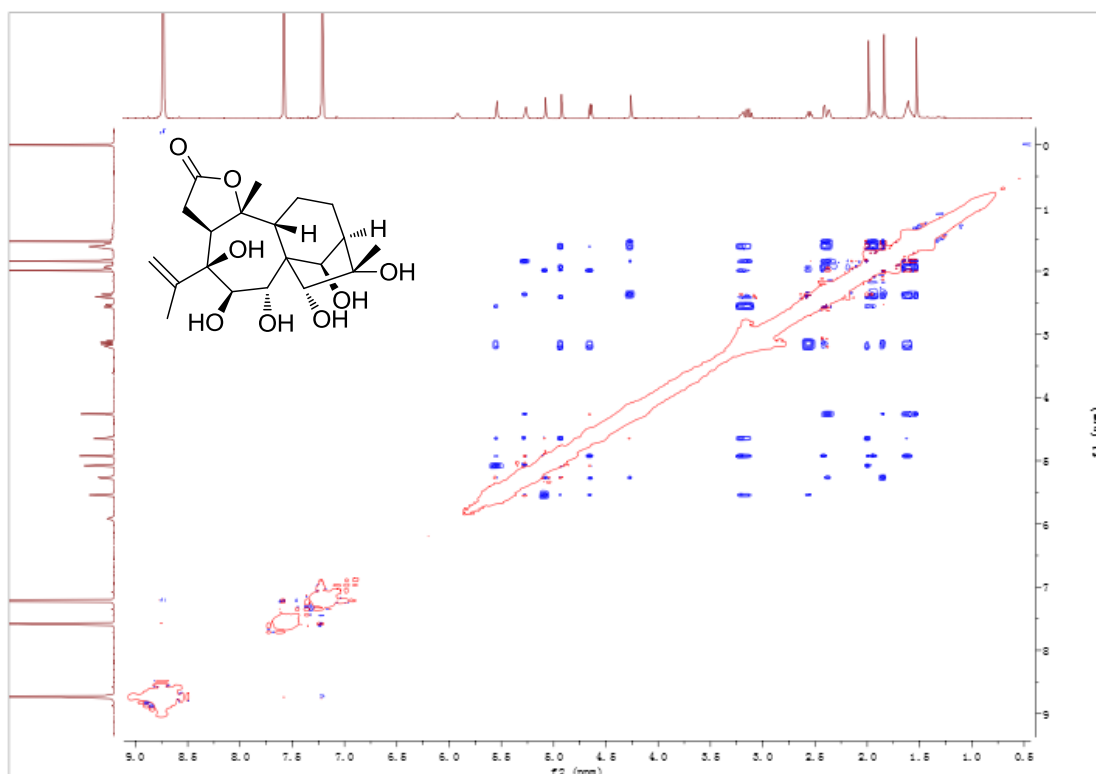


Figure S60. NOESY spectrum of **6** (600 MHz, in C_5D_5N)

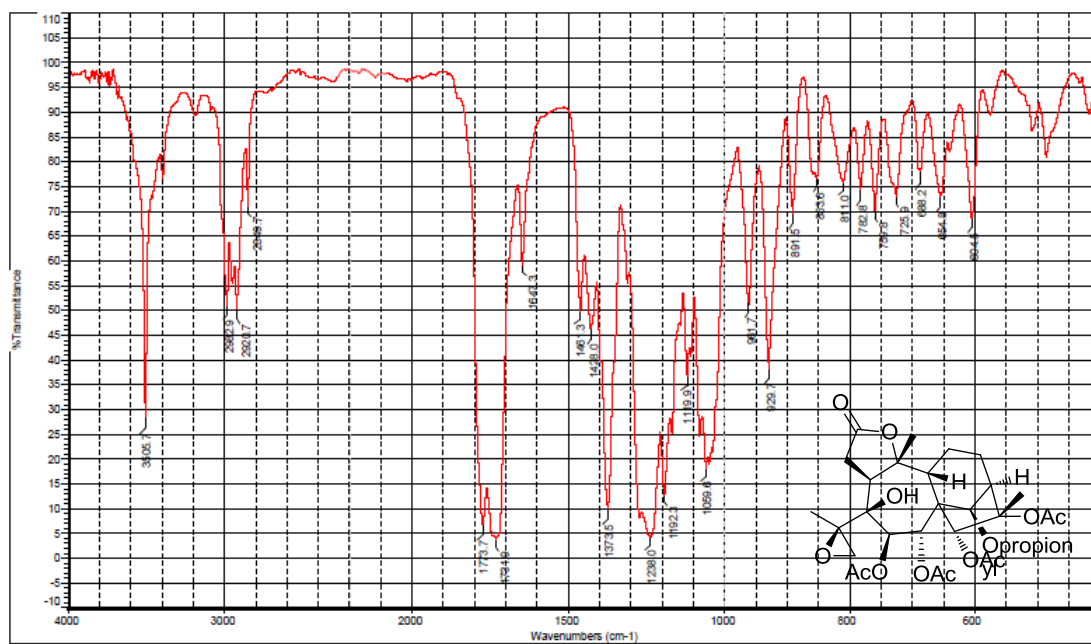


Figure S61. IR spectrum of **7**

MS Formula Results: + Scan (6.499 min) Sub (2015091706.d)

m/z	Ion	Formula	Abundance
661.2478	(M+Na) ⁺	C ₃₁ H ₄₂ NaO ₁₄	882556.8

Ret ¹	Formula (M)	Ion Formula	Score	Cross sco	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
+	[-]	C ₃₁ H ₄₂ NaO ₁₄	99.99		638.2585	638.2575	661.2487	-1.7	1.7	99.9	99.98	99.89	11
+	[-]	C ₃₂ H ₃₈ NaO ₁₀	99.83		638.2585	638.2588	661.248	0.38	0.38	100	99.49	99.92	16
+	[-]	C ₂₇ H ₃₈ NaO ₁₂	99.35		638.2585	638.2546	661.244	-5.94	5.94	88.84	99.71	99.98	12
+	[-]	C ₂₀ H ₄₂ NaO ₁₇	98.11		638.2585	638.2606	661.2499	3.26	3.26	99.65	91.99	99.99	3
+	[-]	C ₄₄ H ₃₄ N ₂ O ₃	97.08		638.2585	638.2569	661.2462	-2.51	2.51	99.79	90.25	99.85	29
+	[-]	C ₄₉ H ₃₄ O	95.45		638.2585	638.281	661.2922	3.8	3.8	99.52	85.02	99.82	33

Figure S62. (+)-HRESIMS data of **7**

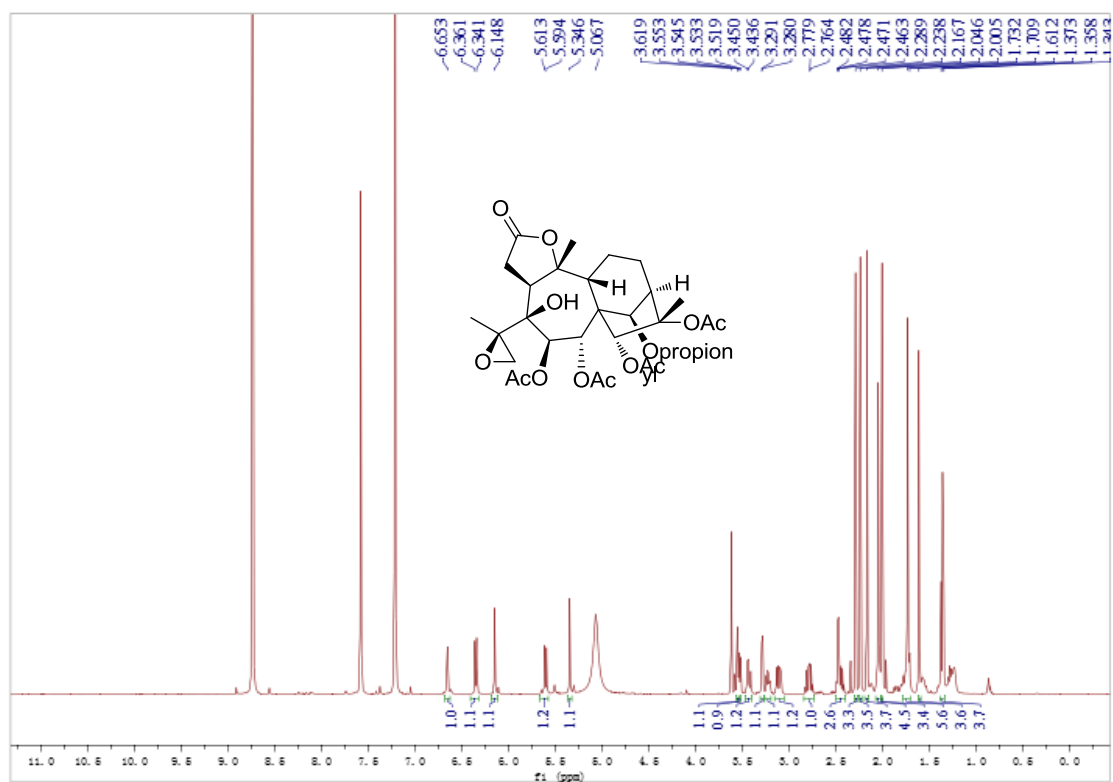


Figure S63. ^1H NMR spectrum of **7** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

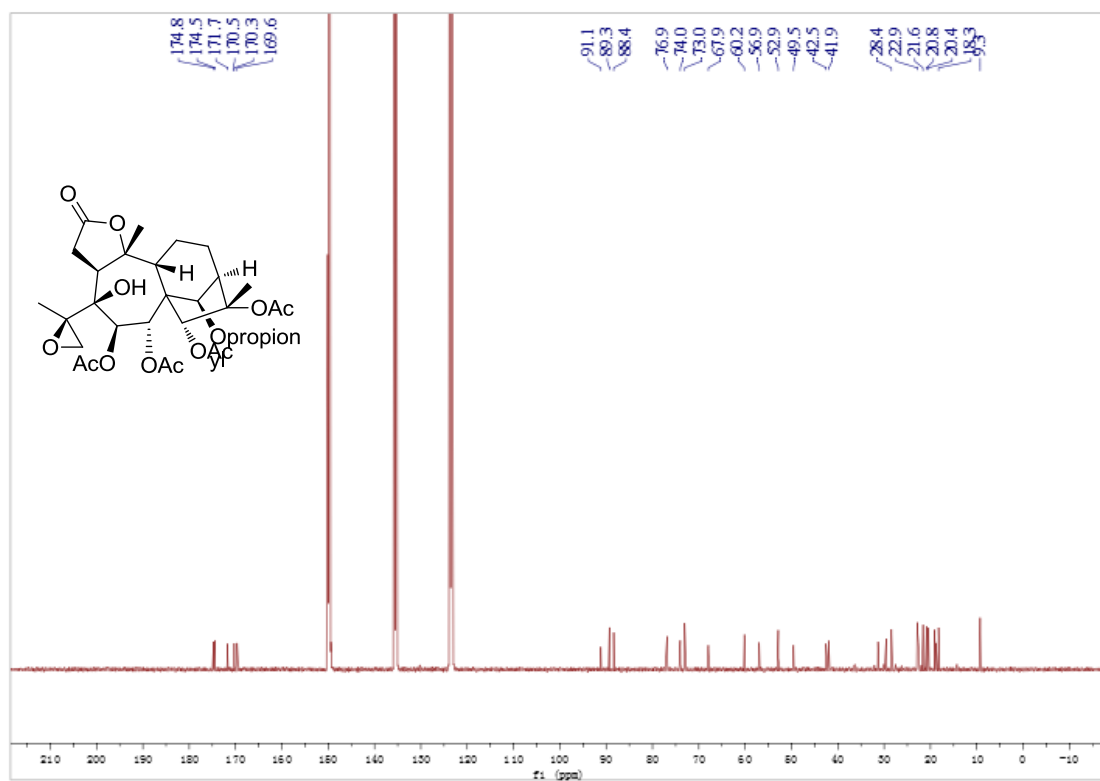


Figure S64. ^{13}C NMR spectrum of **7** (125 MHz, in $\text{C}_5\text{D}_5\text{N}$)

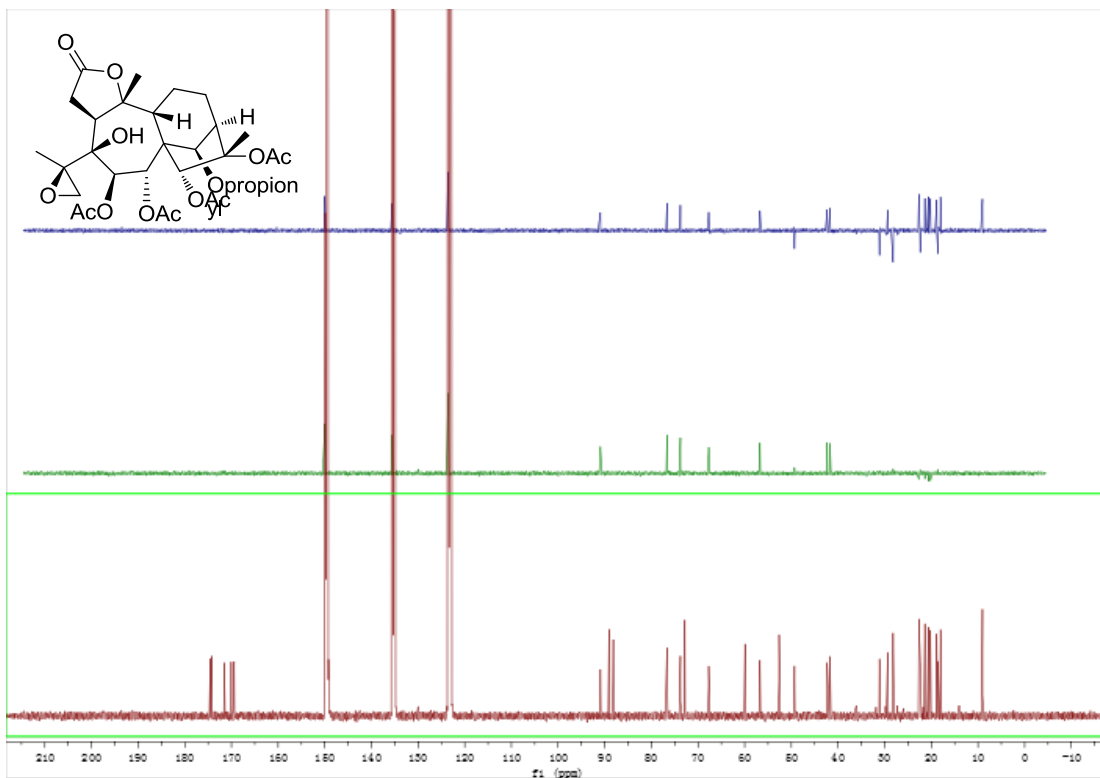


Figure S65. DEPT spectrum of **7** (125 MHz, in C_5D_5N)

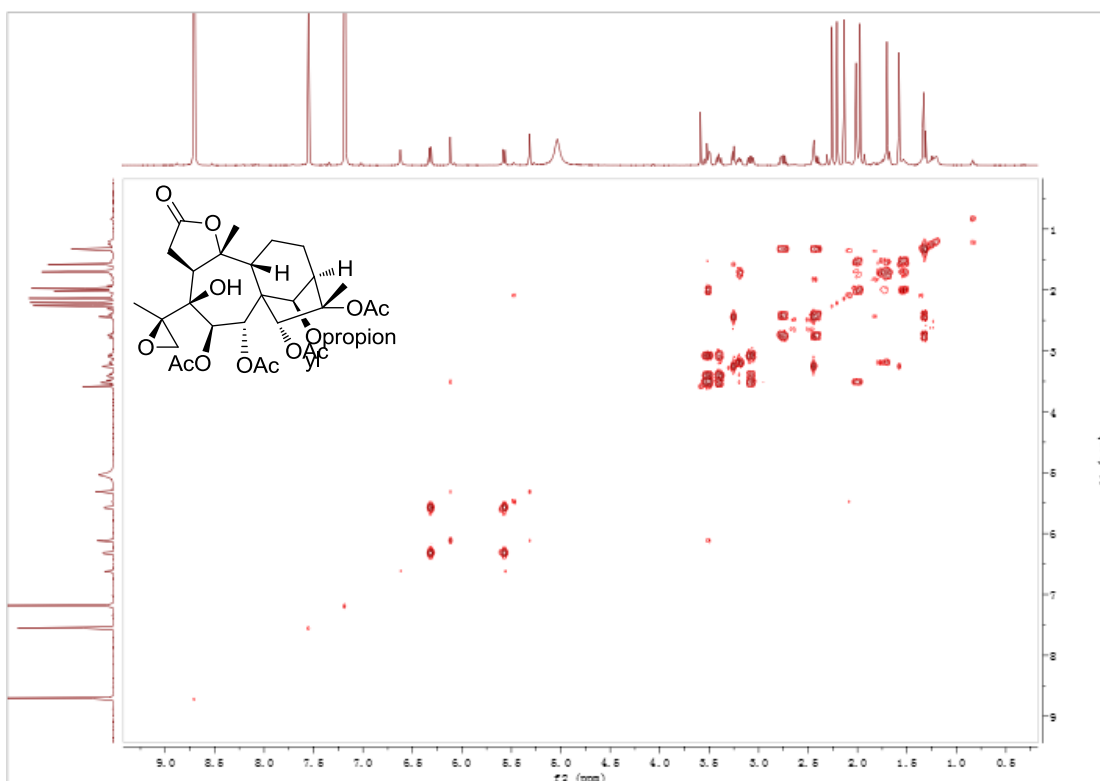


Figure S66. 1H - 1H COSY spectrum of **7** (500 MHz, in C_5D_5N)

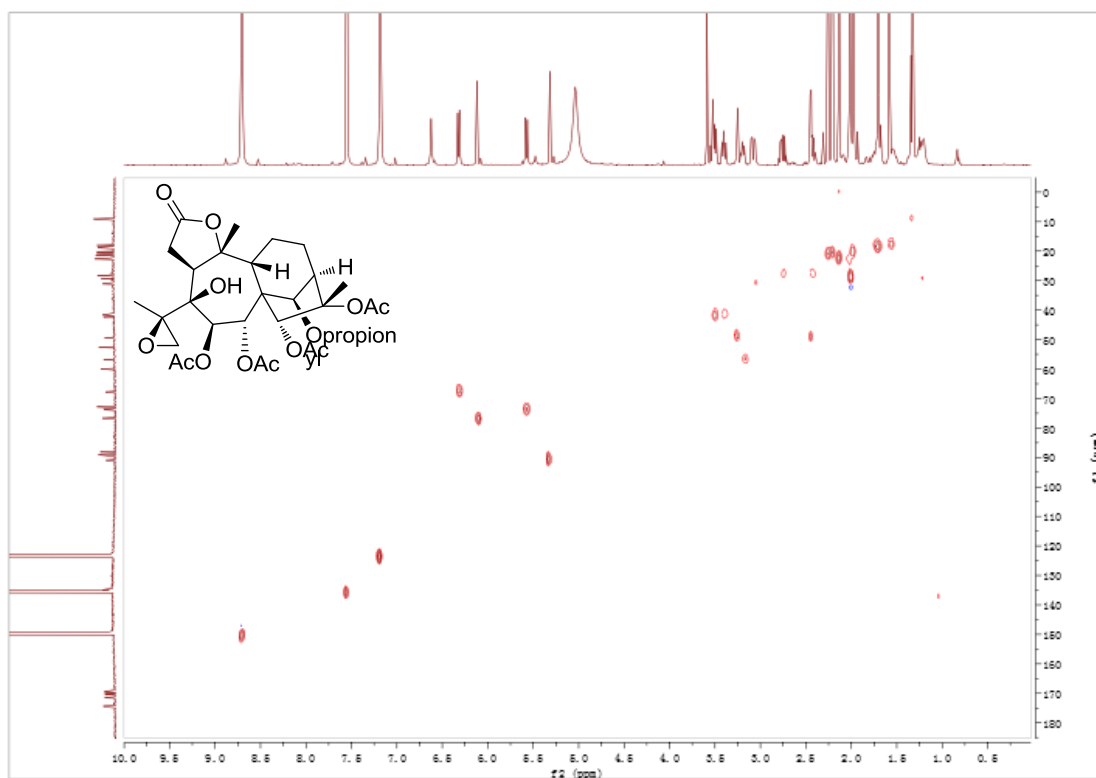


Figure S67. HSQC spectrum of **7** (500 MHz, in C₅D₅N)

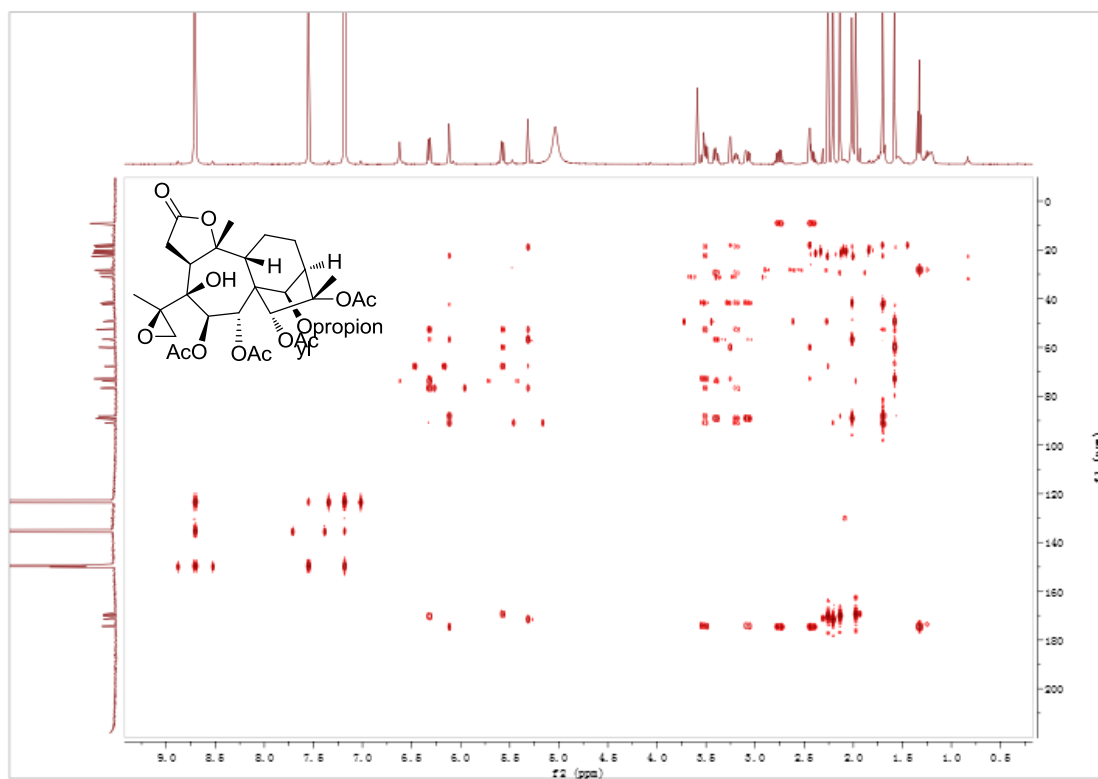


Figure S68. HMBC spectrum of **7** (500 MHz, in C₅D₅N)

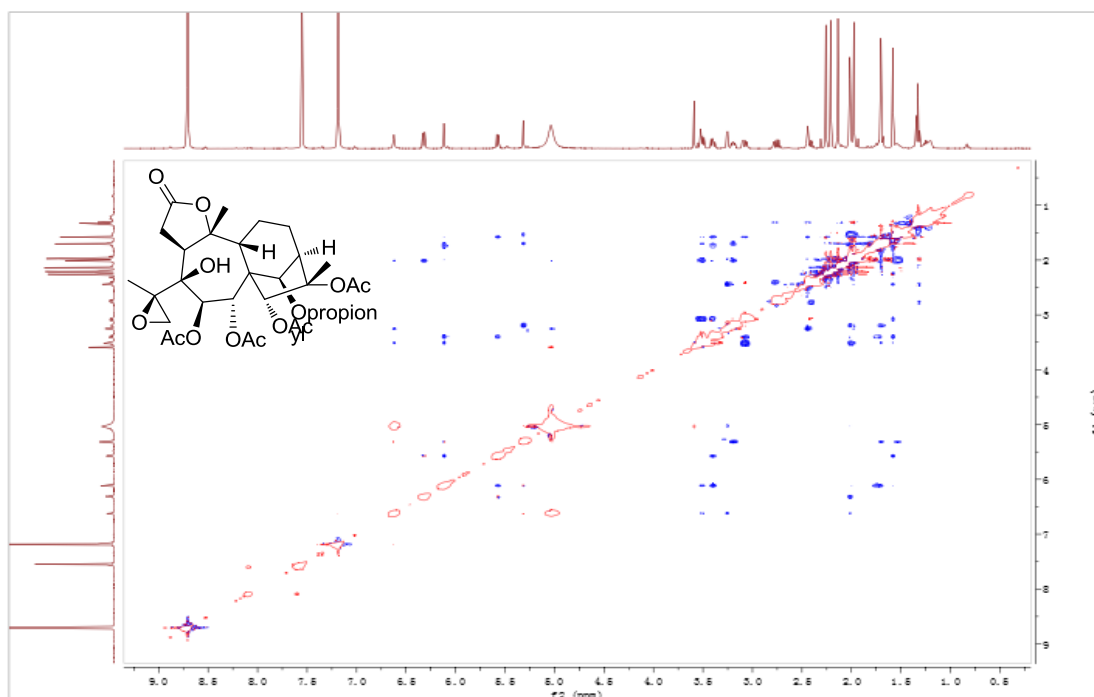


Figure S69. NOESY spectrum of **7** (500 MHz, in C_5D_5N)

Table S2. Crystal data and structure refinement for **7**

Identification code	exp_3590
Empirical formula	$C_{32}H_{42}O_{15}$.26177
Formula weight	670.84
Temperature/K	102.8
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a / Å, b / Å, c / Å	12.7605(3), 15.5108(5), 16.9324(4)
$\alpha/^\circ, \beta/^\circ, \gamma/^\circ$	90, 90, 90
Volume/Å ³	3351.35(16)
Z	4
$\rho_{\text{calc}}/\text{mg mm}^{-3}$	1.330
μ/mm^{-1}	0.900
F(000)	1424
Crystal size/mm ³	0.450 × 0.400 × 0.400
2 θ range for data collection	7.73 to 141.822°
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 16, -12 ≤ l ≤ 20
Reflections collected	12021
Independent reflections	6334[R(int) = 0.0234 (inf-0.9Å)]
Data/restraints/parameters	6334/0/462
Goodness-of-fit on F ²	1.031
Final R indexes [I > 2 σ (I) i.e. F _o > 4 σ (F _o)]	R ₁ = 0.0366, wR ₂ = 0.0931
Final R indexes [all data]	R ₁ = 0.0388 wR ₂ = 0.0951
Largest diff. peak/hole/e Å ⁻³	0.199/-0.300
Flack Parameters	0.04(7)
Completeness	1.000

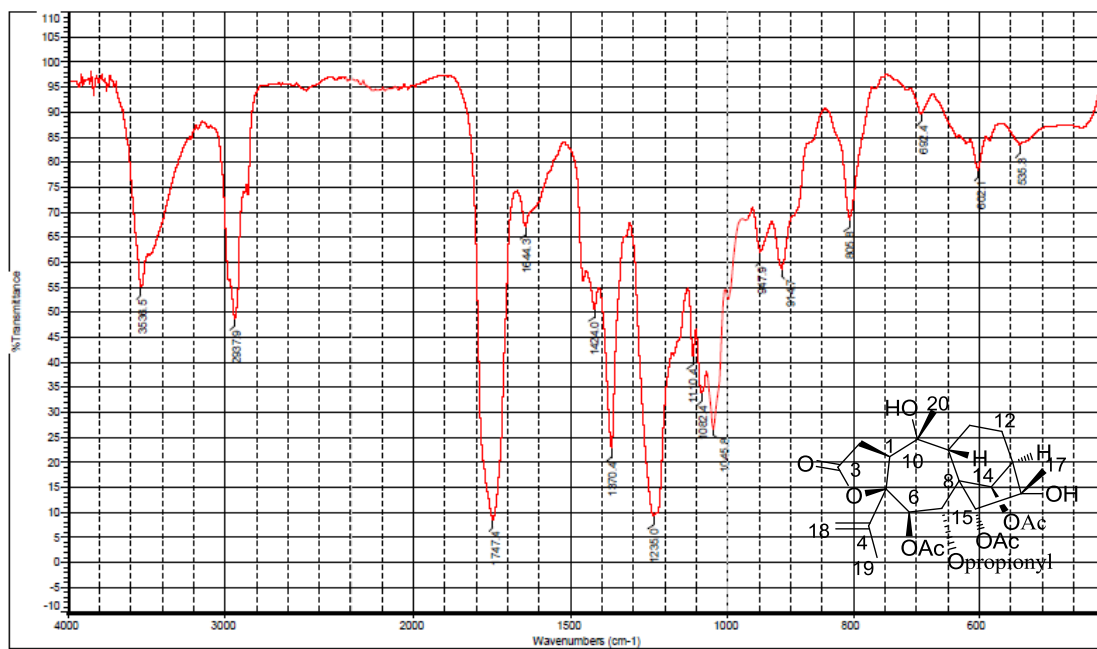


Figure S70. IR spectrum of **8**

MS Formula Results: + Scan (6.106 min) Sub (2015070701.d)

m/z	Ion	Formula	Abundance
603.2398	(M+Na) ⁺	C ₂₉ H ₄₀ NaO ₁₂	176758

Beat	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C ₂₉ H ₄₀ O ₁₂	C ₂₉ H ₄₀ NaO ₁₂	99.89		580.2506	580.252	603.2412	2.35	2.35	99.82	99.98	99.95	10
+	C ₂₅ H ₃₆ N ₆ O ₁₀	C ₂₅ H ₃₆ N ₆ NaO ₁₀	99.77		580.2506	580.2493	603.2385	-2.3	2.3	99.83	99.6	99.67	11
+	C ₃₀ H ₃₆ N ₄ O ₈	C ₃₀ H ₃₆ N ₄ NaO ₈	99.5		580.2506	580.2533	603.2425	4.64	4.64	99.3	99.48	99.91	15
+	C ₂₄ H ₄₀ N ₂ O ₁₄	C ₂₄ H ₄₀ N ₂ NaO ₁₄	99.24		580.2506	580.248	603.2372	-4.99	4.99	99.32	98.95	99.93	6
+	C ₃₇ H ₃₂ N ₄ O ₃	C ₃₇ H ₃₂ N ₄ NaO ₃	97.63		580.2506	580.2474	603.2367	-5.48	5.48	99.03	94.47	99.91	24
+	C ₄₂ H ₃₂ N ₂ O	C ₄₂ H ₃₂ N ₂ NaO	96.97		580.2506	580.2515	603.2407	1.46	1.46	99.93	89.57	99.91	28

Figure S71. (+)-HRESIMS data of **8**

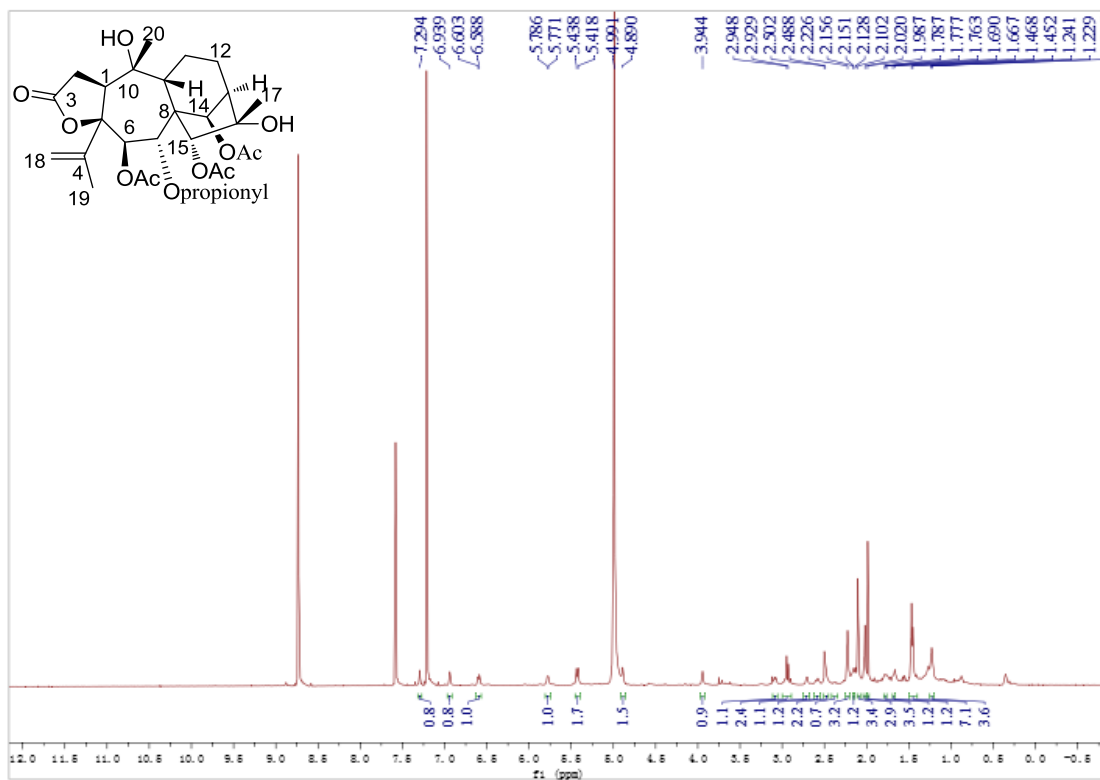


Figure S72. ¹H NMR spectrum of **8** (600 MHz, in C₅D₅N)

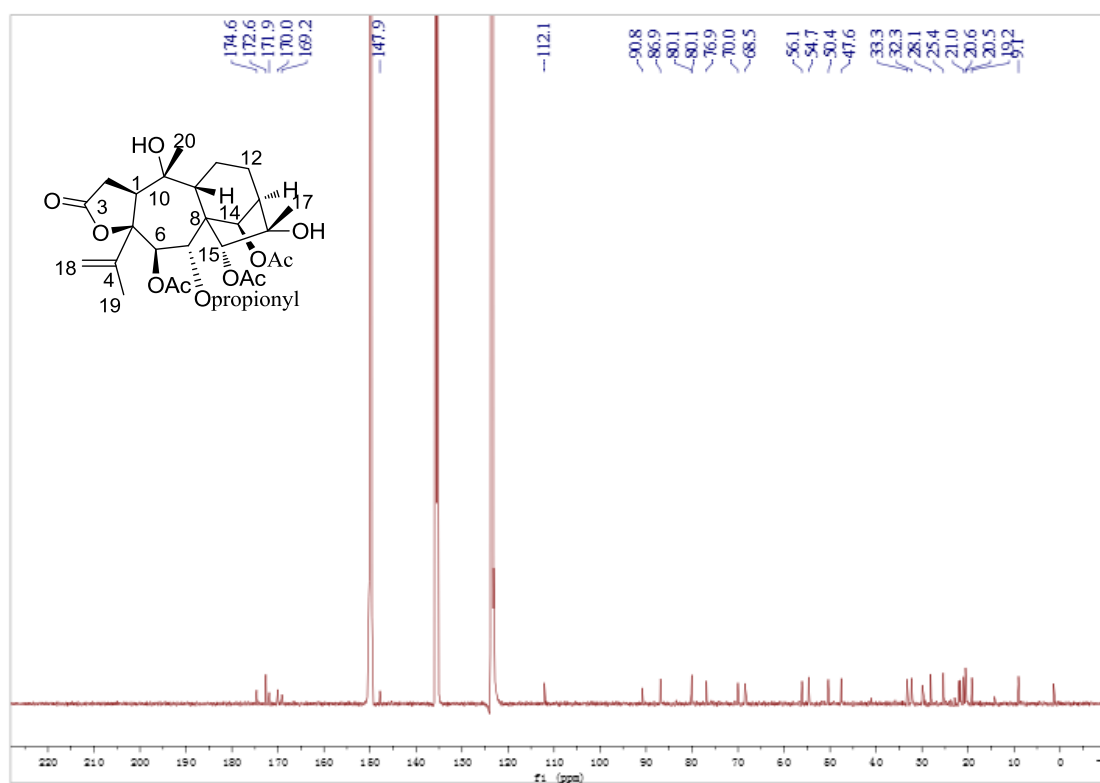


Figure S73. ¹³C NMR spectrum of **8** (150 MHz, in C₅D₅N)

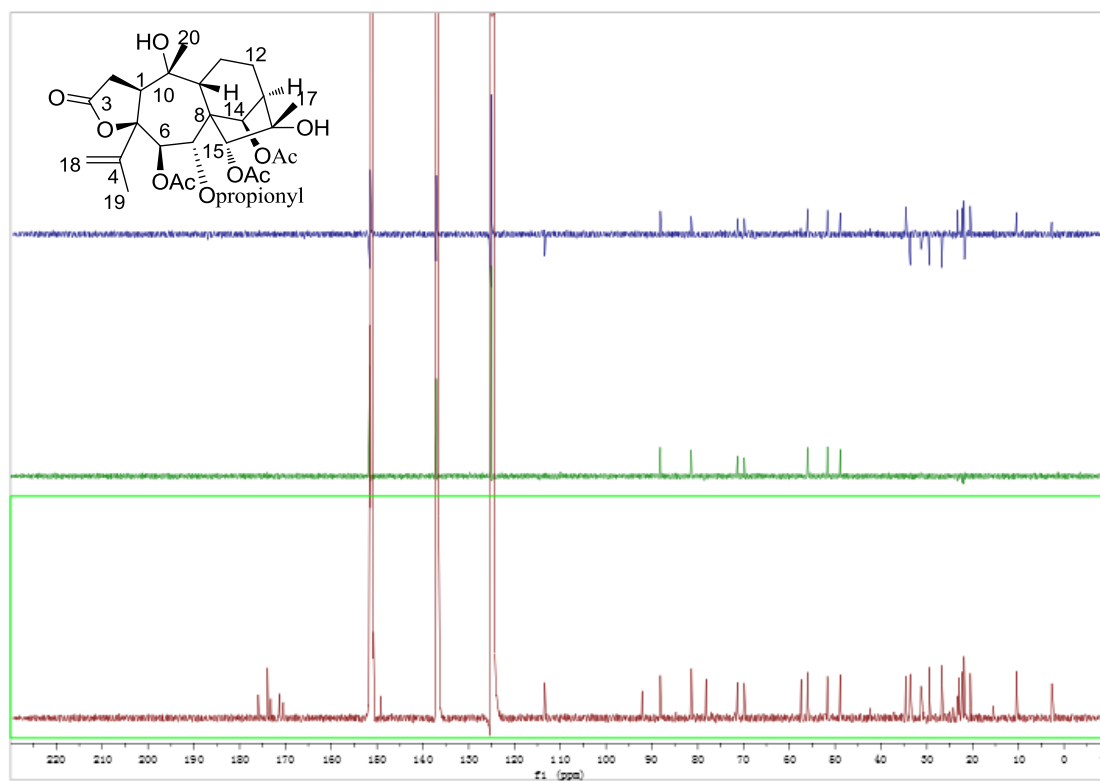


Figure S74. DEPT spectrum of **8** (150 MHz, in C₅D₅N)

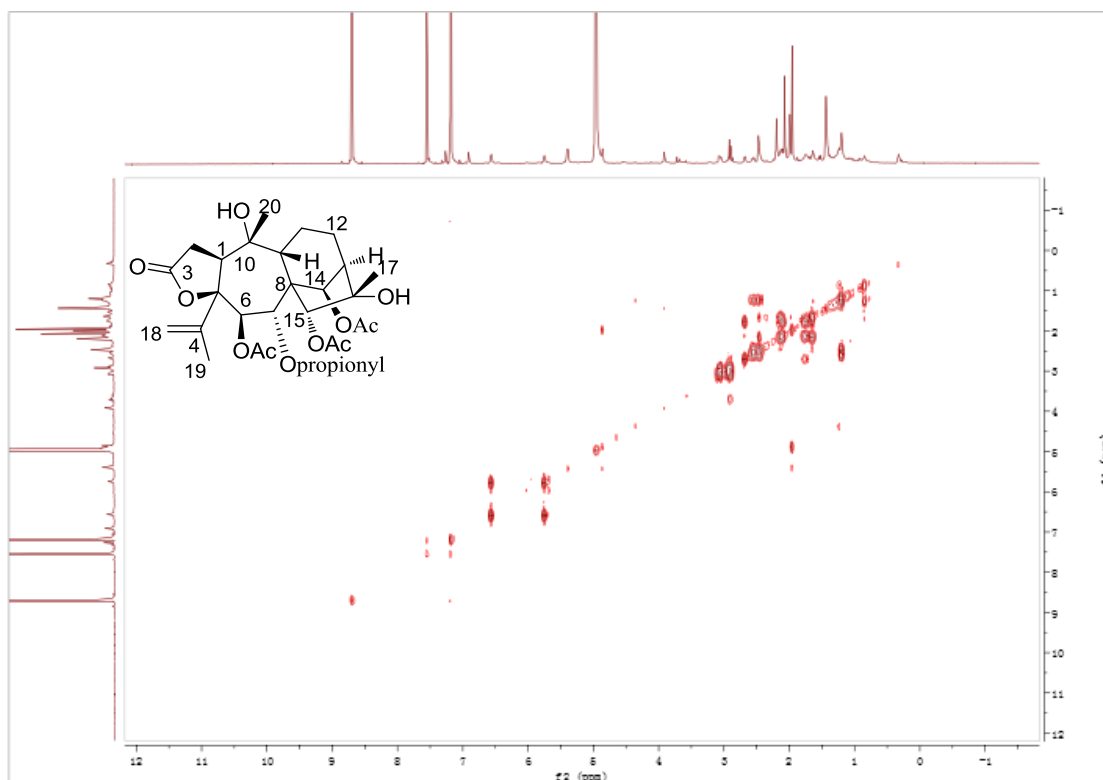


Figure S75. ^1H - ^1H COSY spectrum of **8** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

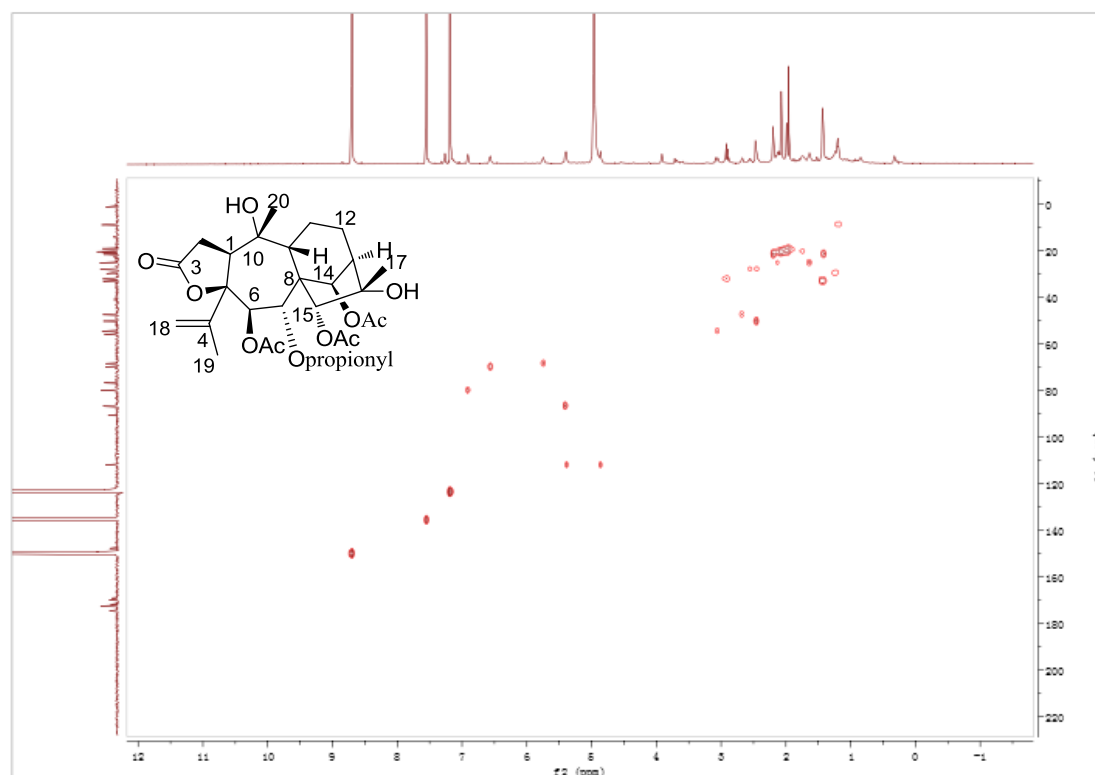


Figure S76. HSQC spectrum of **8** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

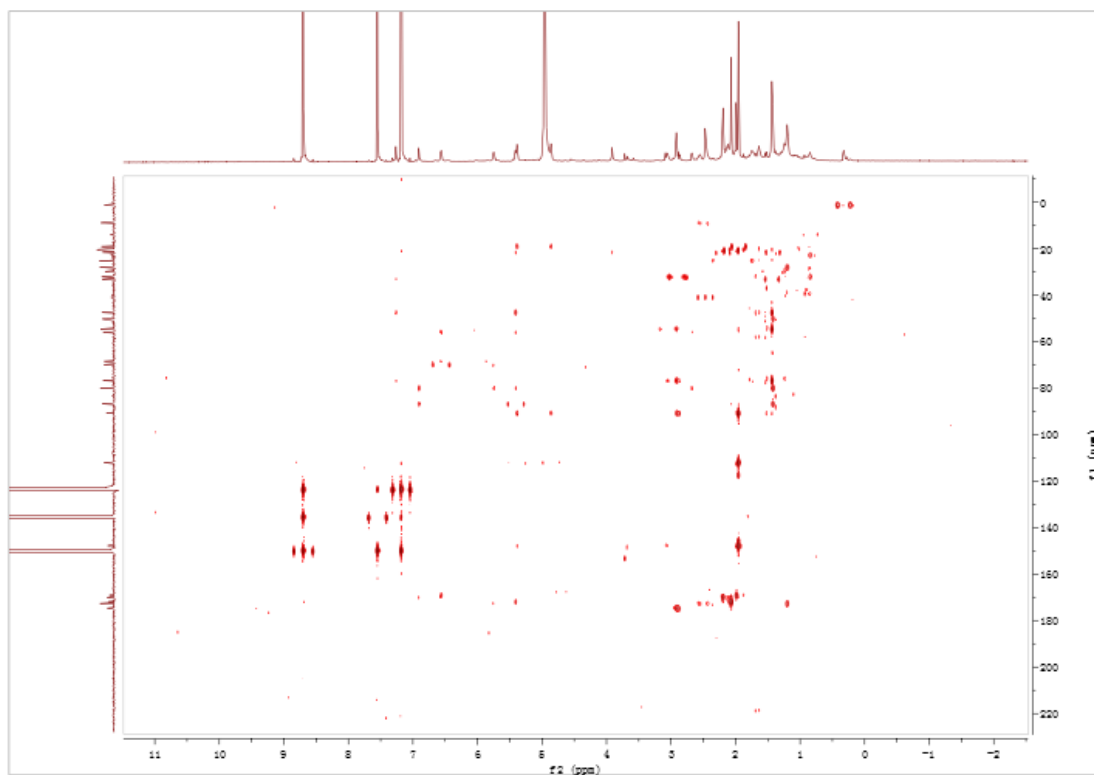


Figure S77. HMBC spectrum of **8** (600 MHz, in C₅D₅N)

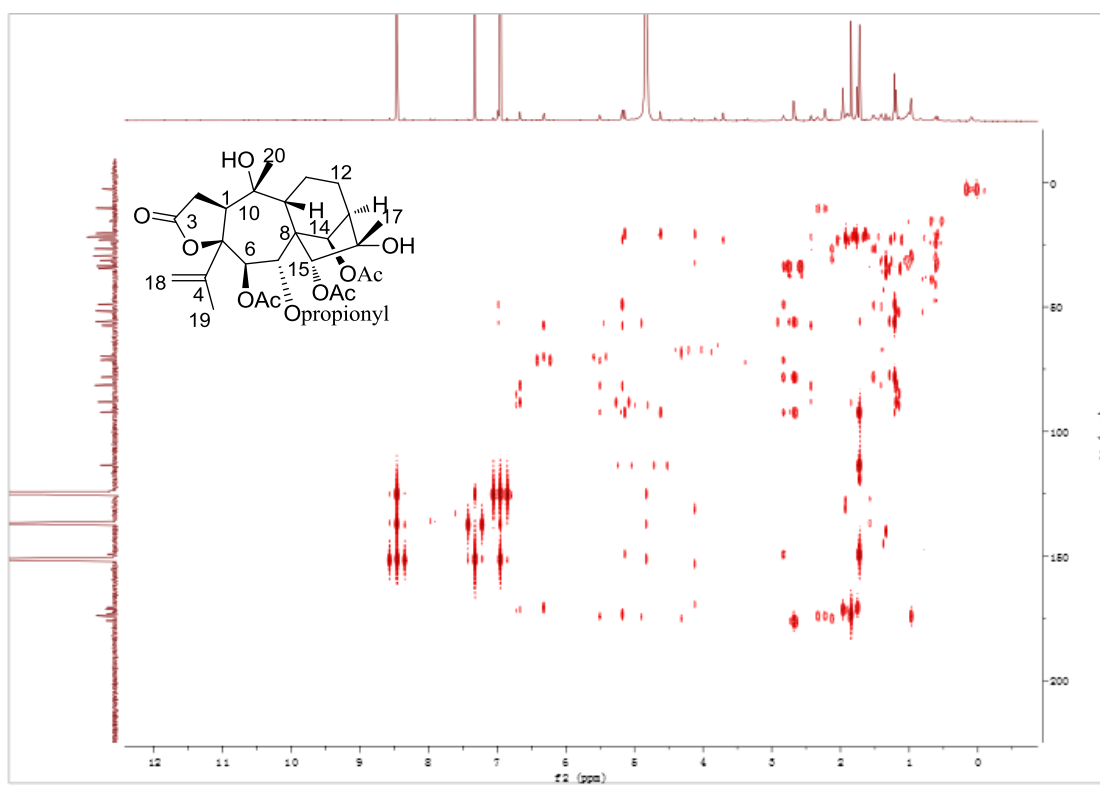


Figure S78. HMBC spectrum of **8** (800 MHz, in C₅D₅N)

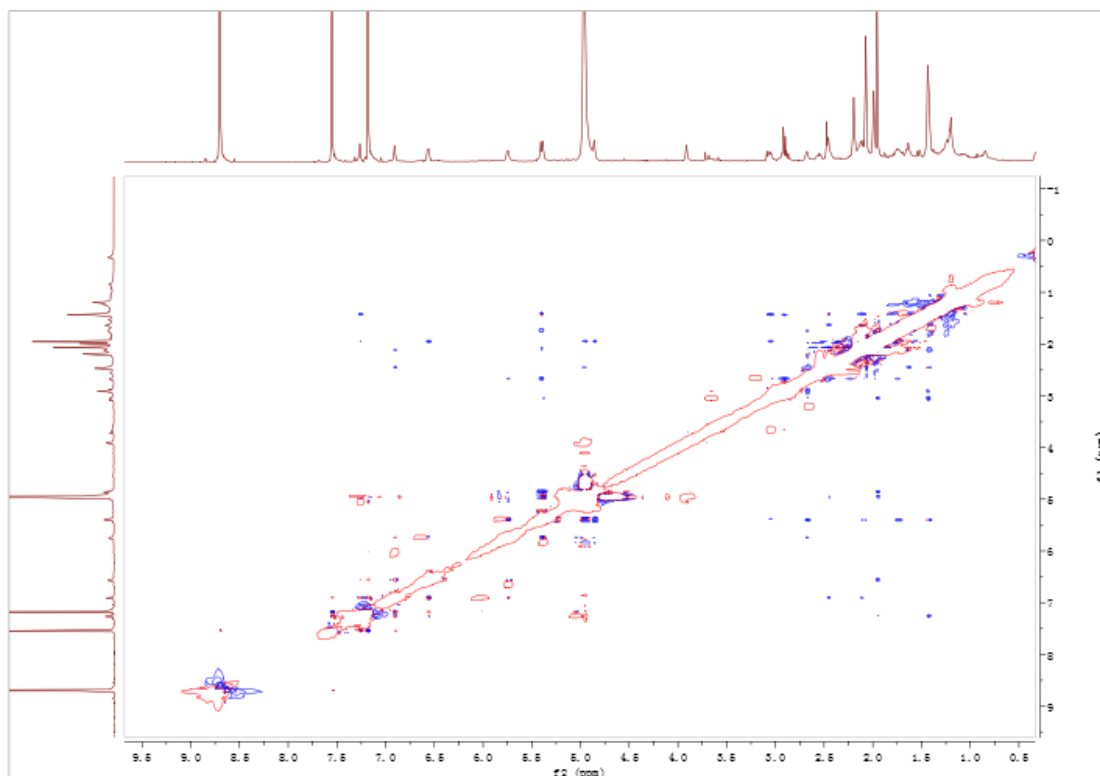


Figure S79. NOESY spectrum of **8** (600 MHz, in C_5D_5N)

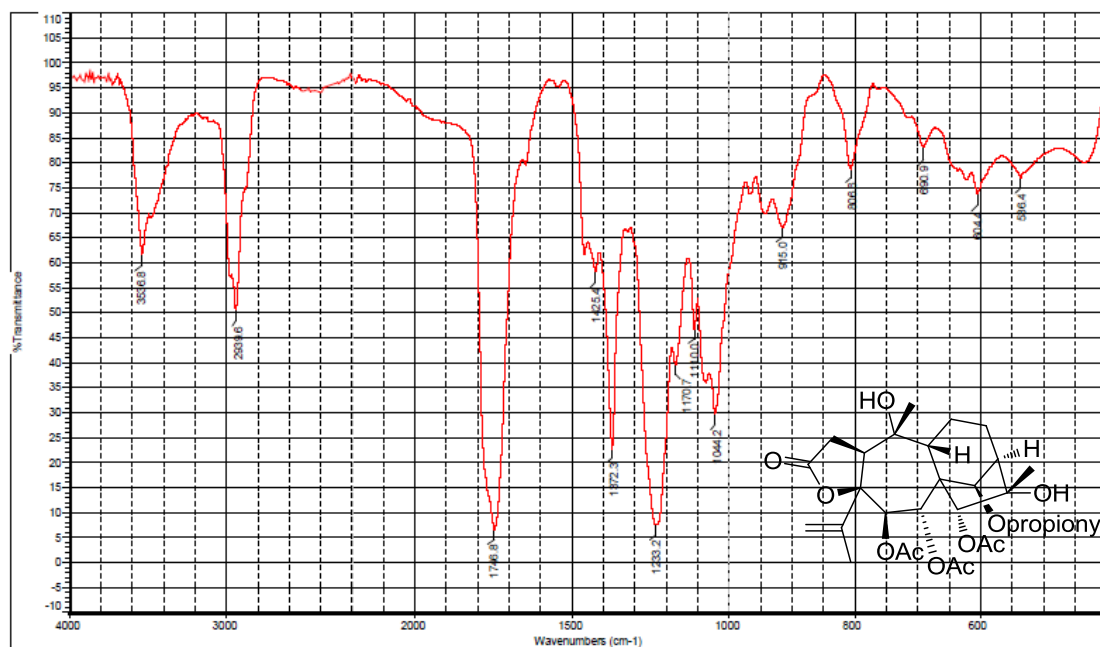


Figure S80. IR spectrum of **9**

MS Formula Results: + Scan (6.135 min) Sub (2015092209.d)

m/z	Ion	Formula	Abundance										
603.2417	(M+Na) ⁺	C29 H40 Na O12	236158.1										
Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
+	C29 H40 O12	C29 H40 Na O12	99.91		580.2525	580.252	603.2412	-0.9	0.9	99.97	99.77	99.95	10
+	C30 H36 N4 O4	C30 H36 Na O4	99.93		580.2525	580.2533	603.2435	1.38	1.38	99.94	98.79	99.93	15
+	C25 H36 N6 O10	C25 H36 Na O10	99.46		580.2525	580.2493	603.2385	-5.55	5.55	99	99.85	99.92	11
+	C18 H40 N6 O15	C18 H40 Na O15	98.28		580.2525	580.2502	603.2444	4.56	4.56	99.32	96.1	99.91	2
+	C42 H32 N2 O	C42 H32 Na O	96.2		580.2525	580.2515	603.2407	-1.79	1.79	99.9	86.94	99.91	28
+	C41 H37 Cl O	C41 H37 Cl Na O	85.79		580.2525	580.2533	603.2425	1.36	1.36	99.94	50.87	99.39	23
+	C38 H37 Cl N2 O3	C38 H37 Cl N2 Na O3	85.39		580.2525	580.2493	603.2385	-5.58	5.58	98.99	51.12	99.31	19
+	C28 H41 Cl N2 O8	C28 H41 Cl N2 Na O8	84.87		580.2525	580.2551	603.2444	4.55	4.55	99.33	48.8	99.22	10
+	C24 H41 Cl N4 O10	C24 H41 Cl N4 Na O10	84.3		580.2525	580.2511	603.2403	-2.4	2.4	99.81	46.08	99.13	6
+	C23 H45 Cl O14	C23 H45 Cl Na O14	83.24		580.2525	580.2498	603.239	-4.68	4.68	99.29	43.19	99.18	1
+	C38 H42 Cl2 O3	C38 H42 Cl2 Na O3	76.35		580.2525	580.2511	603.2403	-2.42	2.42	99.81	18.28	99.1	14
+	C24 H42 Cl2 N6 O6	C24 H42 Cl2 N6 Na O6	75.3		580.2525	580.2543	603.2435	3.05	3.05	99.7	14.93	98.93	6
+	C23 H46 Cl2 N2 O10	C23 H46 Cl2 N2 Na O10	75.06		580.2525	580.253	603.2422	0.77	0.77	99.98	13.59	98.98	1

Figure S81. (+)-HRESIMS data of **9**

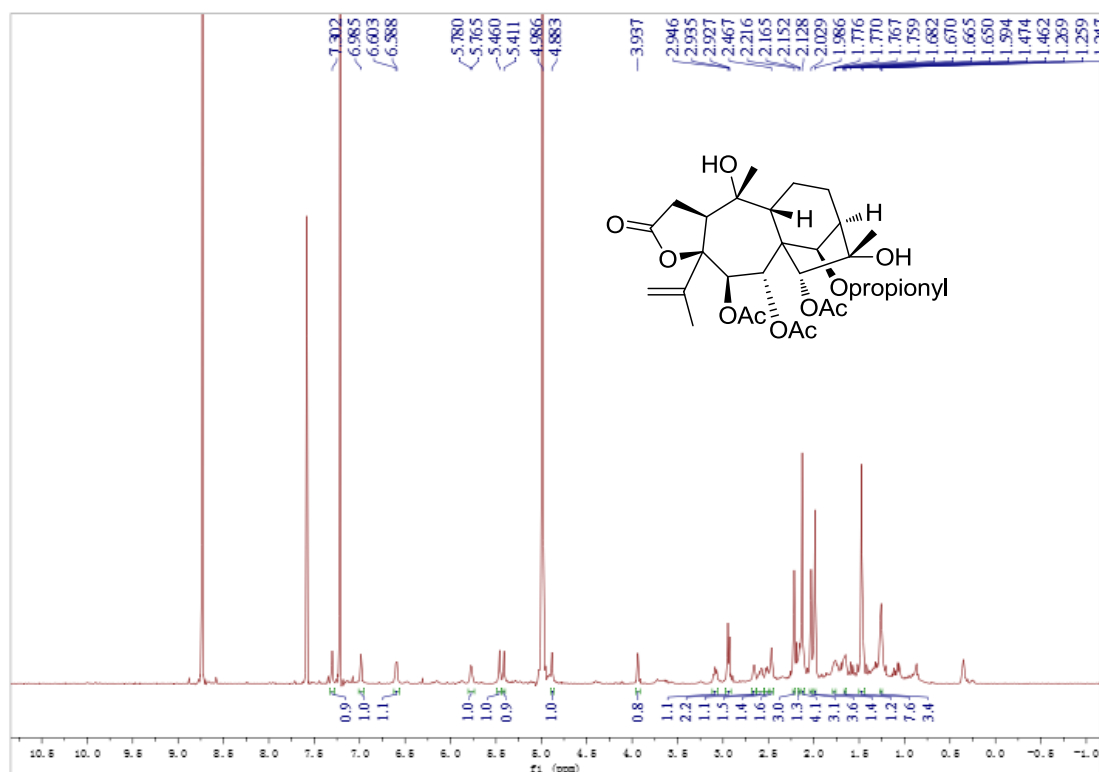


Figure S82. ¹H NMR spectrum of **9** (600 MHz, in C₅D₅N)

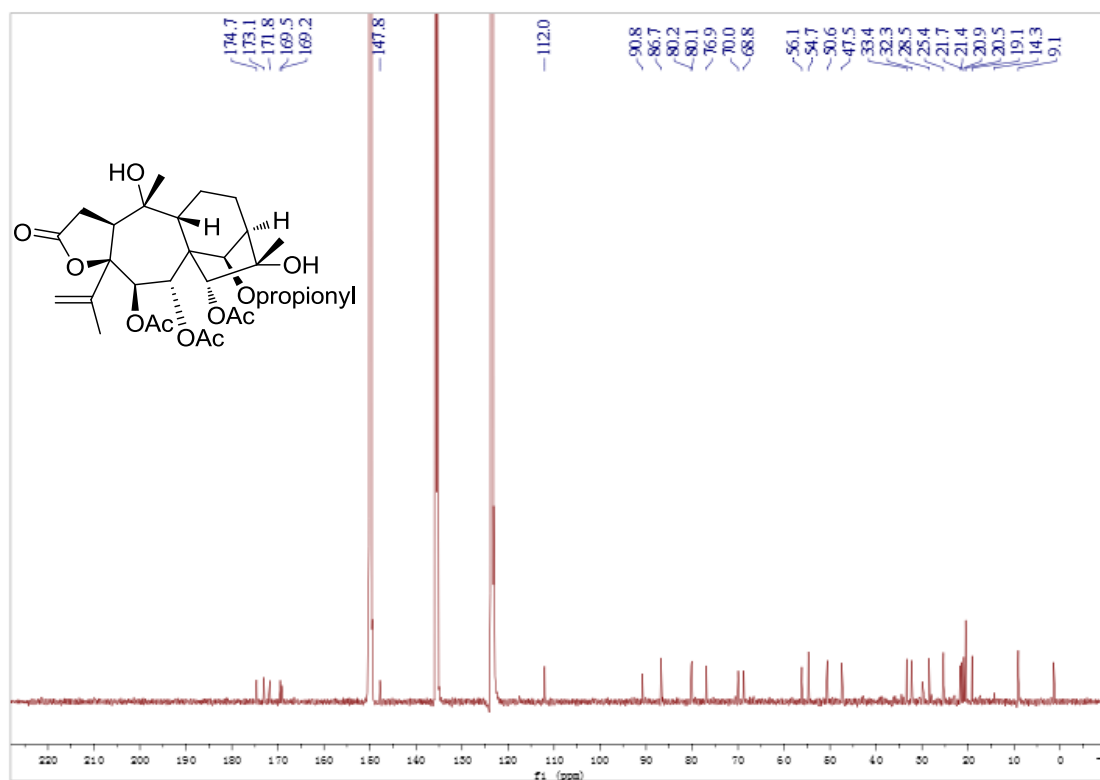


Figure S83. ^{13}C NMR spectrum of **9** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

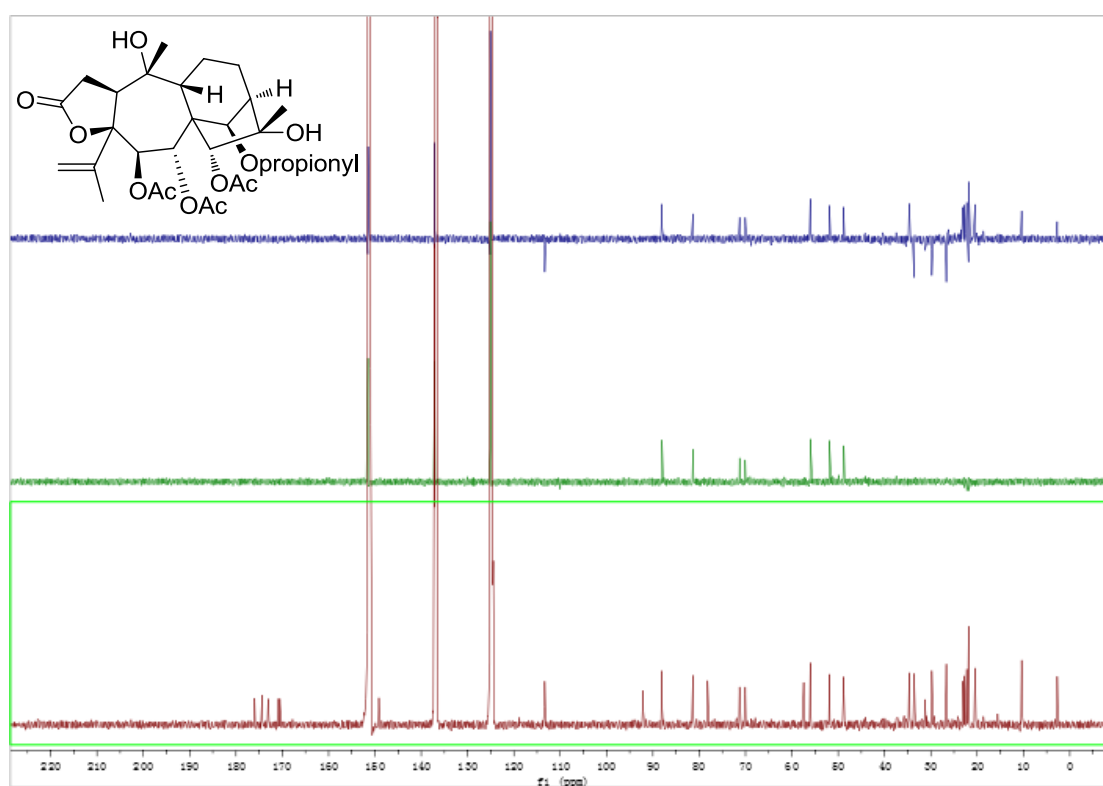


Figure S84. DEPT spectrum of **9** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

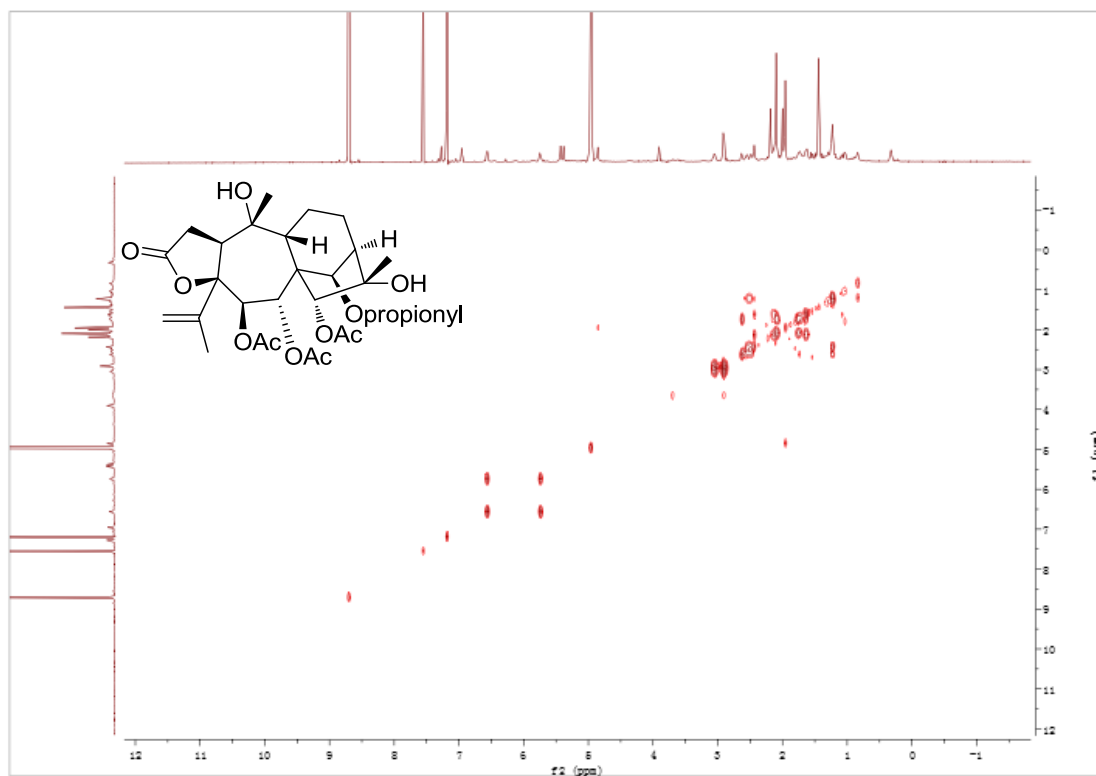


Figure S85. ^1H - ^1H COSY spectrum of **9** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

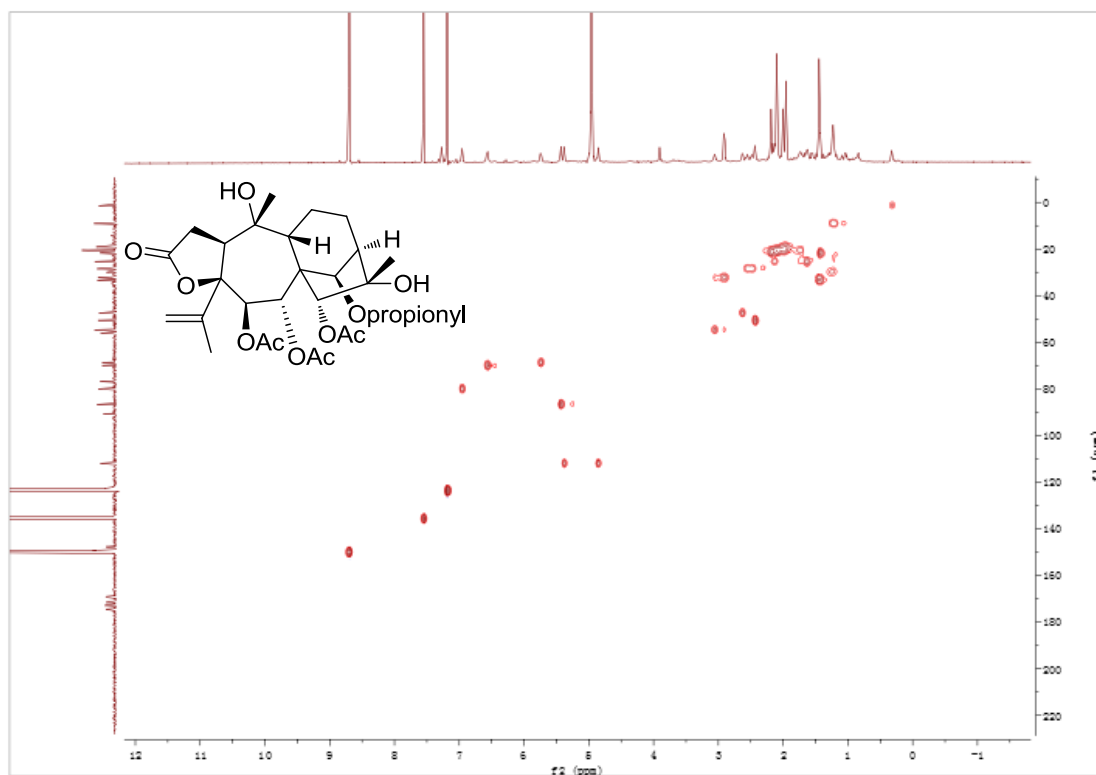


Figure S86. HSQC spectrum of **9** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

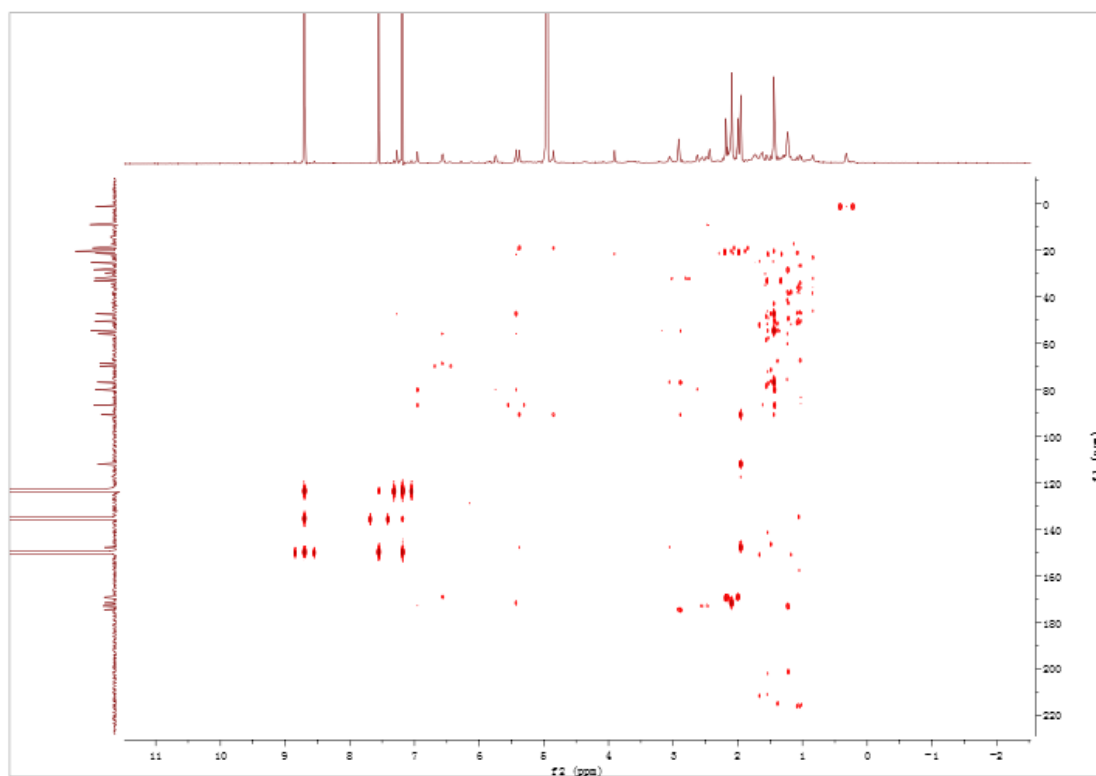


Figure S87. HMBC spectrum of **9** (600 MHz, in C_5D_5N)

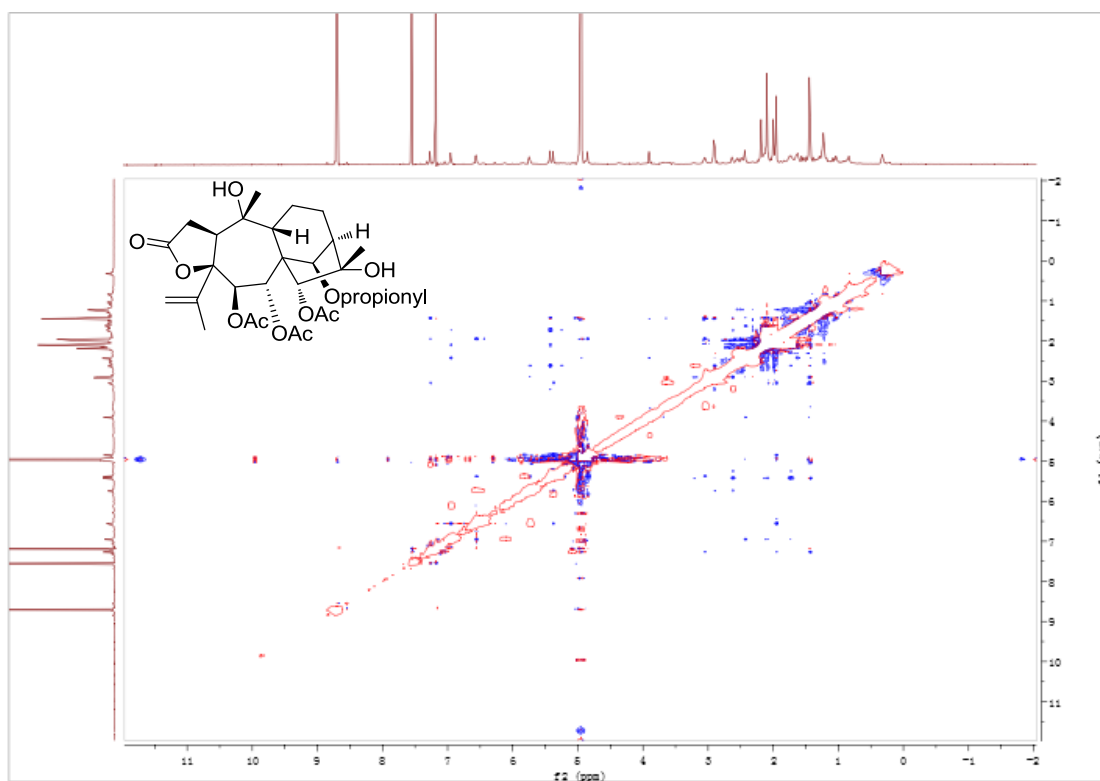


Figure S88. NOESY spectrum of **9** (600 MHz, in C_5D_5N)

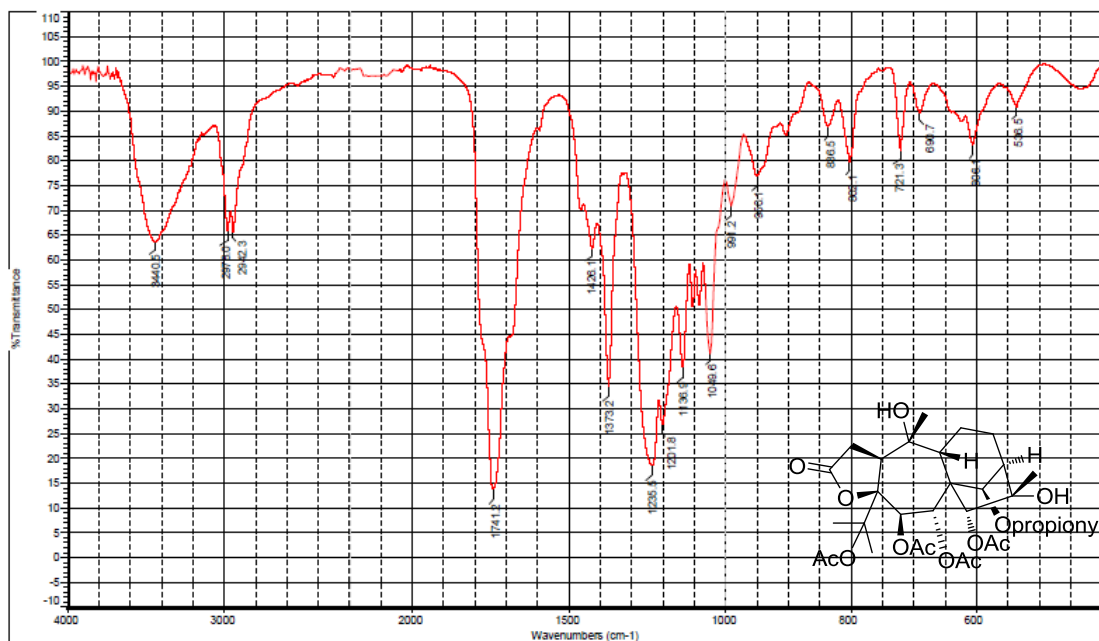


Figure S89. IR spectrum of **10**

MS Formula Results: + Scan (6.026 min) Sub (2015052002.d)

Peak	m/z	Ion	Formula	Abundance
	663.2618	(M+Na) ⁺	C31H44NaO14	141701.8
1	663.2618	✓	C31H44NaO14	99.92
2	663.2618	✓	C32H40NaO10	99.81
3	663.2618	✓	C27H40NaO12	99.58
4	663.2618	✓	C28H44NaO16	98.87
5	663.2618	✓	C44H36NaO9	97.39
6	663.2618	✓	C20H44NaO17	97.18

Peak	Formula (M)	Ion Formula	Score	Cross Sec	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abn Diff (ppm)	Mass Match	Abund Match	Spacing Match	DDC
1	C31H44NaO14	C31H44NaO14	99.92		640.2726	640.2731	663.2623	0.84	0.84	99.98	99.86	99.86	10
2	C32H40NaO10	C32H40NaO10	99.81		640.2726	640.2744	663.2637	2.91	2.91	99.72	99.89	99.9	15
3	C27H40NaO12	C27H40NaO12	99.58		640.2726	640.2704	663.2596	-3.39	3.39	99.62	99.22	99.34	11
4	C28H44NaO16	C28H44NaO16	98.87		640.2726	640.3591	663.3583	-5.46	5.46	99.62	97.76	99.91	6
5	C44H36NaO9	C44H36NaO9	97.39		640.2726	640.2726	662.2618	0.03	0.03	100	92.36	99.83	26
6	C20H44NaO17	C20H44NaO17	97.18		640.2726	640.2763	663.2855	5.78	5.78	98.9	92	99.97	3

Figure S90. (+)-HRESIMS data of **10**

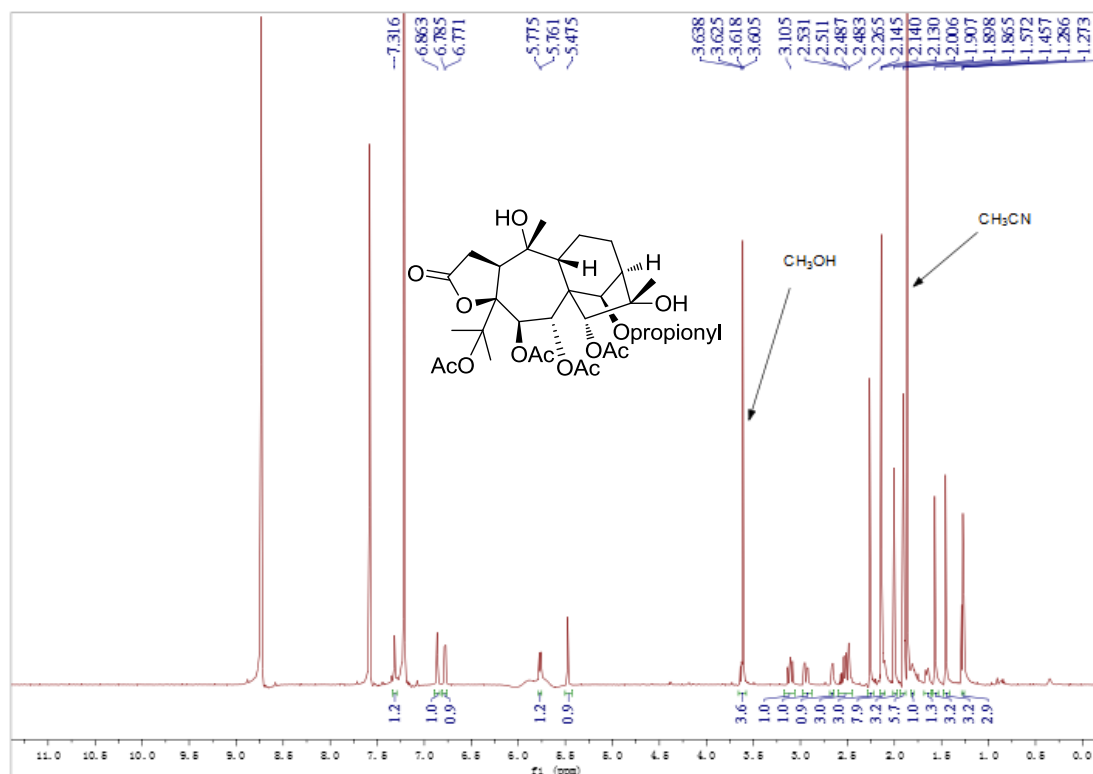


Figure S91. ¹H NMR spectrum of **10** (600 MHz, in C₅D₅N)

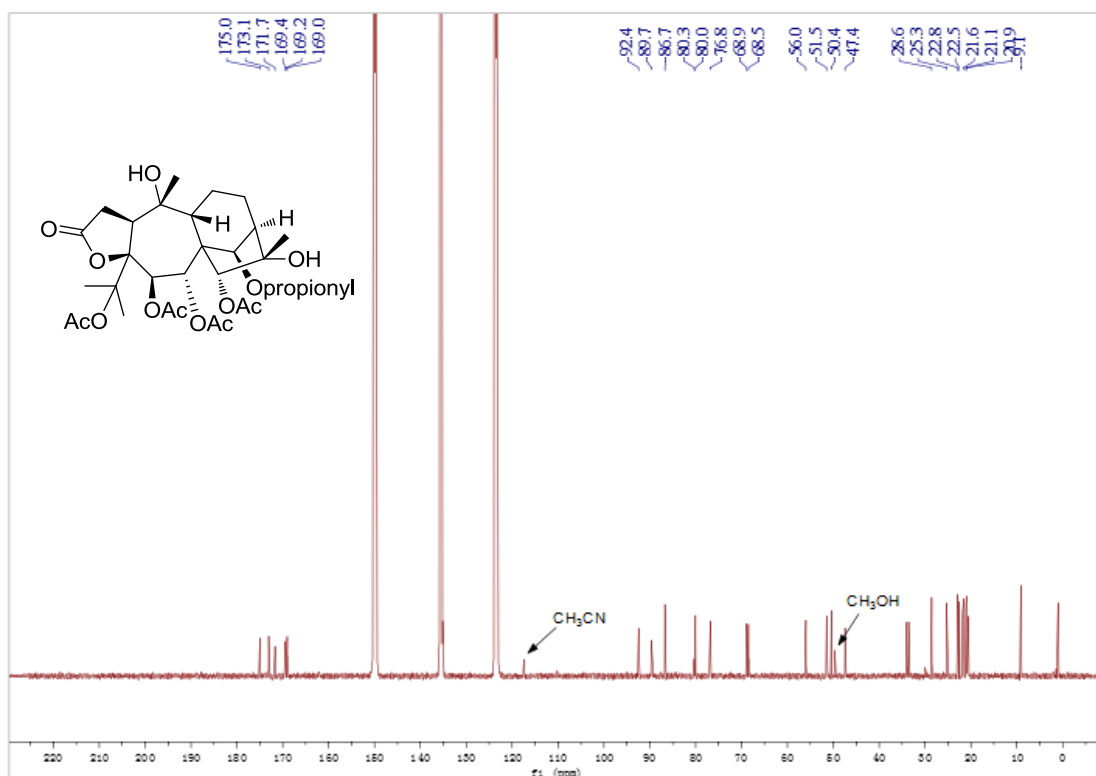


Figure S92 ^{13}C NMR spectrum of **10** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

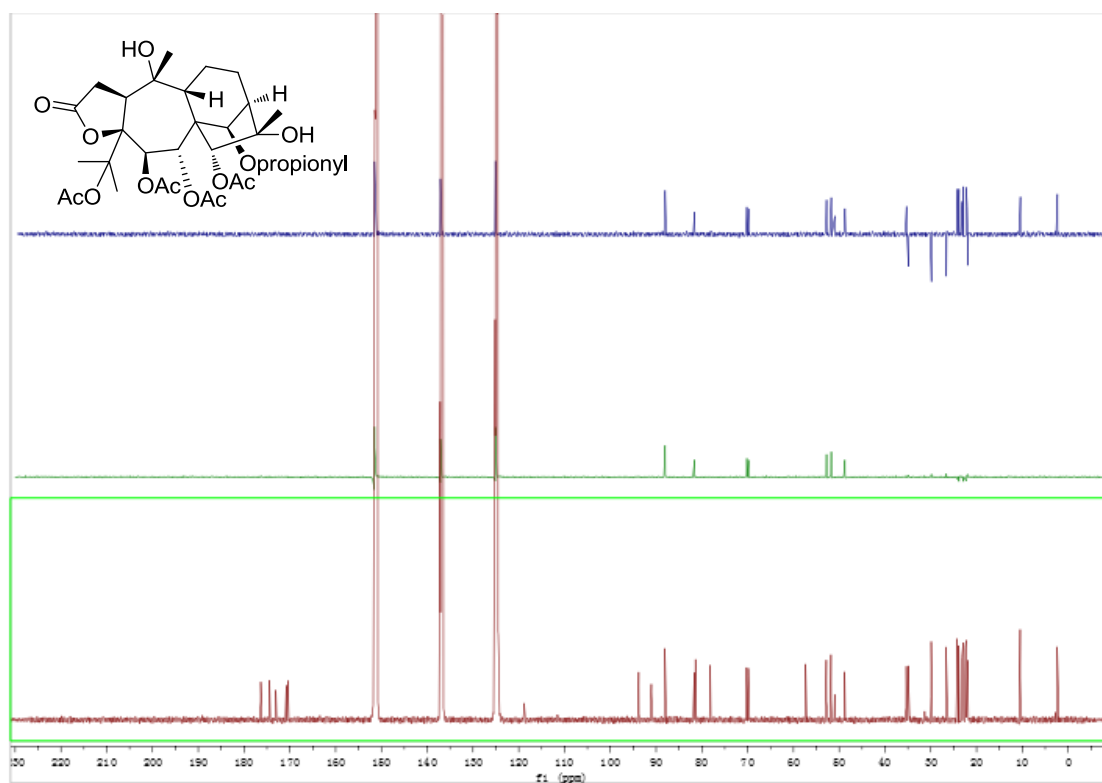


Figure S93. DEPT spectrum of **10** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

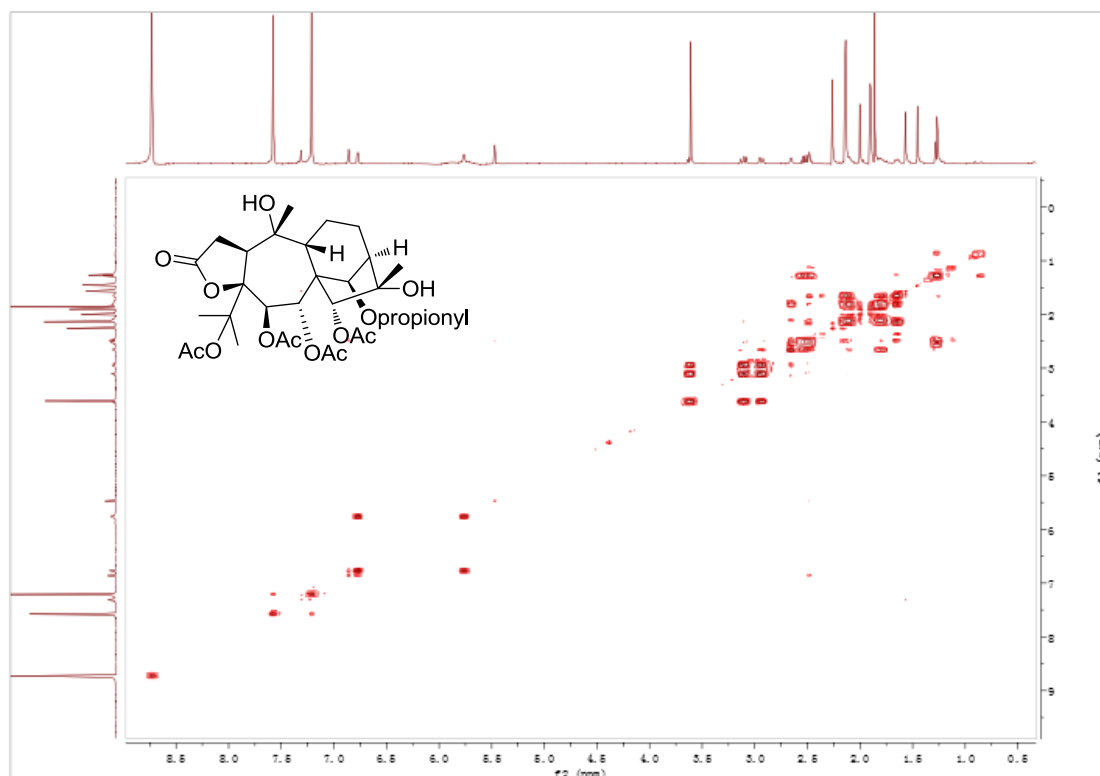


Figure S94. ^1H - ^1H COSY spectrum of **10** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

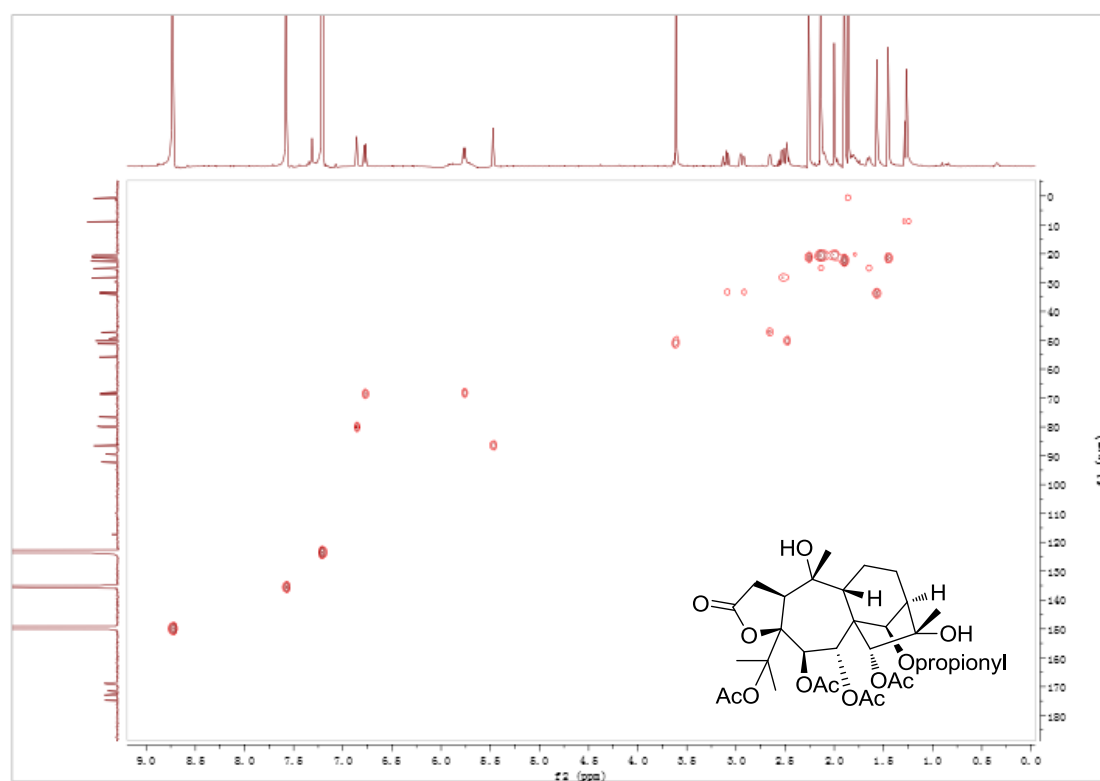


Figure S95. HSQC spectrum of **10** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

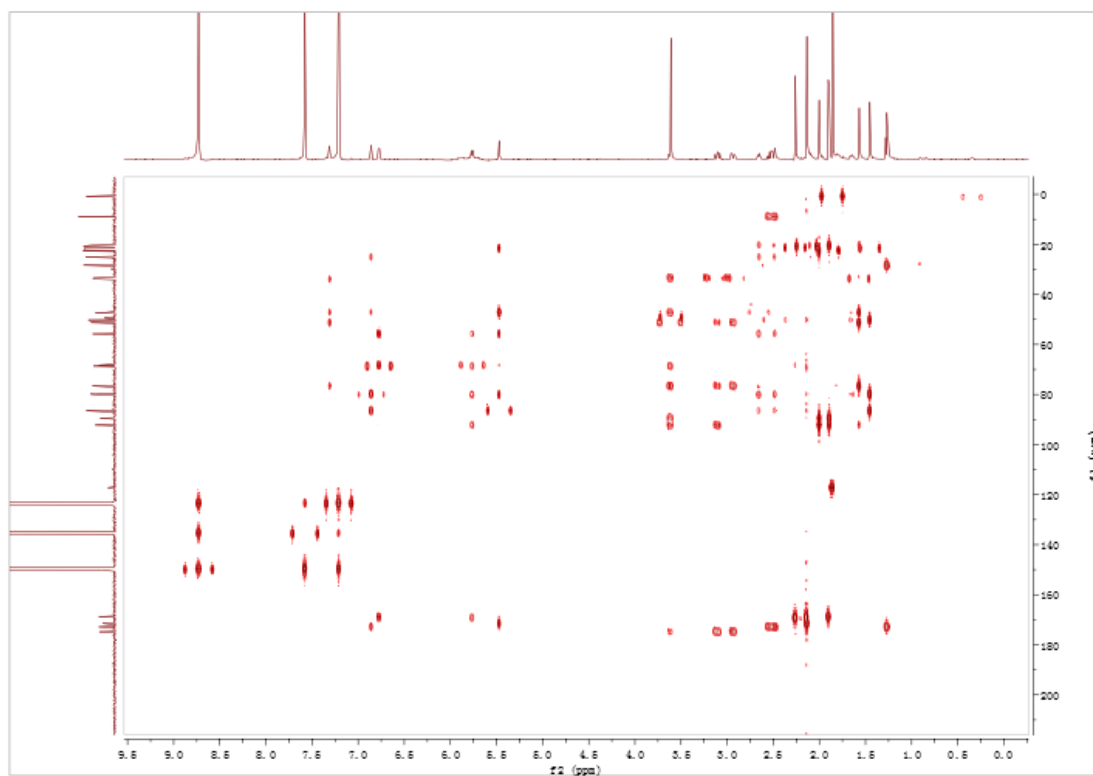


Figure S96. HMBC spectrum of **10** (600 MHz, in C₅D₅N)

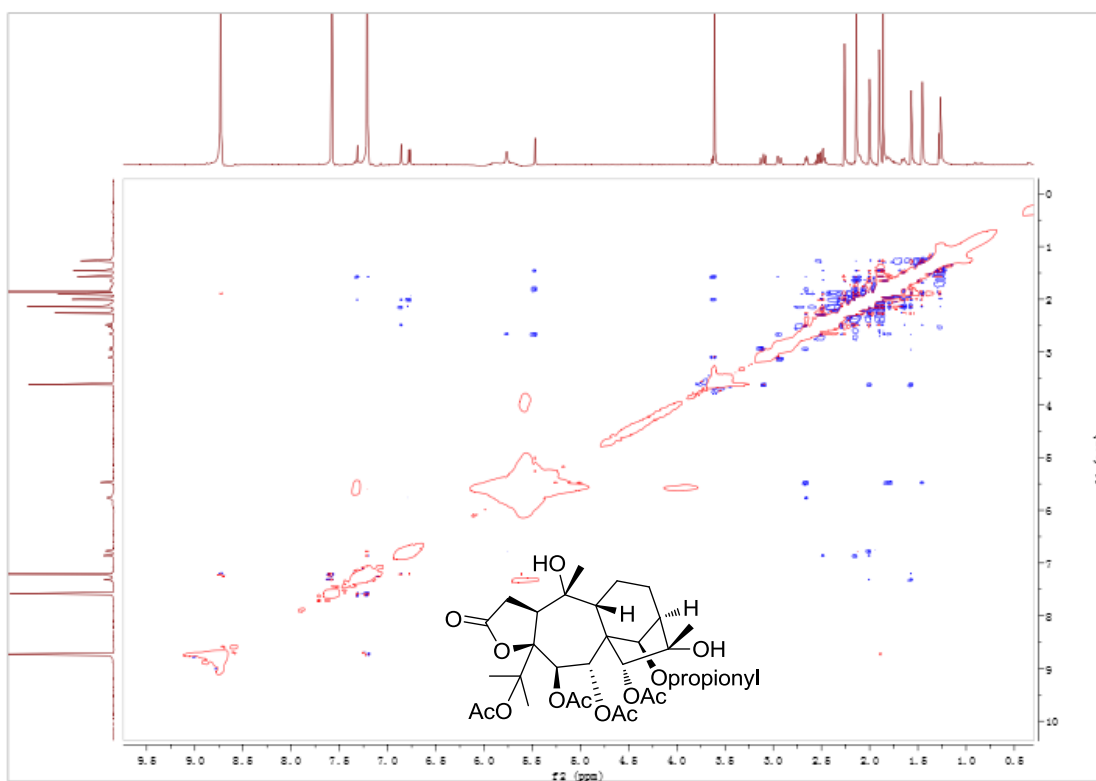


Figure S97. NOESY spectrum of **10** (600 MHz, in C₅D₅N)

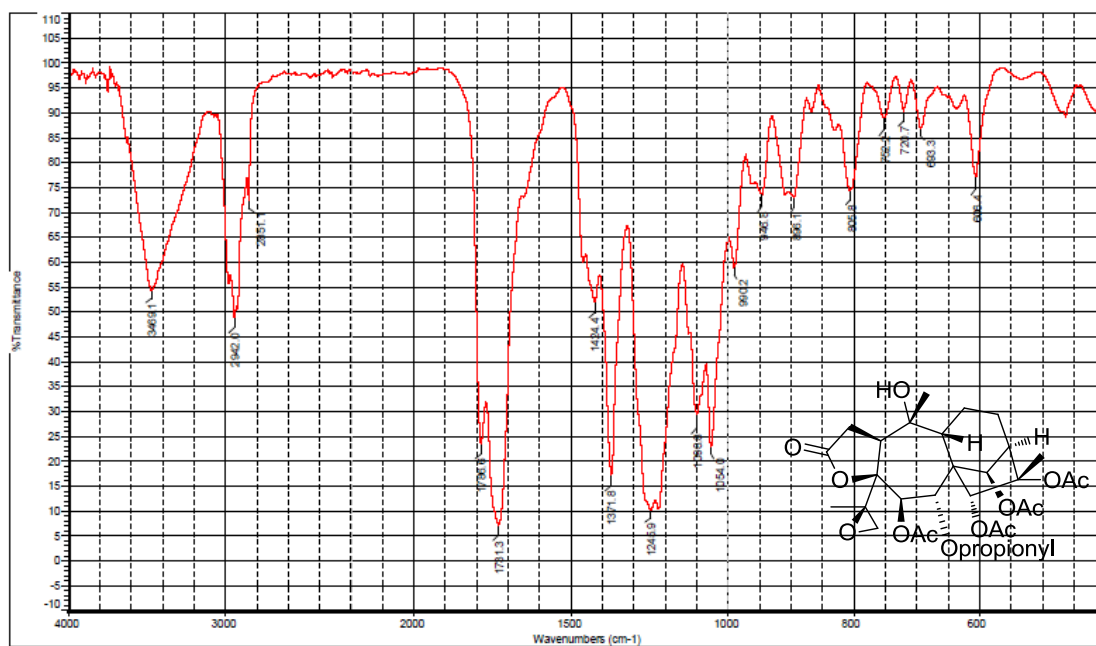


Figure S98. IR spectrum of **11**

MS Formula Results: + Scan (6.407 min) Sub (2015061101.d)

m/z	Ion	Formula	Abundance
661.2469	(M+Na) ⁺	C31 H42 Na O14	84935.9

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C31 H42 O14	C31 H42 Na O14	99.91		638.2576	638.2576	661.2467	-0.27	0.27	100	99.71	99.97	11
	C39 H38 Na O15	C39 H38 Na O15	99.8		638.2576	638.2588	661.2448	1.81	1.81	99.89	99.85	99.99	16
	C27 H38 N6 O12	C27 H38 N6 Na O12	99.32		638.2576	638.2548	661.2444	-4.51	4.51	99.33	98.75	99.99	12
	C44 H34 N2 O3	C44 H34 N2 Na O3	98.07		638.2576	638.2569	661.2462	-1.08	1.08	99.96	93.32	99.97	29
	C20 H42 N6 O17	C20 H42 N6 Na O17	97.08		638.2577	638.2606	661.2499	4.68	4.68	99.28	91.02	99.98	3
	C49 H34 O	C49 H34 Na O	96.98		638.2576	638.261	661.2502	5.23	5.23	99.1	88.81	99.95	33

Figure S99. (+)-HRESIMS data of **11**

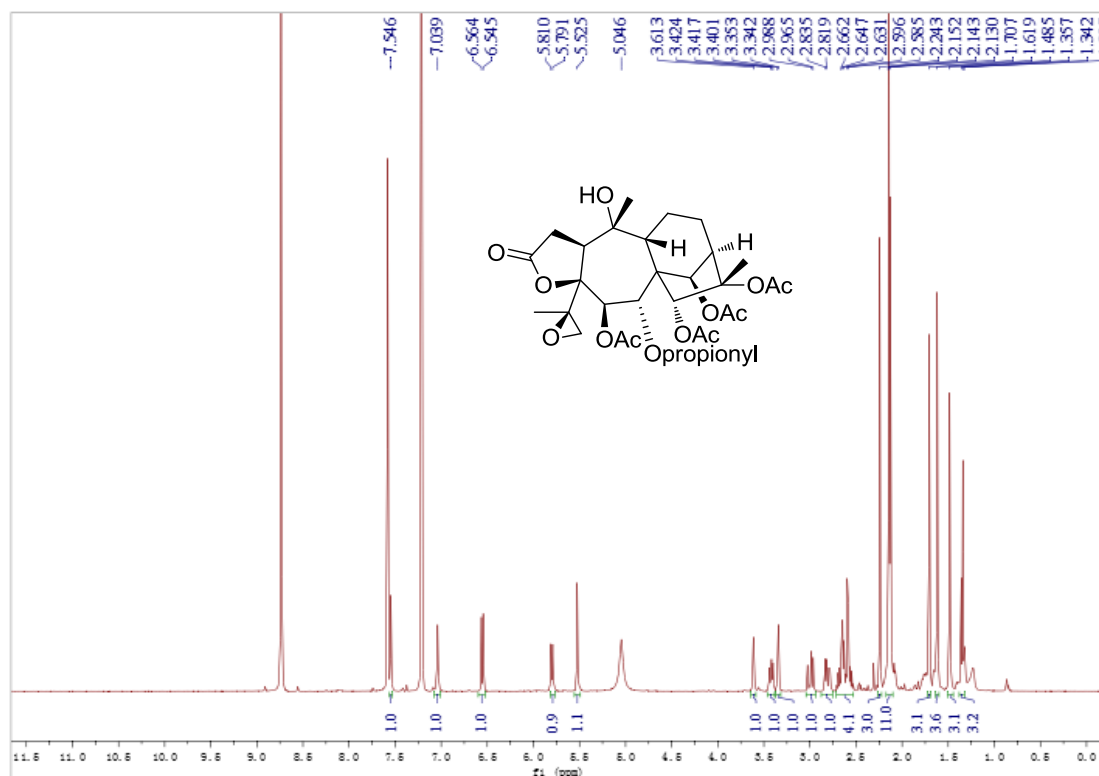


Figure S100. ¹H NMR spectrum of **11** (500 MHz, in C₅D₅N)

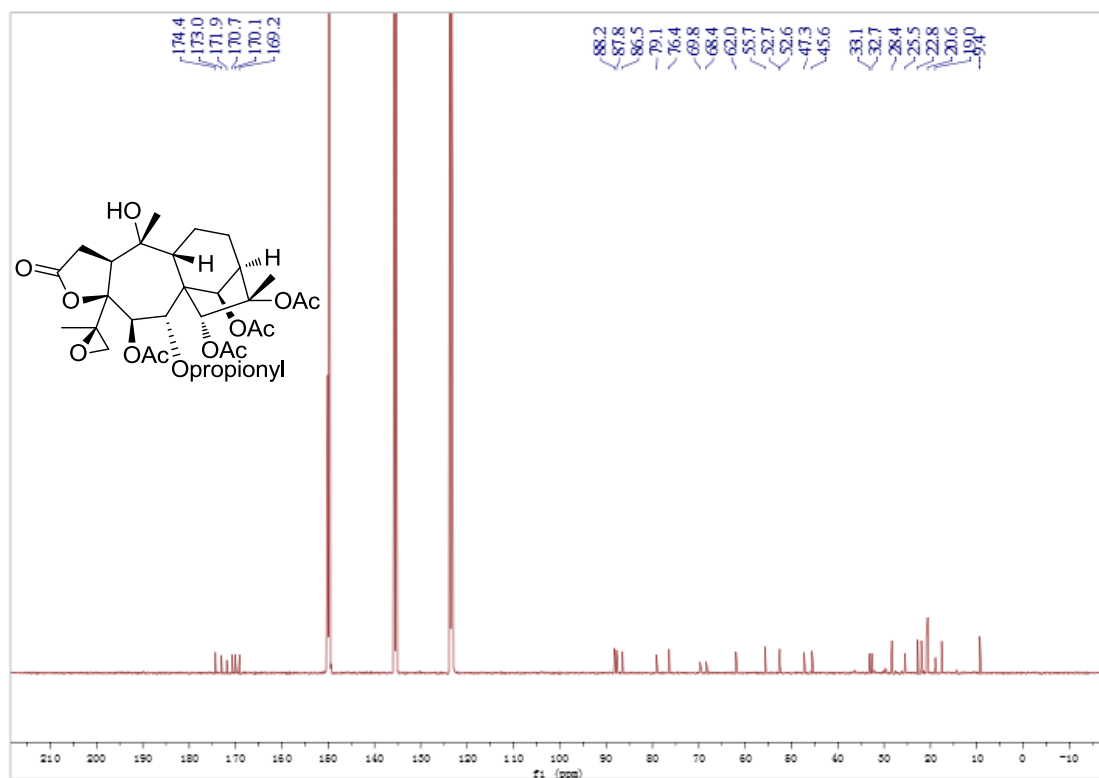


Figure S101. ^{13}C NMR spectrum of **11** (125 MHz, in $\text{C}_5\text{D}_5\text{N}$)

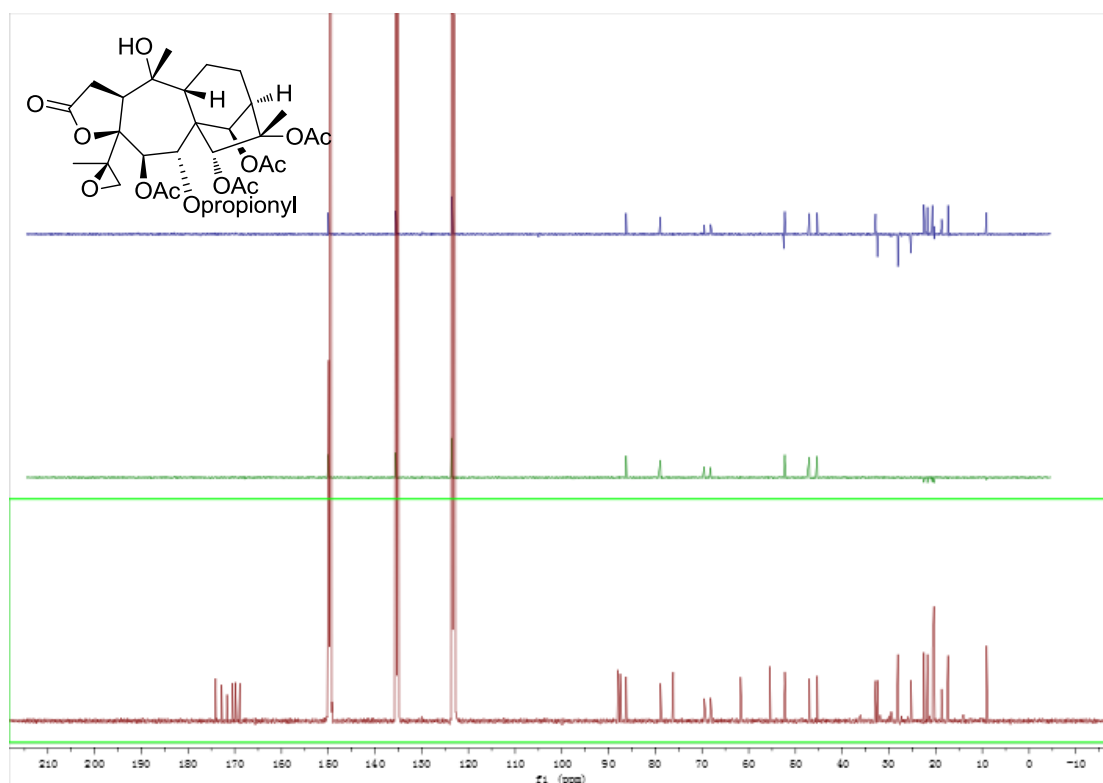


Figure S102. DEPT spectrum of **11** (125 MHz, in $\text{C}_5\text{D}_5\text{N}$)

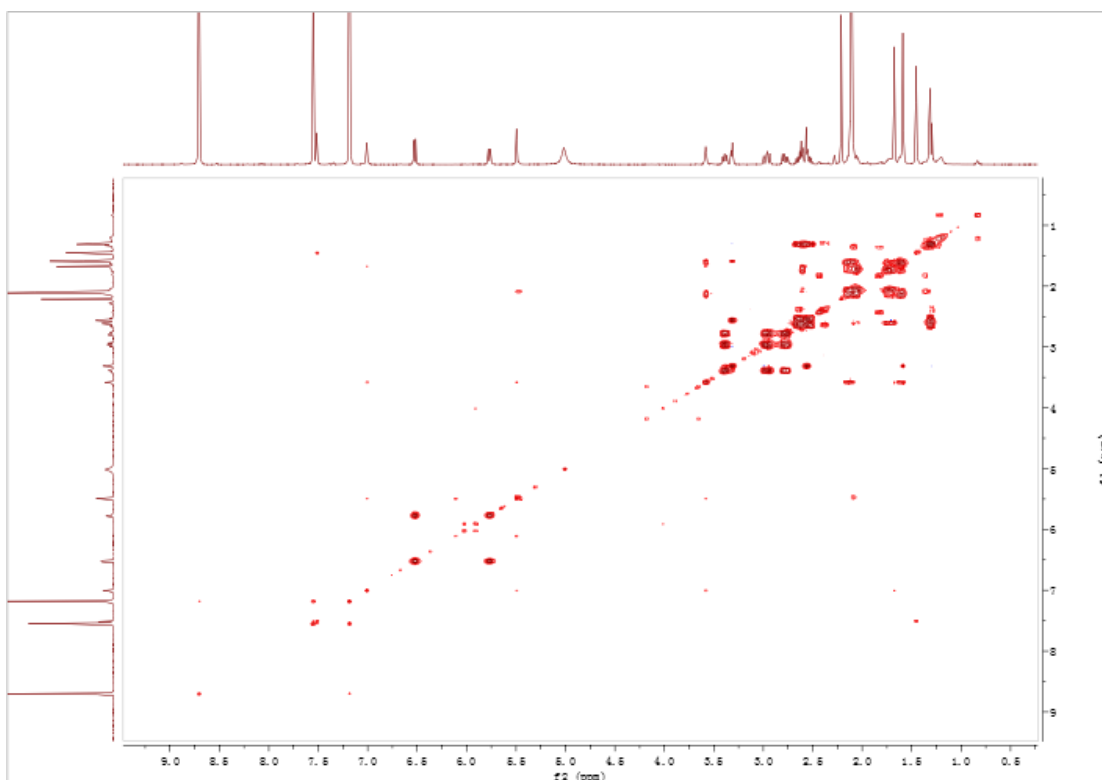


Figure S103. ^1H - ^1H COSY spectrum of **11** (500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

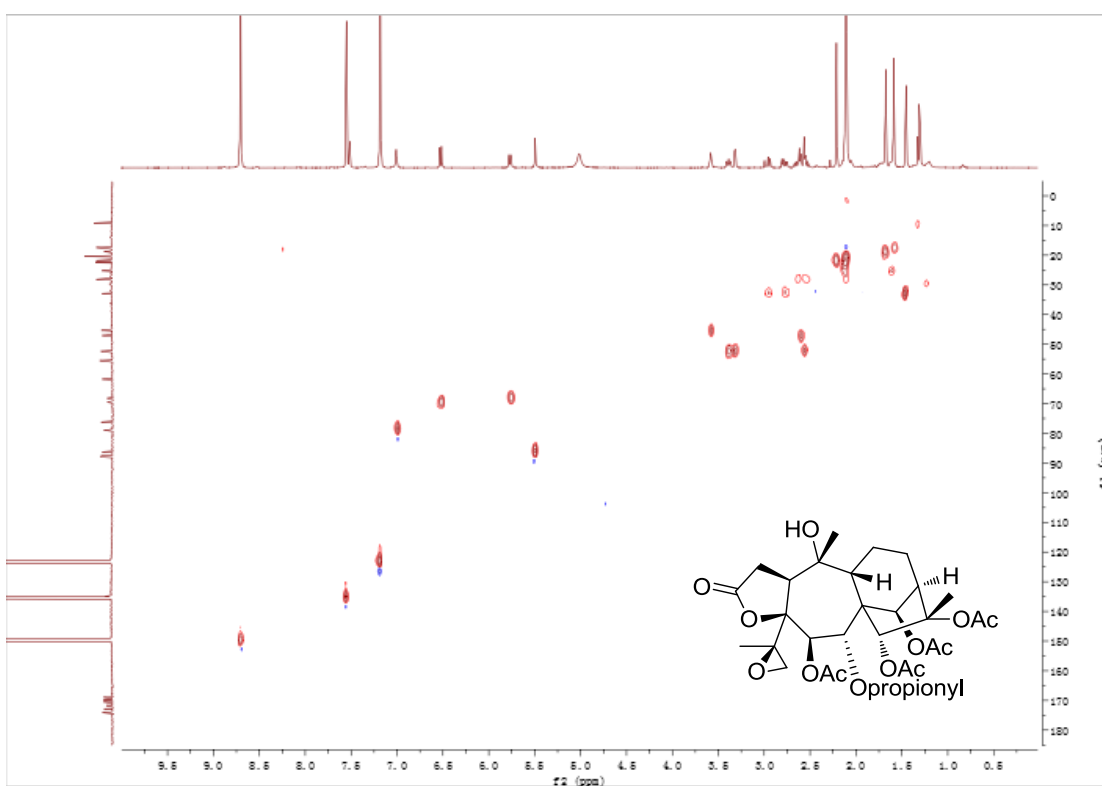


Figure S104. HSQC spectrum of **11**(500 MHz, in $\text{C}_5\text{D}_5\text{N}$)

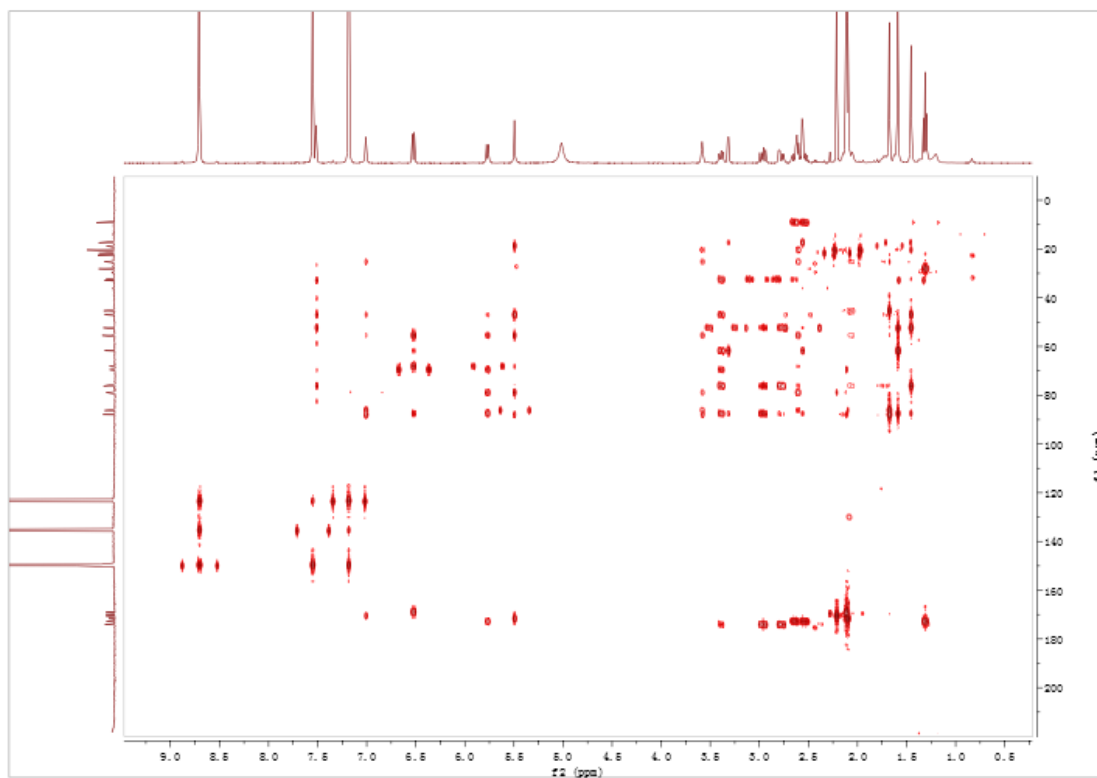


Figure S105. HMBC spectrum of **11** (500 MHz, in C₅D₅N)

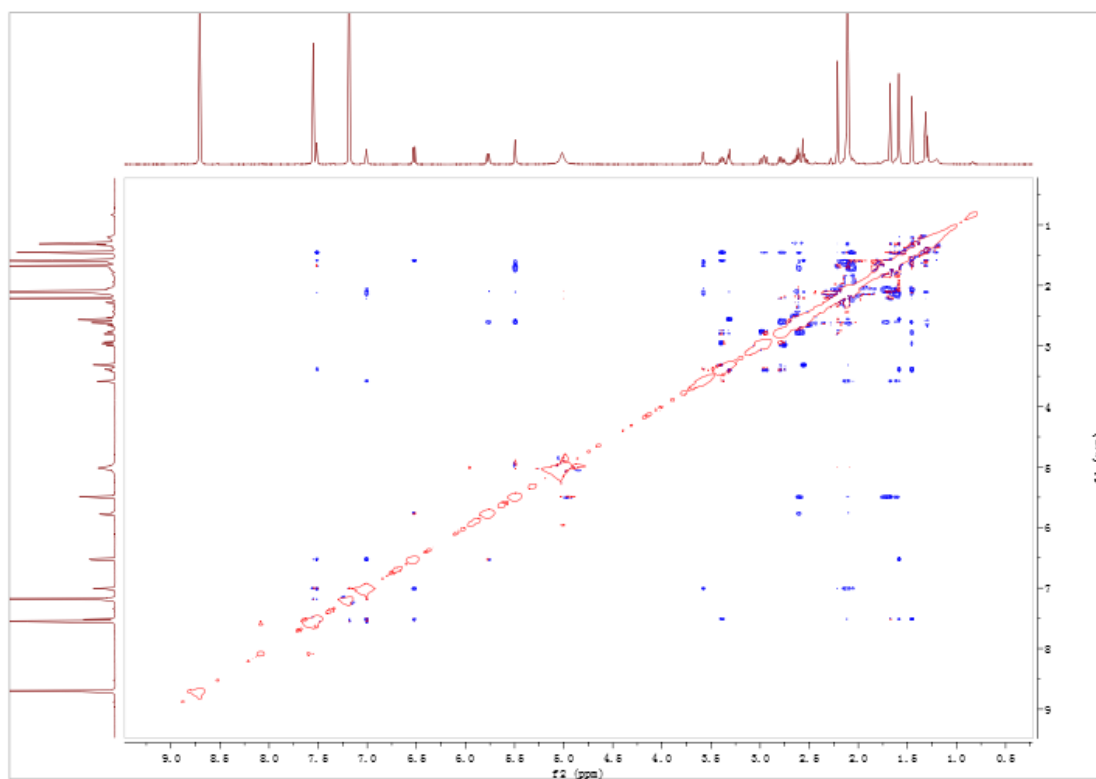
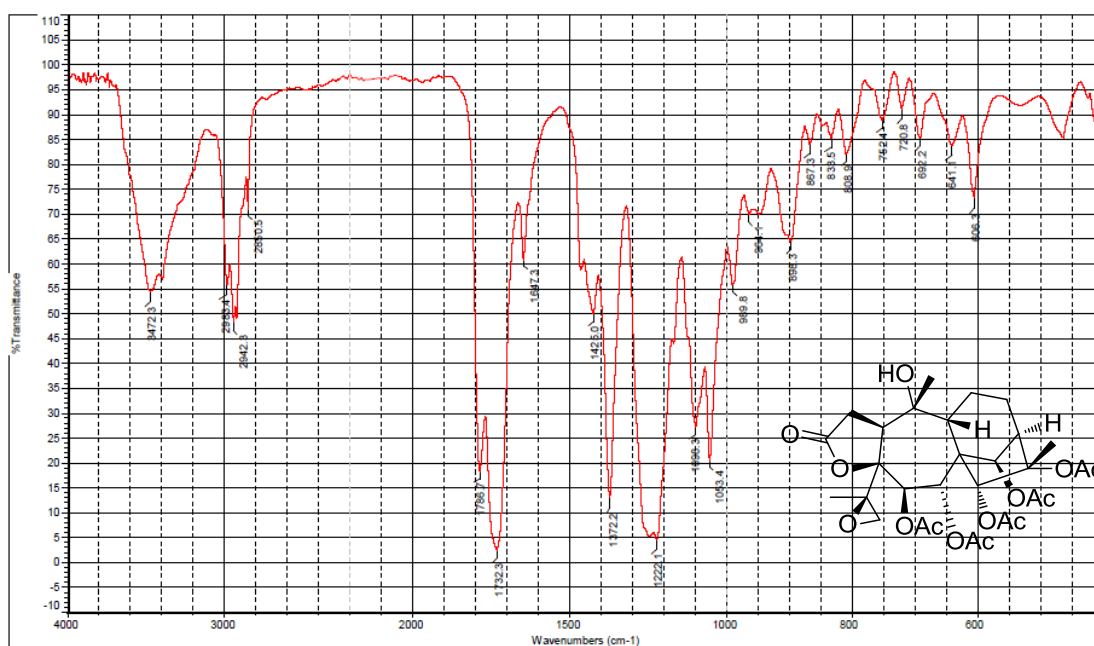


Figure S106. NOESY spectrum of **11** (500 MHz, in C₅D₅N)

Table S3. Crystal data and structure refinement for **11**

Identification code	exp_3589
Empirical formula	C ₃₂ H ₄₈ O ₁₆
Formula weight	688.70
Temperature/K	102.8
Crystal system	monoclinic
Space group	P2 ₁
a / Å, b / Å, c / Å	12.8374(3), 10.8913(3), 24.3599(6)
α/°, β/°, γ/°	90.00, 99.441(2), 90.00
Volume/Å ³	3359.79(14)
Z	4
ρ _{calc} /mg mm ⁻³	1.362
μ/mm ⁻¹	0.925
F(000)	1472
Crystal size/mm ³	0.17 × 0.15 × 0.05
2θ range for data collection	7.34 to 142.17°
Index ranges	-15 ≤ h ≤ 15, -12 ≤ k ≤ 13, -29 ≤ l ≤ 29
Reflections collected	28272
Independent reflections	11987[R(int) = 0.0299 (inf-0.9Å)]
Data/restraints/parameters	11987/1/883
Goodness-of-fit on F ²	1.038
Final R indexes [I > 2σ (I) i.e. F _o > 4σ (F _o)]	R ₁ = 0.0592, wR ₂ = 0.1599
Final R indexes [all data]	R ₁ = 0.0635 wR ₂ = 0.1658
Largest diff. peak/hole/e Å ⁻³	0.168/-0.616
Flack Parameters	-0.07(15)
Completeness	0.990

**Figure S107.** IR spectrum of **12**

MS Formula Results: + Scan (5.921 min) Sub (2015051802.d)

m/z	Ion	Formula	Abundance										
847.2307	(M+Na) ⁺	C30 H40 Na O14	178238.7										
Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
+	C30 H40 Na O14	C30 H40 Na O14	99.95		824.2415	824.2418	847.231	0.55	0.55	99.99	99.95	99.87	11
+	C28 H36 Na O12	C28 H36 Na O12	99.69		824.2415	824.2381	847.2283	-3.77	3.77	99.53	99.76	99.82	12
+	C31 H36 Na O10	C31 H36 Na O10	99.67		824.2415	824.3431	847.2324	2.68	2.68	99.76	99.31	99.91	16
+	C25 H40 N2 O16	C25 H40 N2 Na O16	98.13		824.2415	824.2378	847.227	-5.9	5.9	98.88	98.87	98.88	7
+	C19 H40 N6 O17	C19 H40 N6 Na O17	97.83		824.2415	824.245	847.2342	5.63	5.63	98.96	94.24	99.9	3
+	C43 H32 N2 O3	C43 H32 N2 Na O3	96.88		824.2415	824.2413	847.2305	-0.28	0.28	100	89.21	99.9	29

Figure S108. (+)-HRESIMS data of **12**

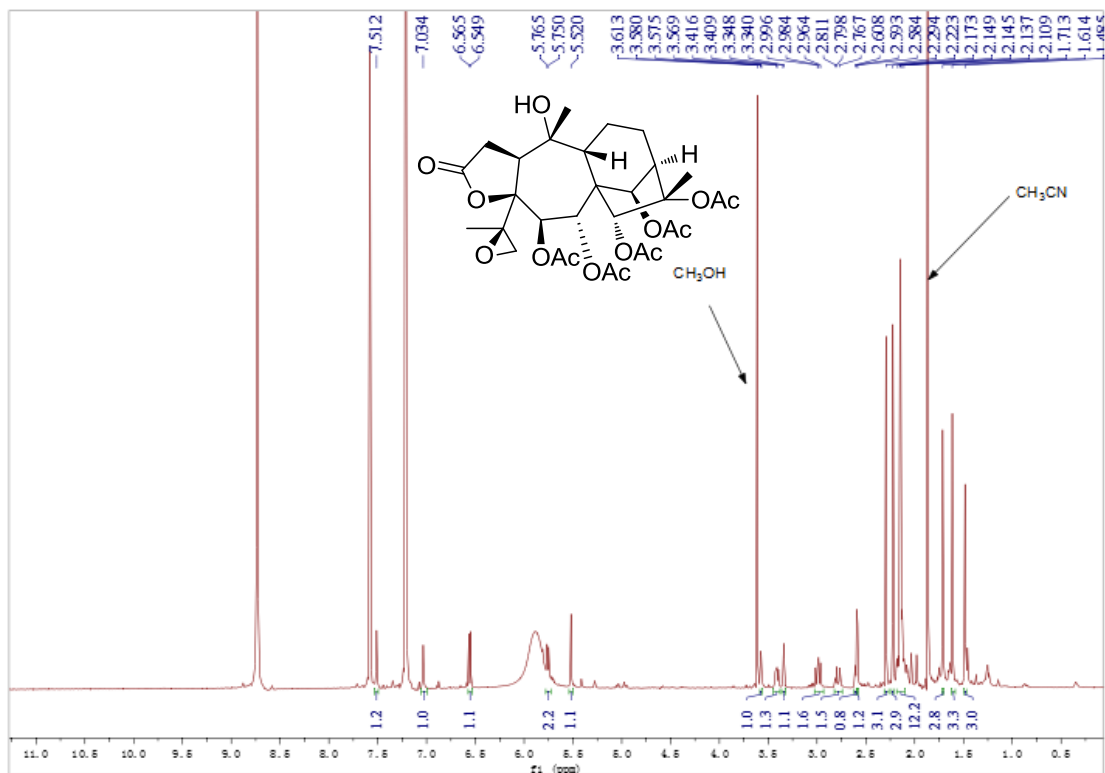


Figure S109. ¹H NMR spectrum of **12** (600 MHz, in C₅D₅N)

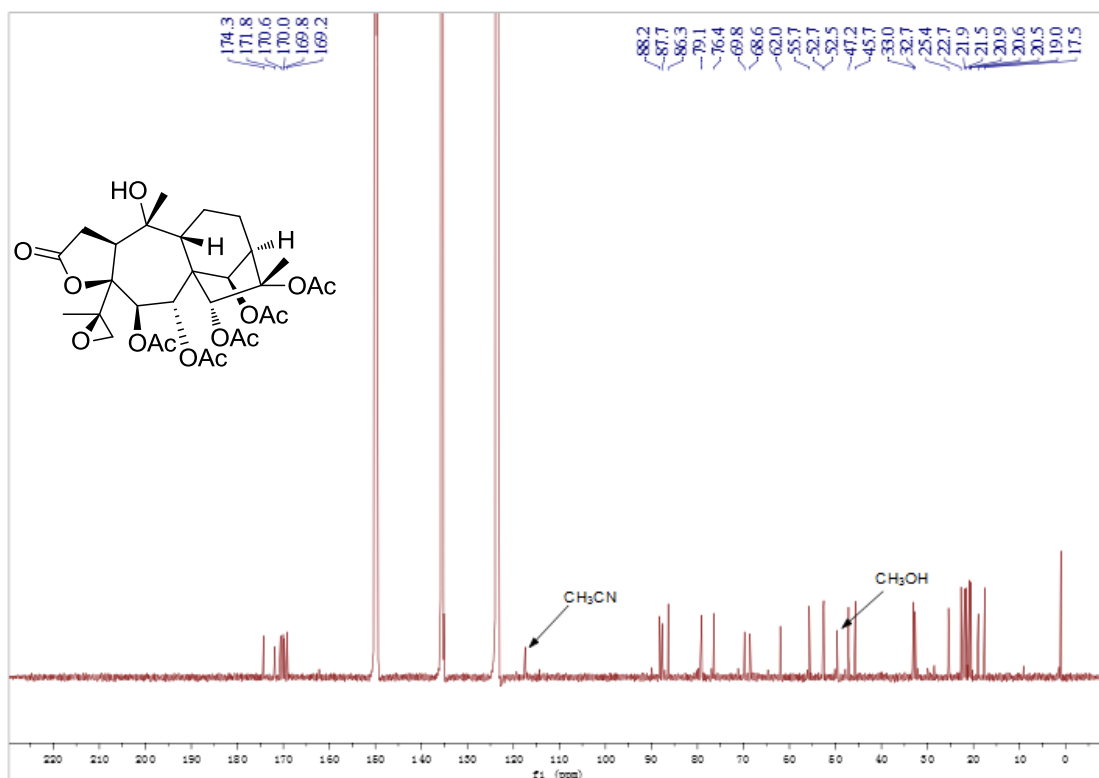


Figure S110. ^{13}C NMR spectrum of **12** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

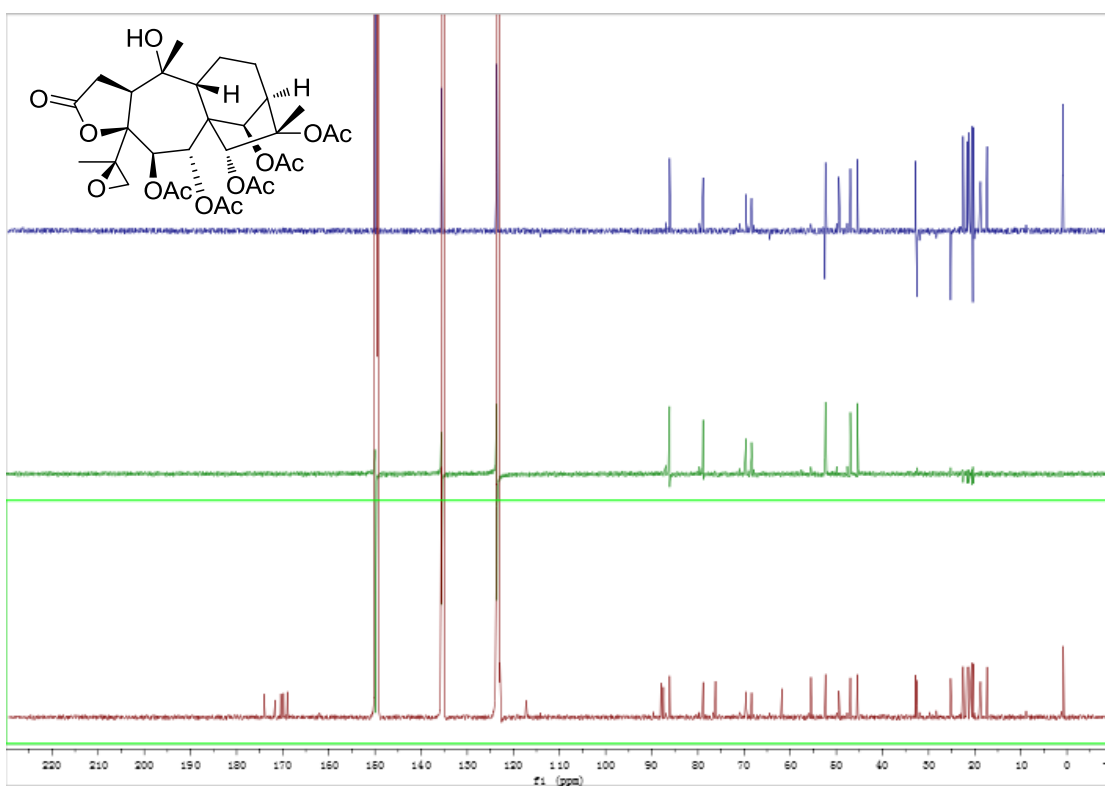


Figure S111. DEPT spectrum of **12** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

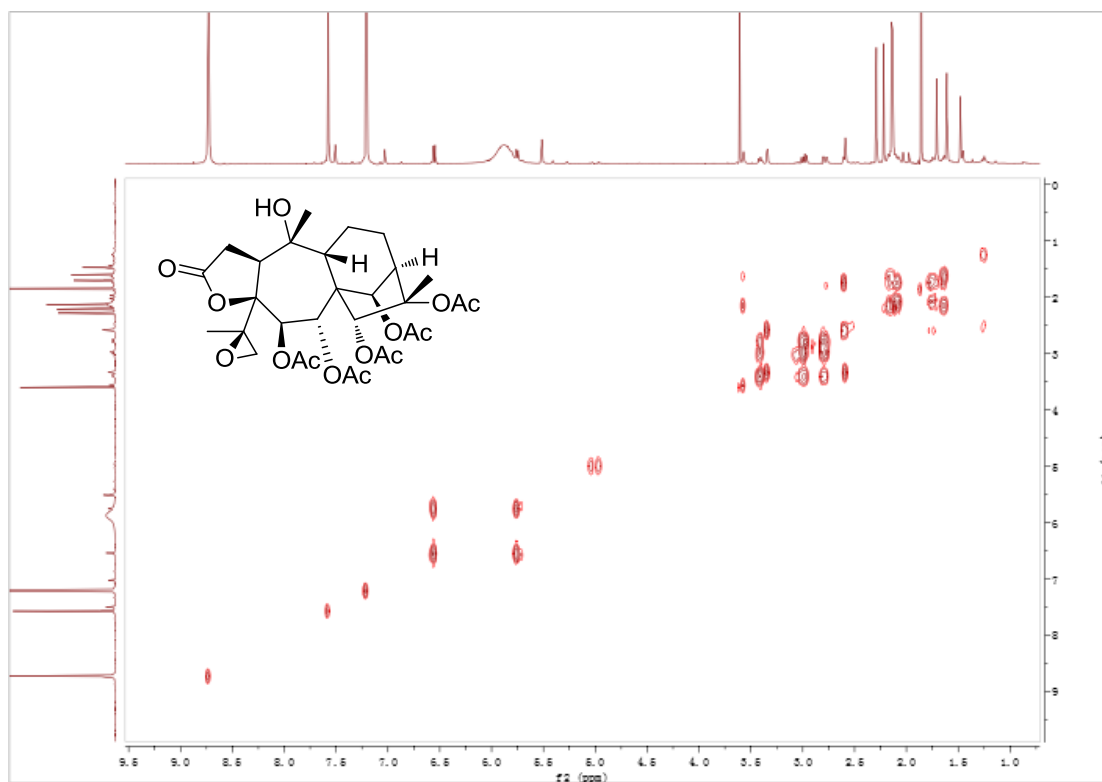


Figure S112. ^1H - ^1H COSY spectrum of **12** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

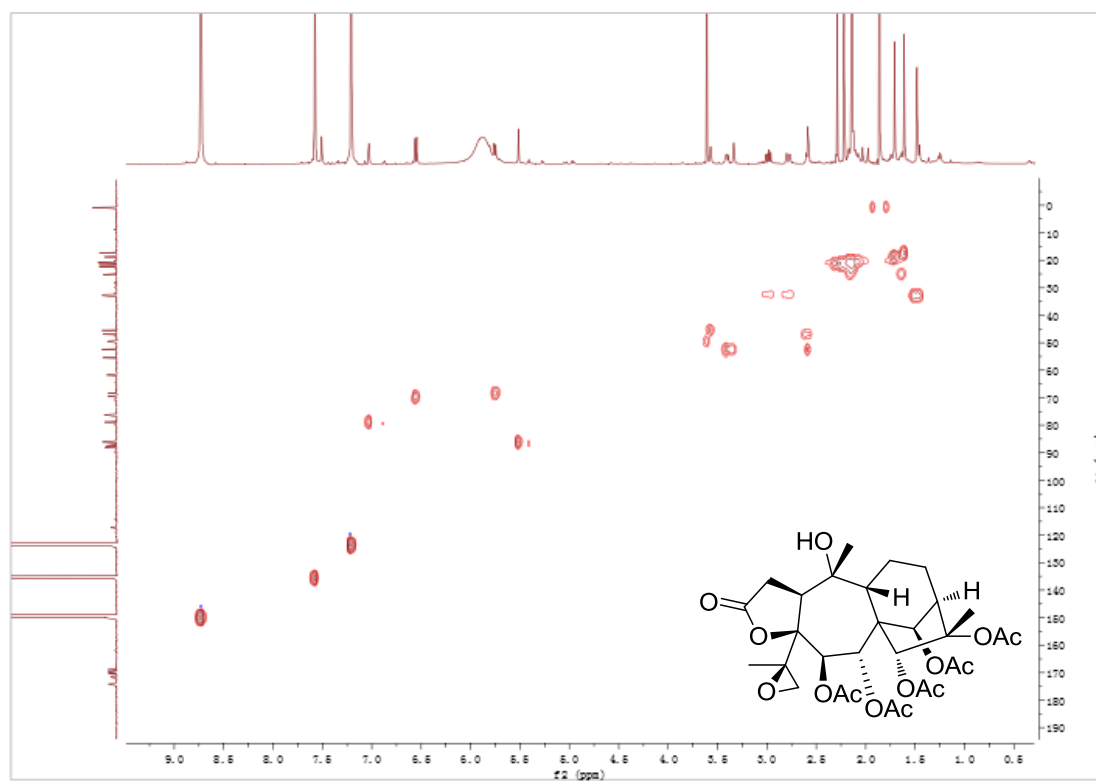


Figure S113. HSQC spectrum of **12** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

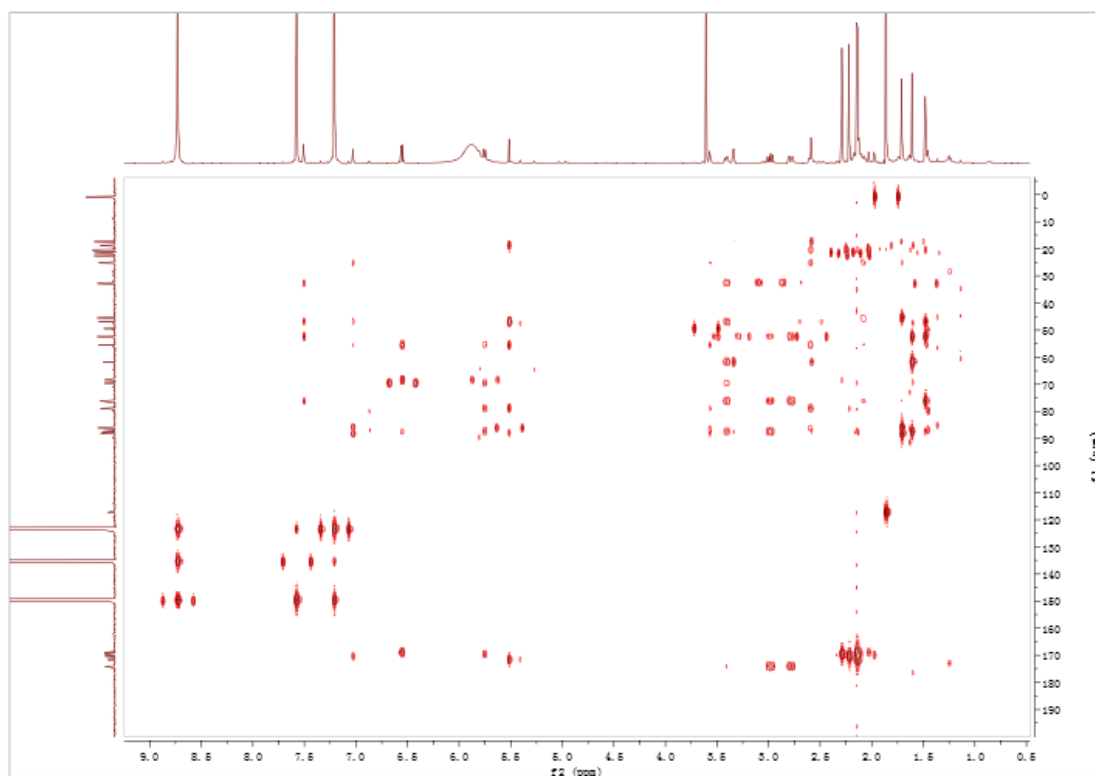


Figure S114. HMBC spectrum of **12** (600 MHz, in C_5D_5N)

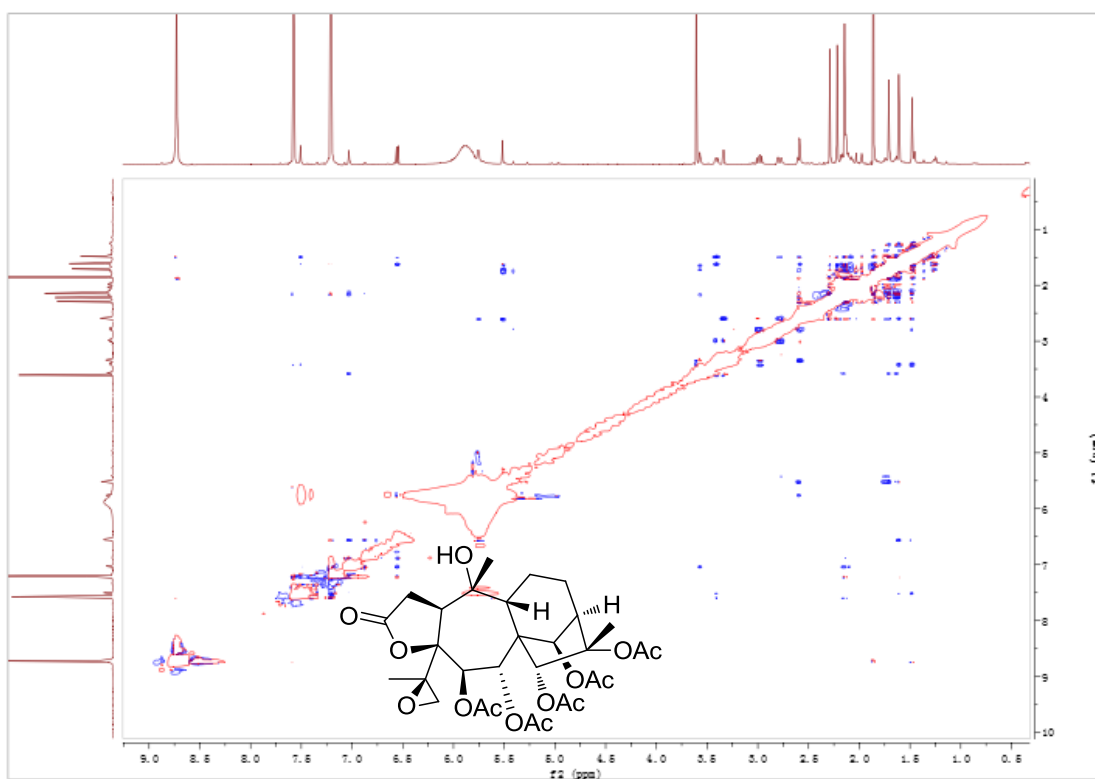


Figure S115. NOESY spectrum of **12** (600 MHz, in C_5D_5N)

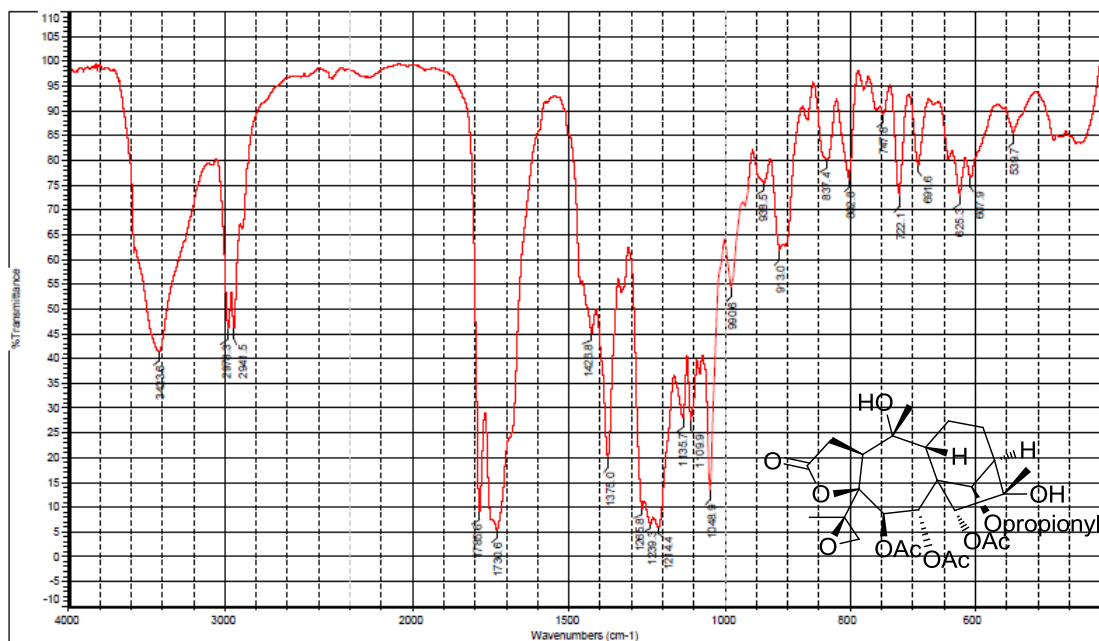


Figure S116. IR spectrum of 13

MS Formula Results: + Scan (5.911 min) Sub (2016090607.d)

m/z	Ion	Formula	Abundance
618.2355	(M+Na) ⁺	C29 H40 Na O13	10644.9

Best	Formula (M)	Ion Formula	Score	Cross Sci	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DfE
✓	C29 H40 O13	C29 H40 Na O13	99.48		596.2463	596.2469	619.2361	-1.03	1.03	99.97	99.65	99.31	10
	C24 H40 N2 O15	C24 H40 N2 Na O15	98.78		596.2463	596.2429	619.2321	-5.73	5.73	96.93	99.01	98.21	6
	C33 H40 O8 S	C33 H40 Na O8 S	97.9		596.2463	596.2444	619.2336	-3.17	3.17	96.67	95.58	97.13	14
	C21 H44 N2 O15 S	C21 H44 N2 Na O15 S	97.59		596.2463	596.2462	619.2355	-0.08	0.08	100	94.36	96.62	1
	C30 H44 O8 S2	C30 H44 Na O8 S2	96.57		596.2463	596.2478	619.2337	2.47	2.47	99.8	91.46	96.22	9
	C25 H44 N2 O10 S2	C25 H44 N2 Na O10 S2	96.35		596.2463	596.2437	619.2333	-4.28	4.28	99.4	91.55	95.99	5
	C42 H32 N2 O2	C42 H32 N2 Na O2	96.08		596.2463	596.2464	619.2356	0.16	0.16	100	87.53	96.51	28
	C39 H36 N2 O2 S	C39 H36 N2 Na O2 S	95.82		596.2463	596.2497	619.2339	5.81	5.81	98.9	89.77	97.36	23
	C34 H44 O3 S3	C34 H44 Na O3 S3	94.07		596.2463	596.2453	619.2345	-1.73	1.73	99.9	82.8	96.81	13
	C22 H48 N2 O10 S3	C22 H48 N2 Na O10 S3	93.8		596.2463	596.2471	619.2363	1.36	1.36	99.94	82.22	95.41	0

Figure S117. (+)-HRESIMS data of 13

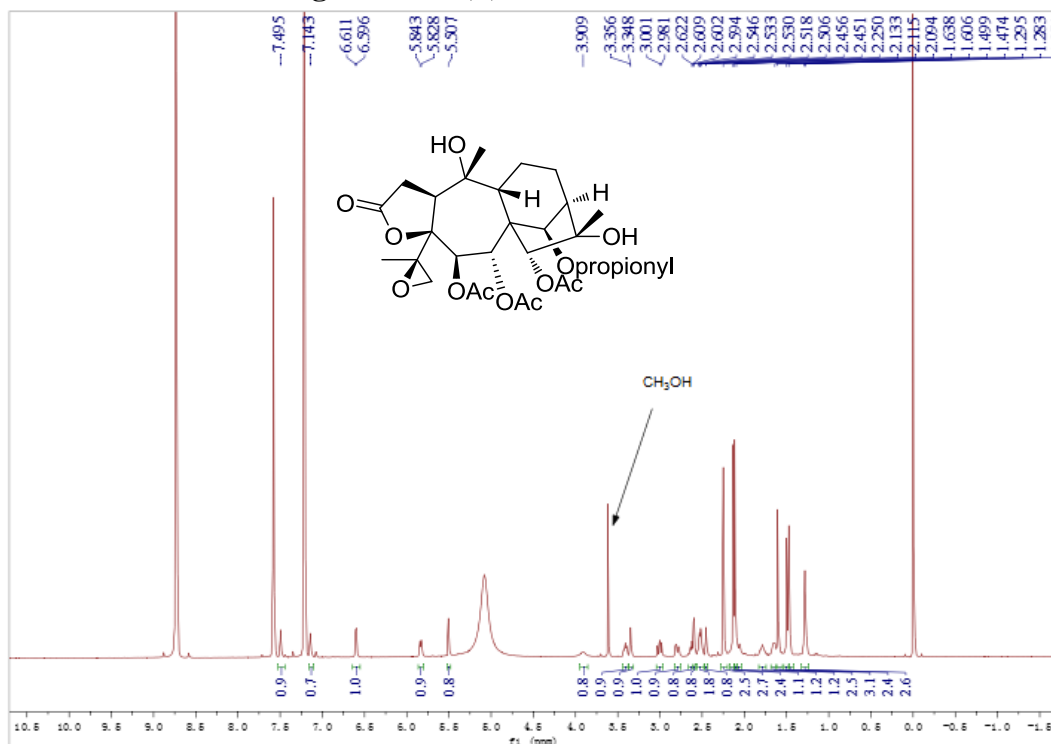


Figure S118. ¹H NMR spectrum of 13 (600 MHz, in C₅D₅N)

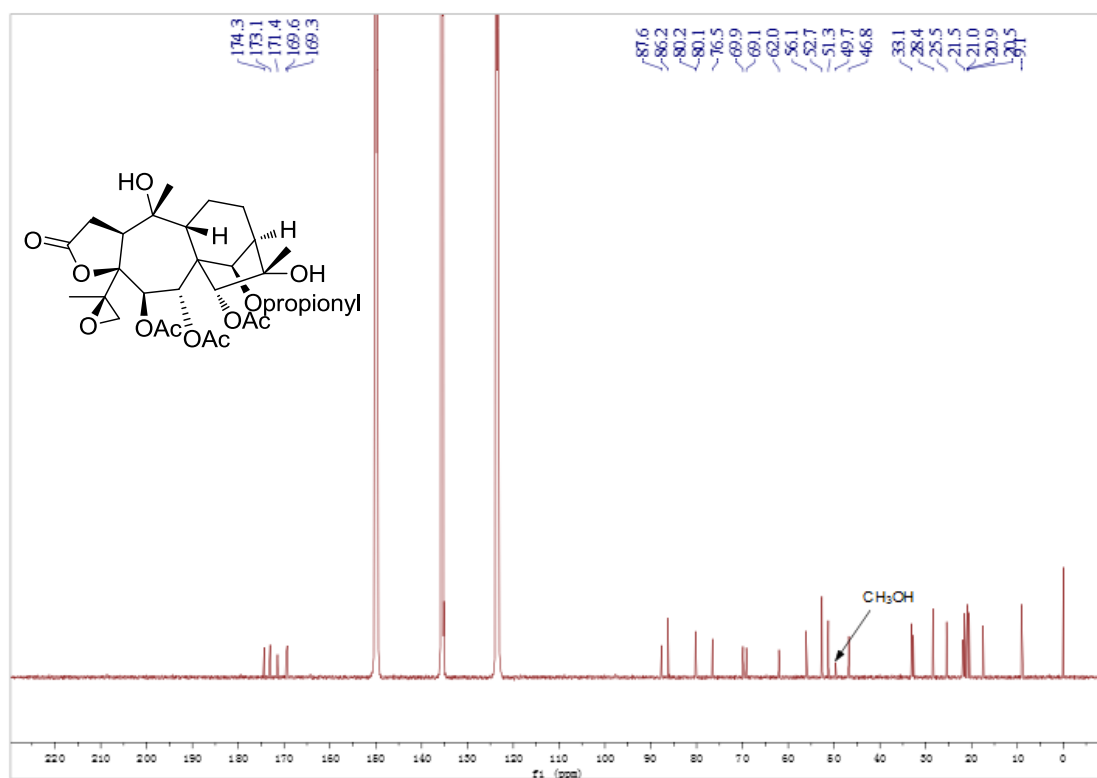


Figure S119. ^{13}C NMR spectrum of **13** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

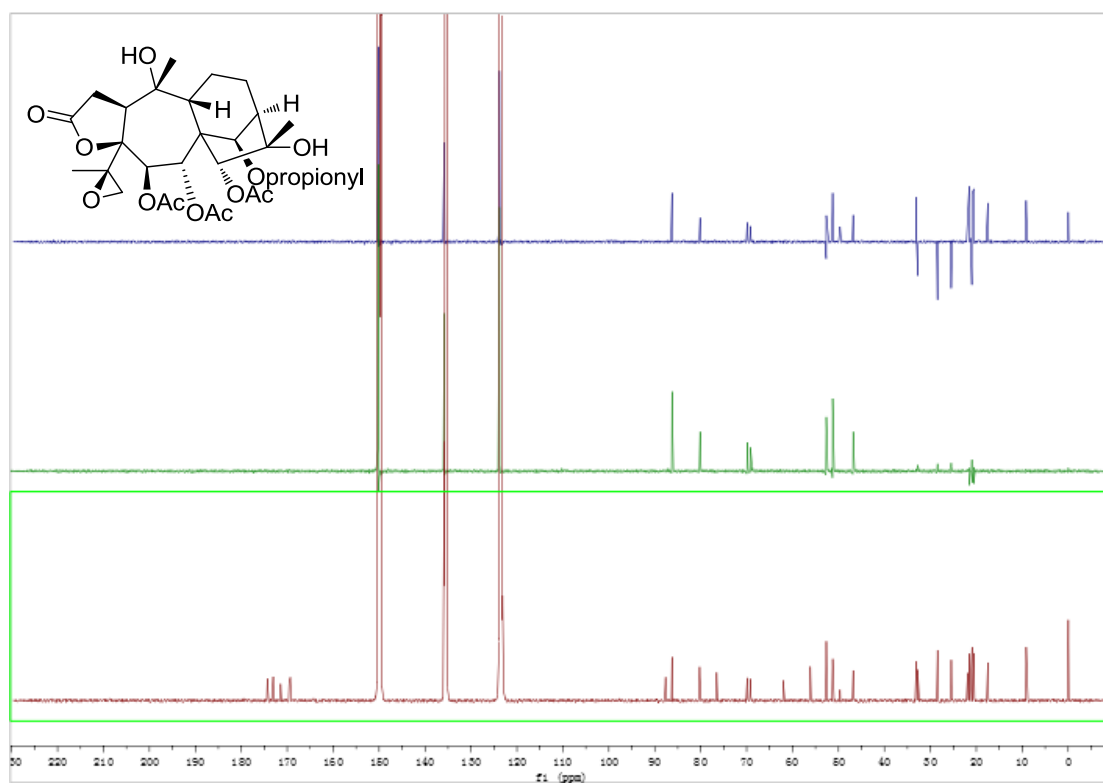


Figure S120. DEPT spectrum of **13** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

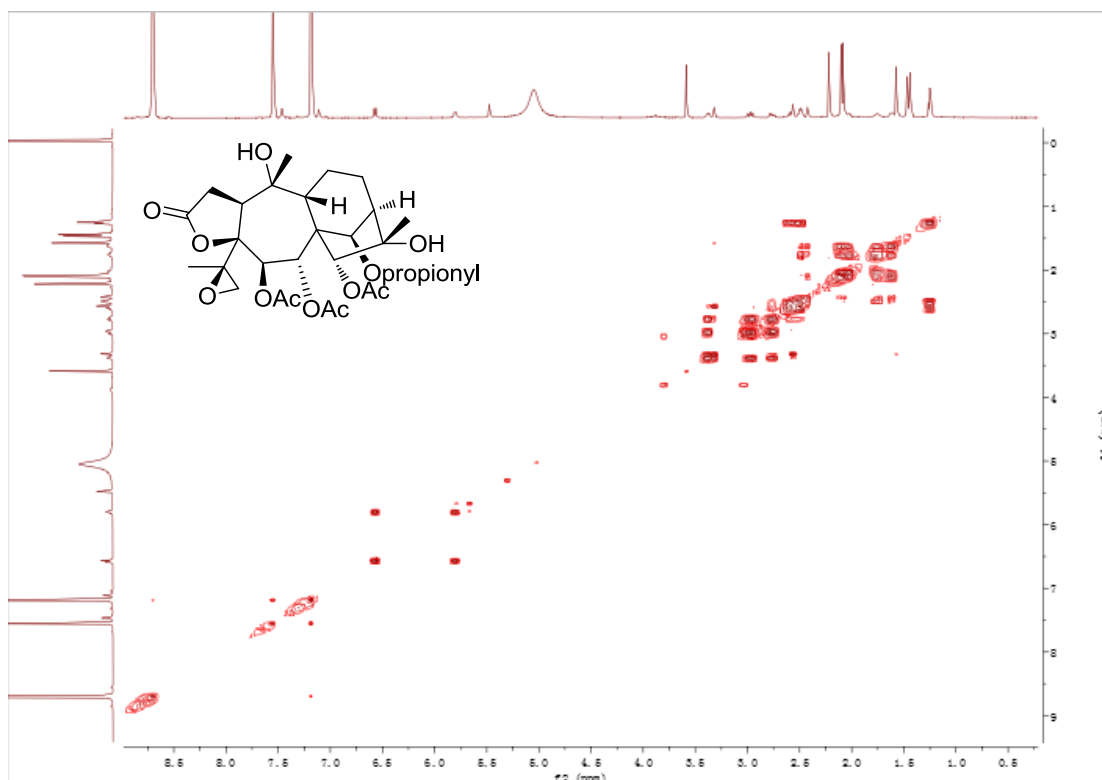


Figure S121. ^1H - ^1H COSY spectrum of **13** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

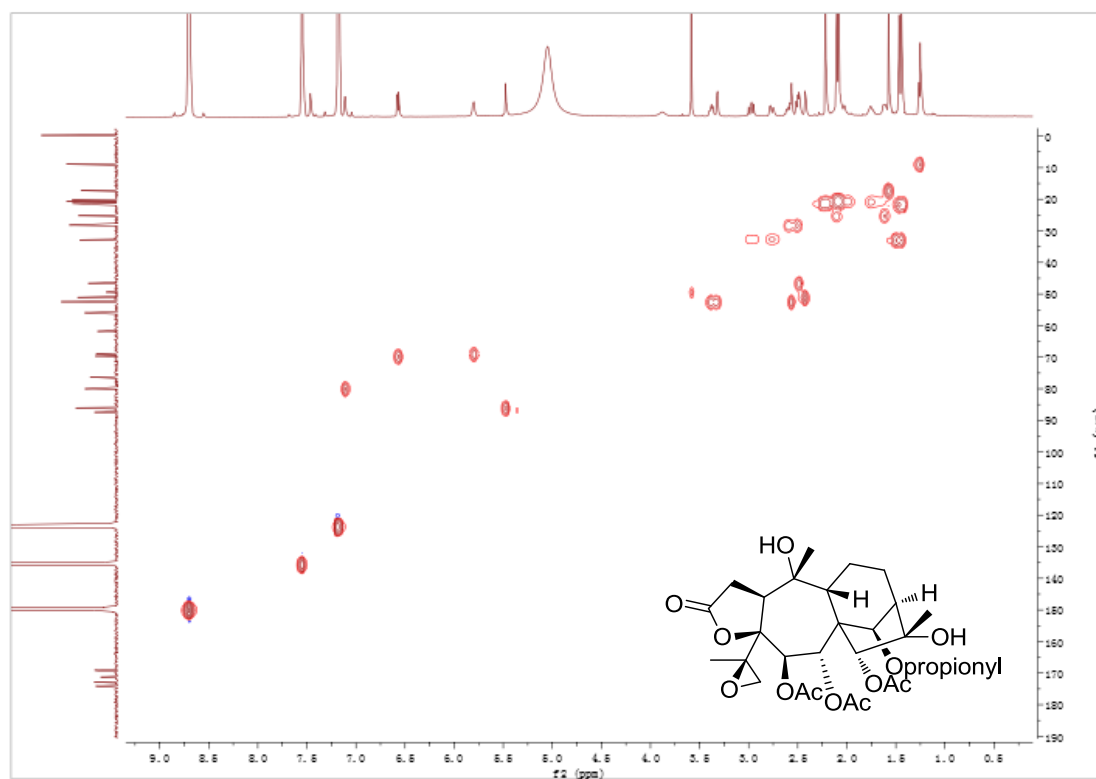


Figure S122. HSQC spectrum of **13** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

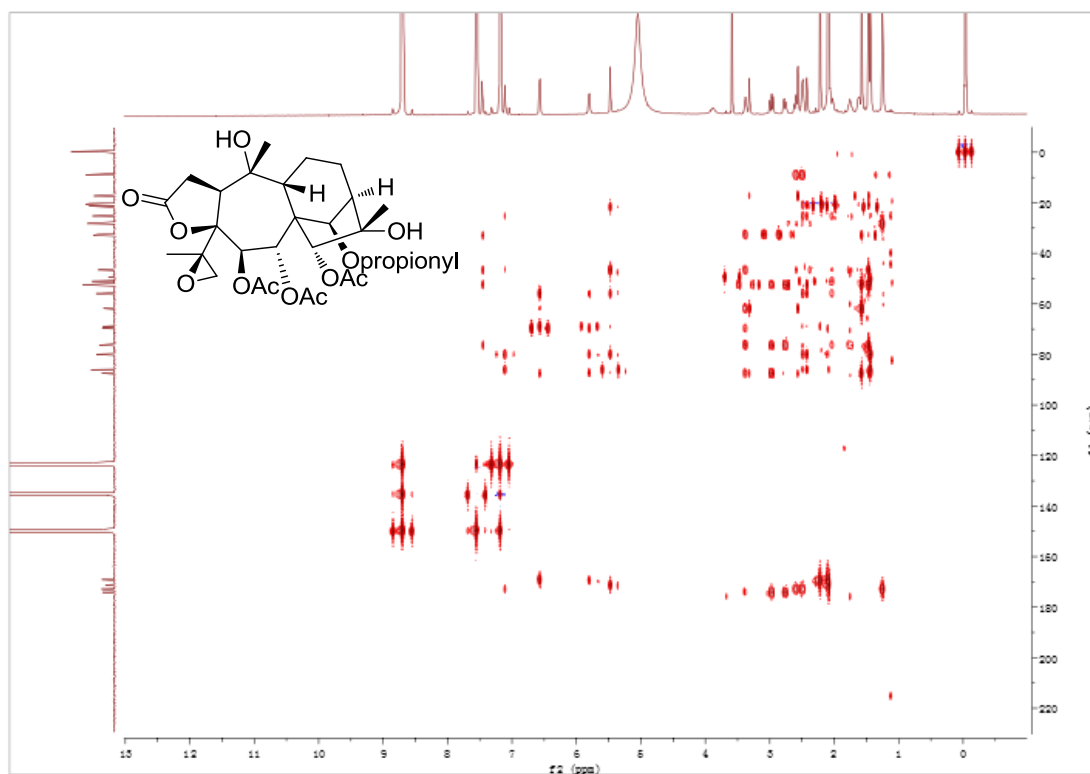


Figure S123. HMBC spectrum of **13** (600 MHz, in C_5D_5N)

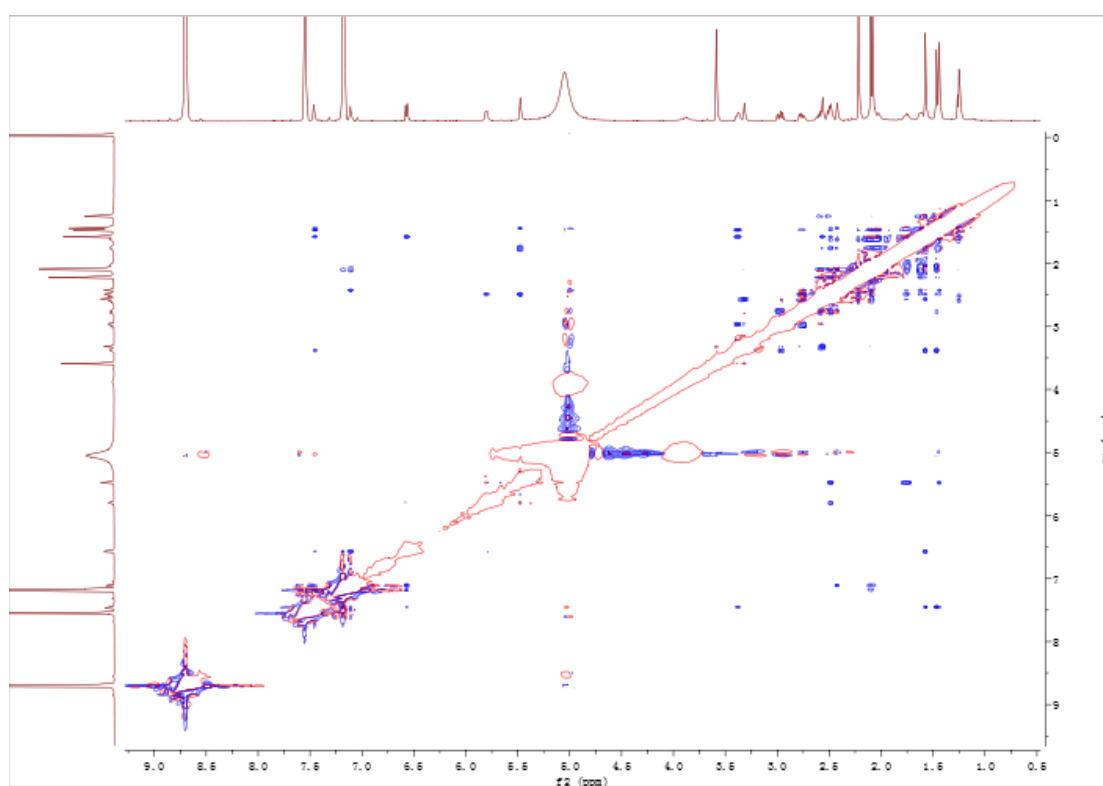


Figure S124. NOESY spectrum of **13** (600 MHz, in C_5D_5N)

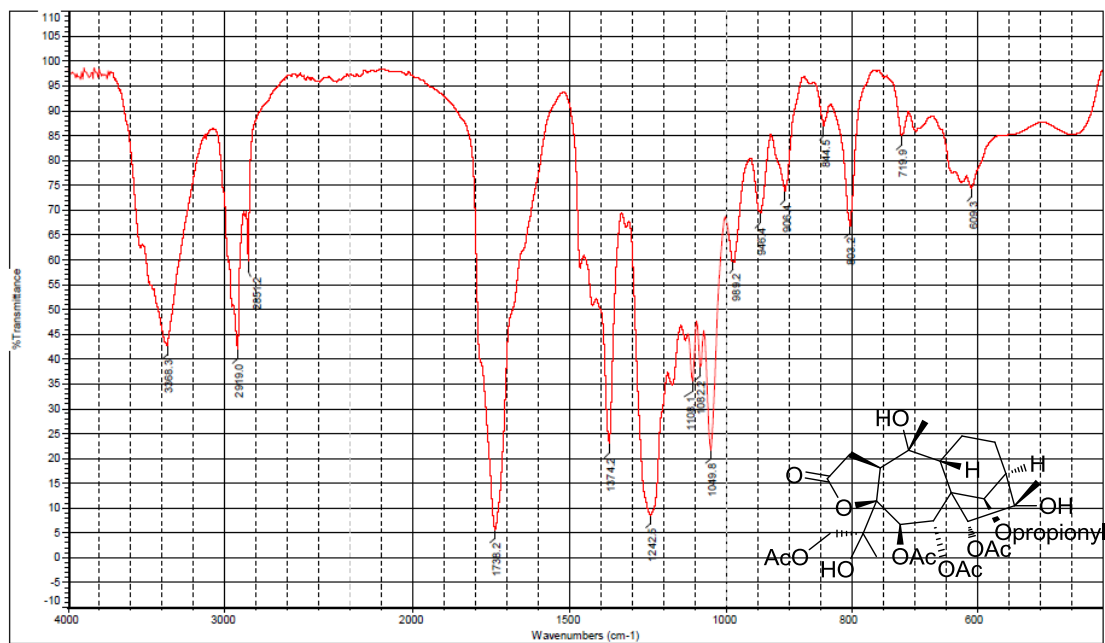


Figure S125. IR spectrum of 14

MS Formula Results: + Scan (5.946 min) Sub (2015060902.d)

m/z	Ion	Formula	Abundance										
678.2572	(M+Na) ⁺	C31 H44 Na O15	428789.7										
Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
14	☑	C31 H44 Na O15	99.93		656.268	656.268	678.2572	0.1	0.1	100	99.88	99.88	10
15	☐	C32 H40 Na O11	99.85		656.268	656.2694	678.2586	2.12	2.12	99.85	99.8	99.92	15
16	☐	C27 H40 N6 O13	99.48		656.268	656.2653	678.2546	-4.02	4.02	99.46	90.11	99.96	11
17	☐	C44 H36 N2 O4	97.81		656.268	656.2675	678.2567	-0.69	0.69	99.98	92.5	99.86	28
18	☐	C20 H44 N6 O18	97.34		656.268	656.2712	678.2604	4.92	4.92	98.7	92.03	98.98	2
19	☐	C45 H32 N6	97.05		656.268	656.2688	678.2581	1.33	1.33	99.94	89.86	99.9	33
20	☐	C49 H36 O2	96		656.268	656.2715	678.2608	5.45	5.45	99.02	87.8	99.82	32

Figure S126. (+)-HRESIMS data of 14

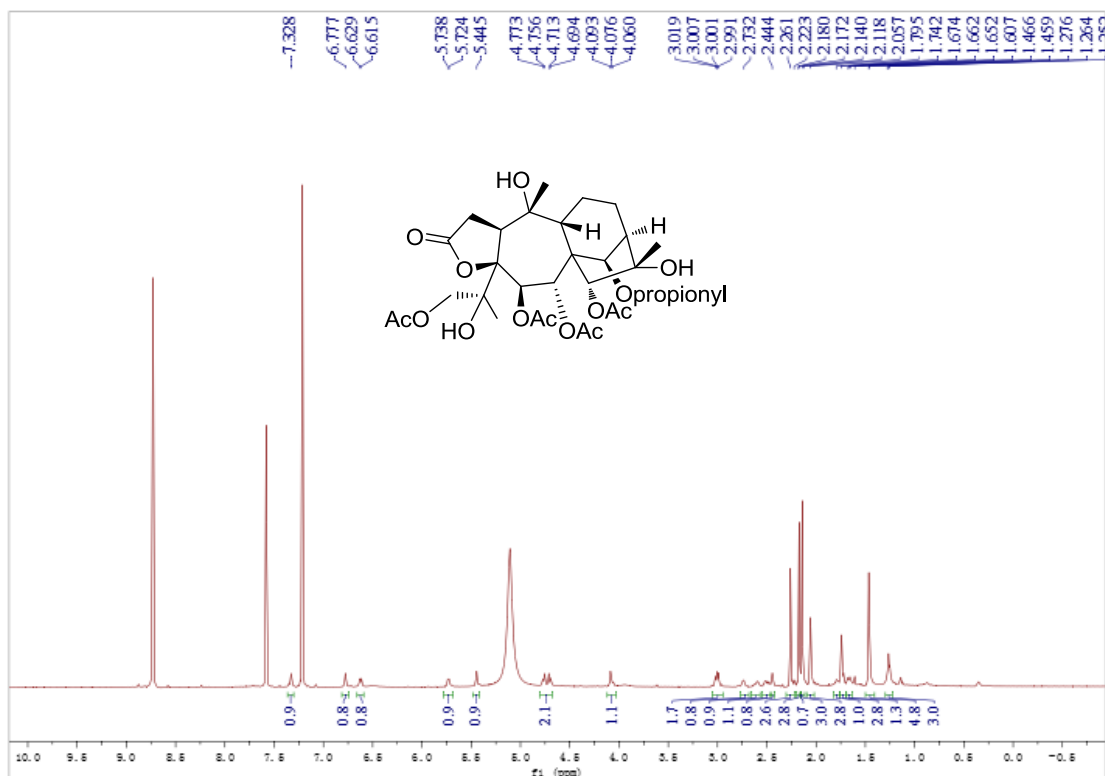


Figure S127. ¹H NMR spectrum of 14 (600 MHz, in C₅D₅N)

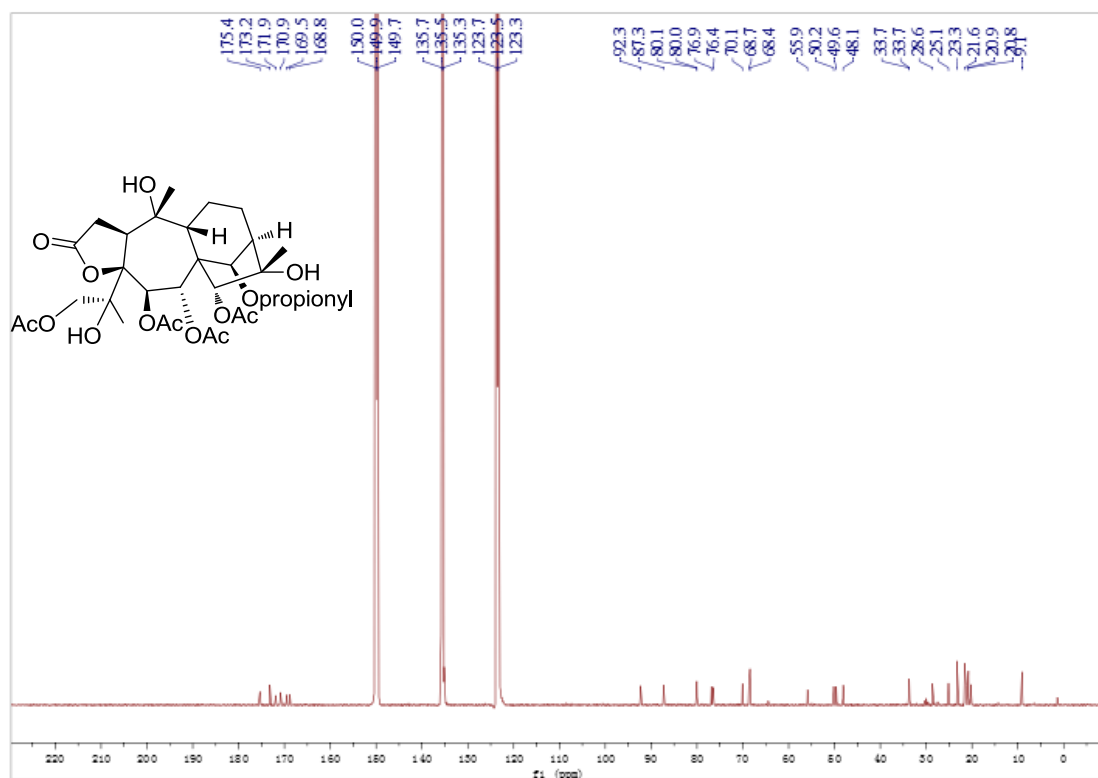


Figure S128. ^{13}C NMR spectrum of **14** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

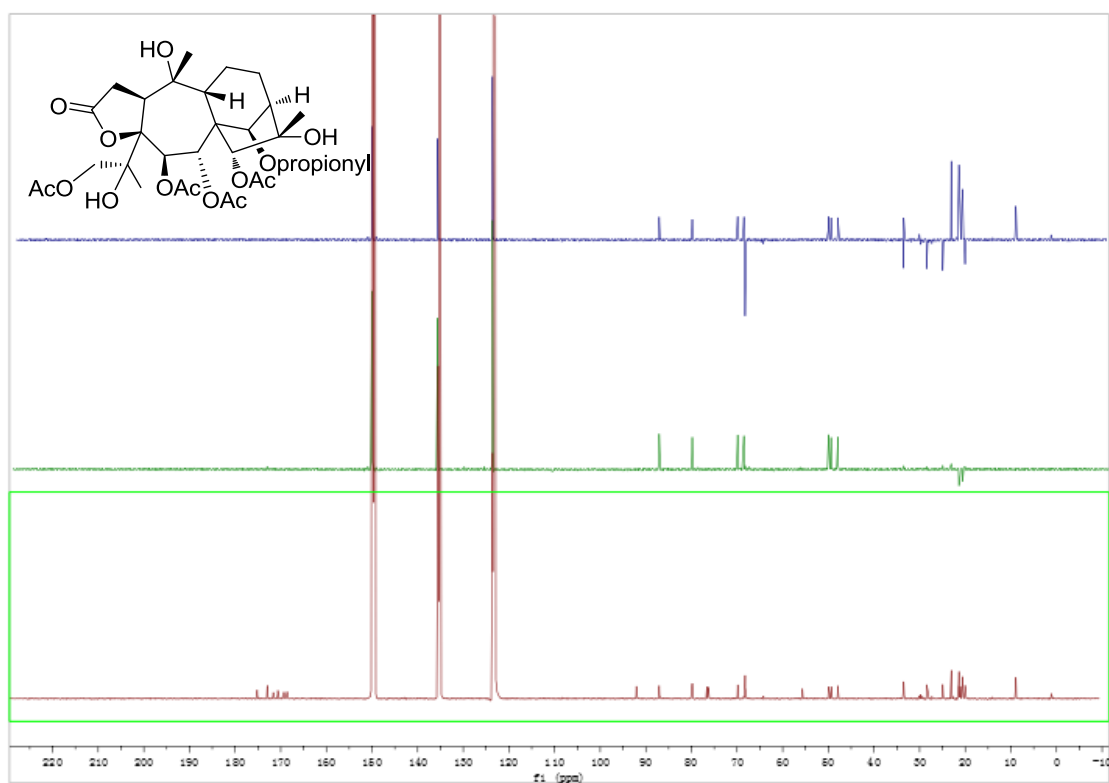


Figure S129. DEPT spectrum of **14** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

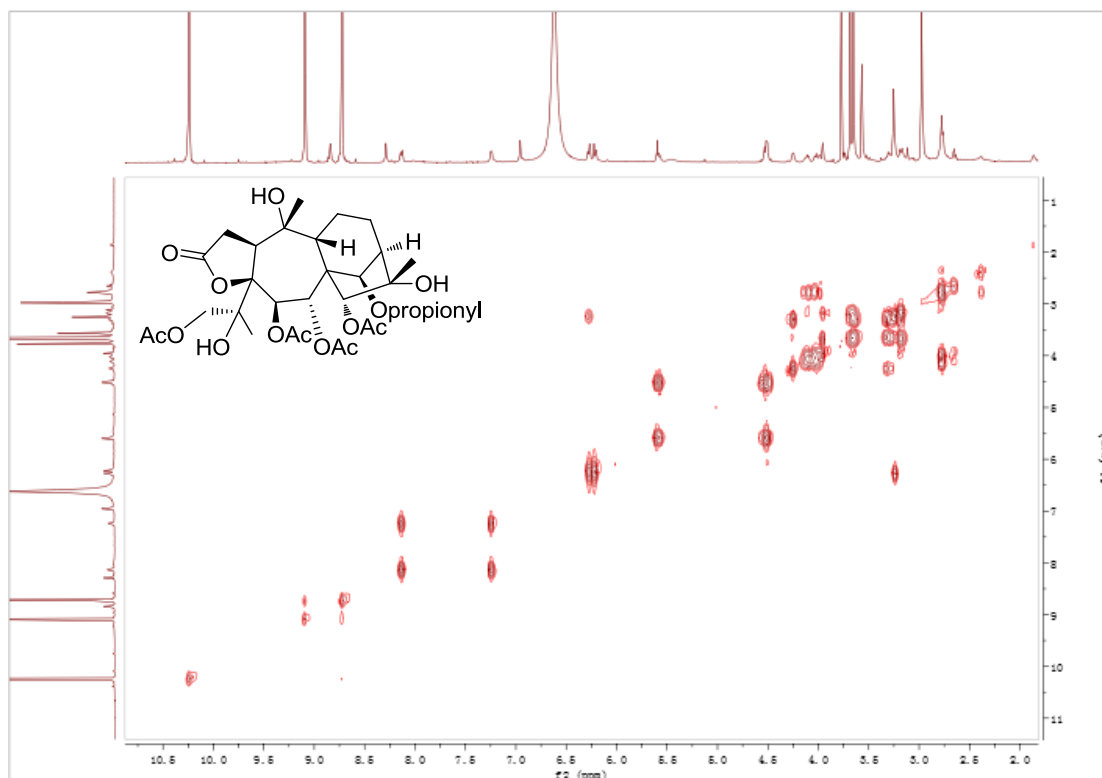


Figure S130. ^1H - ^1H COSY spectrum of **14** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

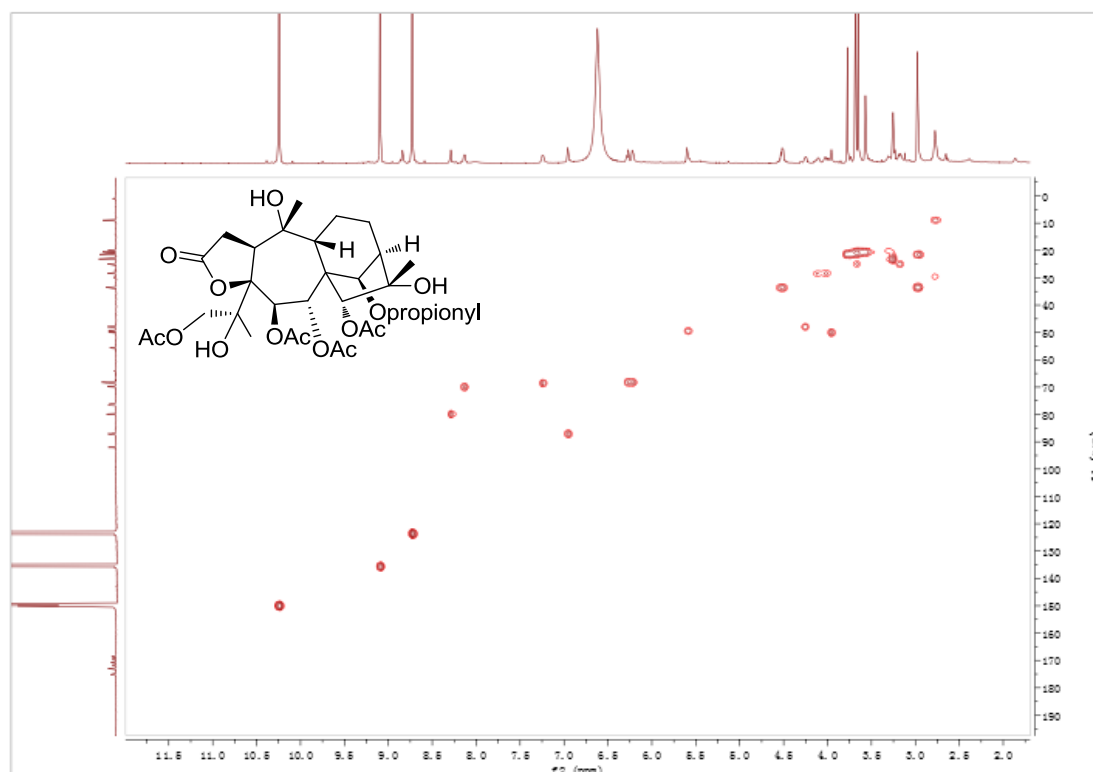


Figure S131. HSQC spectrum of **14** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

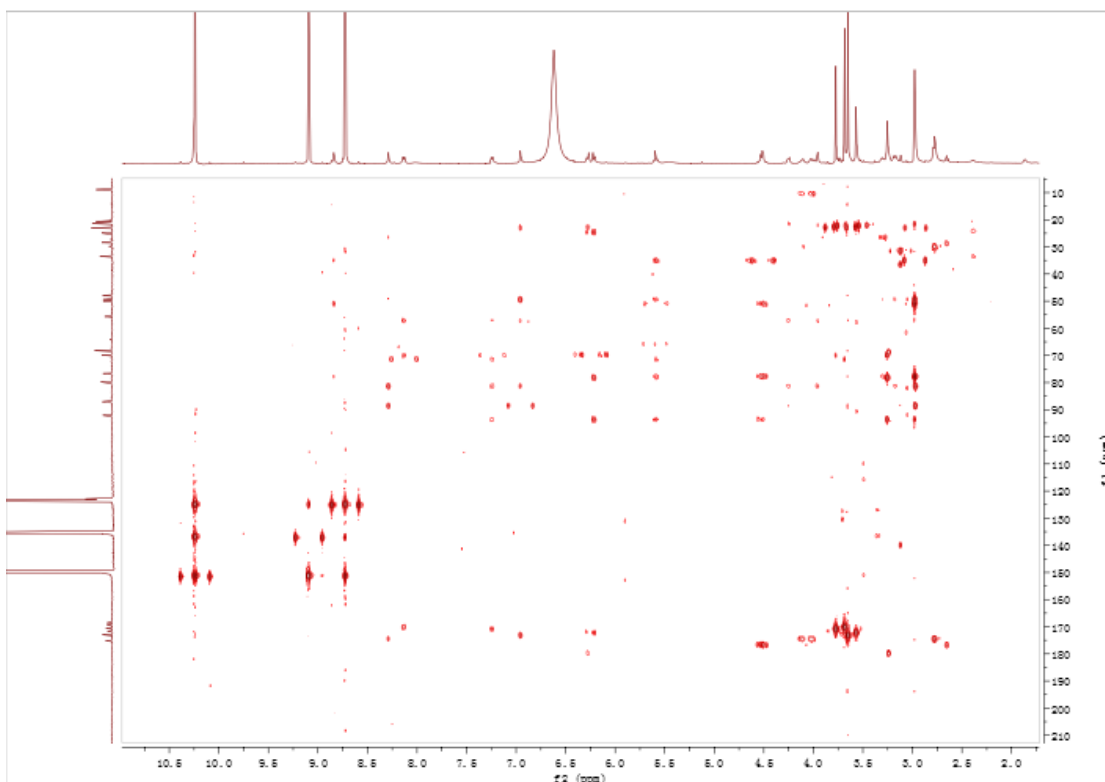


Figure S132. HMBC spectrum of **14** (600 MHz, in C_5D_5N)

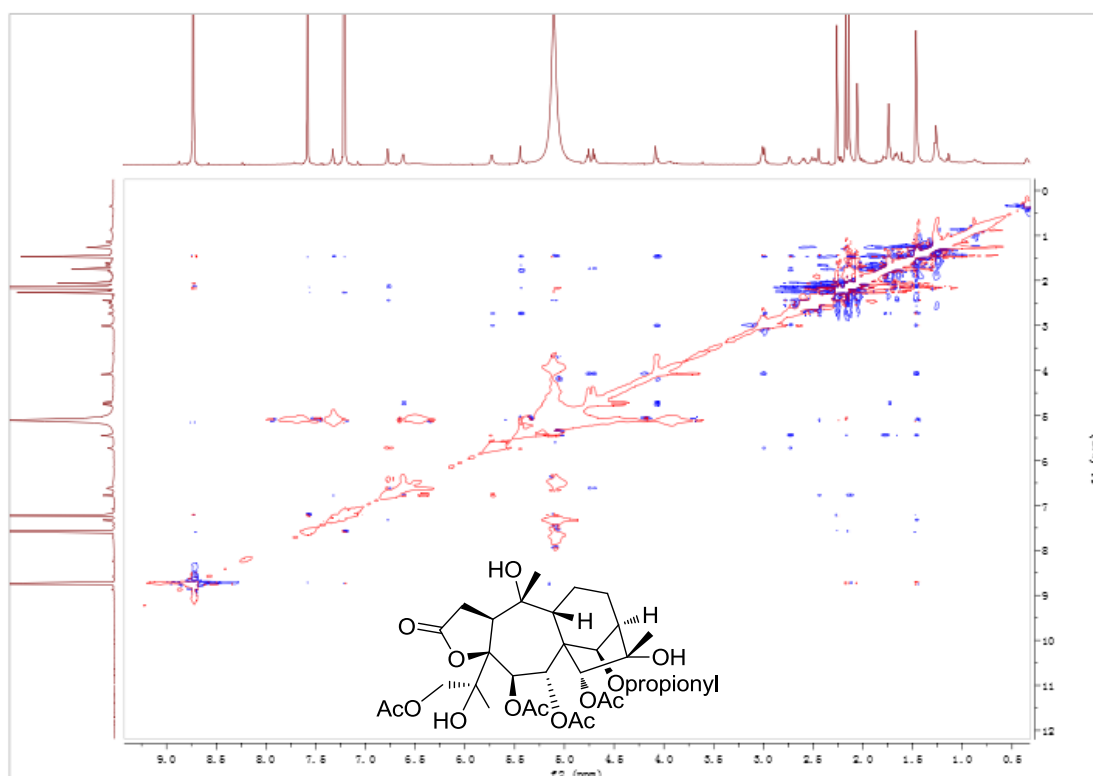
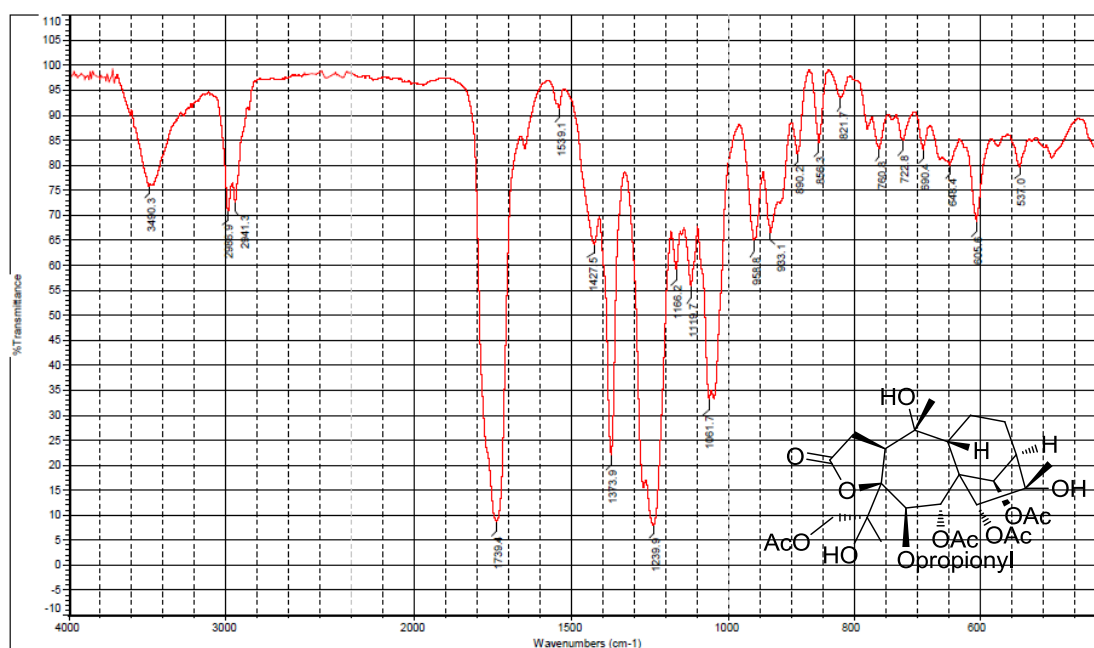


Figure S133. NOESY spectrum of **14** (600 MHz, in C_5D_5N)

Table S4. Crystal data and structure refinement for **14**

Identification code	exp_3672
Empirical formula	C ₃₁ H ₄₆ O ₁₆
Formula weight	674.68
Temperature/K	102.3
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a / Å, b / Å, c / Å	11.0687(2), 12.2272(4), 23.8020(5)
α /°, β /°, γ /°	90.00, 90.00, 90.00
Volume/Å ³	3221.34(15)
Z	4
ρ_{calc} /mg mm ⁻³	1.391
μ /mm ⁻¹	0.954
F(000)	1440
Crystal size/mm ³	0.15 × 0.14 × 0.12
2 θ range for data collection	7.42 to 142.62°
Index ranges	-13 ≤ h ≤ 8, -14 ≤ k ≤ 14, -28 ≤ l ≤ 22
Reflections collected	11345
Independent reflections	6114[R(int) = 0.0316 (inf-0.9Å)]
Data/restraints/parameters	6114/0/435
Goodness-of-fit on F ²	1.051
Final R indexes [I > 2 σ (I) i.e. F _o > 4 σ (F _o)]	R ₁ = 0.0480, wR ₂ = 0.1234
Final R indexes [all data]	R ₁ = 0.0512 wR ₂ = 0.1273
Largest diff. peak/hole/e Å ⁻³	0.456/-0.250
Flack Parameters	0.04(16)
Completeness	0.987

**Figure S134.** IR spectrum of **15**

MS Formula Results: + Scan (5.952 min) Sub (2015060901.d)

m/z	Ion	Formula	Abundance
679.2572	(M-Na) ⁺	C31 H44 Na O15	208514.9

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C31 H44 O15	C31 H44 Na O15	99.9		656.268	656.268	679.2572	0.09	0.09	100	99.76	99.85	10
✓	C30 H40 Na O11	C30 H40 Na O11	95.6		656.268	656.264	679.2586	2.11	2.11	95.85	98.96	99.88	15
✓	C27 H40 N6 O13	C27 H40 N6 Na O13	99.58		656.268	656.2653	679.2546	-4.03	4.03	99.46	99.49	99.92	11
✓	C20 H44 N6 O18	C20 H44 N6 Na O18	98.06		656.268	656.2712	679.2604	4.91	4.91	99.2	94.6	99.95	2
✓	C44 H36 N3 O4	C44 H36 N3 Na O4	98.88		656.268	656.2675	679.2597	-0.71	0.71	99.98	99.3	99.79	26
✓	C45 H32 N6	C45 H32 N6 Na	98		656.268	656.2688	679.2581	1.33	1.33	99.94	88.36	99.82	33
✓	C49 H36 O2	C49 H36 Na O2	94.93		656.268	656.2715	679.2608	5.43	5.43	99.02	84.11	99.74	32

Figure S135. (+)-HRESIMS data of **15**

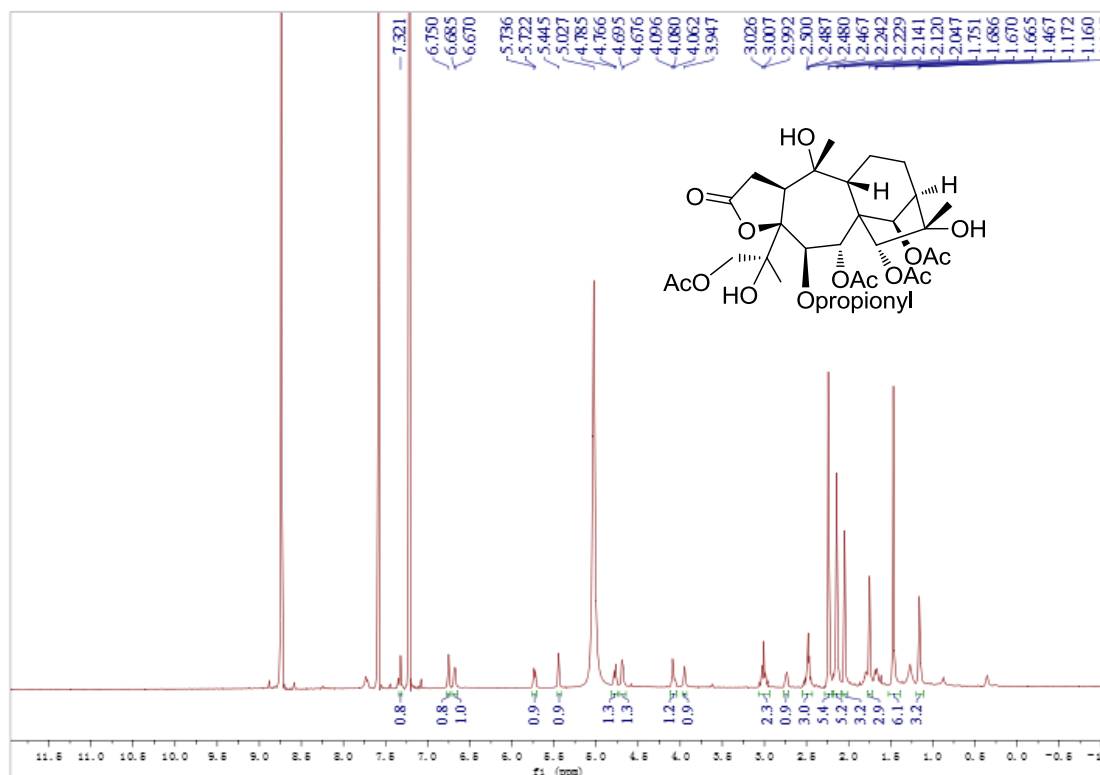


Figure S136. ¹H NMR spectrum of **15** (600 MHz, in C₅D₅N)

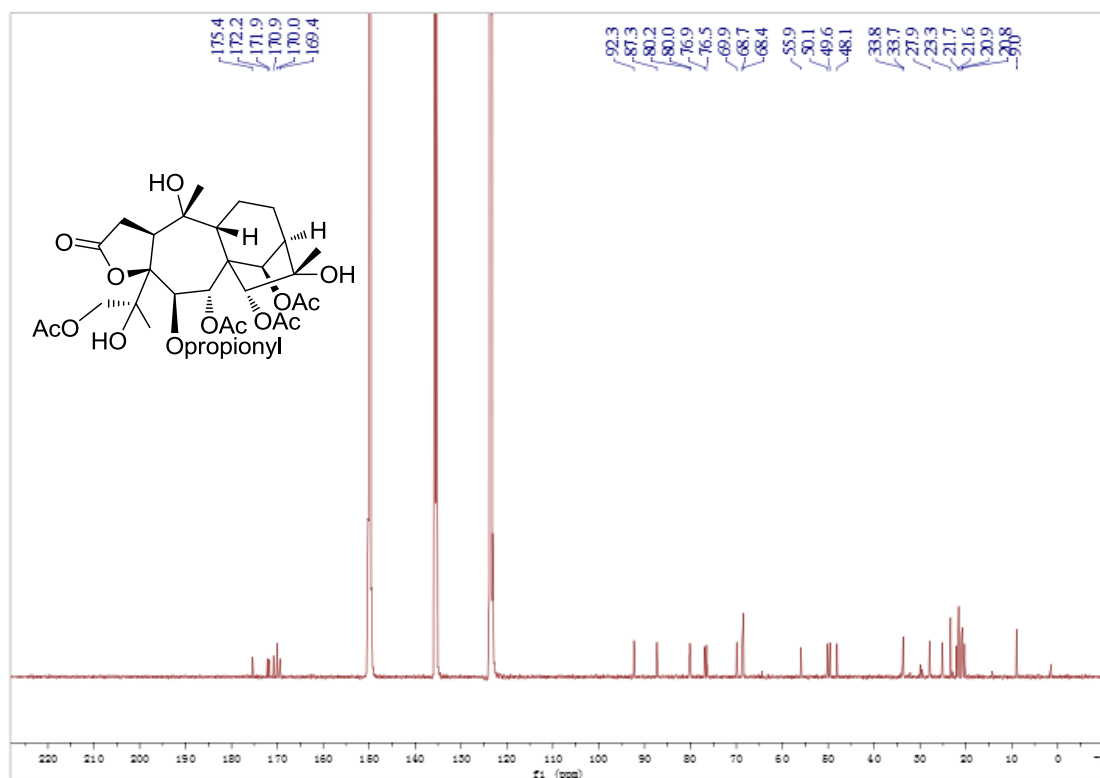


Figure S137. ^{13}C NMR spectrum of **15** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

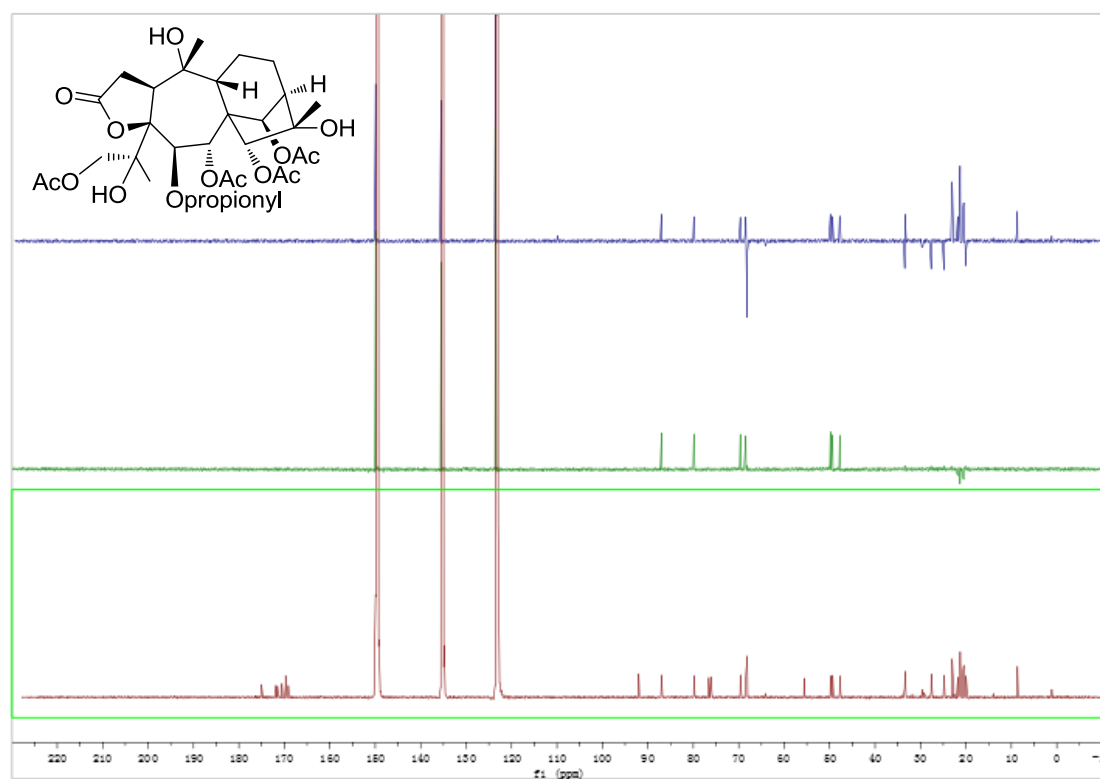


Figure S138. DEPT spectrum of **15** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

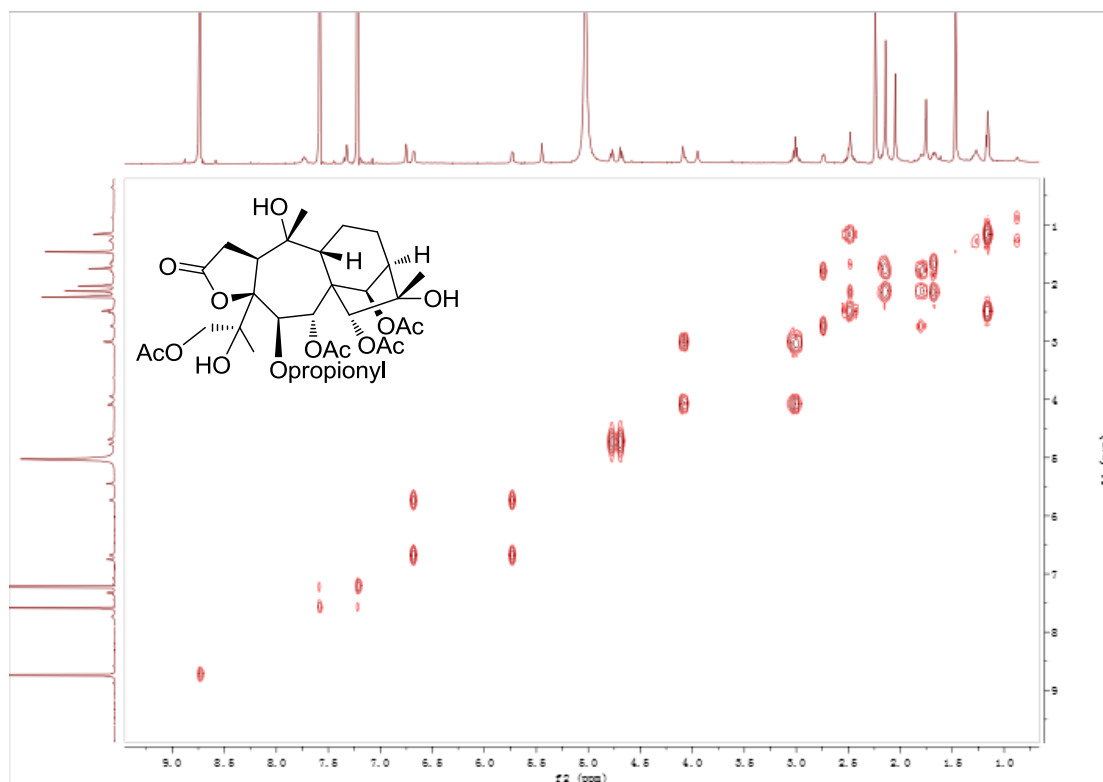


Figure S139. ^1H - ^1H COSY spectrum of **15** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

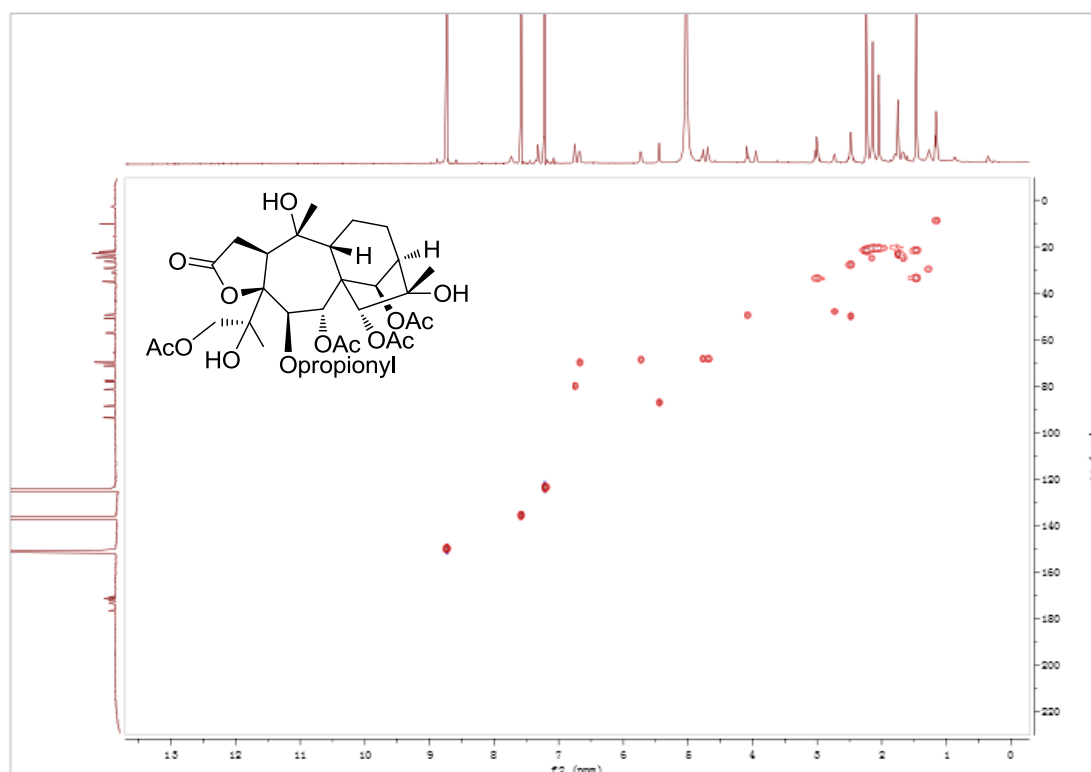


Figure S140. HSQC spectrum of **15** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

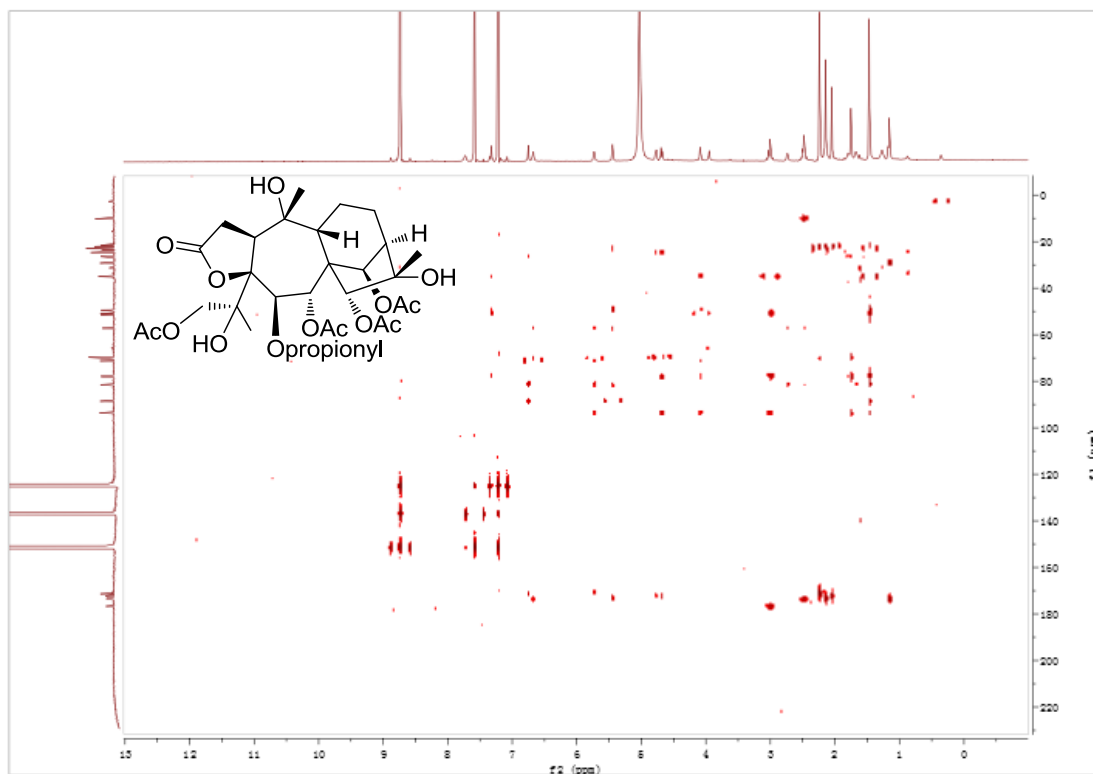


Figure S141. HMBC spectrum of **15** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

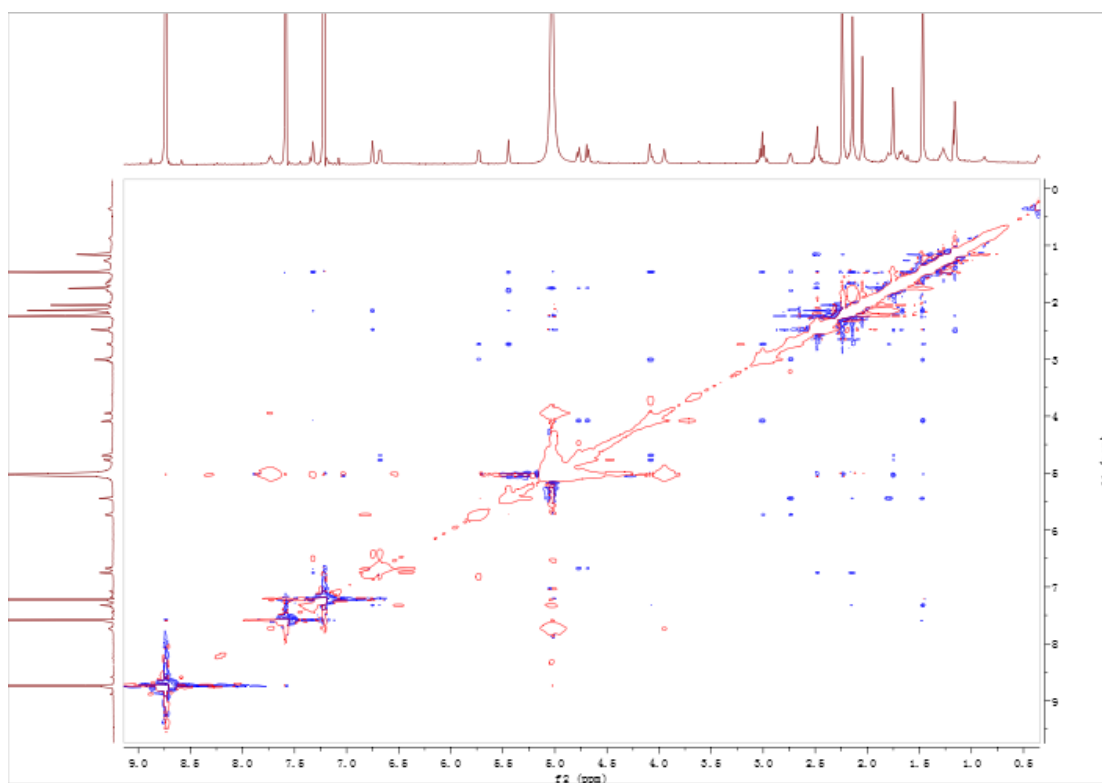


Figure S142. NOESY spectrum of **15** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

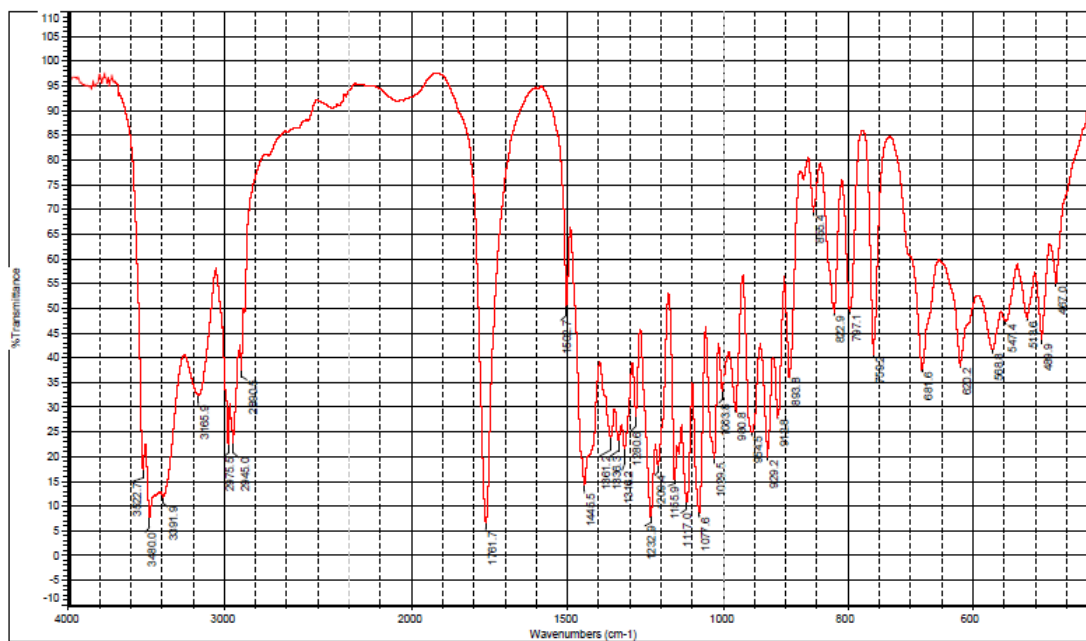


Figure S143. IR spectrum of 16

MS Formula Results: + Scan (3.247 min) Sub (2016111404.d)

m/z	Ion	Formula	Abundance
417.2123	(M+H) ⁺	C20 H33 O9	841007.5

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abs. Diff (ppm)	Mass Match	Abund. Match	Spacing Match	DBE
✓	C20 H32 O9	C20 H33 O9	99.98		416.205	416.2046	417.2118	-0.95	0.95	99.97	99.92	99.97	5
□	C21 H38 O4 S2	C21 H37 O4 S2	97.31		416.205	416.2055	417.2128	1.13	1.13	99.96	90.91	90.89	4

Figure S144. (+)-HRESIMS data of 16

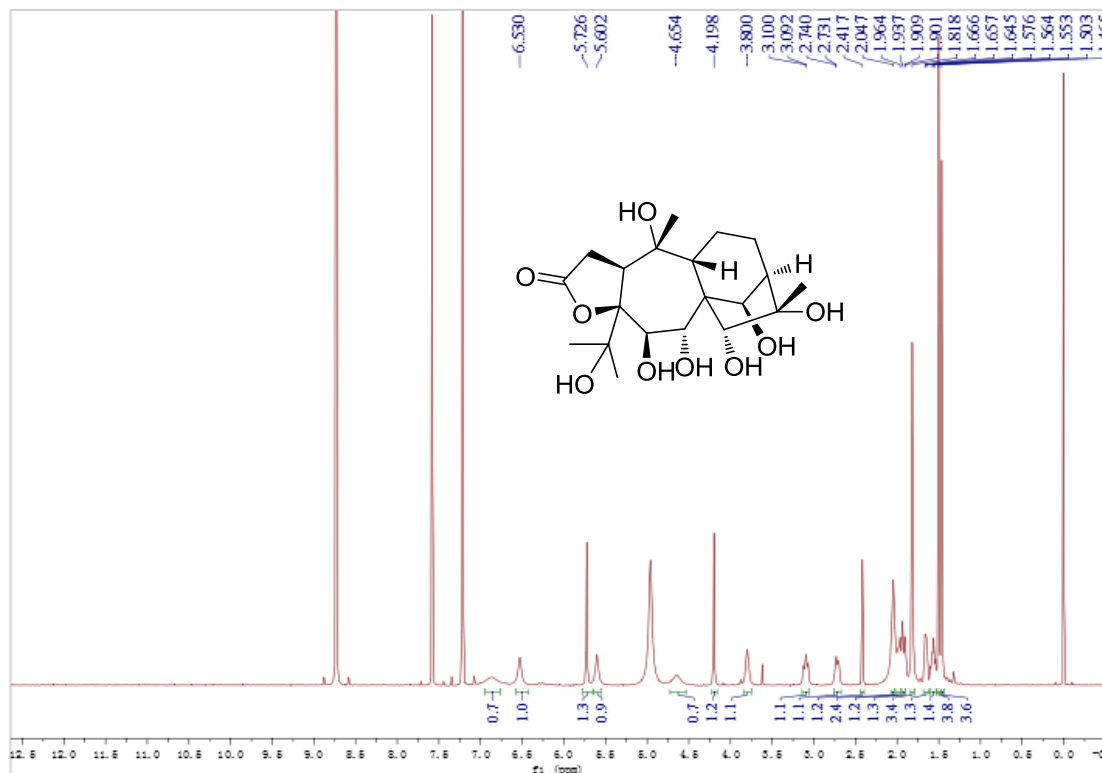


Figure S145. ¹H NMR spectrum of 16 (600 MHz, in C₅D₅N)

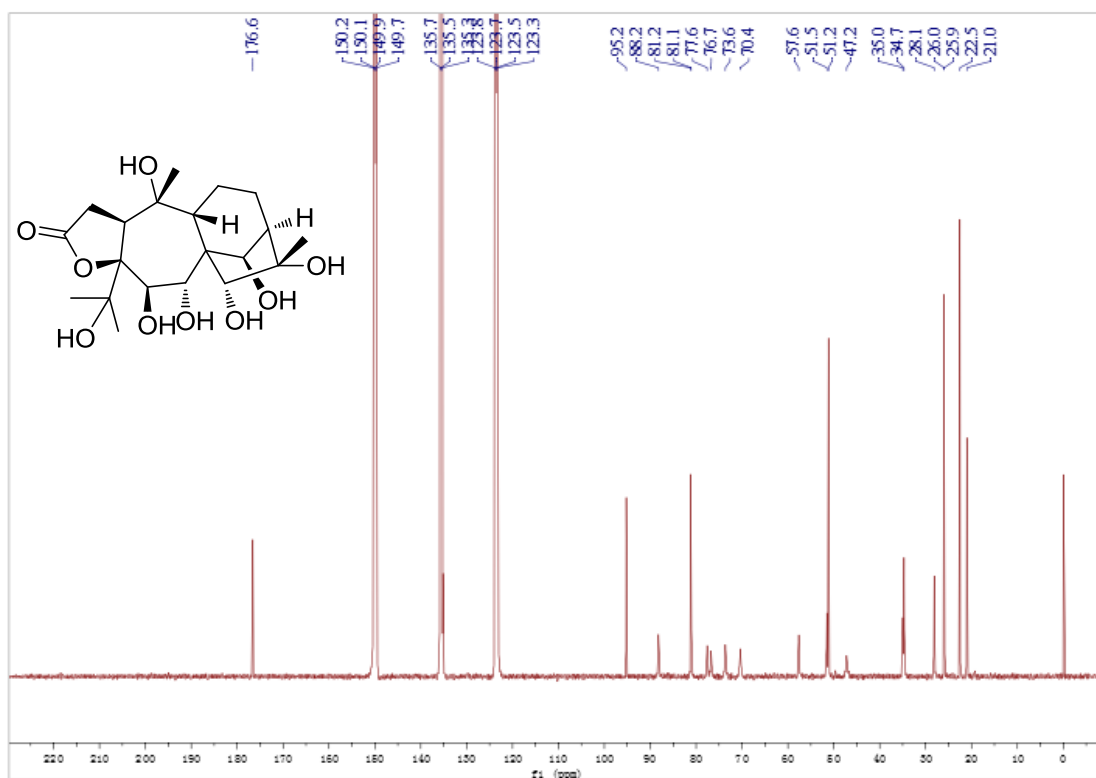


Figure S146. ^{13}C NMR spectrum of **16** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

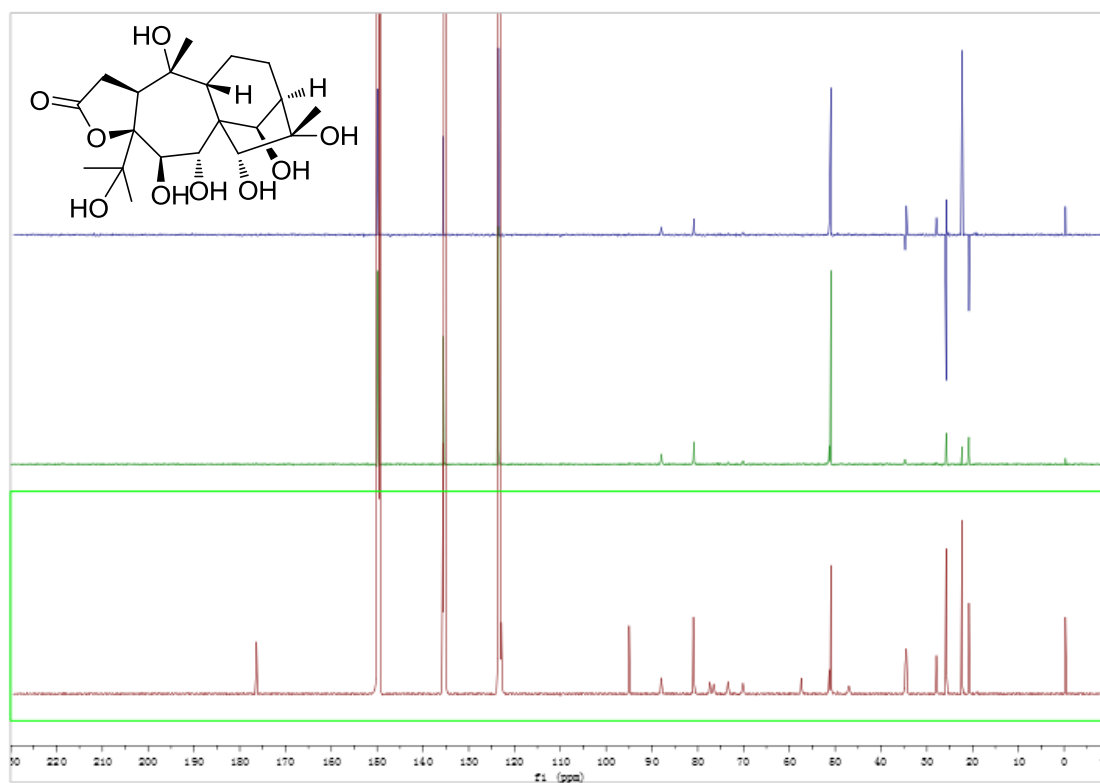


Figure S147. DEPT spectrum of **16** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

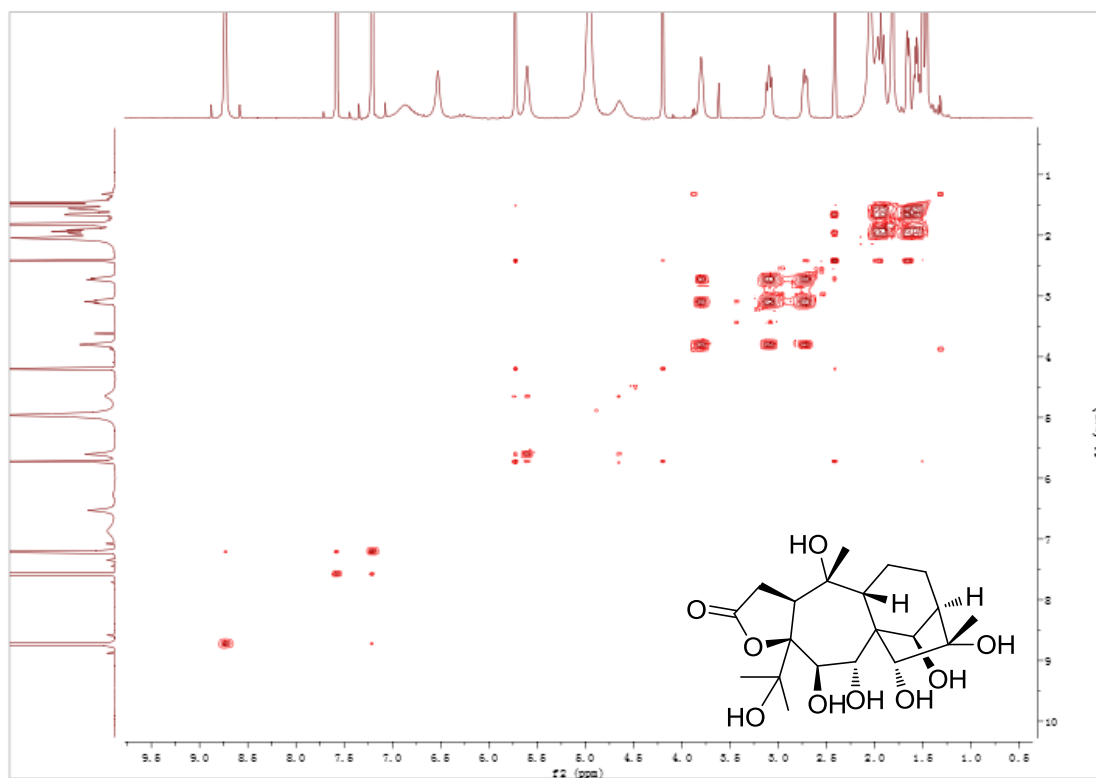


Figure S148. ^1H - ^1H COSY spectrum of **16** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

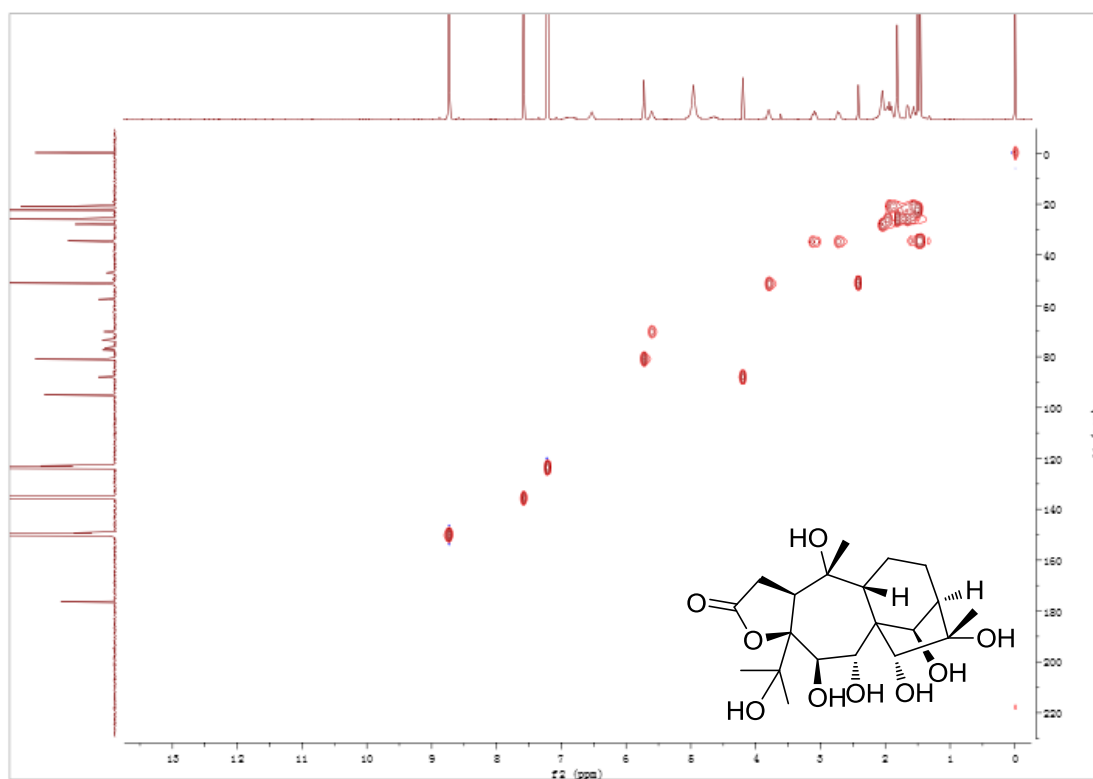


Figure S149. HSQC spectrum of **16** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

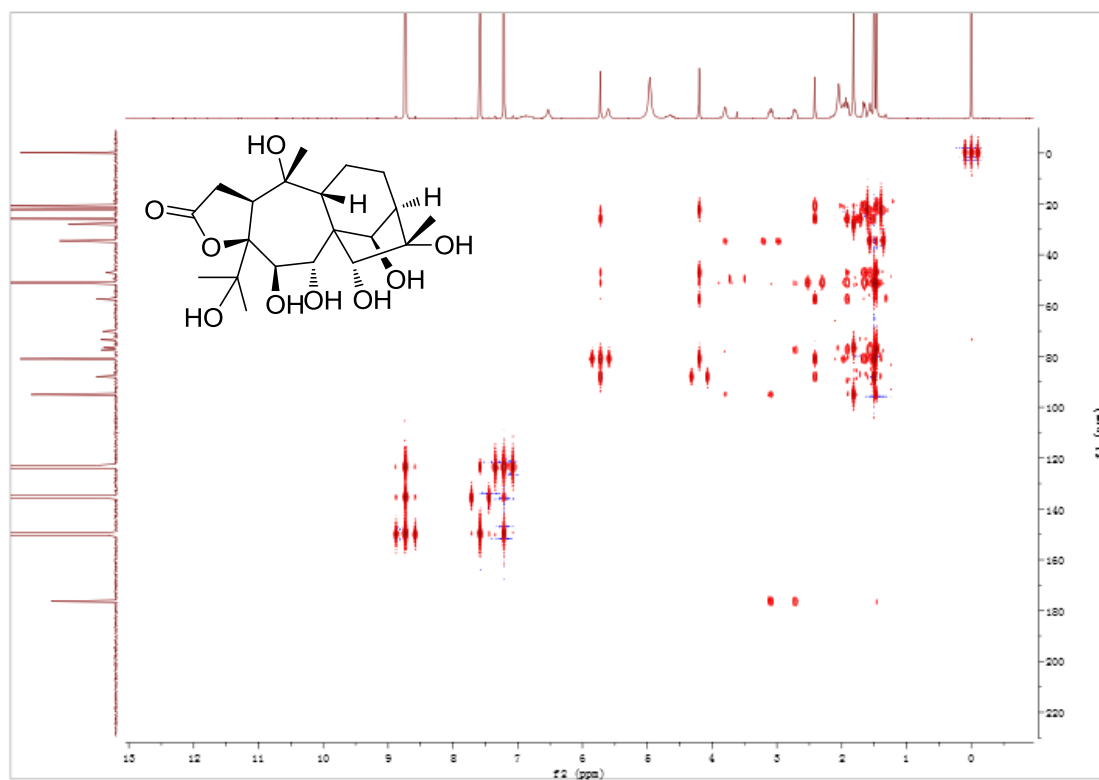


Figure S150. HMBC spectrum of **16** (600 MHz, in C_5D_5N)

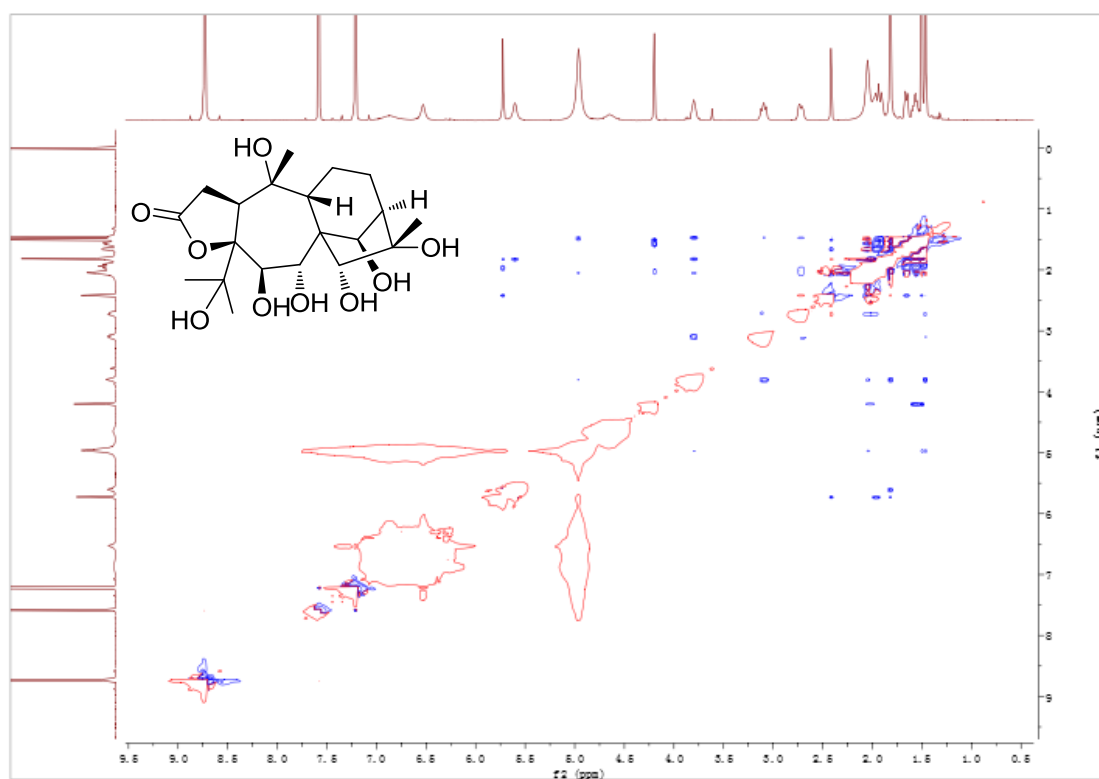


Figure S151. NOESY spectrum of **16** (600 MHz, in C_5D_5N)

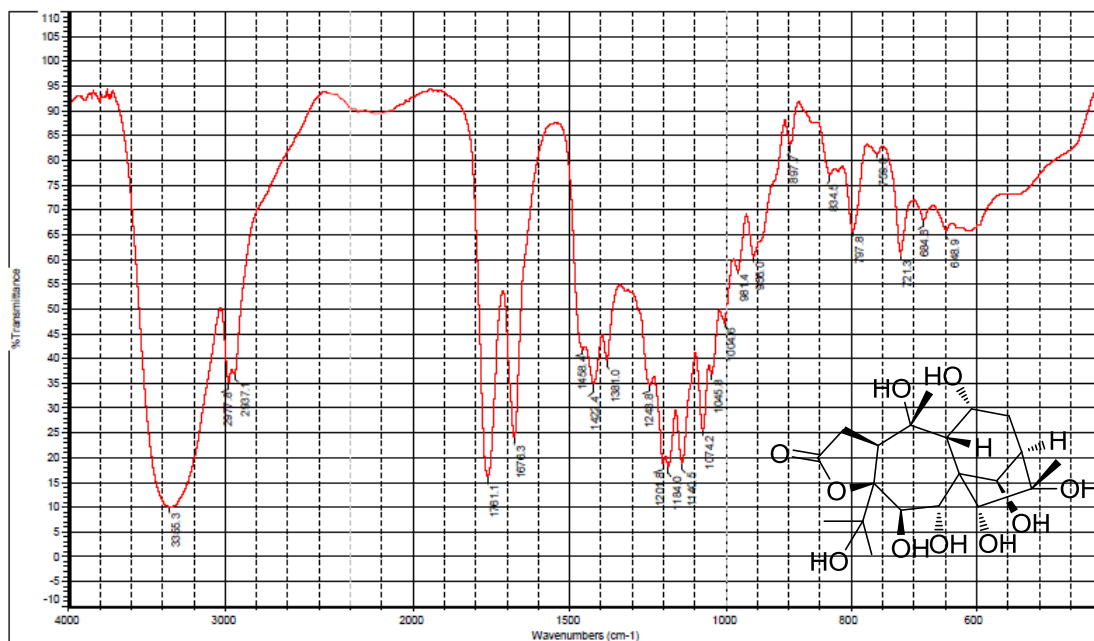


Figure S152. IR spectrum of 17

MS Formula Results: + Scan (2.928 min) Sub (2016111703.d)

m/z	Ion	Formula	Abundance
433.2065	(M+H) ⁺	C29 H33 O10	281379.6

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc. Mass	Calc. m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C20 H32 O10	C20 H33 O10	99.95		432.1992	432.1995	433.2058	0.72	0.72	99.98	99.85	100	5
✓	C24 H32 O5 G	C24 H33 O5 G	98.3		432.1992	432.197	433.2043	6.07	6.07	99.14	96.88	99.76	6
✓	C21 H36 O5 S2	C21 H37 O5 S2	97.43		432.1992	432.2004	433.2077	2.72	2.72	99.75	91.86	99.46	4
✓	C25 H36 S3	C25 H37 S3	94.73		432.1992	432.1979	433.2052	-3.07	3.07	99.69	82.63	99.35	9

Figure S153. (+)-HRESIMS data of 17

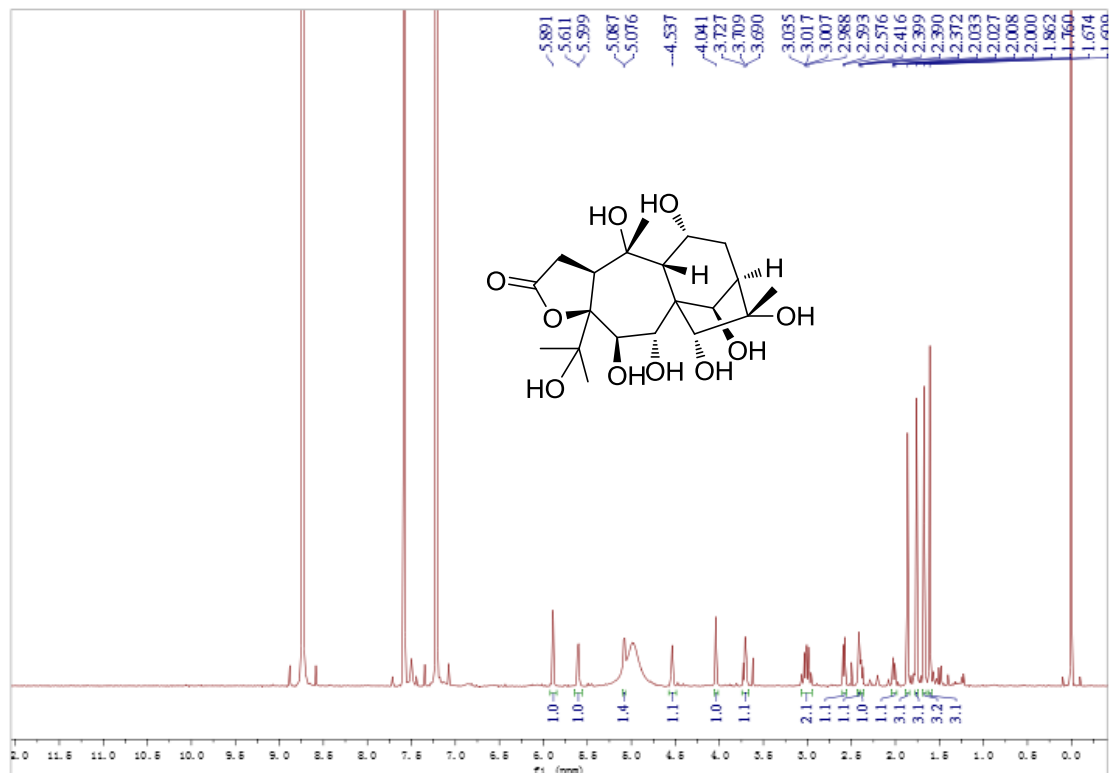


Figure S154. ¹H NMR spectrum of 17 (600 MHz, in C₅D₅N)

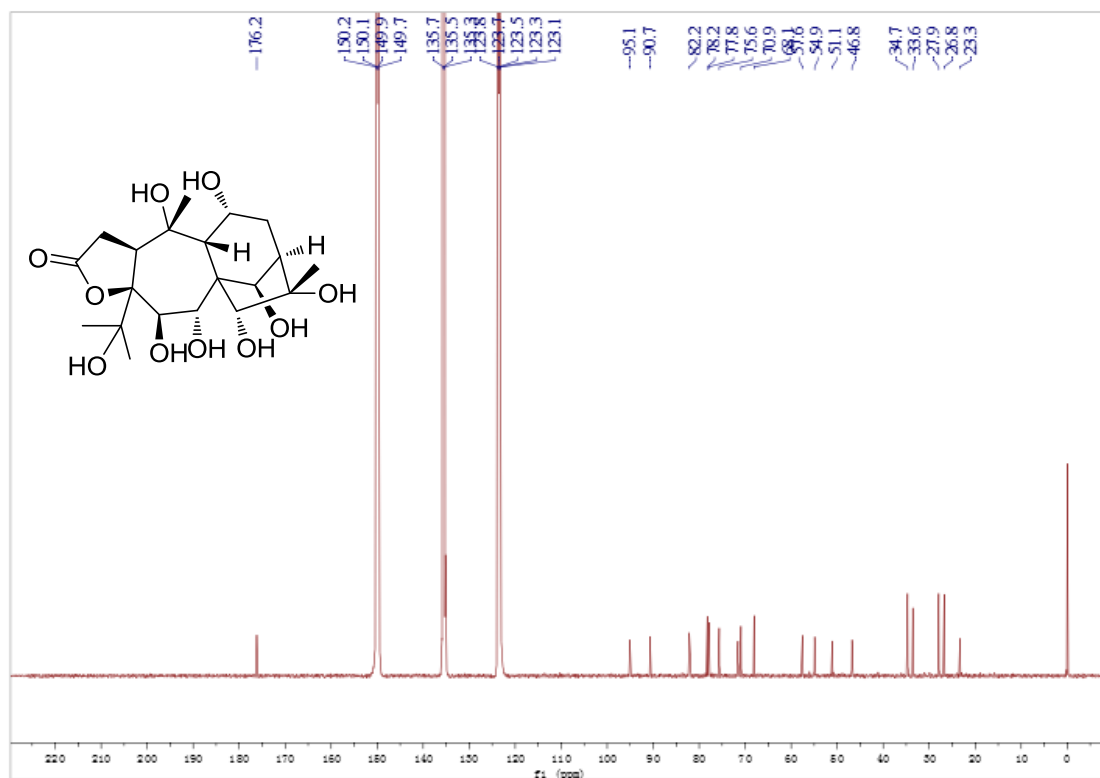


Figure S155. ^{13}C NMR spectrum of **17** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

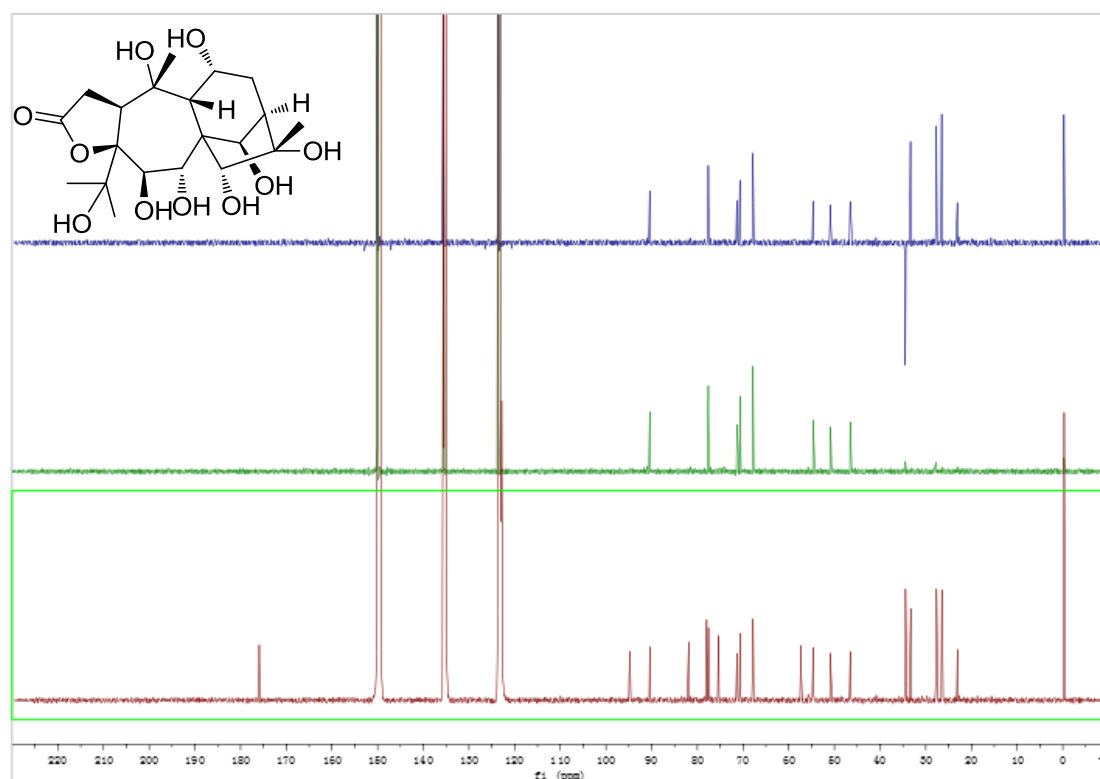


Figure S156. DEPT spectrum of **17** (150 MHz, in $\text{C}_5\text{D}_5\text{N}$)

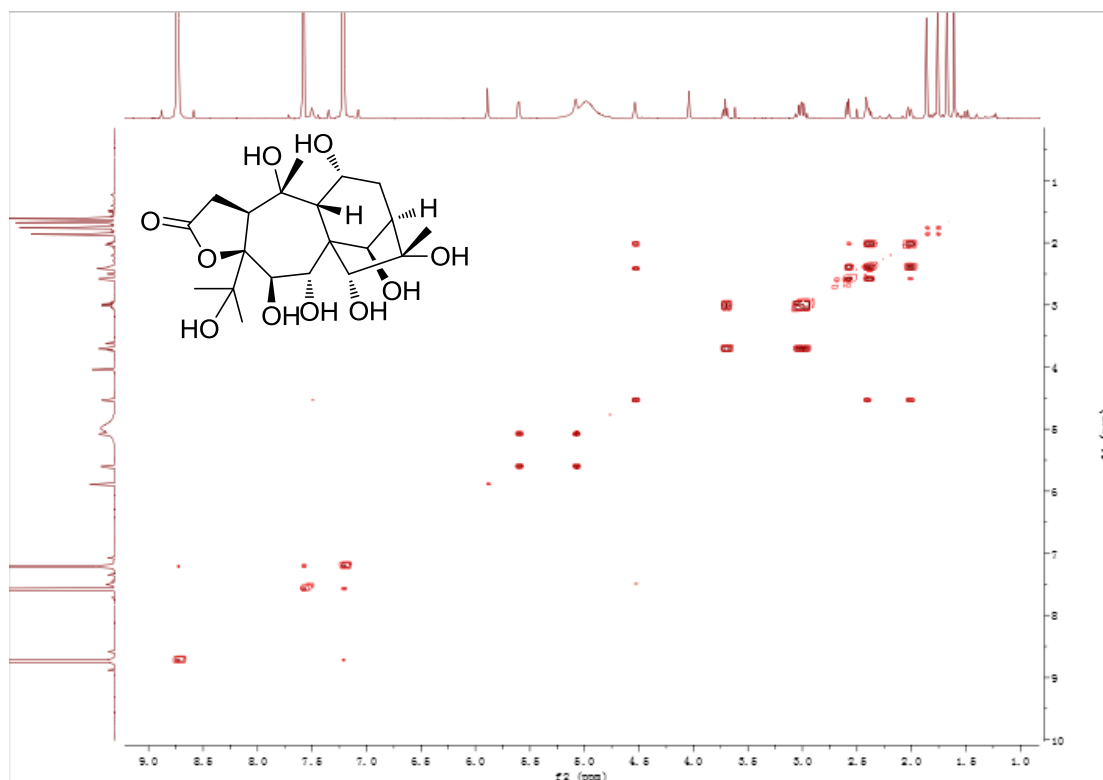


Figure S157. ^1H - ^1H COSY spectrum of **17** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

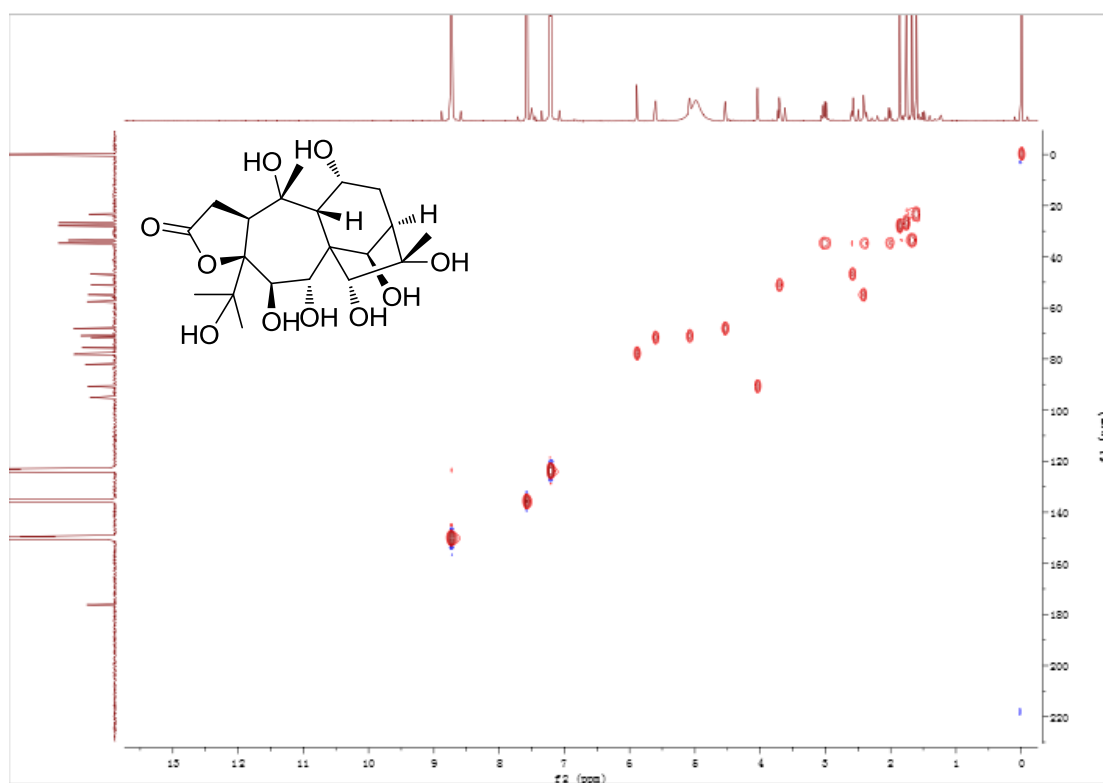


Figure S158. HSQC spectrum of **17** (600 MHz, in $\text{C}_5\text{D}_5\text{N}$)

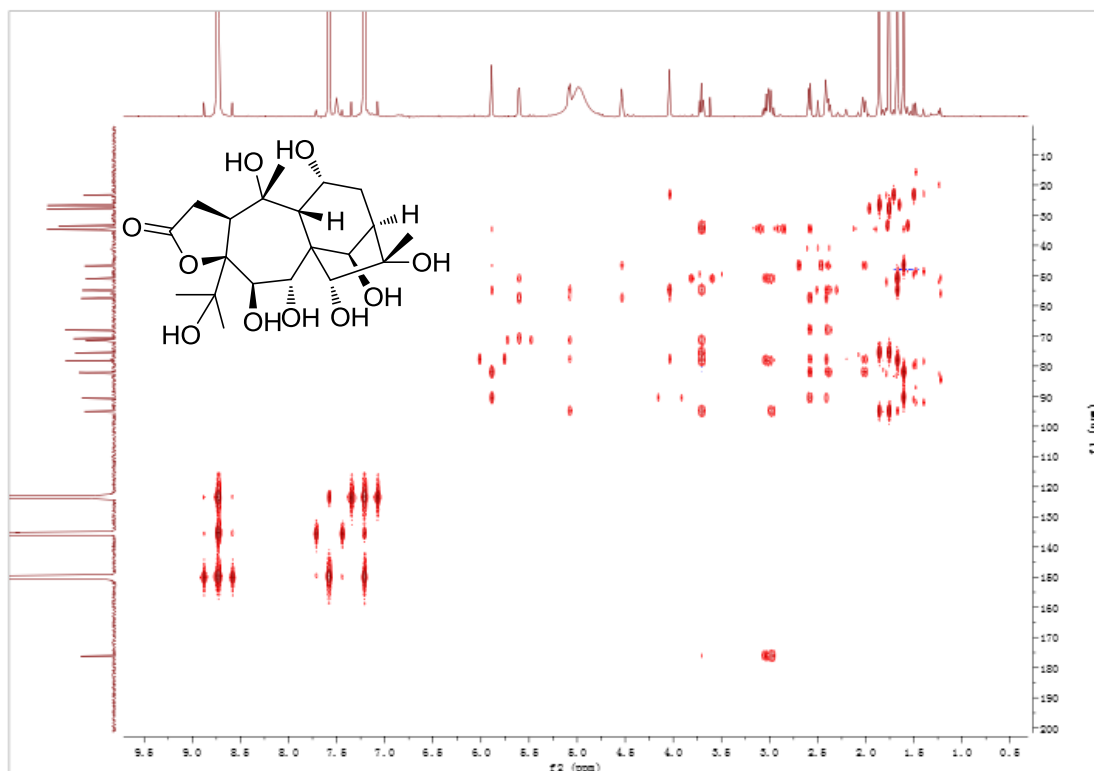


Figure S159. HMBC spectrum of **17** (600 MHz, in C_5D_5N)

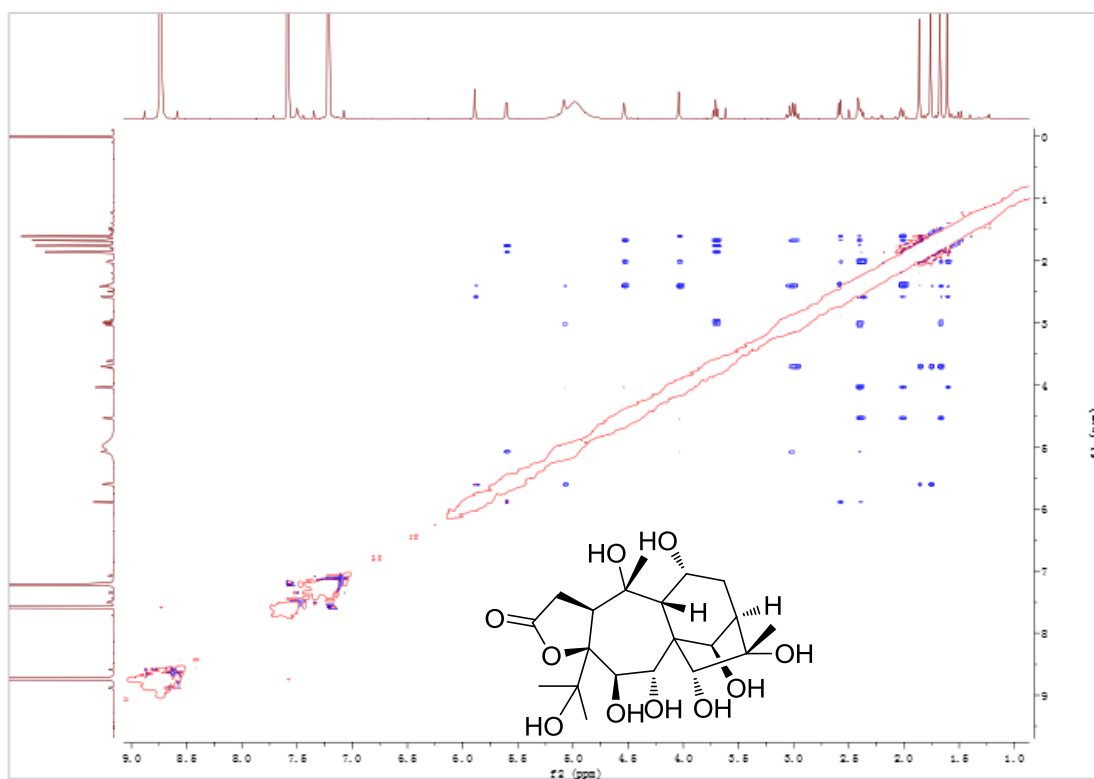


Figure S160. NOESY spectrum of **17** (600 MHz, in C_5D_5N)