

Supplementary Materials for

Secondary Metabolites with Anti-inflammatory Activity from *Laurencia majuscula* Collected in the Red Sea

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Table S1. ¹³C and ¹H NMR data (δ in ppm, *J* in Hz) of compounds **23–26**.

Position	23		24		25		26	
	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H
1	78.0	3.23 (d, 2.3)	78.9	3.28 (d, 2.3)	78.0	3.24 (d, 2.1)	78.0	3.23 (d, 2.1)
2	84.6	-	84.5	-	84.5	-	84.5	-
3	111.5	5.63 (t, 2.3)	111.7	5.66 (t, 2.1)	111.7	5.65 (t, 2.2)	111.5	5.63 (t, 2.2)
4	141.4	5.95 (t, 10.5)	140.3	5.85 (t, 10.5)	141.6	5.97 (t, 10.5)	141.8	6.17 (t, 10.7)
5	58.2	4.78 (t, 10.5)	58.7	4.85 (t, 10.5)	58.2	4.77 (m)	58.7	4.85 (m)
6	51.5	2.89 (dd, 10.5, 1.7)	51.2	2.03 (m)	51.5	2.90 (m)	51.2	2.03 (m)
7	77.8	4.80 (d, 5.2)	78.2	4.76 (d, 5.2)	77.4	4.79 (d, 5.2)	78.2	4.77 (d, 5.0)
8	38.8	1.91 (m), 1.67 (m)	40.3	1.80 (m), 1.61 (m)	38.8	1.91 (m), 1.67 (m)	40.3	1.84 (m), 1.66 (m)
9	78.6	4.41 (dd, 7.8, 4.9)	77.2	4.48 (dd, 6.7, 4.5)	78.6	4.41 (dd, 7.8, 4.9)	78.8	4.57 (dd, 7.0, 4.6)
10	83.4	5.02 (t, 4.9)	84.4	5.41 (t, 4.5)	83.1	4.96 (t, 5.0)	83.3	5.32 (t, 5.0)
11	50.0	2.45 (brd, 5.3)	49.8	2.30 (dd, 4.6, 2.3)	48.2	2.37 (brd, 5.0)	53.6	2.35 (dd, 4.9, 2.3)
12	104.4	-	104.4	-	104.8	-	105.4	-
13	66.4	3.75 (dd, 11.2, 2.4)	64.9	4.0 (dd, 11.4, 1.6)	67.8	3.79 (dd, 11.0, 2.3)	60.4	3.83 (dd, 10.9, 2.0)
14	25.7	2.05 (m), 1.65 (m)	28.4	2.01 (m), 1.76 (m)	27.4	1.88 (m), 1.65 (m)	24.7	2.17 (m), 1.75 (m)
15	12.7	1.09 (m)	12.7	1.08 (m)	12.7	1.08 (m)	12.7	1.09 (m)
OH		3.00 (brs)		3.01 (brs)		3.12 (brs)		n.d.

¹ Recorded in CDCl₃ at 400MHz. ¹³C chemical shifts were determined through HMBC correlations. n.d.: not determined.

Table S2. Collection and refinement details for compounds **1** and **2**.

	1	2
Colour, habit	Colourless, Triangular plate	Colourless, Plate
Size/mm	0.127 x 0.065 x 0.04	0.35 x 0.23 x 0.048
Empirical formula	C ₁₆ H ₂₀ BrClO ₃	C ₁₆ H ₂₀ BrClO ₃
FW	375.68	375.68
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁	<i>P</i> 2 ₁
<i>a</i> /Å	8.5263(4)	7.4471(2)
<i>b</i> /Å	11.6240(6)	14.1825(3)
<i>c</i> /Å	8.7843(4)	8.1676(2)
α /°	90	90
β /°	107.330(2)	107.6960(10)
γ /°	90	90
<i>V</i> /Å ³	831.09(7)	821.83(3)
<i>Z</i>	4	4
μ /mm ⁻¹	2.640	2.670
<i>T</i> /K	100	100
θ min/max	2.502/ 25.242	2.618/ 25.242
Completeness to θ max (%)	99.9 to 25.242	99.9 to 25.242
Reflections Total/ Independent	5085/4879	4991/4870
Parameters	192	192
<i>R</i> _{int}	0.0567	0.0385
Final <i>R</i> 1, <i>wR</i> 2	0.0238/0.0578	0.0171/0.0422
<i>Goof</i>	1.066	1.035
Largest peak, hole / e.Å ⁻³	0.6/-0.2	0.2/-0.3
ρ_{calc} /g cm ⁻³	1.501	1.518
Flack	-0.010(2)	-0.0090(18)
CCDC Reference	CCDC 2226802	CCDC 2226801

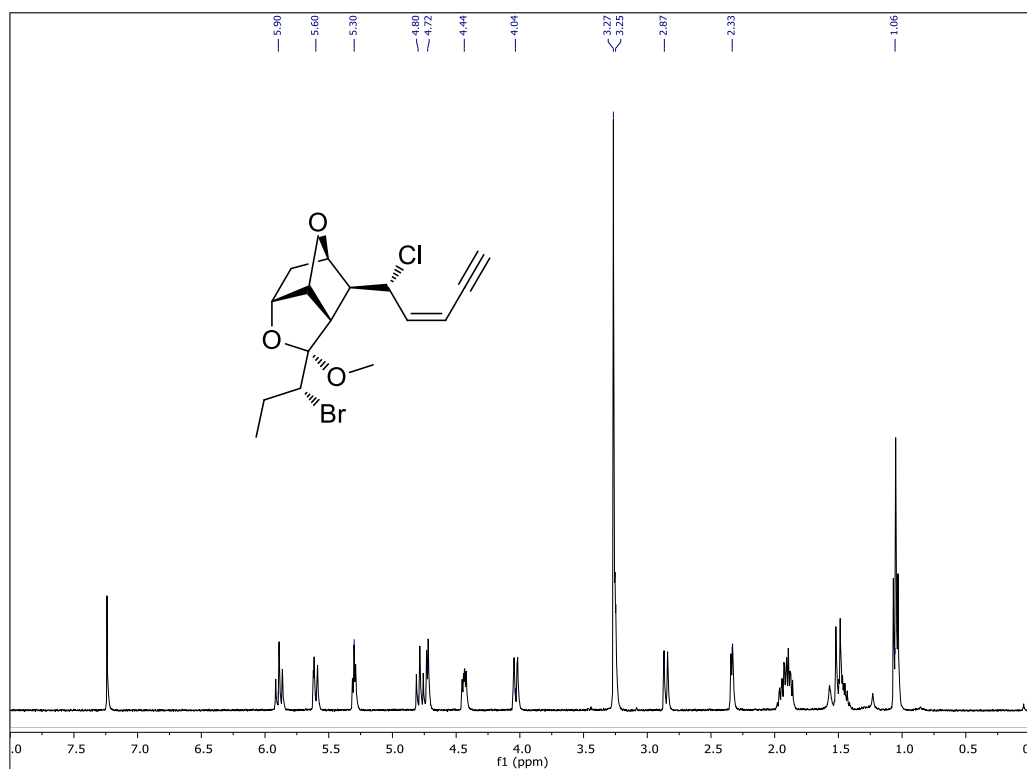


Figure S1. ¹H NMR spectrum (CDCl₃) of compound **1**.

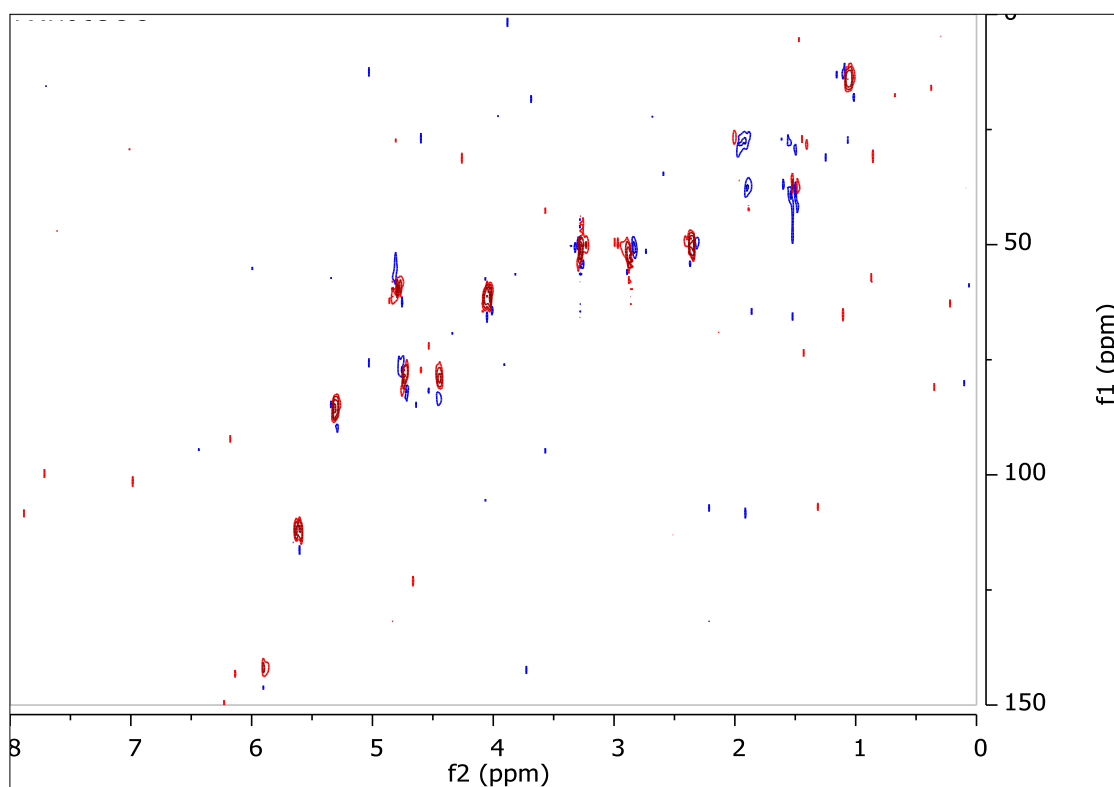


Figure S2. HSQC spectrum (CDCl₃) of compound **1**.

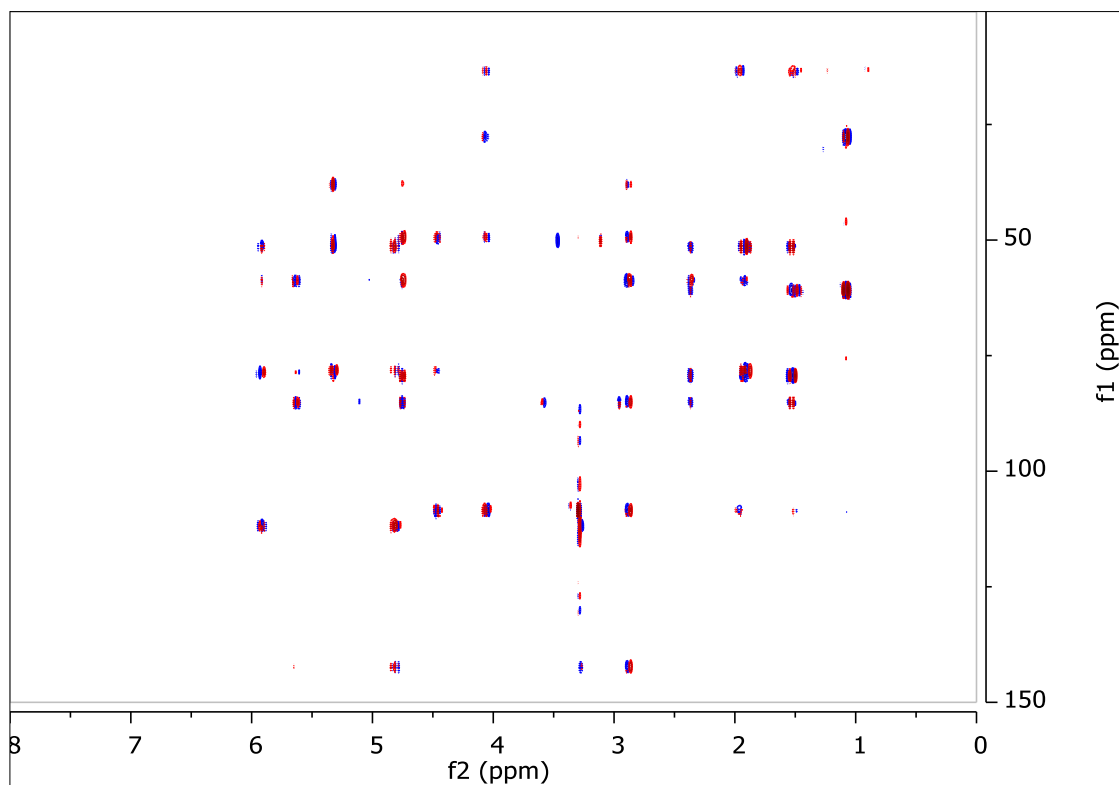


Figure S3. HMBC spectrum (CDCl_3) of compound **1**.

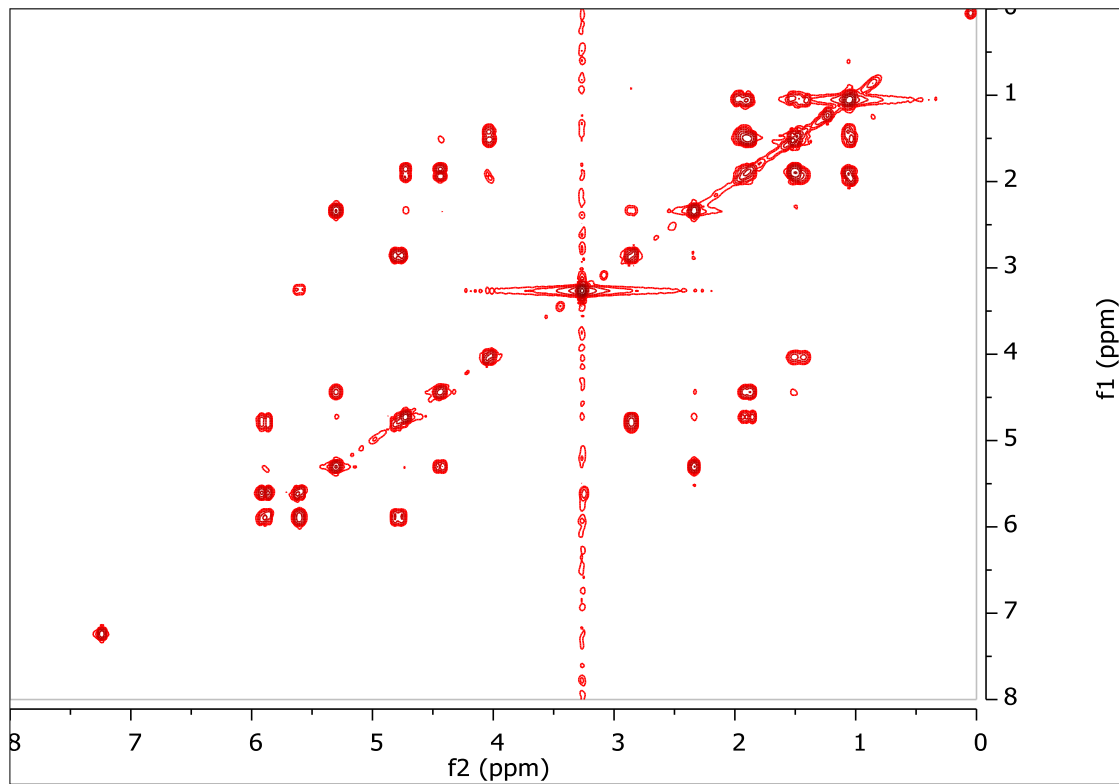


Figure S4. COSY spectrum (CDCl_3) of compound **1**.

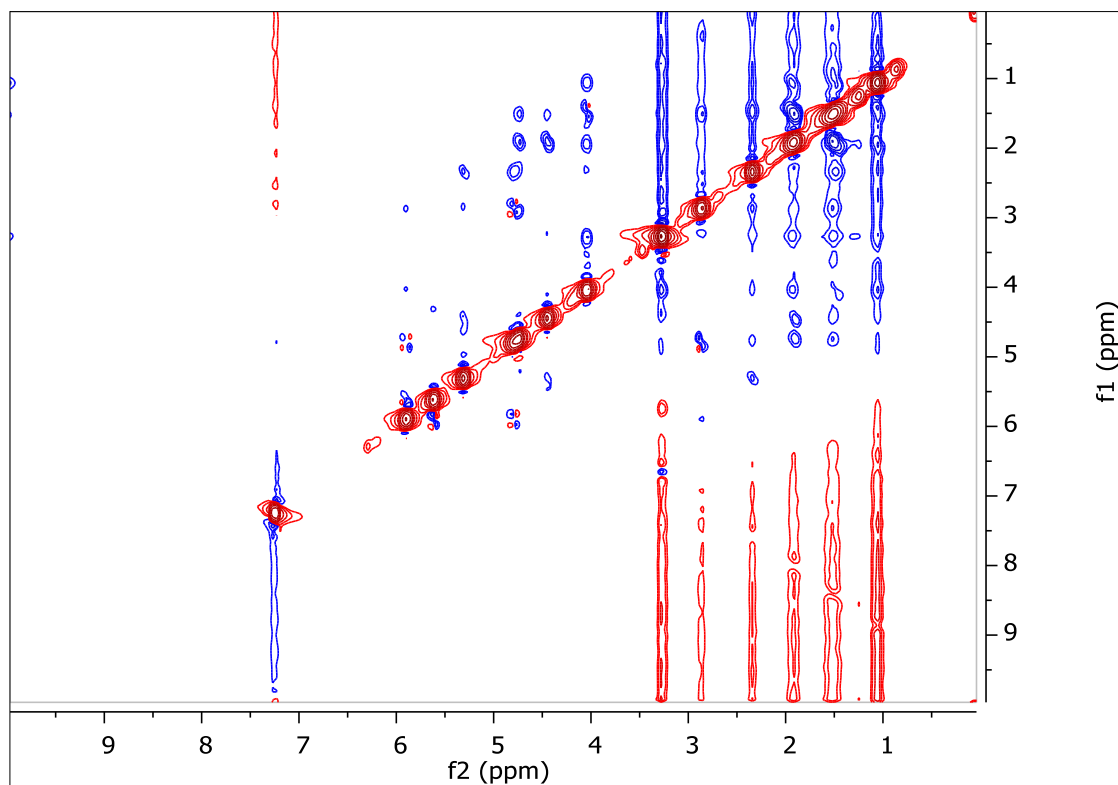


Figure S5. NOESY spectrum (CDCl₃) of compound **1**.

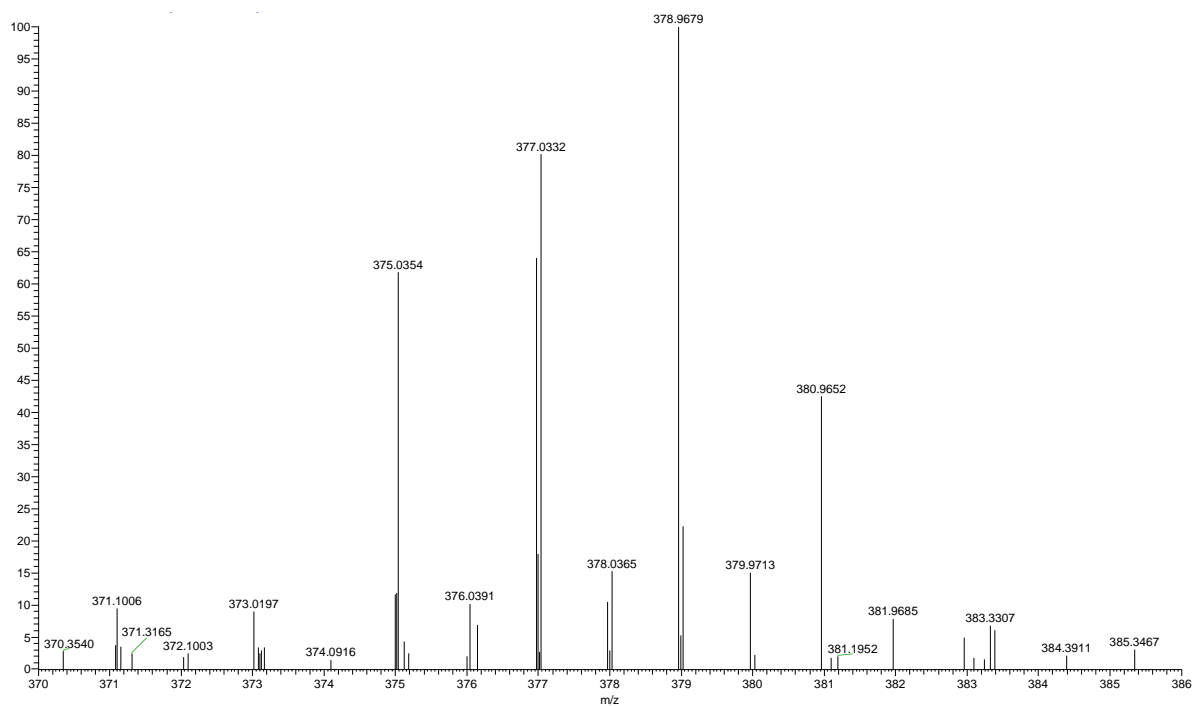


Figure S6. Mass spectrum (HR-APCIMS) of compound **1**.

[M + H]⁺ observed at m/z 375.0354, consistent with C₁₆H₂₁⁷⁹Br³⁵ClO₃

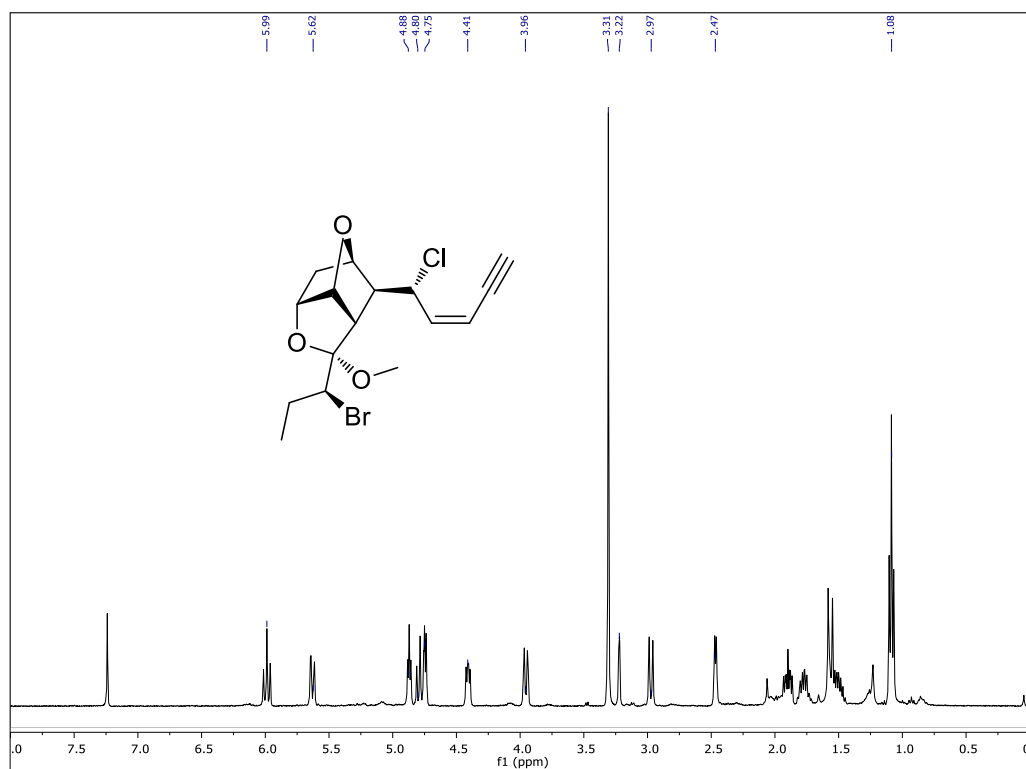


Figure S7. ^1H NMR spectrum (CDCl_3) of compound 2.

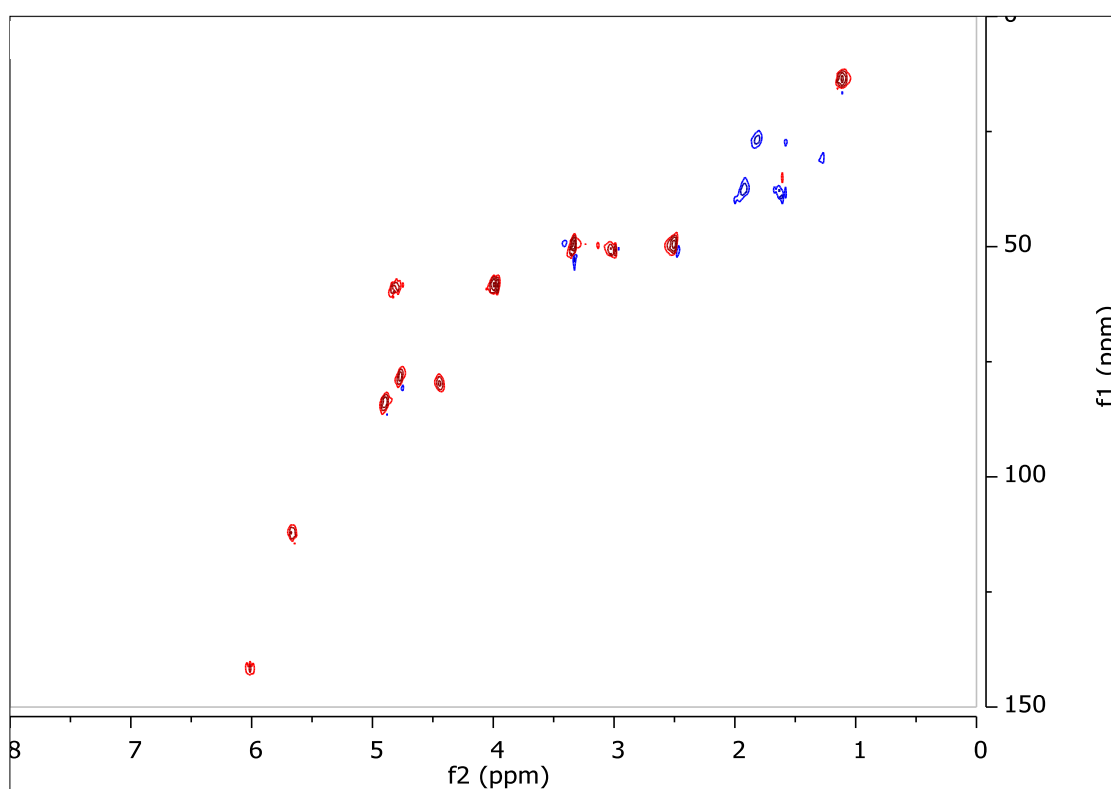


Figure S8. HSQC spectrum (CDCl_3) of compound 2.

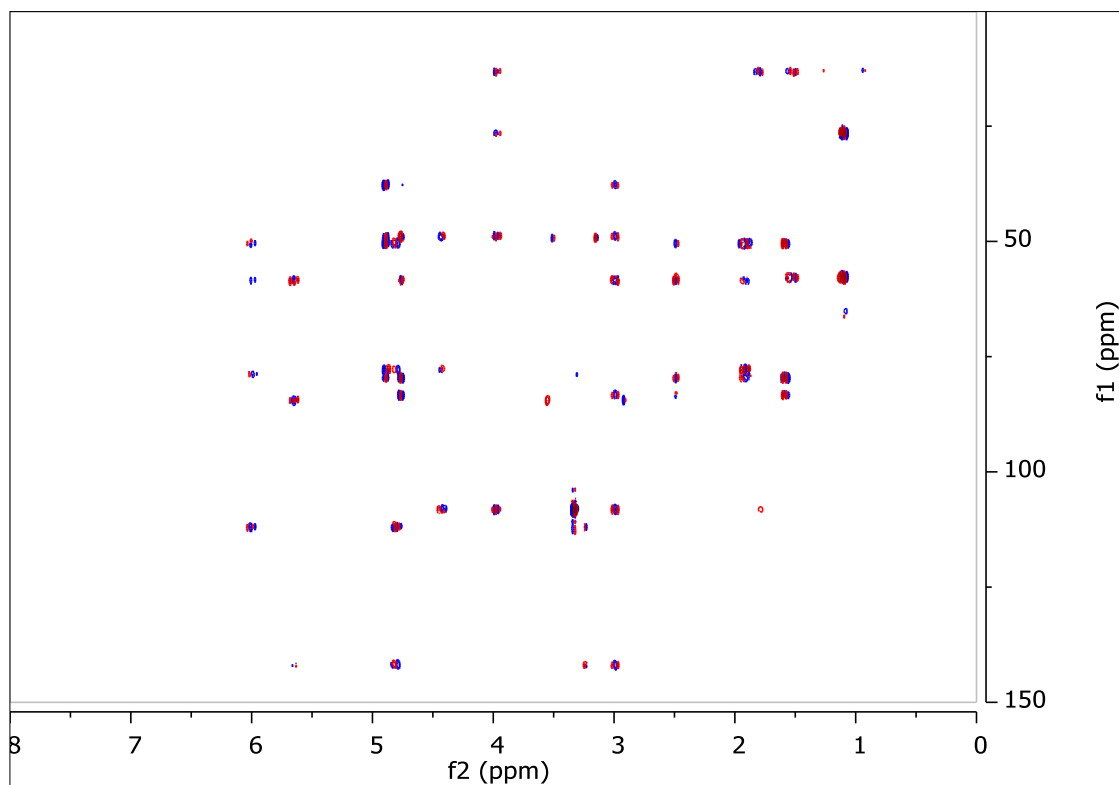


Figure S9. HMBC spectrum (CDCl₃) of compound **2**.

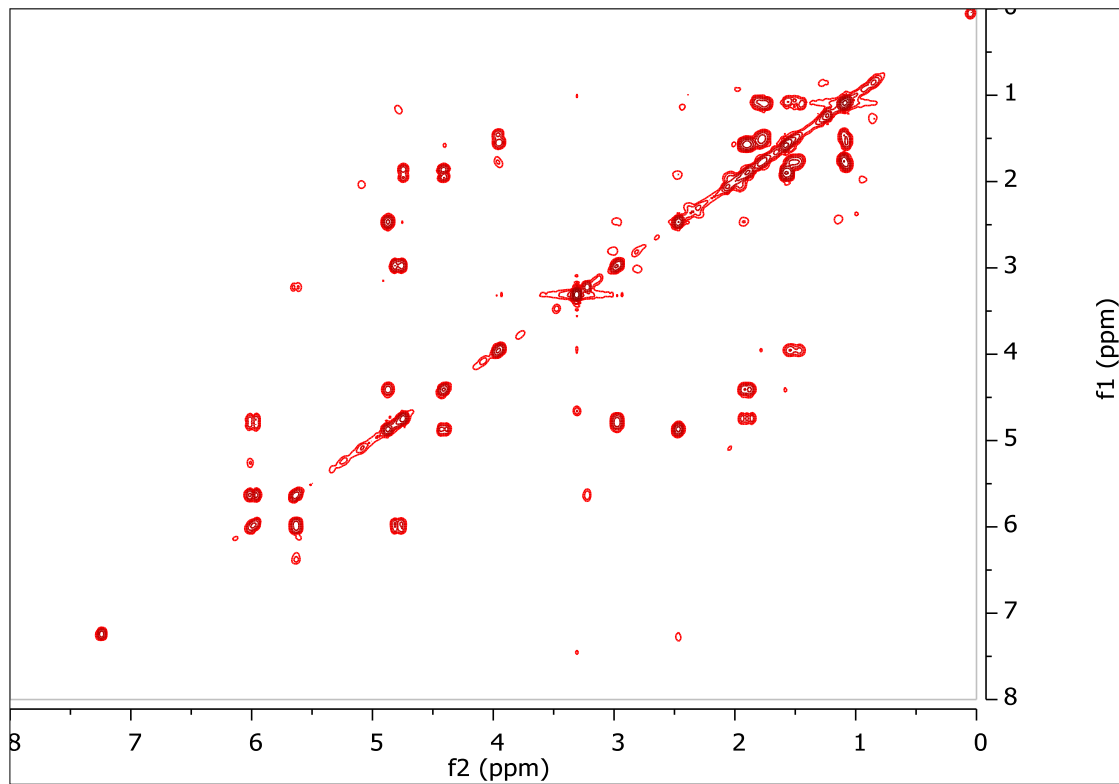


Figure S10. COSY spectrum (CDCl₃) of compound **2**.

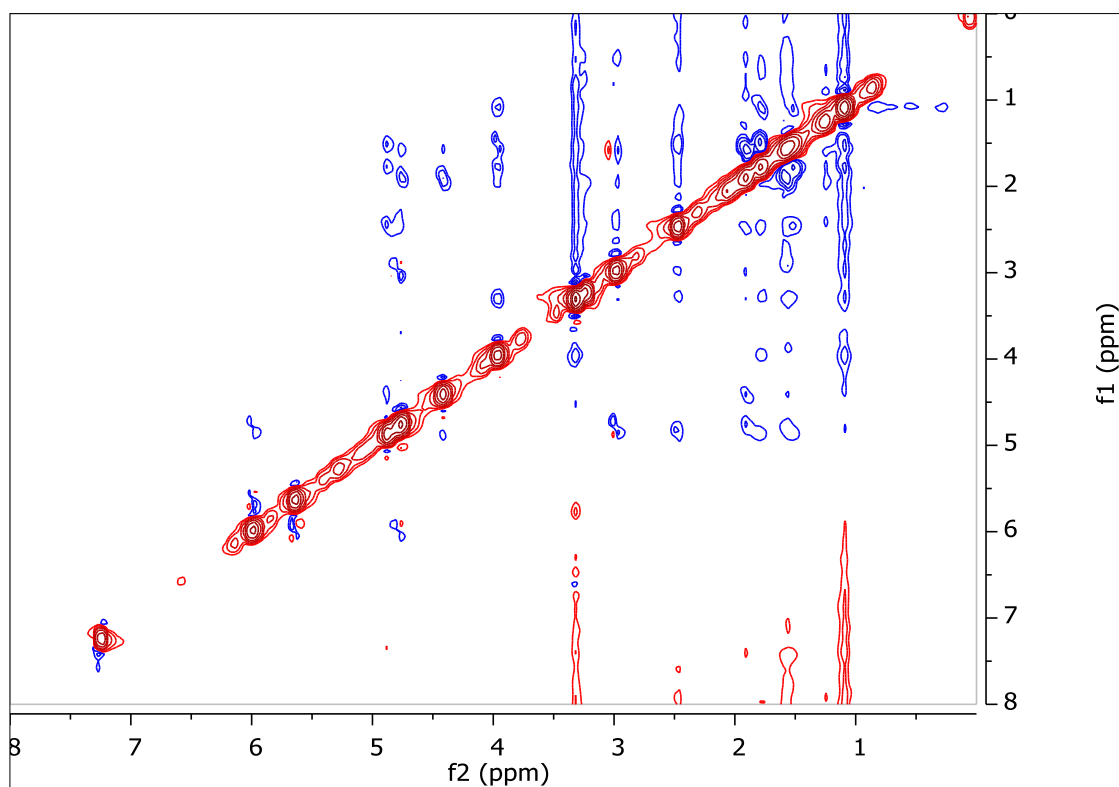


Figure S11. NOESY spectrum (CDCl_3) of compound **2**.

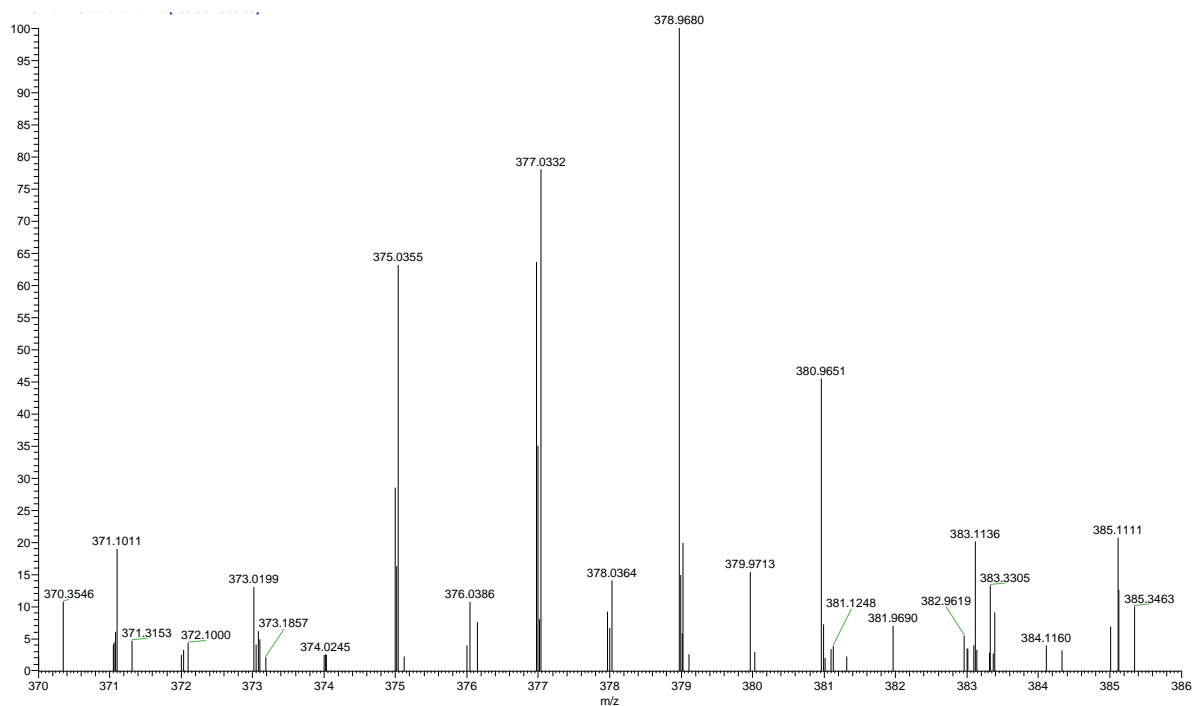


Figure S12. Mass spectrum (HR-APCIMS) of compound **2**.

$[\text{M} + \text{H}]^+$ observed at m/z 375.0355, consistent with $\text{C}_{16}\text{H}_{21}^{79}\text{Br}^{35}\text{ClO}_3$

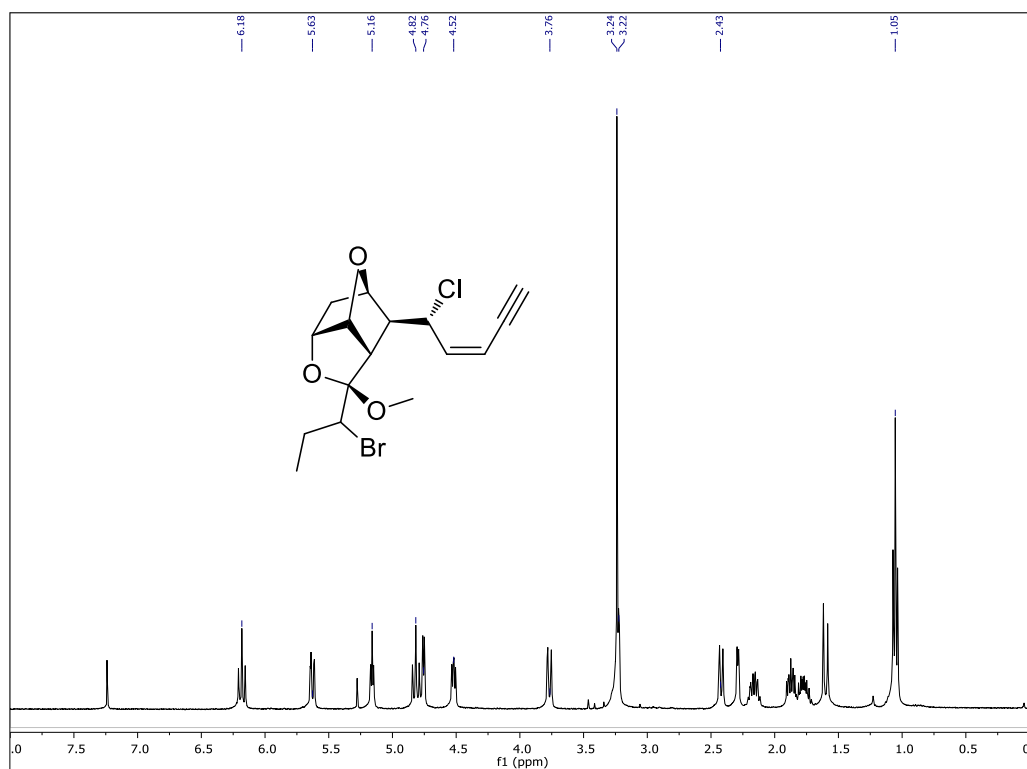


Figure S13. ¹H NMR spectrum (CDCl₃) of compound 3.

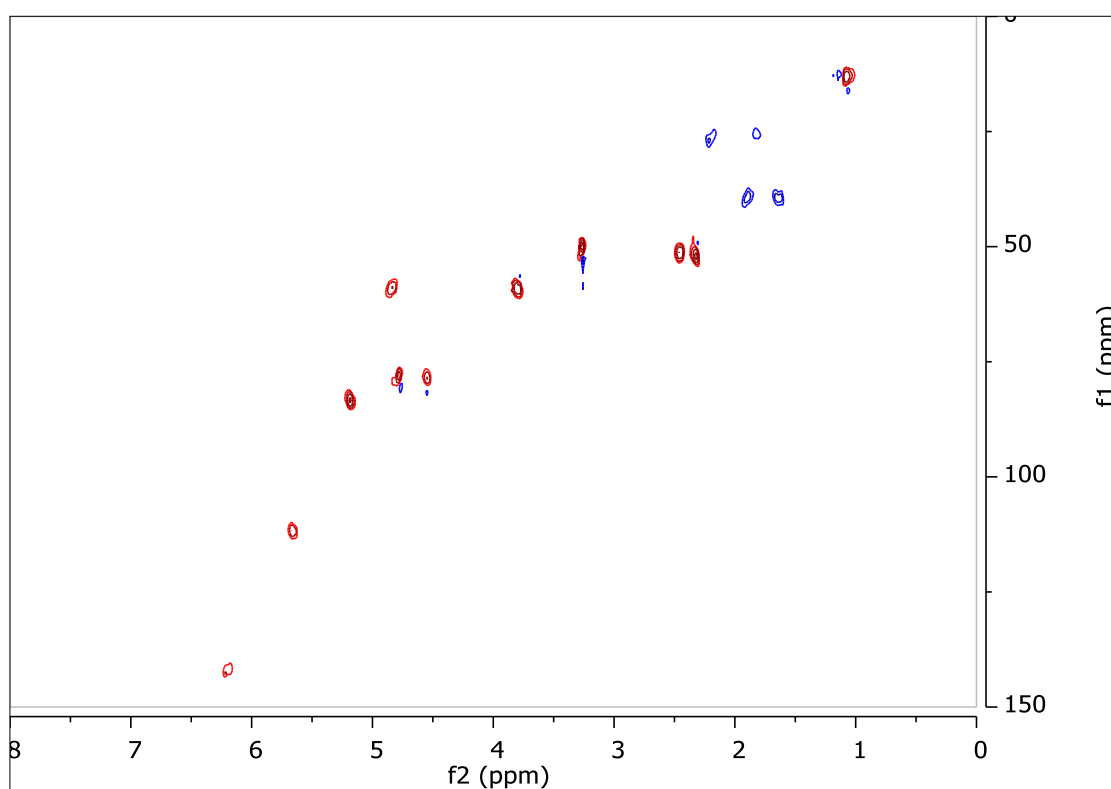


Figure S14. HSQC spectrum (CDCl₃) of compound 3.

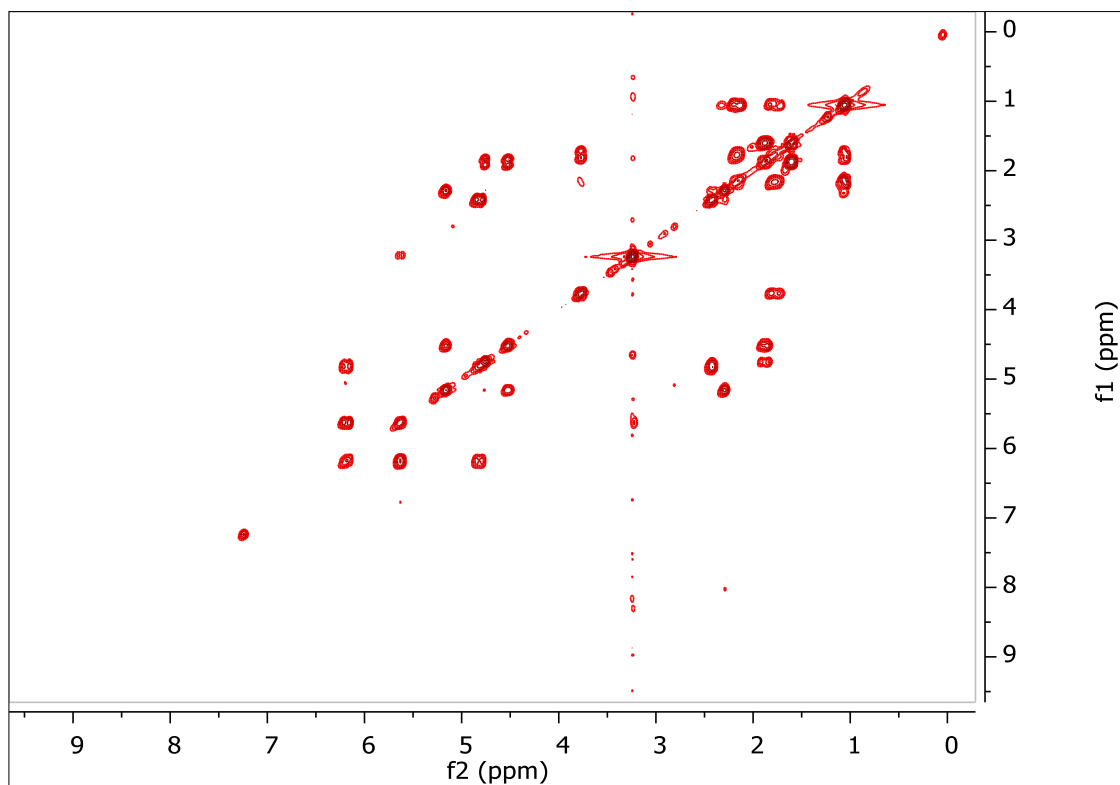


Figure S15. COSY spectrum (CDCl_3) of compound 3.

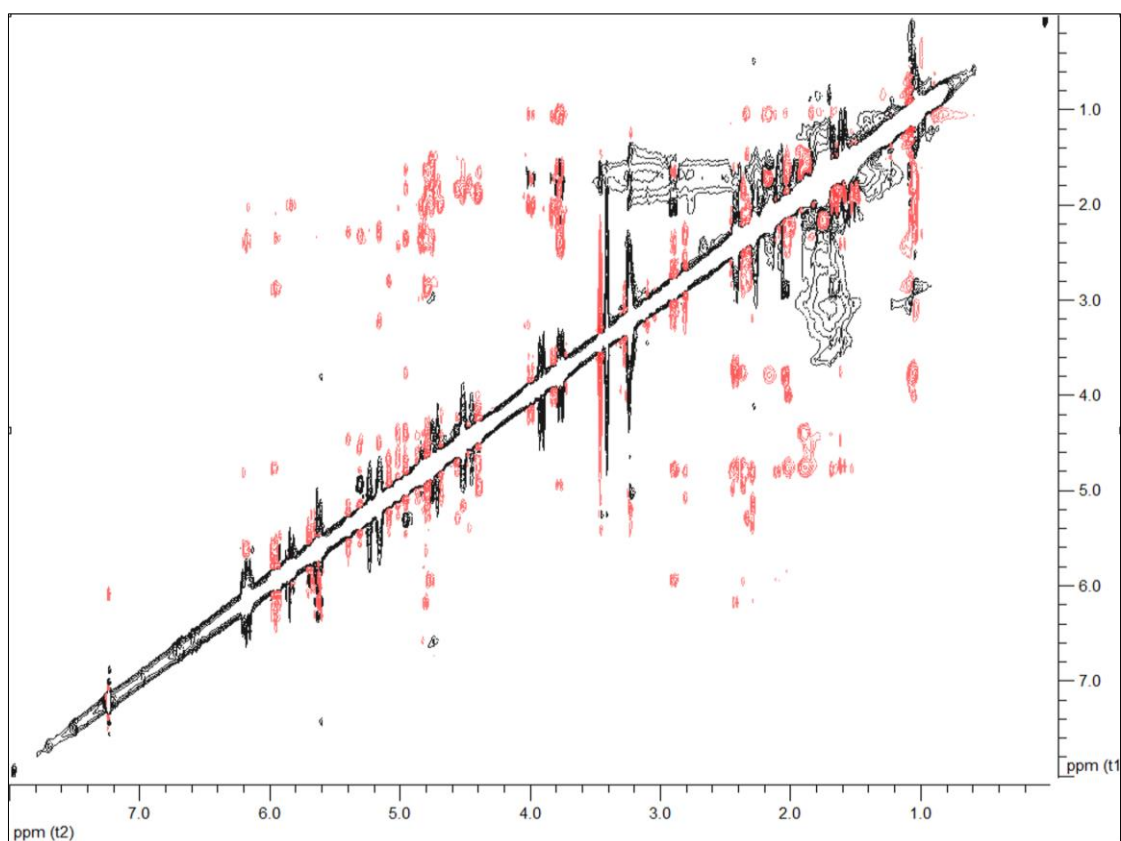


Figure S16. NOESY spectrum (CDCl_3) of compound 3.

*having already started to convert

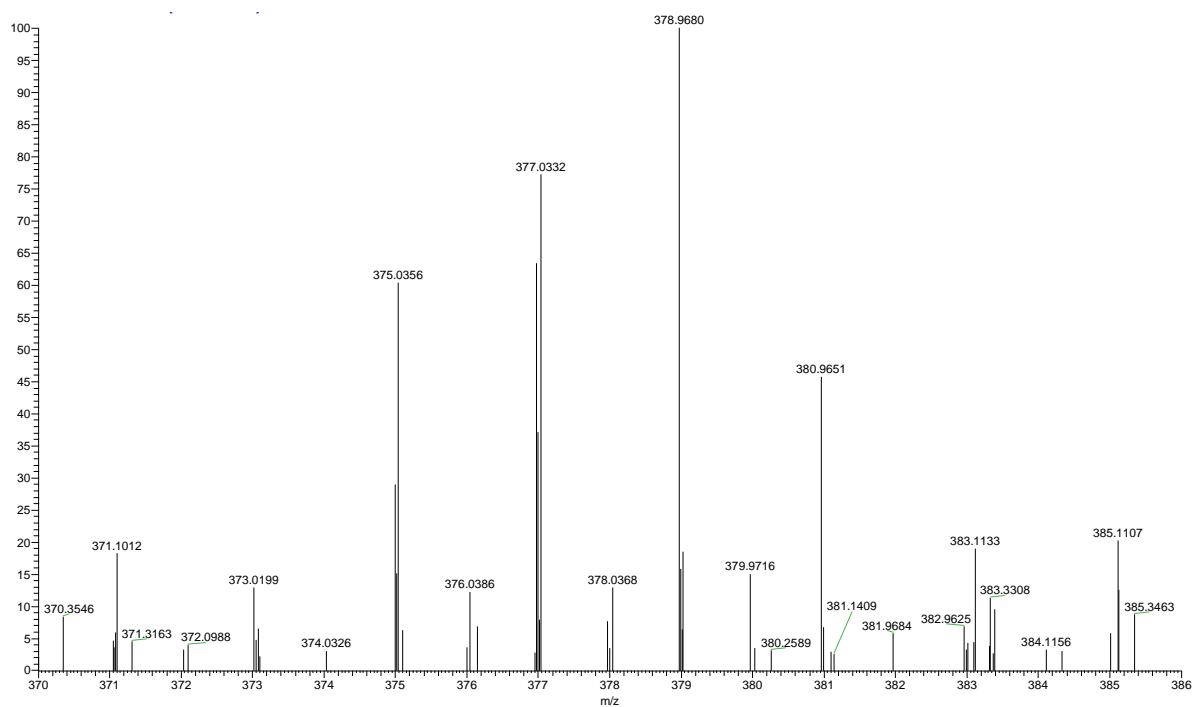


Figure S17. Mass spectrum (HR-APCIMS) of compound **3**.
[M + H]⁺ observed at m/z 375.0356, consistent with C₁₆H₂₁⁷⁹Br³⁵ClO₃

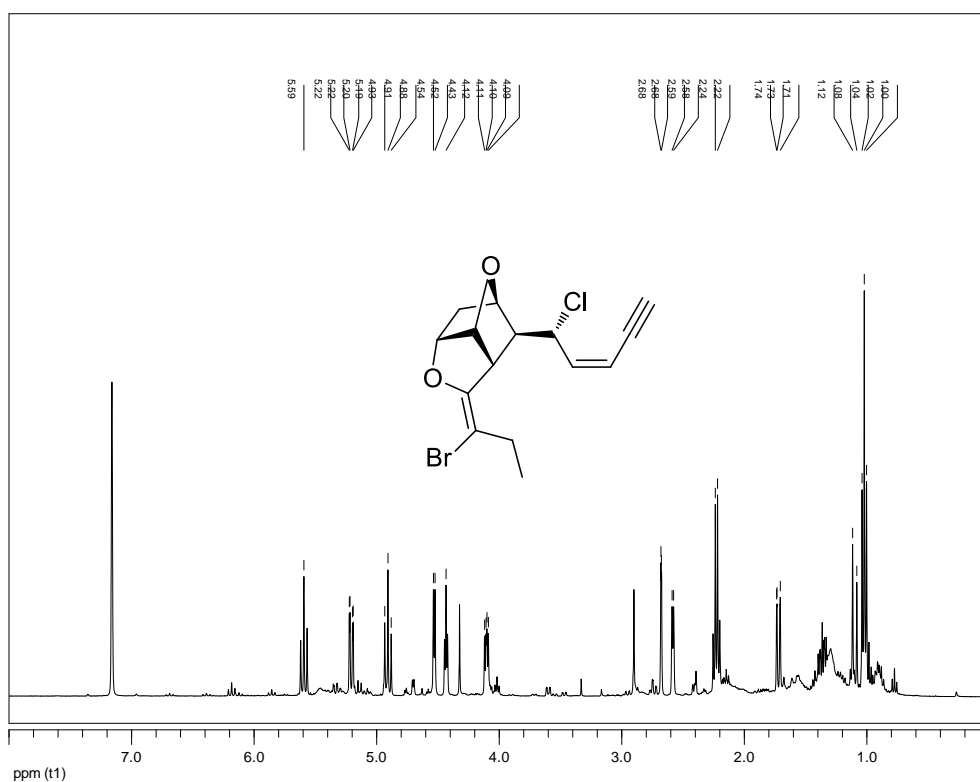


Figure S18. ¹H NMR spectrum (CDCl₃) of compound 4.

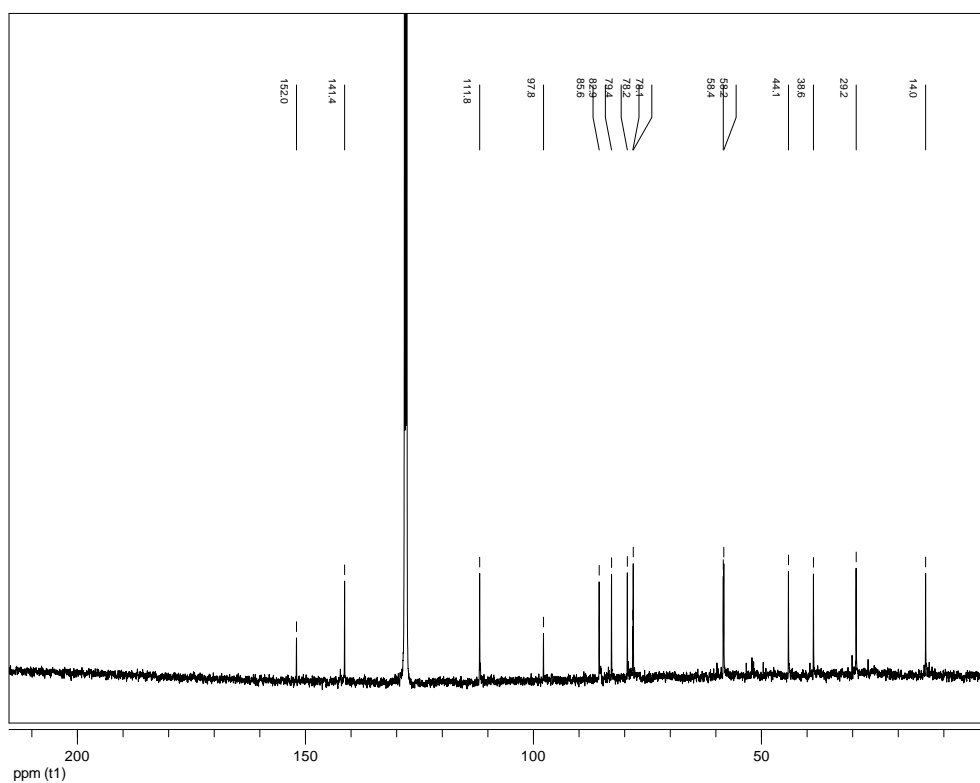


Figure S19. ¹³C NMR spectrum (CDCl₃) of compound 4.

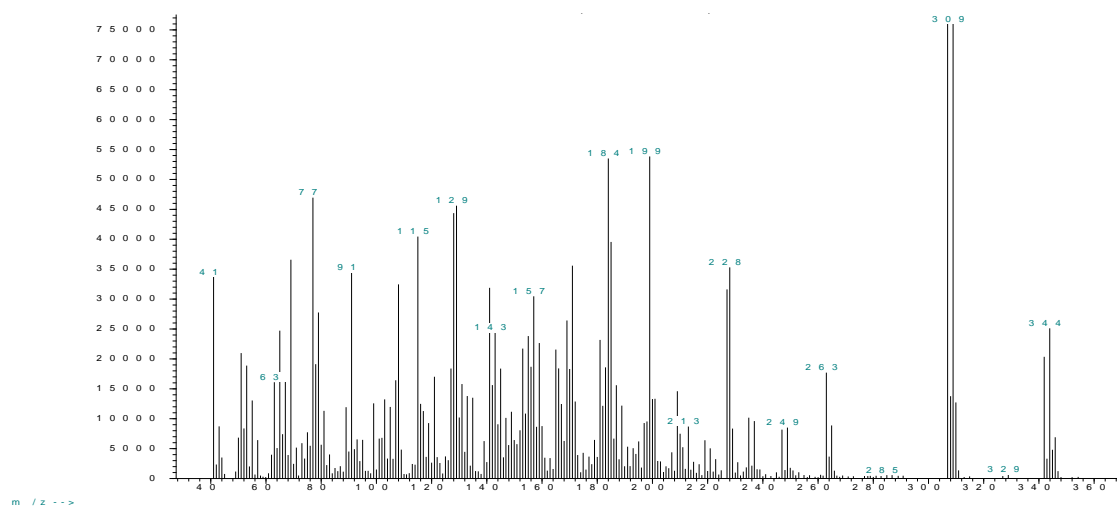


Figure S20. Mass spectrum (LR-EIMS) of compound **4**.

$[M]^+$ observed at m/z 342, 344 and 346

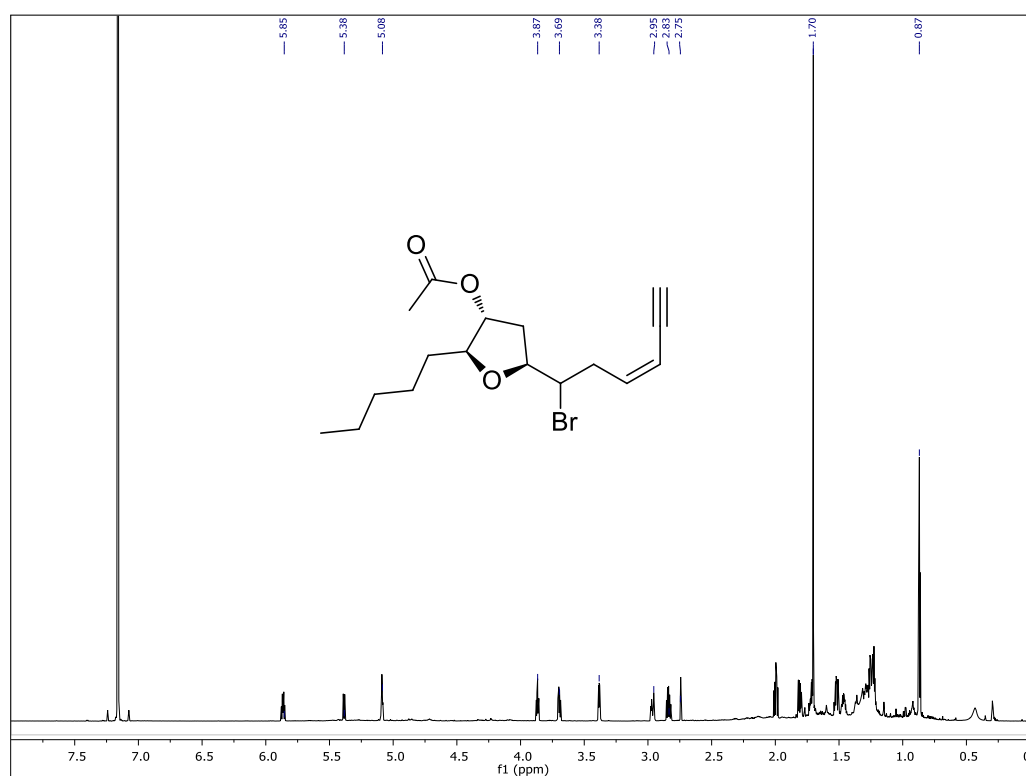


Figure S21. ^1H NMR spectrum (C_6D_6) of compound 5.

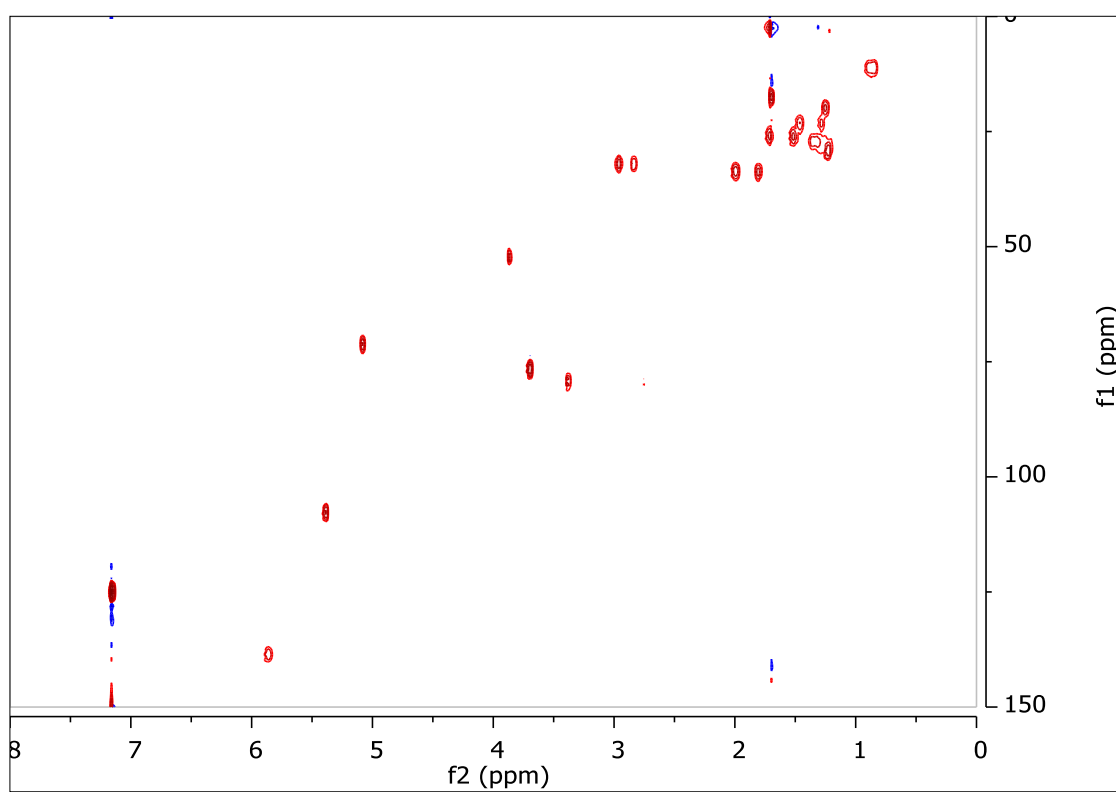


Figure S22. HSQC spectrum (C_6D_6) of compound 5.

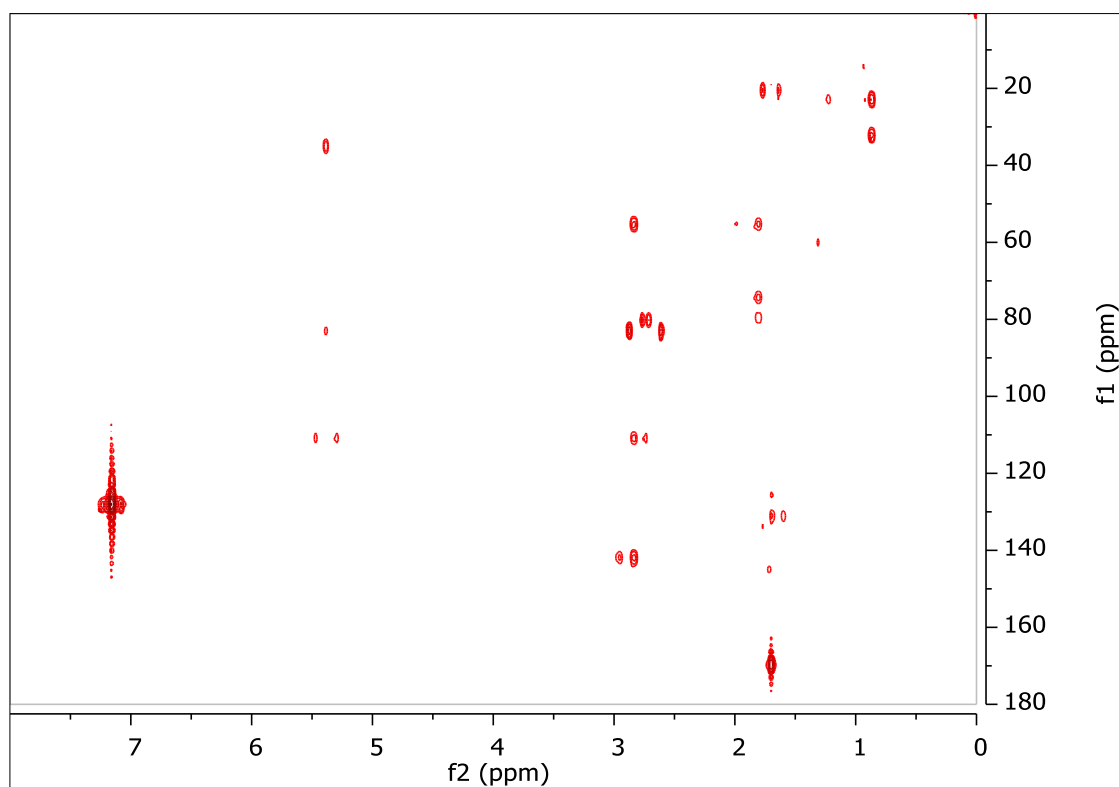


Figure S23. HMBC spectrum (C_6D_6) of compound **5**.

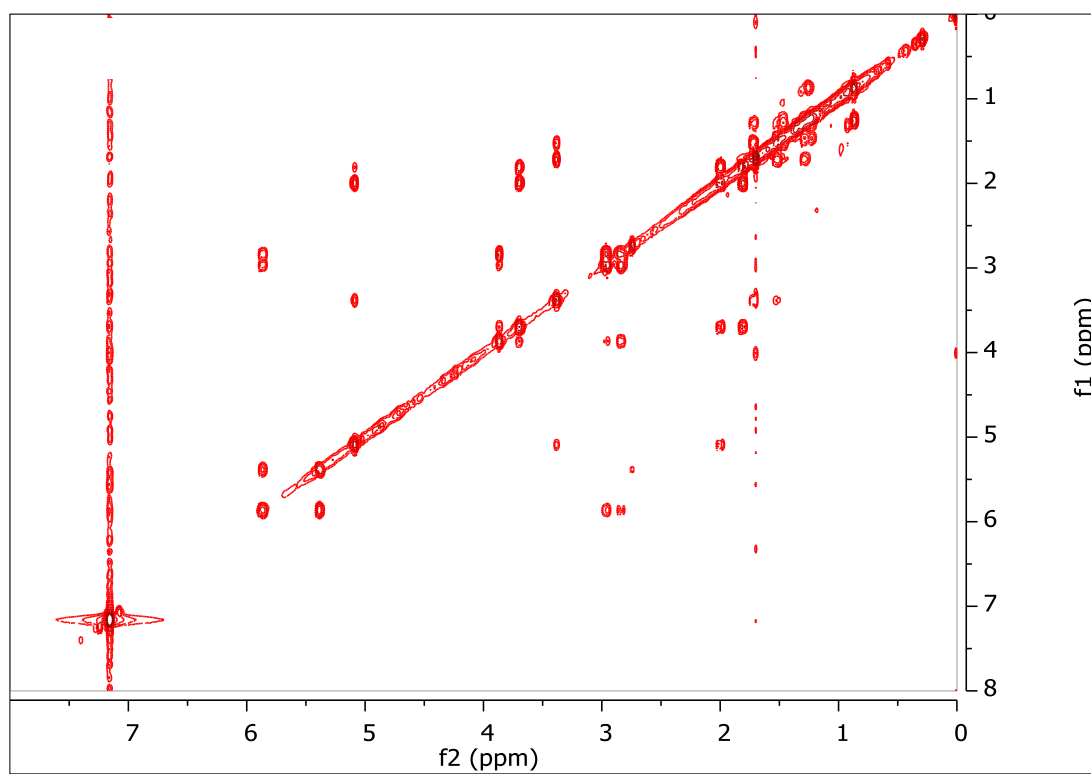


Figure S24. COSY spectrum (C_6D_6) of compound **5**.

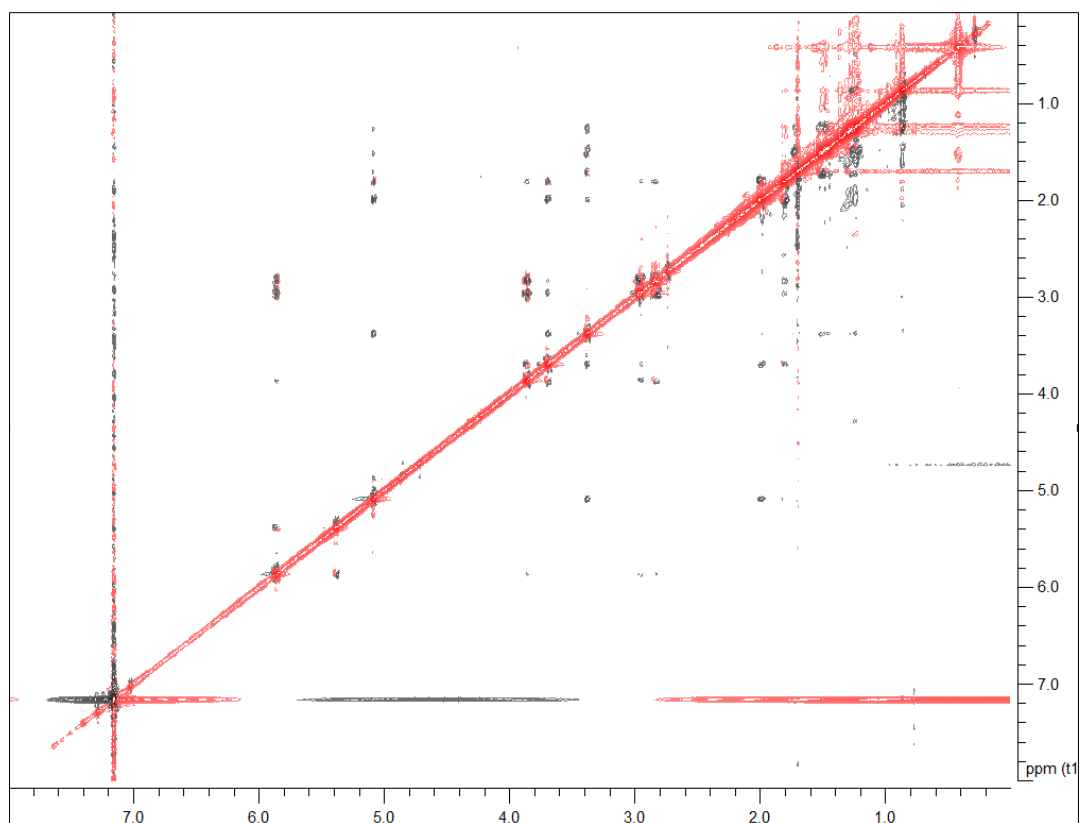


Figure S25. NOESY spectrum (C_6D_6) of compound **5**.

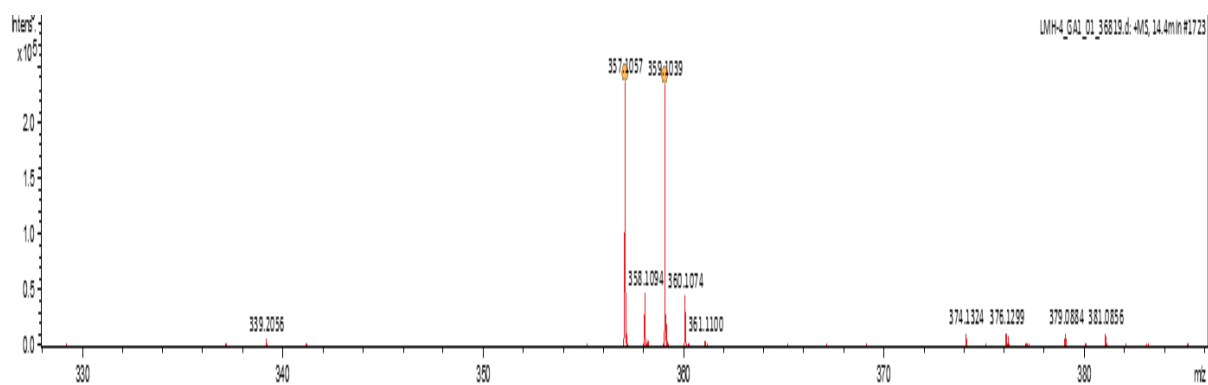


Figure S26. Mass spectrum (HR-ESIMS) of compound **5**.

$[\text{M} + \text{H}]^+$ observed at m/z 357.1057, consistent with $\text{C}_{17}\text{H}_{26}^{79}\text{BrO}_3$

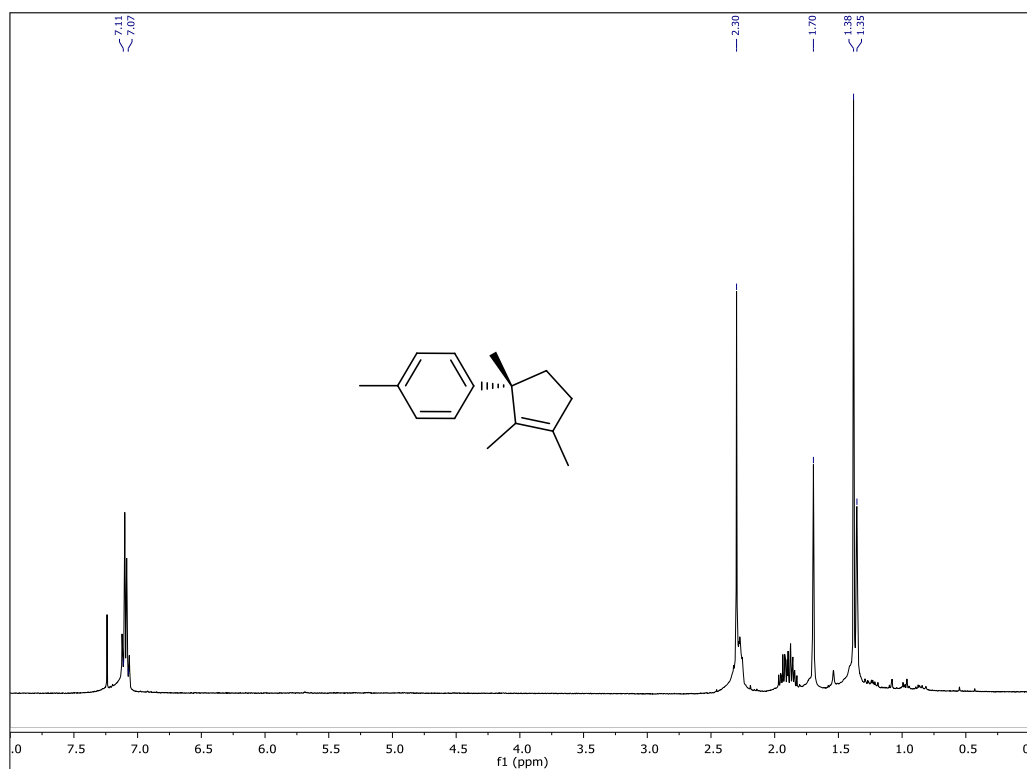


Figure S27. ¹H NMR spectrum (CDCl₃) of compound 6.

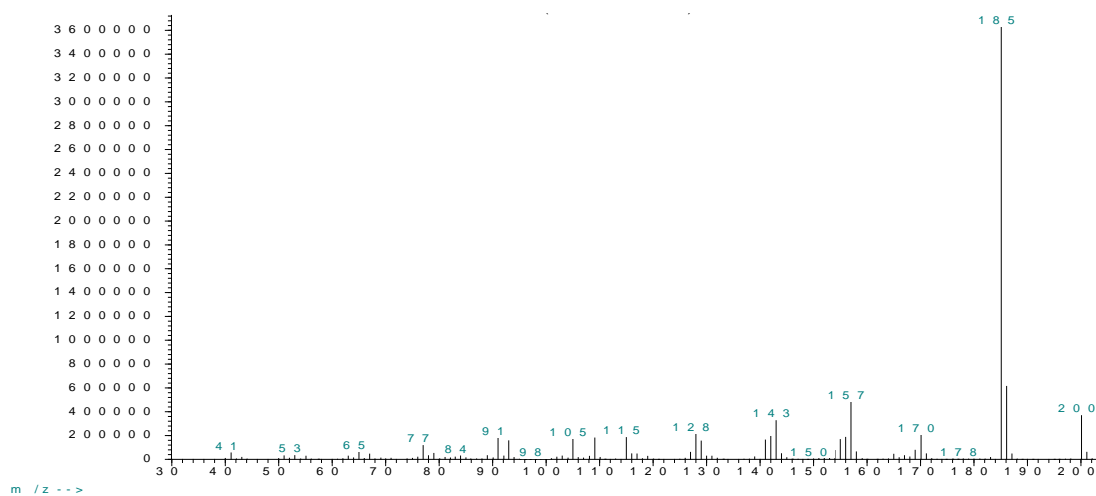


Figure S28. Mass spectrum (LR-EIMS) of compound 6.

[M]⁺ observed at *m/z* 200

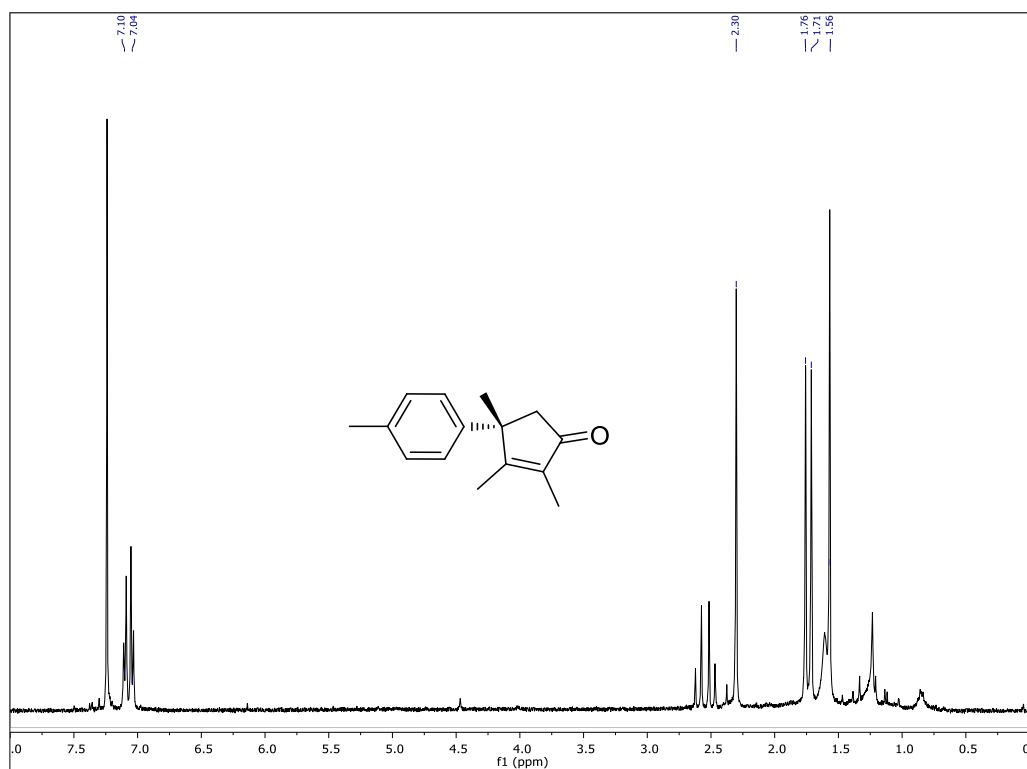


Figure S29. ¹H NMR spectrum (CDCl₃) of compound 7.

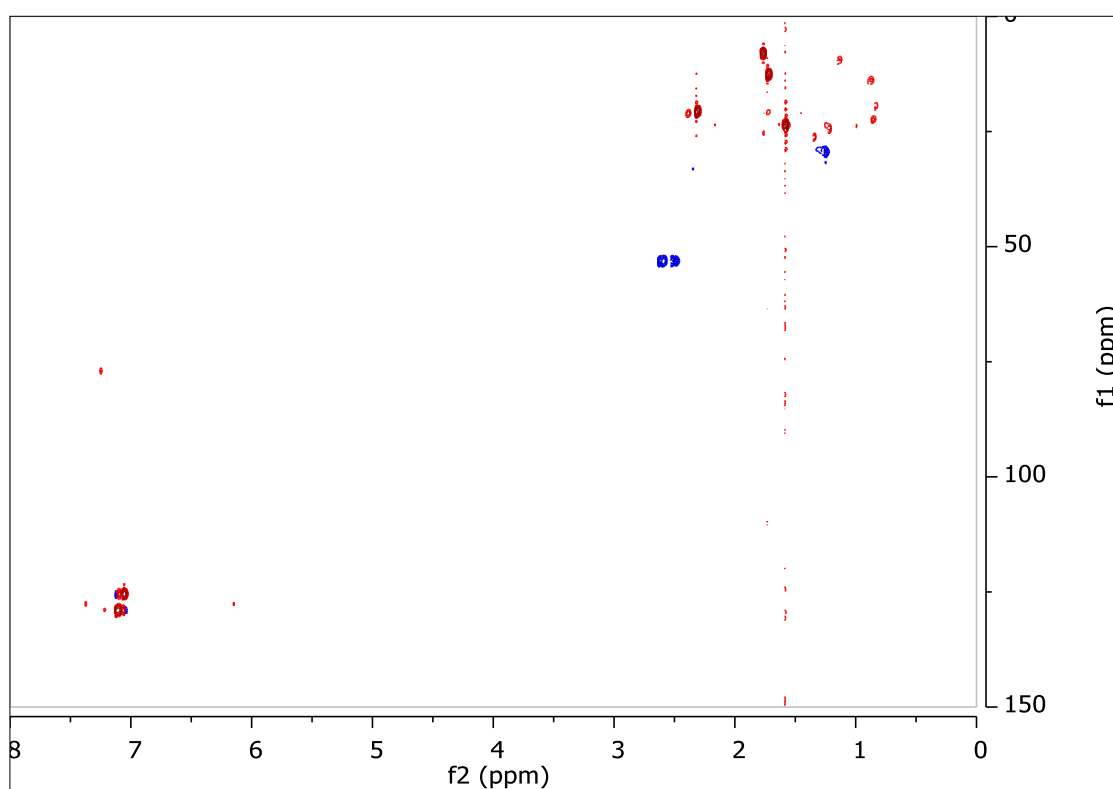


Figure S30. HSQC spectrum (CDCl₃) of compound 7.

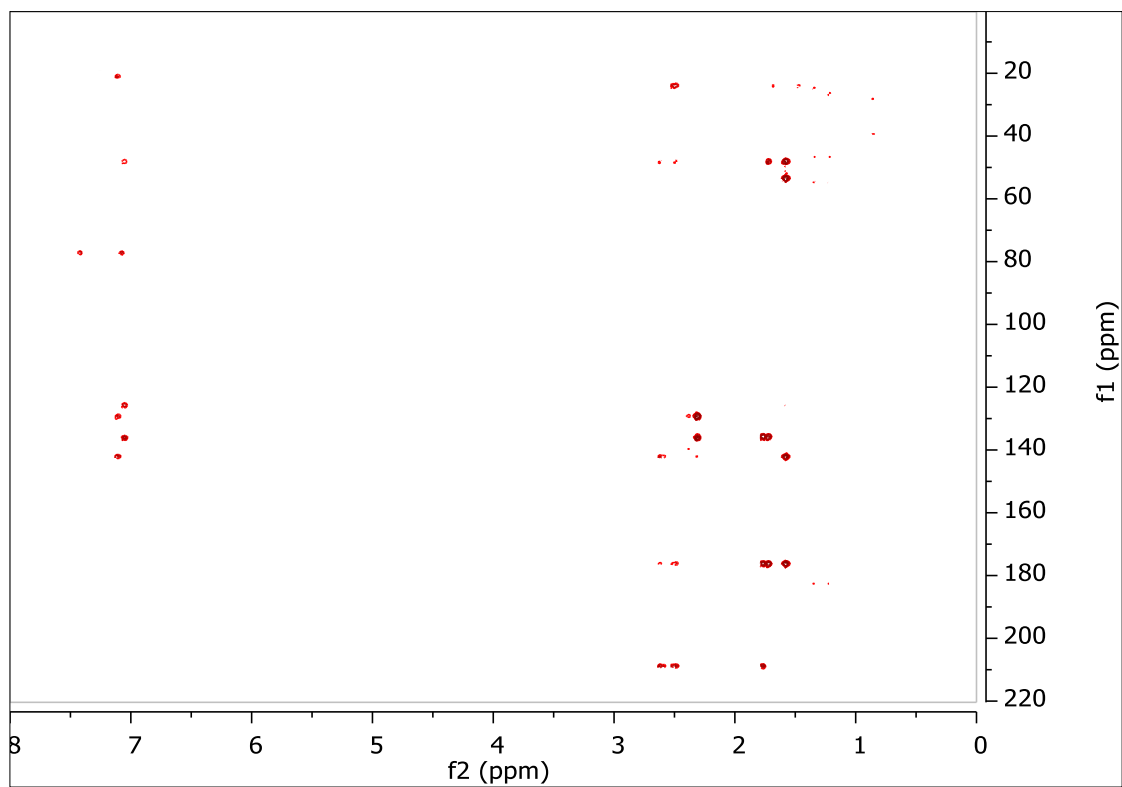


Figure S31. HMBC spectrum (CDCl_3) of compound 7.

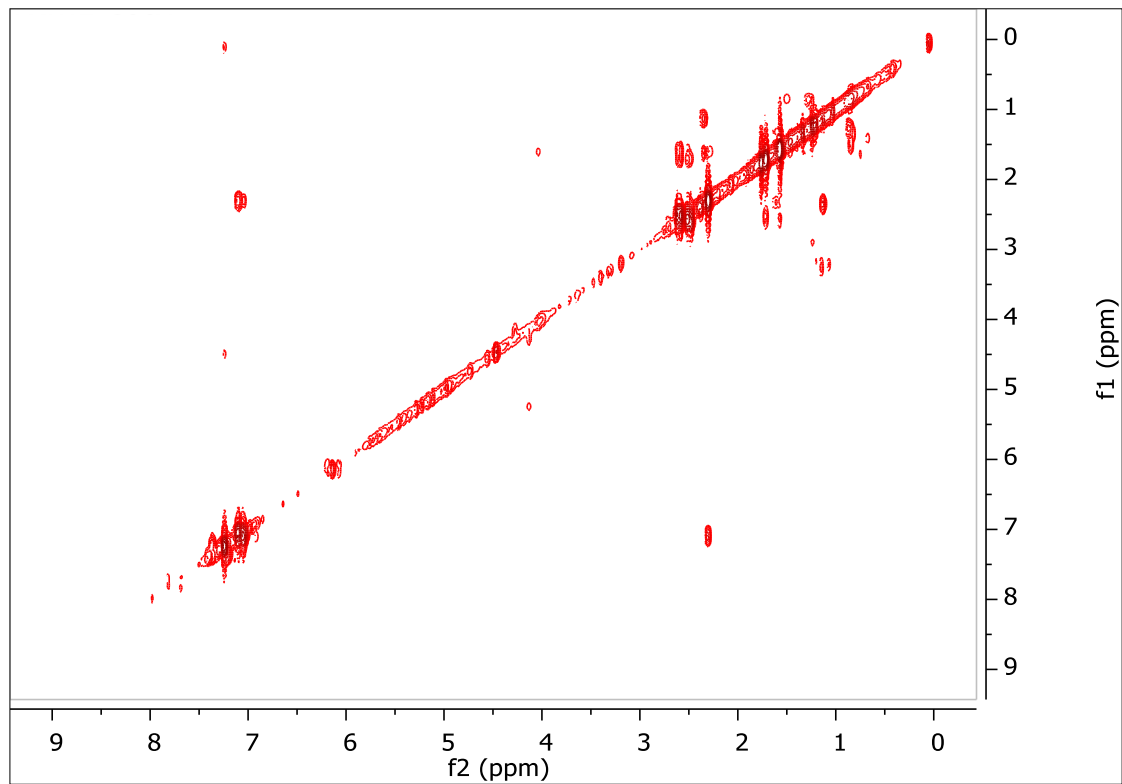


Figure S32. COSY spectrum (CDCl_3) of compound 7.

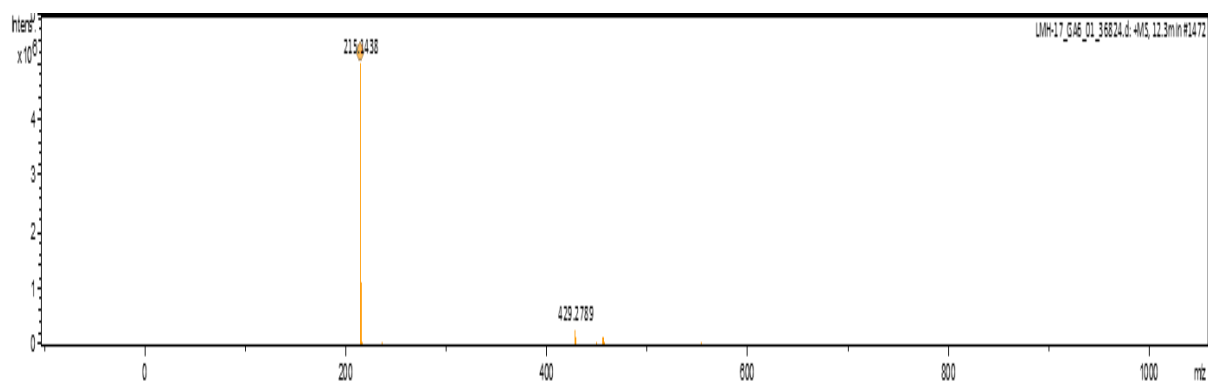


Figure S33. Mass spectrum (HR-ESIMS) of compound 7.
[M + H]⁺ observed at m/z 215.1438, consistent with C₁₅H₁₉O

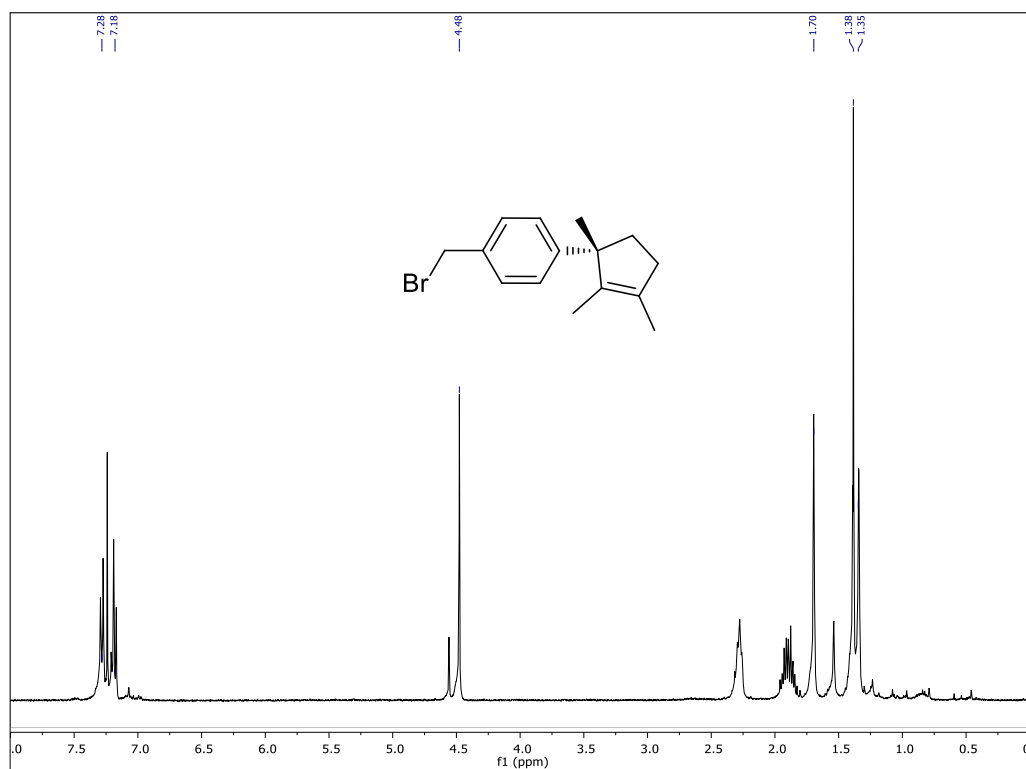


Figure S34. ¹H NMR spectrum (CDCl₃) of compound 8.

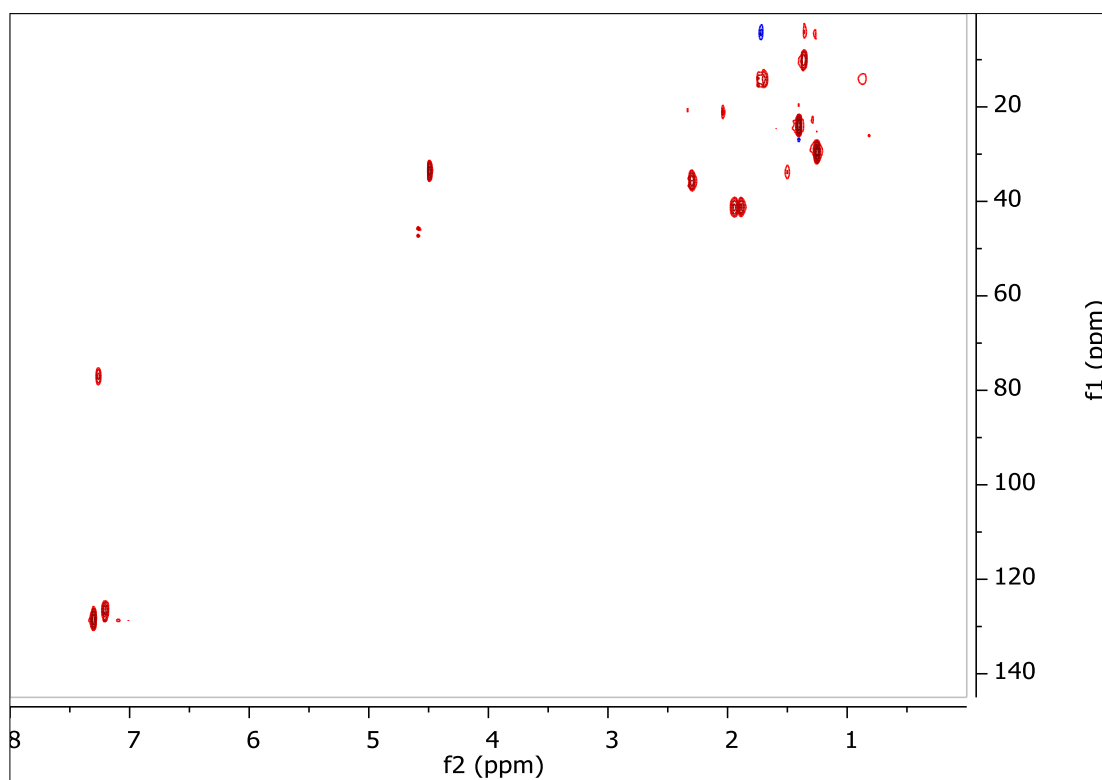


Figure S35. HSQC spectrum (CDCl₃) of compound 8.

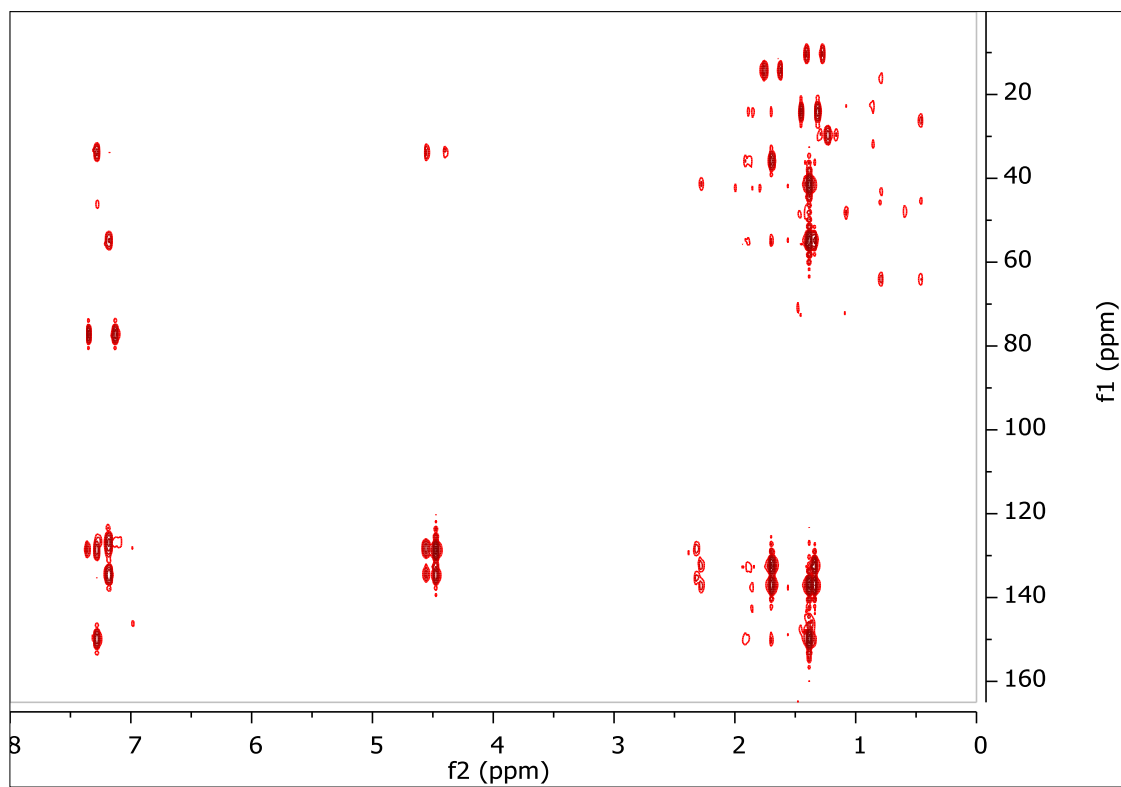


Figure S36. HMBC spectrum (CDCl_3) of compound **8**.

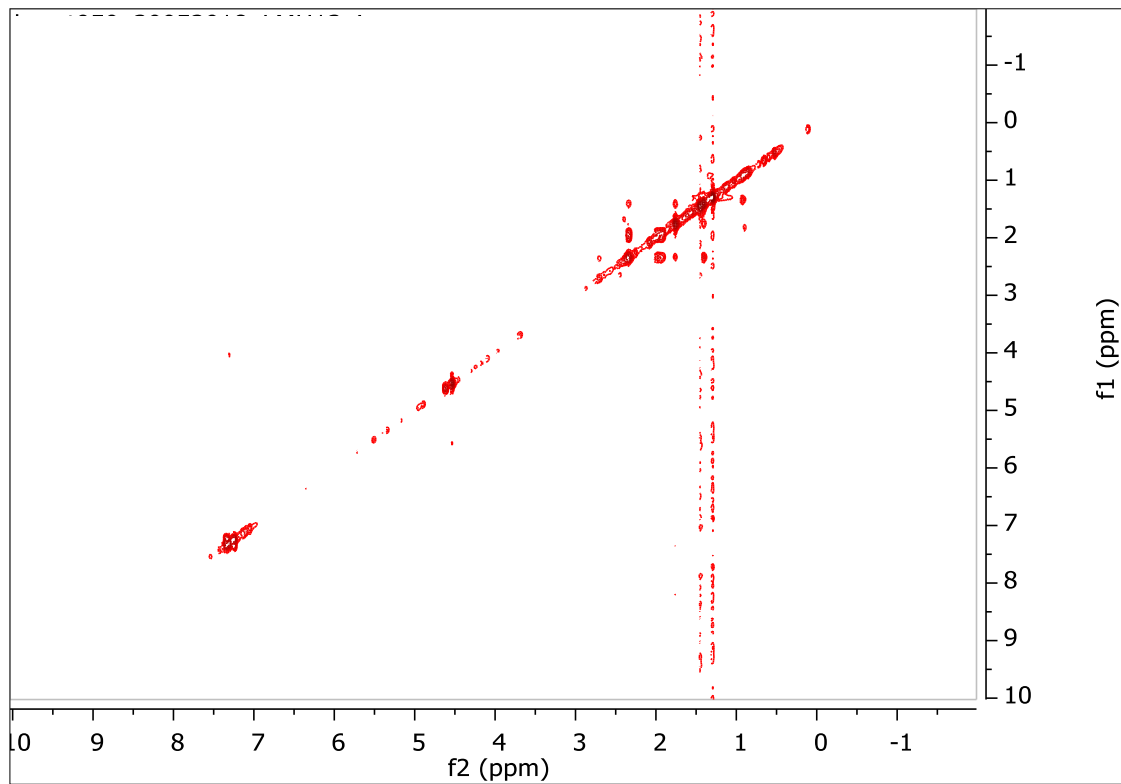


Figure S37. COSY spectrum (CDCl_3) of compound **8**.

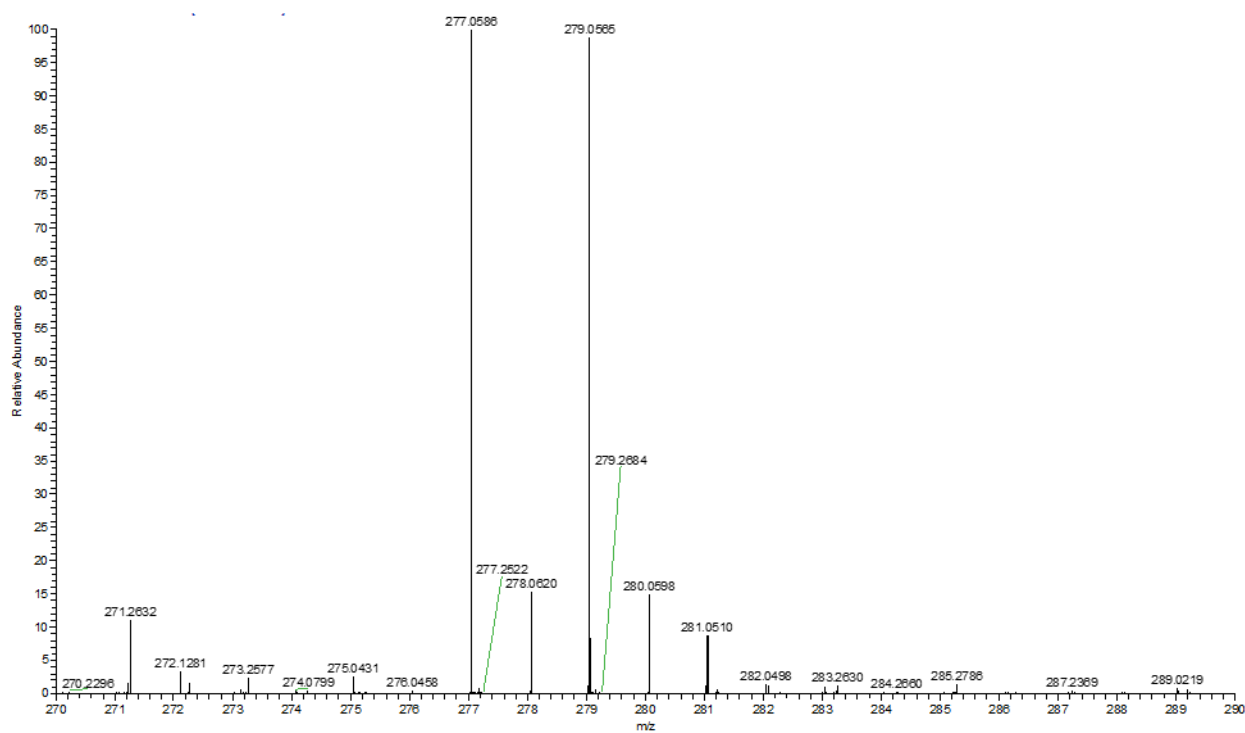


Figure S38. Mass spectrum (HR-APCIMS) of compound 8.

$[M - H]^-$ observed at m/z 277.0586, consistent with $C_{15}H_{18}^{79}Br$

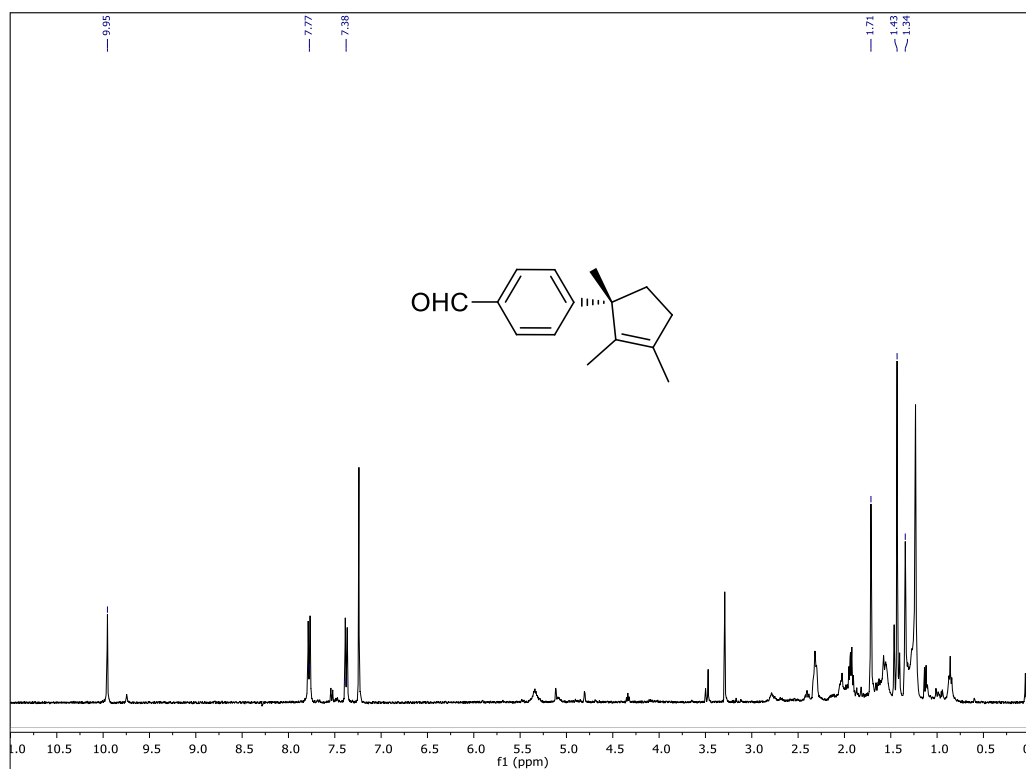


Figure S39. ¹H NMR spectrum (CDCl₃) of compound 9.

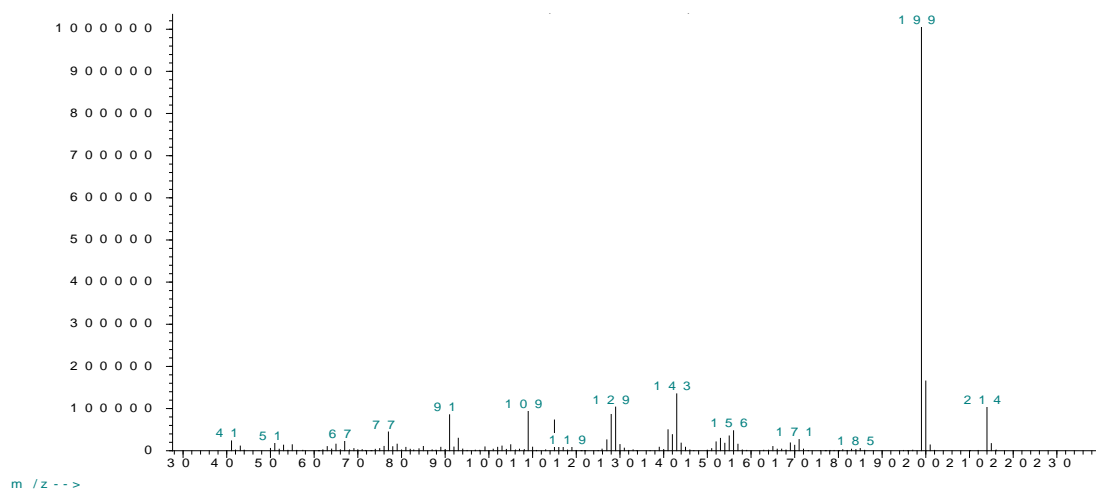


Figure S40. Mass spectrum (LR-EIMS) of compound 9.

[M]⁺ observed at *m/z* 214

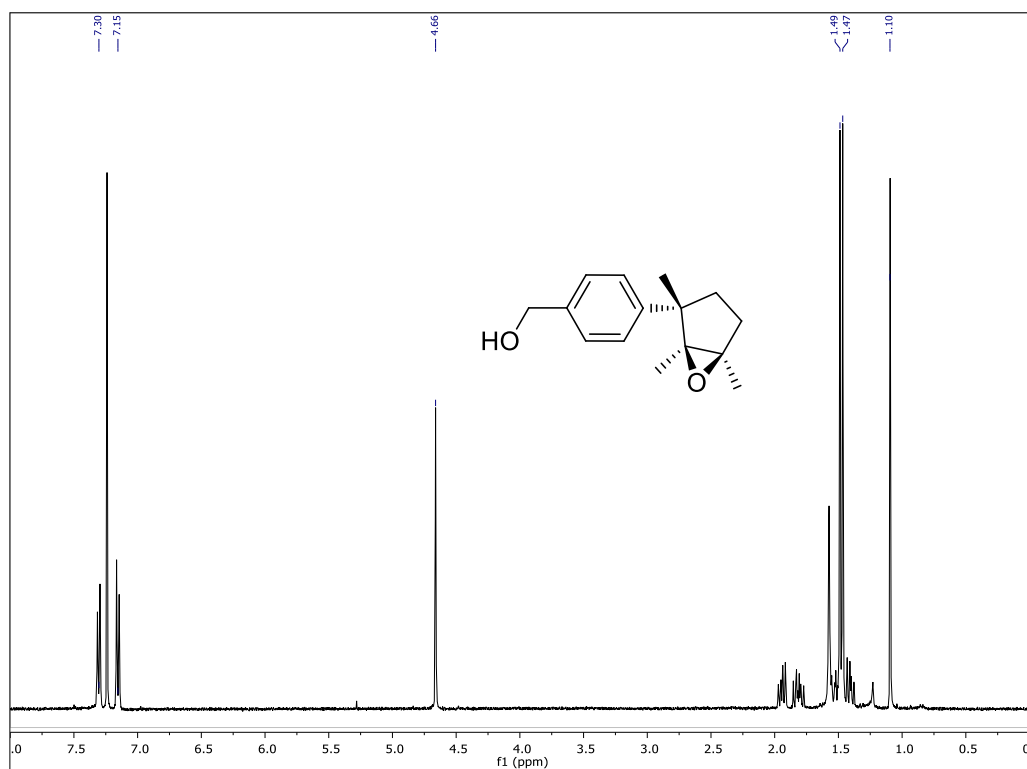


Figure S41. ¹H NMR spectrum (CDCl₃) of compound 10.

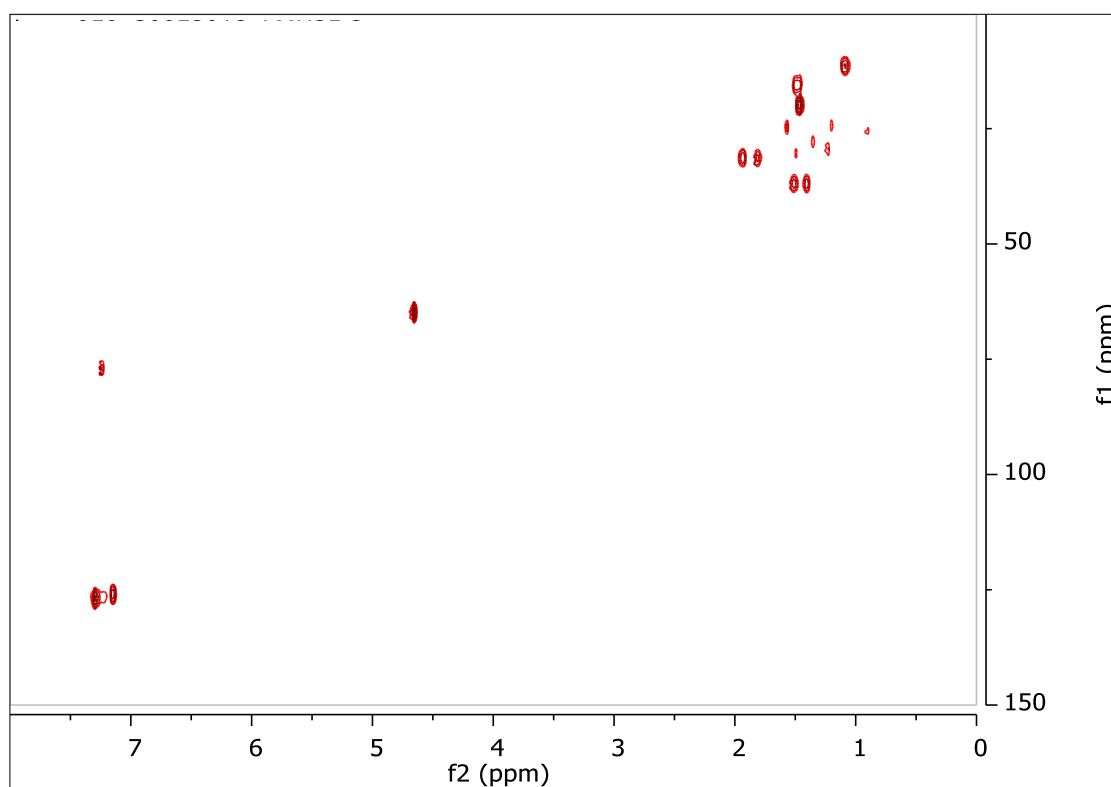


Figure S42. HSQC spectrum (CDCl₃) of compound 10.

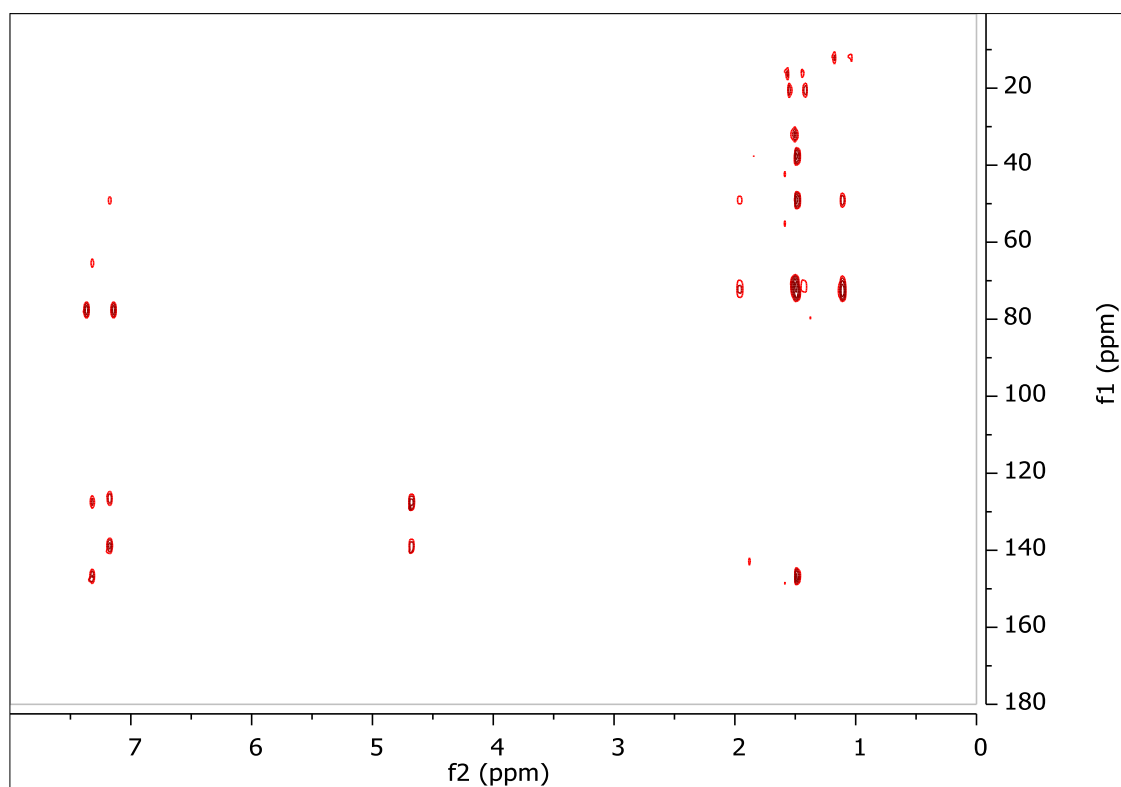


Figure S43. HMBC spectrum (CDCl₃) of compound 10.

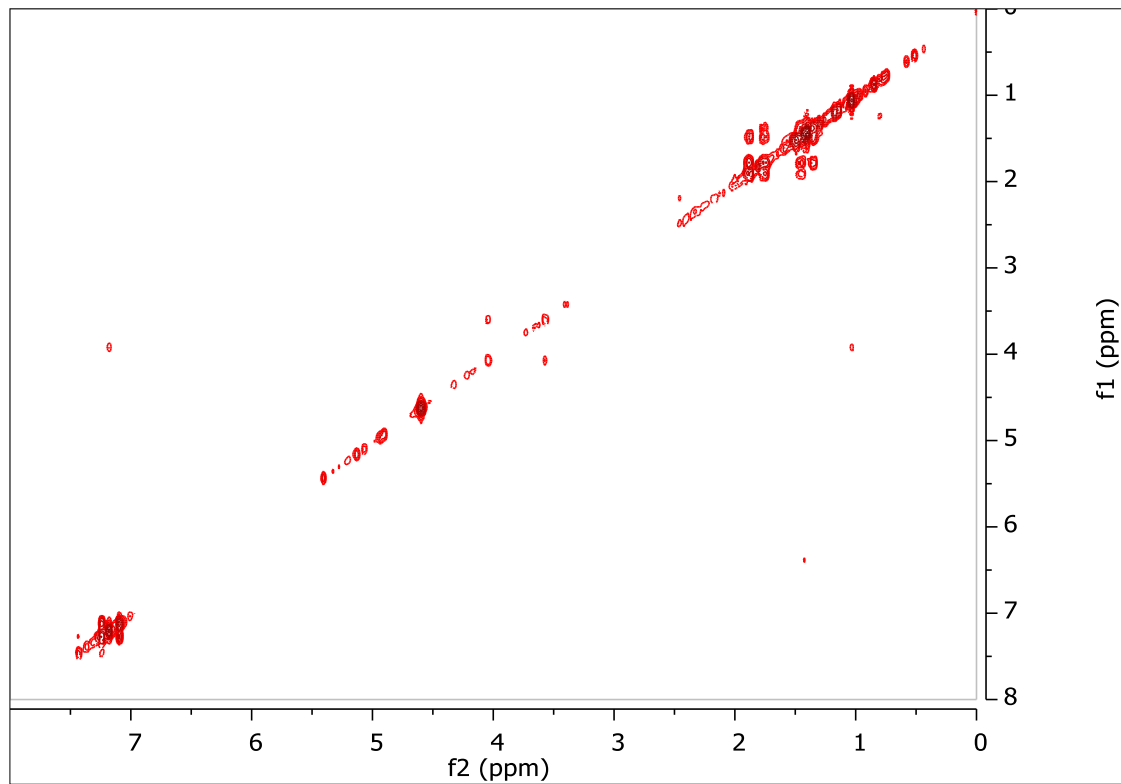


Figure S44. COSY spectrum (CDCl₃) of compound 10.

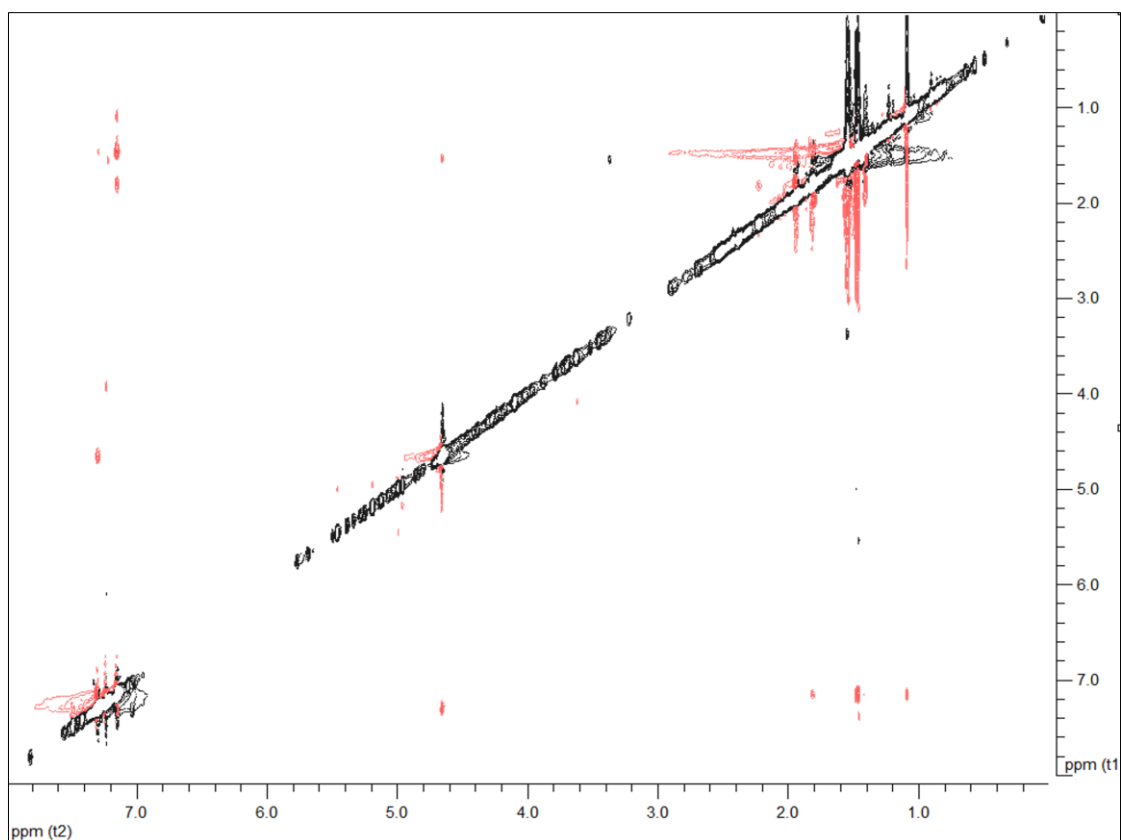


Figure S45. NOESY spectrum (CDCl₃) of compound **10**.

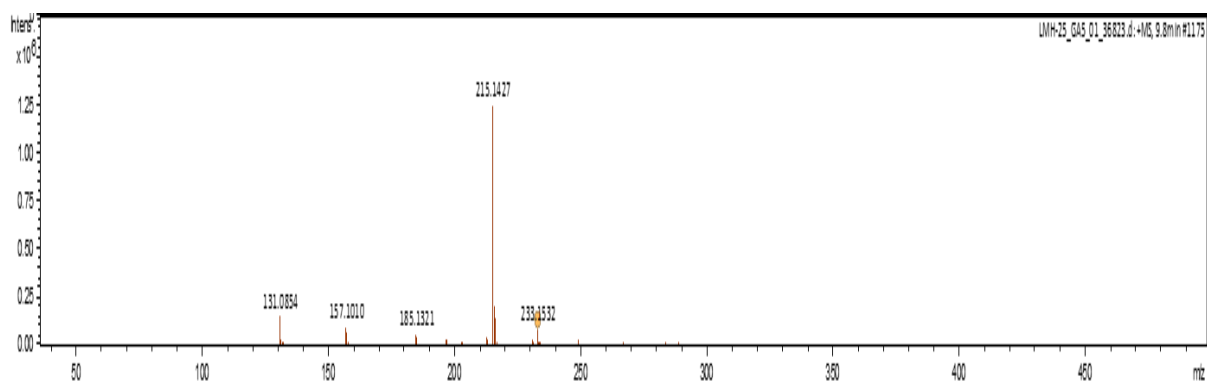


Figure S46. Mass spectrum (HR-ESIMS) of compound **10**.

[M + H]⁺ observed at m/z 233.1532, consistent with C₁₅H₂₁O₂

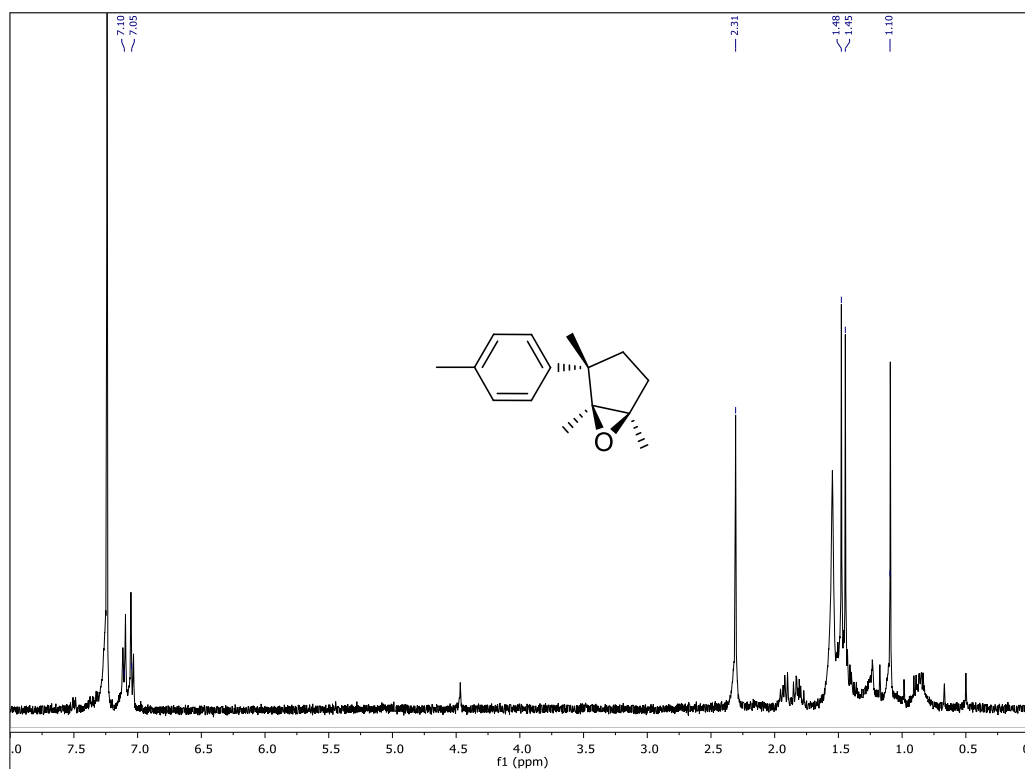


Figure S47. ^1H NMR spectrum (CDCl_3) of compound **11**.

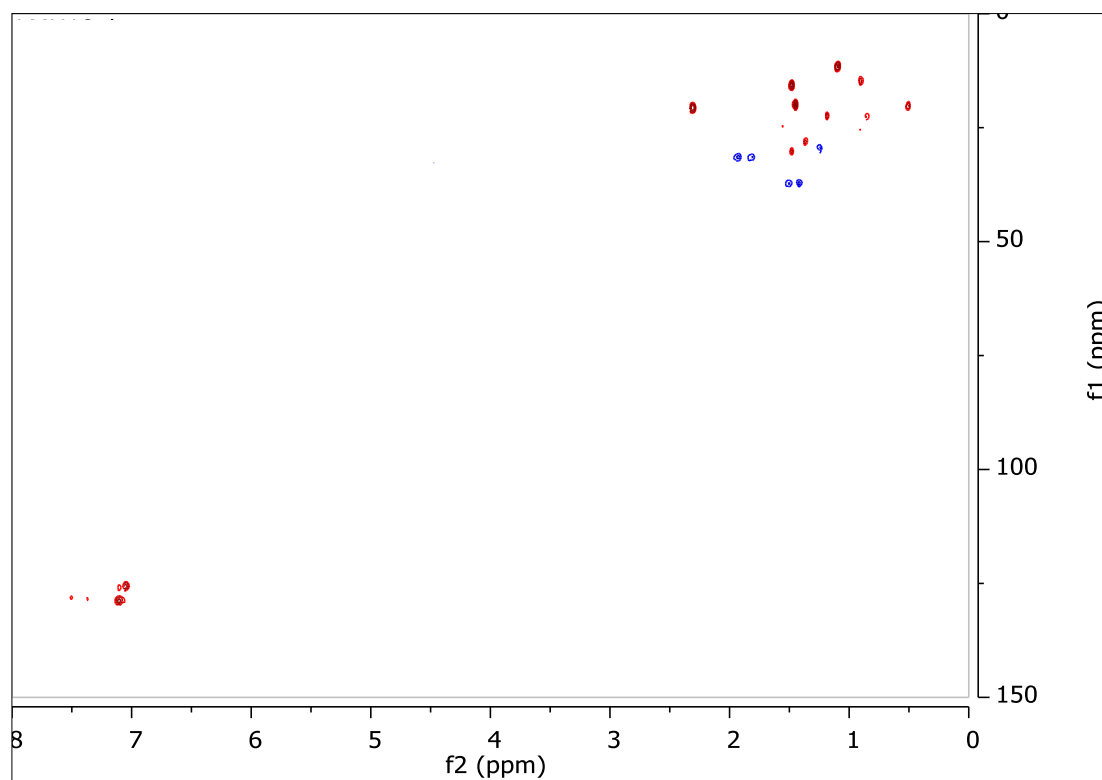


Figure S48. HSQC spectrum (CDCl_3) of compound **11**.

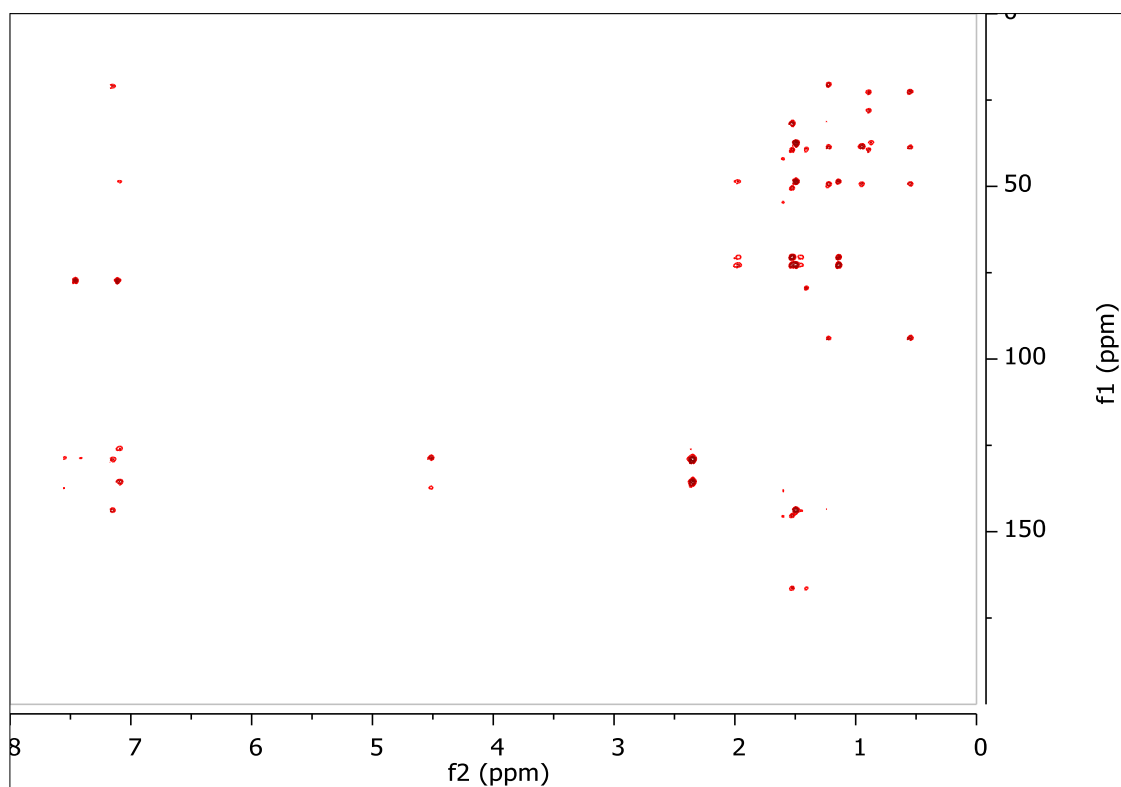


Figure S49. HMBC spectrum (CDCl_3) of compound **11**.

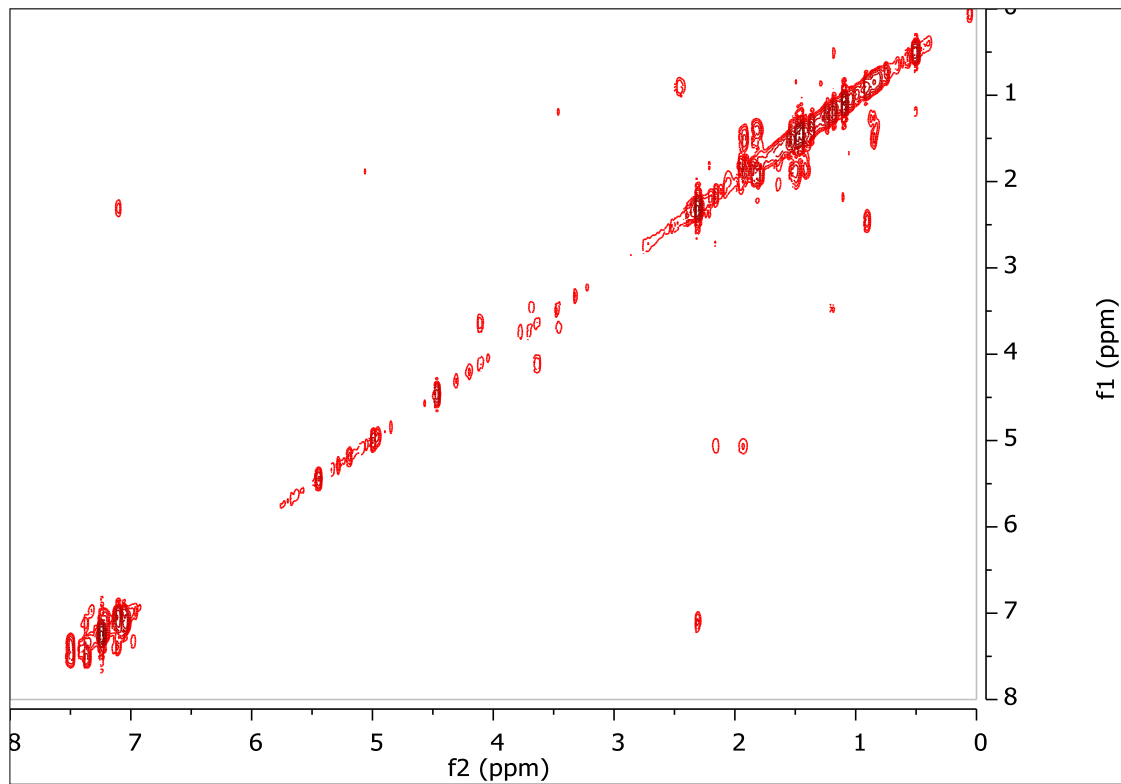


Figure S50. COSY spectrum (CDCl_3) of compound **11**.

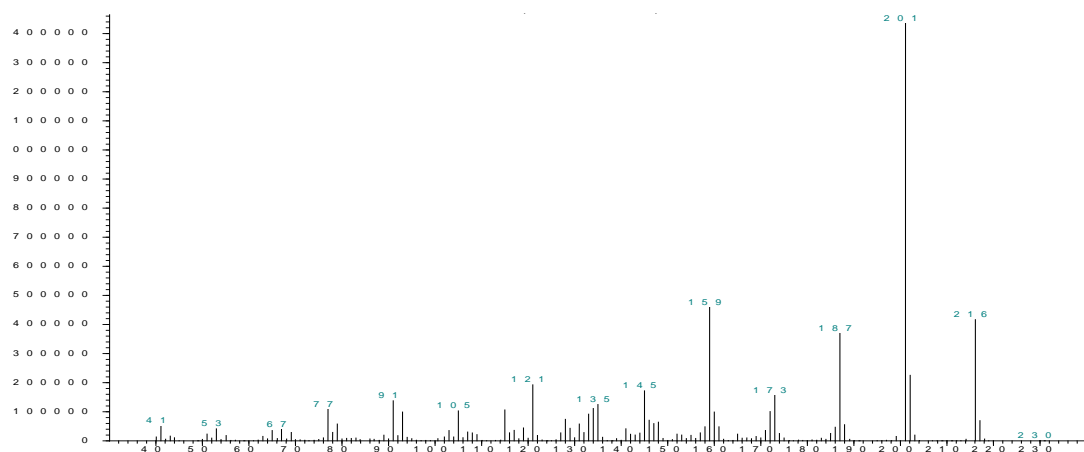


Figure S51. Mass spectrum (LR-EIMS) of compound **11**.

$[M]^+$ observed at m/z 216

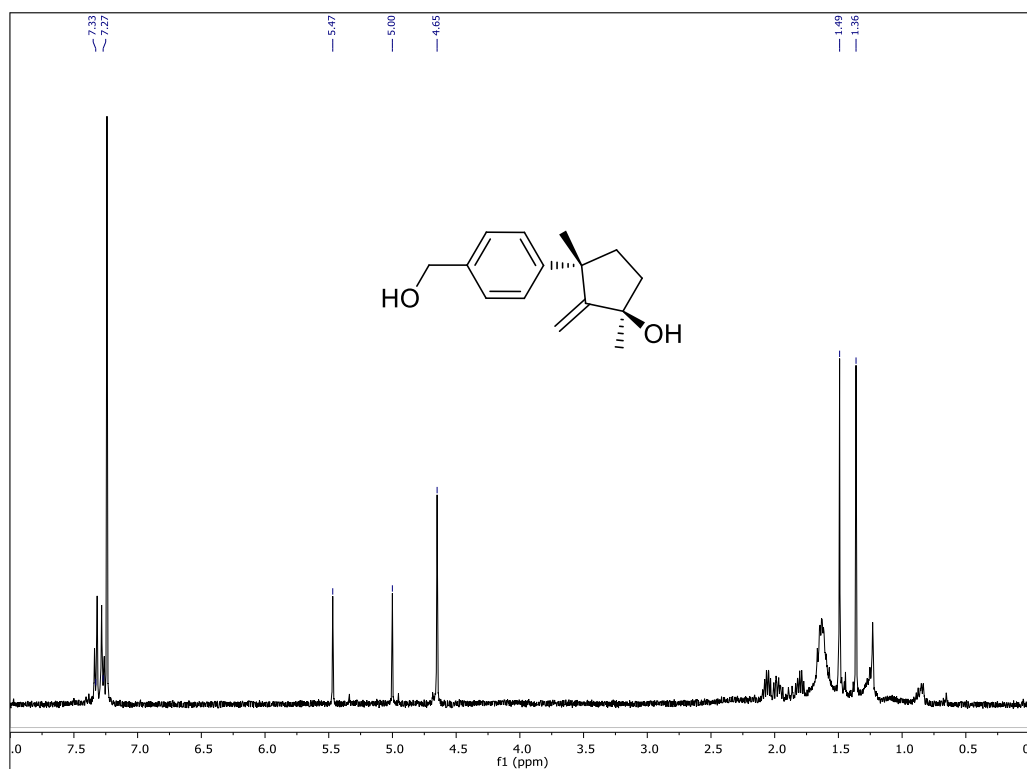


Figure S52. ¹H NMR spectrum (CDCl₃) of compound 12.

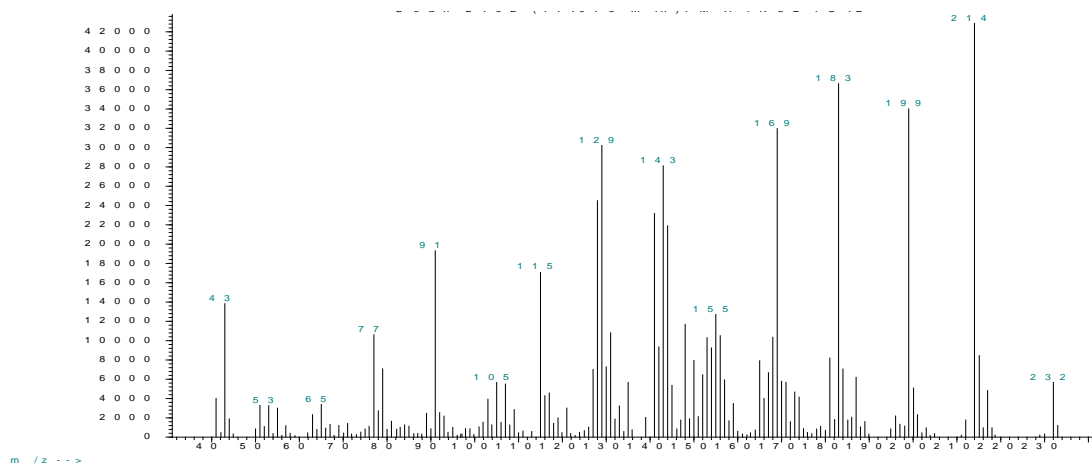


Figure S53. Mass spectrum (LR-EIMS) of compound 12.

[M]⁺ observed at m/z 232

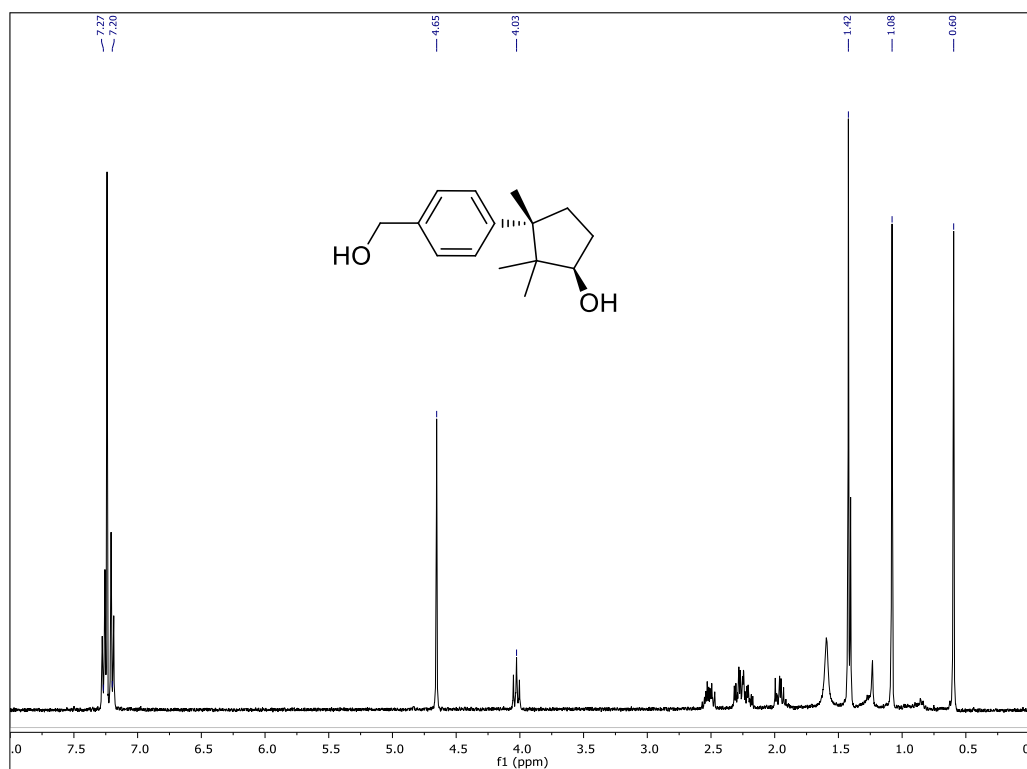


Figure S54. ¹H NMR spectrum (CDCl₃) of compound 13.

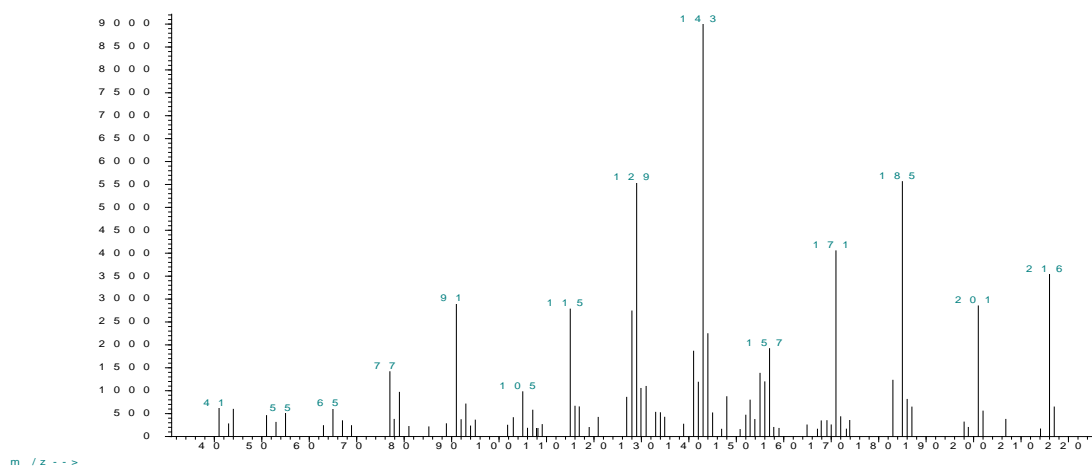


Figure S55. Mass spectrum (LR-EIMS) of compound 13.

[M-H₂O]⁺ observed at *m/z* 216

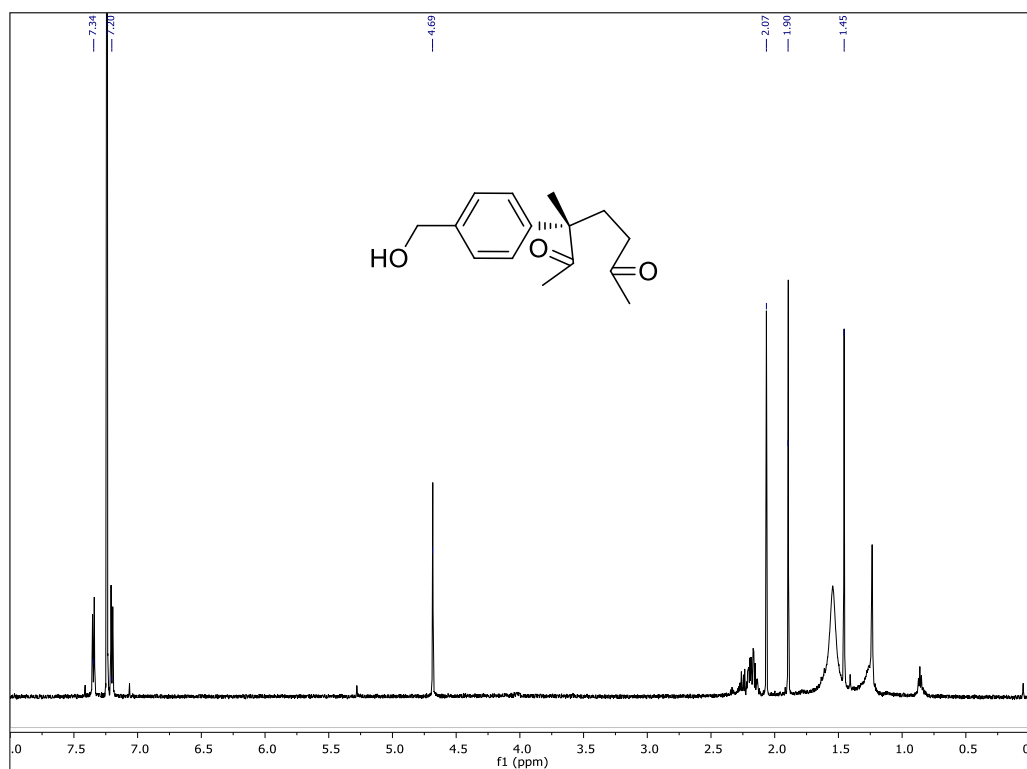


Figure S56. ^1H NMR spectrum (CDCl_3) of compound **14**.

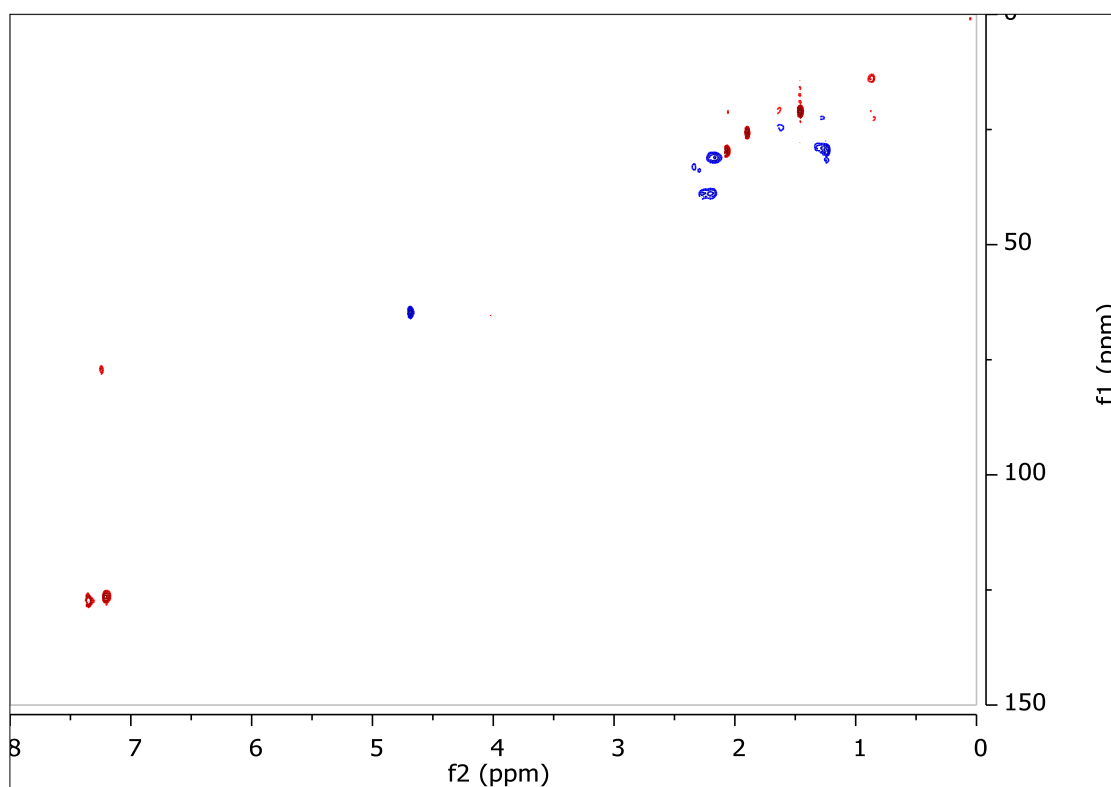


Figure S57. HSQC spectrum (CDCl_3) of compound **14**.

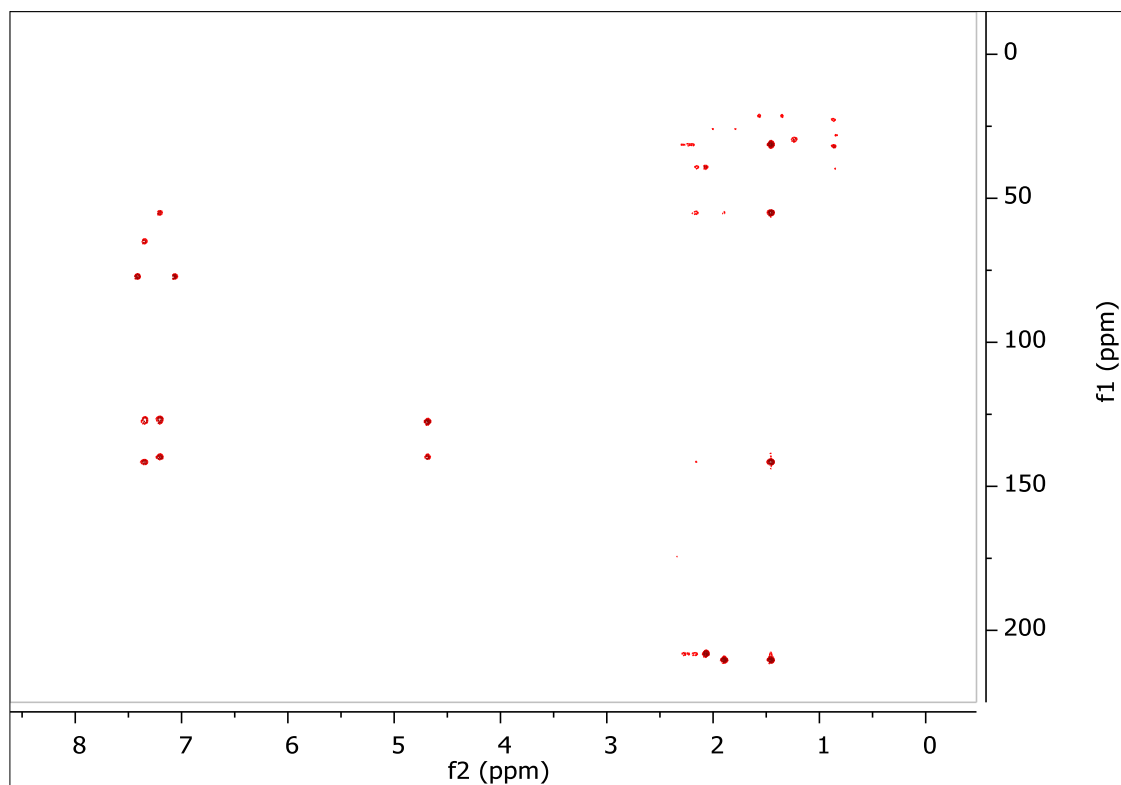


Figure S58. HMBC spectrum (CDCl_3) of compound **14**.

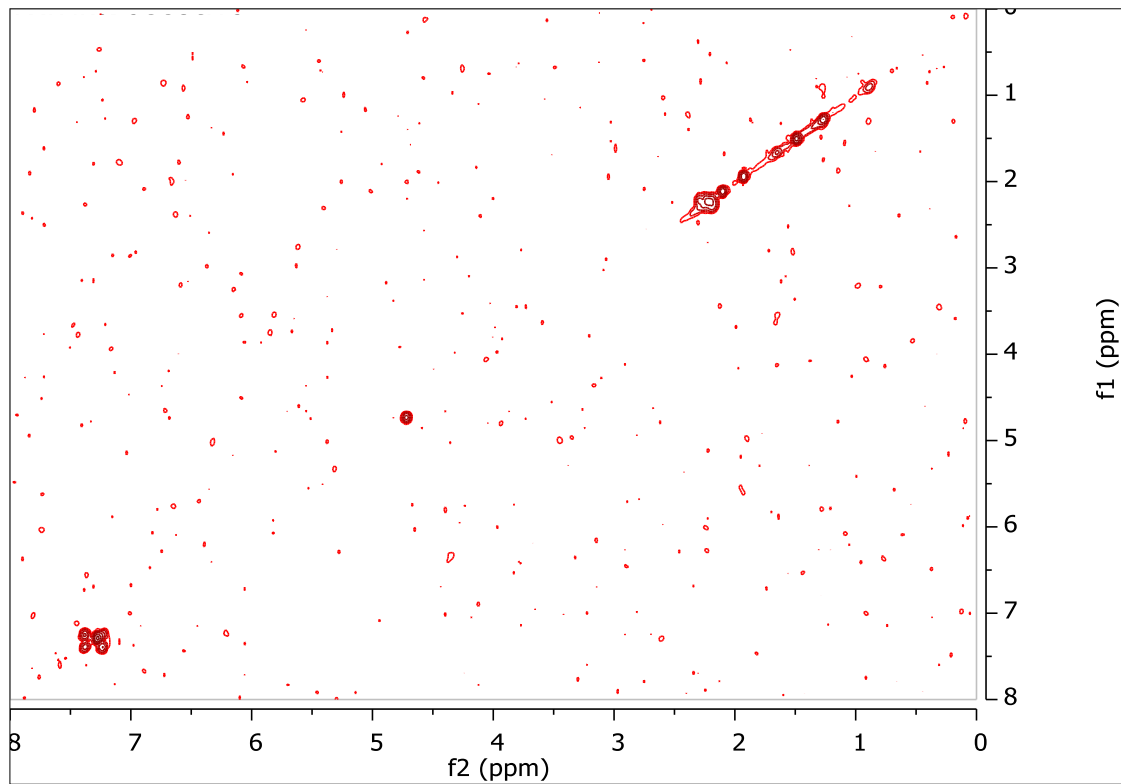


Figure S59. COSY spectrum (CDCl_3) of compound **14**.

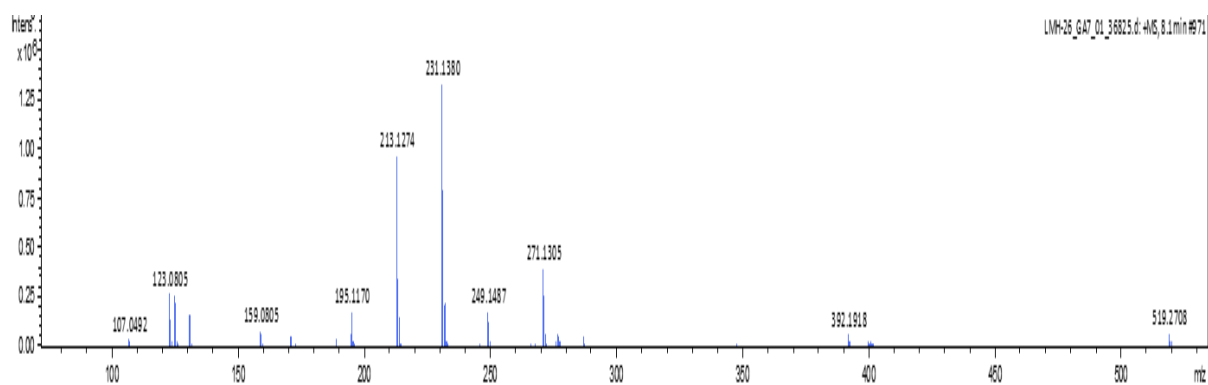


Figure S60. Mass spectrum (HR-ESIMS) of compound **14**.
[M + H]⁺ observed at m/z 249.1487, consistent with C₁₅H₂₁O₃

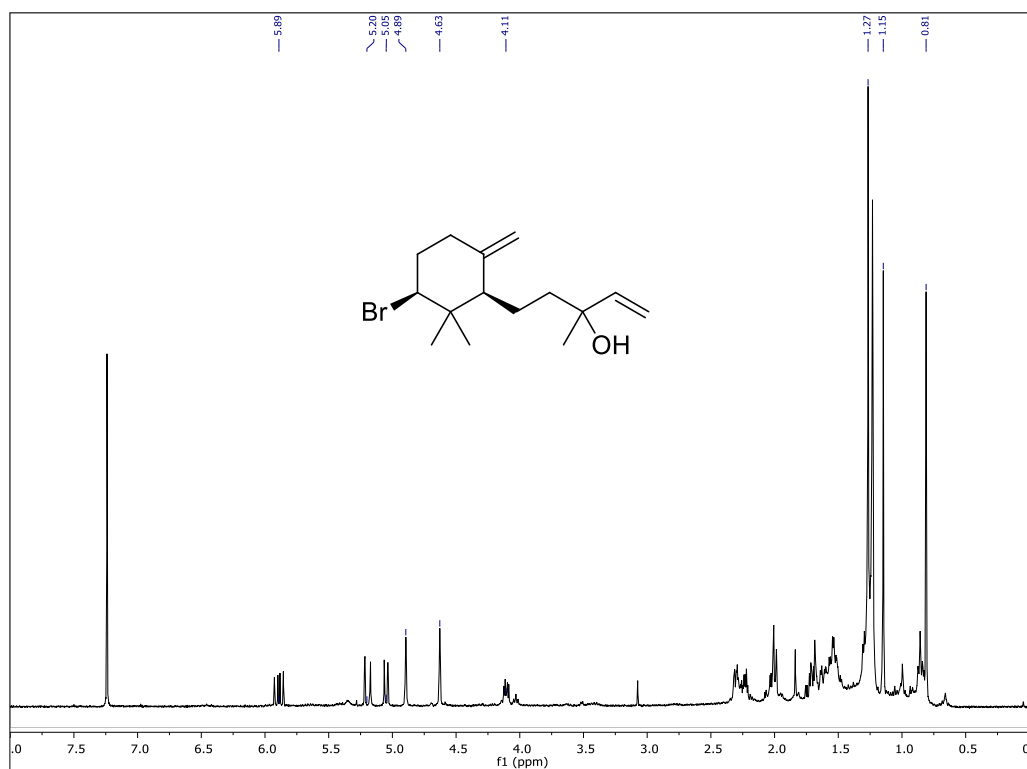


Figure S61. ¹H NMR spectrum (CDCl₃) of compound 15.

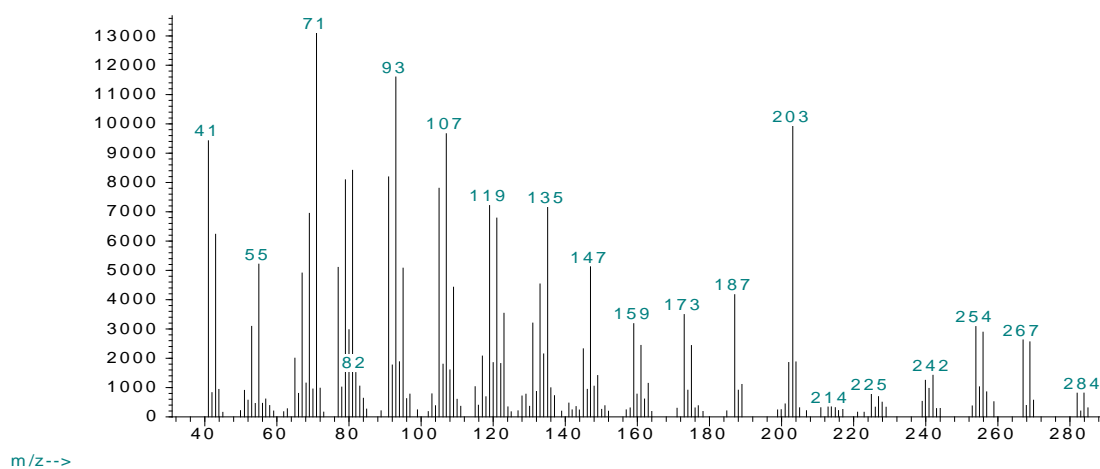


Figure S62. Mass spectrum (LR-EIMS) of compound 15.

[M-H₂O]⁺ observed at *m/z* 282 and 284

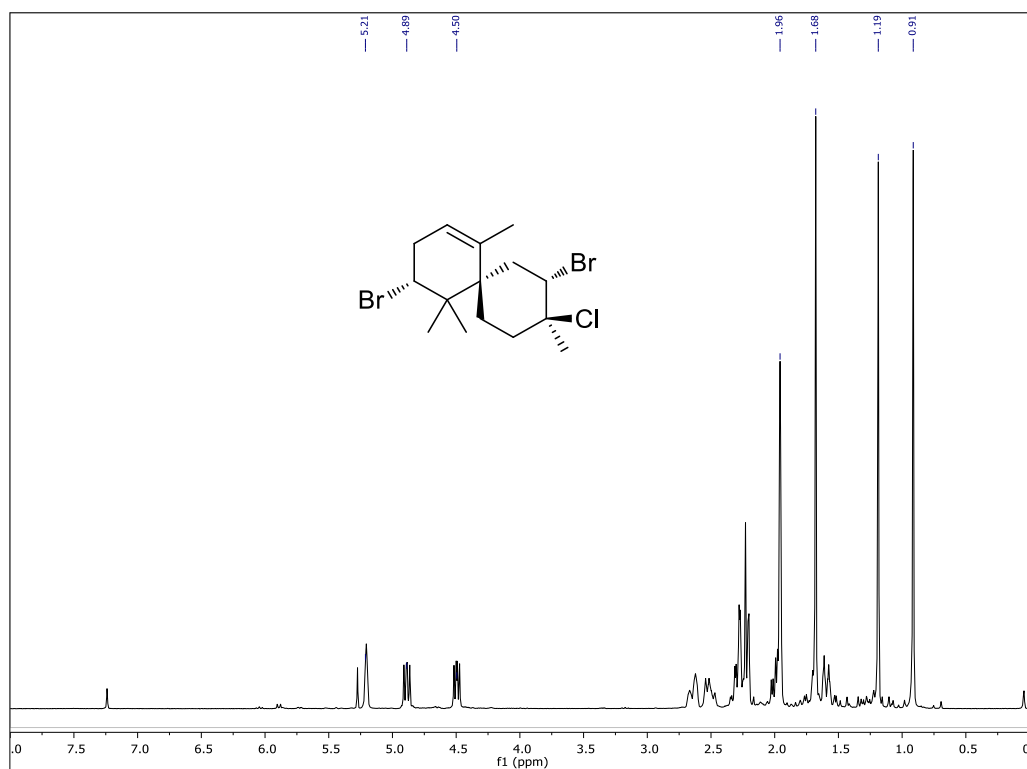


Figure S63. ¹H NMR spectrum (CDCl₃) of compound 16.

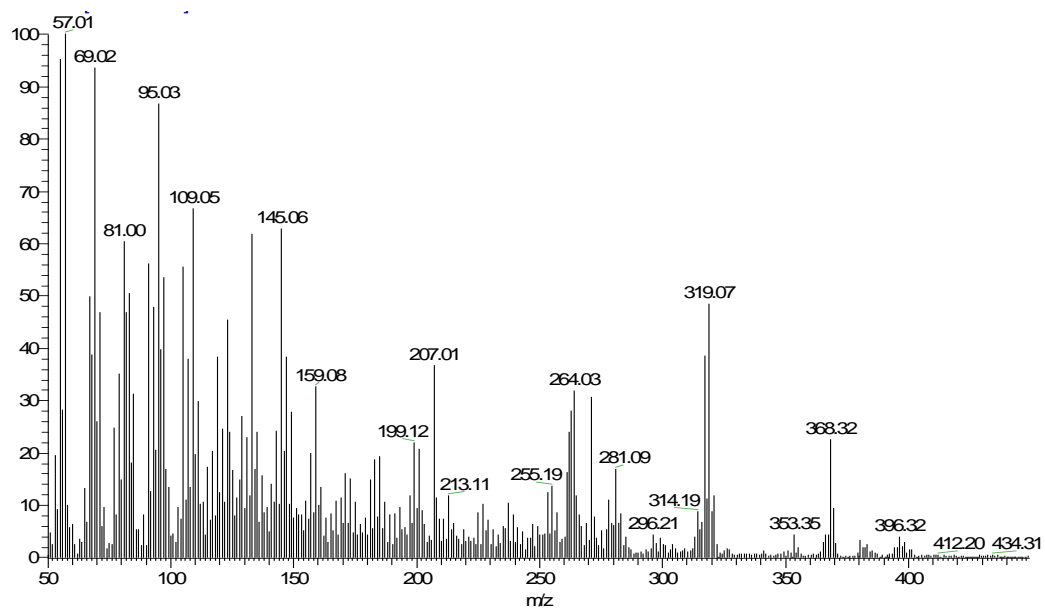


Figure S64. Mass spectrum (LR-EIMS) of compound 16.

[M]⁺ observed at *m/z* 396, 398, 400 and 402

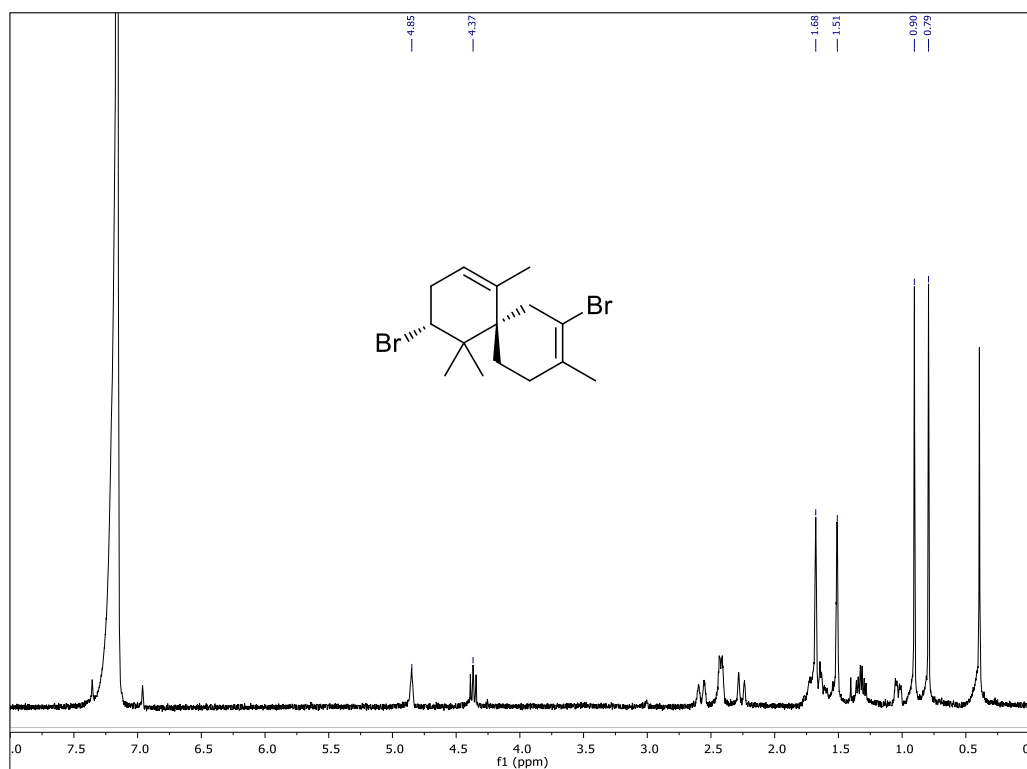


Figure S65. ¹H NMR spectrum (C₆D₆) of compound 17.

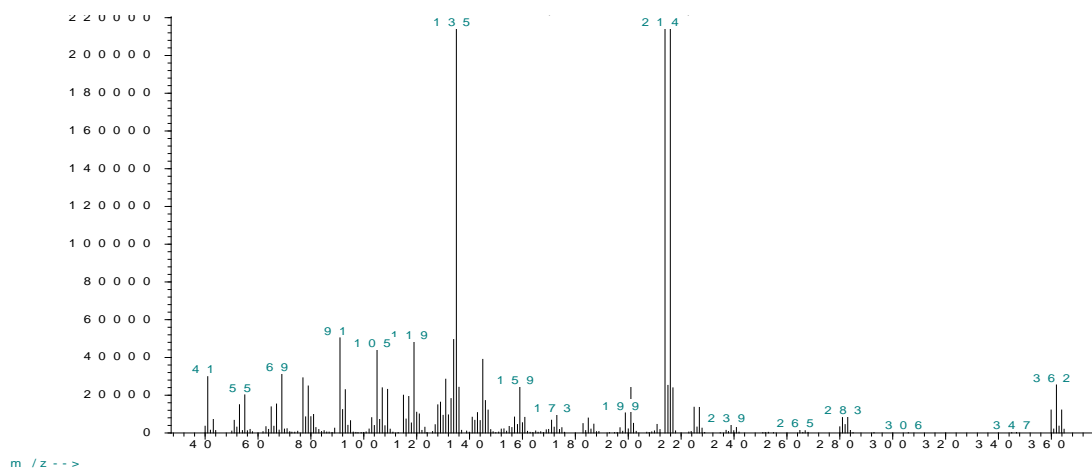


Figure S66. Mass spectrum (LR-EIMS) of compound 17.

[M]⁺ observed at *m/z* 360, 362 and 364

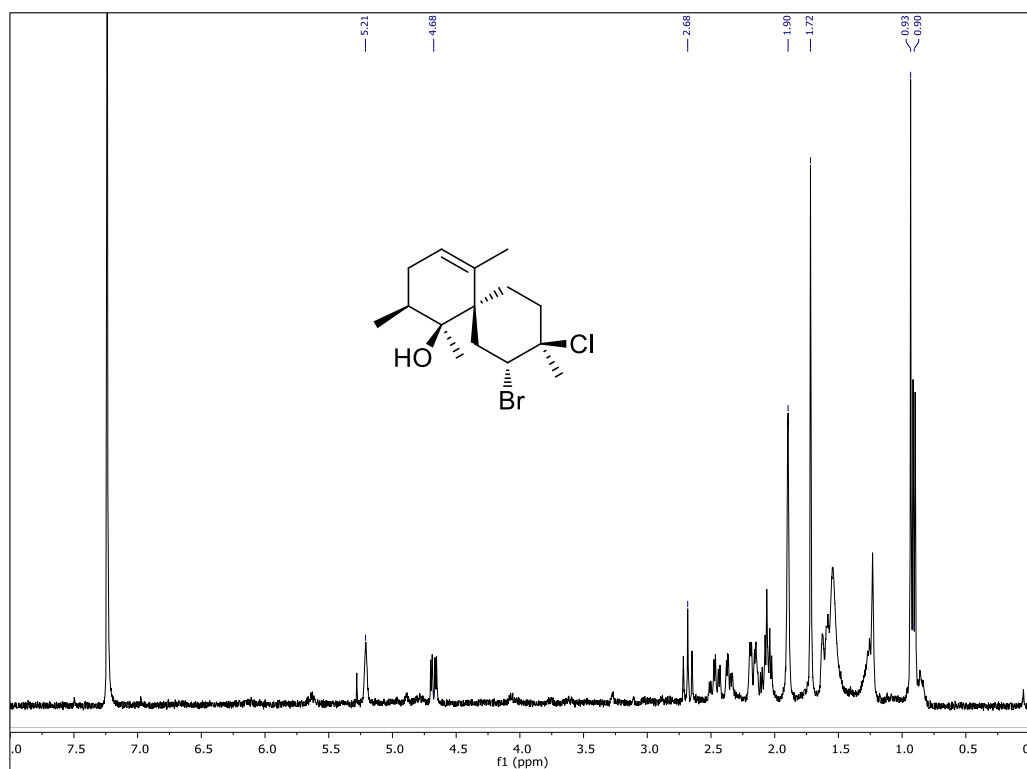


Figure S67. ¹H NMR spectrum (CDCl₃) of compound 18.

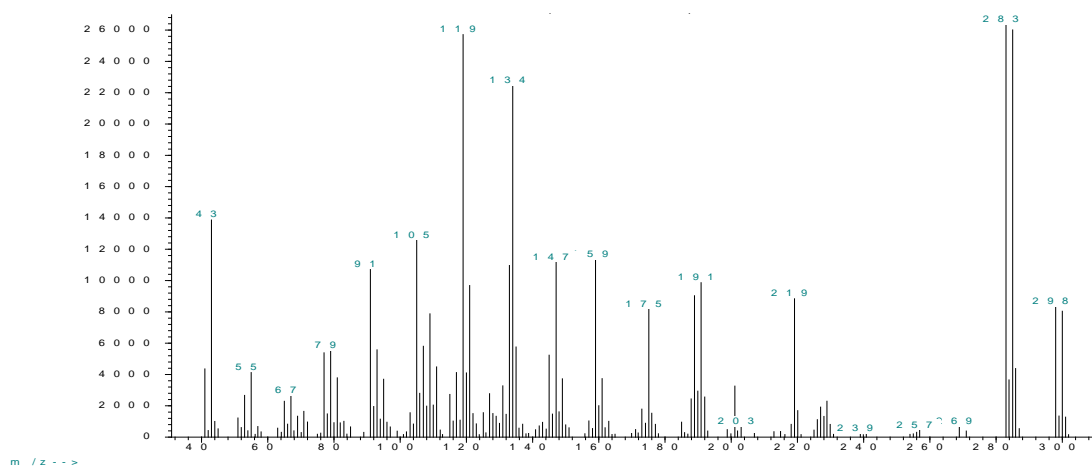


Figure S68. Mass spectrum (LR-EIMS) of compound 18.

[M-HCl]⁺ observed at *m/z* 298 and 300

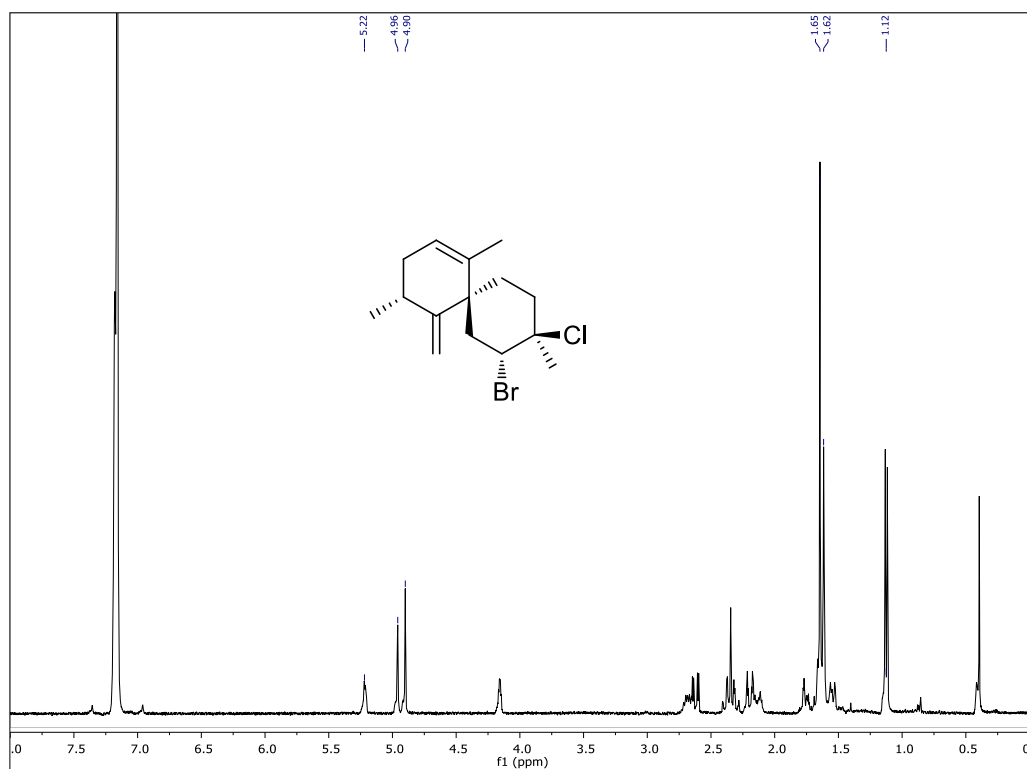


Figure S69. ¹H NMR spectrum (C₆D₆) of compound 19.

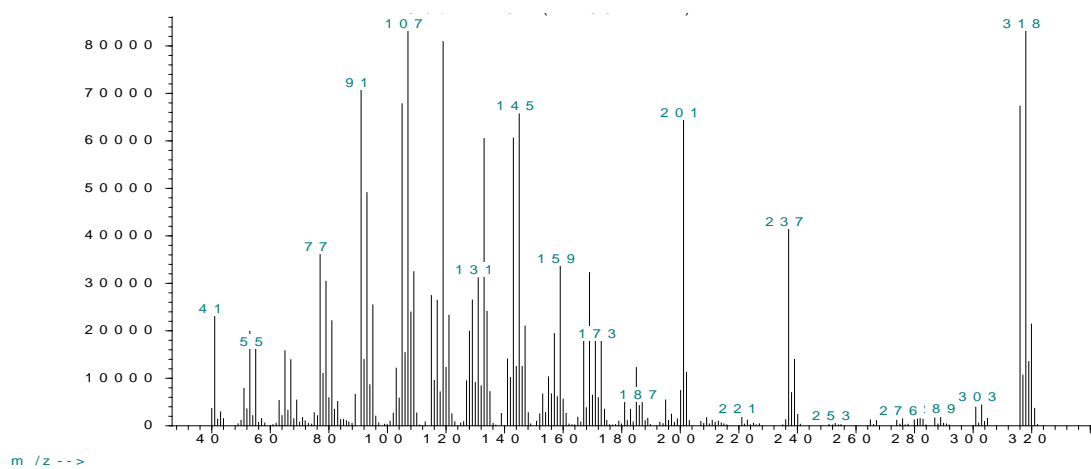


Figure S70. Mass spectrum (LR-EIMS) of compound 19.

[M]⁺ observed at *m/z* 316, 318 and 320

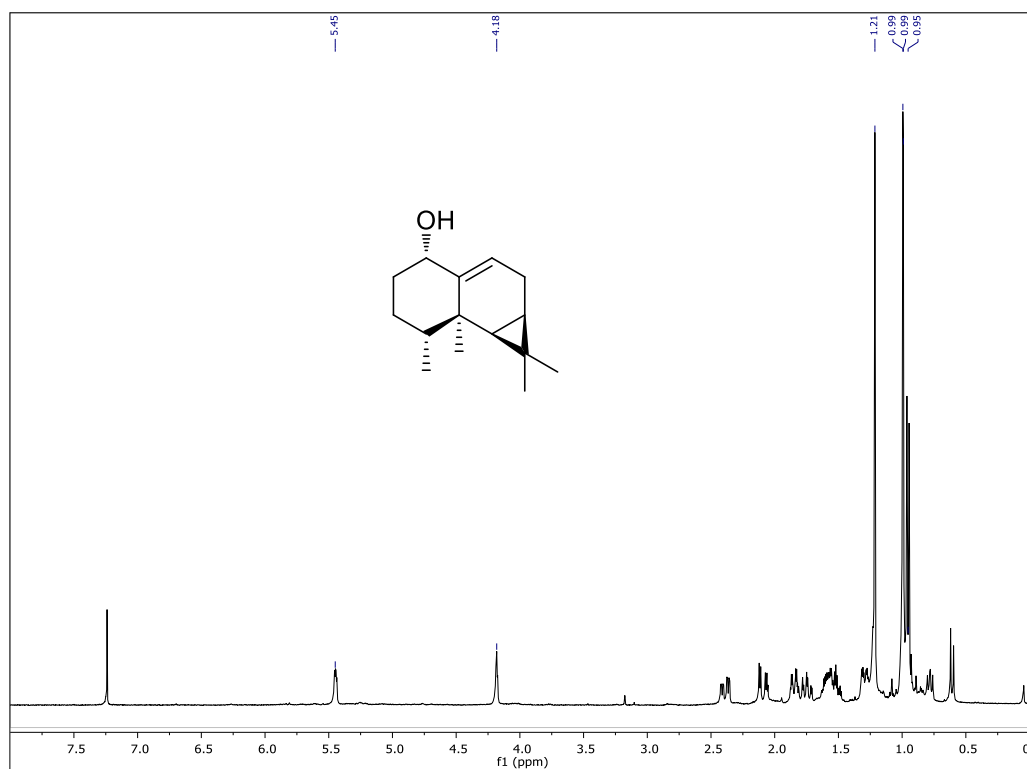


Figure S71. ¹H NMR spectrum (CDCl₃) of compound 20.

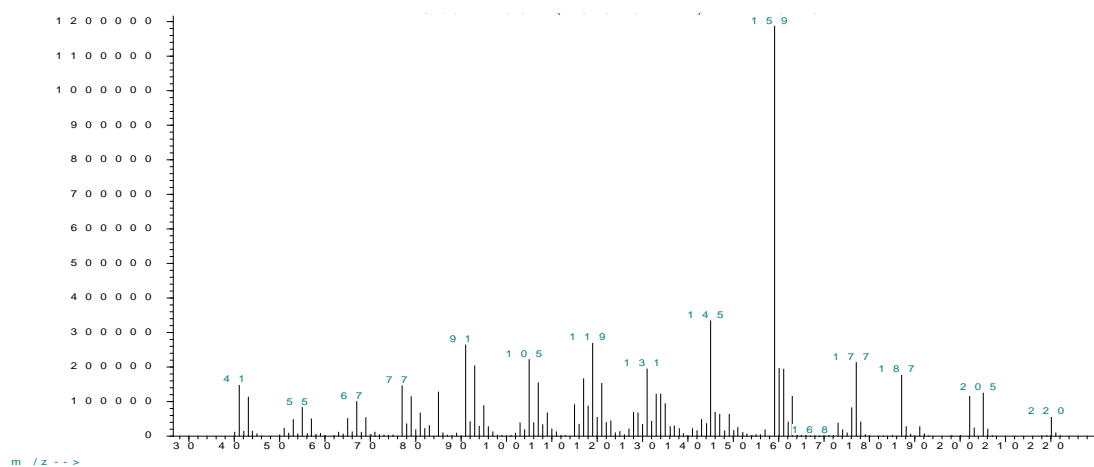


Figure S72. Mass spectrum (LR-EIMS) of compound 20.

[M]⁺ observed at *m/z* 220

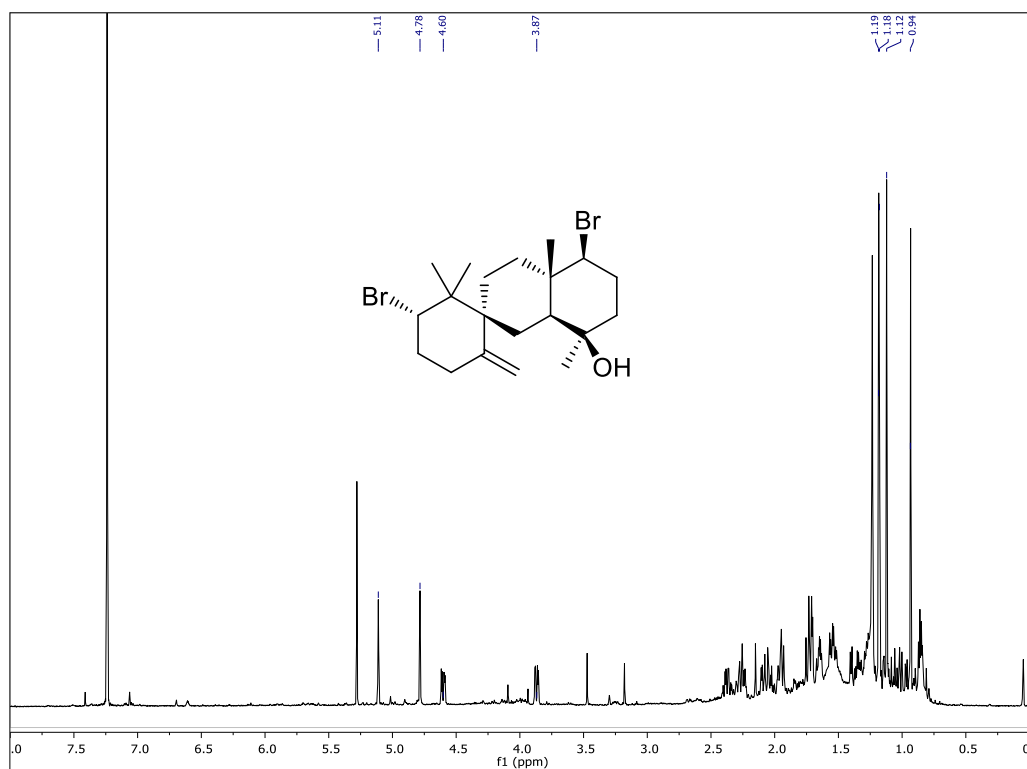


Figure S73. ^1H NMR spectrum (CDCl_3) of compound **21**.

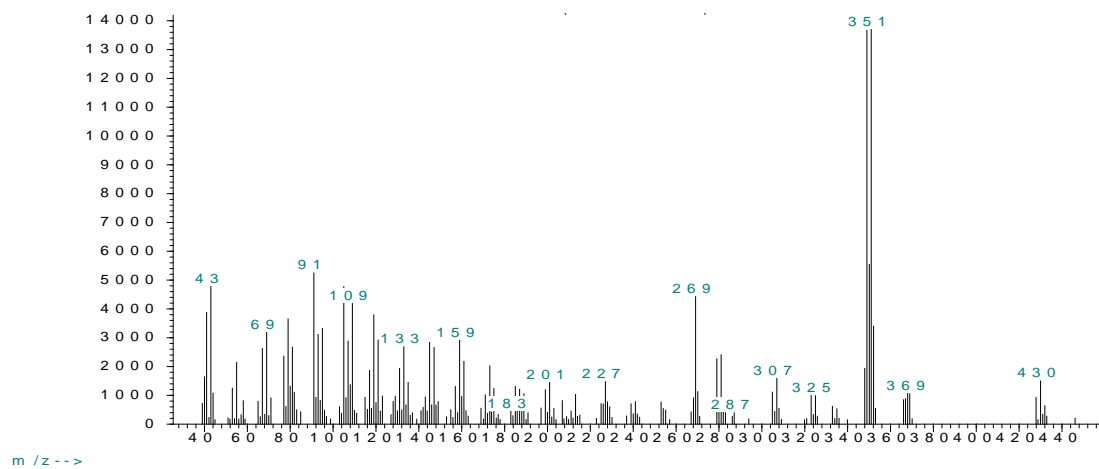


Figure S74. Mass spectrum (LR-EIMS) of compound **21**.

$[\text{M}-\text{H}_2\text{O}]^+$ observed at m/z 428, 430 and 432

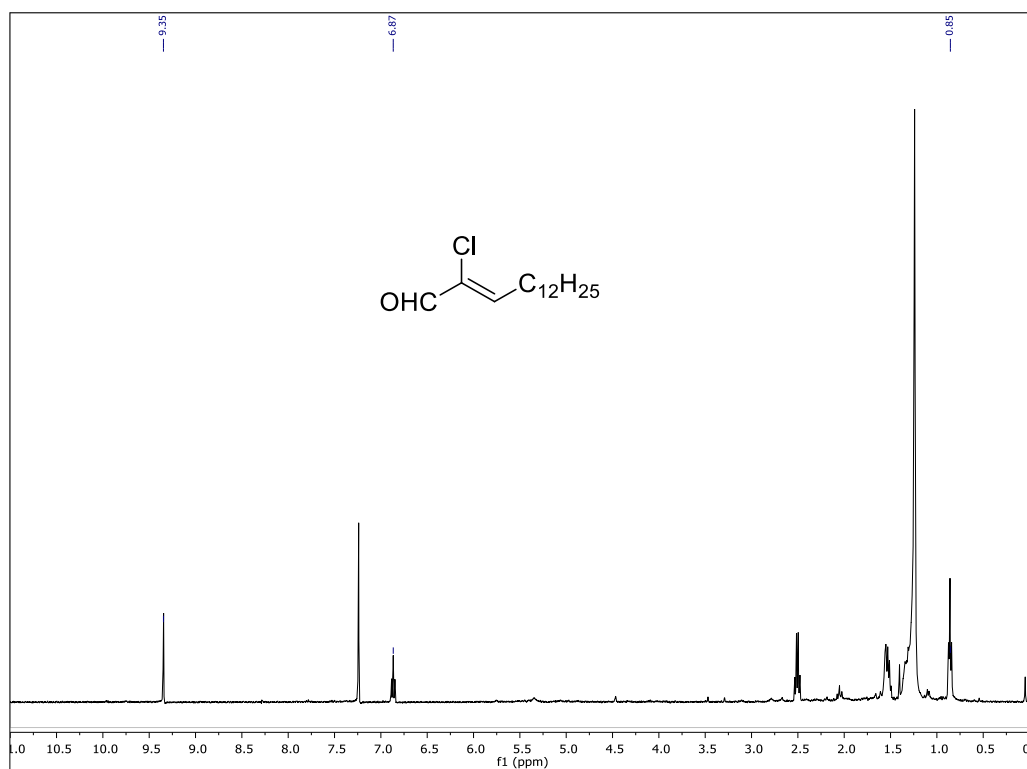


Figure S75. ¹H NMR spectrum (CDCl₃) of compound 22.

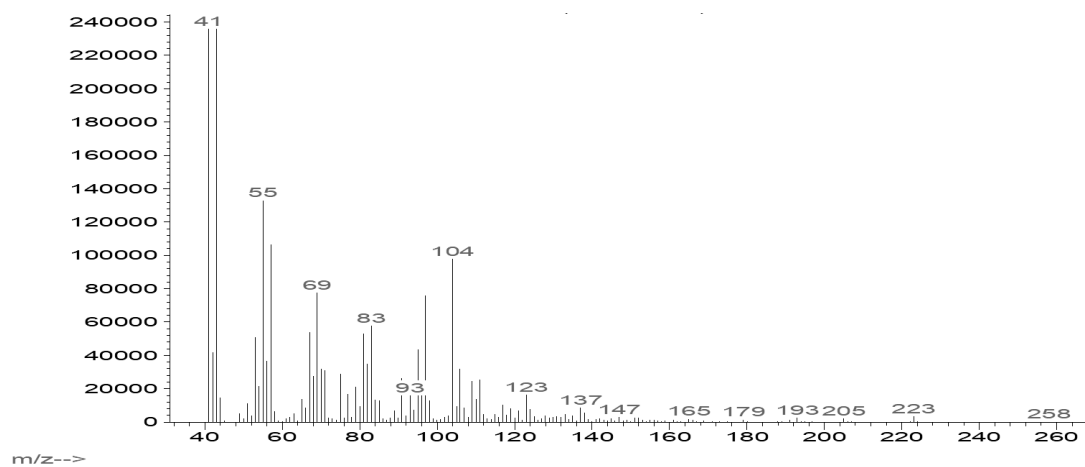


Figure S76. Mass spectrum (LR-EIMS) of compound 22.

[M]⁺ observed at *m/z* 258

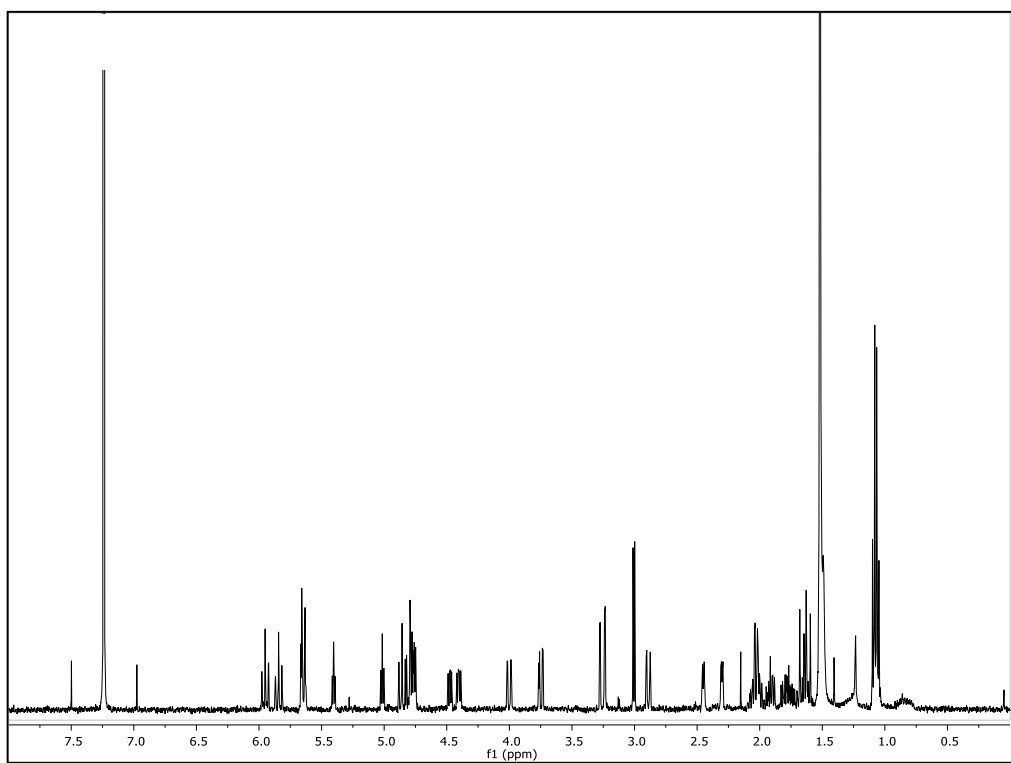


Figure S77. ^1H NMR spectrum (CDCl_3) of compounds **23** and **24** (at a 1:1 ratio).

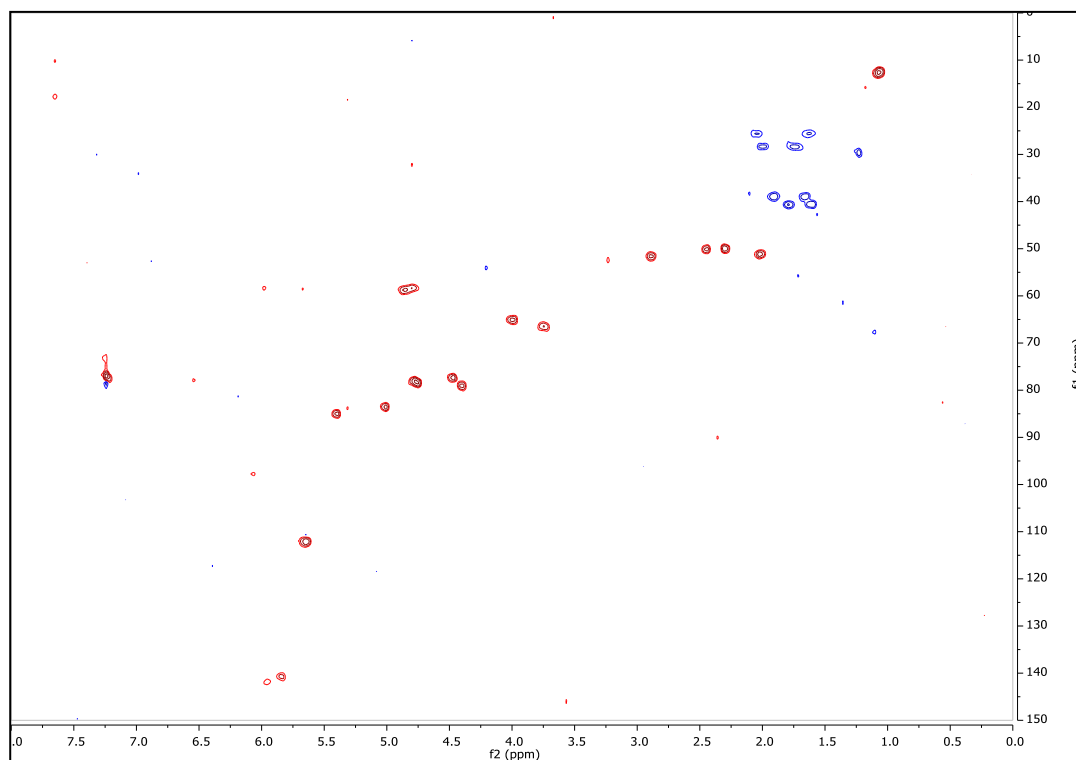


Figure S78. HSQC spectrum (CDCl_3) of compounds **23** and **24** (at a 1:1 ratio).

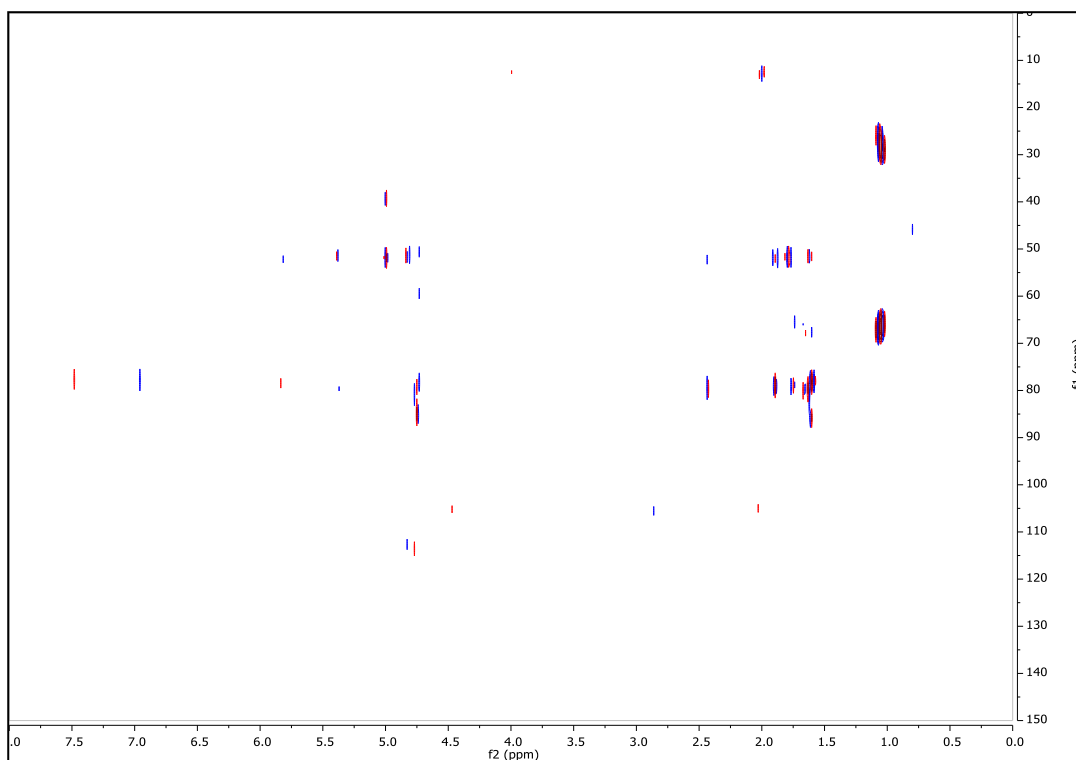


Figure S79. HMBC spectrum (CDCl_3) of compounds **23** and **24** (at a 1:1 ratio).

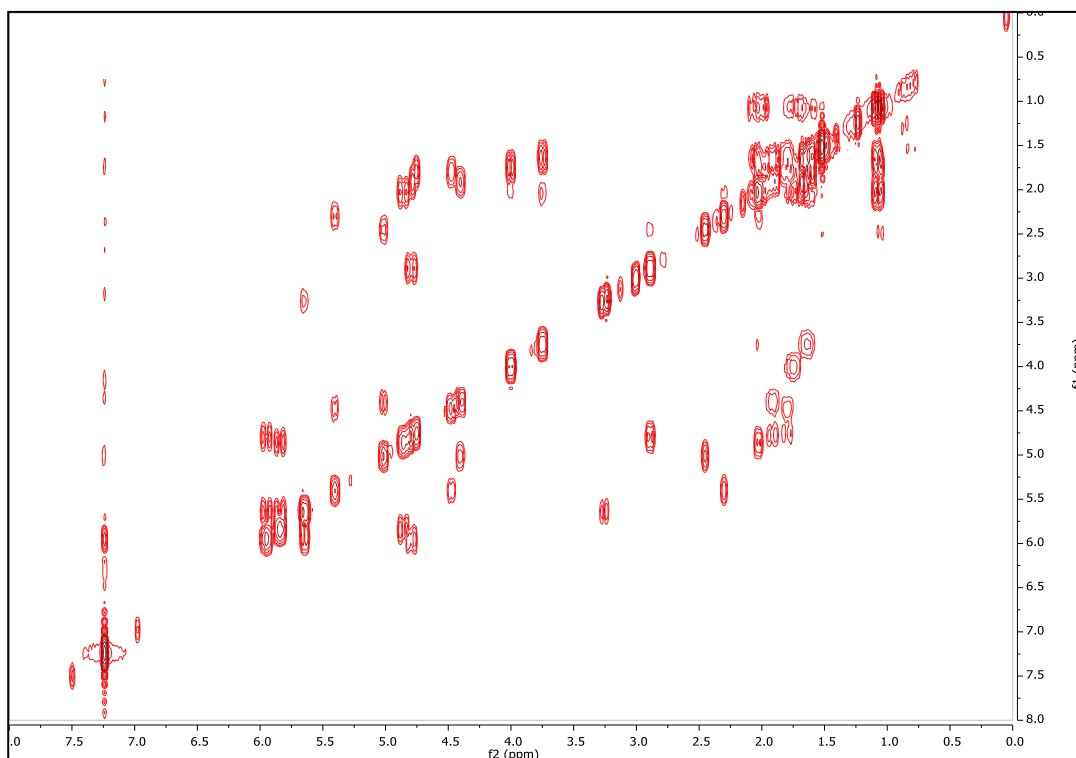


Figure S80. COSY spectrum (CDCl_3) of compounds **23** and **24** (at a 1:1 ratio).

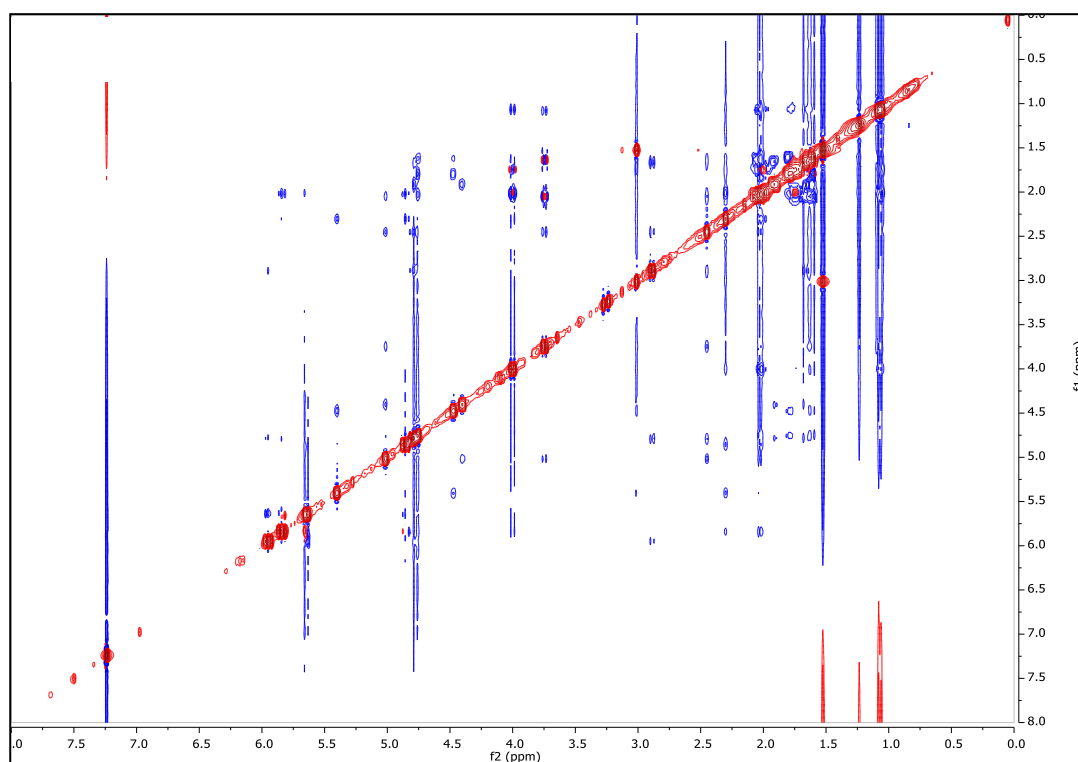


Figure S81. NOESY spectrum (CDCl₃) of compounds **23** and **24** (at a 1:1 ratio).

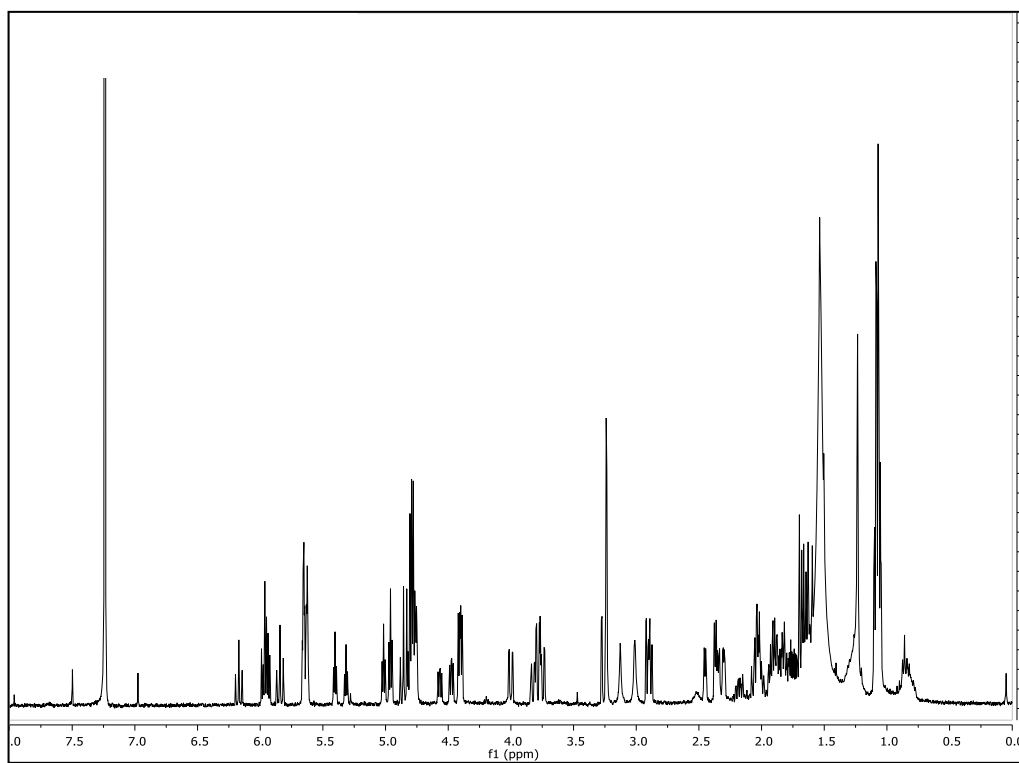


Figure S82. ^1H NMR spectrum (CDCl_3) of compounds **23–26** (at a 1:2:1:2 ratio).

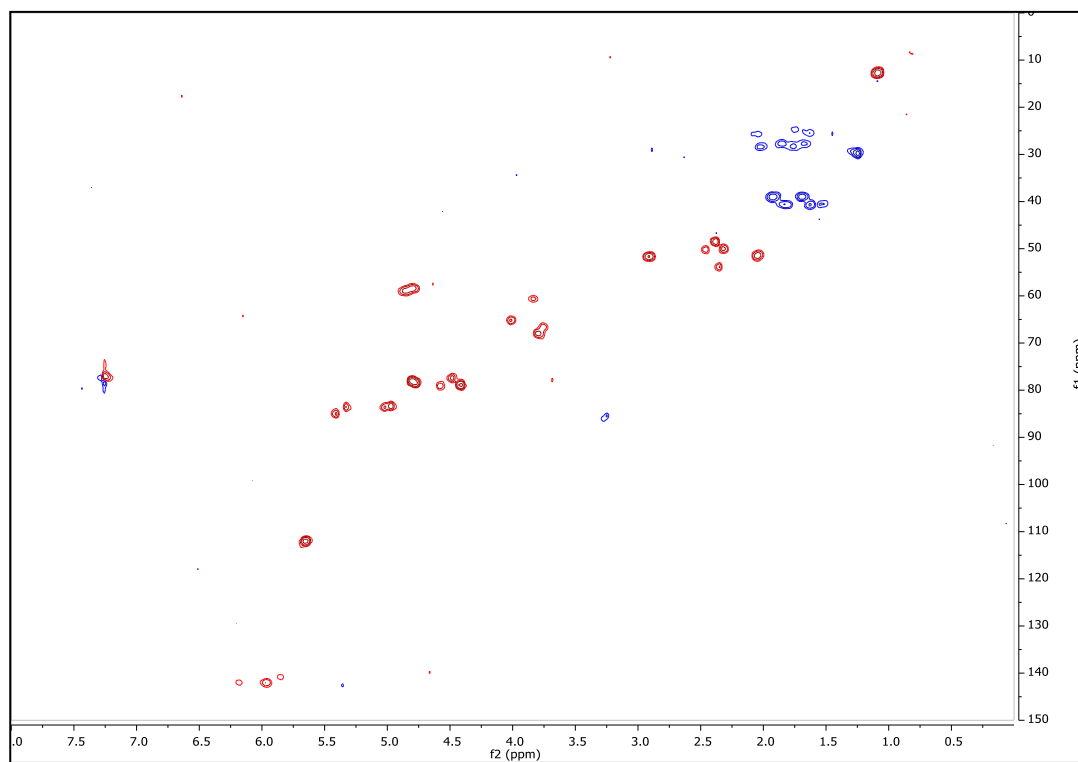


Figure S83. HSQC spectrum (CDCl_3) of compounds **23–26** (at a 1:2:1:2 ratio).

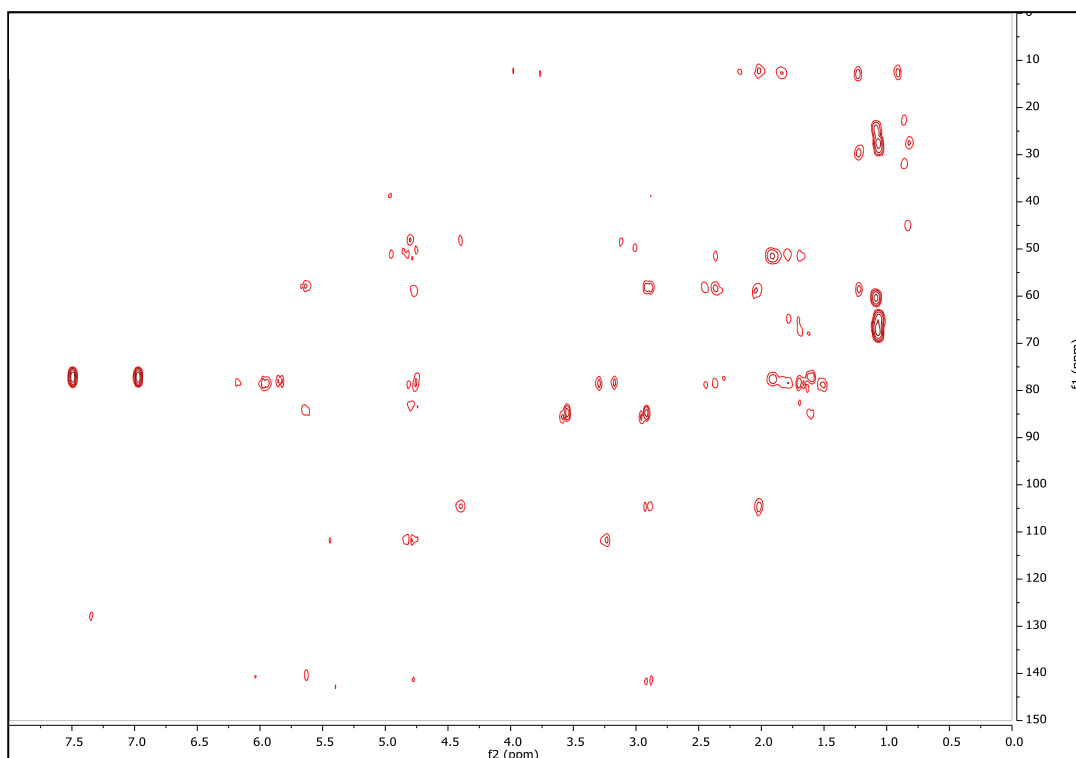


Figure S84. HMBC spectrum (CDCl₃) of compounds **23–26** (at a 1:2:1:2 ratio).

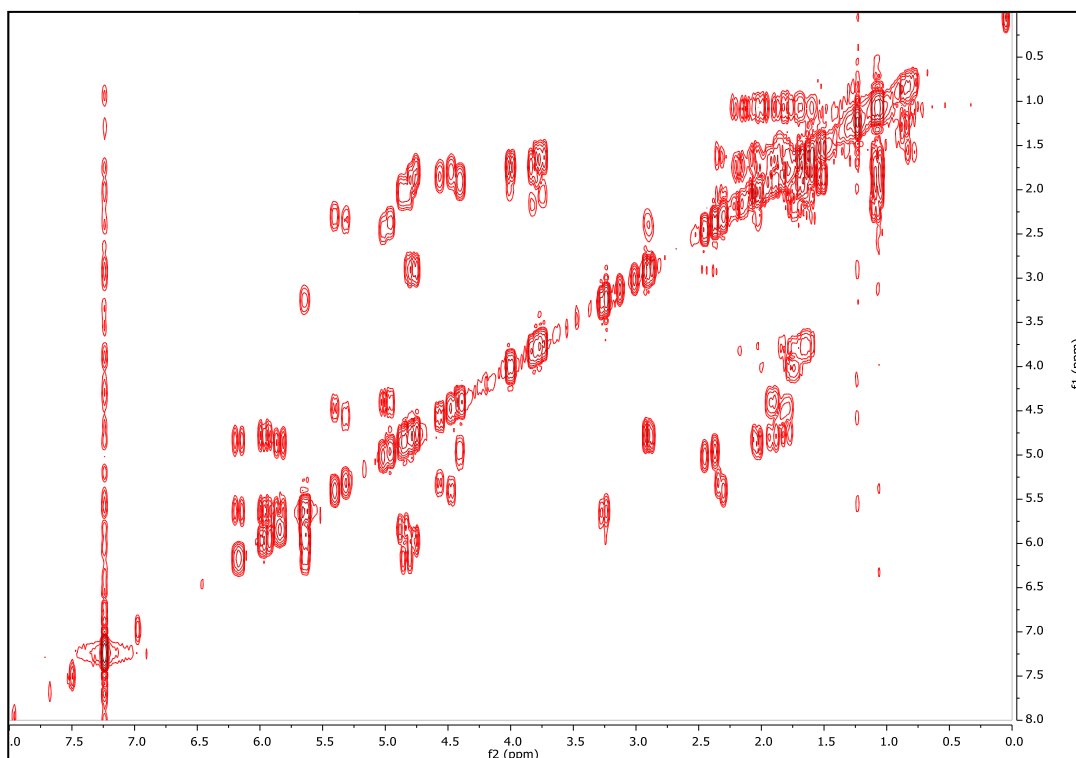


Figure S85. COSY spectrum (CDCl₃) of compounds **23–26** (at a 1:2:1:2 ratio).

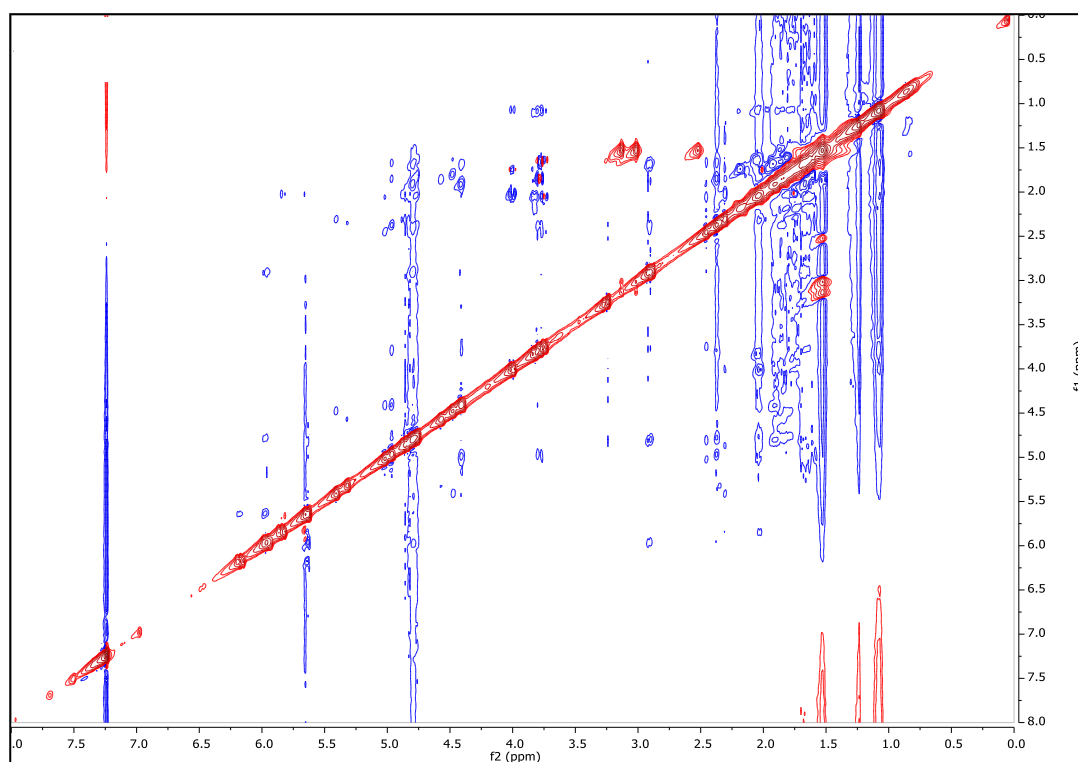


Figure S86. NOESY spectrum (CDCl_3) of compounds **23–26** (at a 1:2:1:2 ratio).