

Bioactive Diterpenes, Norditerpenes, and Sesquiterpenes from a Formosan Soft Coral *Cespitularia* sp.

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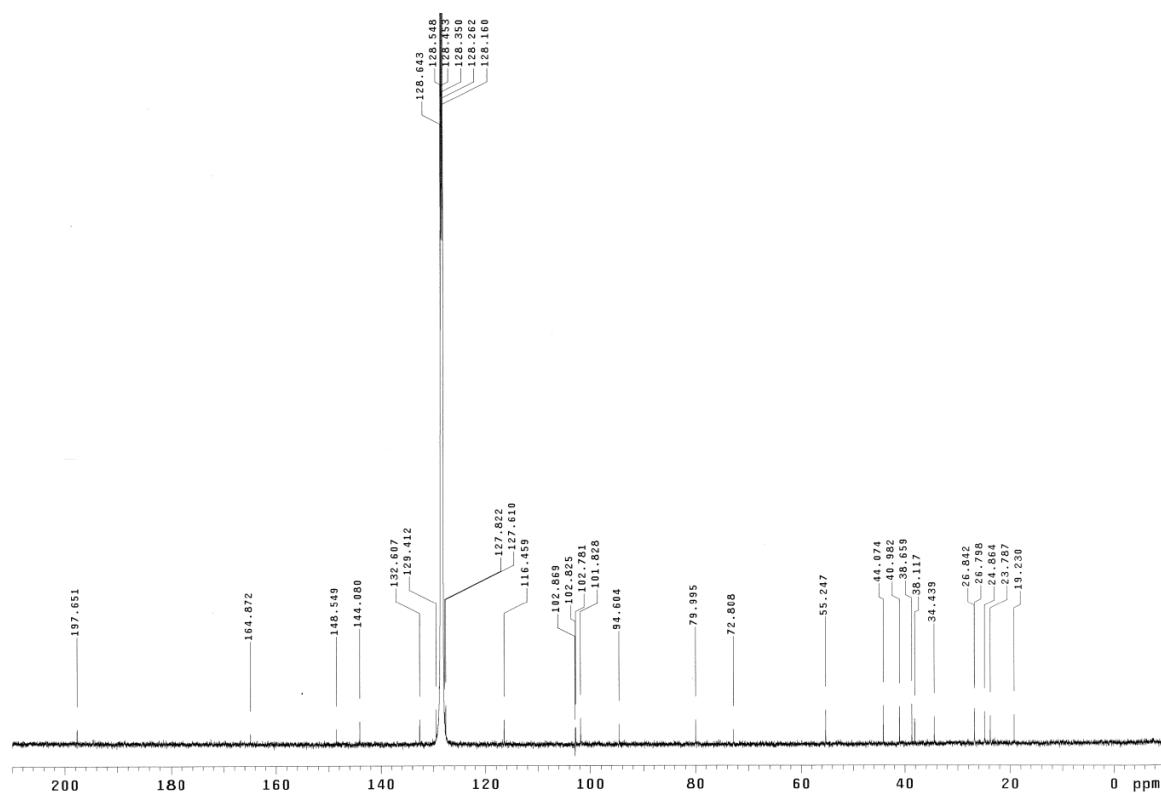


Figure S3. ^{13}C NMR spectrum of **1** in C_6D_6 at 125 MHz

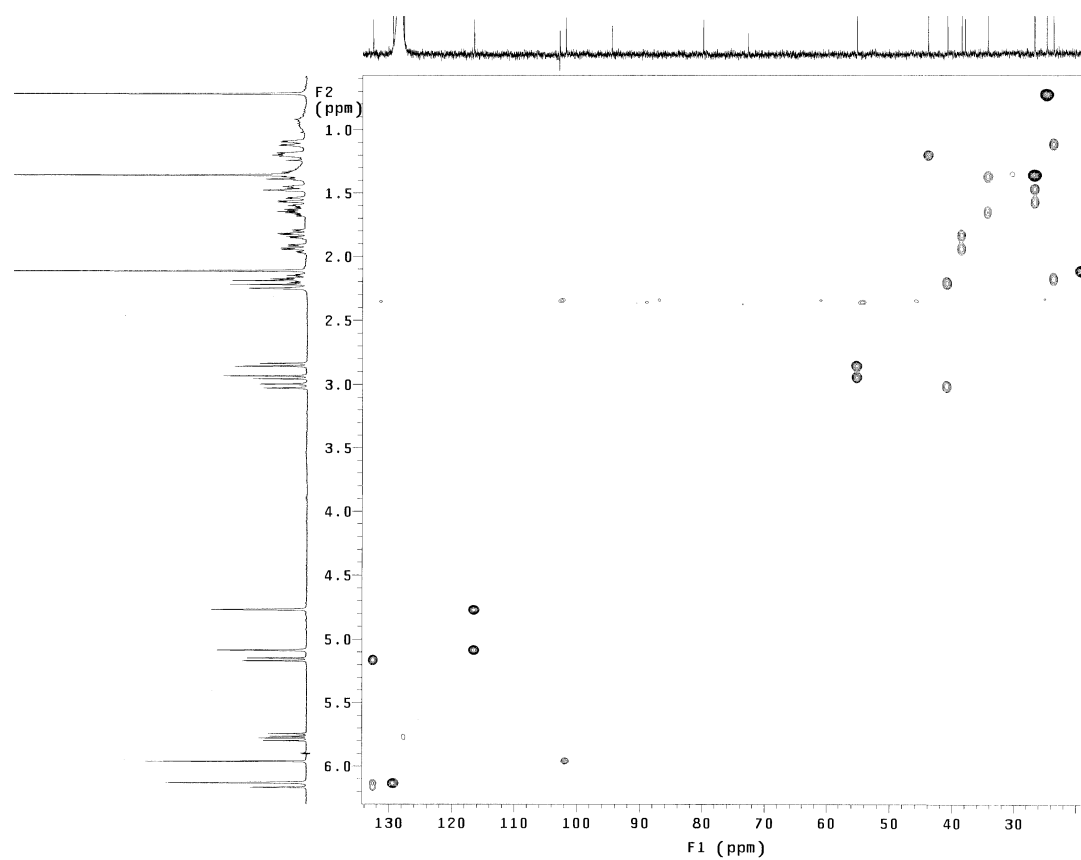


Figure S4. HSQC spectrum of **1** in C_6D_6

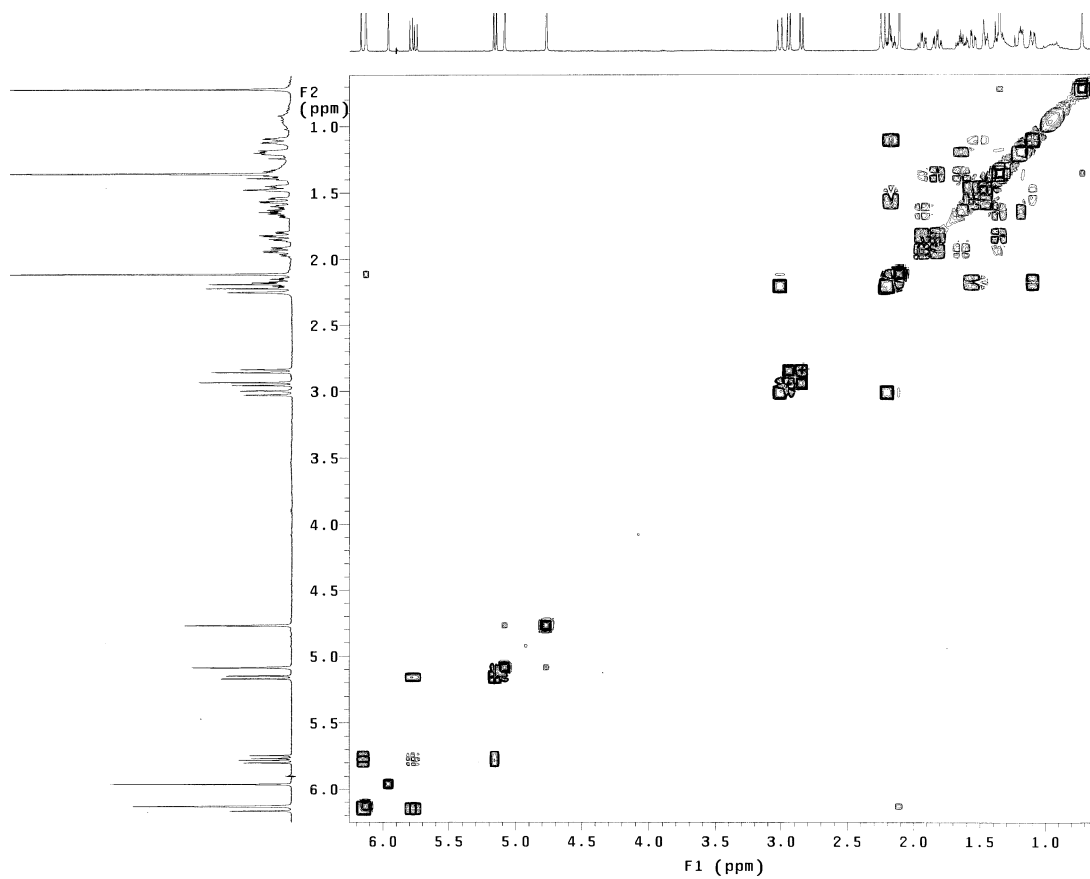


Figure S5. COSY spectrum of **1** in C₆D₆

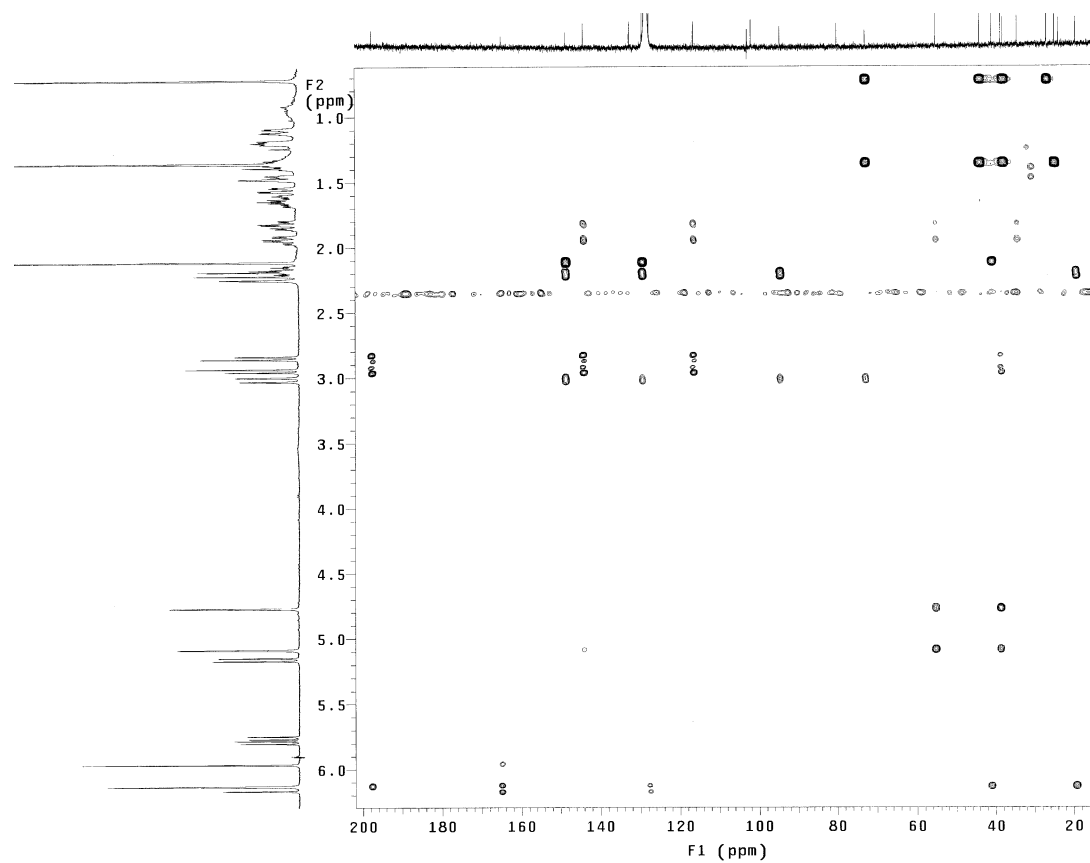


Figure S6. HMBC spectrum of **1** in C₆D₆

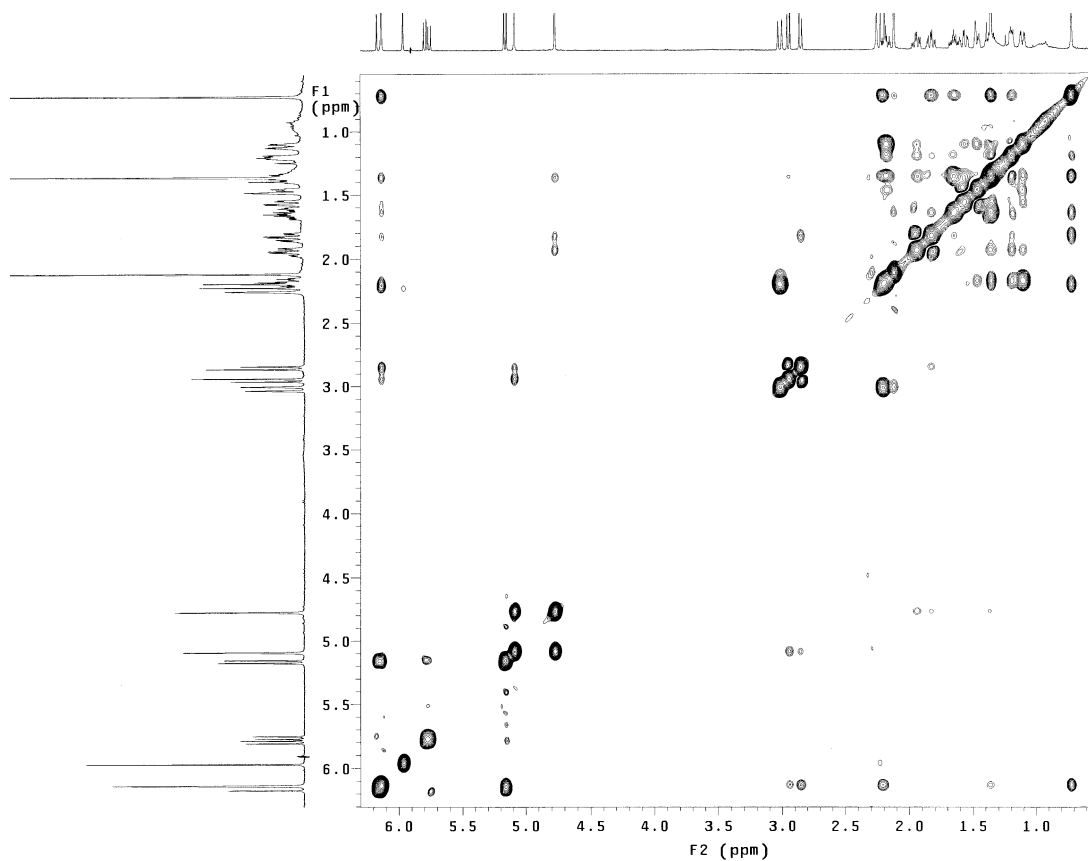


Figure S7. NOESY spectrum of **1** in C₆D₆

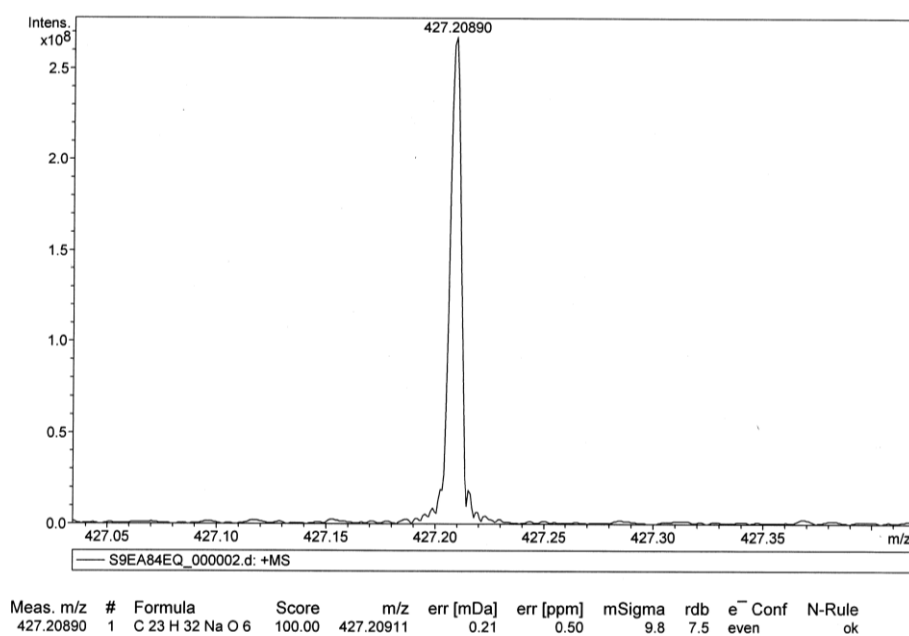


Figure S8. HRESIMS spectrum of **2**

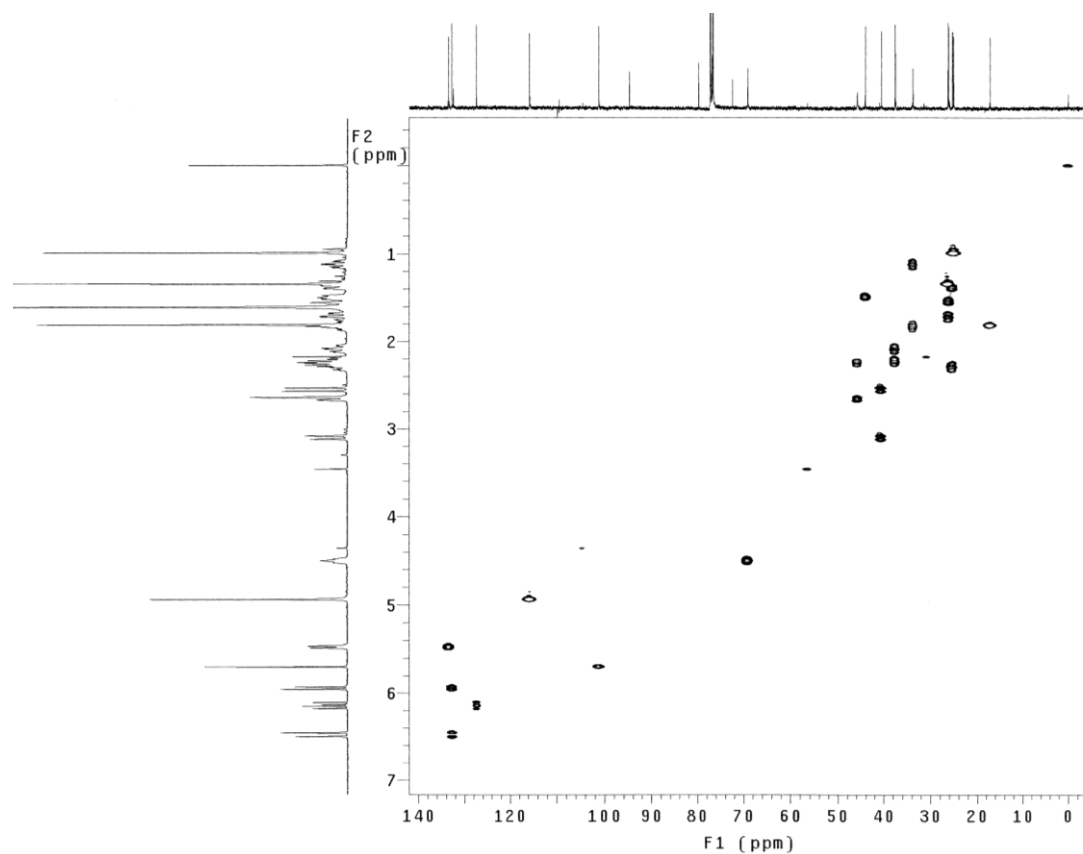


Figure S11. HSQC spectrum of **2** in CDCl₃

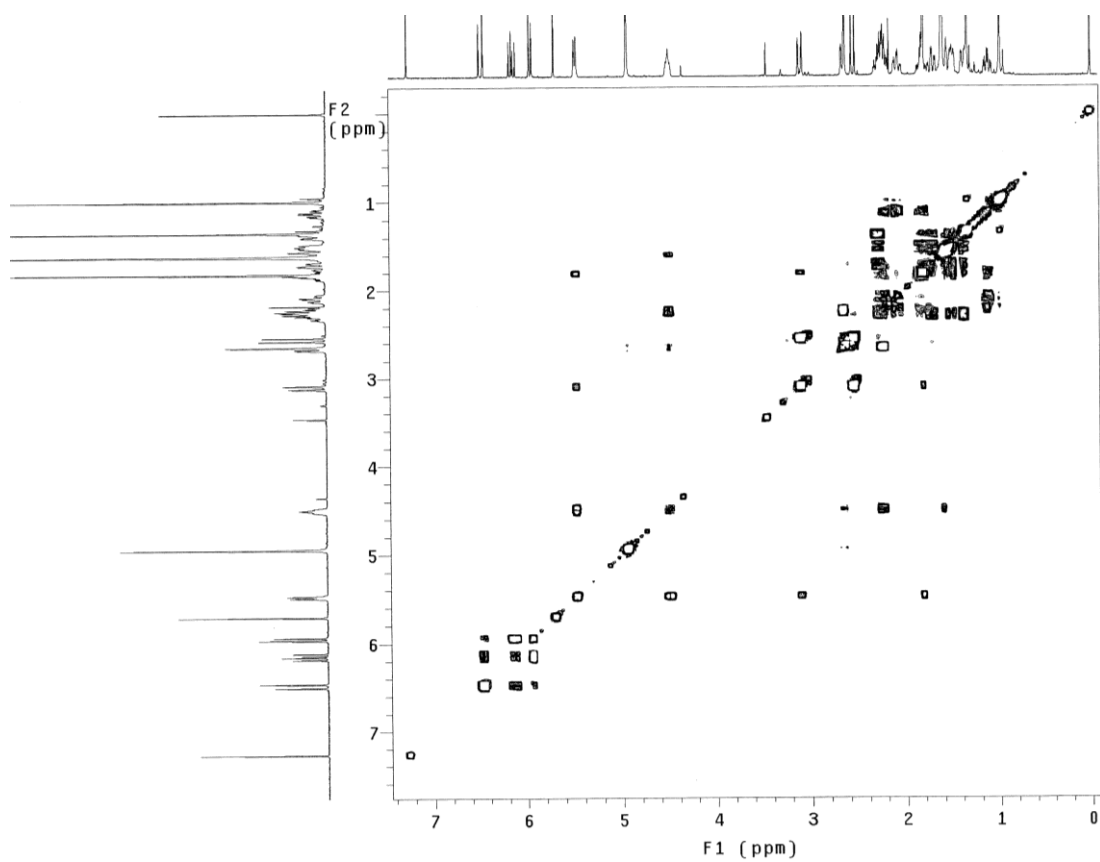


Figure S12. COSY spectrum of **2** in CDCl₃

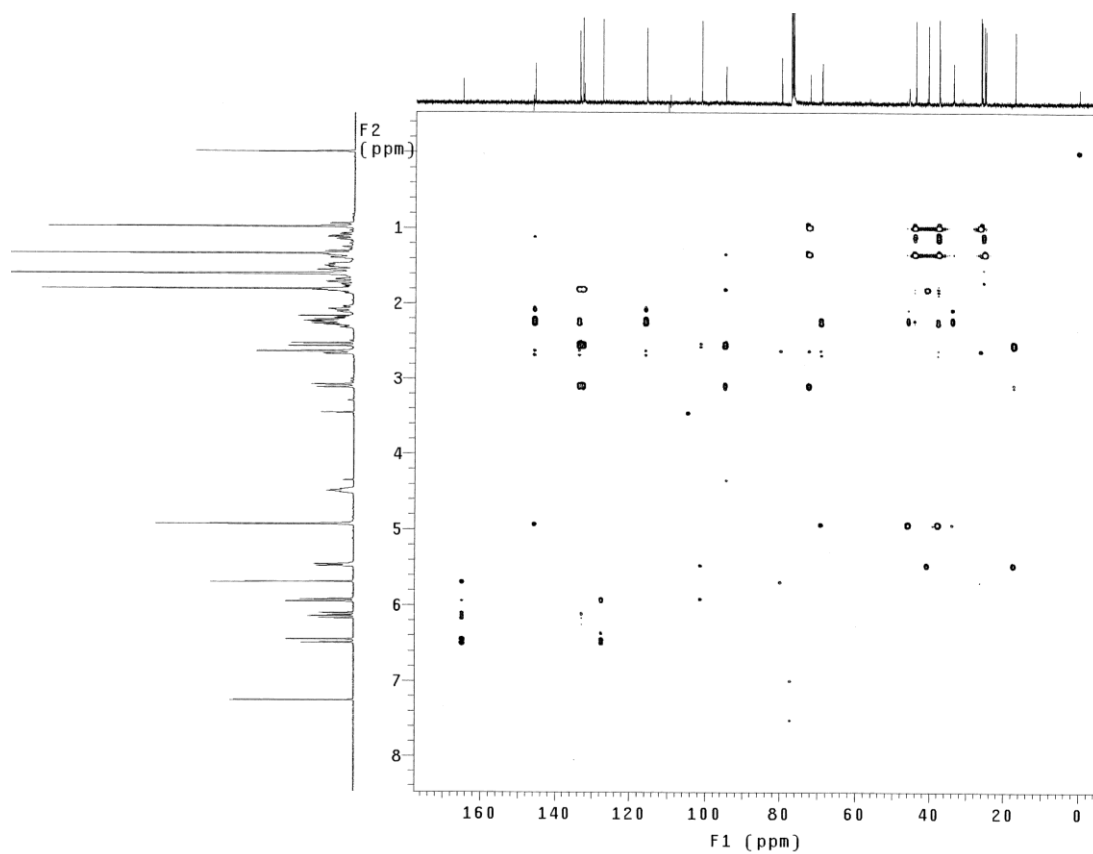


Figure S13. HMBC spectrum of **2** in CDCl₃

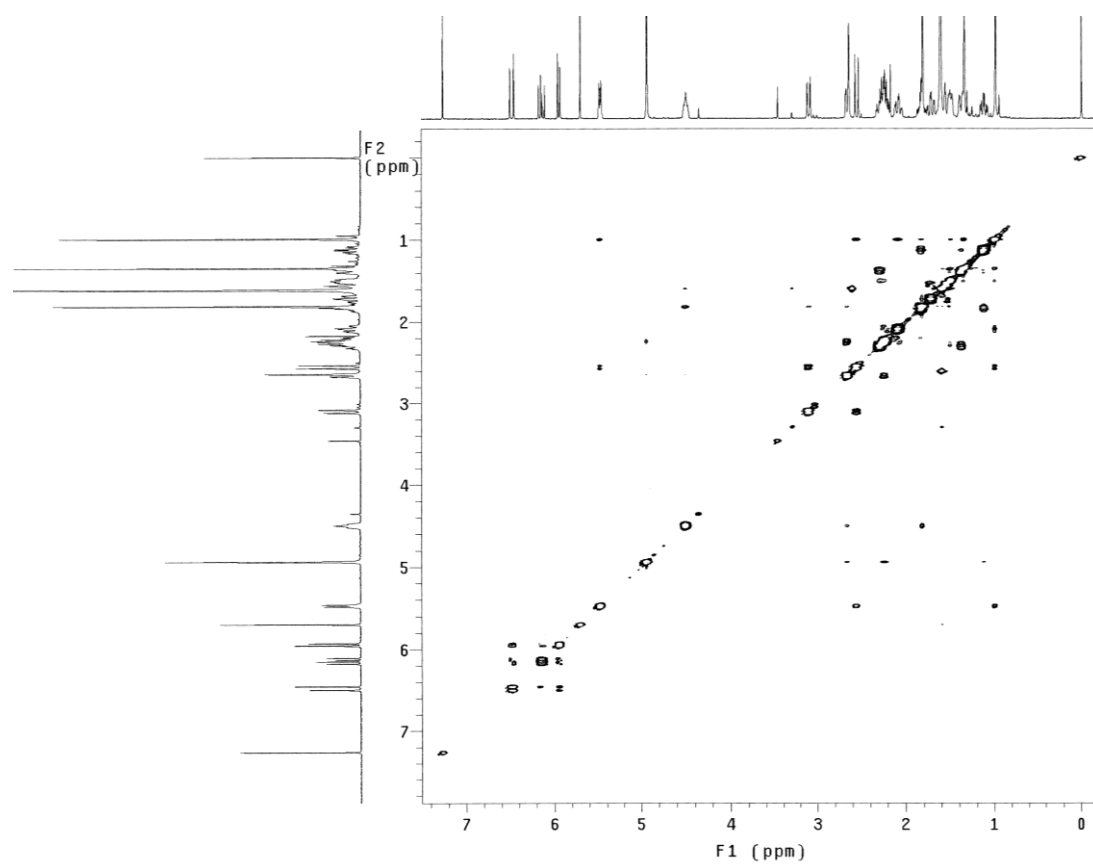
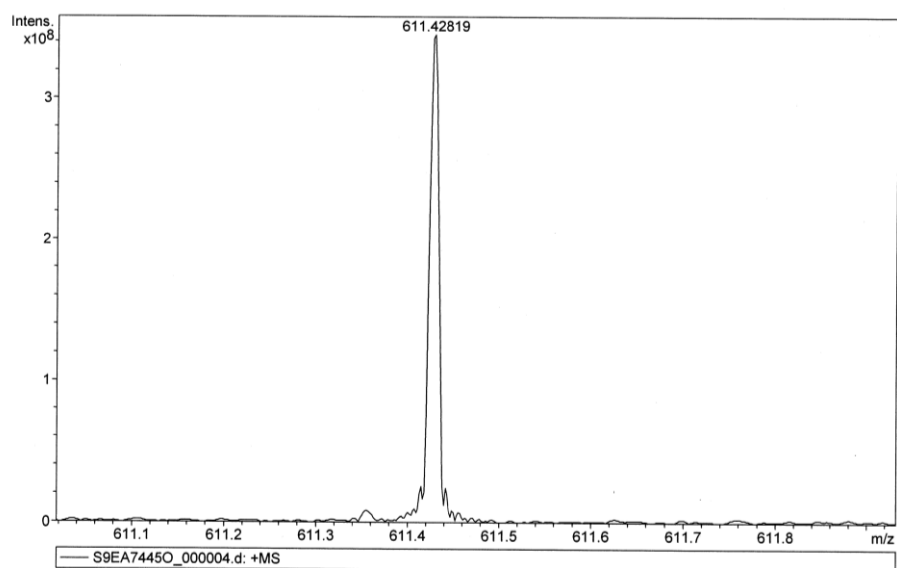


Figure S14. NOESY spectrum of **2** in CDCl₃



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
611.42819	1	C ₃₆ H ₆₀ NaO ₆	100.00	611.42821	0.02	0.04	7.8	6.5	even	ok

Figure S15. HRESIMS spectrum of 3

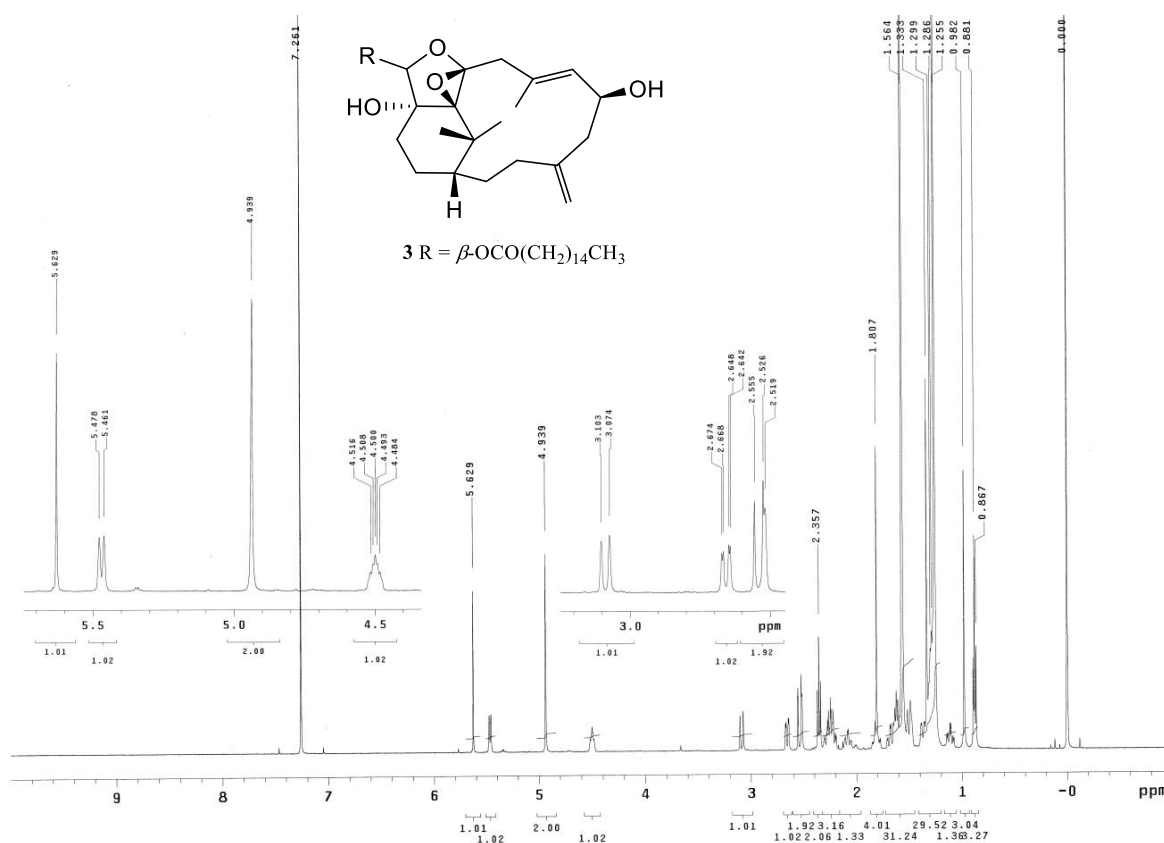


Figure S16. ¹H NMR spectrum of 3 in CDCl₃ at 500 MHz

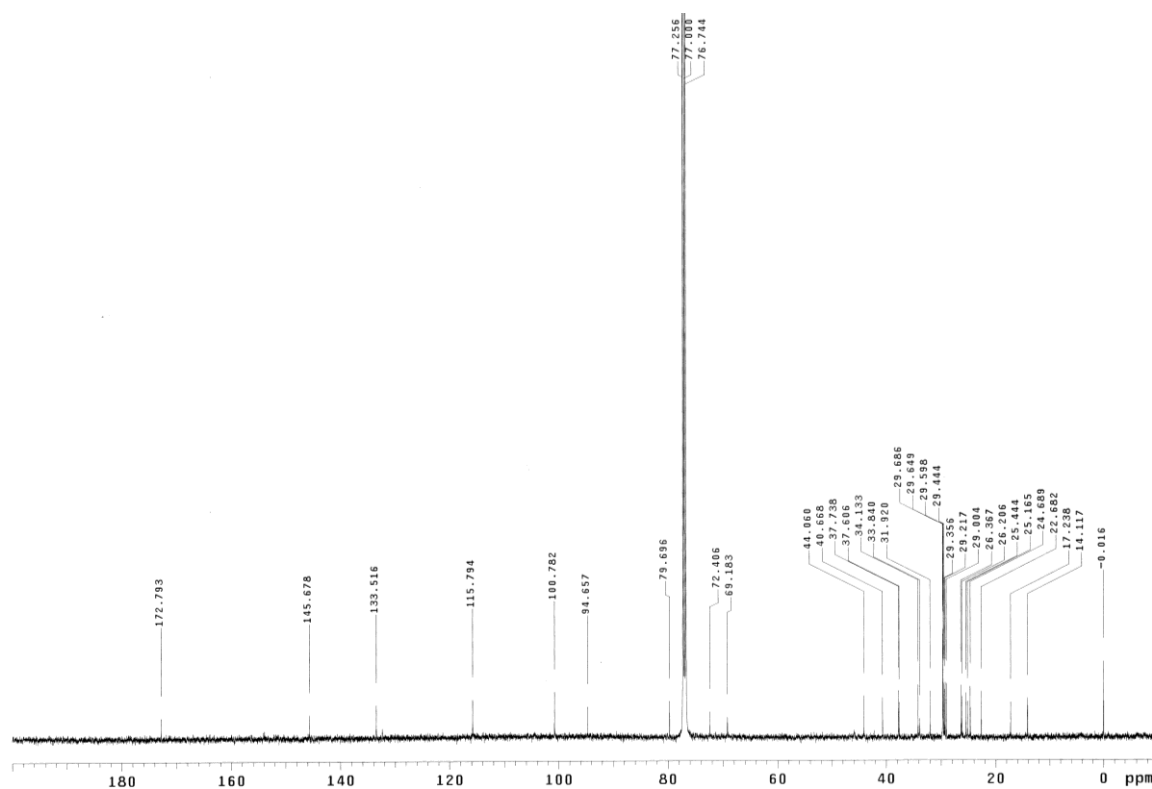


Figure S17. ^{13}C NMR spectrum of **3** in CDCl_3 at 125 MHz

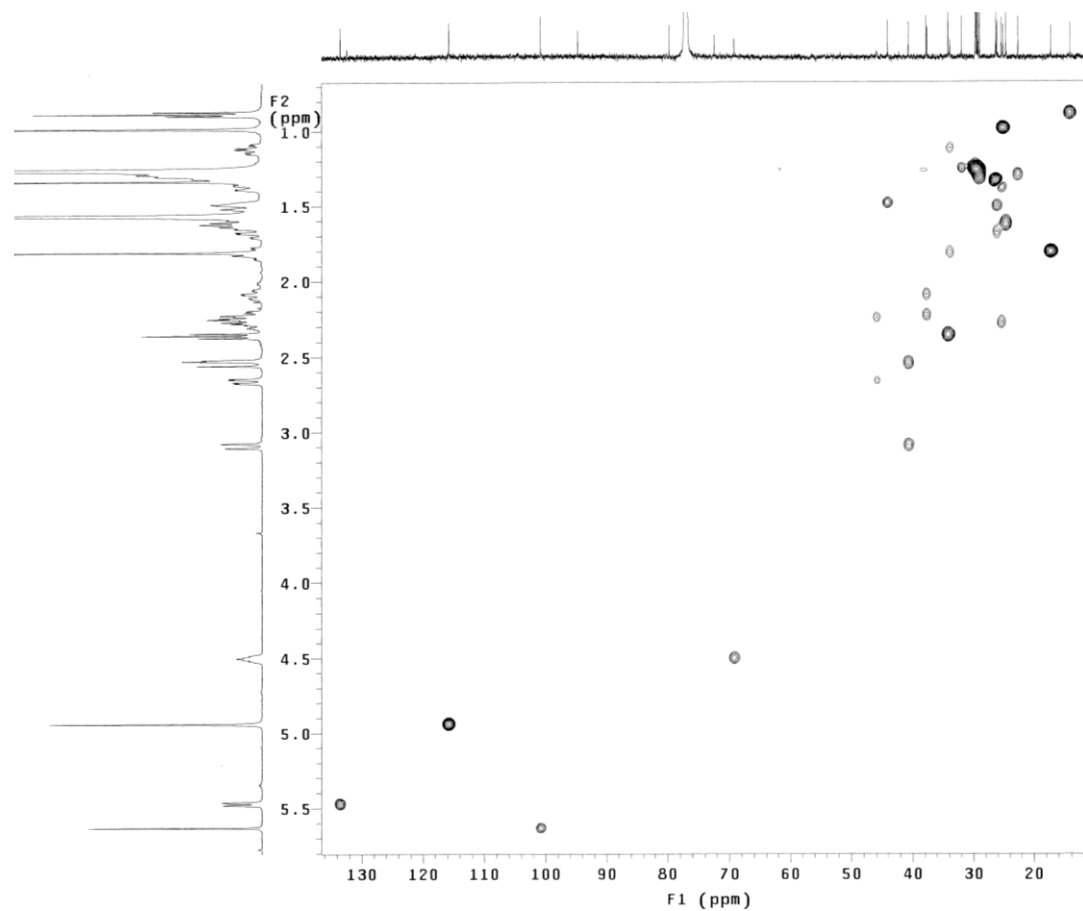


Figure S18. HSQC spectrum of **3** in CDCl_3

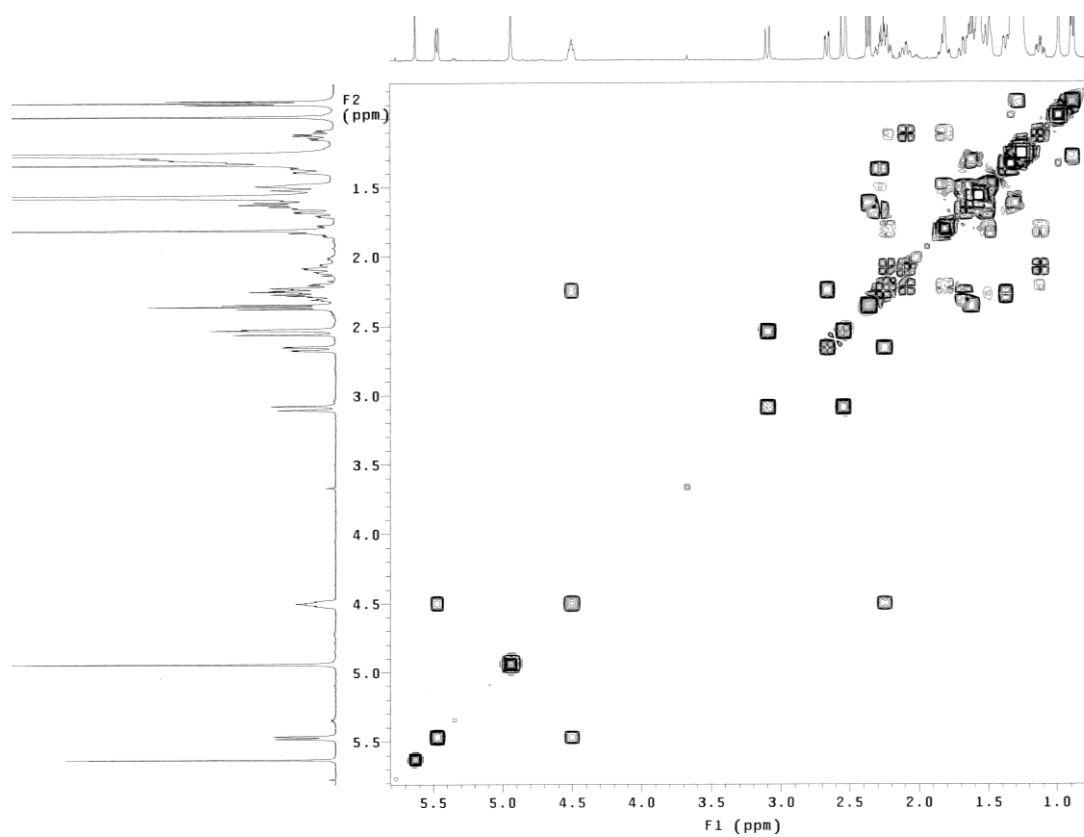


Figure S19. COSY spectrum of **3** in CDCl₃

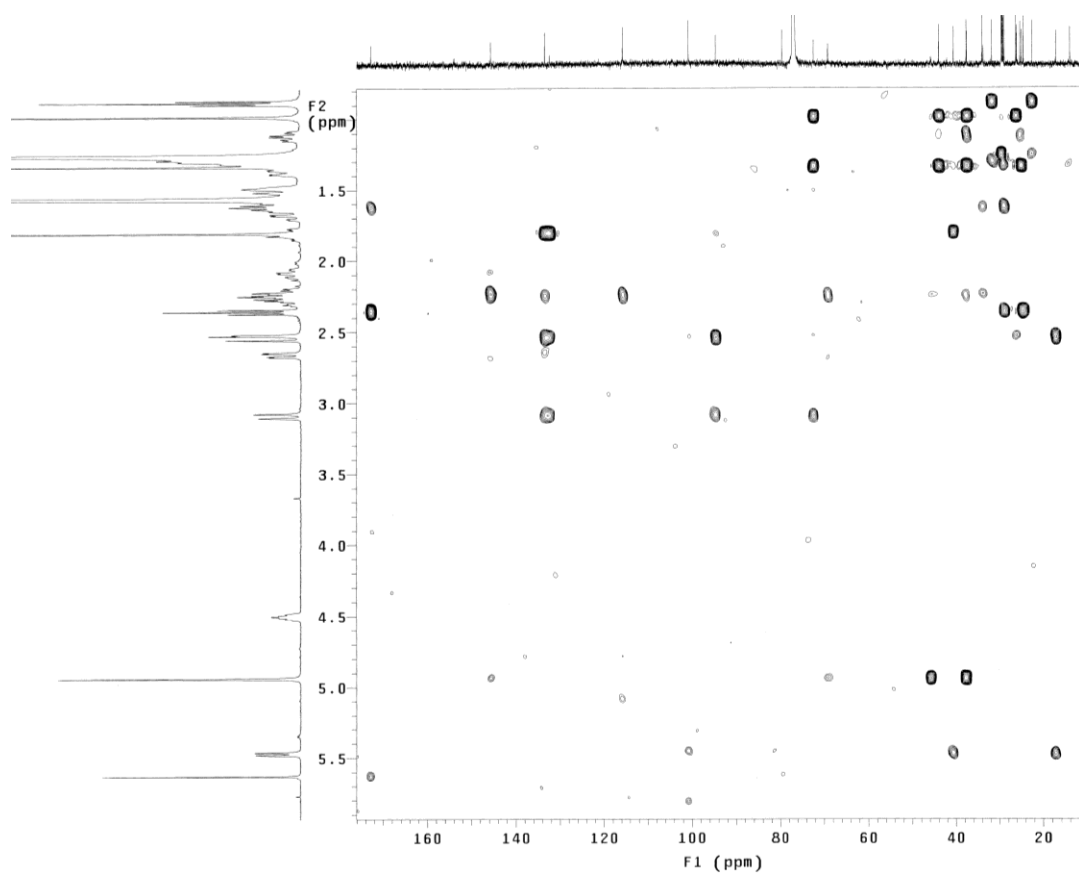


Figure S20. HMBC spectrum of **3** in CDCl₃

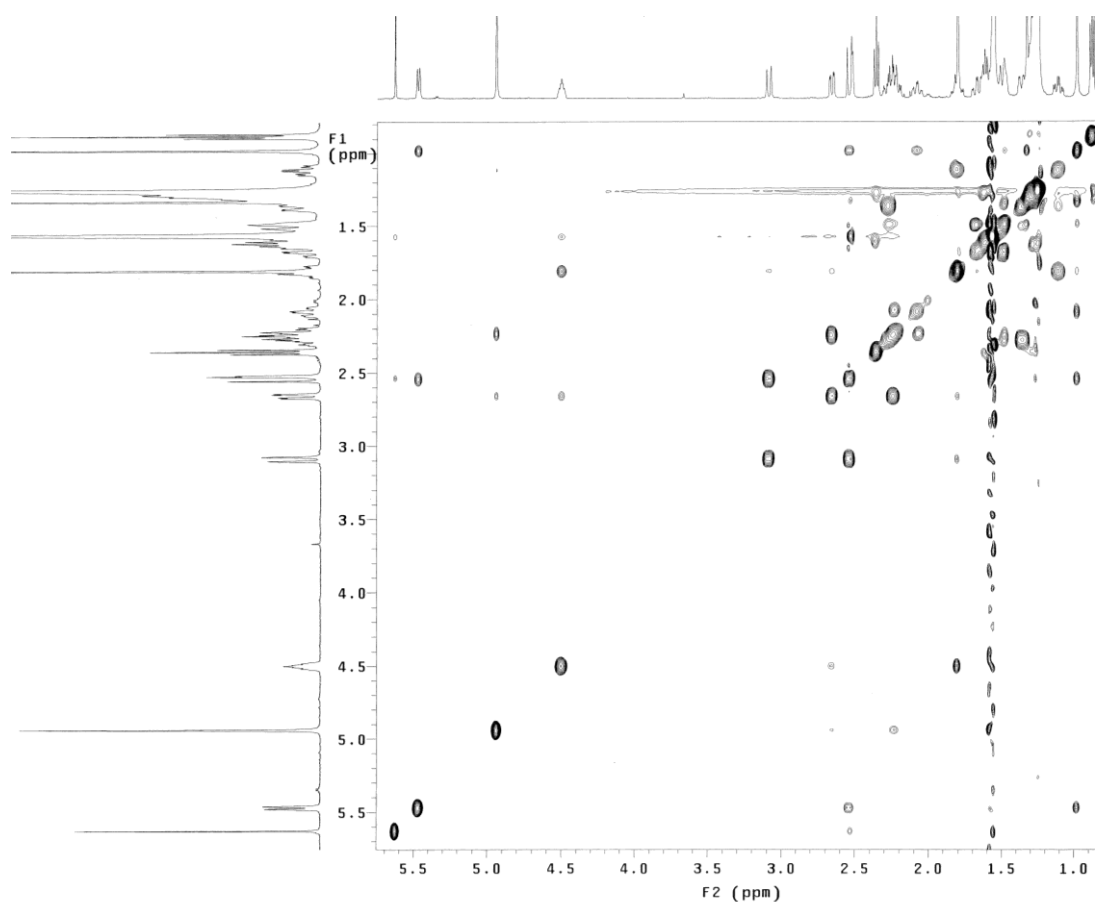
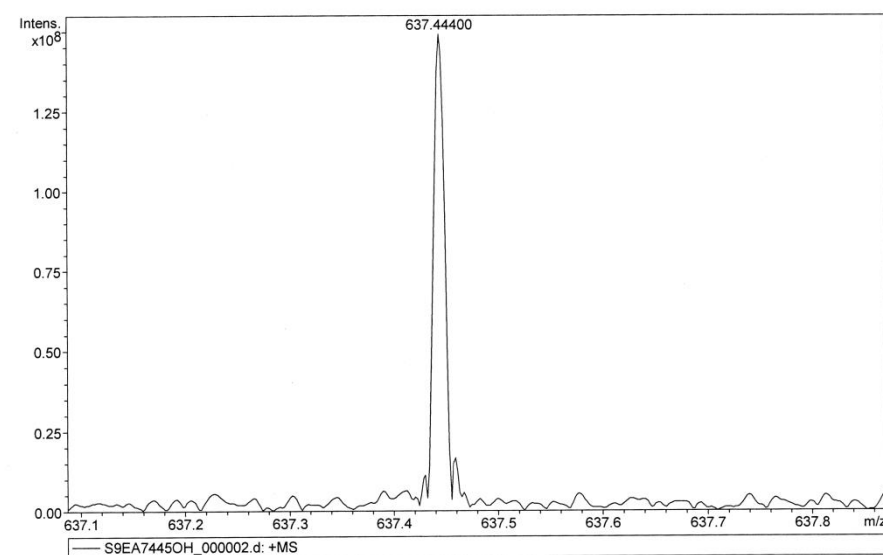


Figure S21. NOESY spectrum of **3** in CDCl₃



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
637.44400	1	C 38 H 62 Na O 6	100.00	637.44386	-0.14	-0.21	24.2	7.5	even		ok

Figure S22. HRESIMS spectrum of **4**

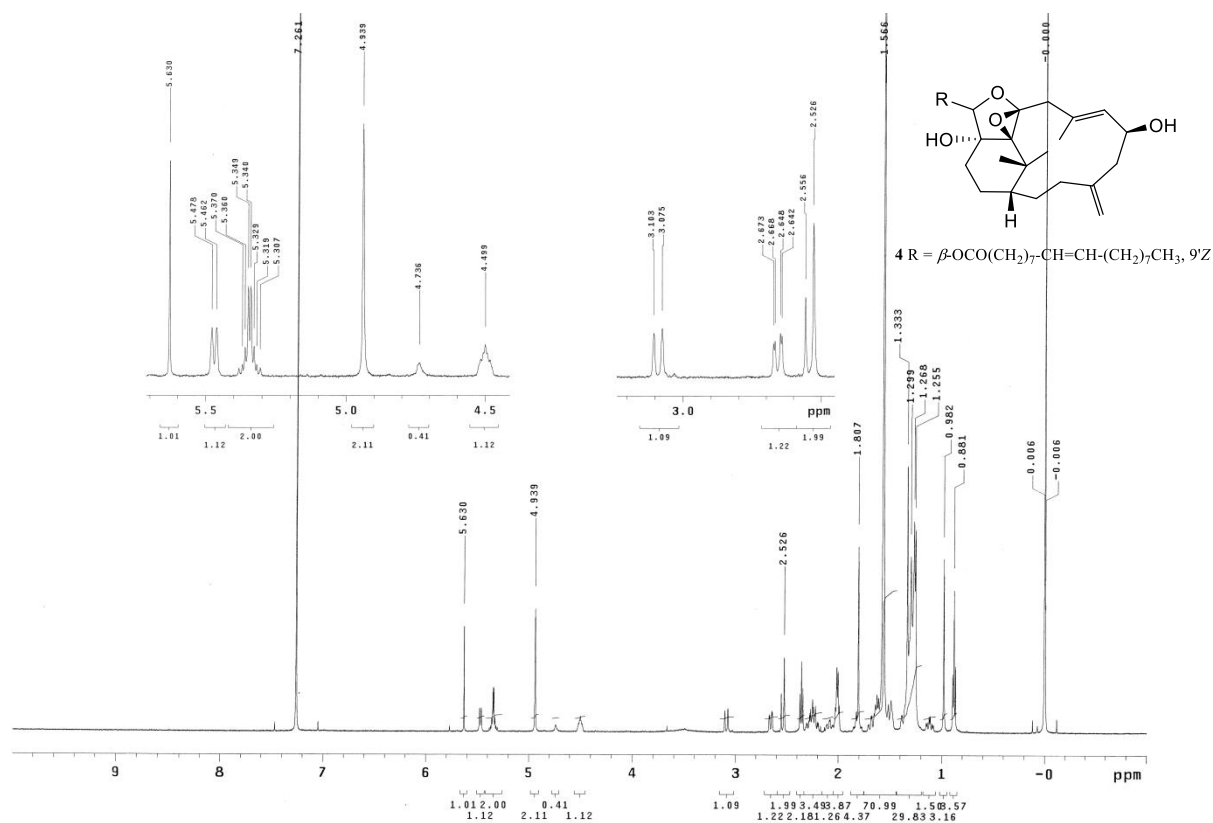


Figure S23. ^1H NMR spectrum of **4** in CDCl_3 at 500 MHz

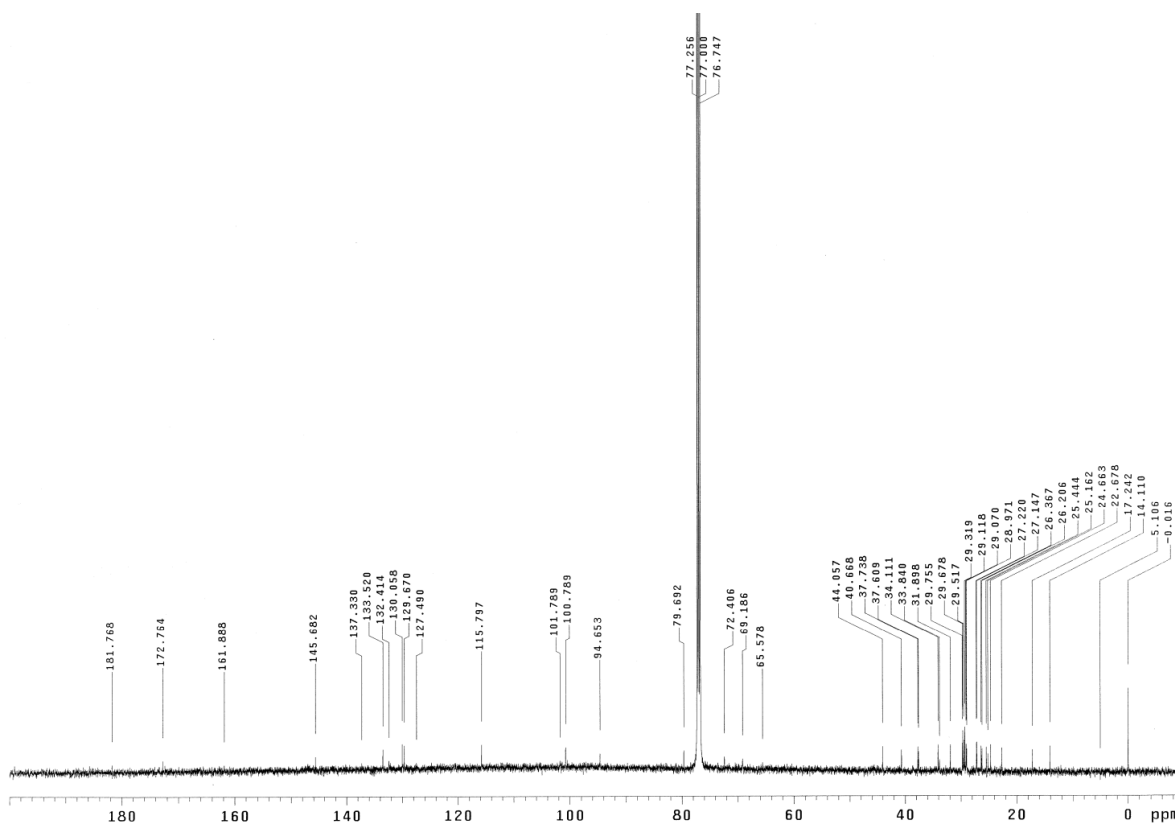


Figure S24. ^{13}C NMR spectrum of **4** in CDCl_3 at 125 MHz

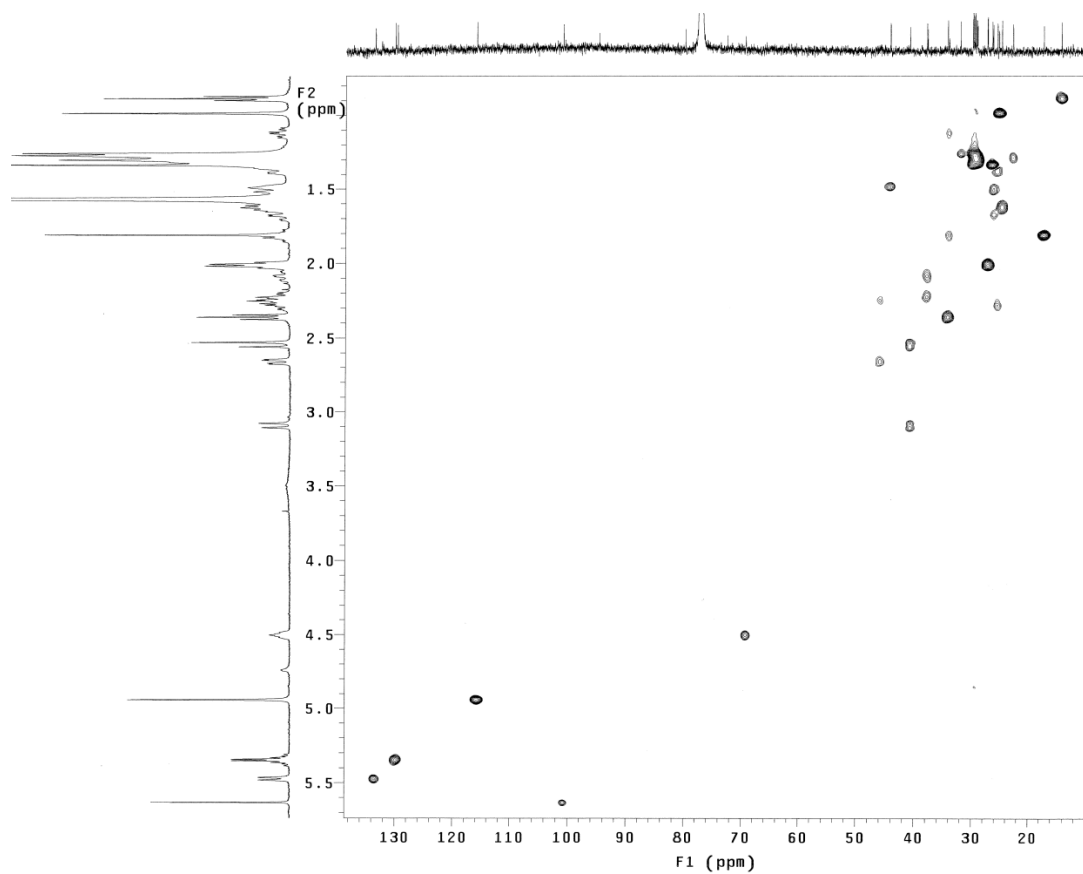


Figure S25. HSQC spectrum of **4** in CDCl₃

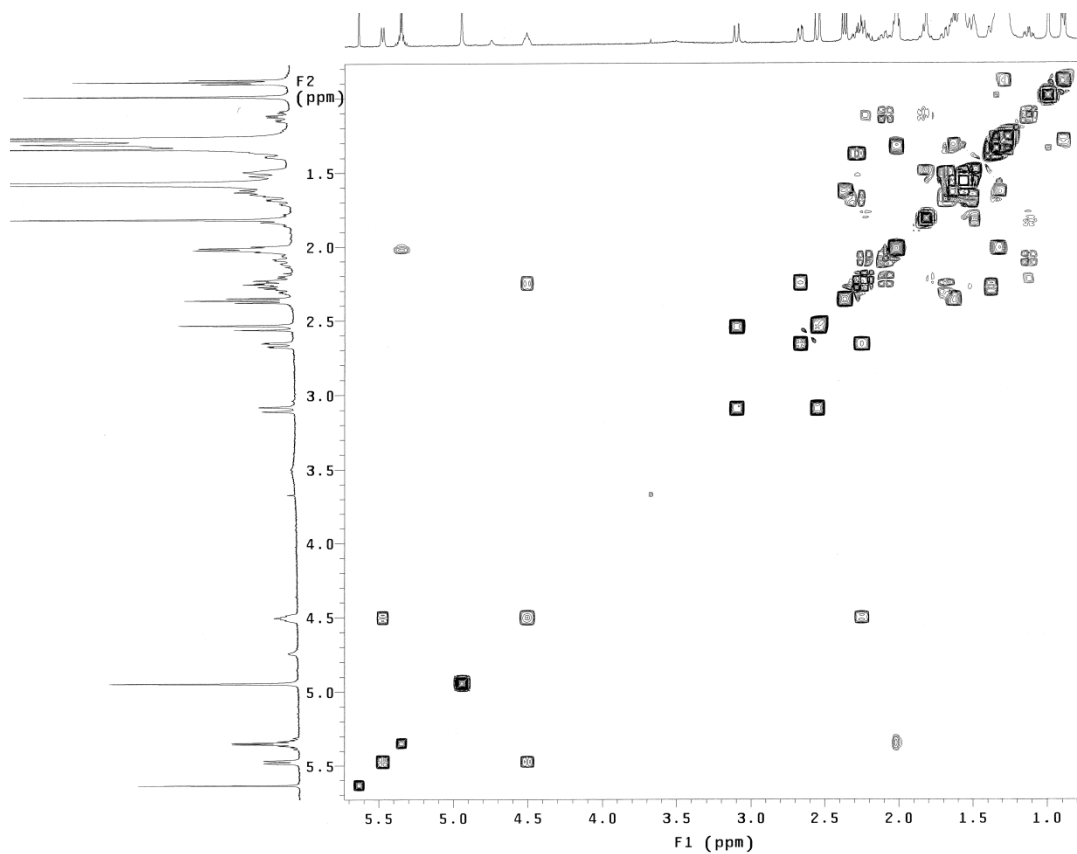


Figure S26. COSY spectrum of **4** in CDCl₃

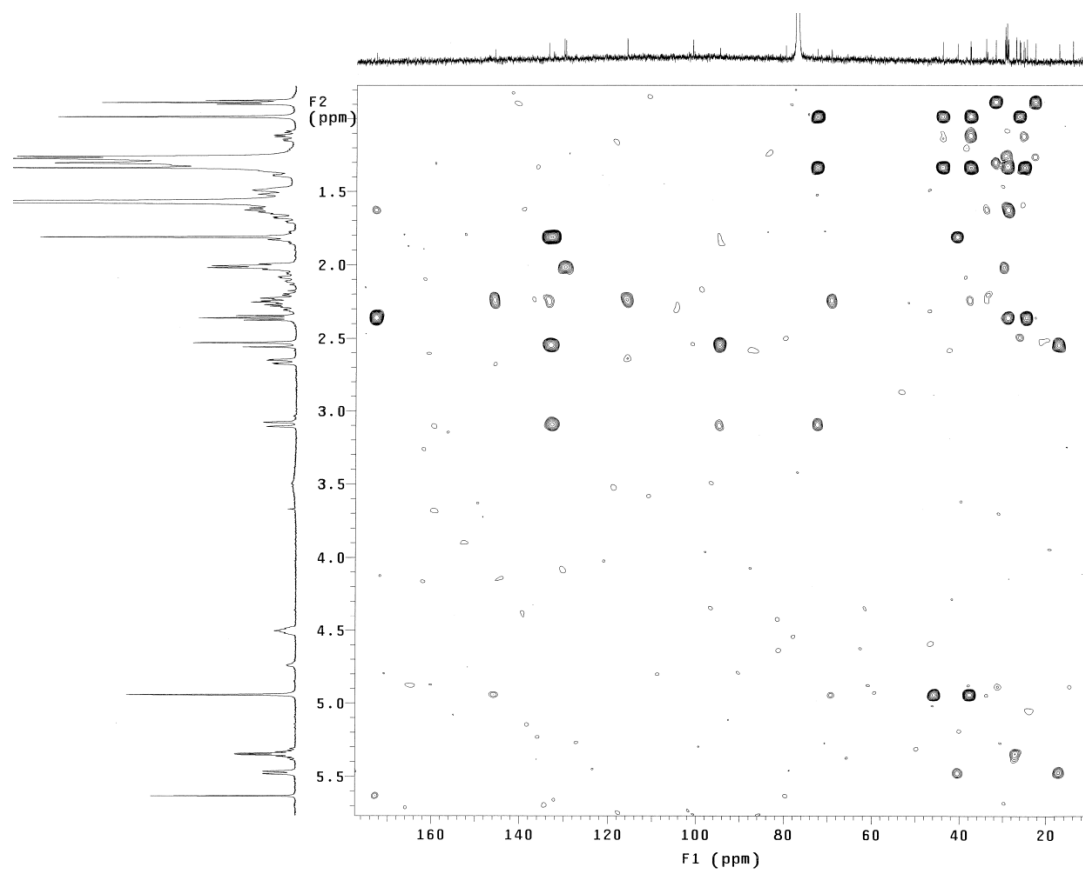


Figure S27. HMBC spectrum of **4** in CDCl₃

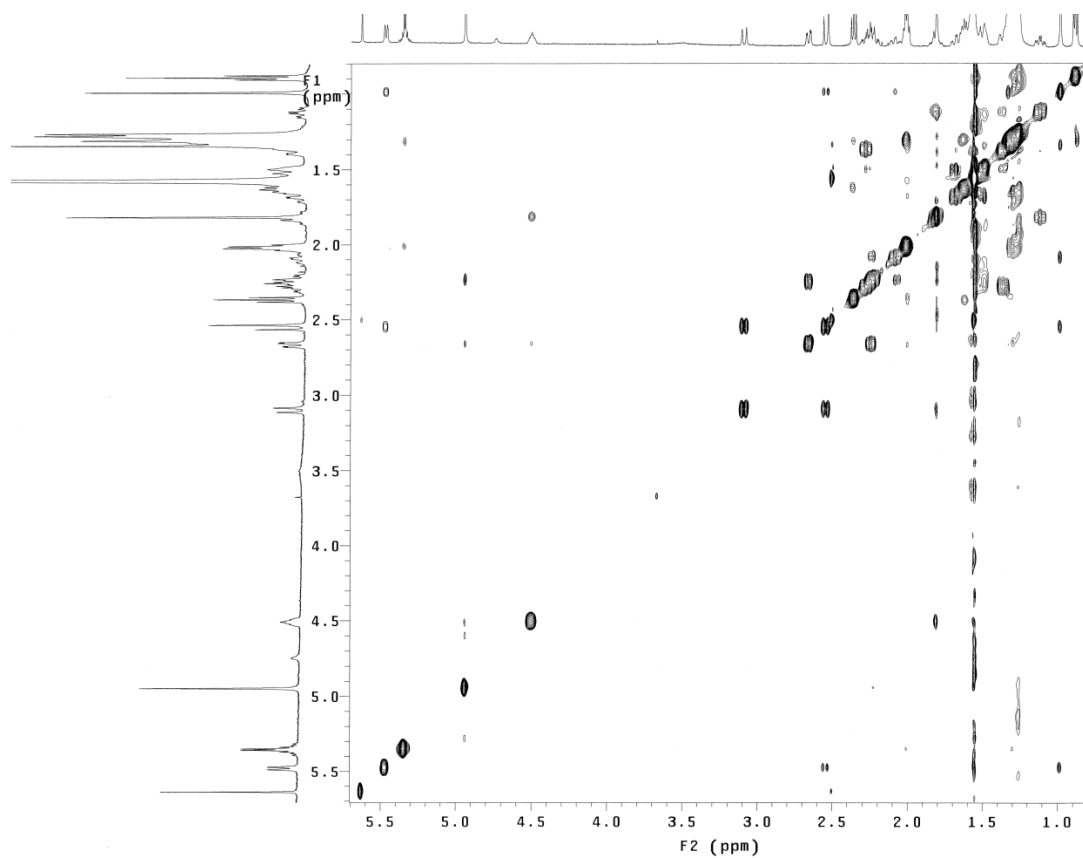


Figure S28. NOESY spectrum of **4** in CDCl₃

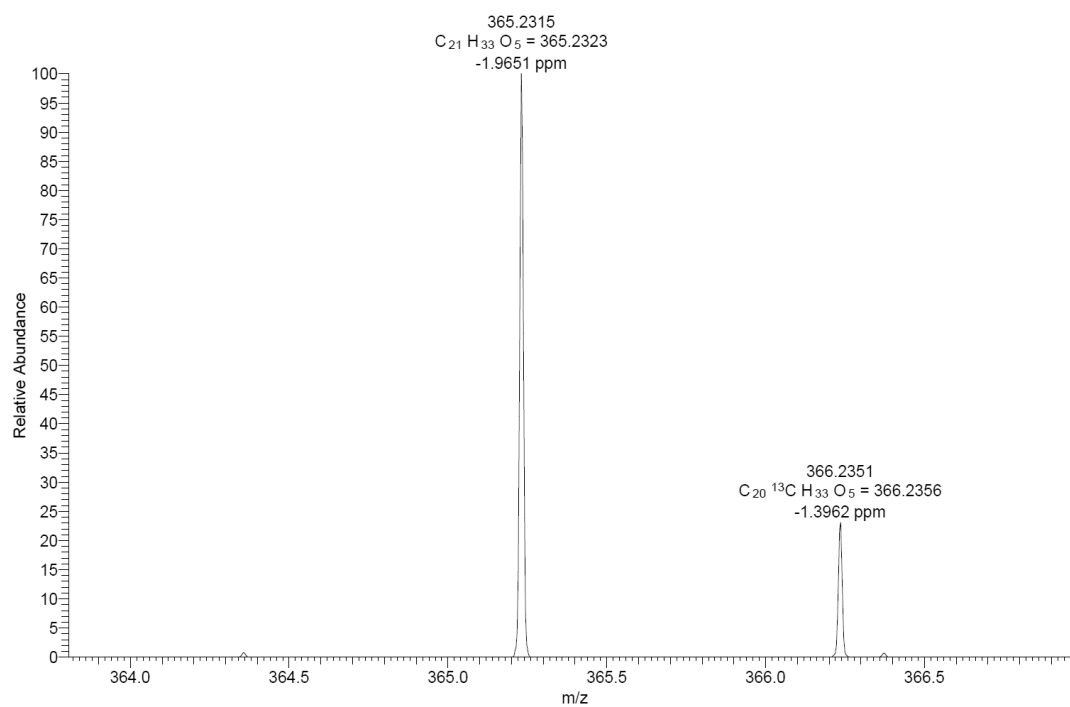


Figure S29. HRESIMS spectrum of 5

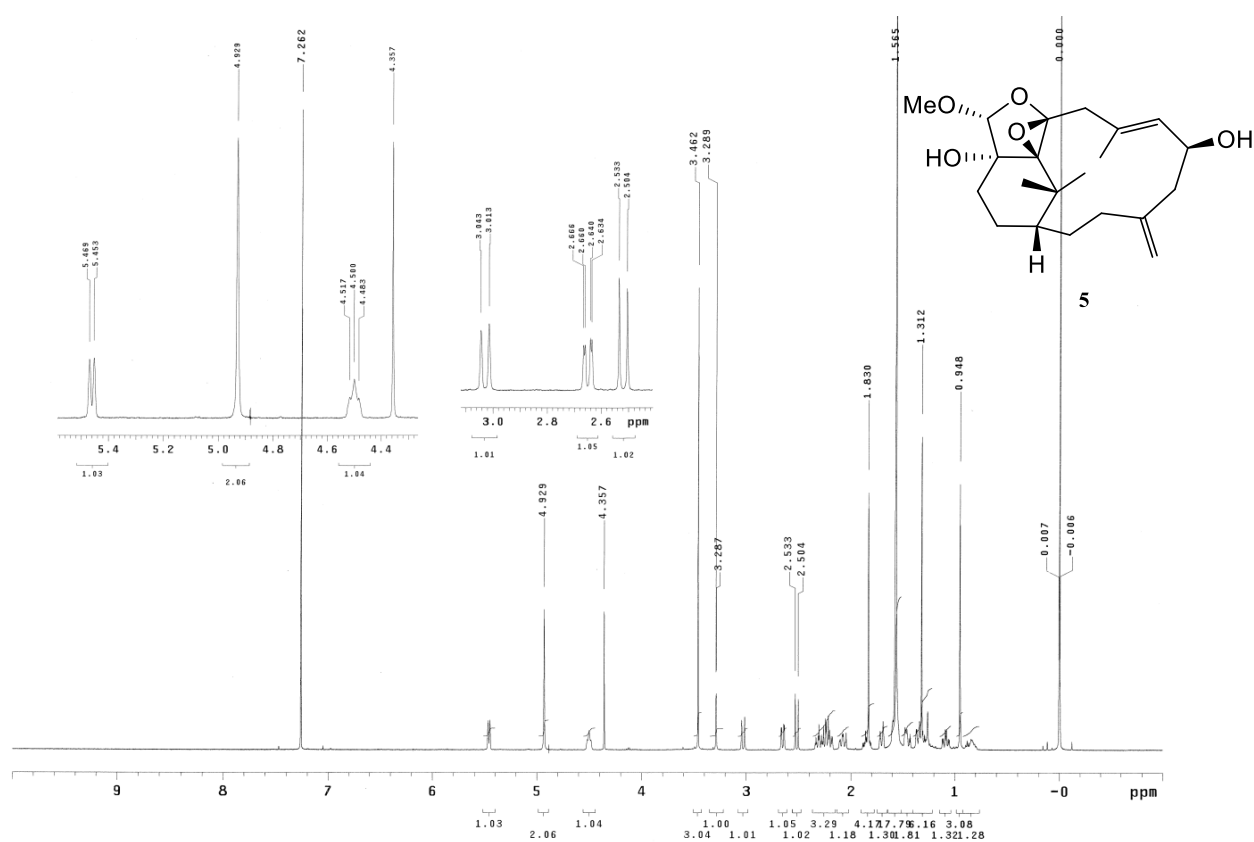


Figure S30. 1H NMR spectrum of 5 in $CDCl_3$ at 500 MHz

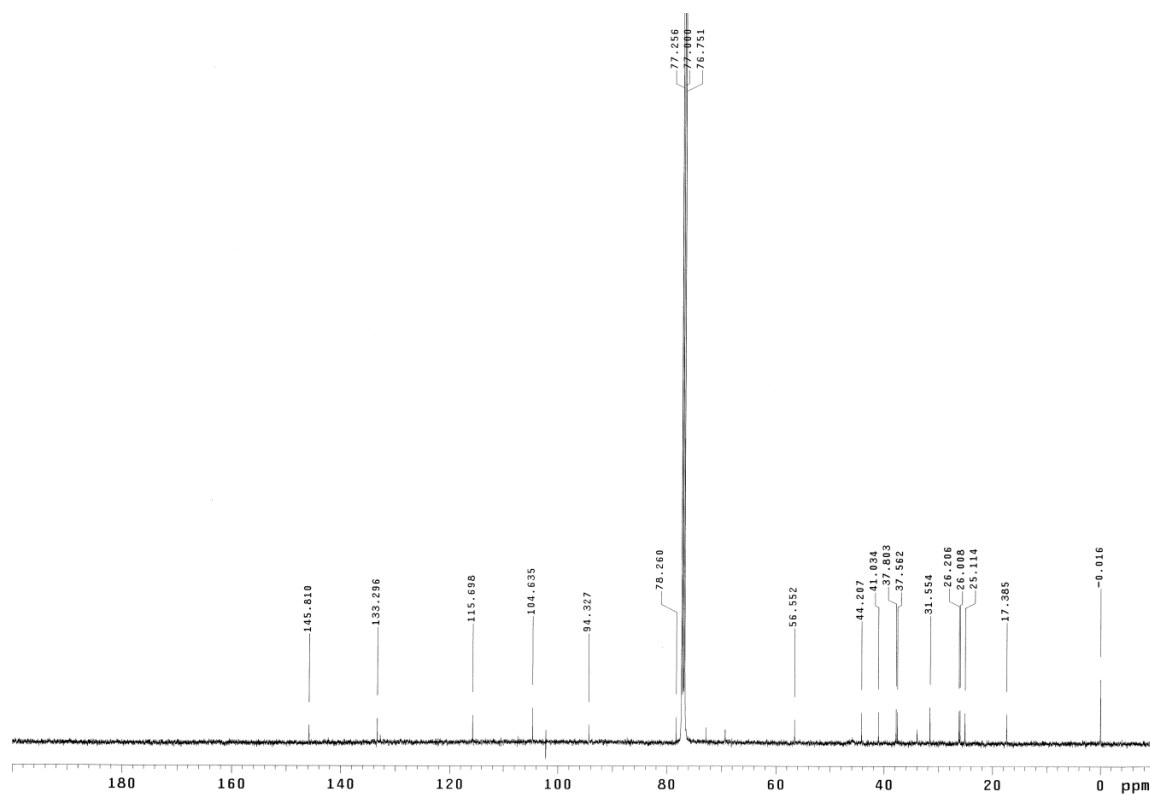


Figure S31. ¹³C NMR spectrum of 5 in CDCl₃ at 125 MHz

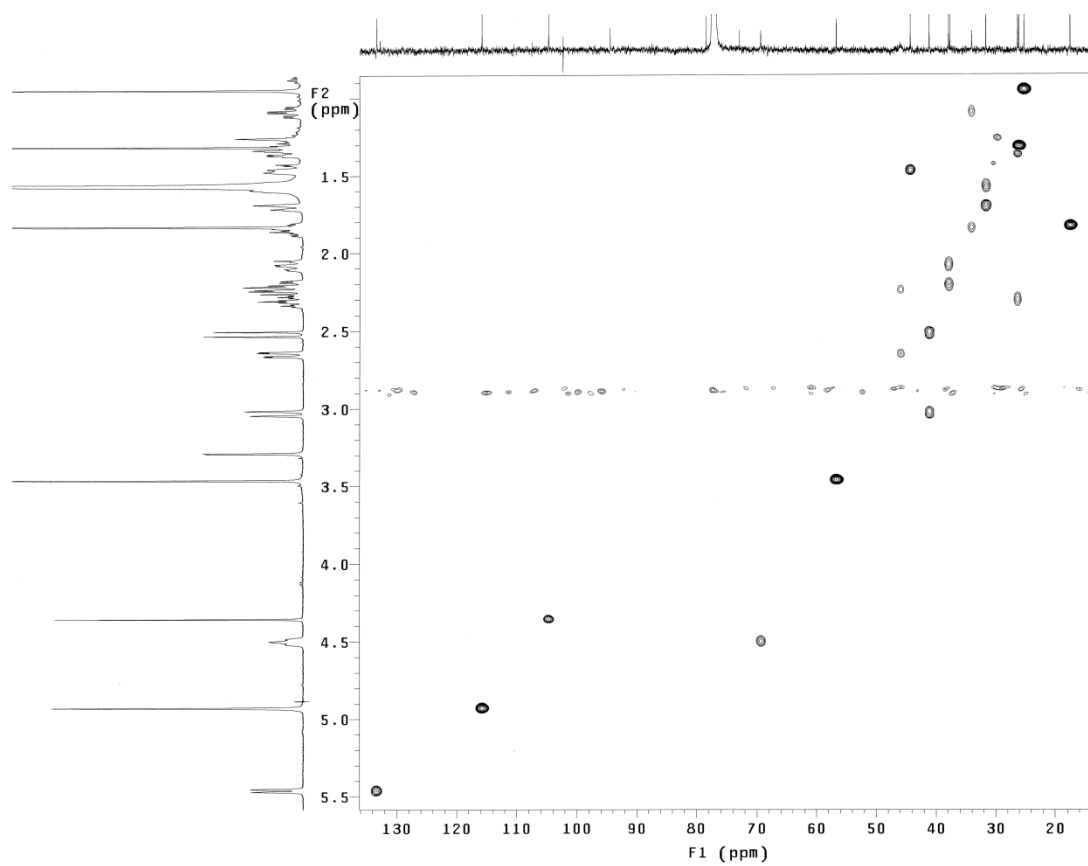


Figure S32. HSQC spectrum of 5 in CDCl₃

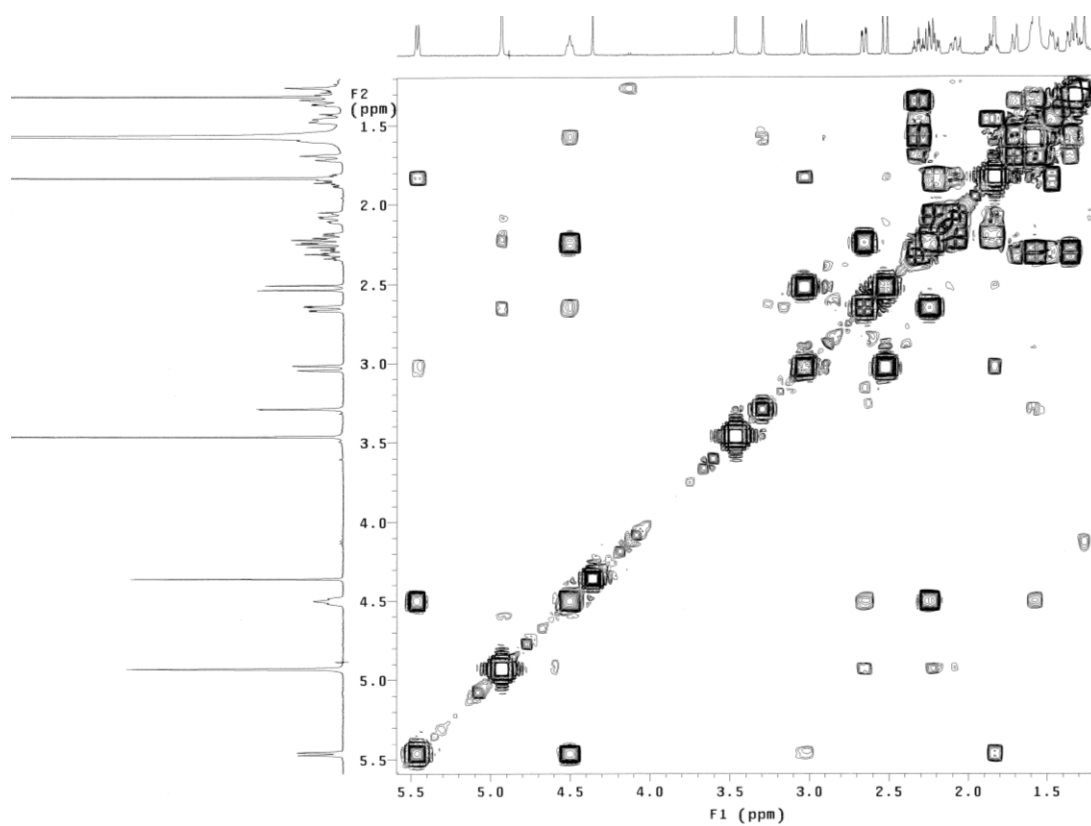


Figure S33. COSY spectrum of **5** in CDCl₃

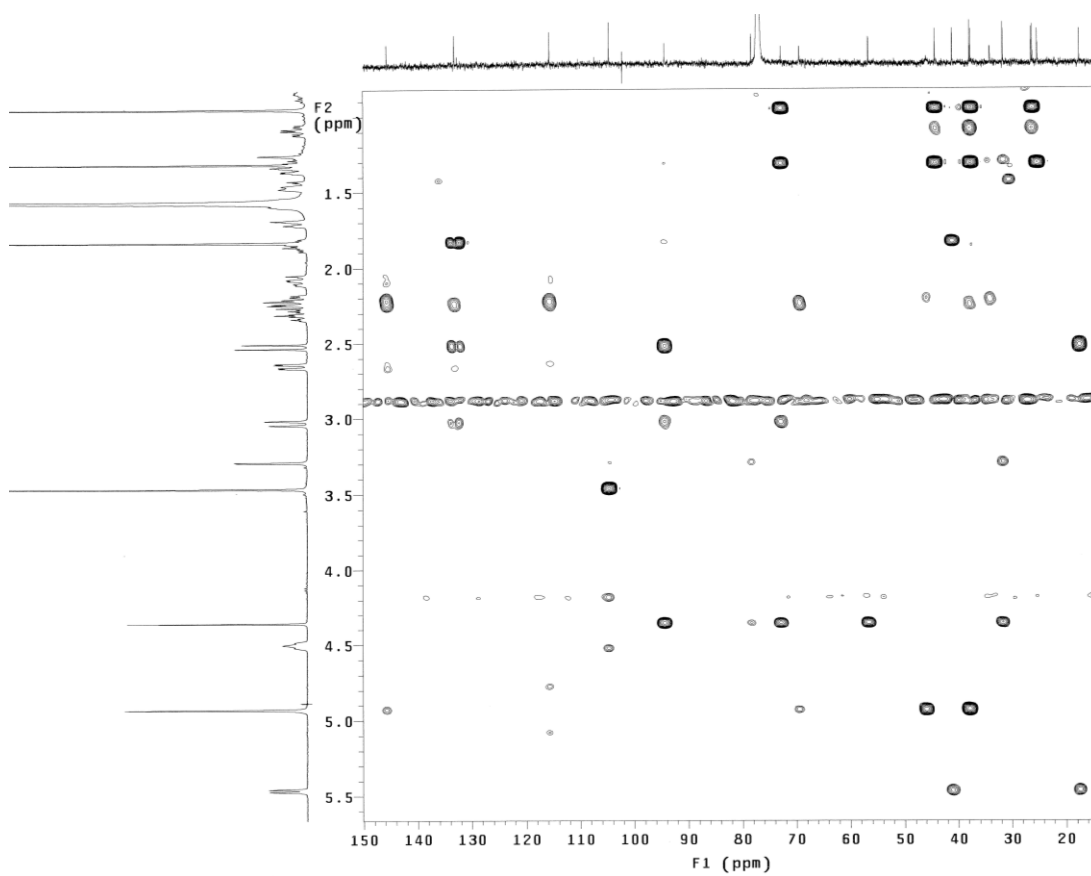


Figure S34. HMBC spectrum of **5** in CDCl₃

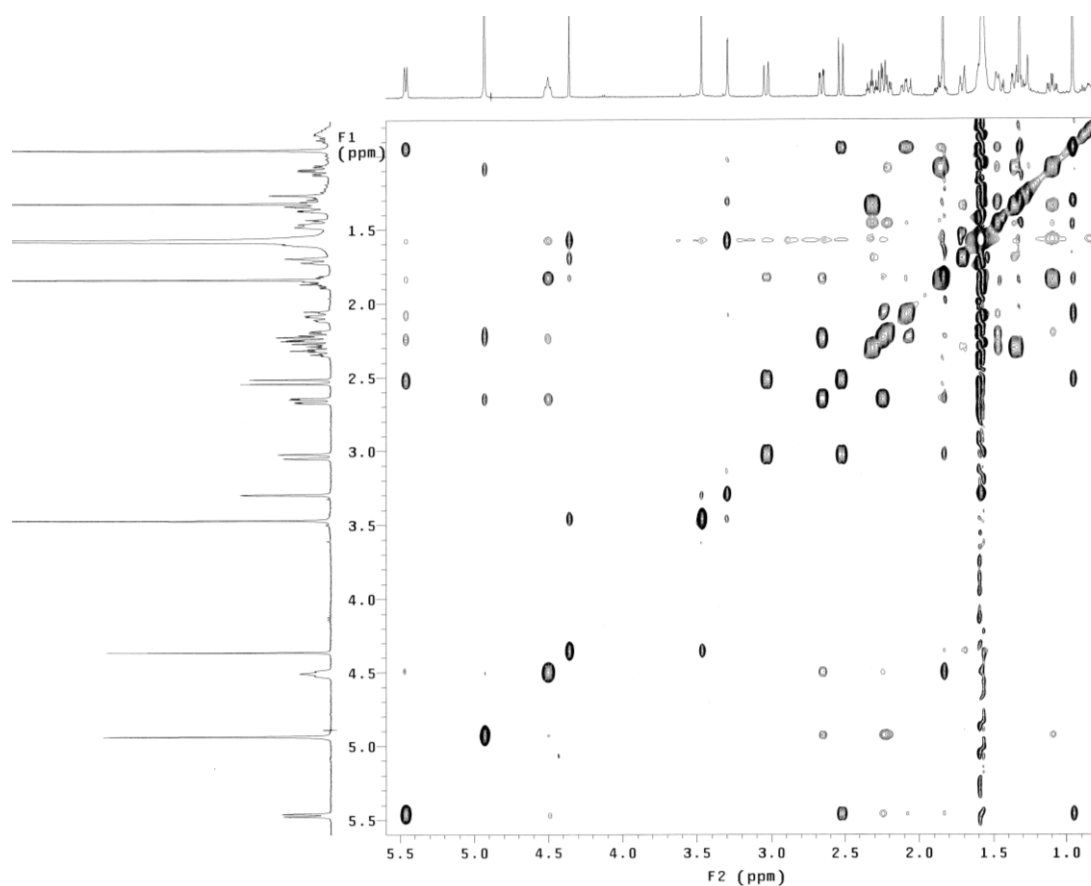
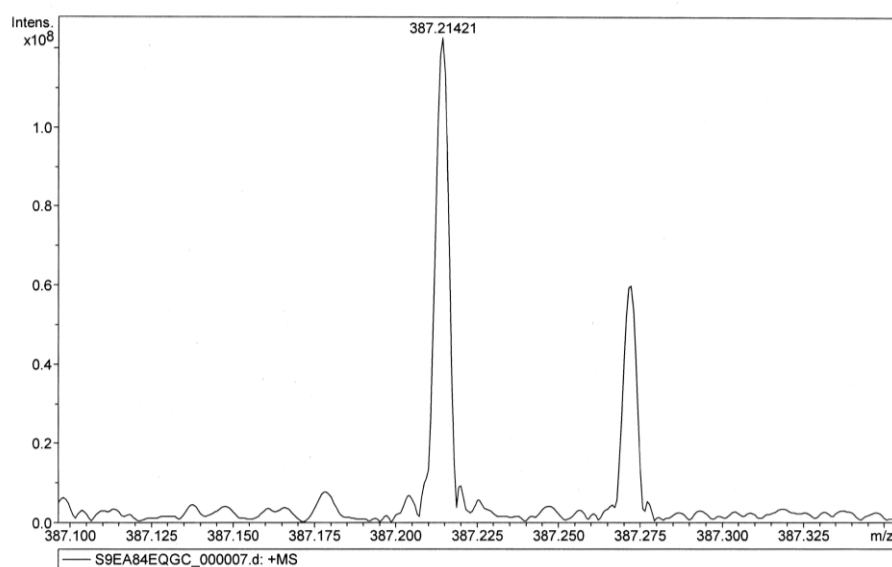


Figure S35. NOESY spectrum of of 5 in CDCl_3



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
387.21421	1	C ₂₁ H ₃₂ NaO ₅	100.00	387.21420	-0.02	-0.04	32.2	5.5	even	ok

Figure S36. HRESIMS spectrum of 6

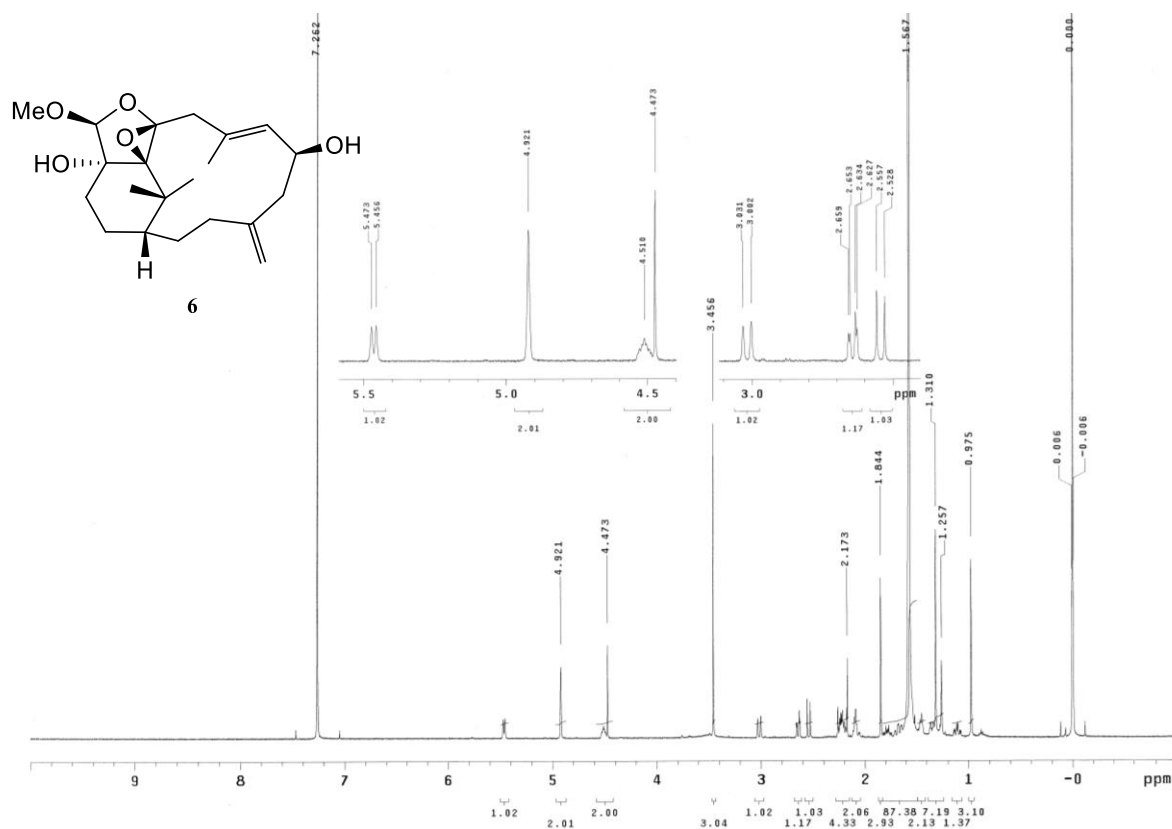


Figure S37. ¹H NMR spectrum of 6 CDCl₃ at 500 MHz

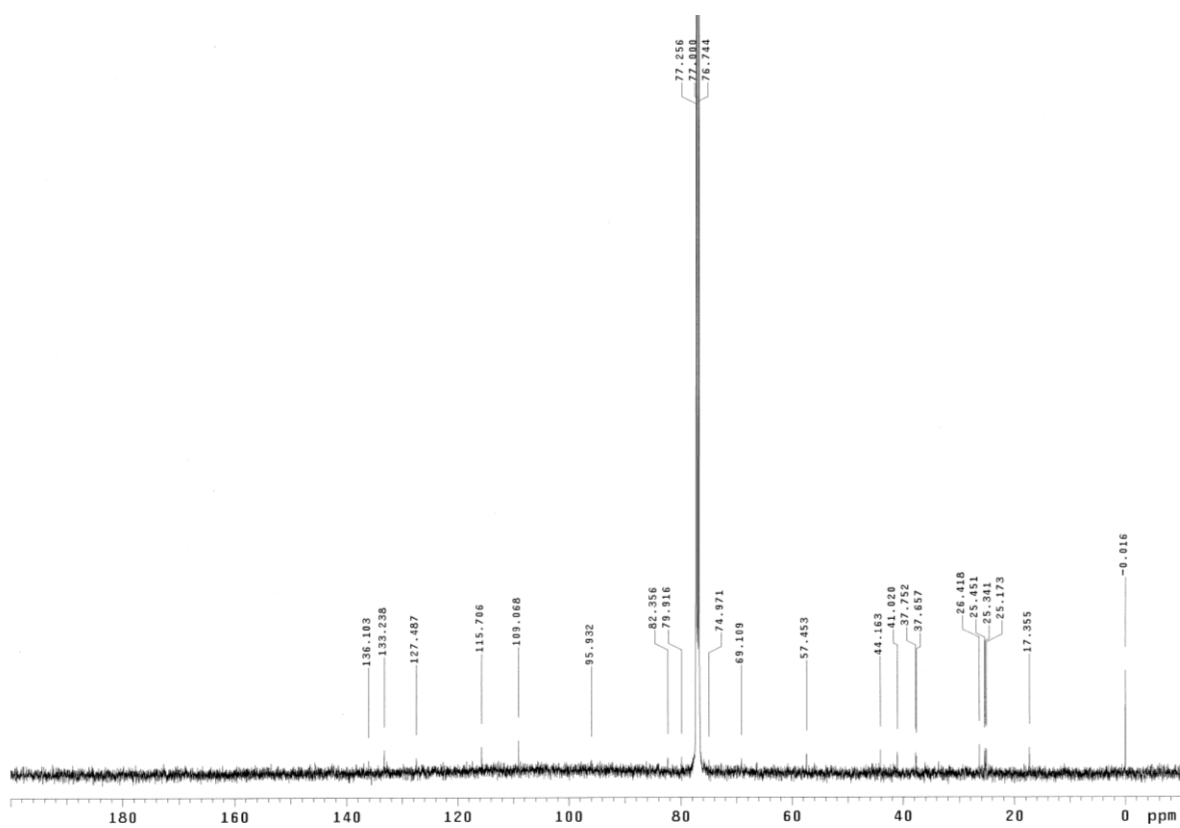


Figure S38. ¹³C NMR spectrum of 6 in CDCl₃ at 125 MHz

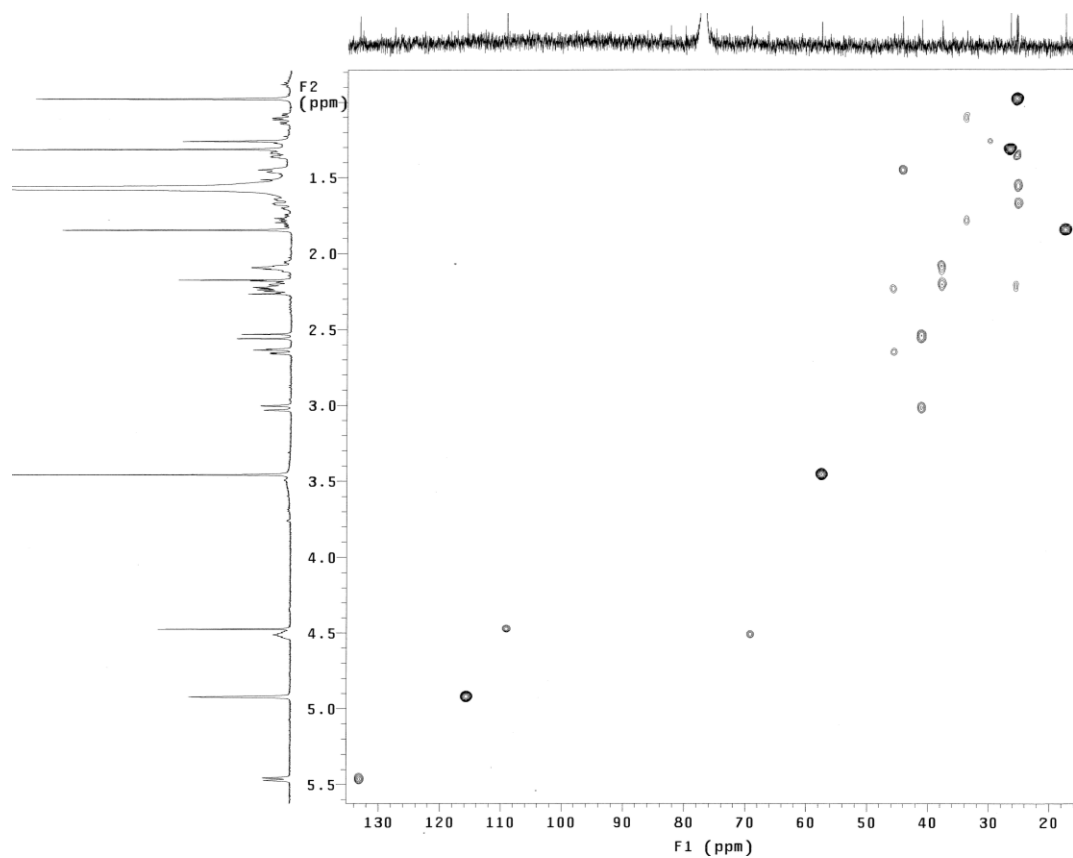


Figure S39. HSQC spectrum of **6** in CDCl_3

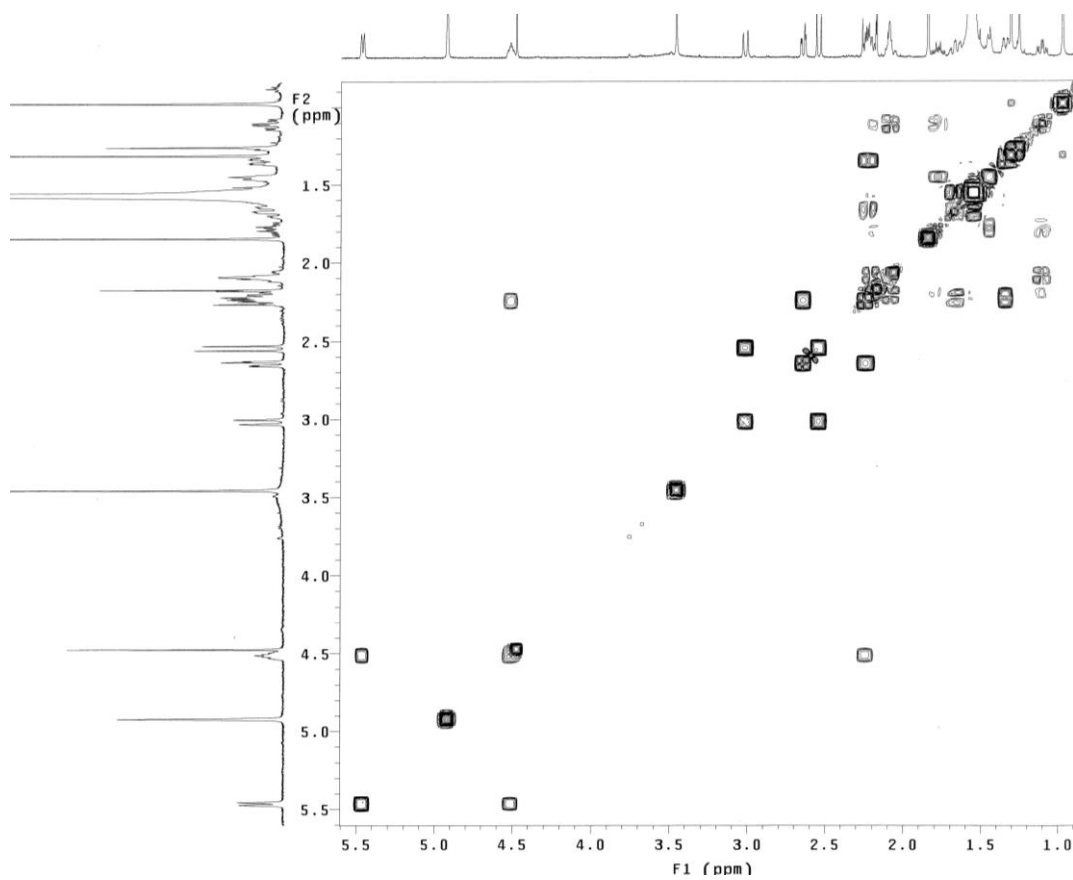


Figure S40. COSY spectrum of **6** in CDCl_3

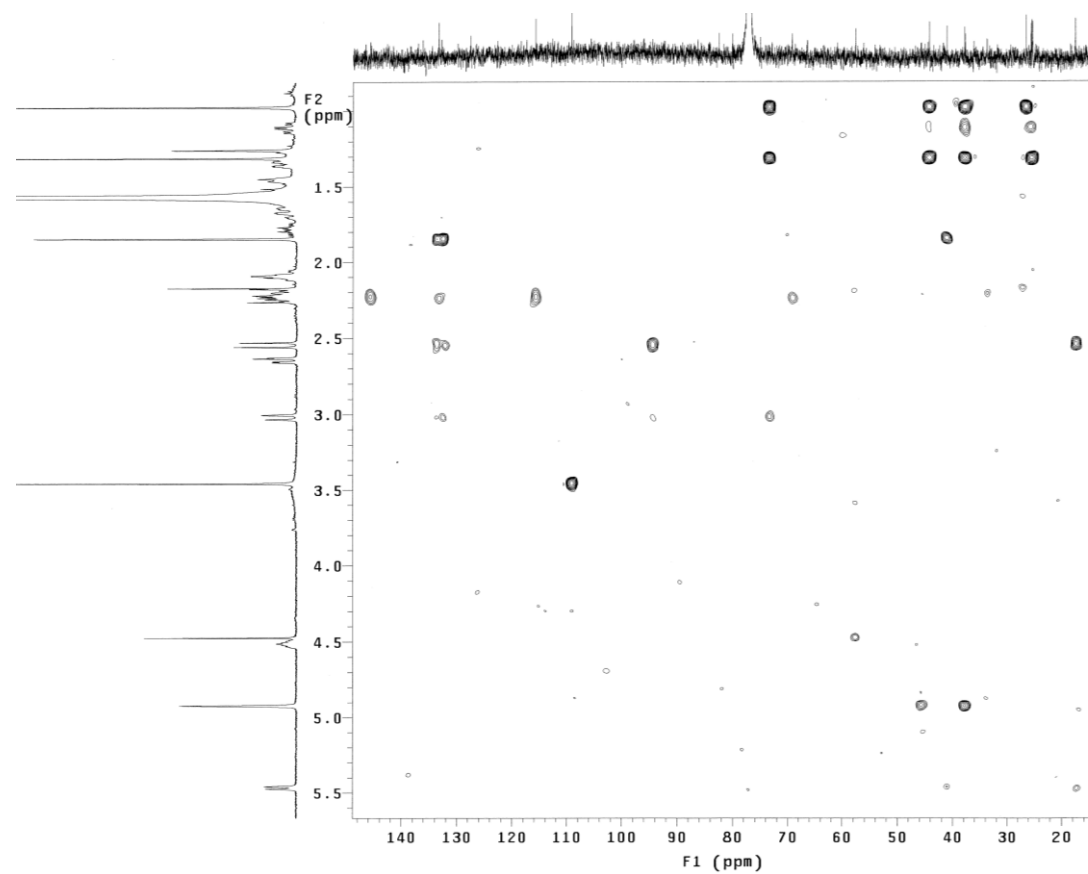


Figure S41. HMBC spectrum of **6** in CDCl_3

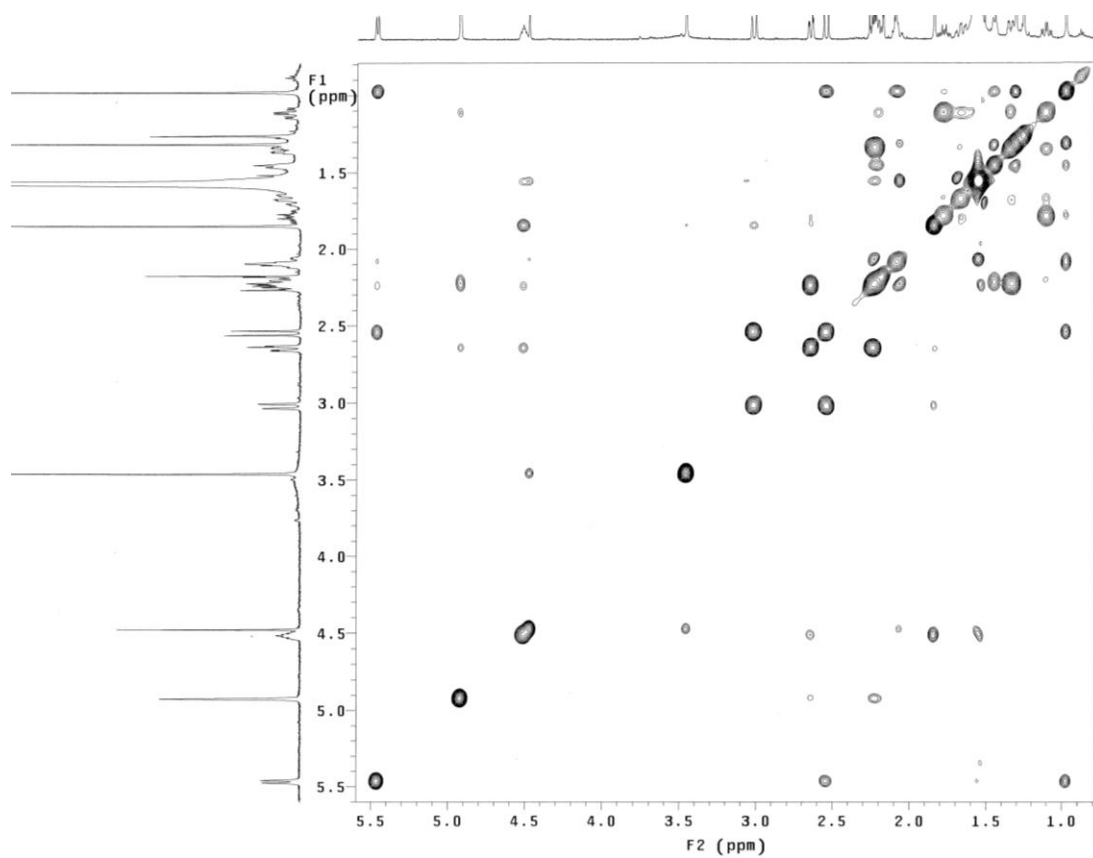


Figure S42. NOESY spectrum of **6** in CDCl_3

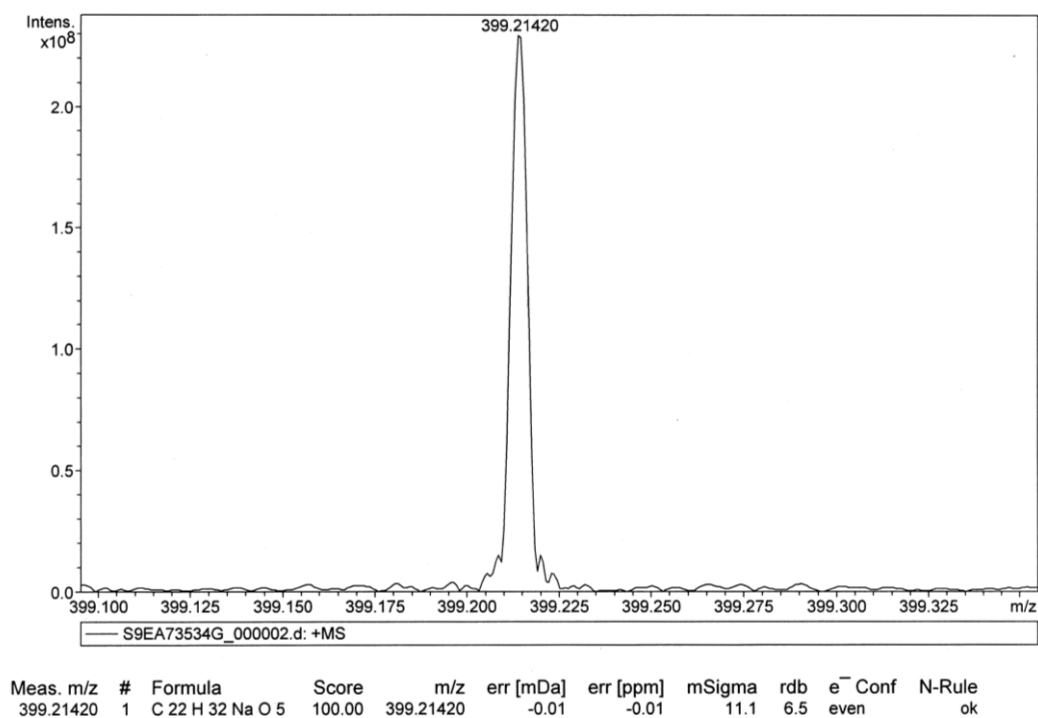


Figure S43. HRESIMS spectrum of 7

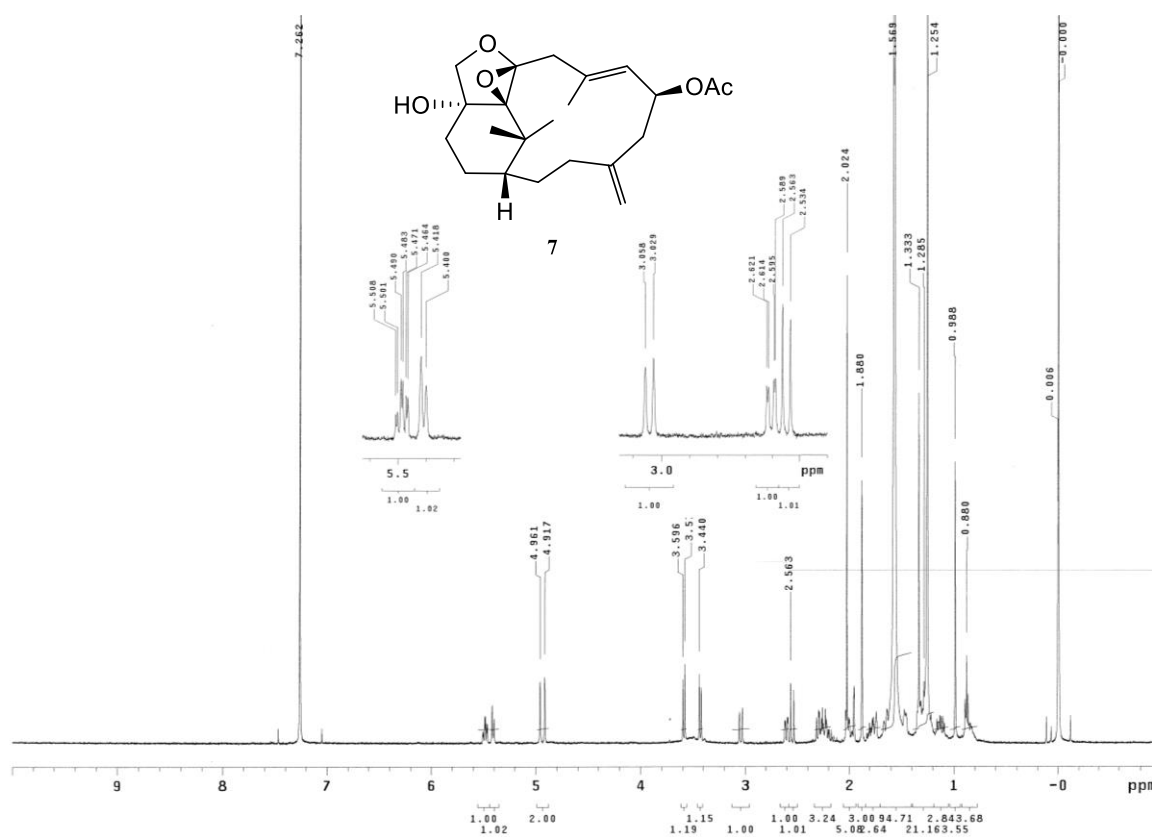


Figure S44. ¹H NMR spectrum of 7 in CDCl₃ at 500 MHz

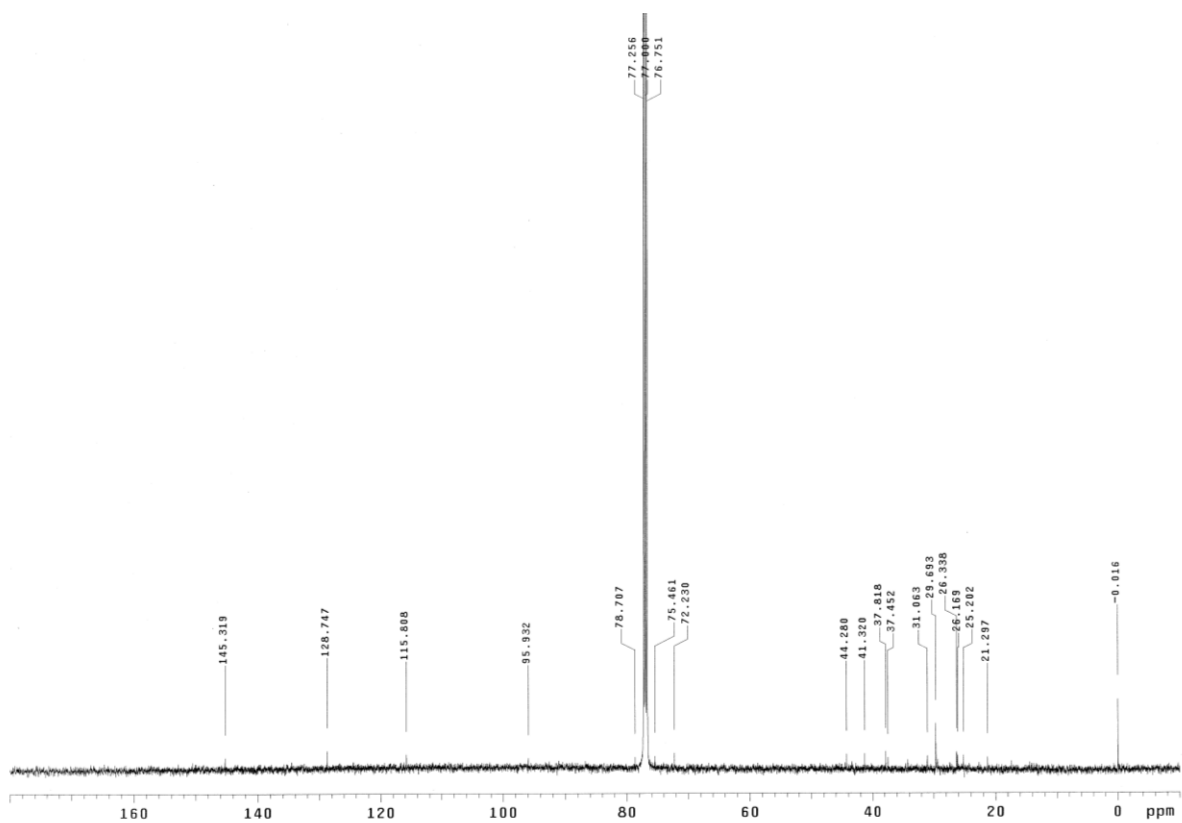


Figure S45. ¹³C NMR spectrum of 7 in CDCl₃ at 125 MHz

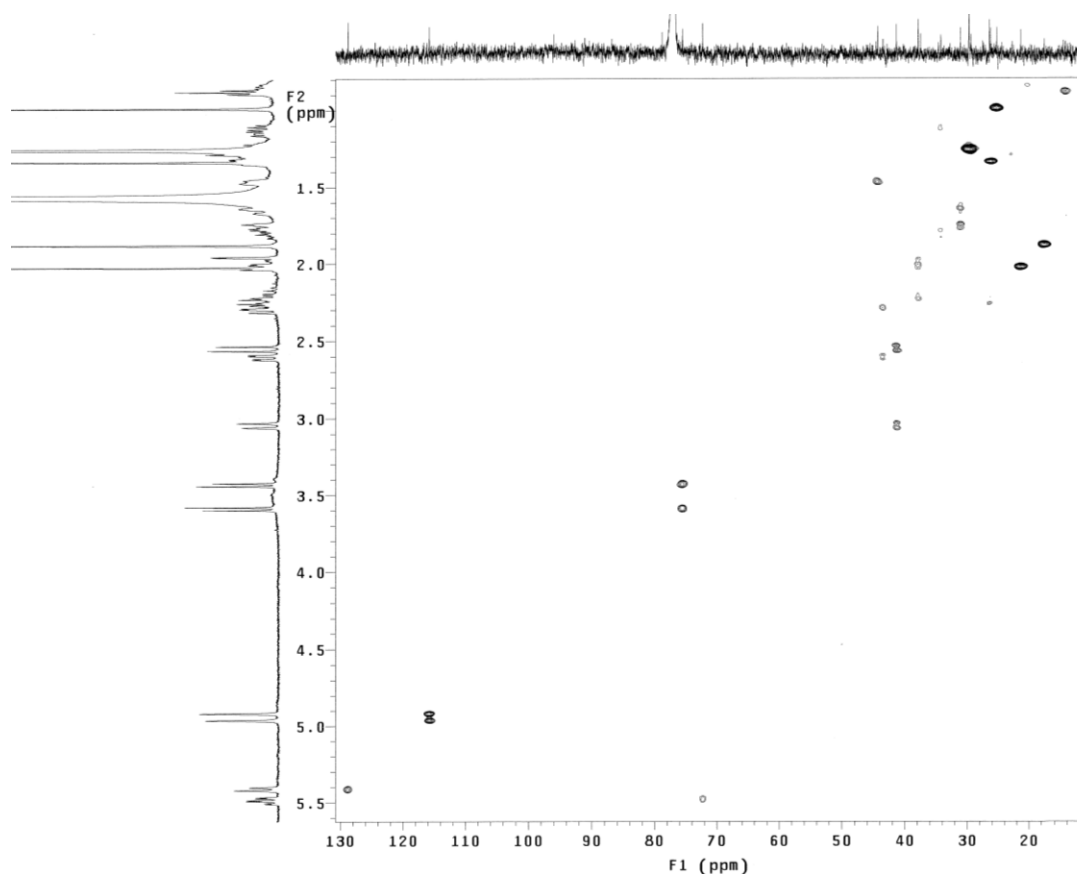


Figure S46. HSQC spectrum of 7 in CDCl₃

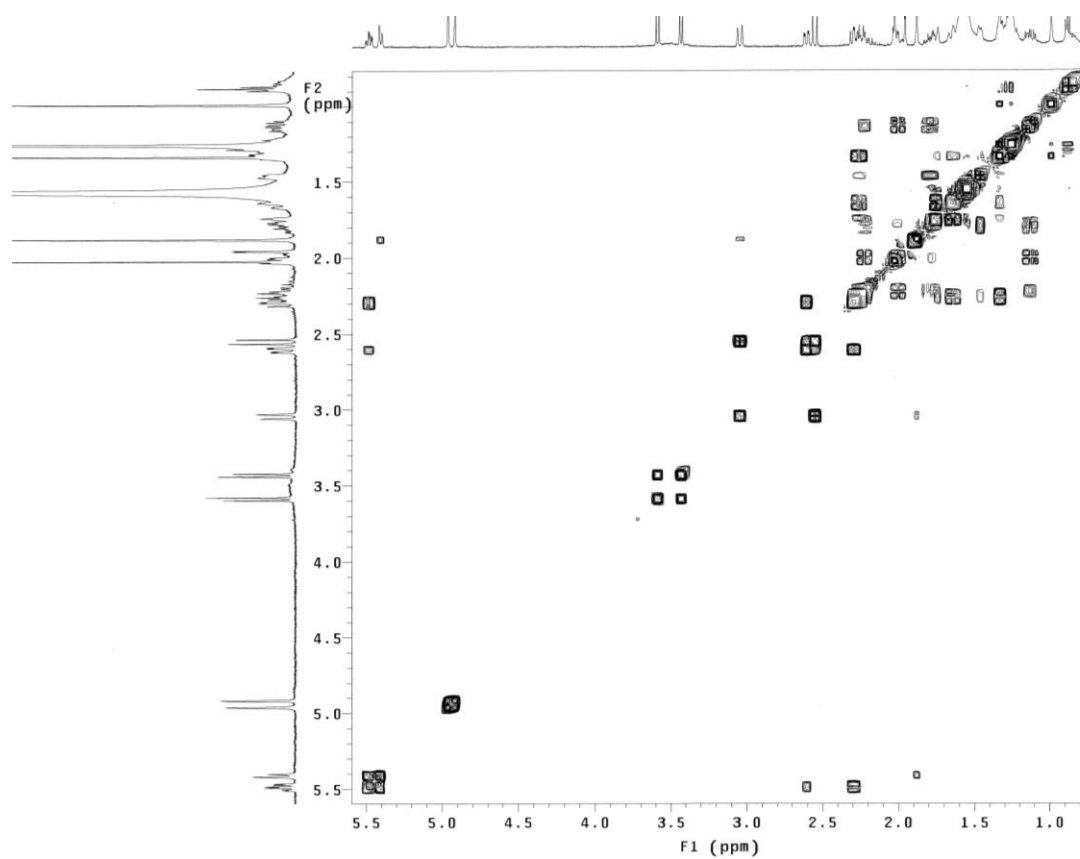


Figure S47. COSY spectrum of **7** in CDCl₃

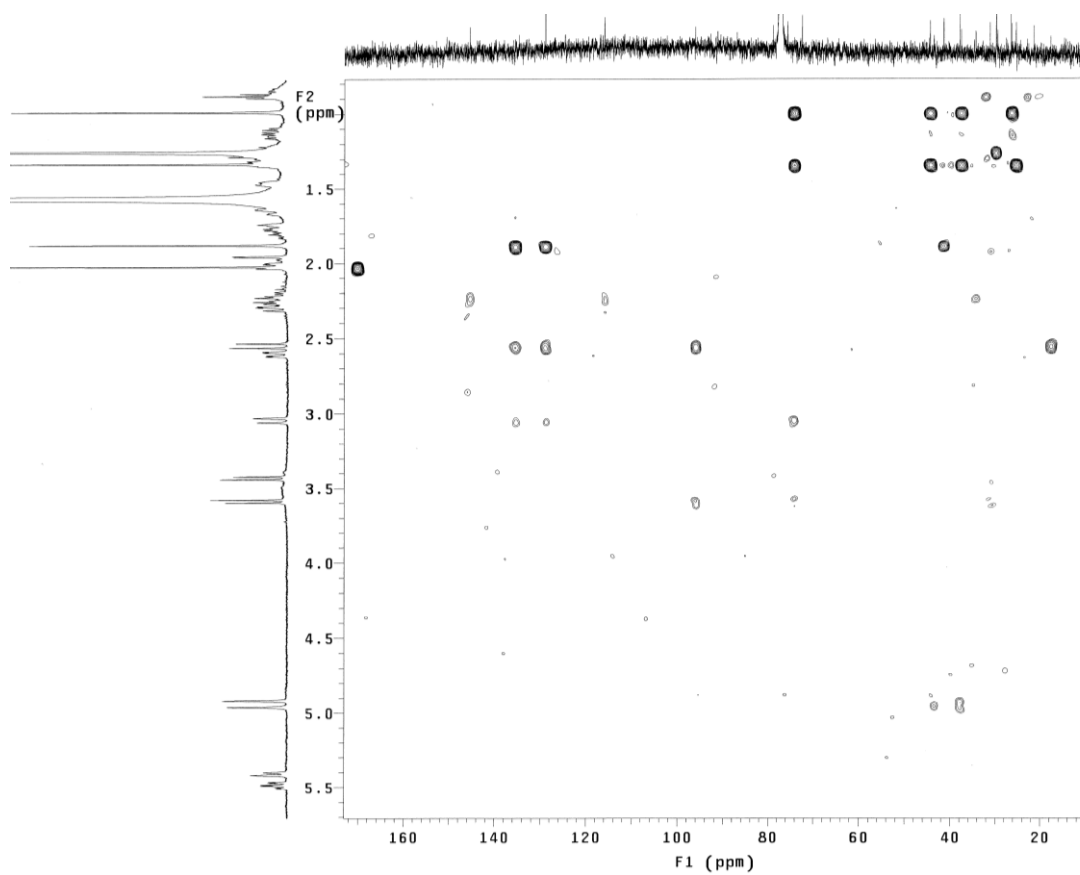


Figure S48. HMBC spectrum of **7** in CDCl₃

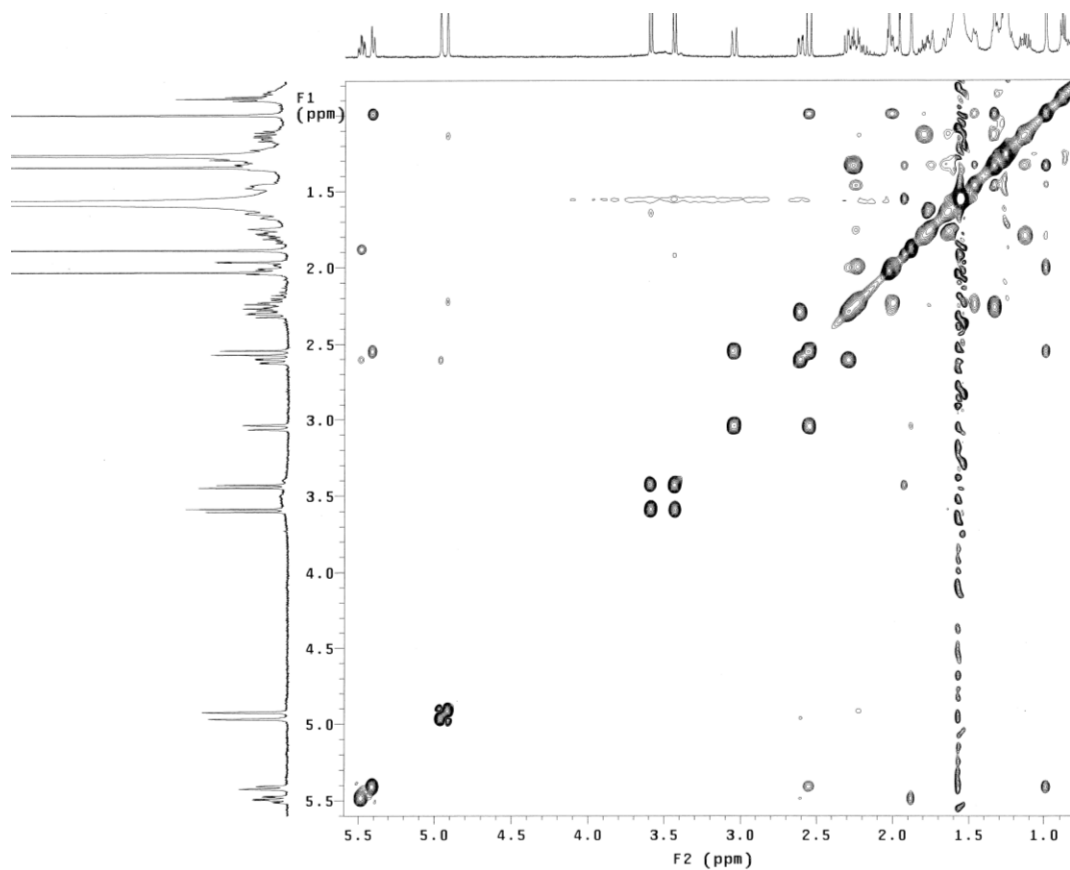


Figure S49. NOESY spectrum of 7 in CDCl_3

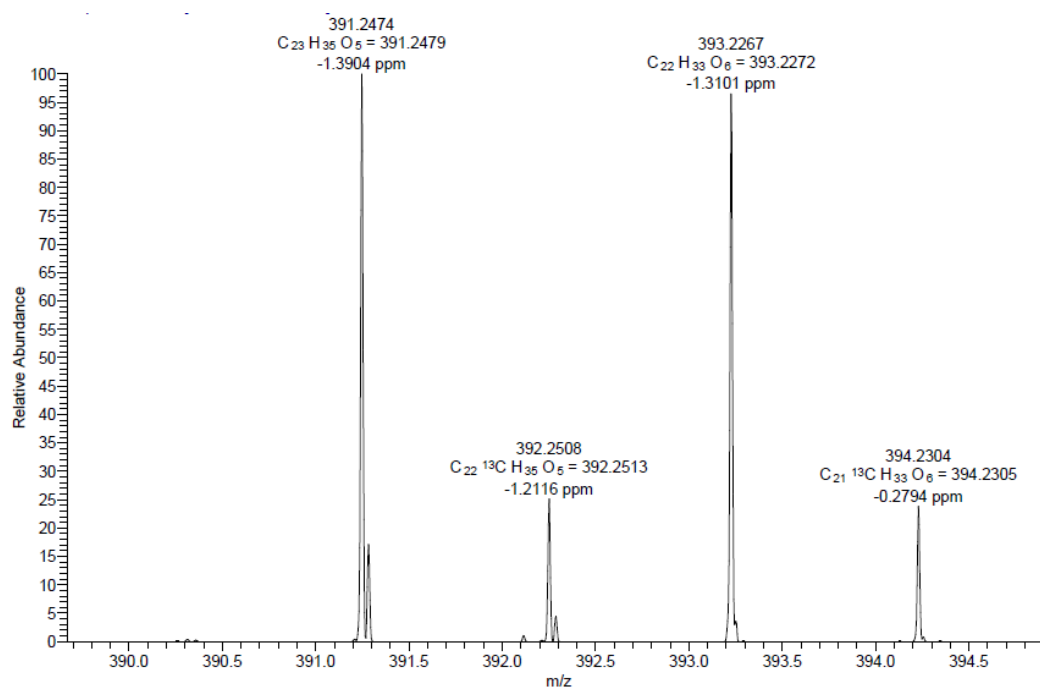


Figure S50. HRESIMS spectrum of 8

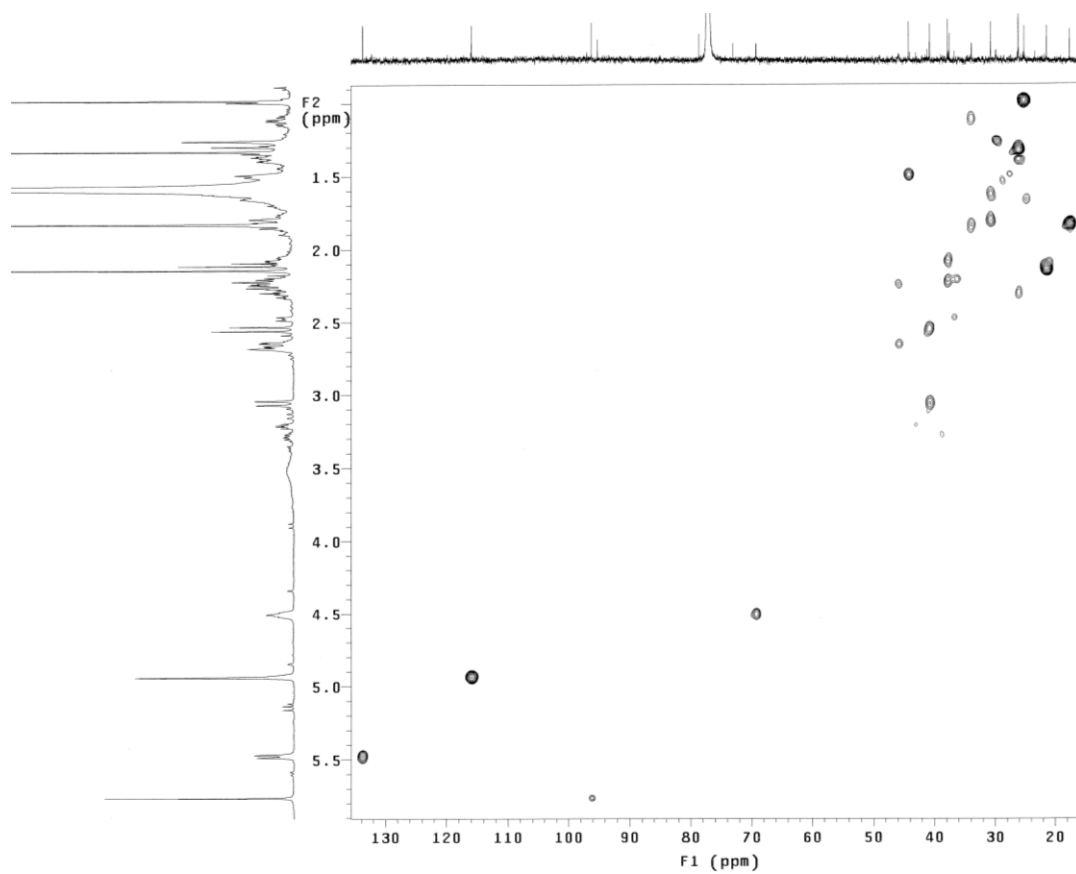


Figure S53. HSQC spectrum of **8** in CDCl_3

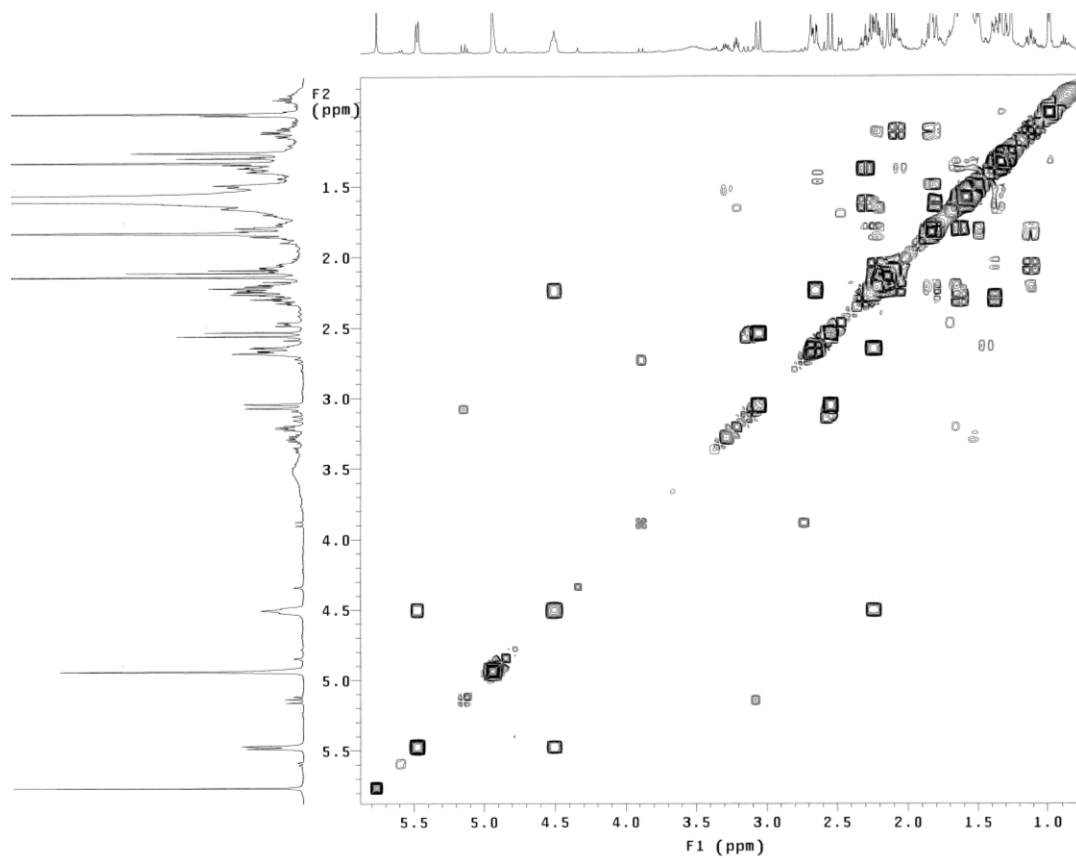


Figure S54. COSY spectrum of **8** in CDCl_3

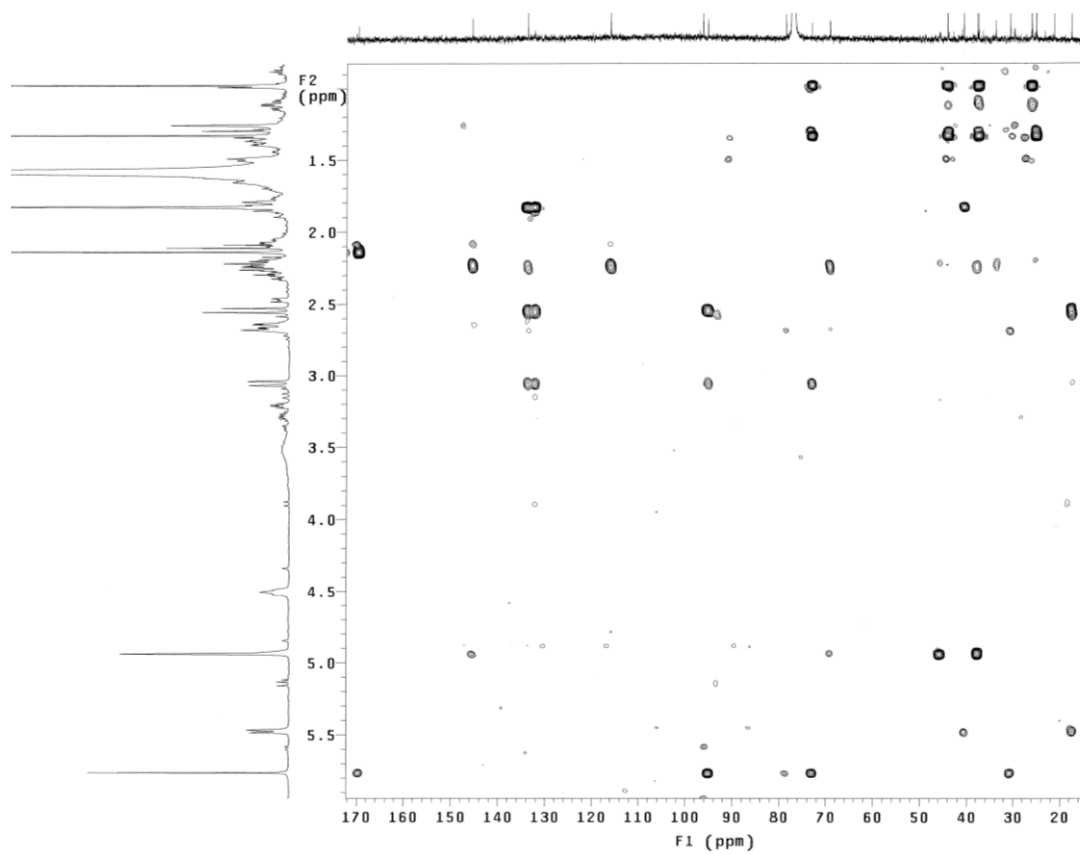


Figure S55. HMBC spectrum of **8** in CDCl_3

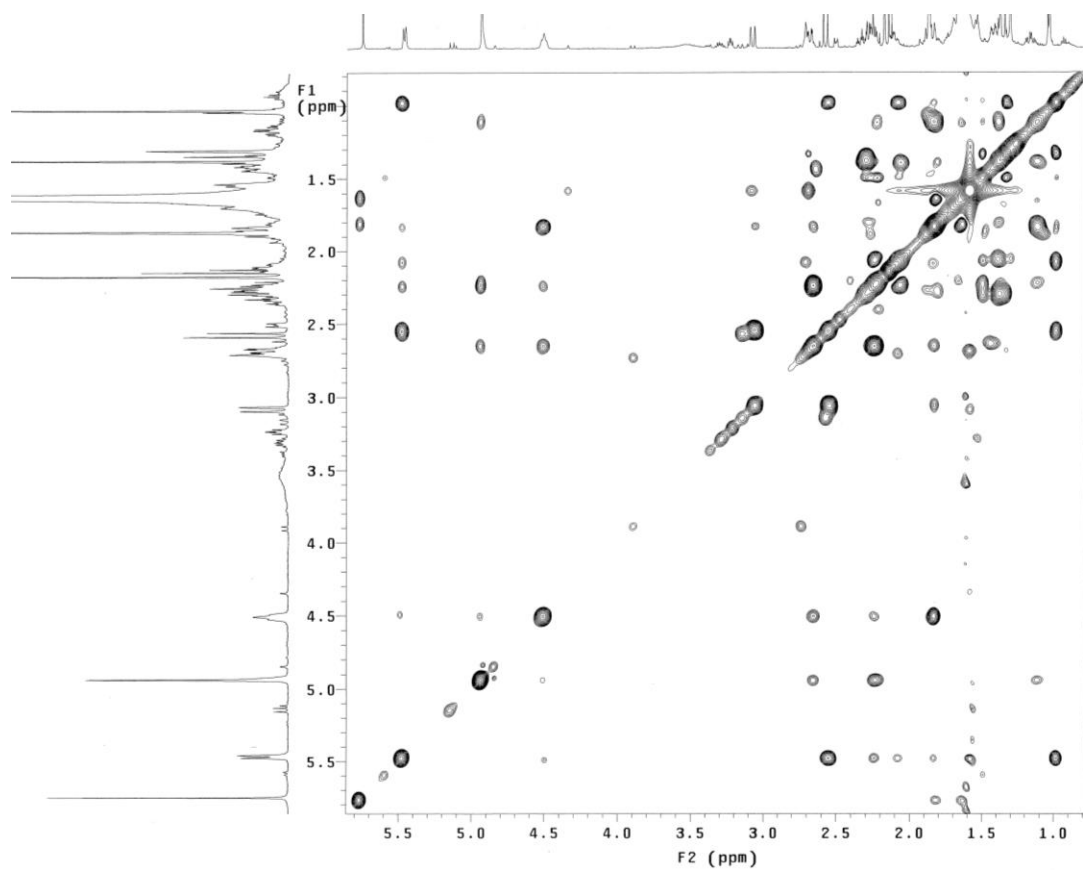
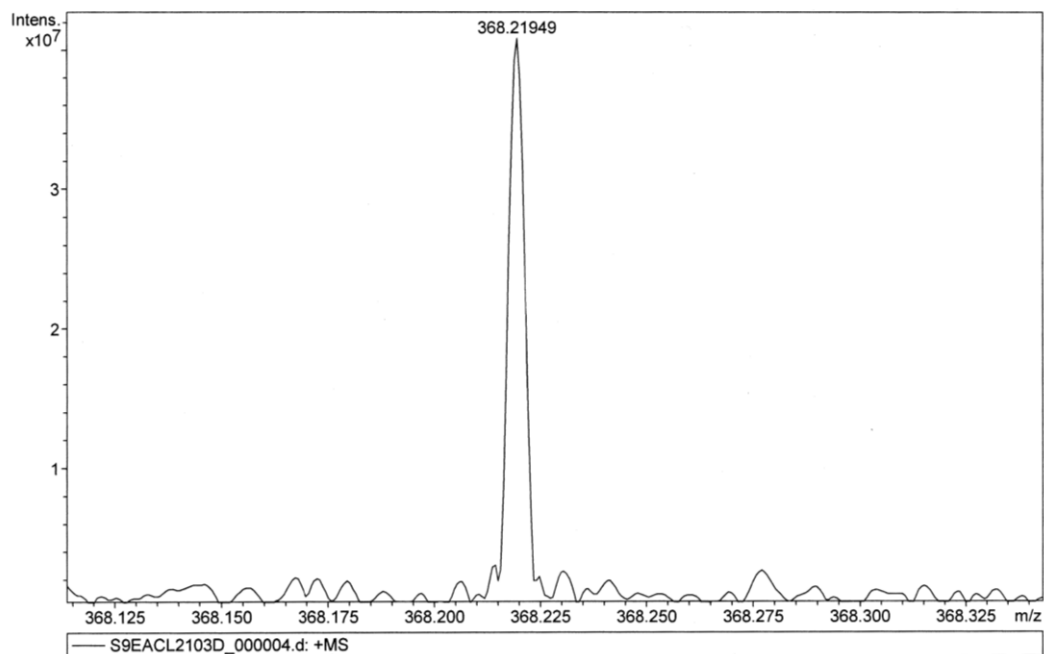


Figure S56. NOESY spectrum of **8** in CDCl_3



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
368.21949	1	C ₂₁ H ₃₁ NNaO ₃	100.00	368.21961	0.13	0.34	25.0	6.5	even	ok

Figure S57. HRESIMS spectrum of 9

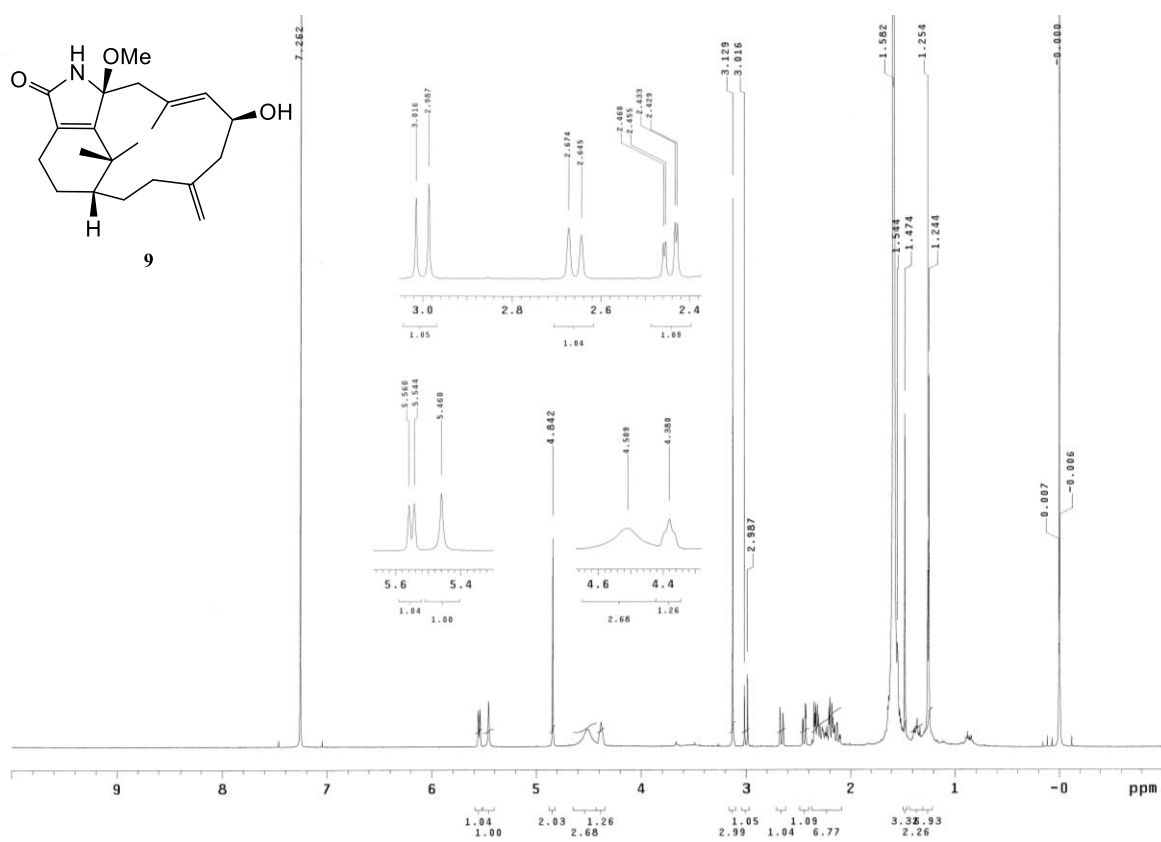


Figure S58. ¹H NMR spectrum of 9 in CDCl₃ at 500 MHz

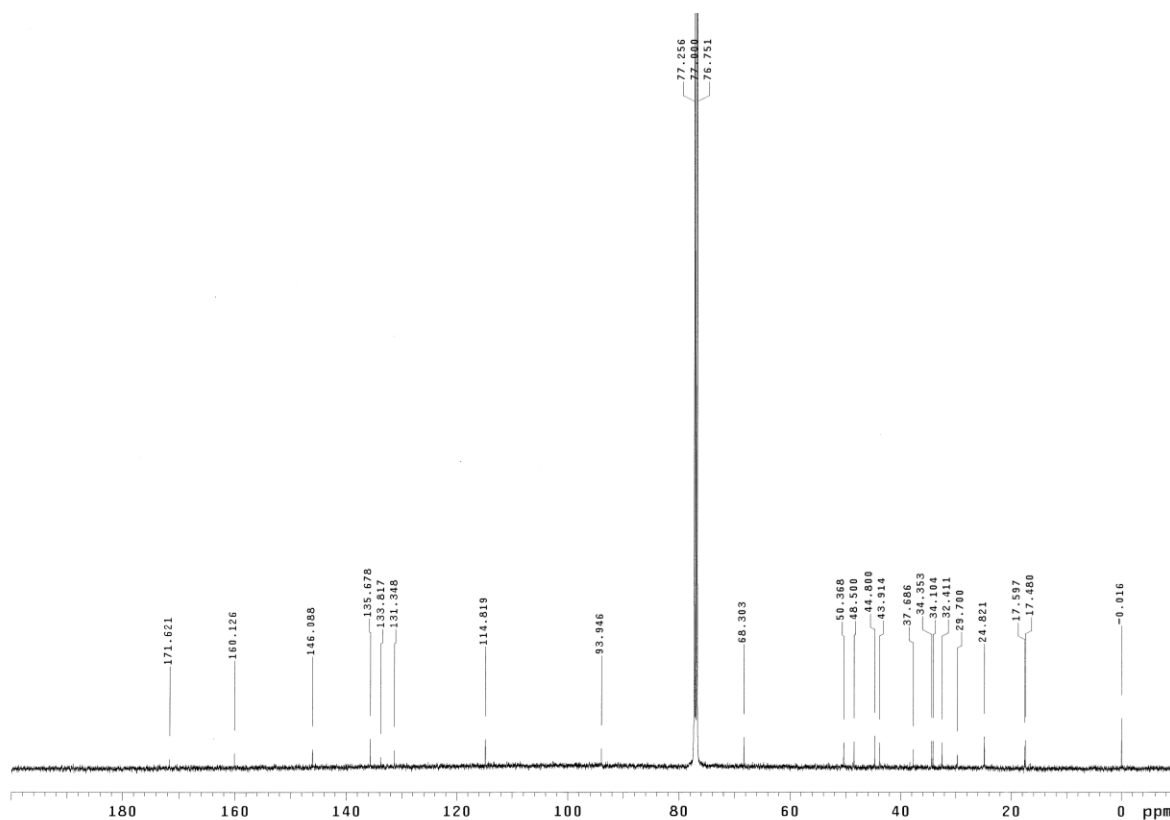


Figure S59. ¹³C NMR spectrum of **9** in CDCl₃ at 125 MHz

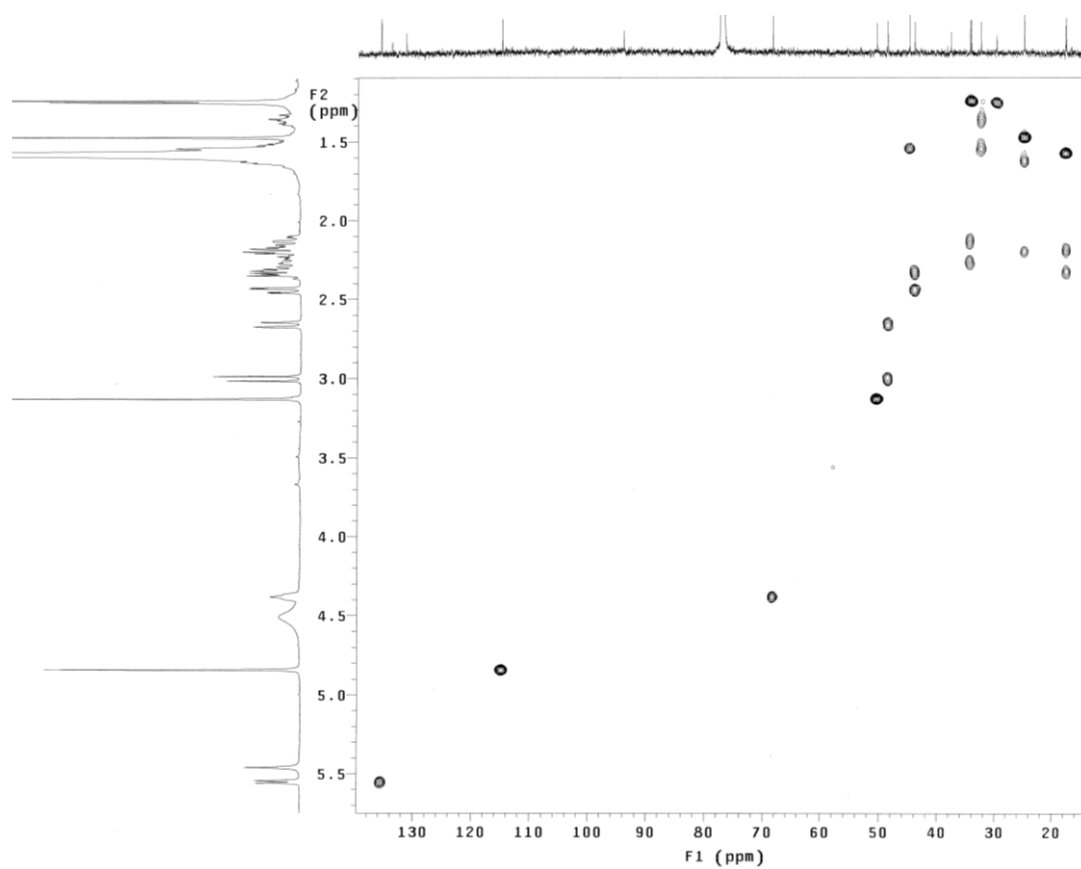


Figure S60. HSQC spectrum of **9** in CDCl₃

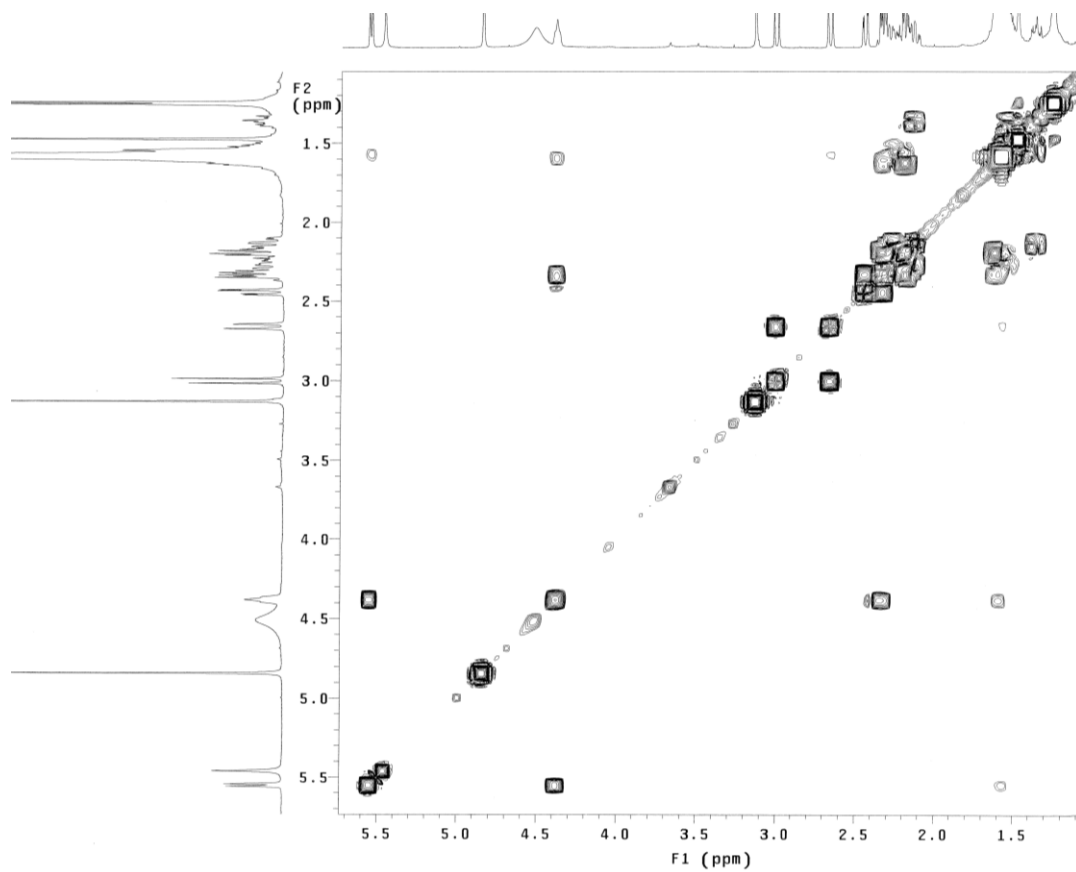


Figure S61. COSY spectrum of **9** in CDCl_3

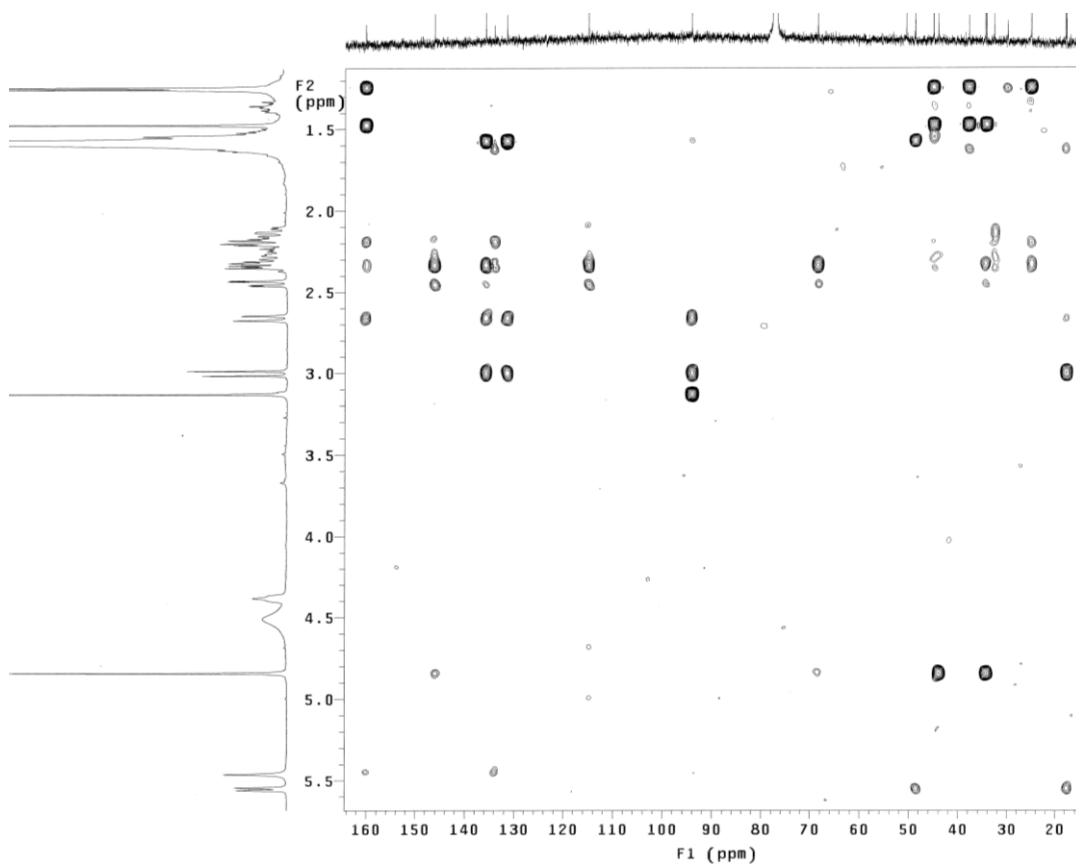


Figure S62. HMBC spectrum of **9** in CDCl_3

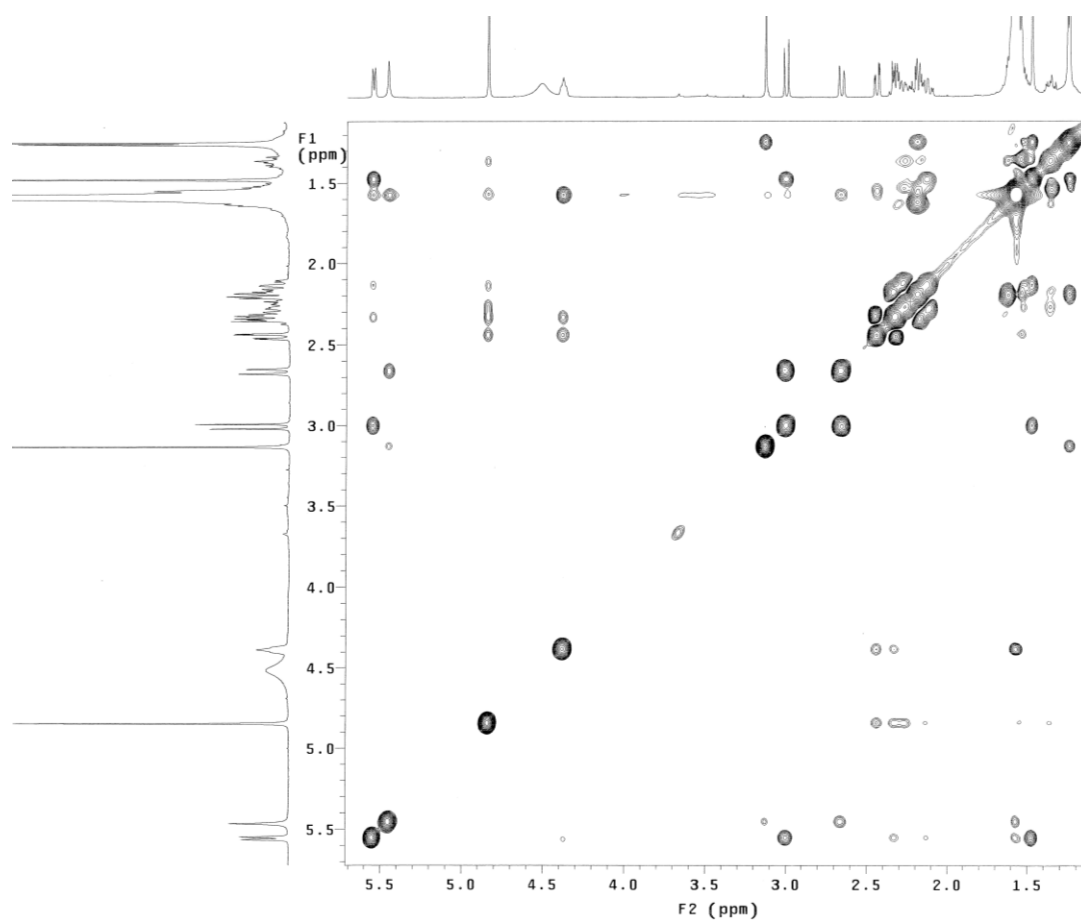


Figure S63. NOESY spectrum of **9** in CDCl_3

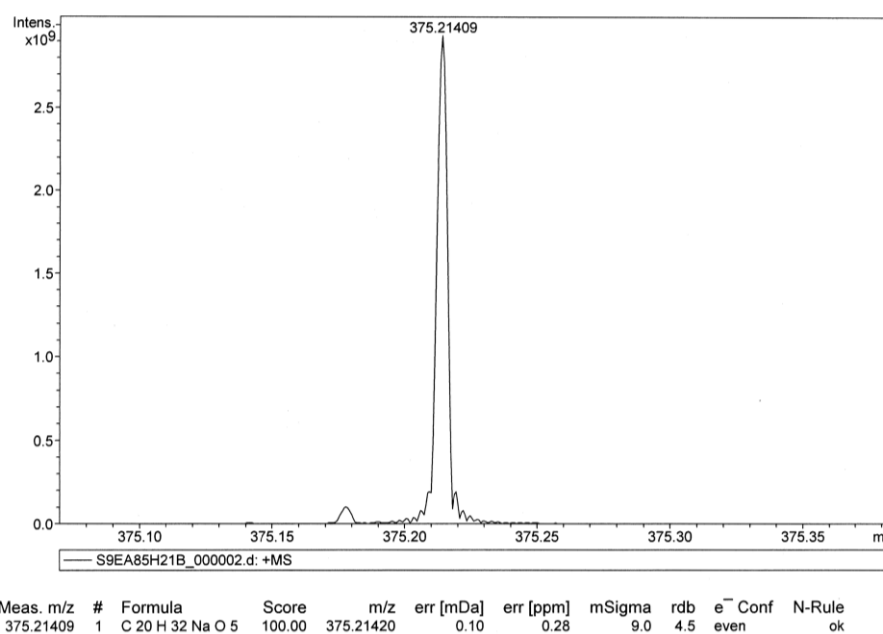


Figure S64. HRESIMS spectrum of **10**

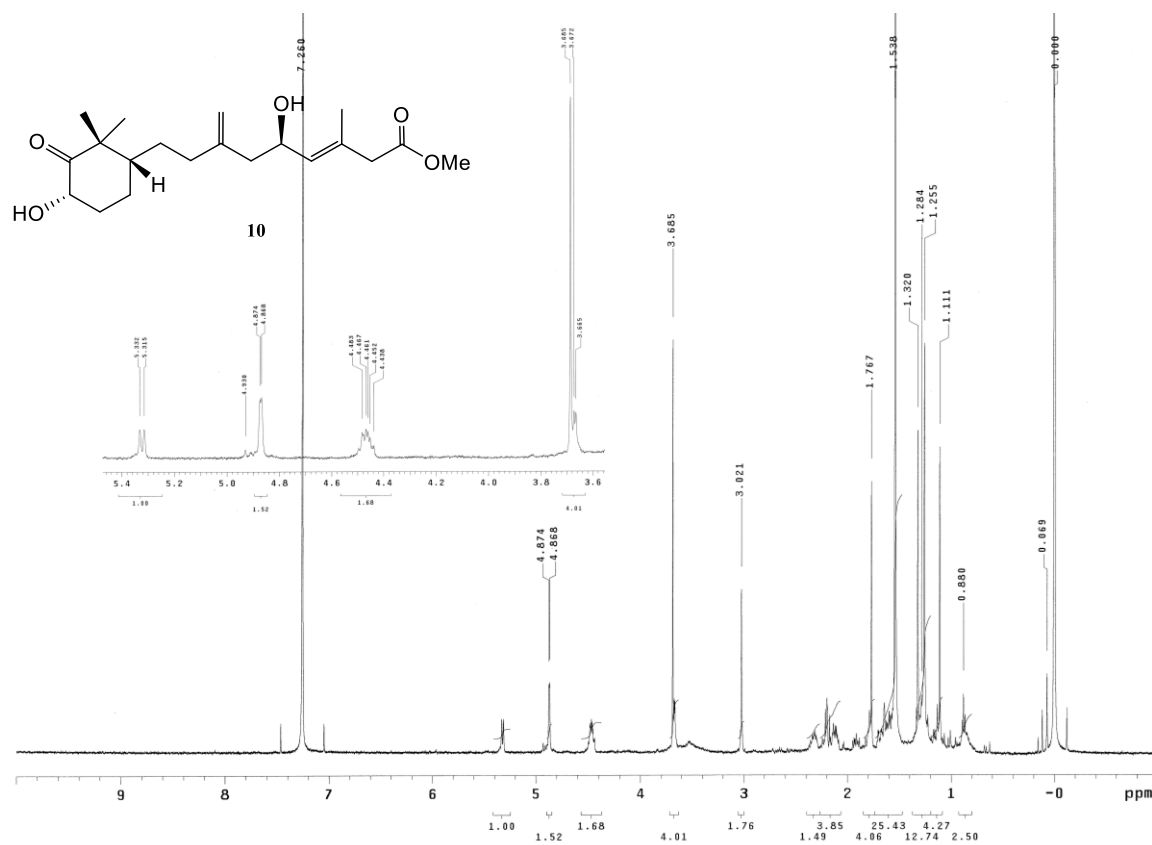


Figure S65. ¹H NMR spectrum of 10 in CDCl₃ at 500 MHz

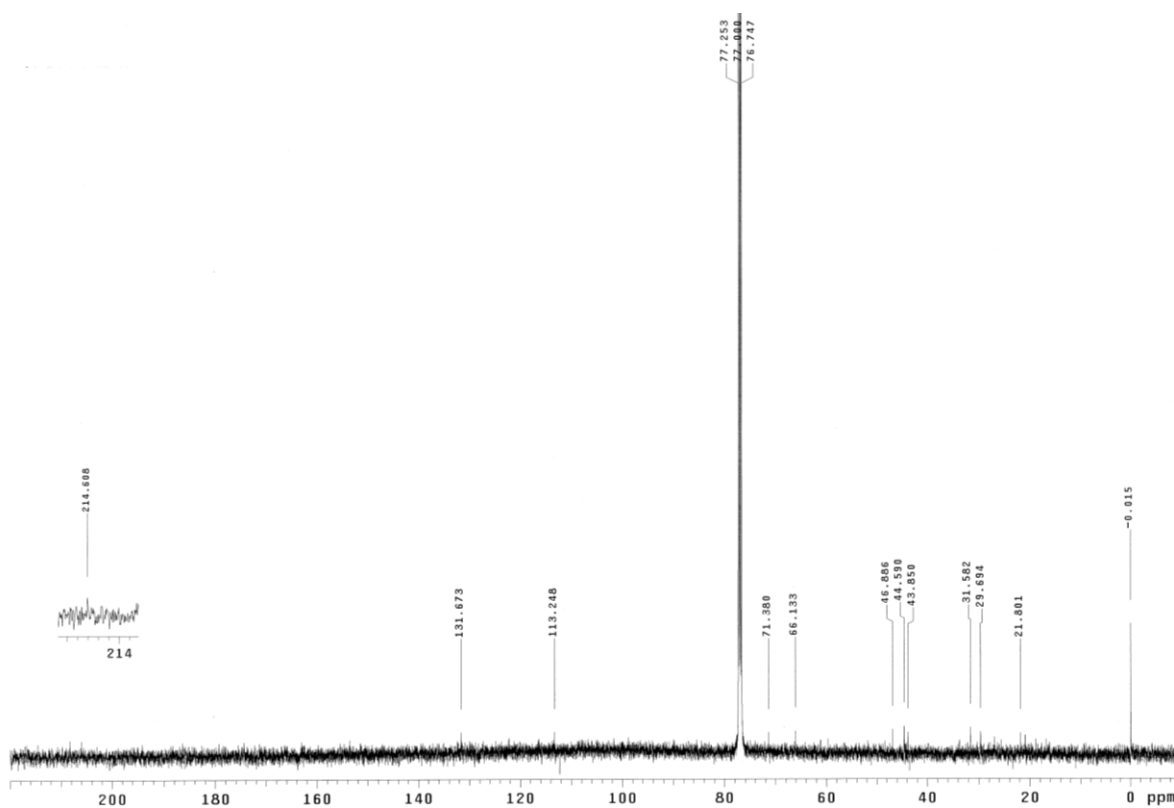


Figure S66. ¹³C NMR spectrum of 10 in CDCl₃ at 125 MHz

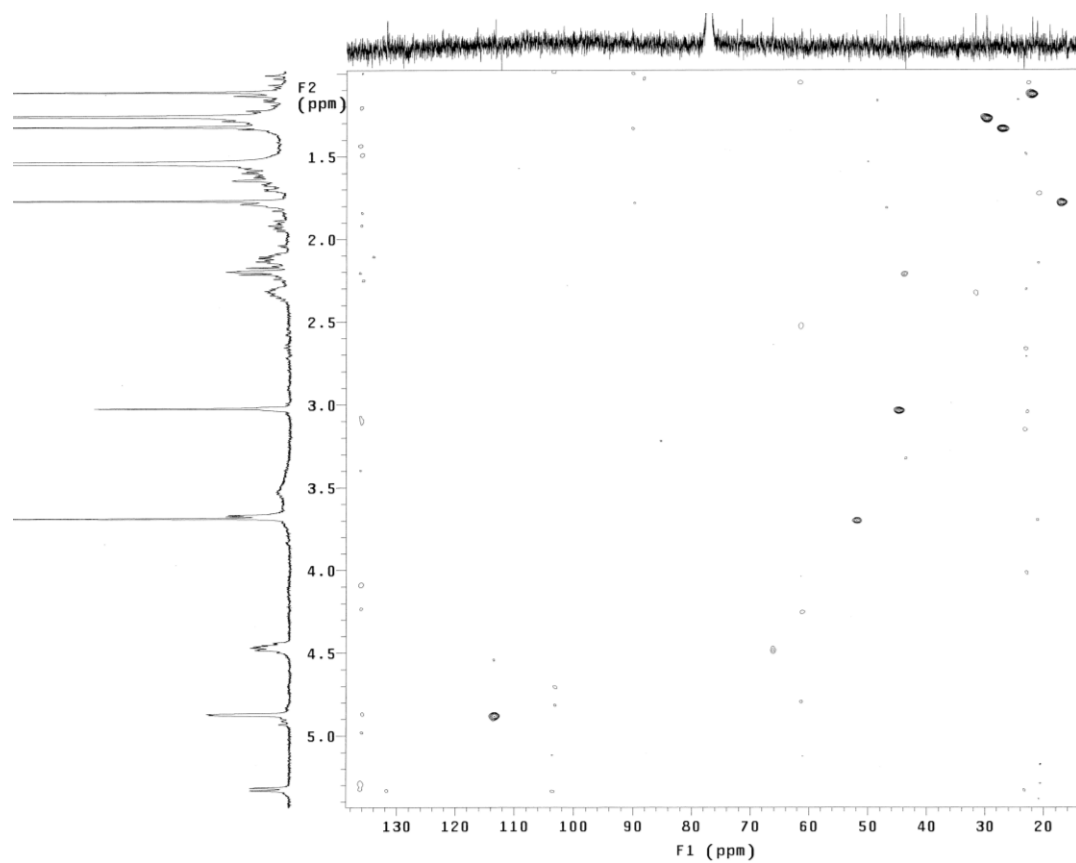


Figure S67. HSQC spectrum of **10** in CDCl_3

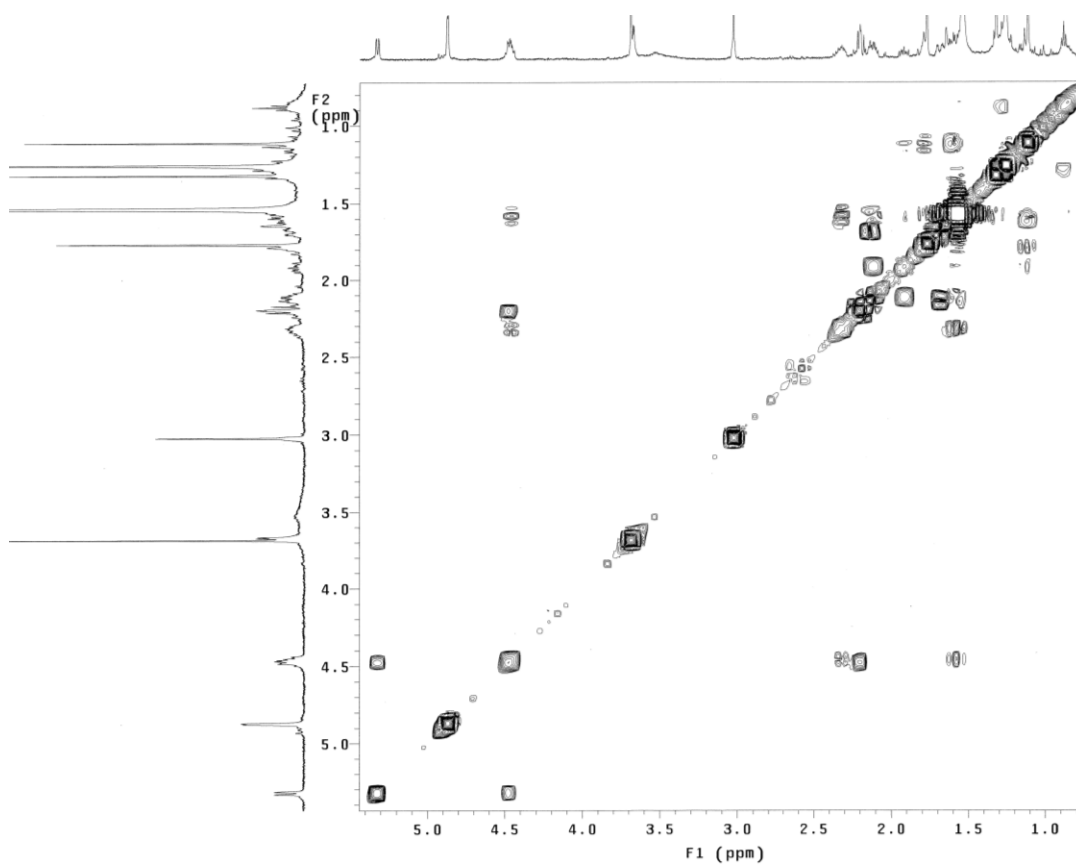


Figure S68. COSY spectrum of **10** in CDCl_3

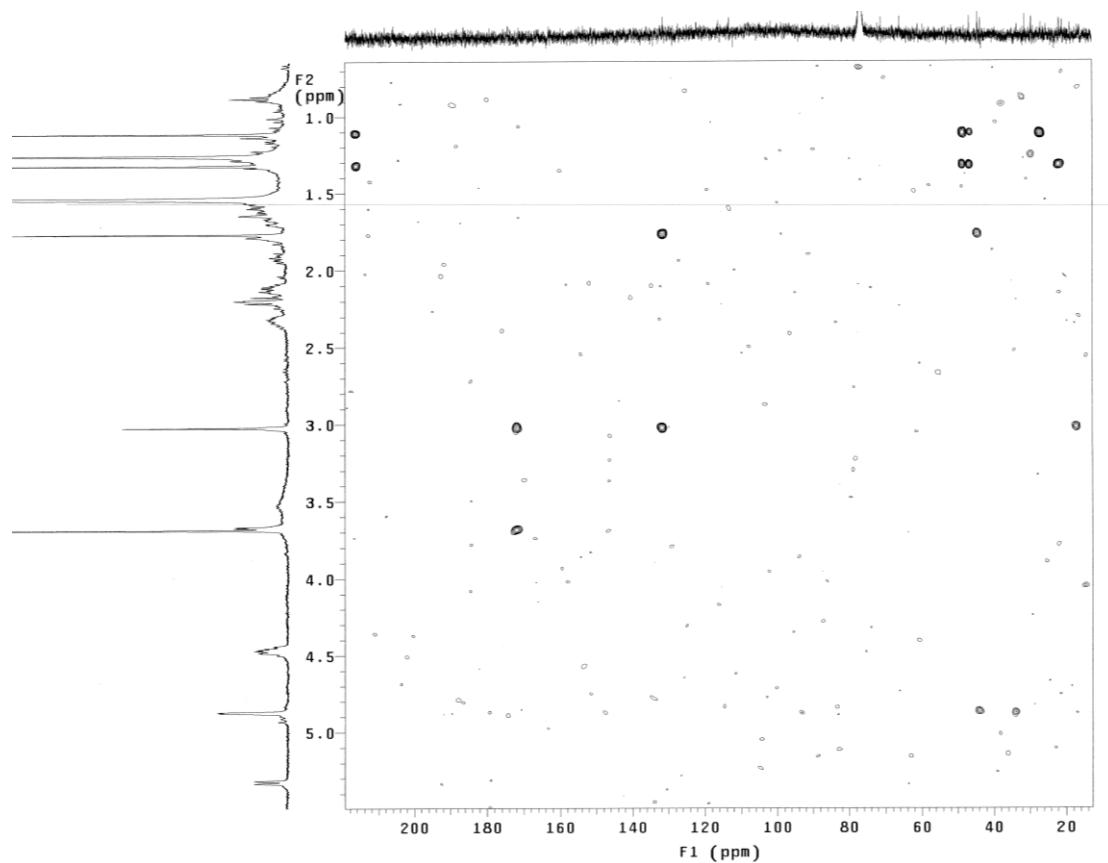


Figure S69. HMBC spectrum of **10** in CDCl₃

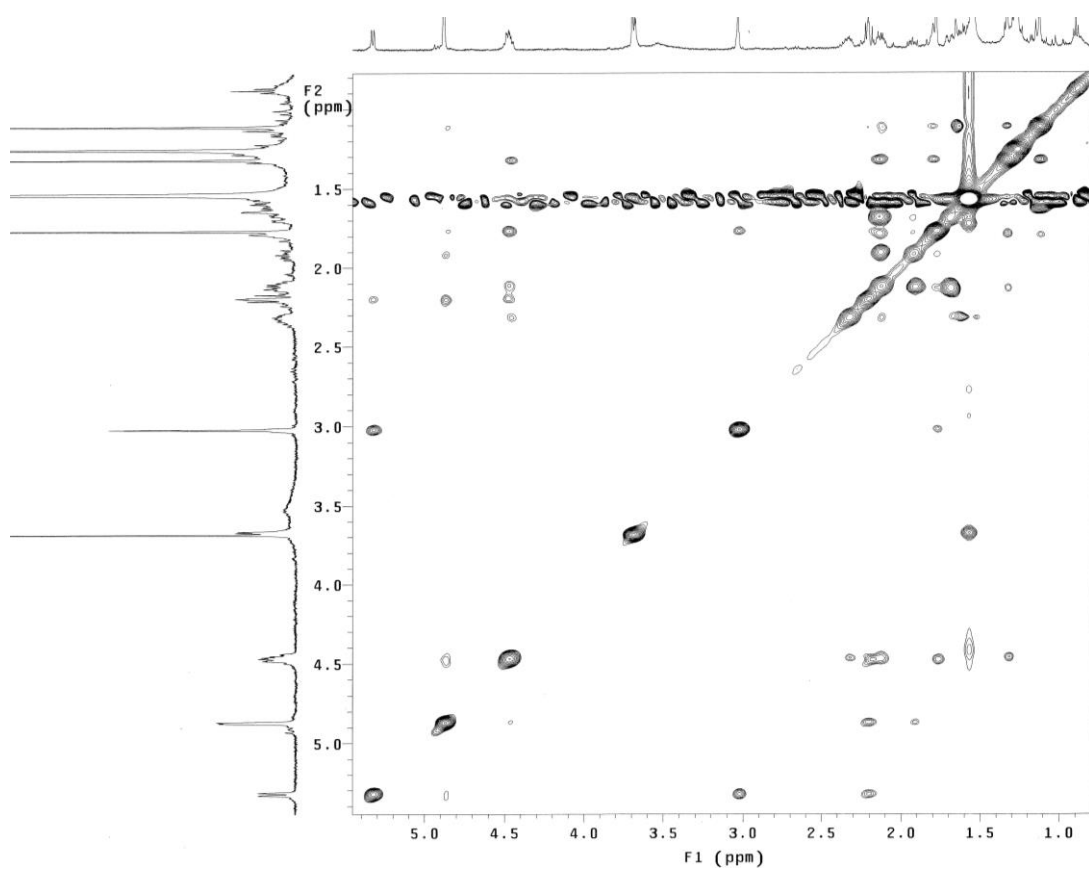


Figure S70. NOESY spectrum of **10** in CDCl₃

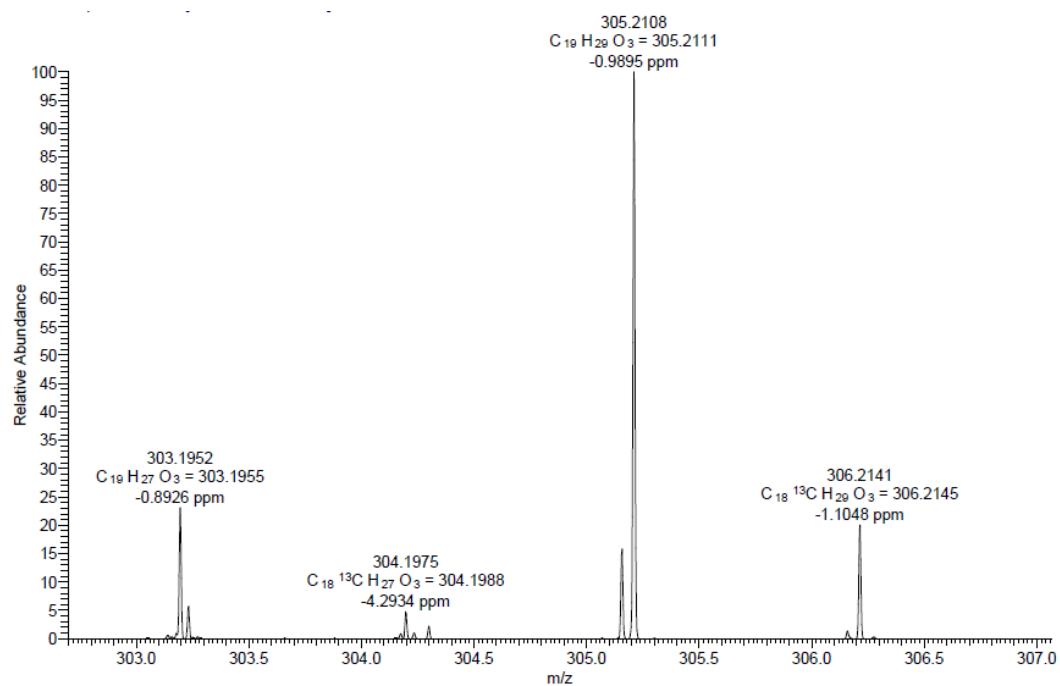


Figure S71. HRESIMS spectrum of **11**

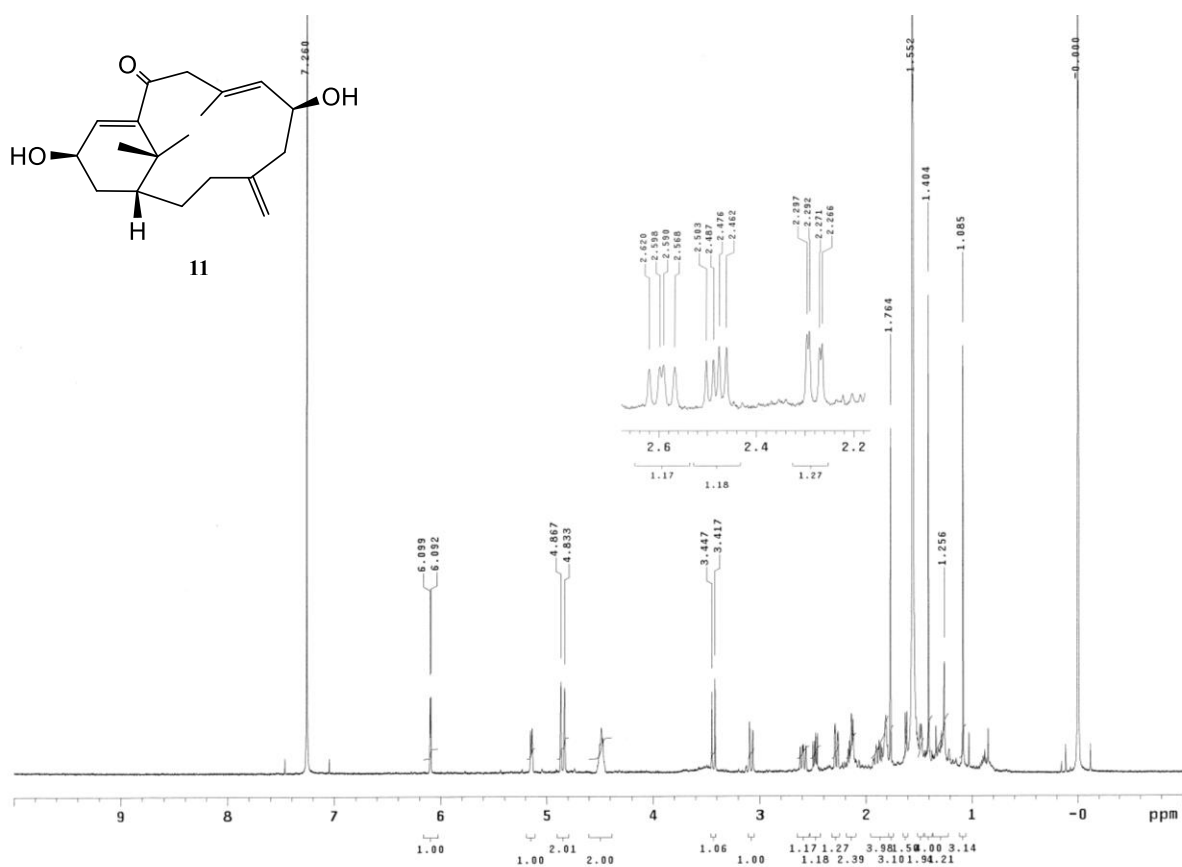


Figure S72. 1H NMR spectrum of **11** in $CDCl_3$ at 500 MHz

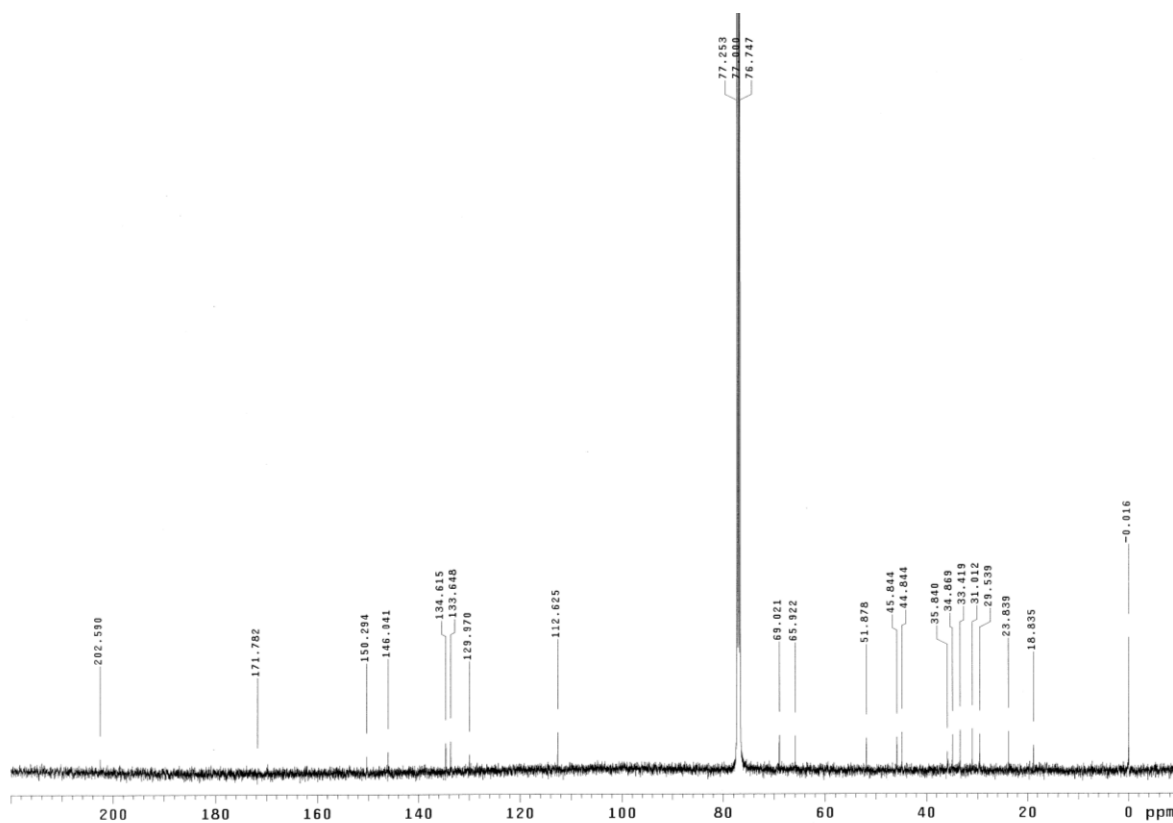


Figure S73. ¹³C NMR spectrum of **11** in CDCl₃ at 125 MHz

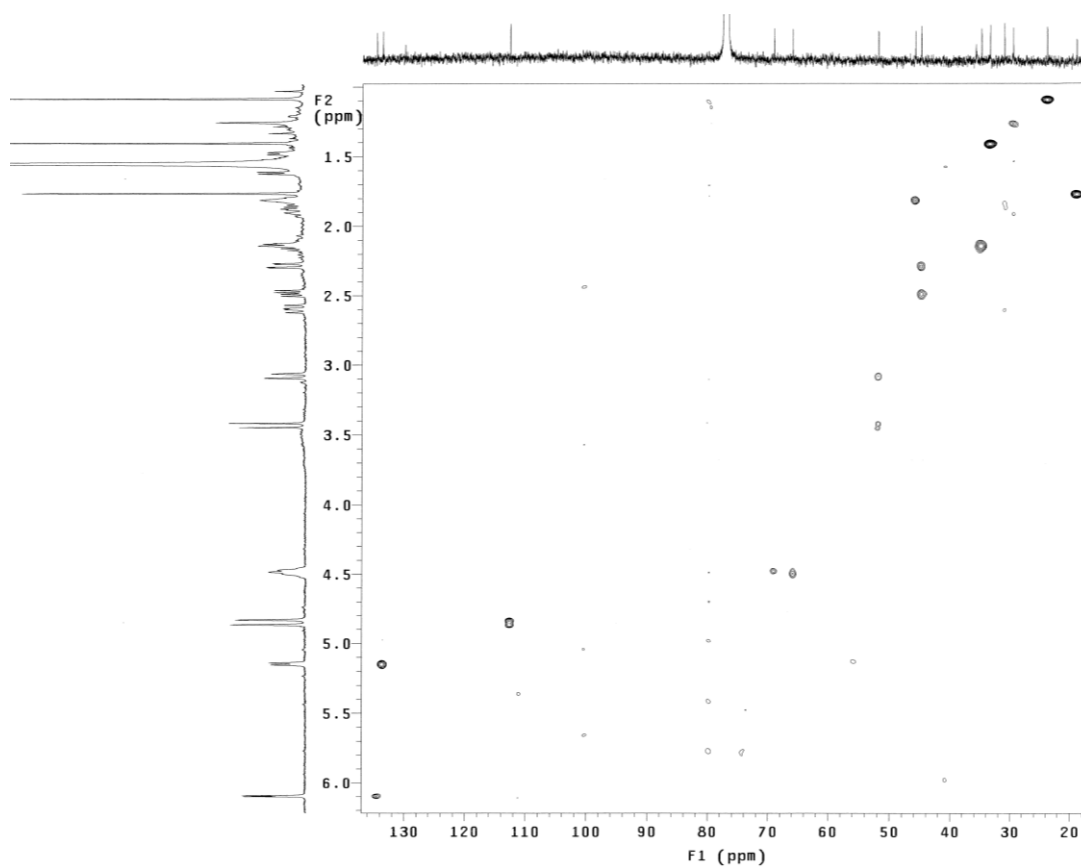


Figure S74. HSQC spectrum of **11** in CDCl₃

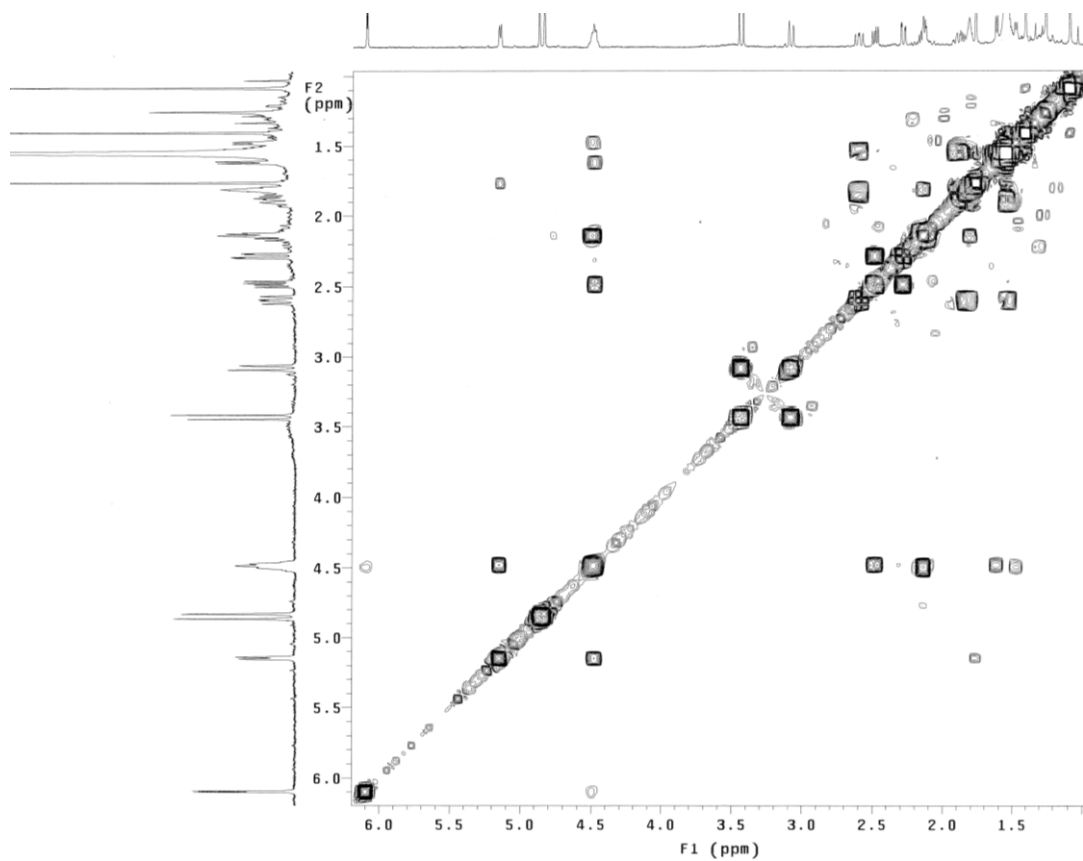


Figure S75. COSY spectrum of **11** in CDCl₃

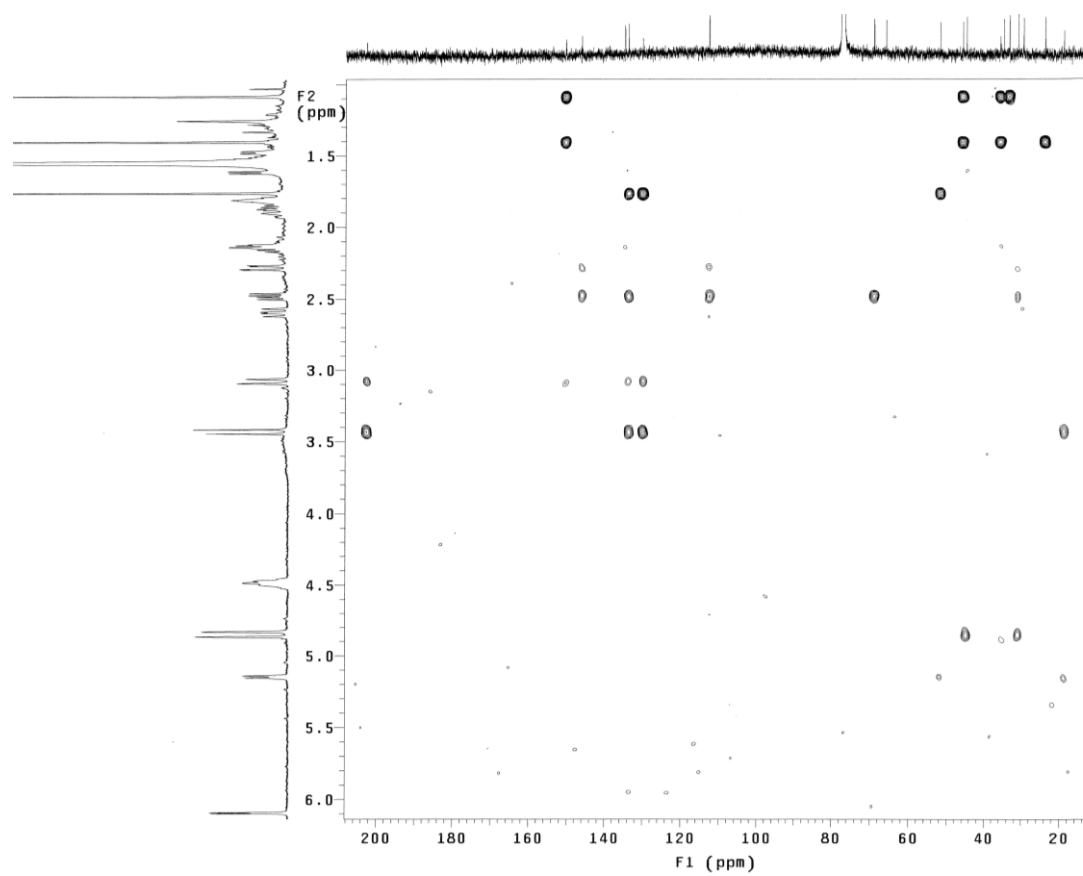


Figure S76. HMBC spectrum of **11** in CDCl₃

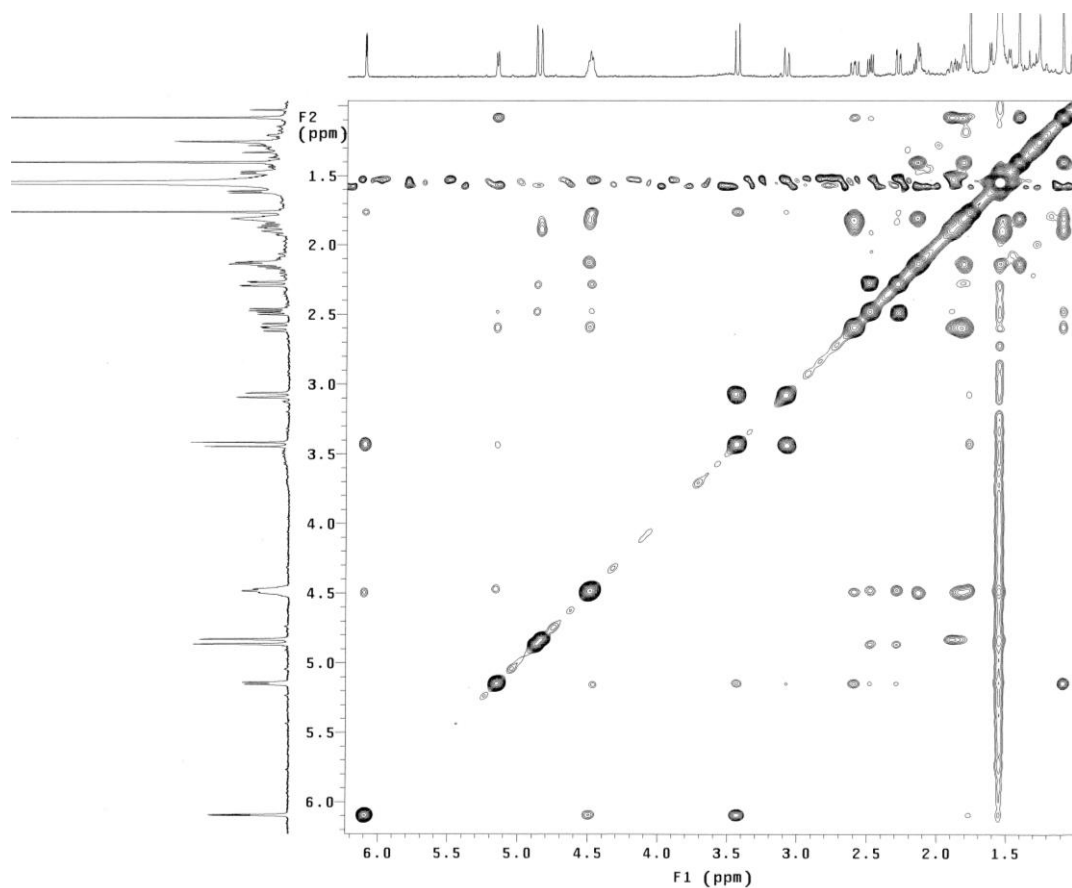
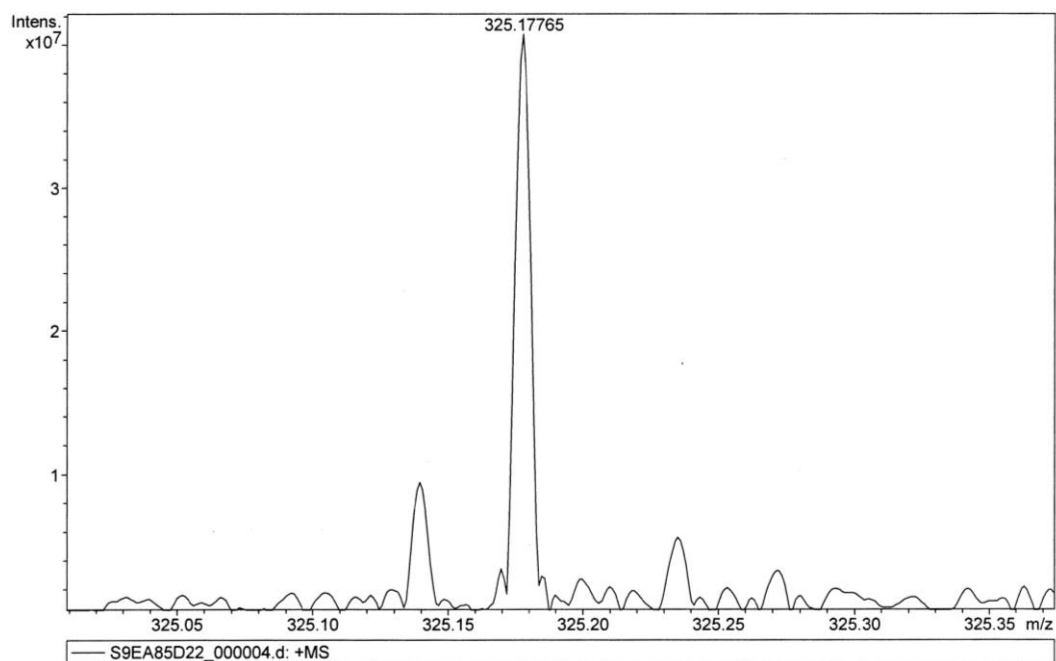


Figure S77. NOESY spectrum of **11** in CDCl_3



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
325.17765	1	C ₁₉ H ₂₆ NaO ₃	100.00	325.17742	-0.24	-0.73	15.1	6.5	even	ok

Figure S78. HRESIMS spectrum of **12**

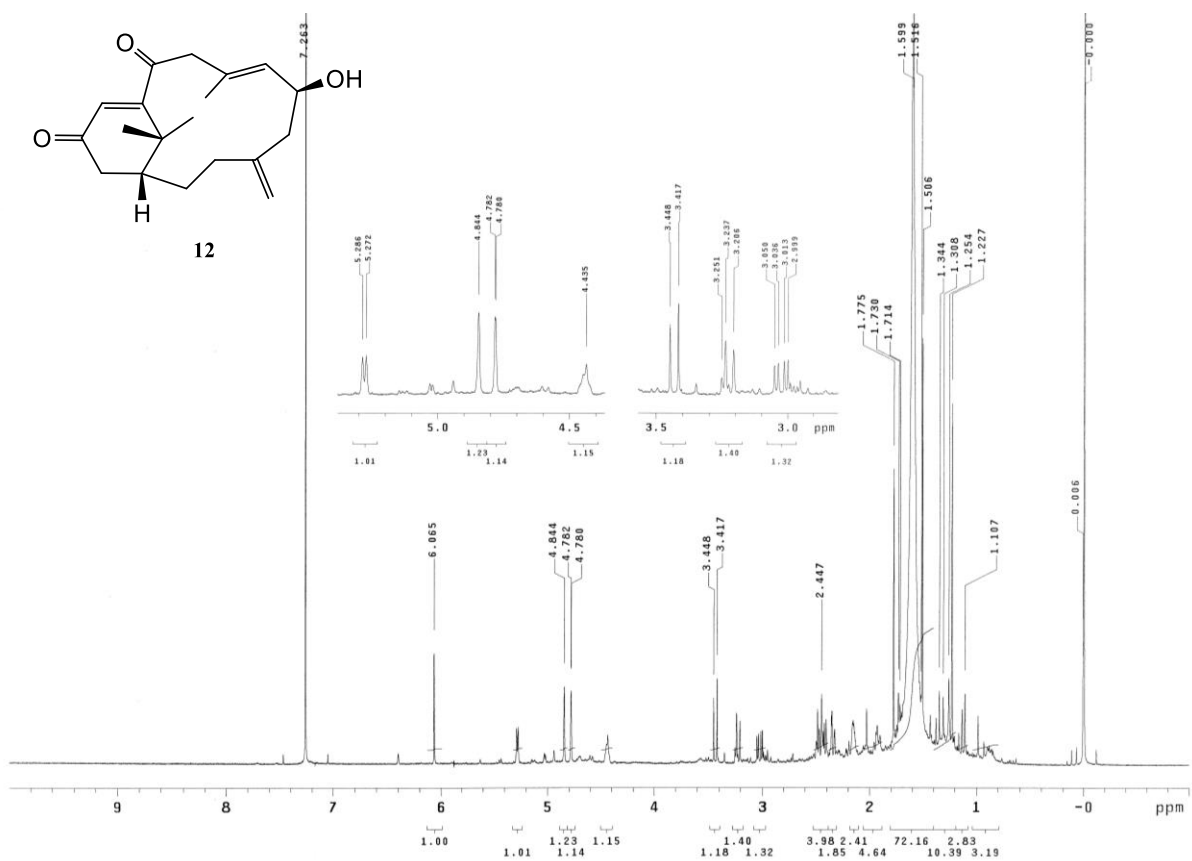


Figure S79. ¹H NMR spectrum of 12 in CDCl₃ at 500 MHz

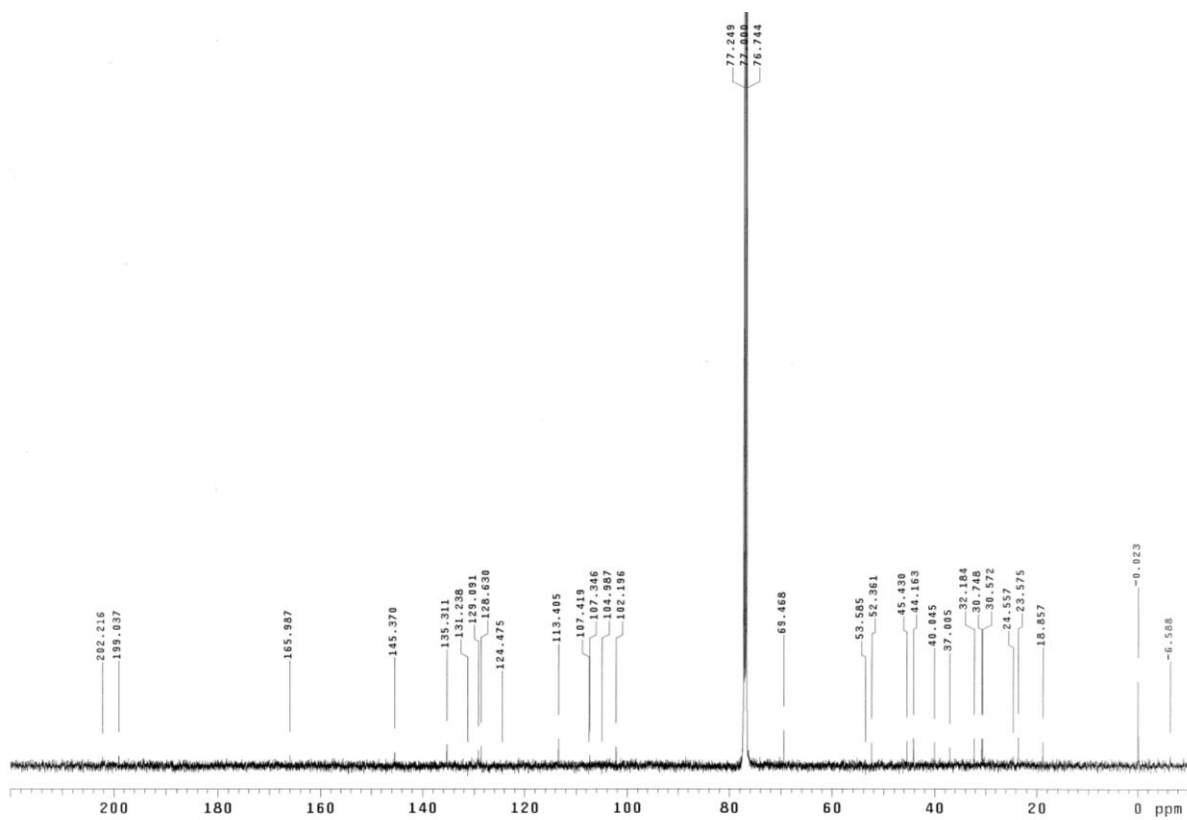


Figure S80. ¹³C NMR spectrum of 12 in CDCl₃ at 125 MHz

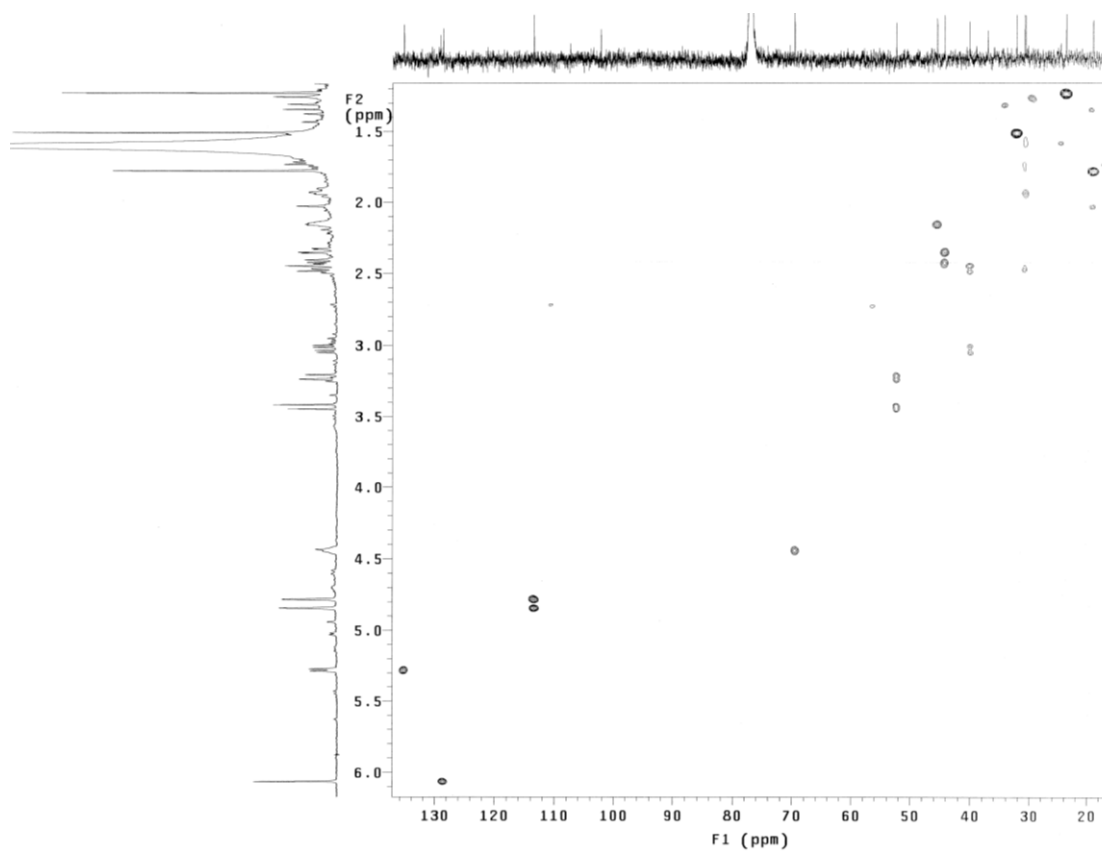


Figure S81. HSQC spectrum of **12** in CDCl₃

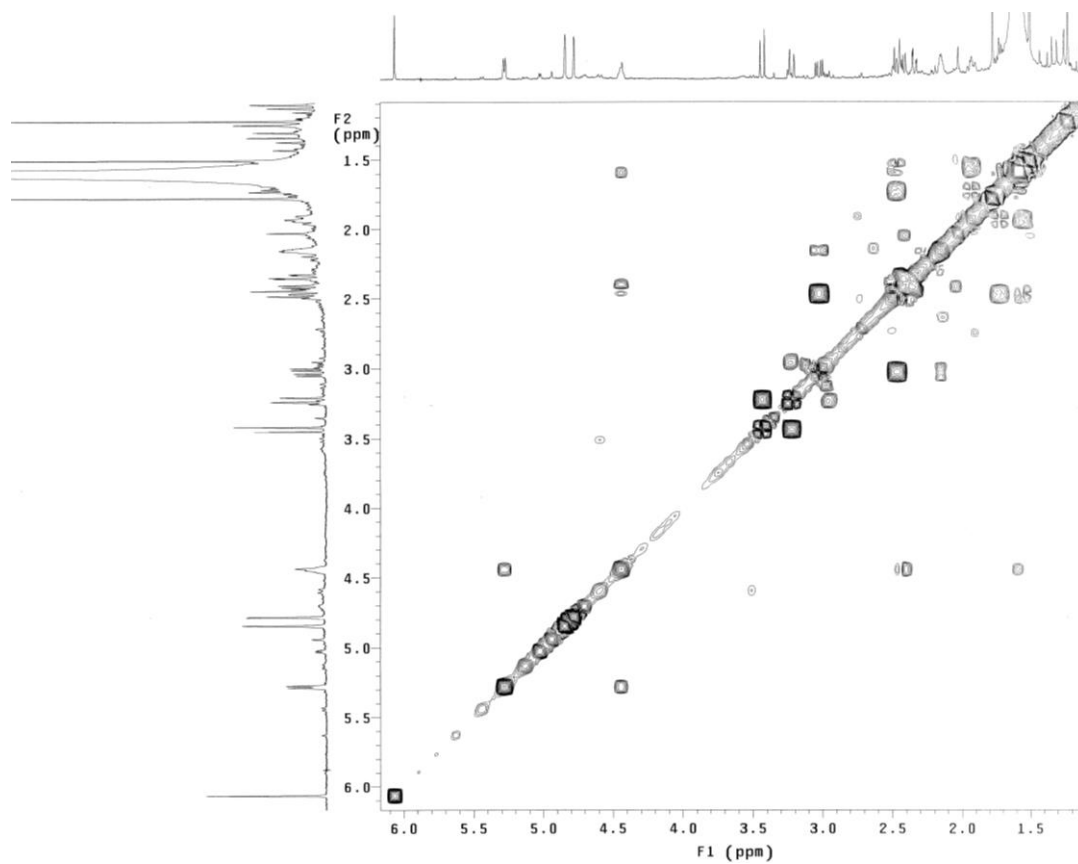


Figure S82. COSY spectrum of **12** in CDCl₃

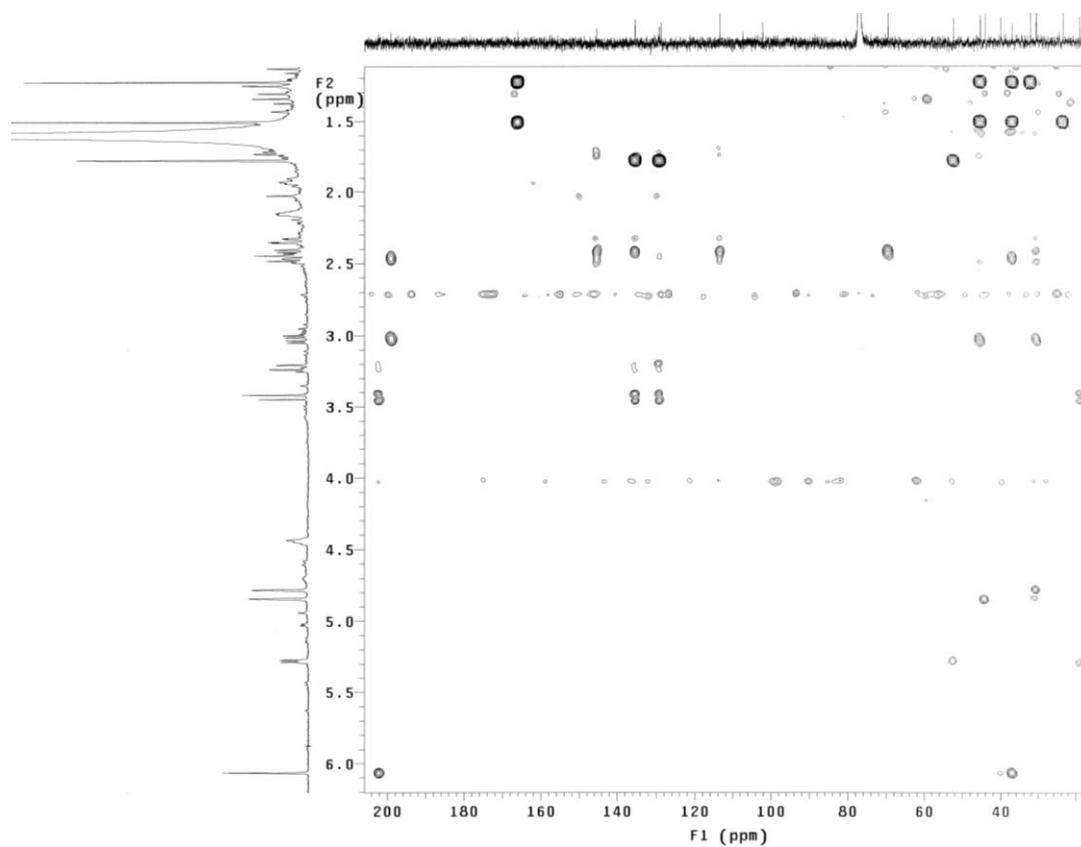


Figure S83. HMBC spectrum of **12** in CDCl_3

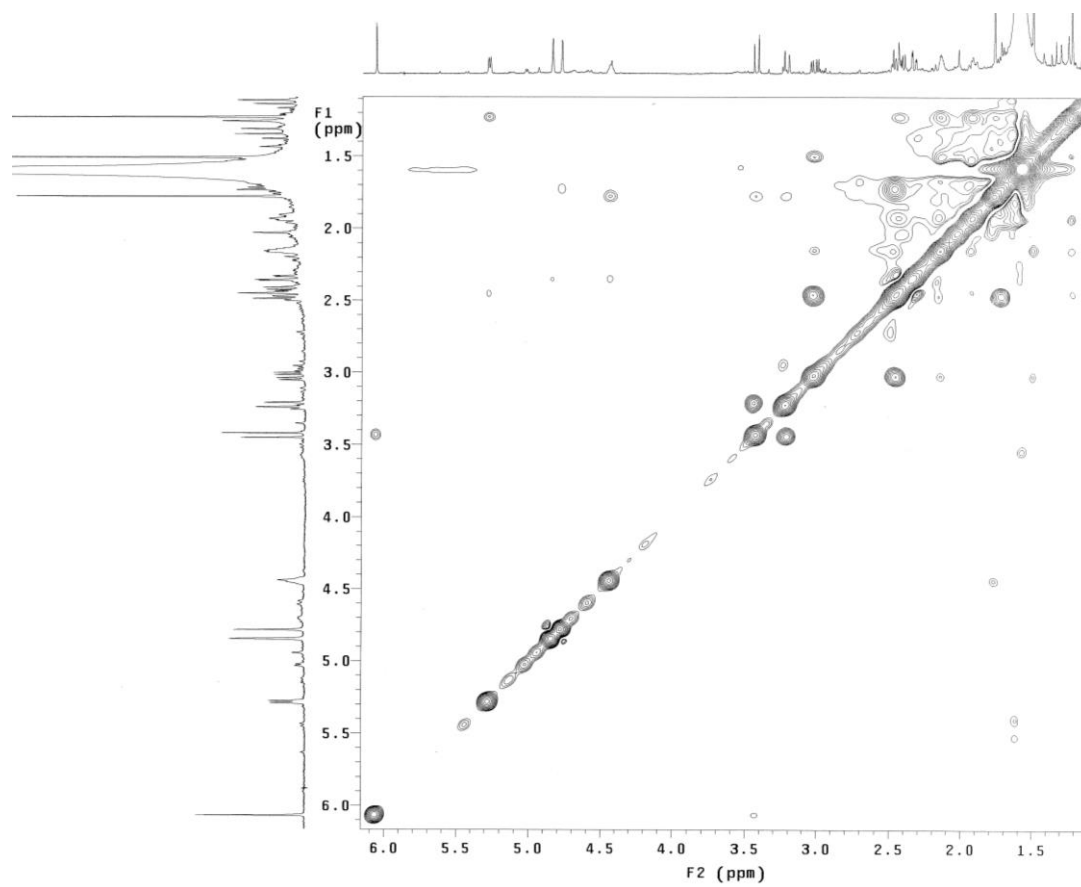


Figure S84. NOESY spectrum of **12** in CDCl_3

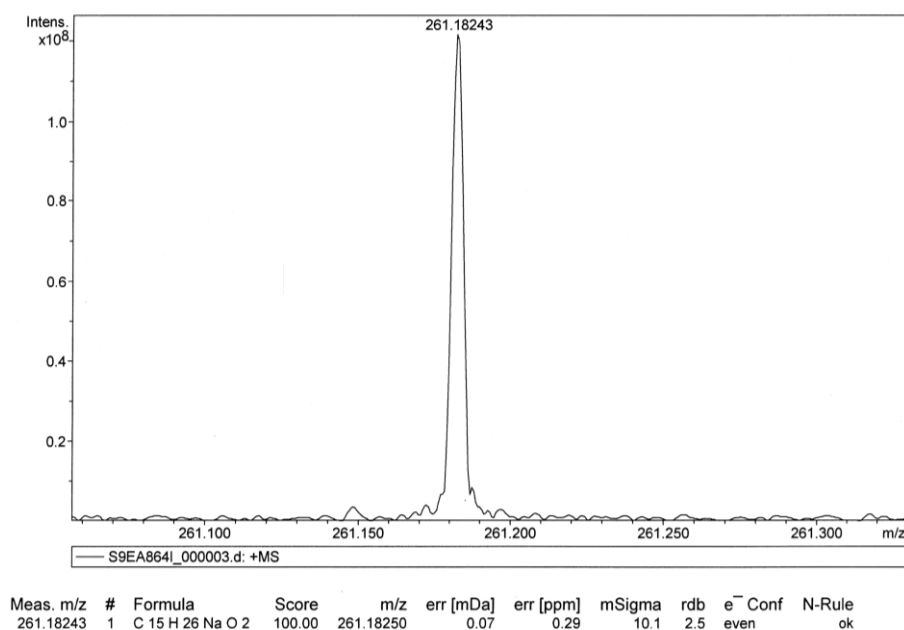


Figure S85. HRESIMS spectrum of **13**

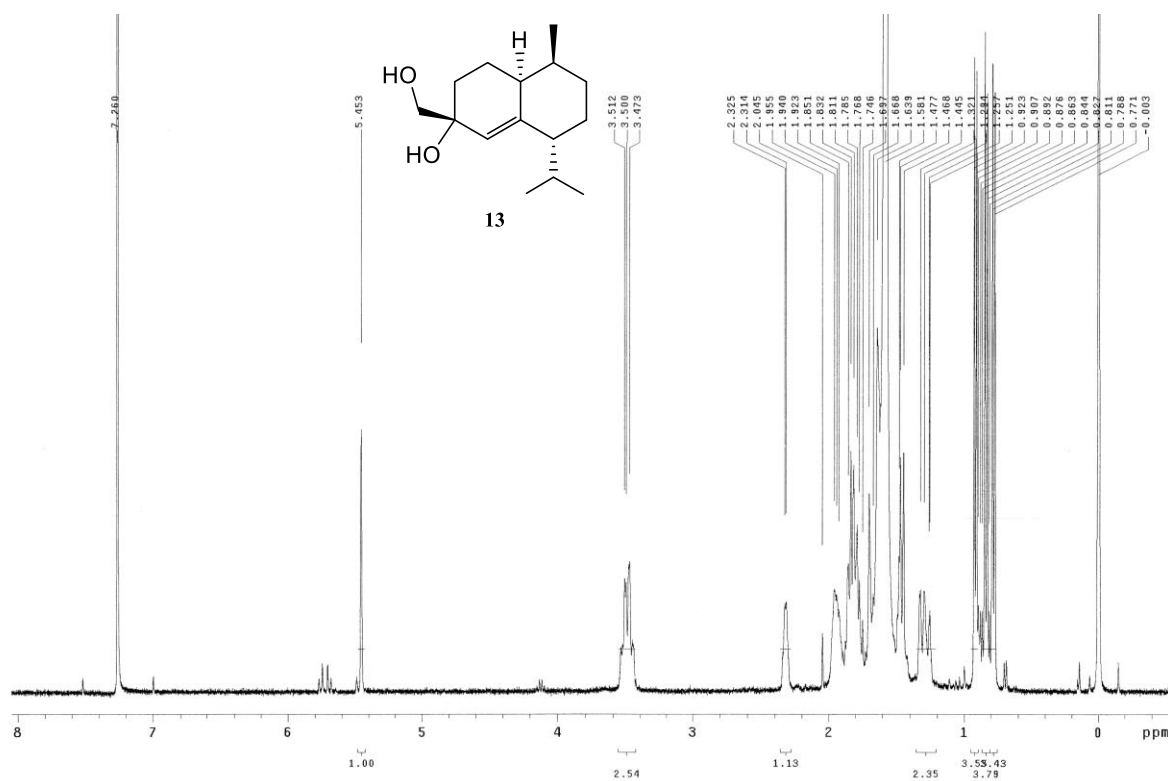


Figure S86. ¹H NMR spectrum of **13** in CDCl₃ at 400 MHz

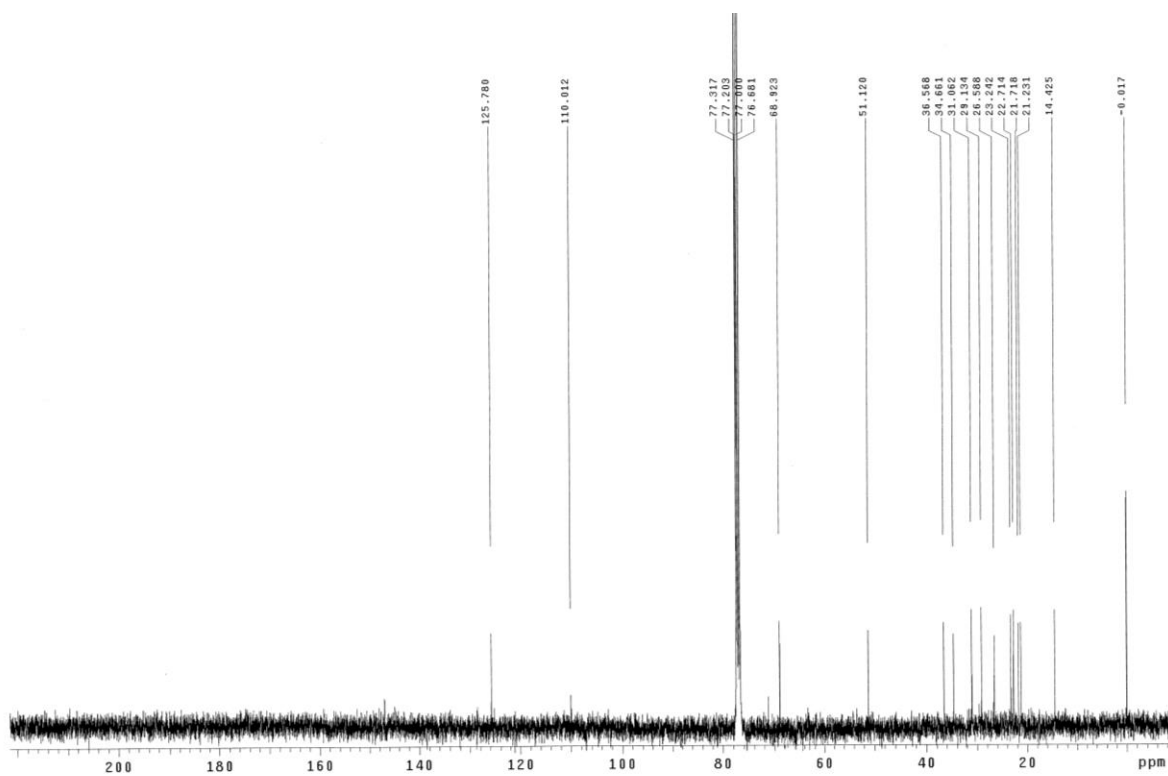


Figure S87. ^{13}C NMR spectrum of **13** in CDCl_3 at 100 MHz

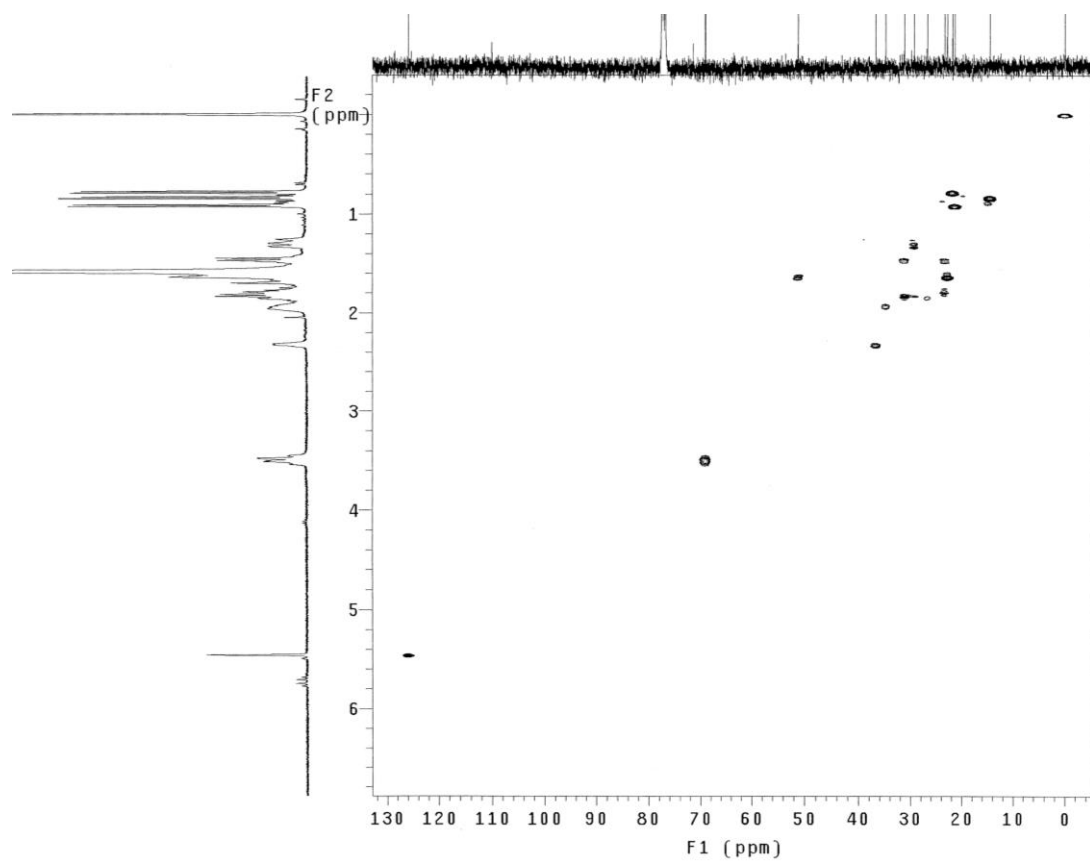


Figure S88. HSQC spectrum of **13** in CDCl_3

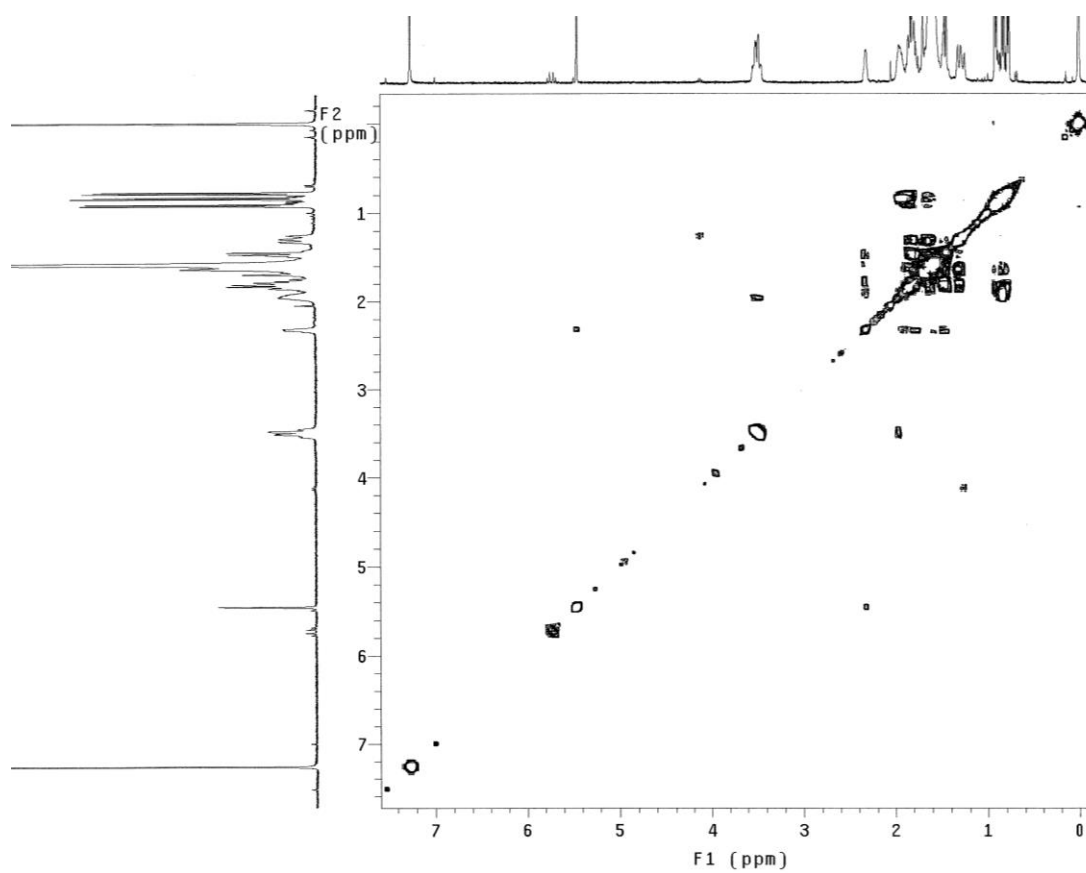


Figure S89. COSY spectrum of **13** in CDCl_3

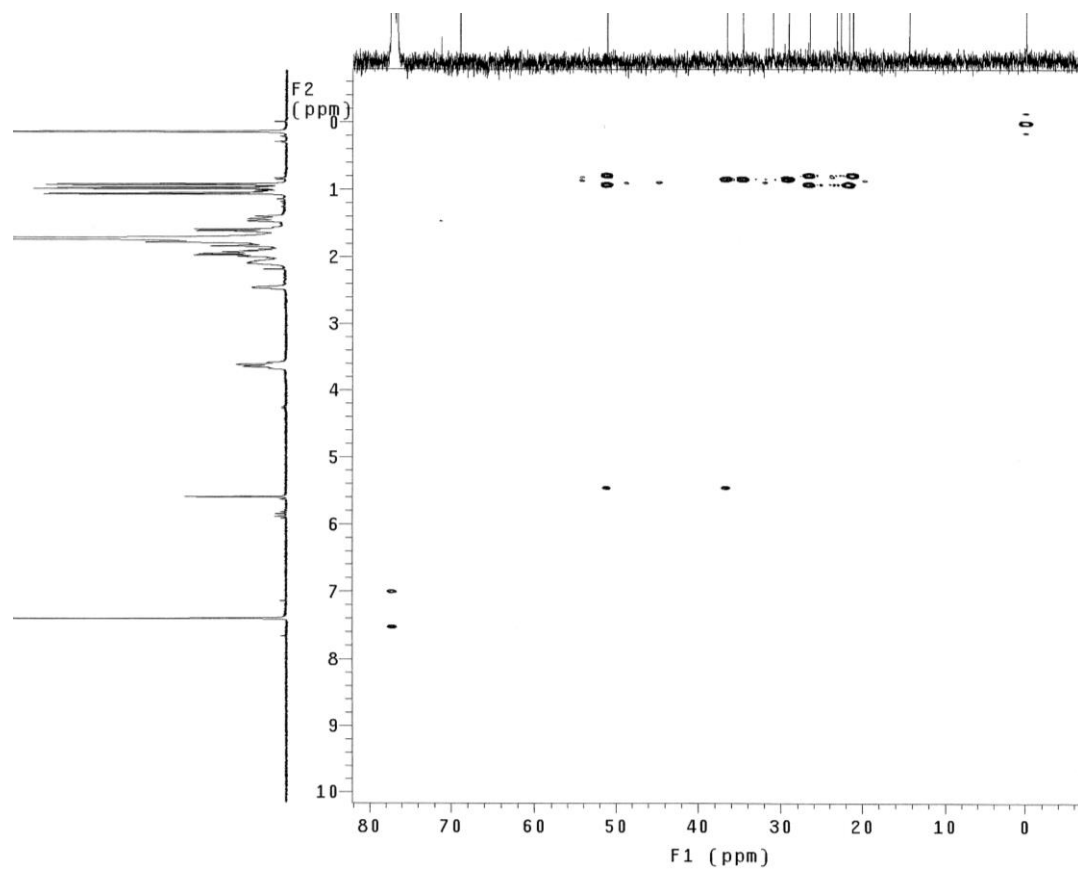


Figure S90. HMBC spectrum of **13** in CDCl_3

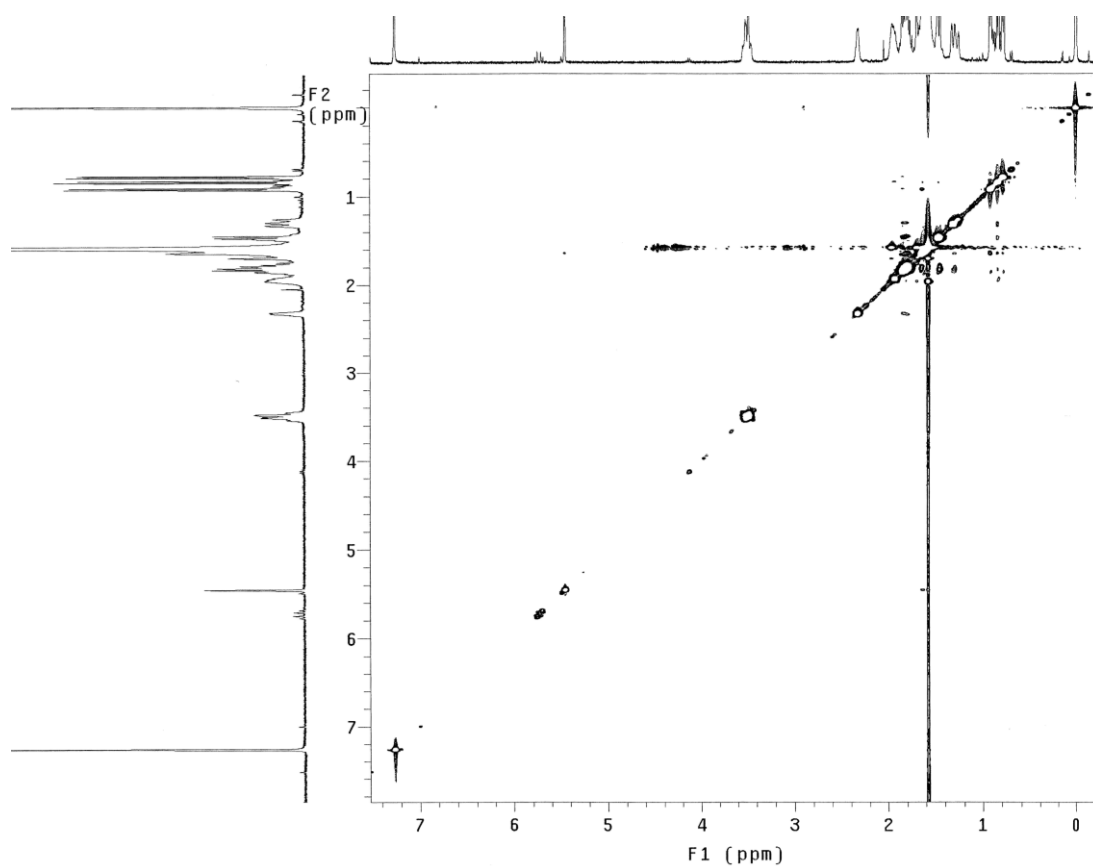


Figure S91. NOESY spectrum of **13** in CDCl_3

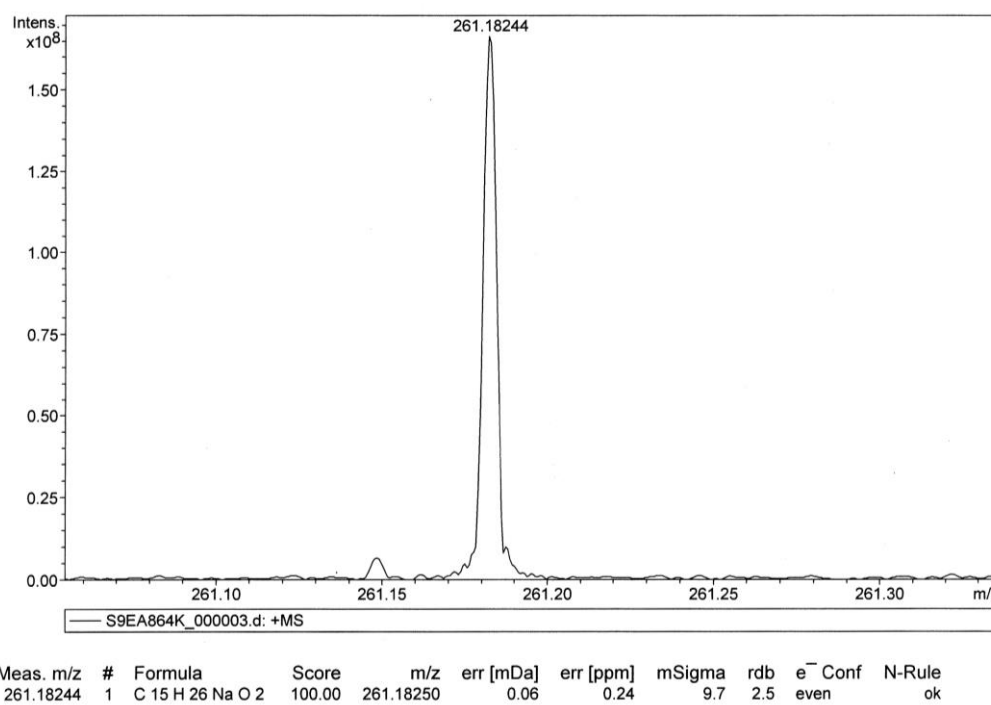


Figure S92. HRESIMS spectrum of **14**

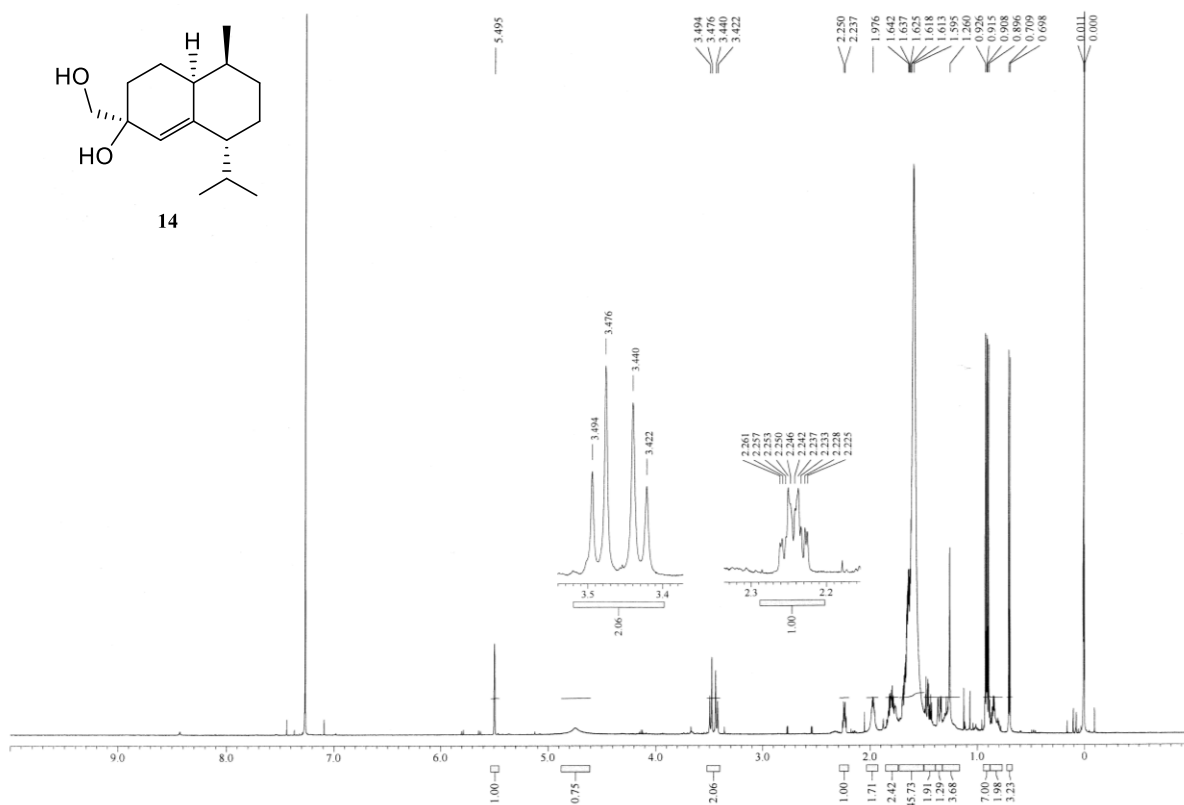


Figure S93. ¹H NMR spectrum of **14** in CDCl₃ at 600 MHz

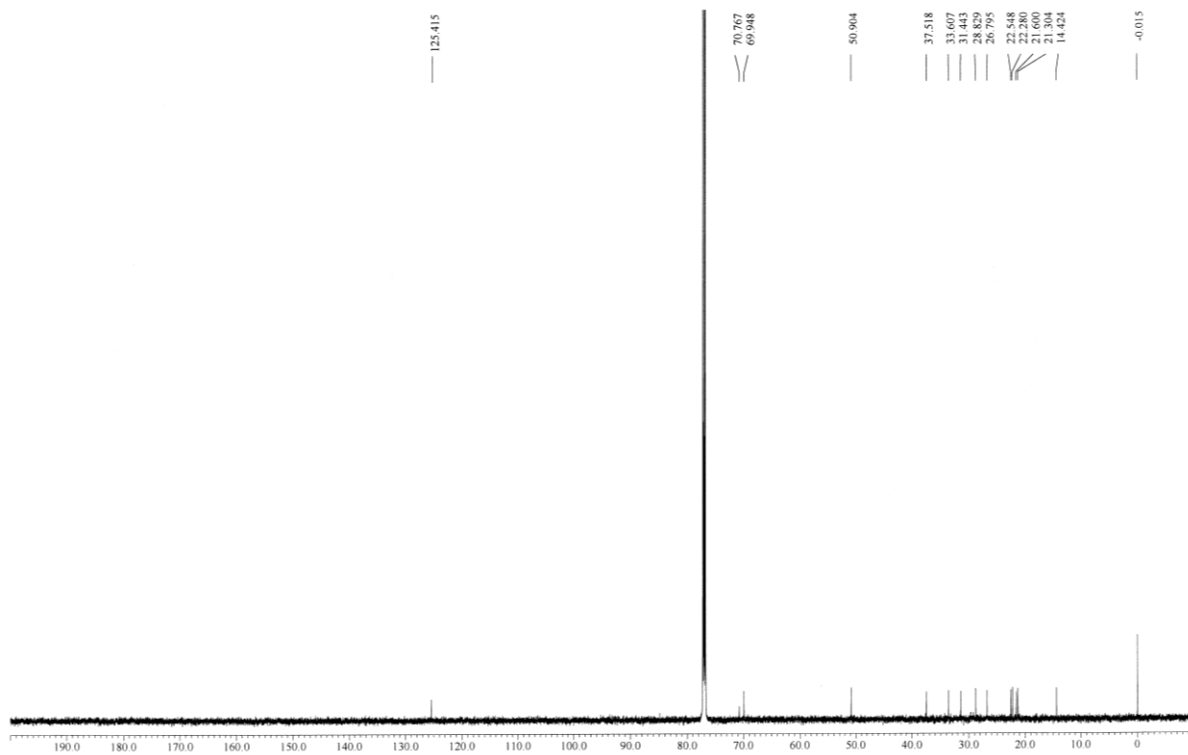


Figure S94. ¹³C NMR spectrum of **14** in CDCl₃ at 150 MHz

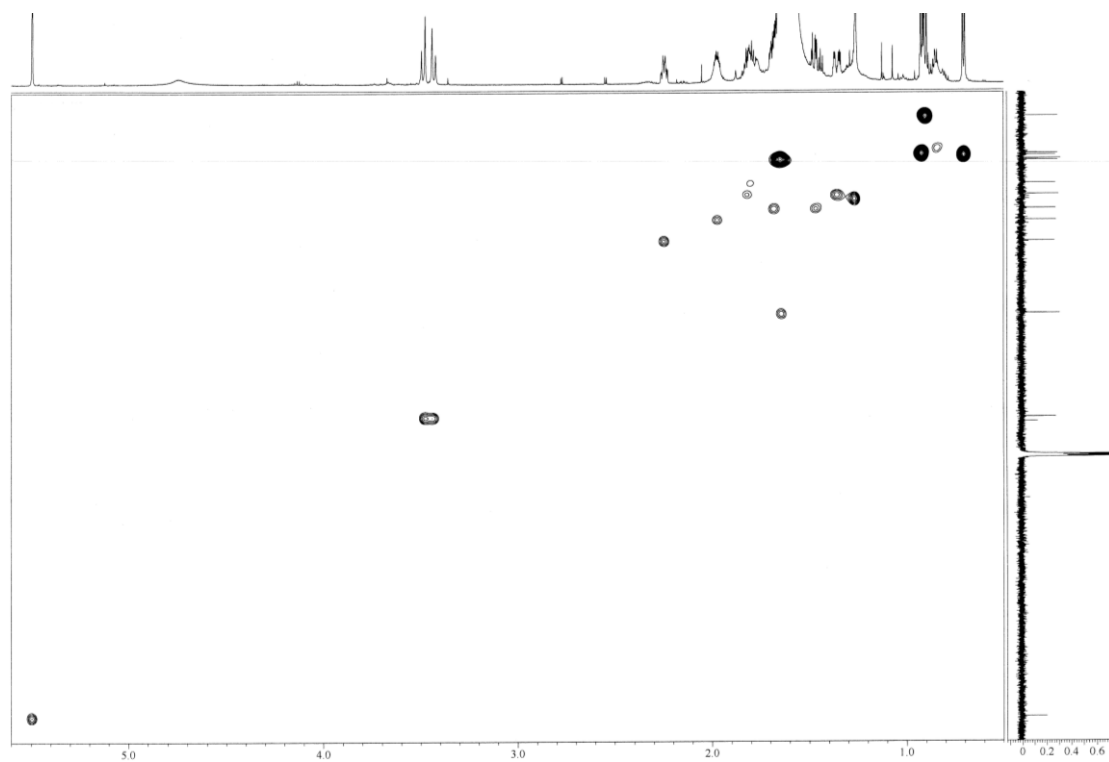


Figure S95. HSQC spectrum of **14** in CDCl₃

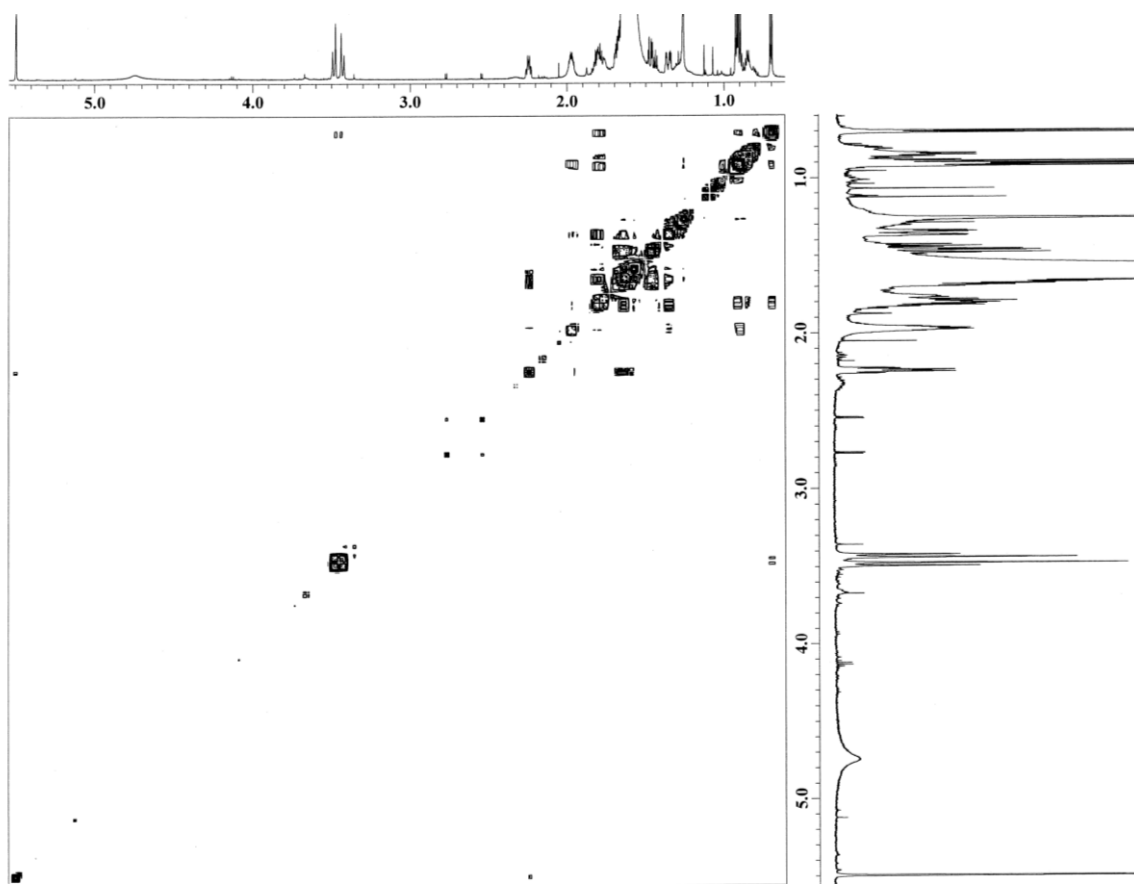


Figure S96. COSY spectrum of **14** in CDCl₃

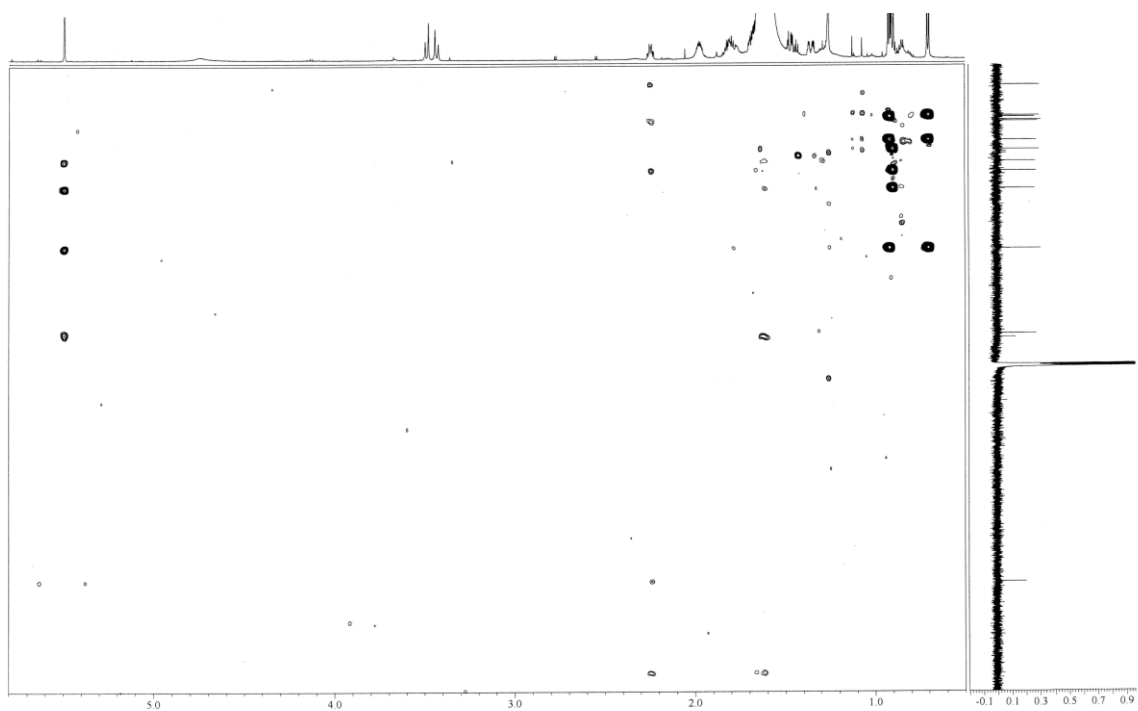


Figure S97. HMBC spectrum of **14** in CDCl₃

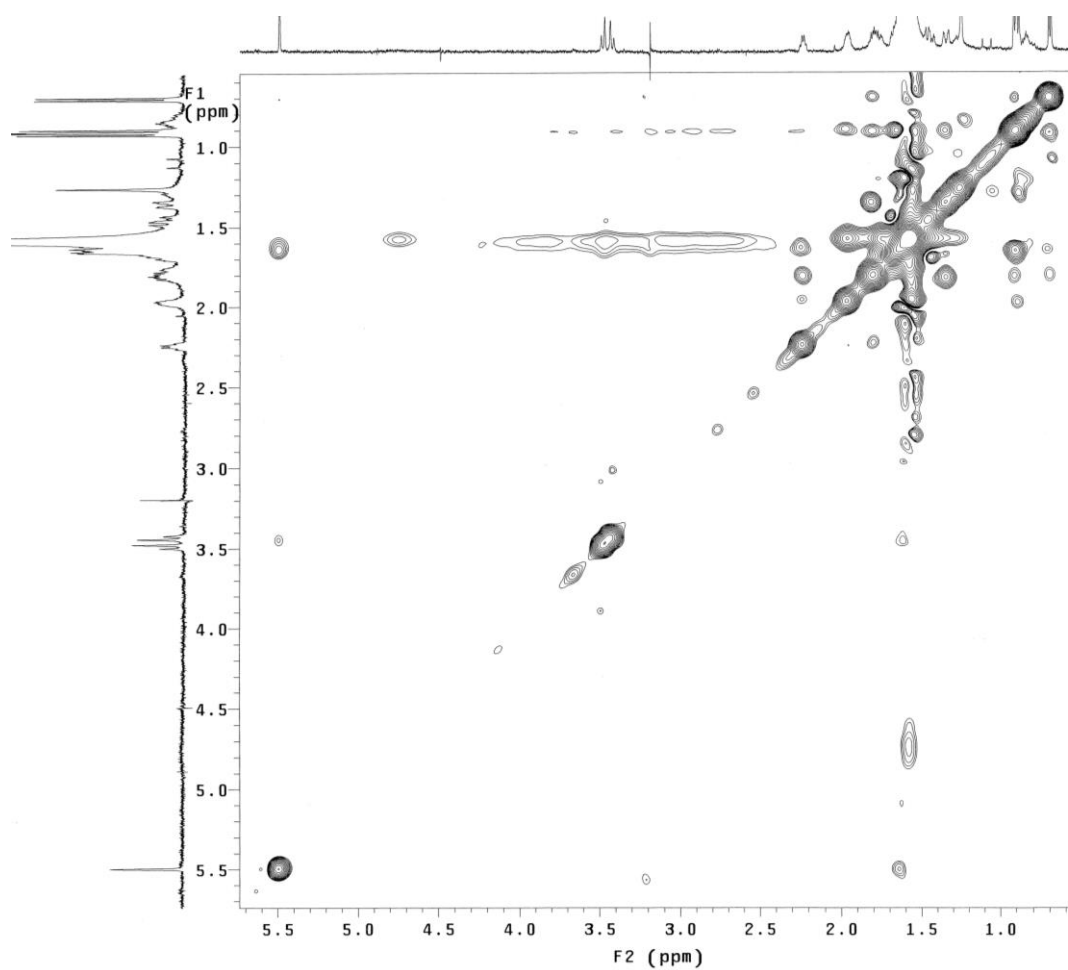


Figure S98. NOESY spectrum of **14** in CDCl₃

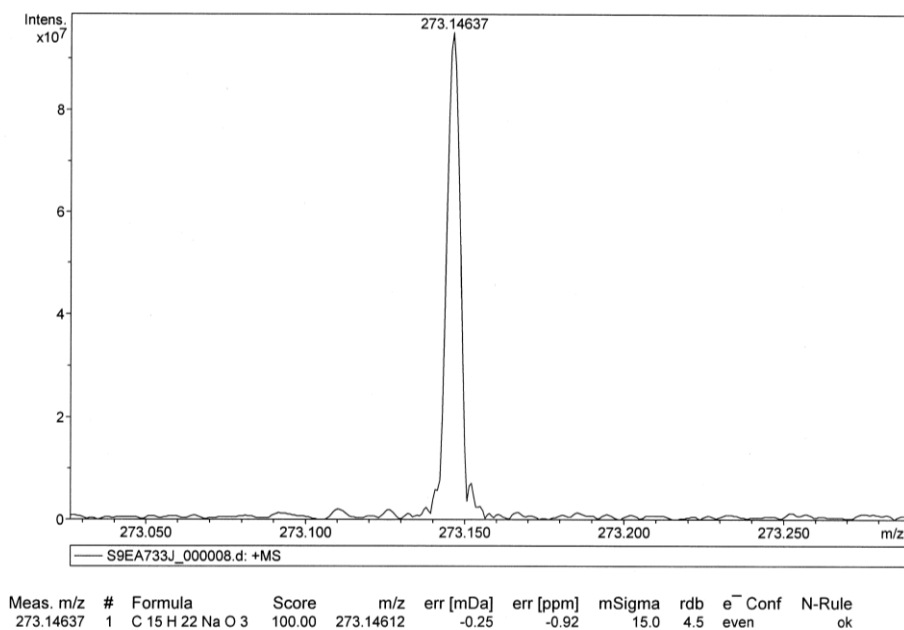


Figure S99. HRESIMS spectrum of **15**

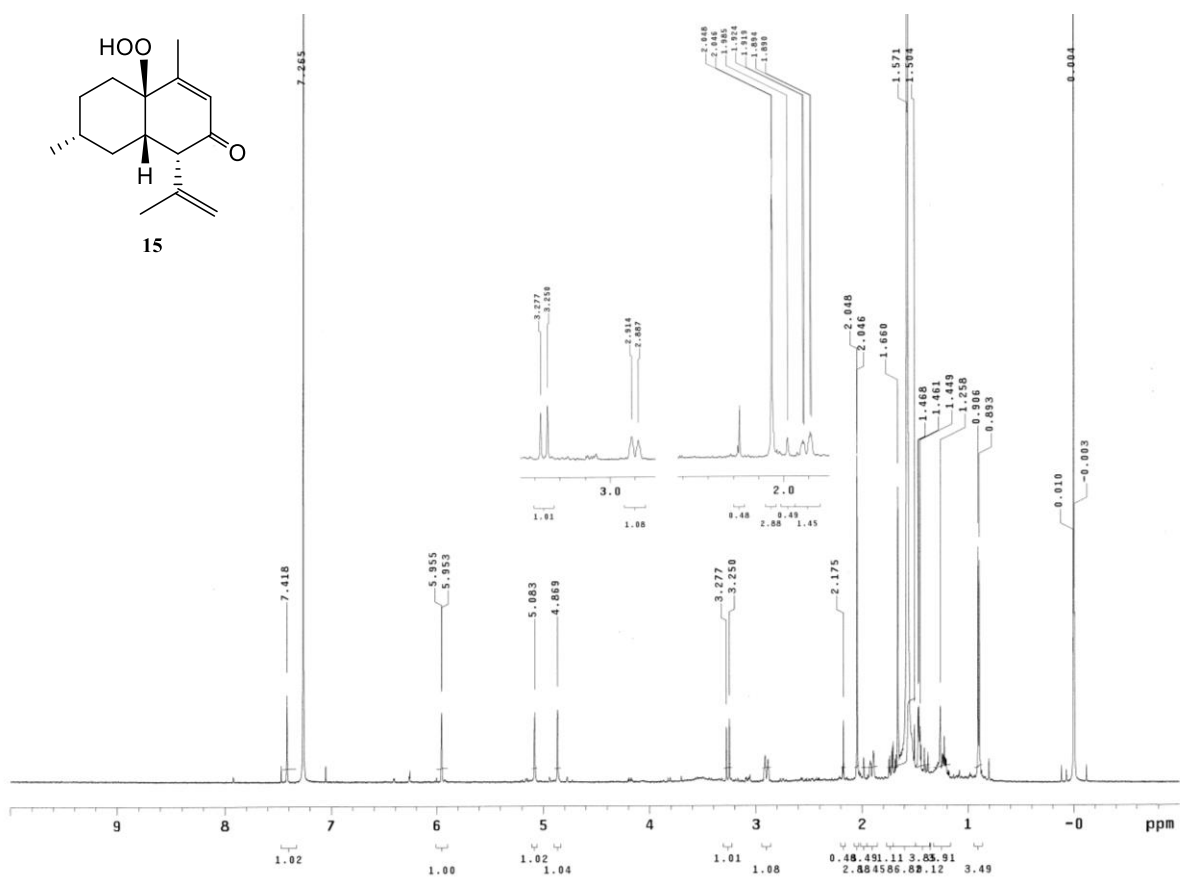


Figure S100. ¹H NMR spectrum of **15** in CDCl₃ at 500 MHz

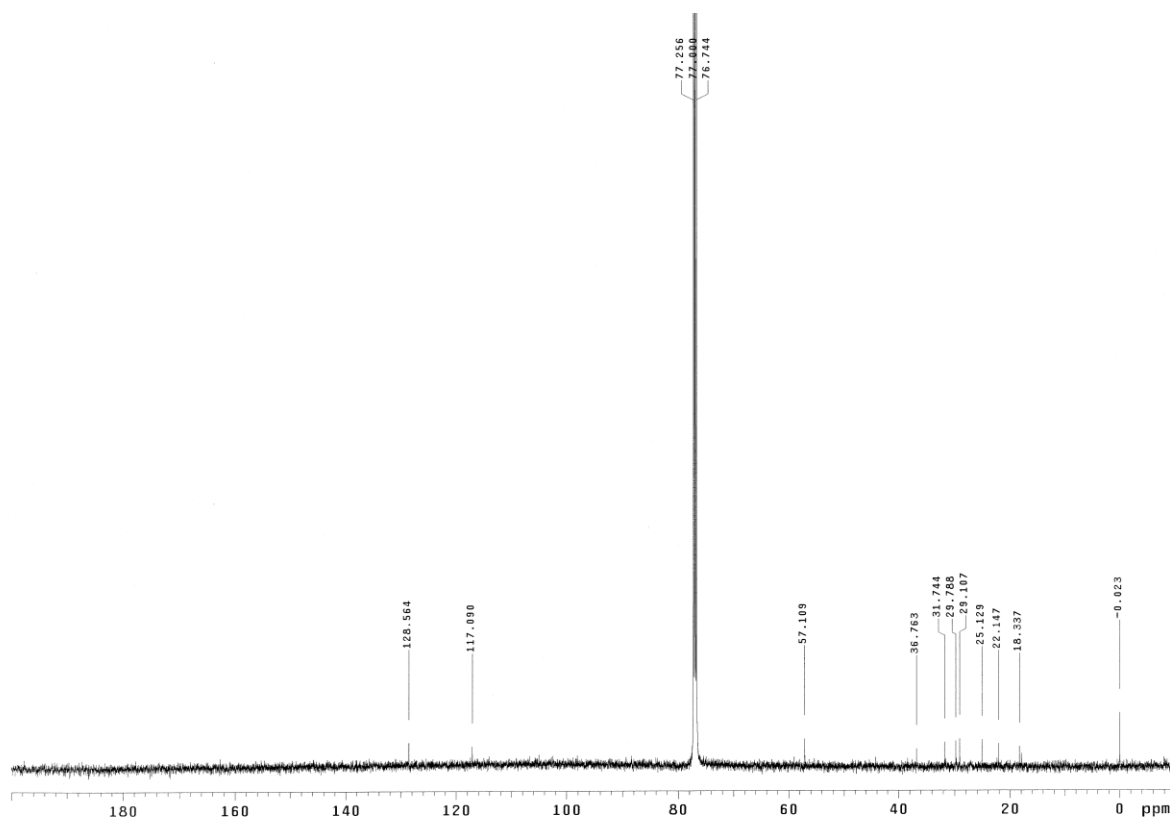


Figure S101. ^{13}C NMR spectrum of **15** in CDCl_3 at 125 MHz

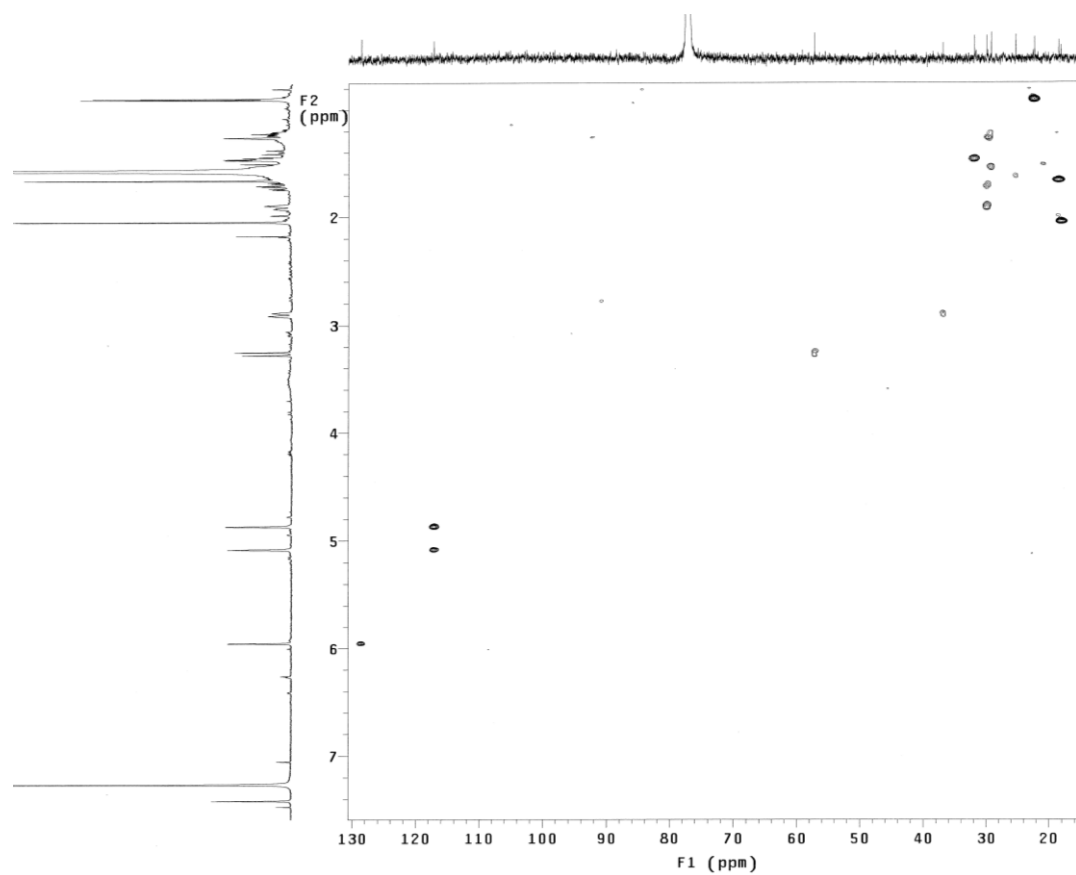


Figure S102. HSQC spectrum of **15** in CDCl_3

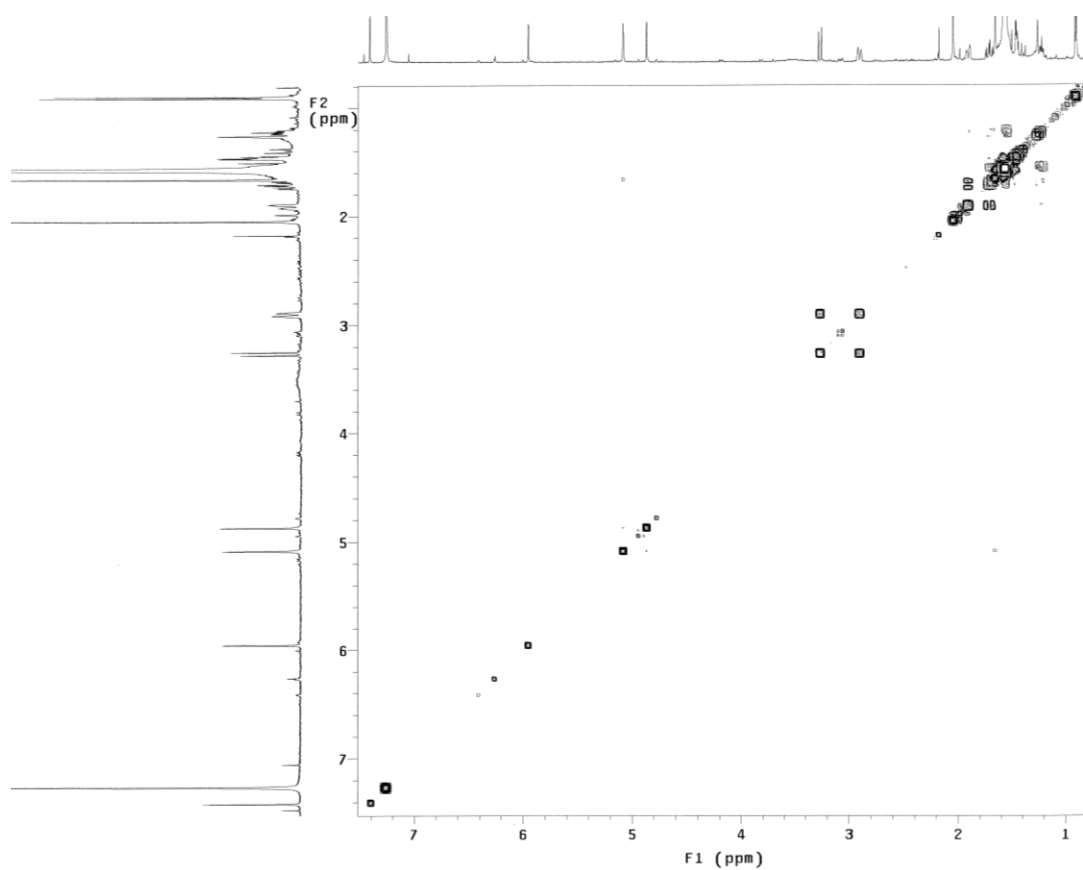


Figure S103. COSY spectrum of **15** in CDCl_3

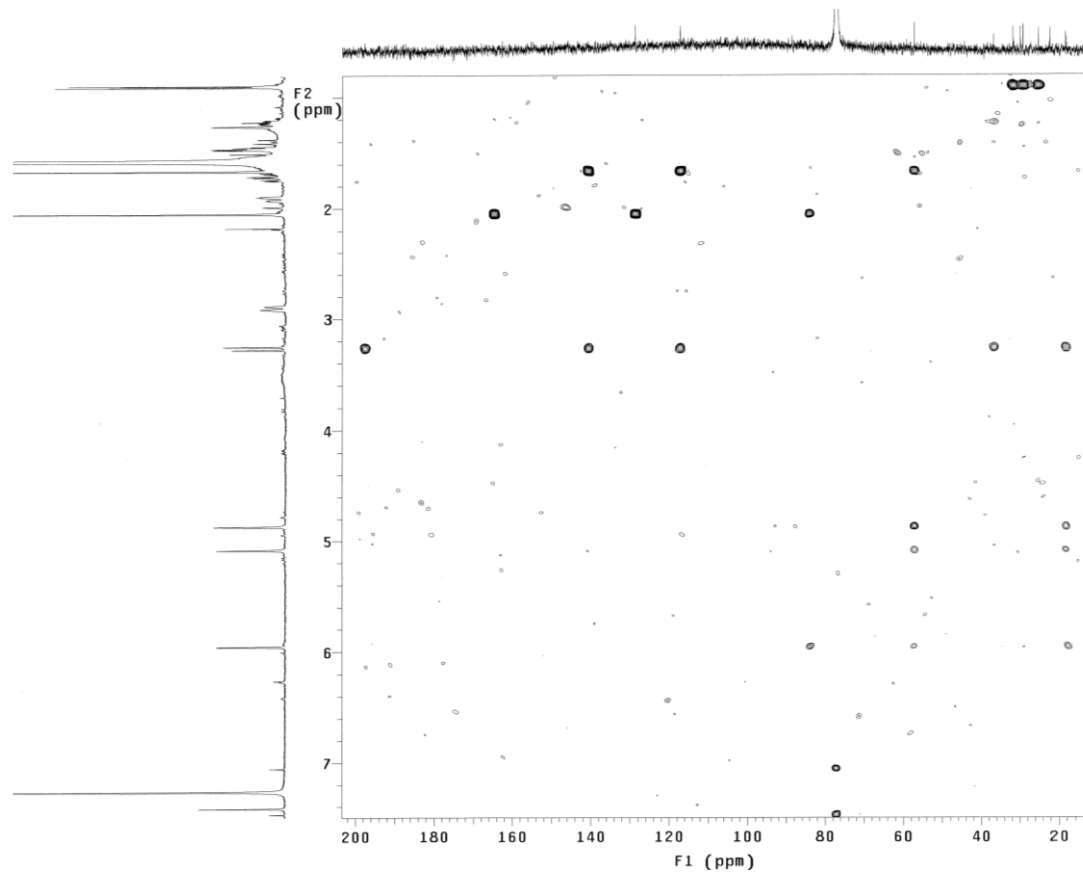


Figure S104. HMBC spectrum of **15** in CDCl_3

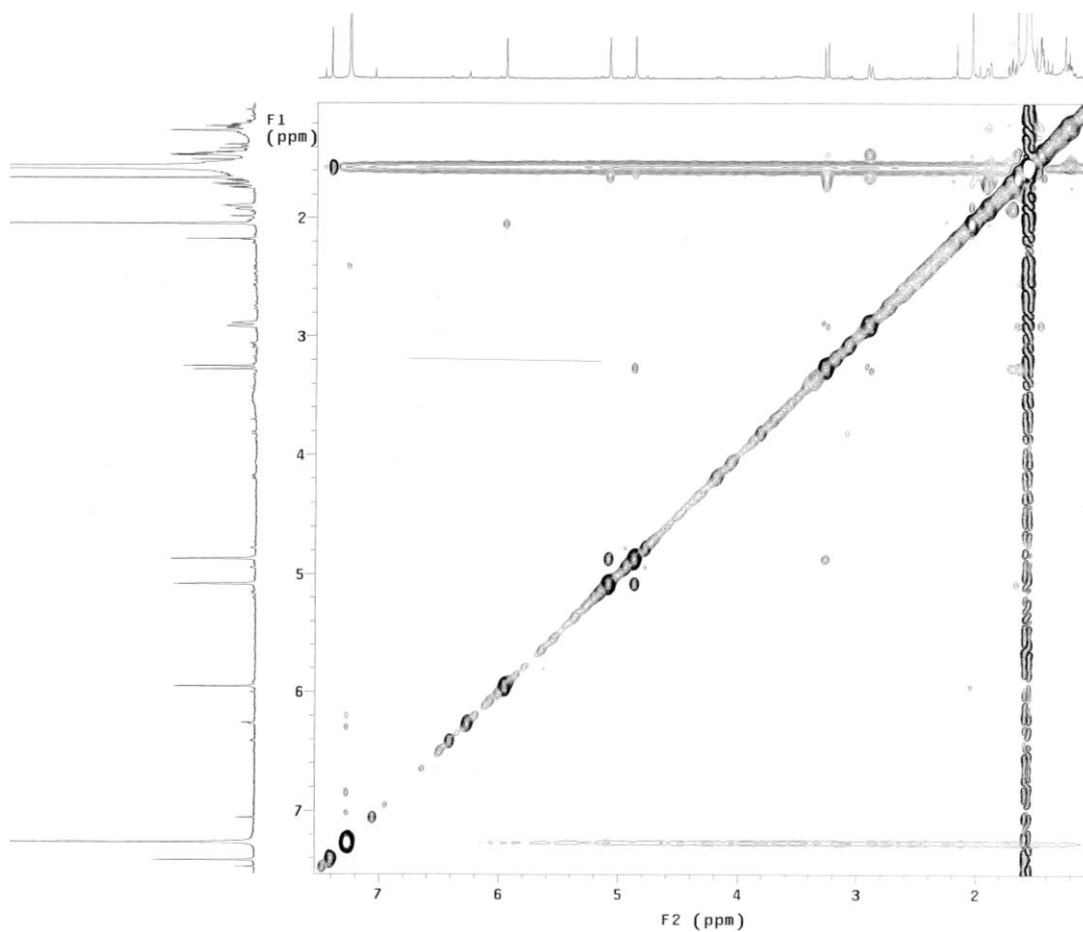


Figure S105. NOESY spectrum of **15** in CDCl₃

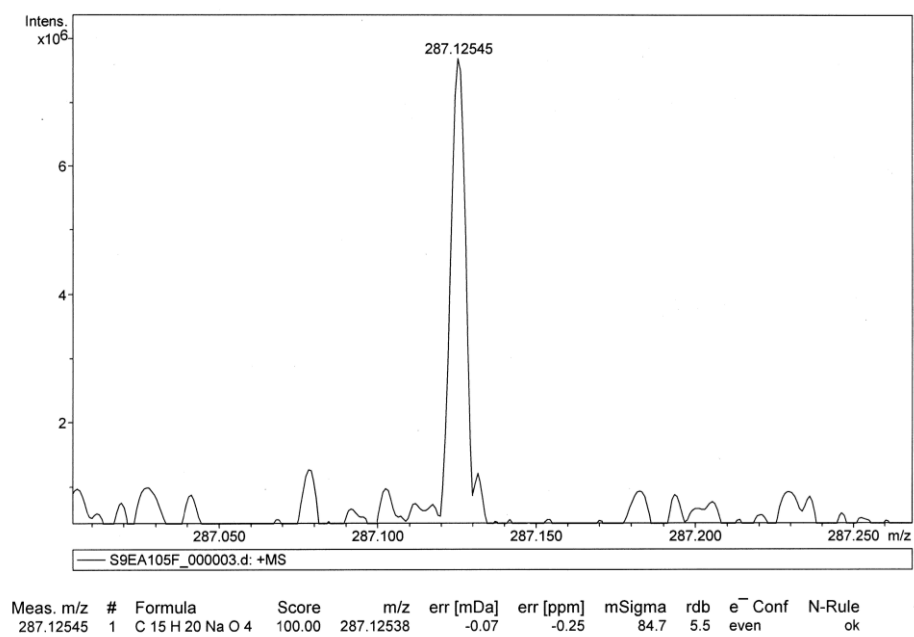


Figure S106. HRESIMS spectrum of **16**

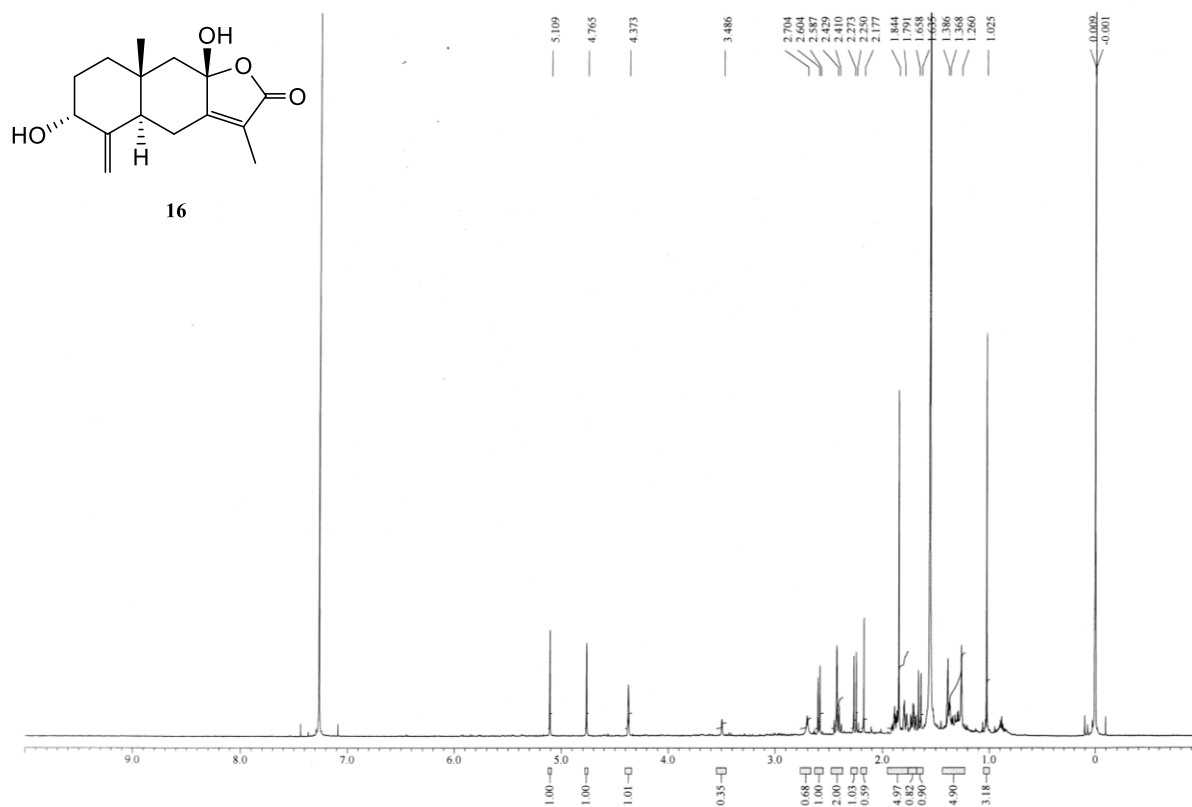


Figure S107. ¹H NMR spectrum of **16** in CDCl₃ at 600 MHz

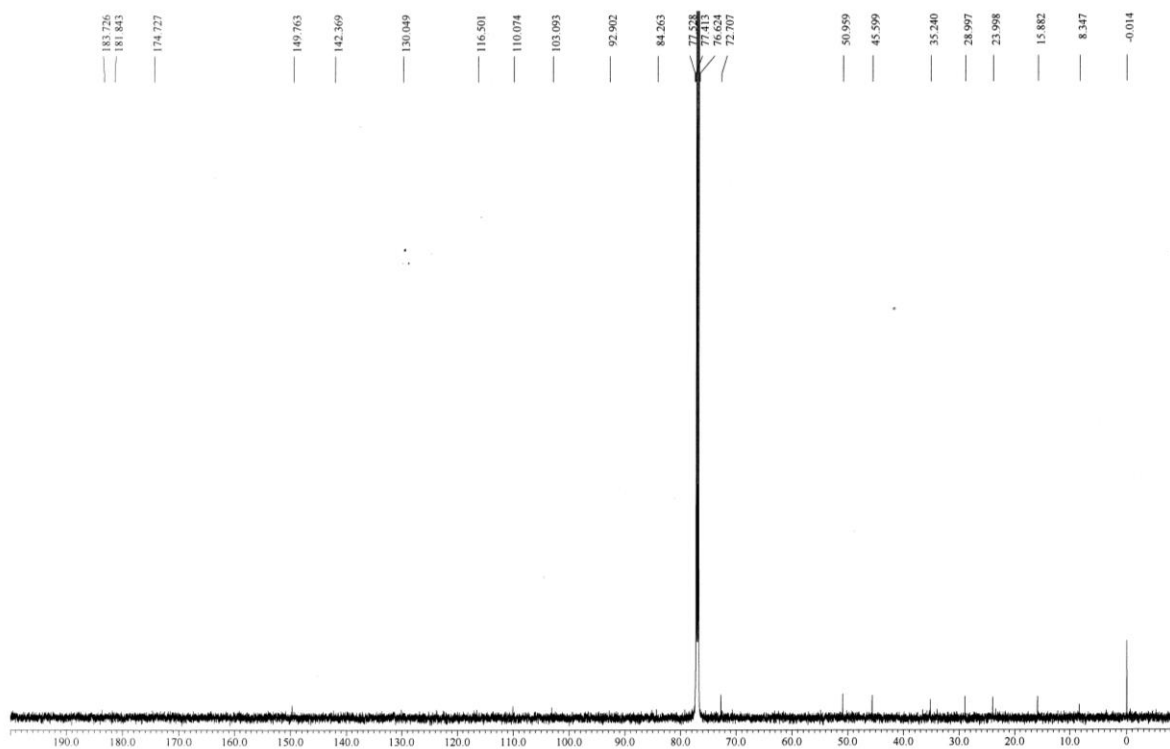


Figure S108. ¹³C NMR spectrum of **16** in CDCl₃ at 150 MHz

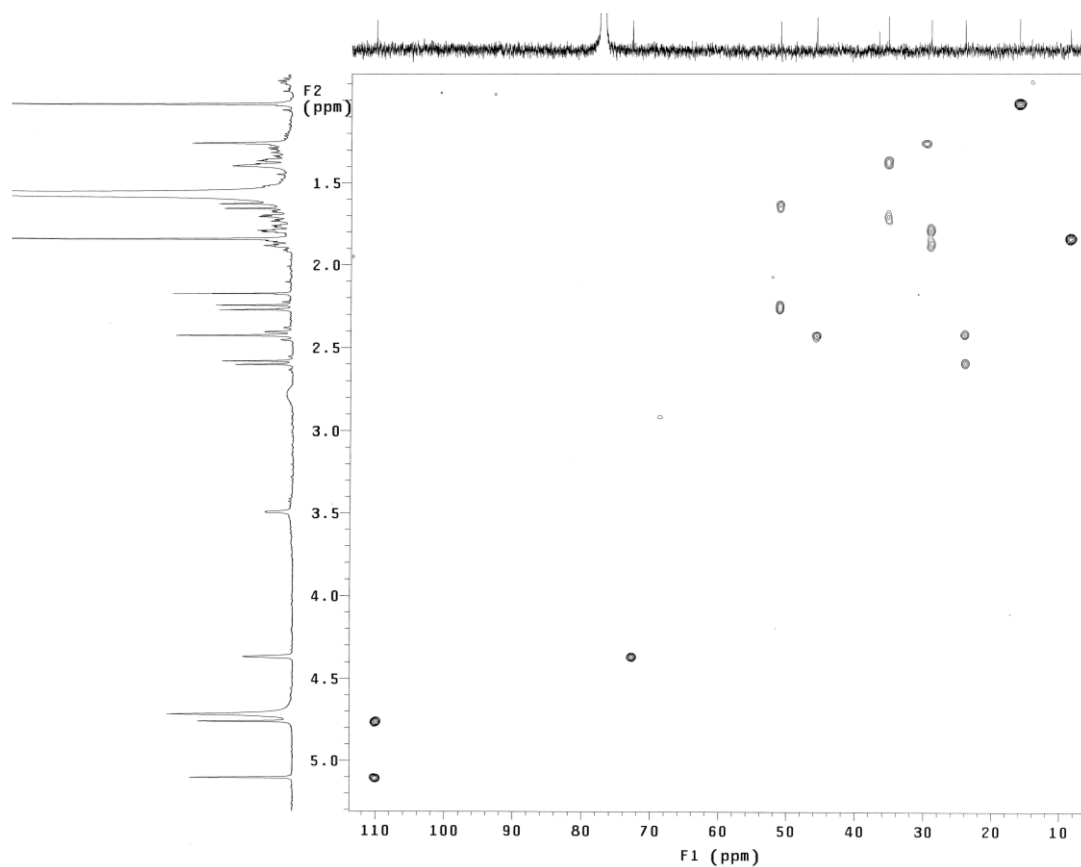


Figure S109. HSQC spectrum of **16** in CDCl₃

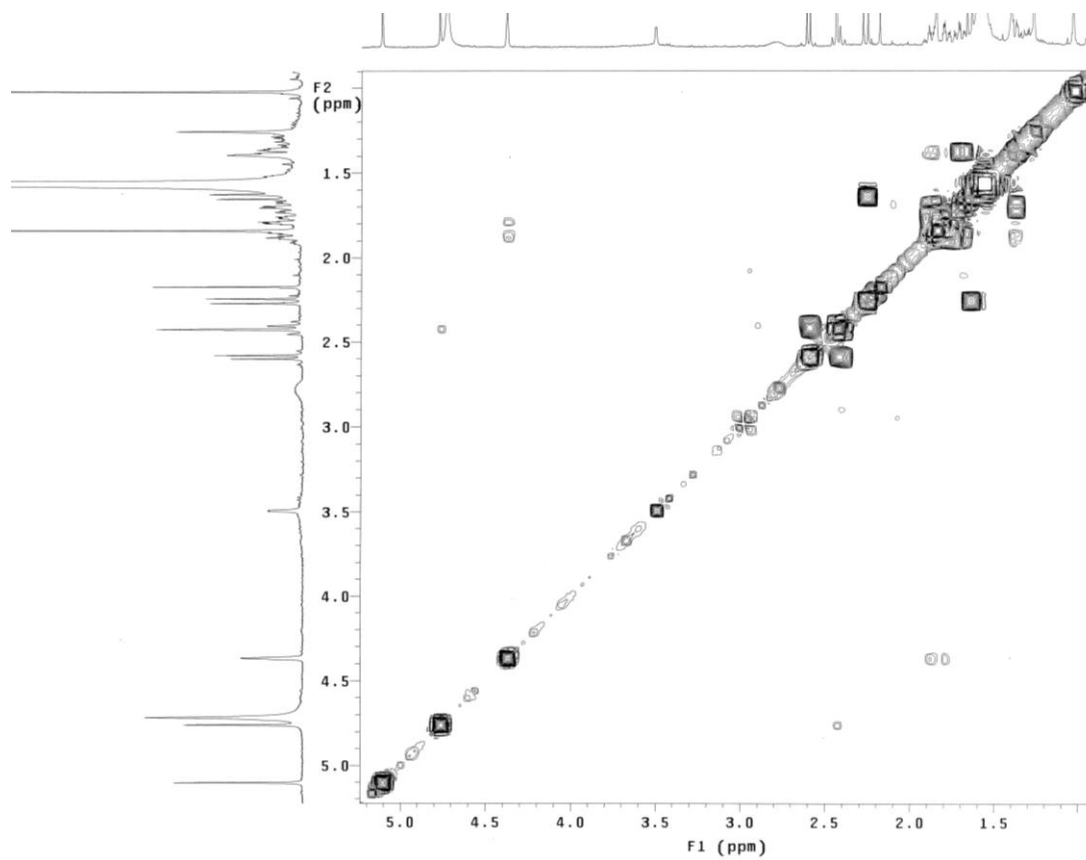


Figure S110. COSY spectrum of **16** in CDCl₃

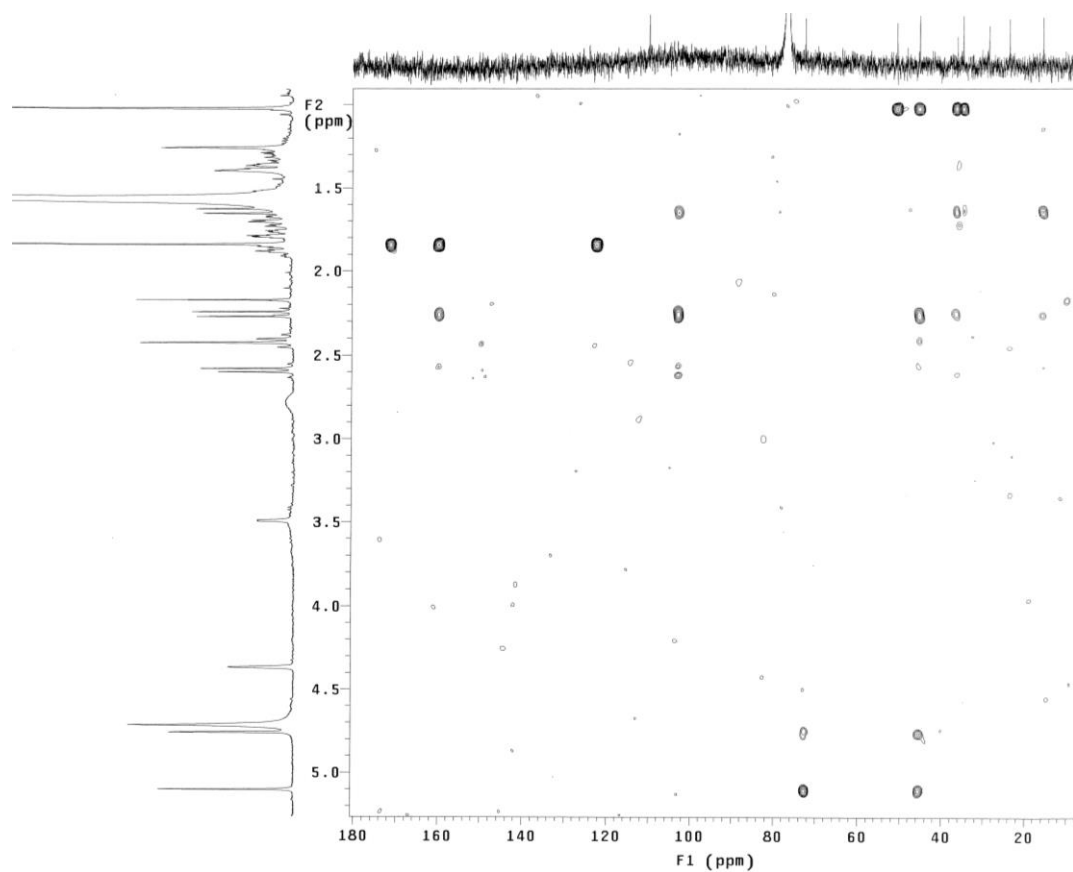


Figure S111. HMBC spectrum of **16** in CDCl_3

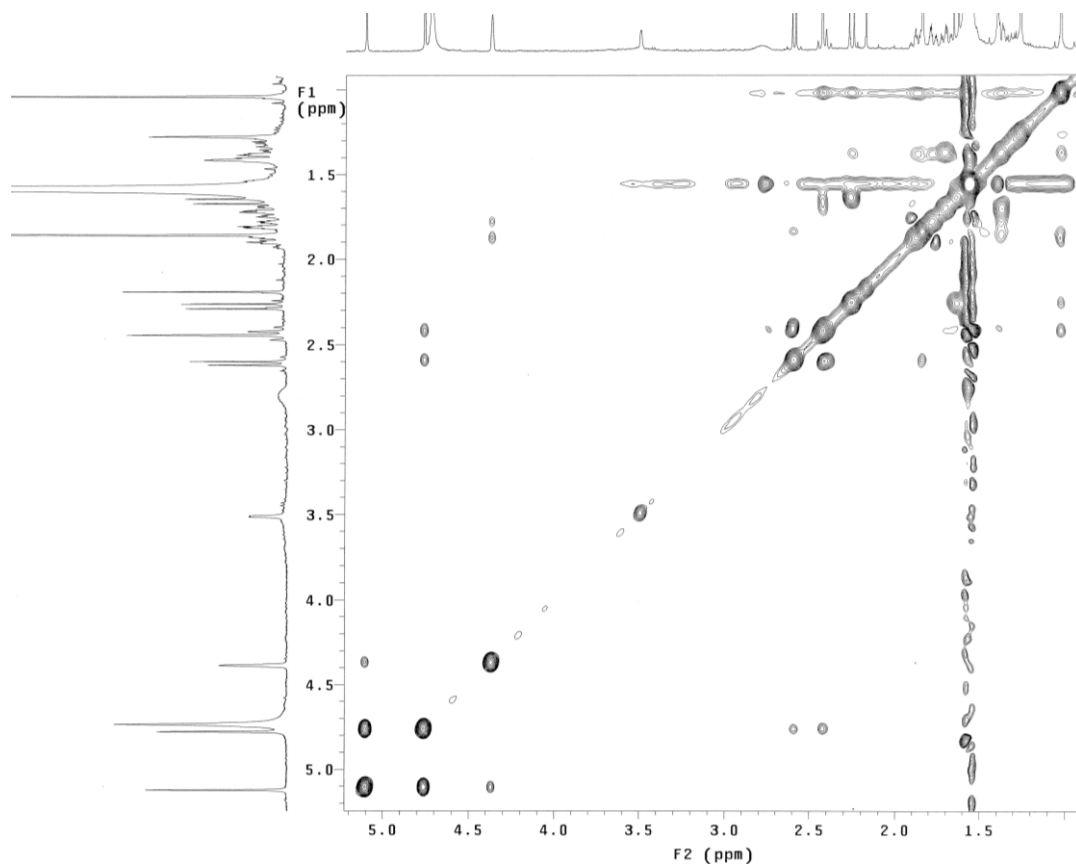


Figure S112. NOESY spectrum of **16** in CDCl_3

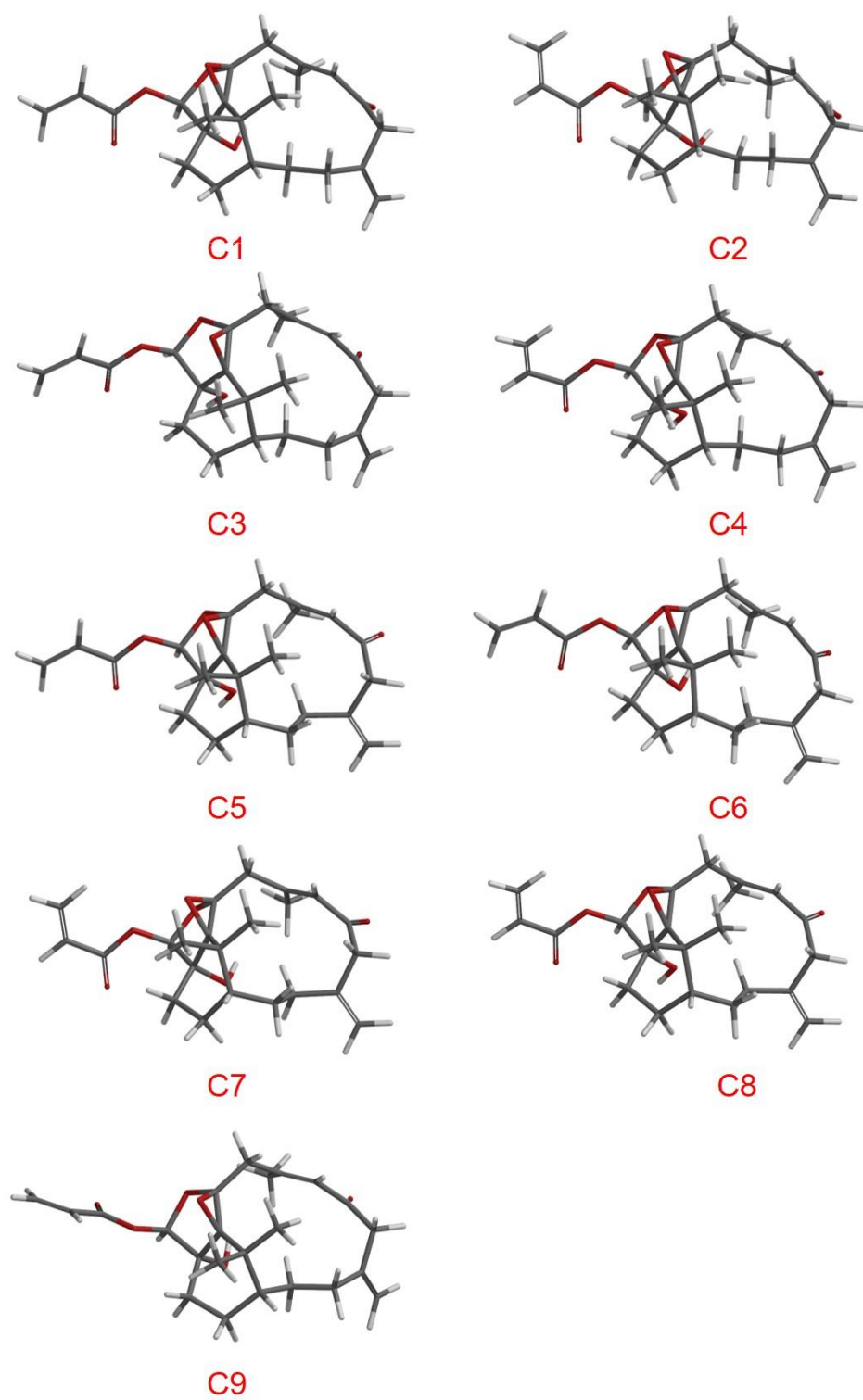


Figure S113. MMFF lowest energy conformers for **1**.

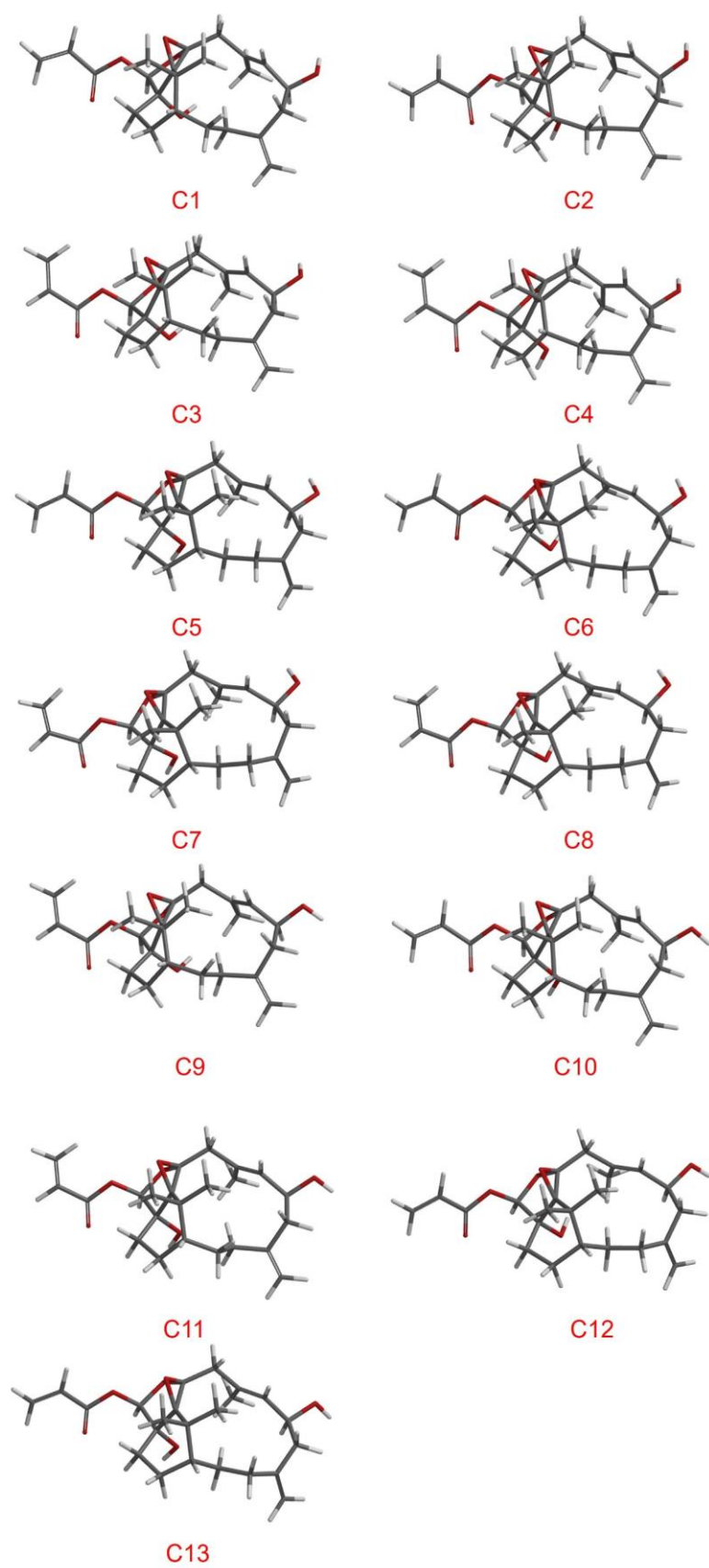


Figure S114. MMFF lowest energy conformers for **2**.

Table S1. ¹H and ¹³C NMR spectroscopic data of compounds **17** and **18**.

No.	17		18	
	¹ H ¹	¹³ C ²	¹ H ³	¹³ C ⁴
1	1.91, m	43.0 (CH) ⁶	1.63, m	43.0 (CH) ⁶
2	1.66, m; 1.57, m	29.0 (CH ₂)	1.95, m; 1.52, m	30.6 (CH ₂)
3	1.99, m; 1.84 m	33.5 (CH ₂)	2.69, t (12.8) ⁵	30.6 (CH ₂)
			1.91, m	
4		146.2 (C)		147.0 (C)
5	2.49, dd (13.5, 2.5) ⁵	44.3 (CH ₂)	2.46, dd (12.8, 2.4)	44.7 (CH ₂)
	2.29, dd (13.5, 9.0)		2.30, dd (12.8, 7.6)	
6	4.48, t (9.0)	68.7 (CH)	4.44, d (6.0)	69.2 (CH)
7	5.40, d (9.0)	134.4 (CH)	5.13, d (7.6)	131.1 (CH)
8		130.5 (C)		130.8 (C)
9	3.23, d (13.5)	46.3 (CH ₂)	3.43, d (15.6)	51.0 (CH ₂)
	2.86, d (13.5)		3.04, d (15.6)	
10		169.7 (C)		202.2 (C)
11		211.1 (C)		147.9 (C)
12	5.08, dd (6.0, 4.0)	72.2 (CH)	6.21, br s	135.5 (CH)
13	2.40, dt (22.0, 7.0)	26.4 (CH ₂)	2.29, 2H, m	23.9 (CH ₂)
	1.89, m			
14	1.97, m; 1.65, m	20.4 (CH ₂)	2.24, m; 1.66, m	22.9 (CH ₂)
15		47.6 (C)		35.3 (C)
16	1.23, 3H, s	27.8 (CH ₃)	1.28, 3H, s	32.8 (CH ₃)
17	1.17, 3H, s	23.1 (CH ₃)	1.15, 3H, s	24.5 (CH ₃)
18	4.87, 4.85, both s	112.2 (CH ₂)	4.84, 4.81, both s	112.6 (CH ₂)
19	1.74, 3H, s	16.9 (CH ₃)	1.75, 3H, s	18.9 (CH ₃)

¹ Spectrum recorded at 500 MHz in CDCl₃.² Spectrum recorded at 125 MHz in CDCl₃.³ Spectrum recorded at 400 MHz in CDCl₃.⁴ Spectrum recorded at 100 MHz in CDCl₃.⁵ J values are in Hz.⁶ Attached protons were deduced by HSQC experiments**Table S2.** Energy analysis for MMFF conformational searching of compounds **1** and **2**

Conf.	1		2	
	rel. E (kcal/mol)	Boltzmann Dist.	rel. E (kcal/mol)	Boltzmann Dist.
C1	0.00	0.223	0.00	0.261
C2	0.31	0.133	0.30	0.156
C3	0.33	0.127	0.96	0.052
C4	0.71	0.067	1.16	0.037
C5	1.08	0.036	1.21	0.034
C6	1.11	0.034	1.48	0.021
C7	1.40	0.021	1.59	0.018
C8	1.45	0.019	1.80	0.013
C9	1.83	0.010	2.07	0.008
C10			2.18	0.007
C11			2.56	0.003
C12			2.81	0.002
C13			2.99	0.002