

Supporting Information

Chemical Epigenetics Alters the Secondary Metabolite Composition of Guttate Excreted by an Atlantic-Forest-Soil-Derived *Penicillium citreonigrum*.

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Figure S32. 1D NOE NMR (500 MHz, CDCl₃) of pencolide methyl ester (**8**)

Table S1. Crystal data and structure refinement for atlantinone A (**9**).

Empirical formula	(C ₂₆ H ₃₄ O ₆) (C H ₄ O)
	C ₂₇ H ₃₈ O ₇
Formula weight	474.57
Crystal system	Orthorhombic
Space group	<i>P</i> 212121
Unit cell dimensions	<i>a</i> = 12.0199(6) Å = 90° <i>b</i> = 13.7713(6) Å = 90° <i>c</i> = 14.8276(8) Å = 90°
Volume	2454.4(2) Å ³
Z, Z'	4, 1
Density (calculated)	1.284 Mg/m ³
Wavelength	1.54178 Å
Temperature	100(2) K
<i>F</i> (000)	1024
Absorption coefficient	0.746 mm ⁻¹
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.832 and 0.694
Theta range for data collection	4.38 to 69.53°
Reflections collected	26979
Independent reflections	4555 [R(int) = 0.0476]
Data / restraints / parameters	4555 / 0 / 314
<i>wR</i> (<i>F</i> ² all data)	<i>wR</i> ² = 0.0802
<i>R</i> (<i>F</i> obsd data)	<i>R</i> ¹ = 0.0327
Goodness-of-fit on	<i>F</i> ² 1.001
Observed data	[<i>I</i> > 2(<i>I</i>)] 4244
Absolute structure parameter	0.01(14)
Extinction coefficient	0.0040(2)
Largest and mean shift / s.u.	0.000 and 0.000
Largest diff. peak and hole	0.216 and -0.201 e/Å ³

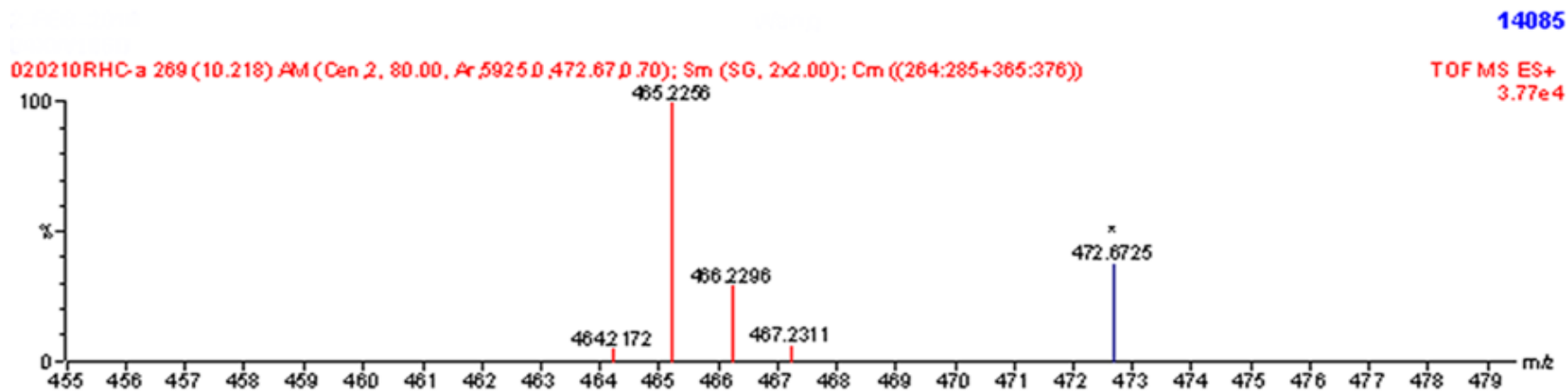


Figure S1. HRESIMS of atlantinone A (**9**)

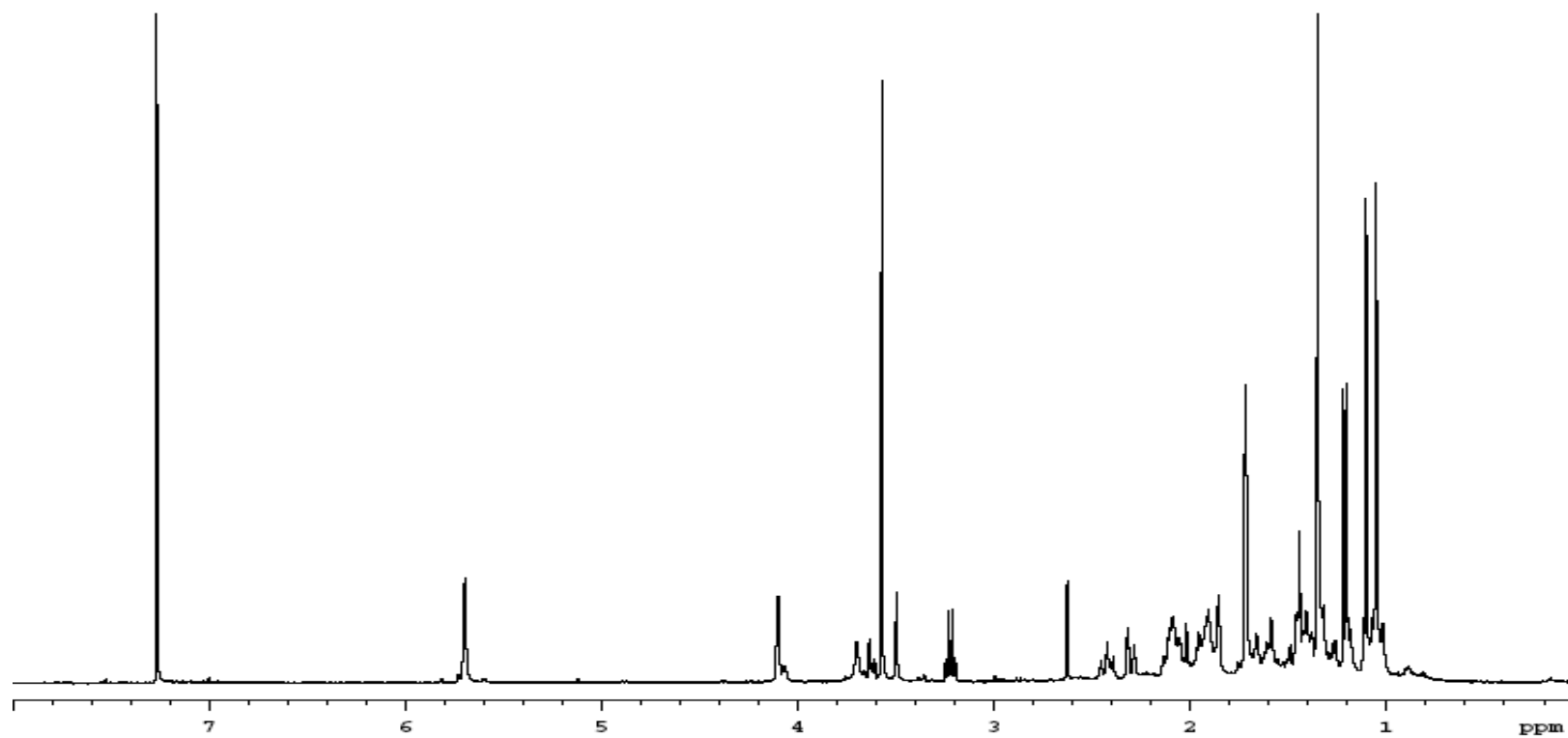


Figure S2. ^1H -NMR spectrum (500 MHz, CDCl_3) of atlantinone A (**9b**)

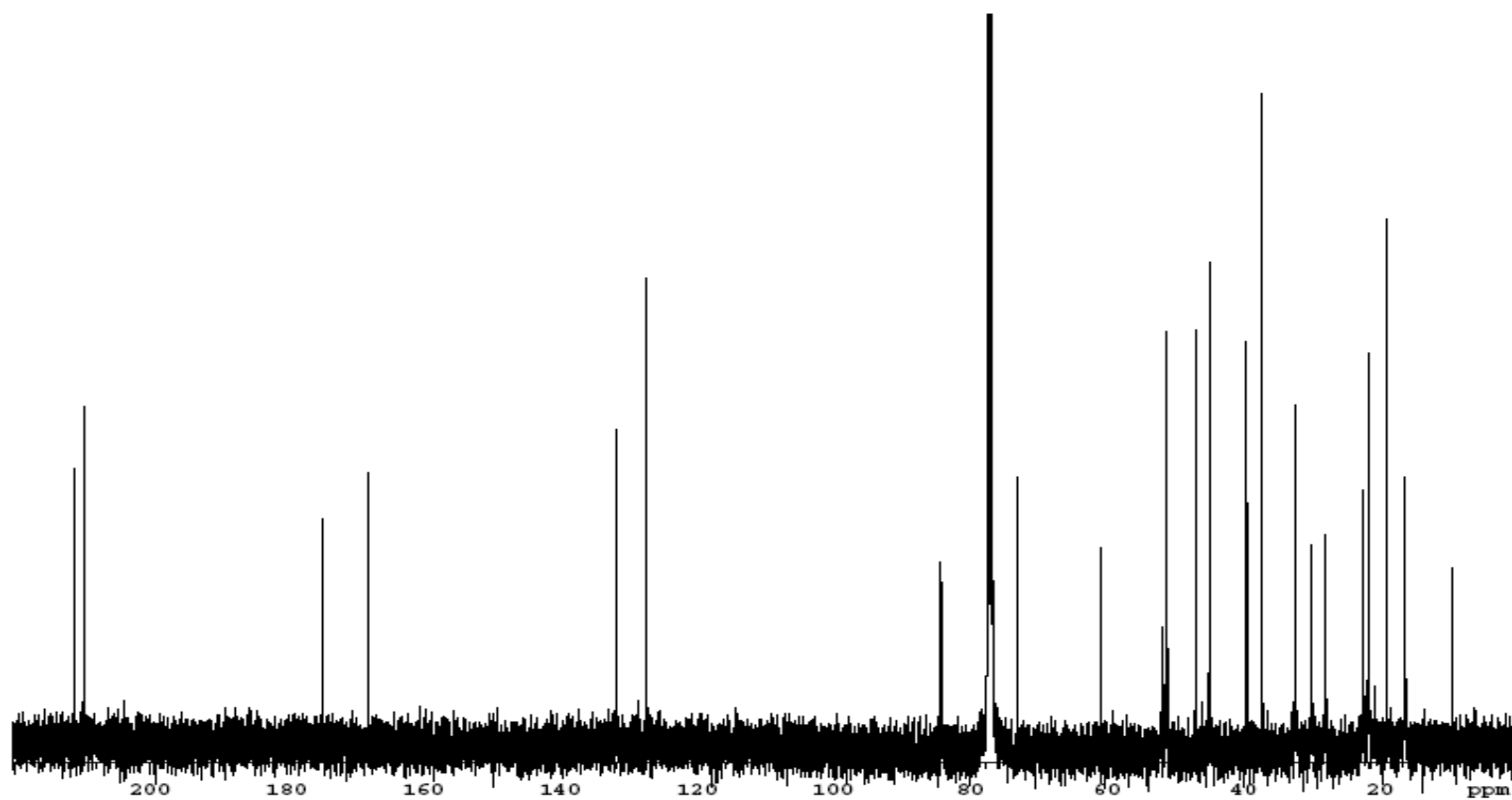


Figure S3. ^{13}C -NMR spectrum (125 MHz, CDCl_3) of atlantinone A (**9b**)

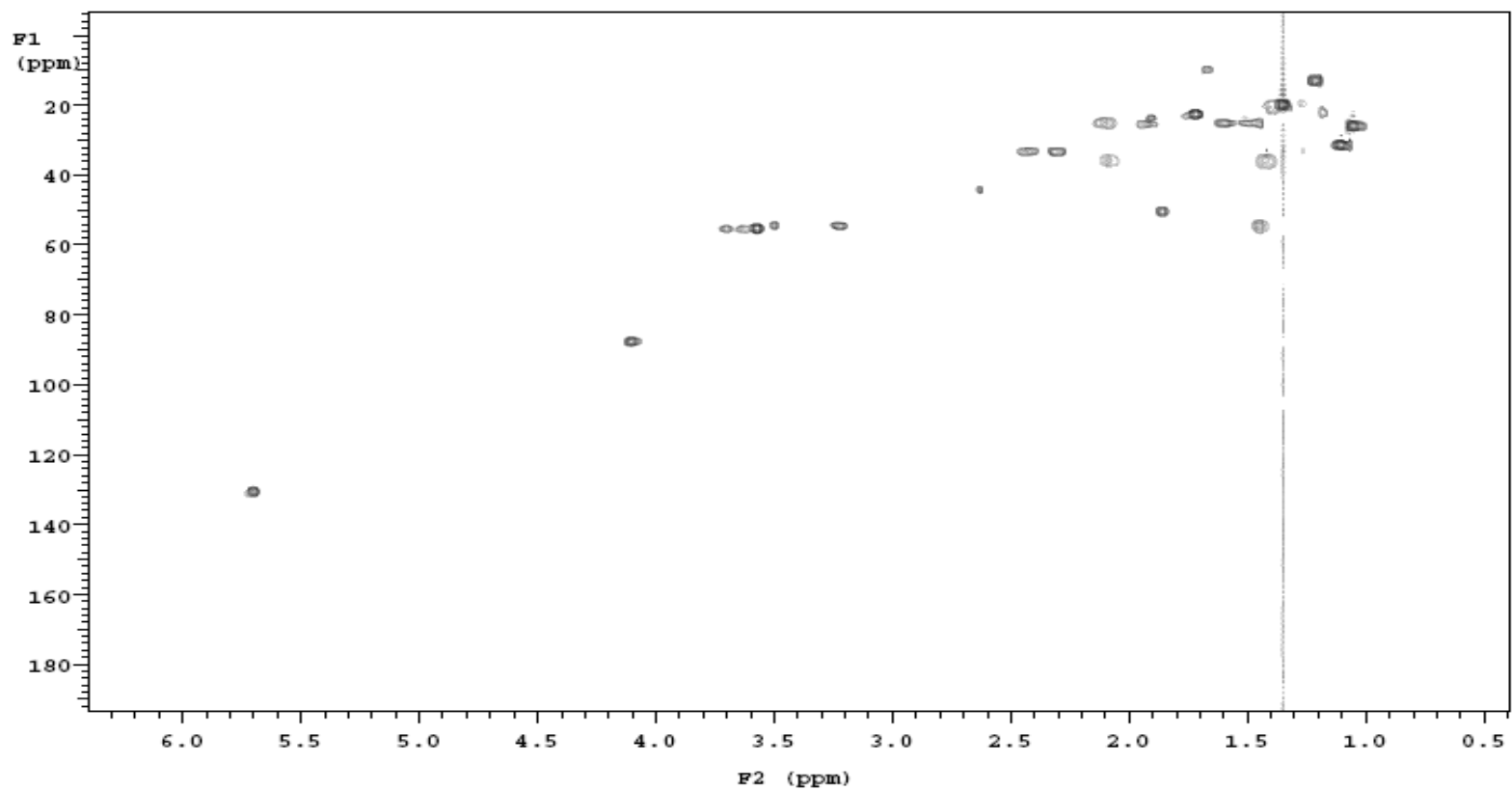


Figure S4. HSQC-NMR spectrum (500 MHz, CDCl₃) of atlantinone A (**9b**)

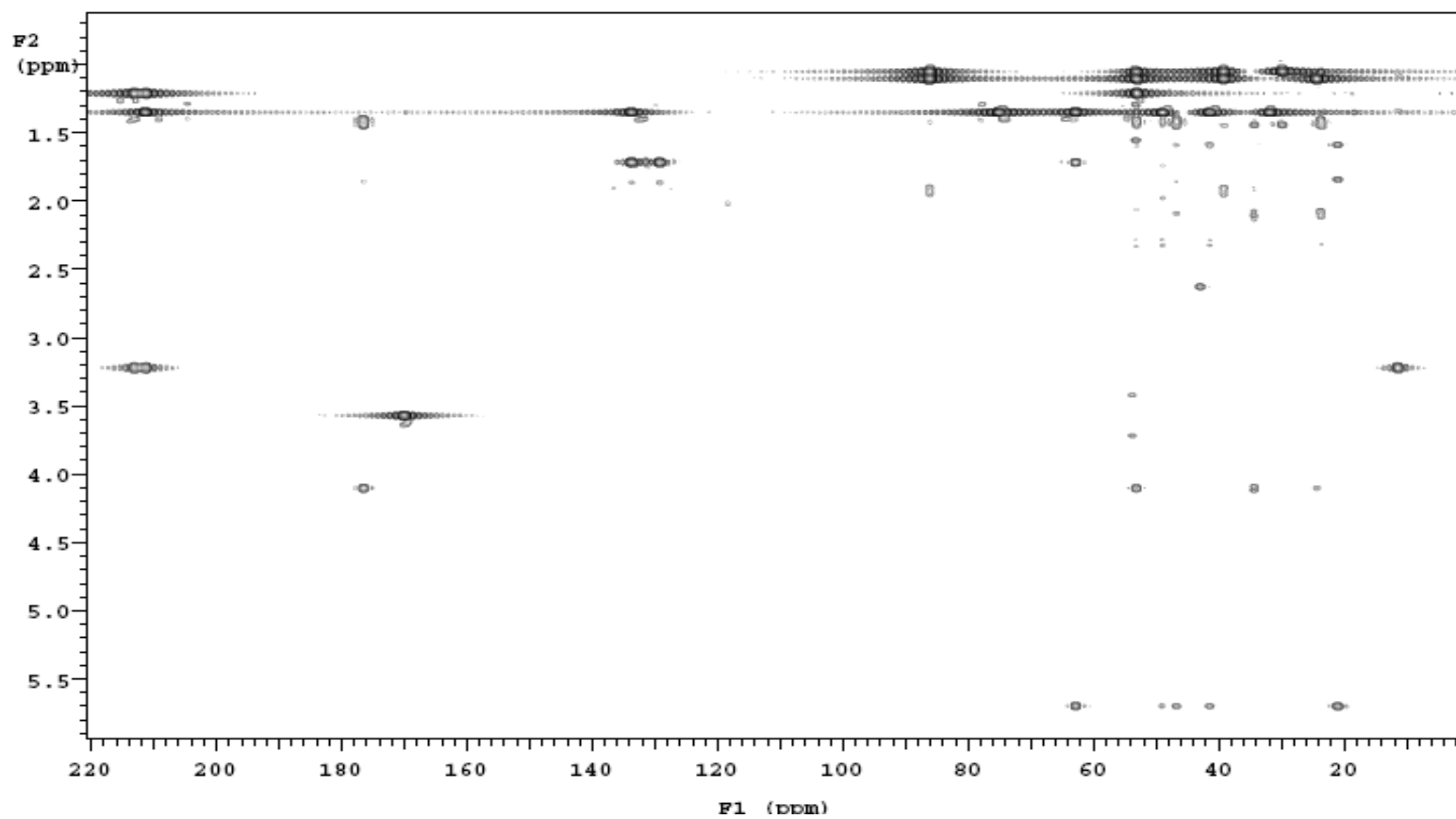


Figure S5. HMBC-NMR spectrum (500 MHz, CDCl₃) of atlantinone A (**9b**)

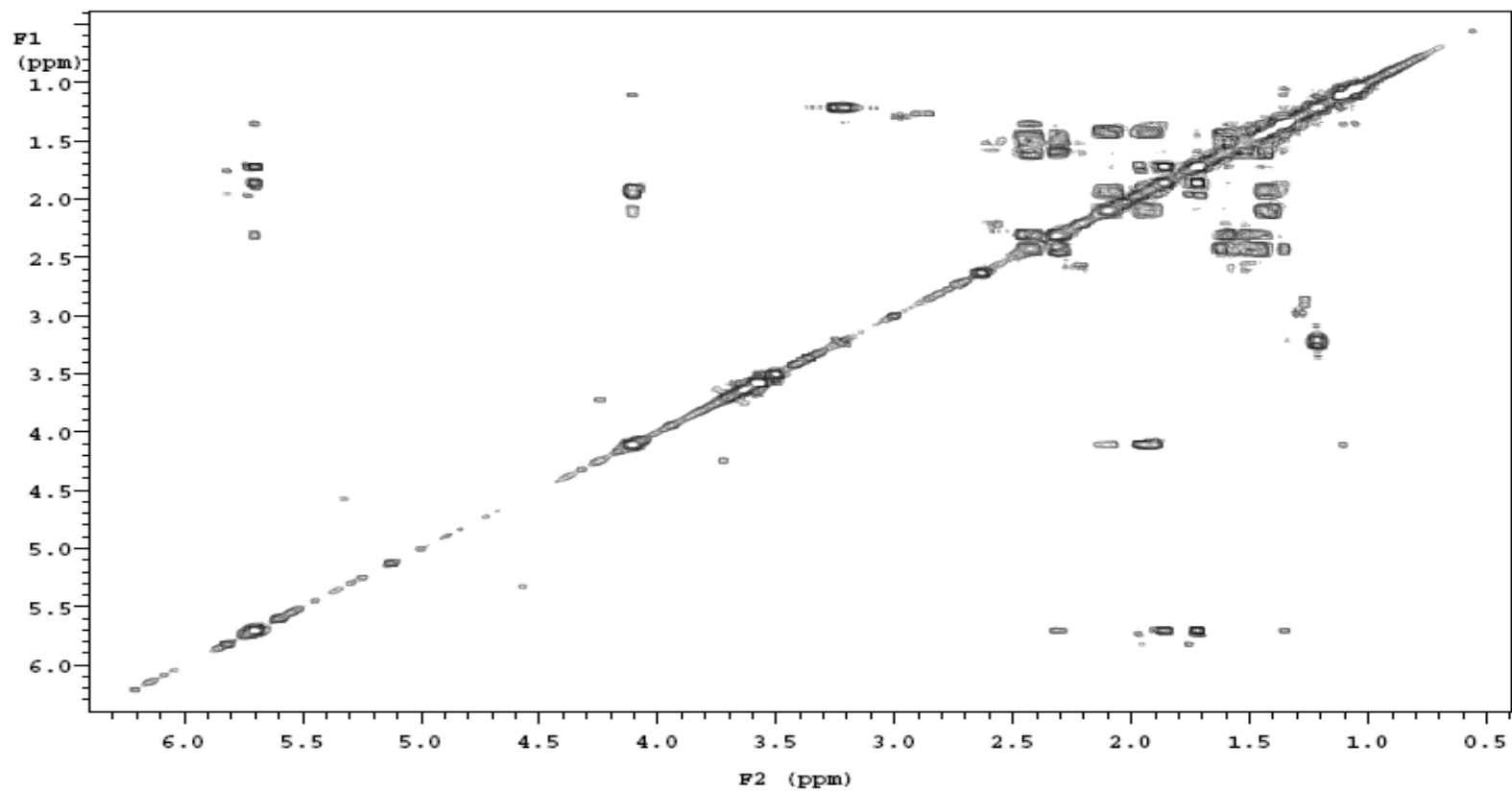


Figure S6. COSY-NMR spectrum (500 MHz, CDCl₃) of atlantinone A (**9b**)

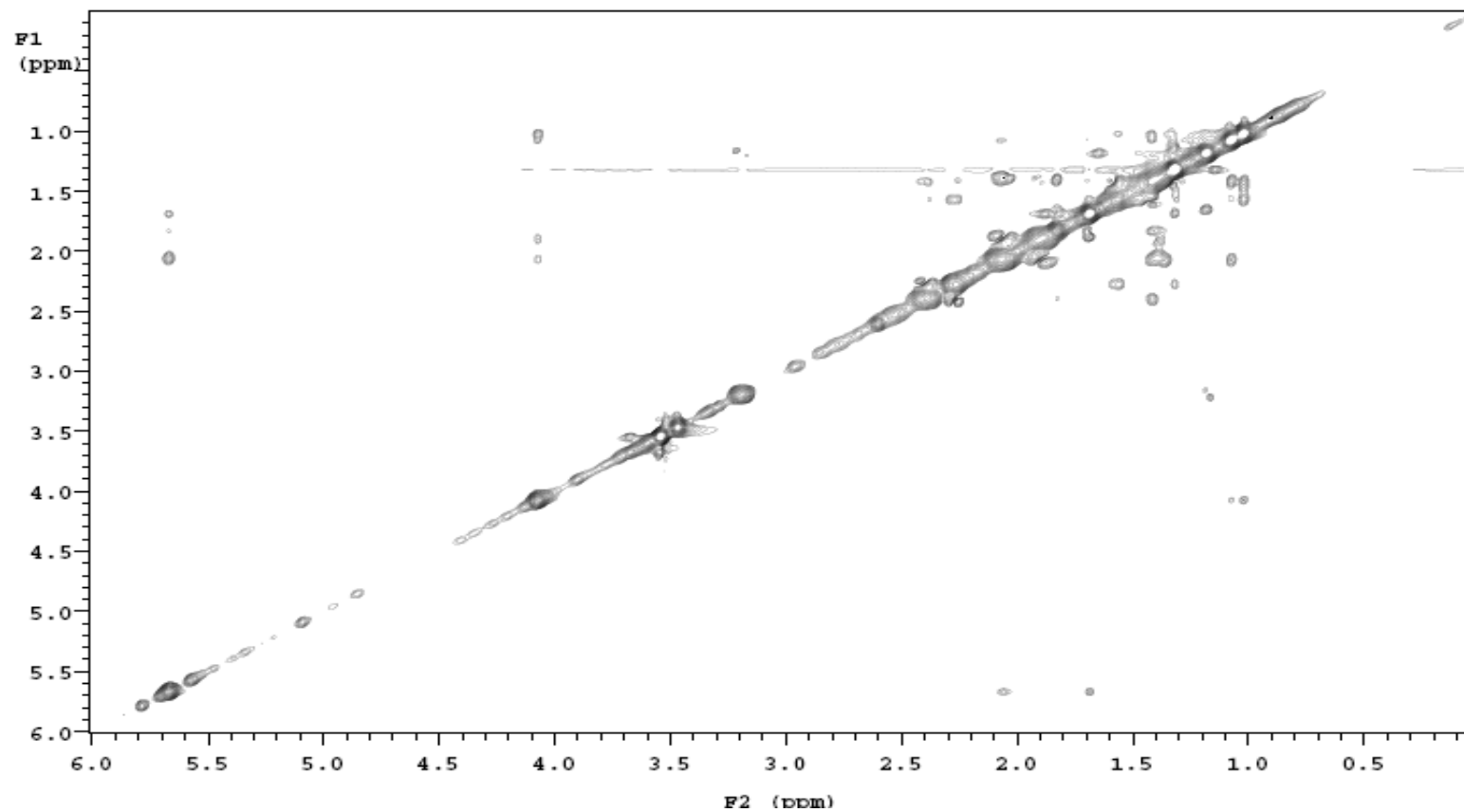


Figure S7. ROESY-NMR spectrum (400 MHz, CDCl₃) of atlantinone A (**9b**)

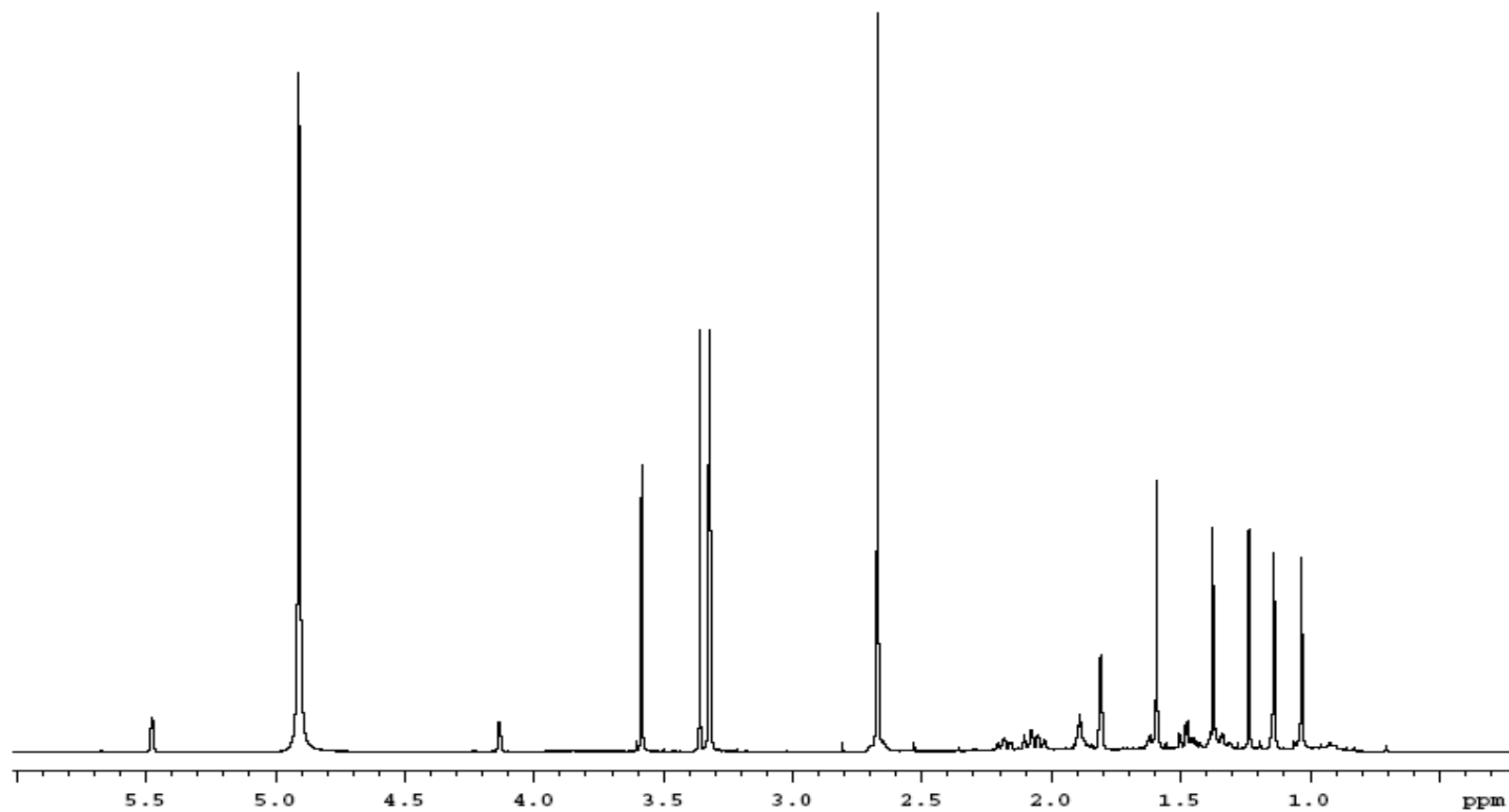


Figure S8. ^1H -NMR spectrum (500 MHz, CD_3OD) of atlantinone A (**9a**)

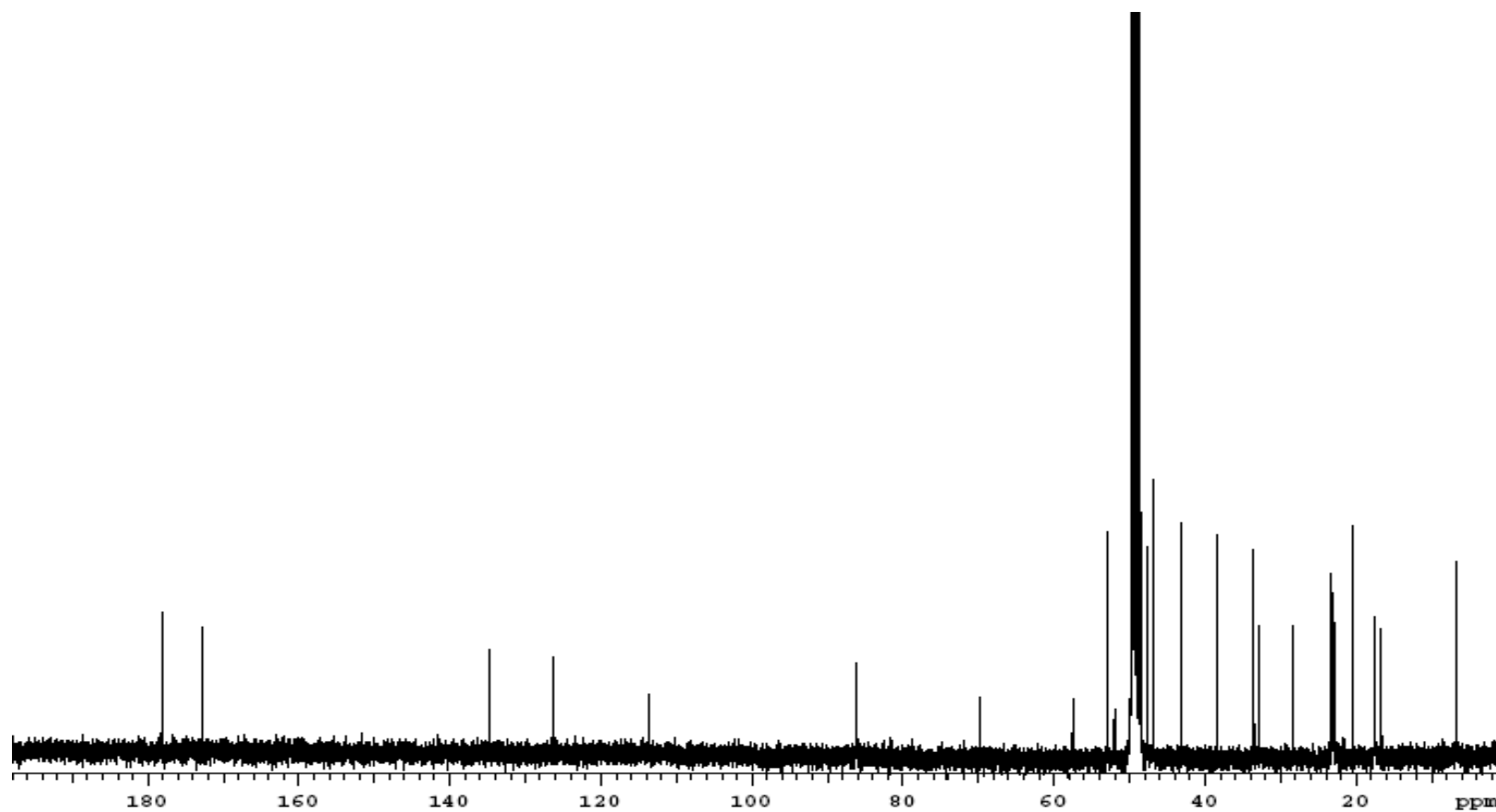


Figure S9. ^{13}C -NMR spectrum (125 MHz, CD_3OD) of atlantinone A (**9a**)

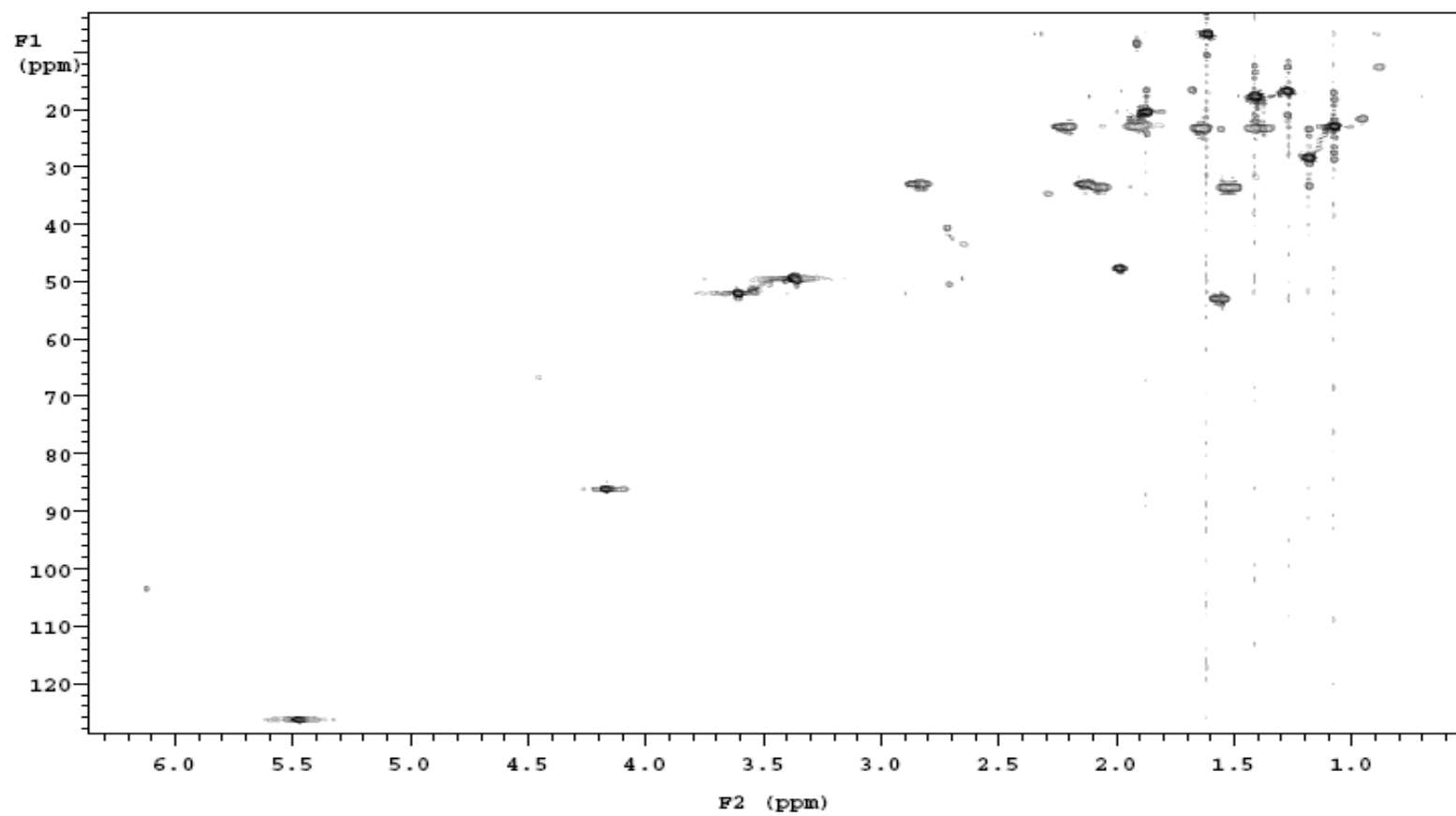


Figure S10. HSQC-NMR spectrum (500 MHz, CD₃OD) of atlantinone A (**9a**)

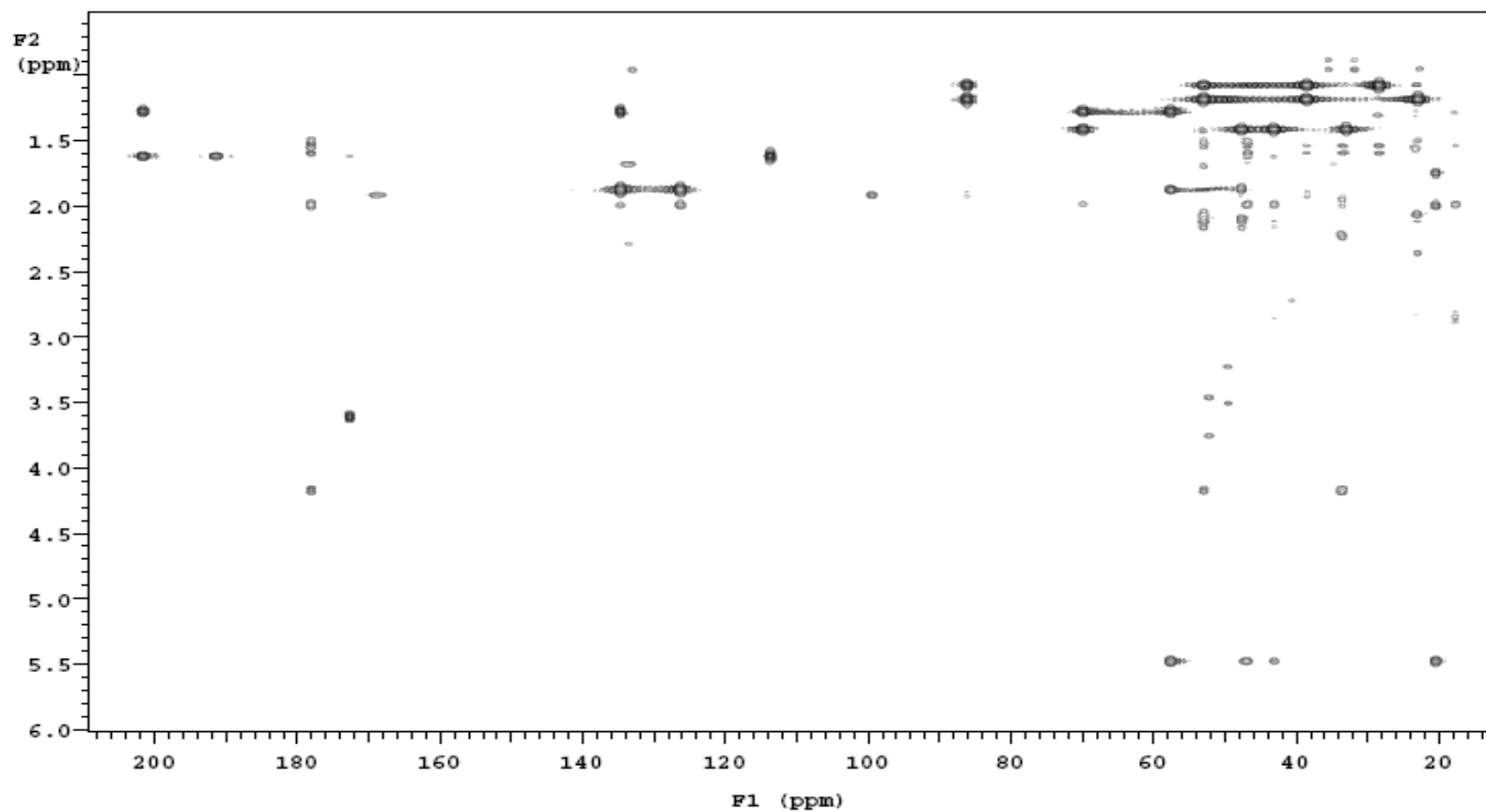


Figure S11. HMBC-NMR spectrum (500 MHz, CD₃OD) of atlantinone A (**9a**)

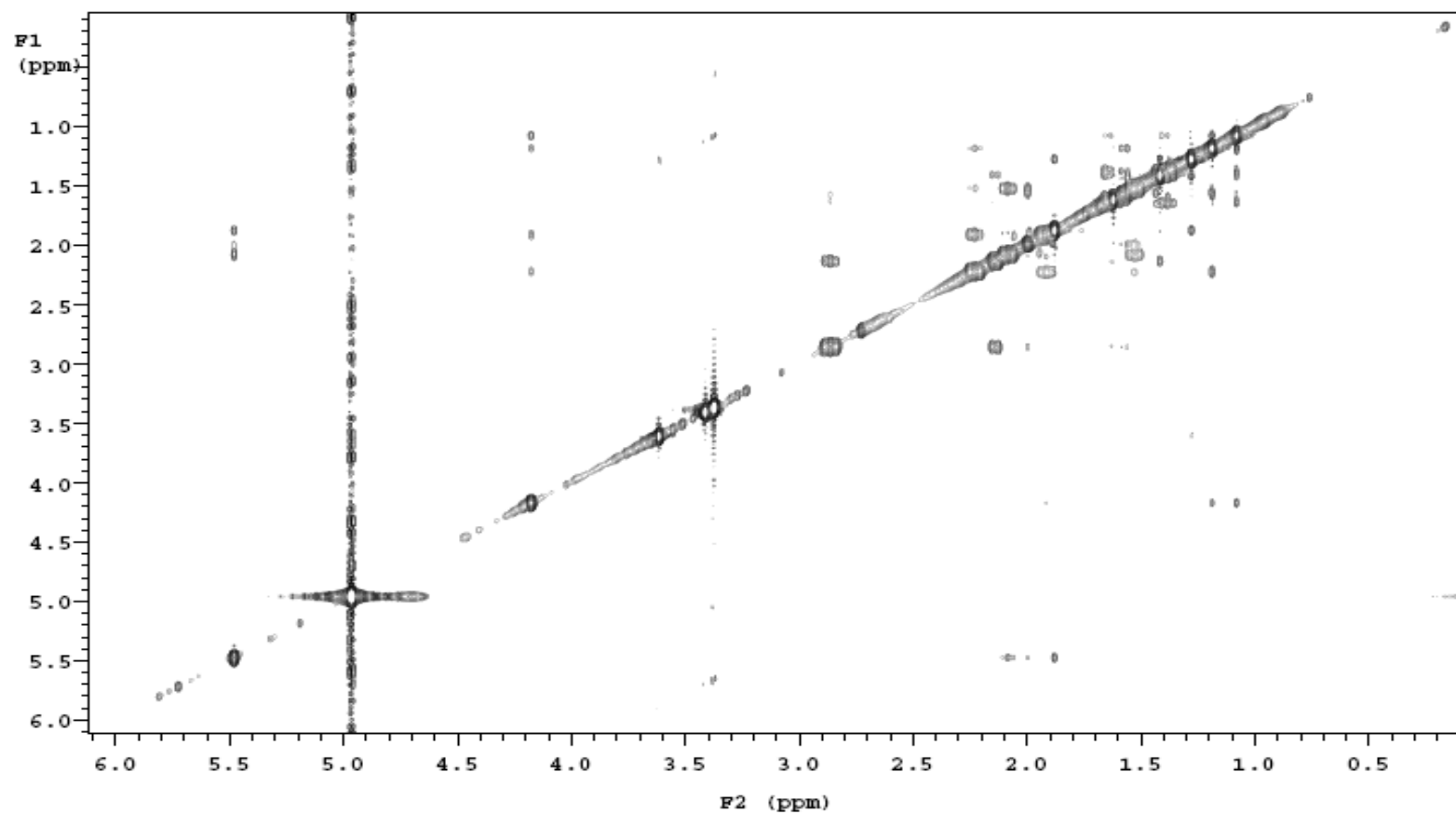


Figure S12. ROESY-NMR spectrum (500 MHz, CD₃OD) of atlantinone A (**9a**)

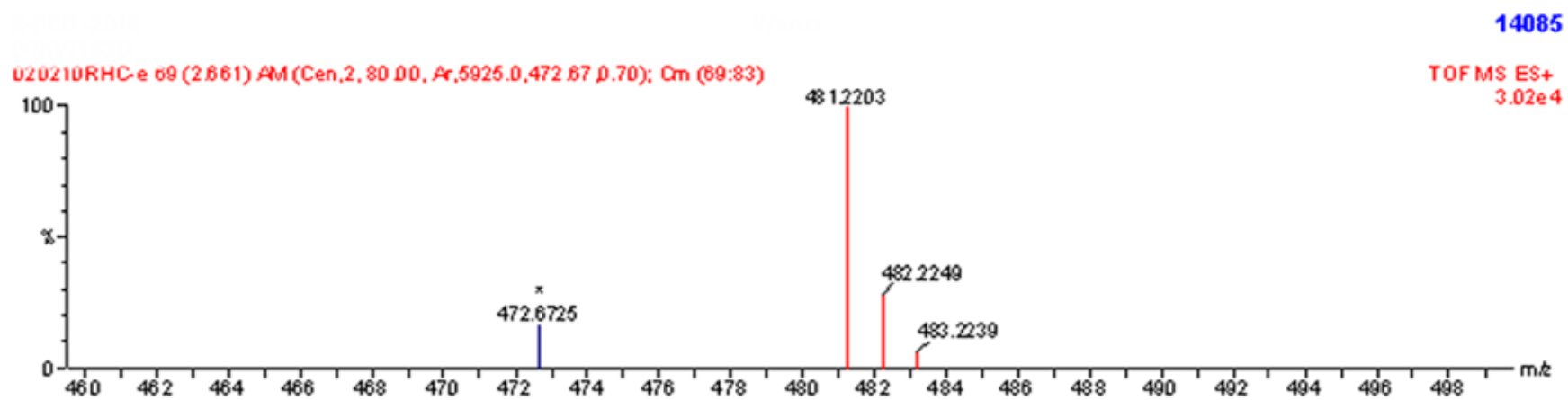


Figure S13. HRESIMS of atlantinone B (10)

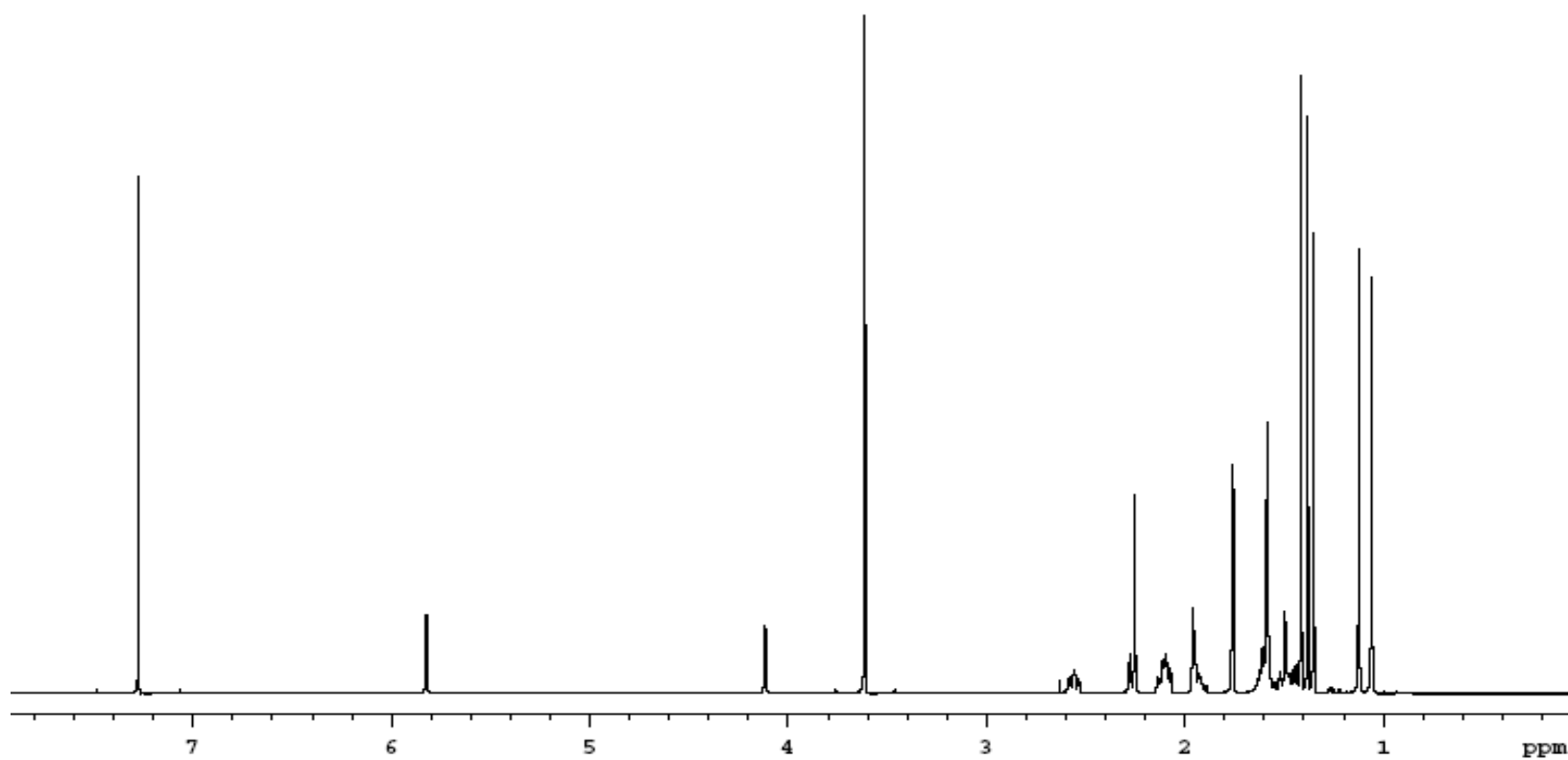


Figure S14. ^1H -NMR spectrum (500 MHz, CDCl_3) of atlantinone B (**10**)

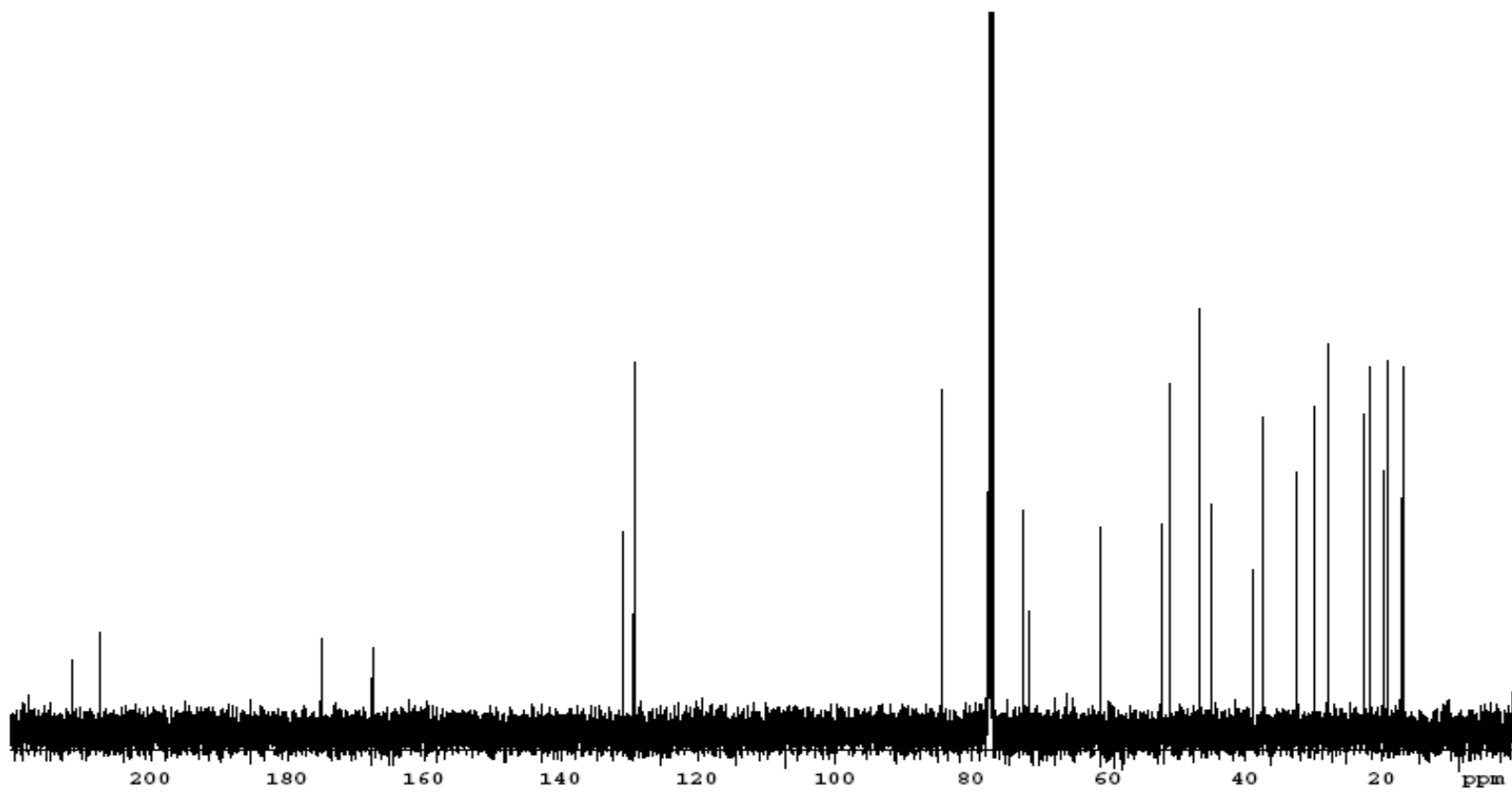


Figure S15. ^{13}C -NMR (125 MHz, CDCl_3) of atlantinone B (**10**)

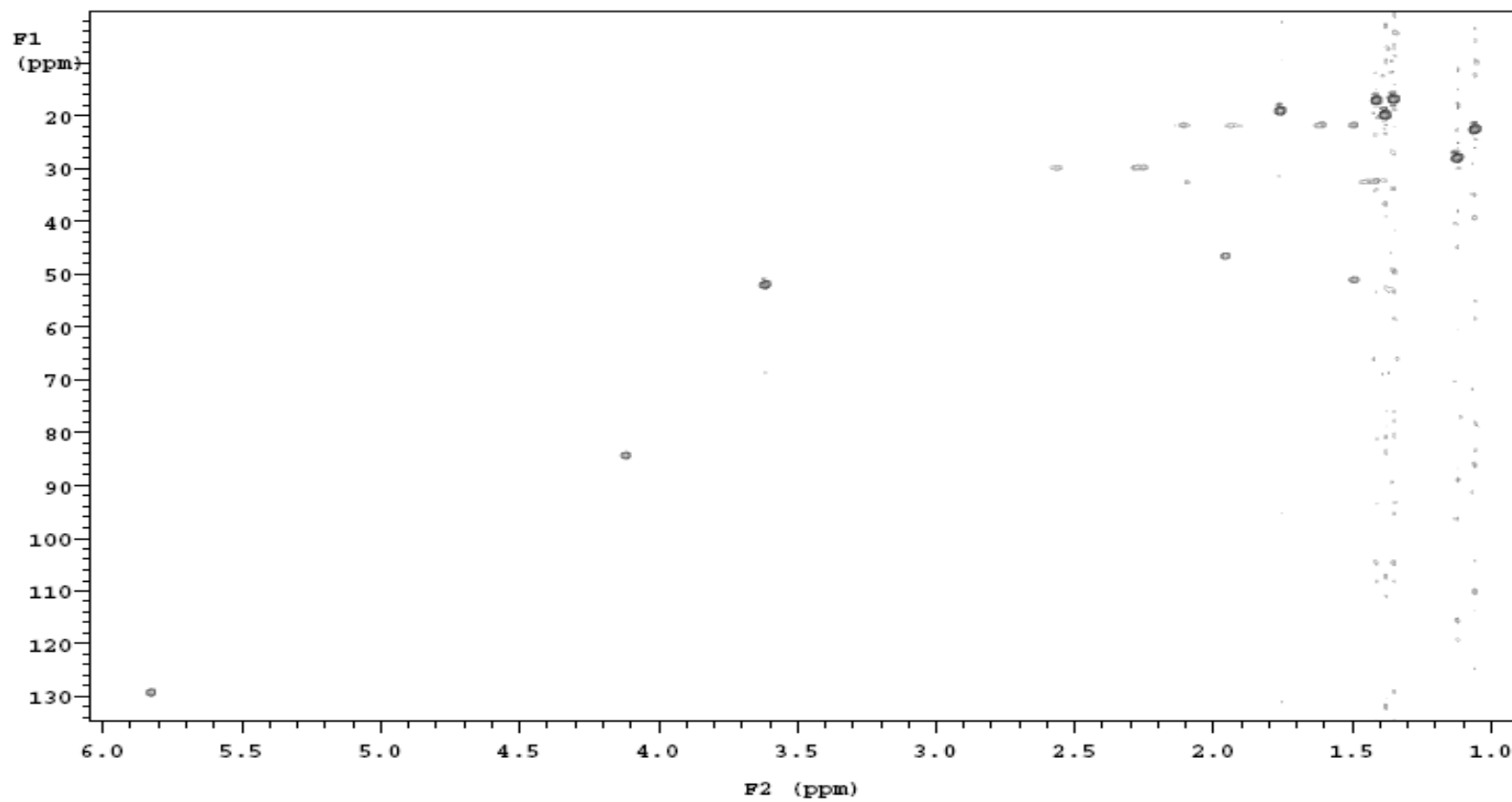


Figure S16. HSQC-NMR spectrum (500 MHz, CDCl₃) of atlantinone B (**10**)

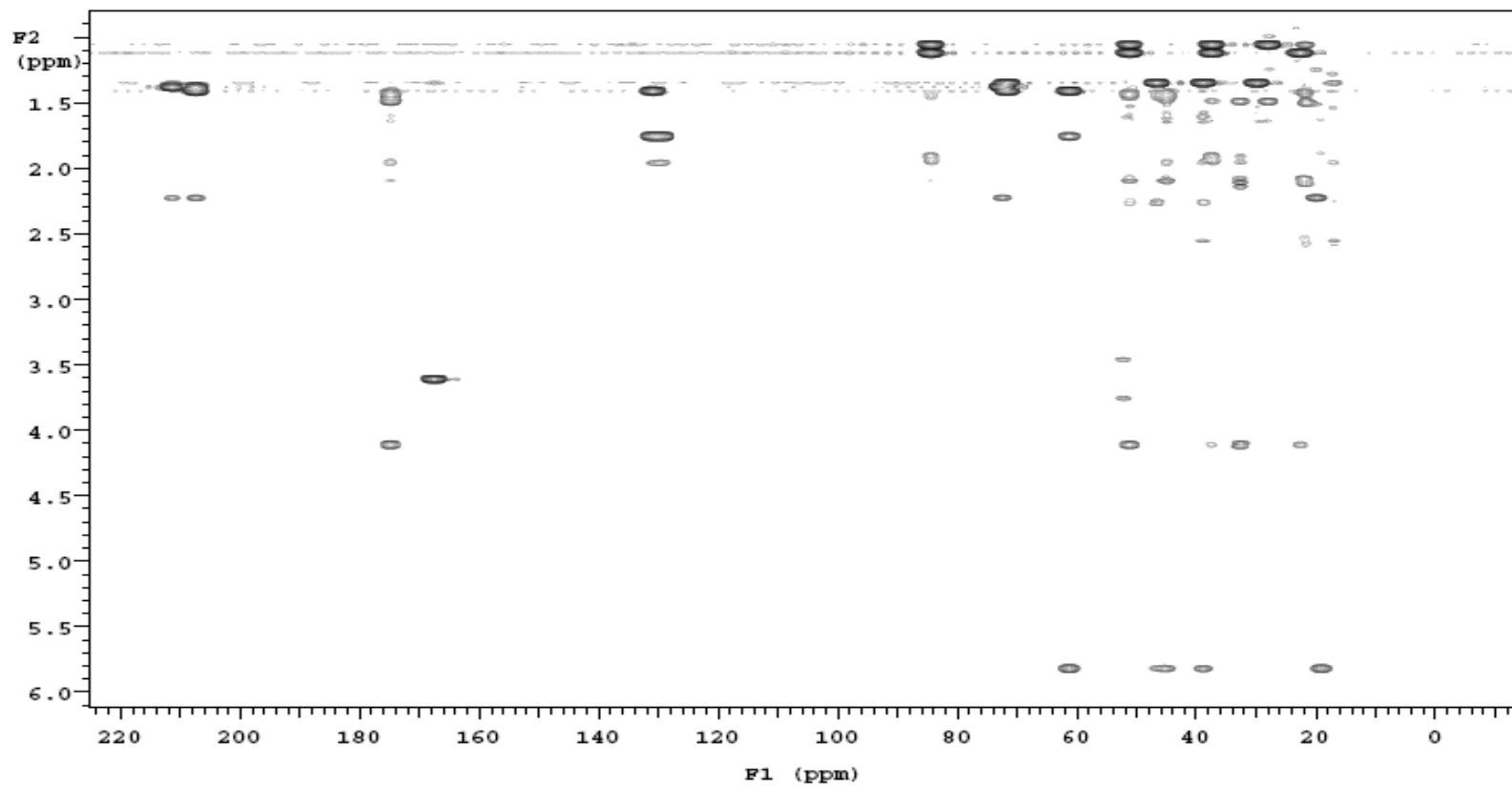


Figure S17. HMBC-NMR spectrum (500 MHz, CDCl₃) of atlantinone B (**10**)

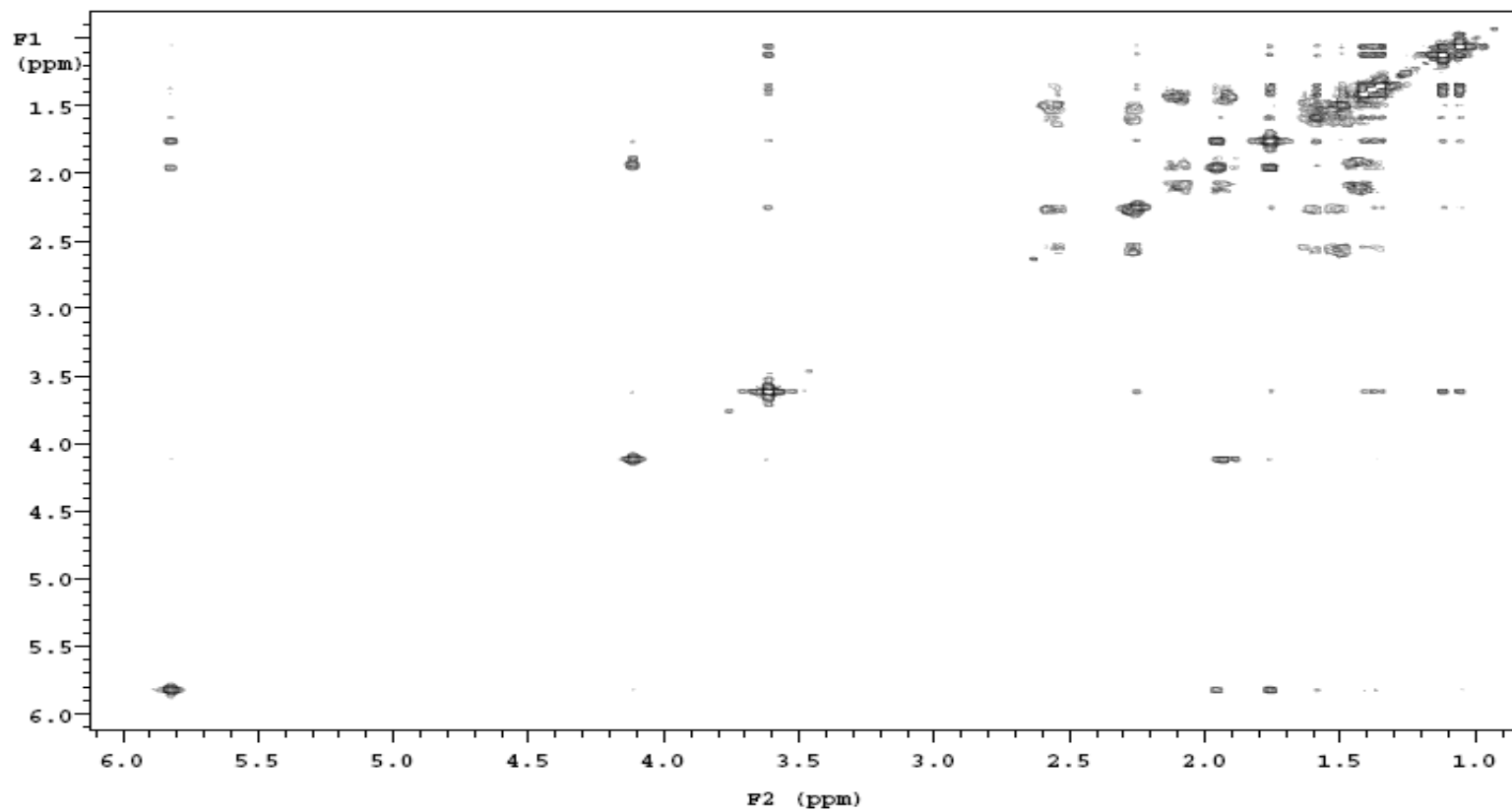


Figure S18. COSY-NMR spectrum (500 MHz, CDCl_3) of atlantinone B (**10**)

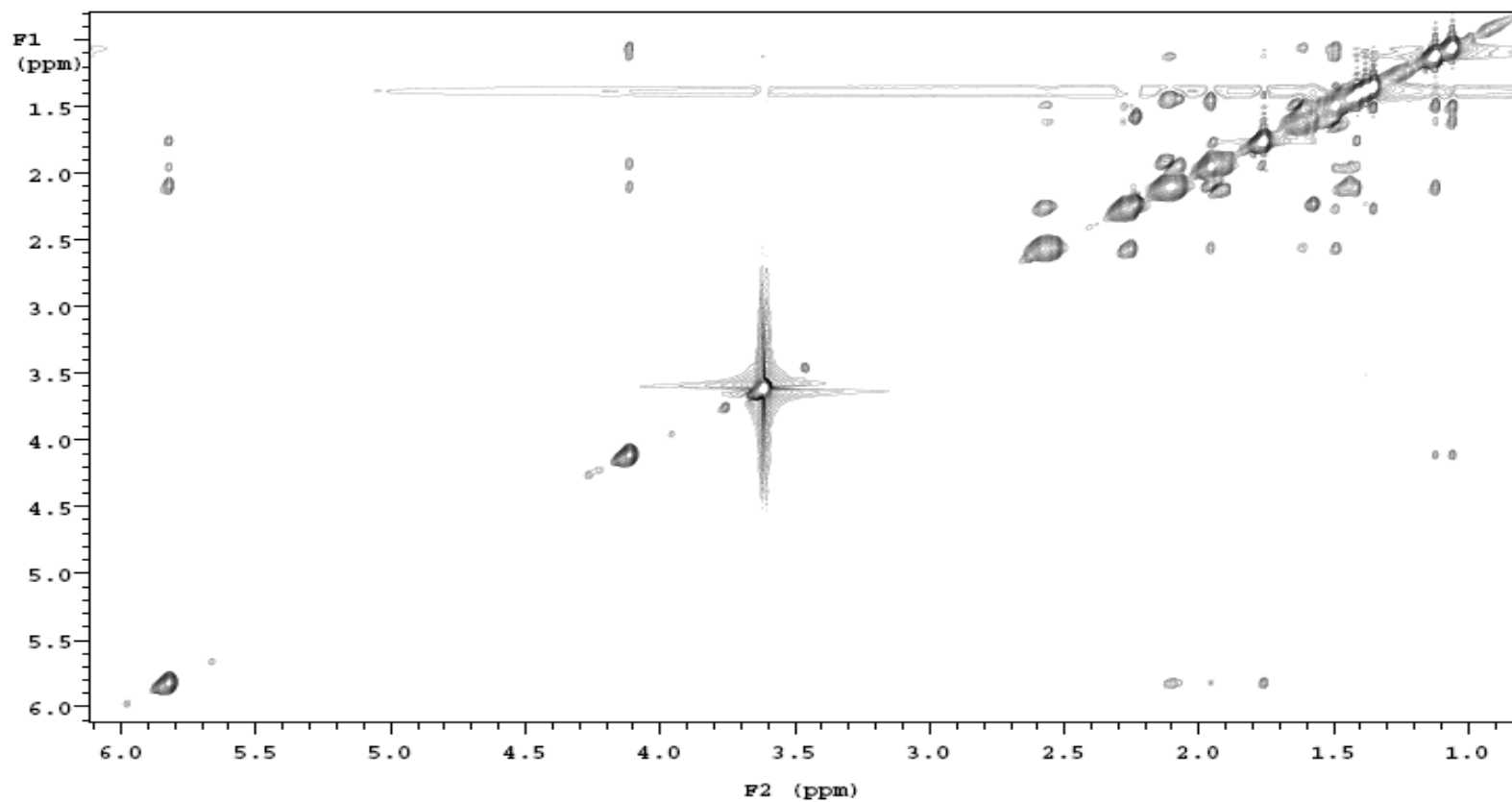


Figure S19. ROESY-NMR spectrum (500 MHz, CDCl₃) of atlantinone B (**10**)

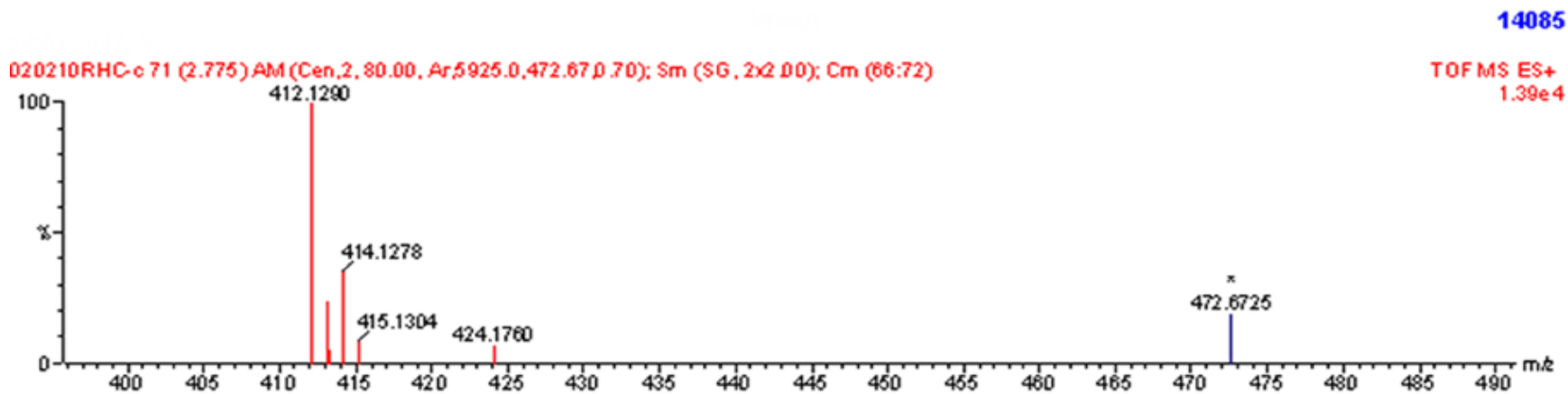


Figure S20. HRESIMS of sclerotioramine (**6**)

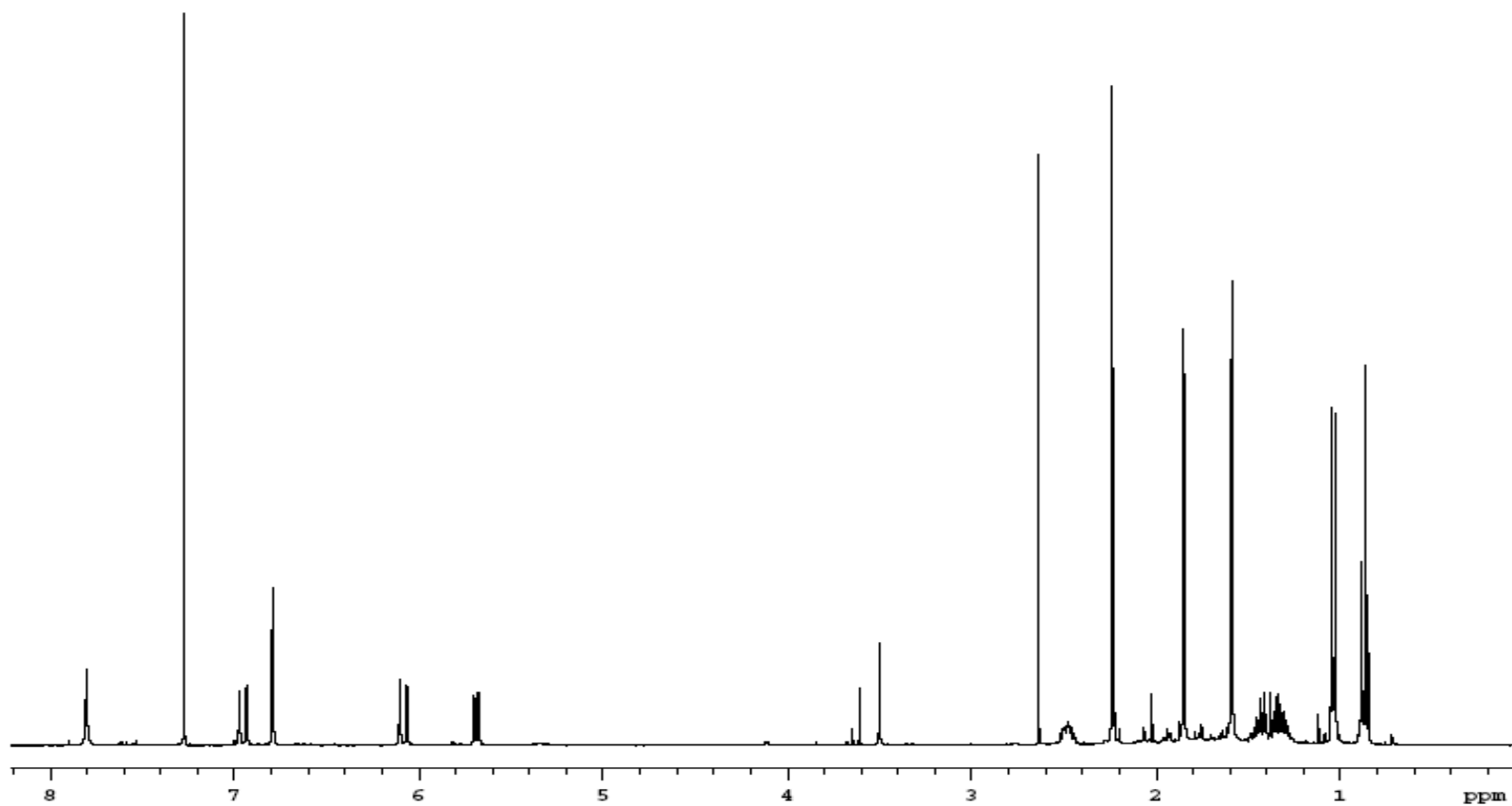


Figure S21. ^1H -NMR (400 MHz, CDCl_3) of sclerotioramine (**6**)

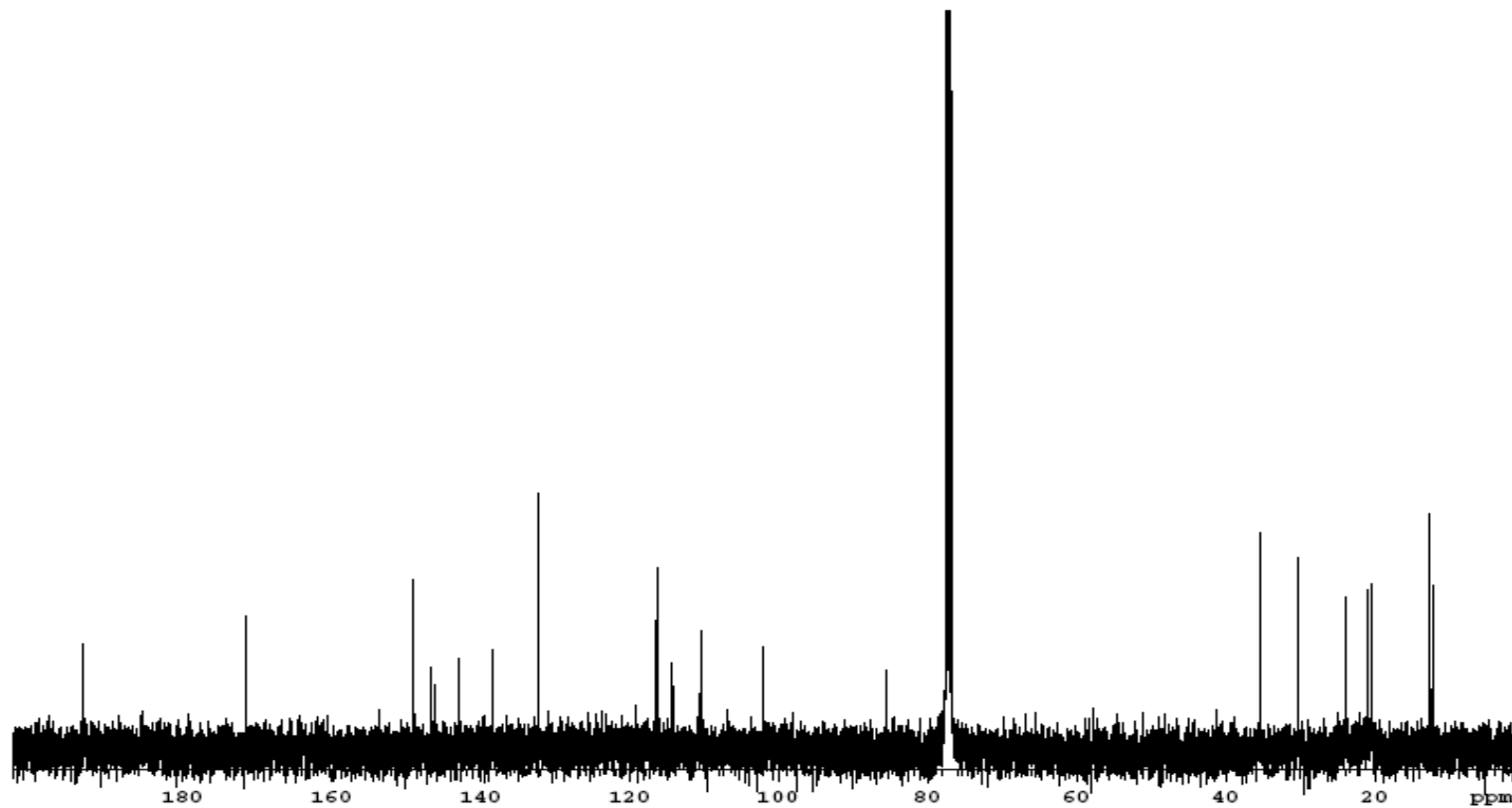


Figure S22. ^{13}C -NMR (100 MHz, CDCl_3) of sclerotioramine (**6**)

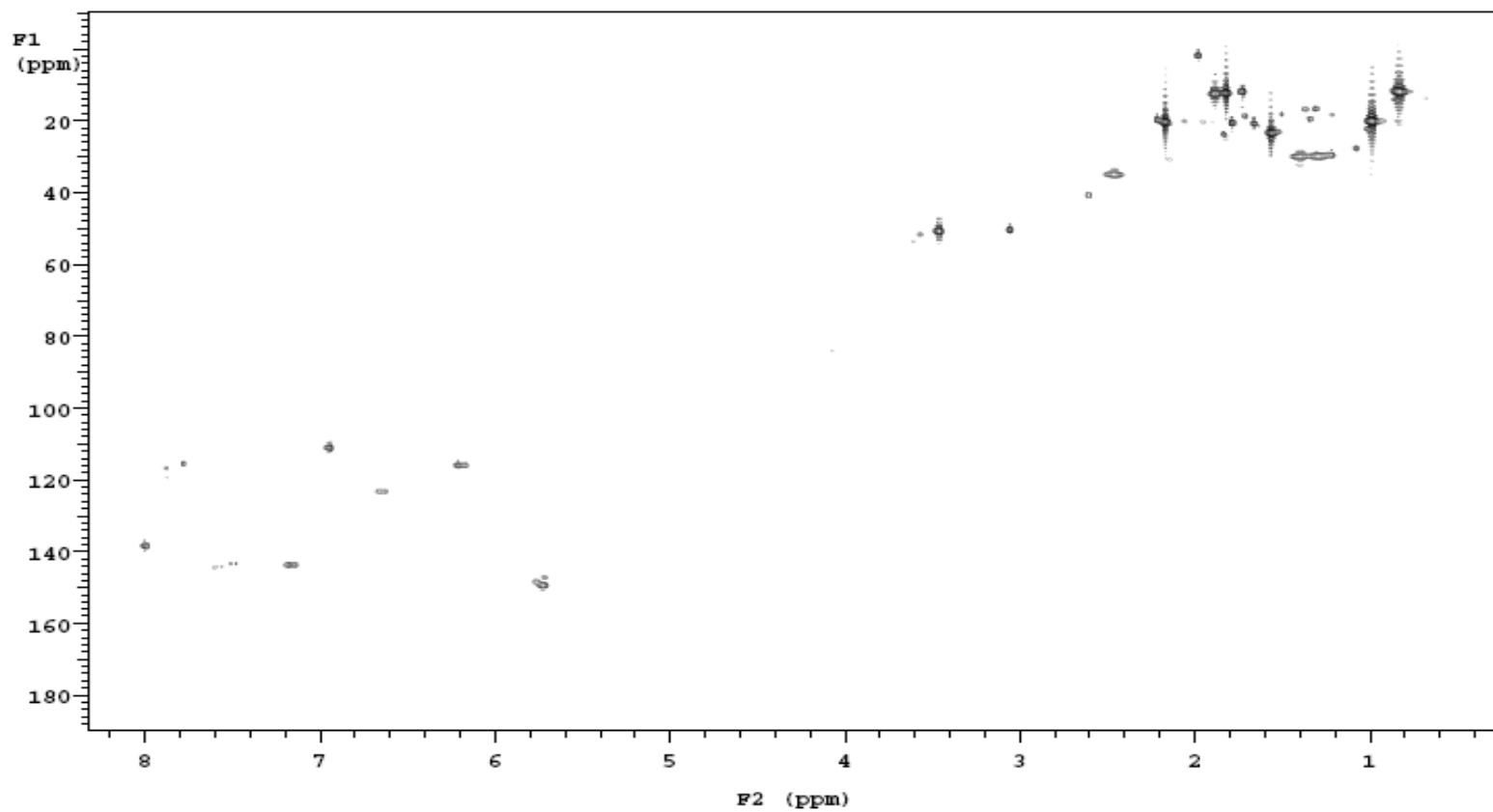


Figure S23. HSQC-NMR (500 MHz, CDCl₃) of sclerotioramine (**6**)

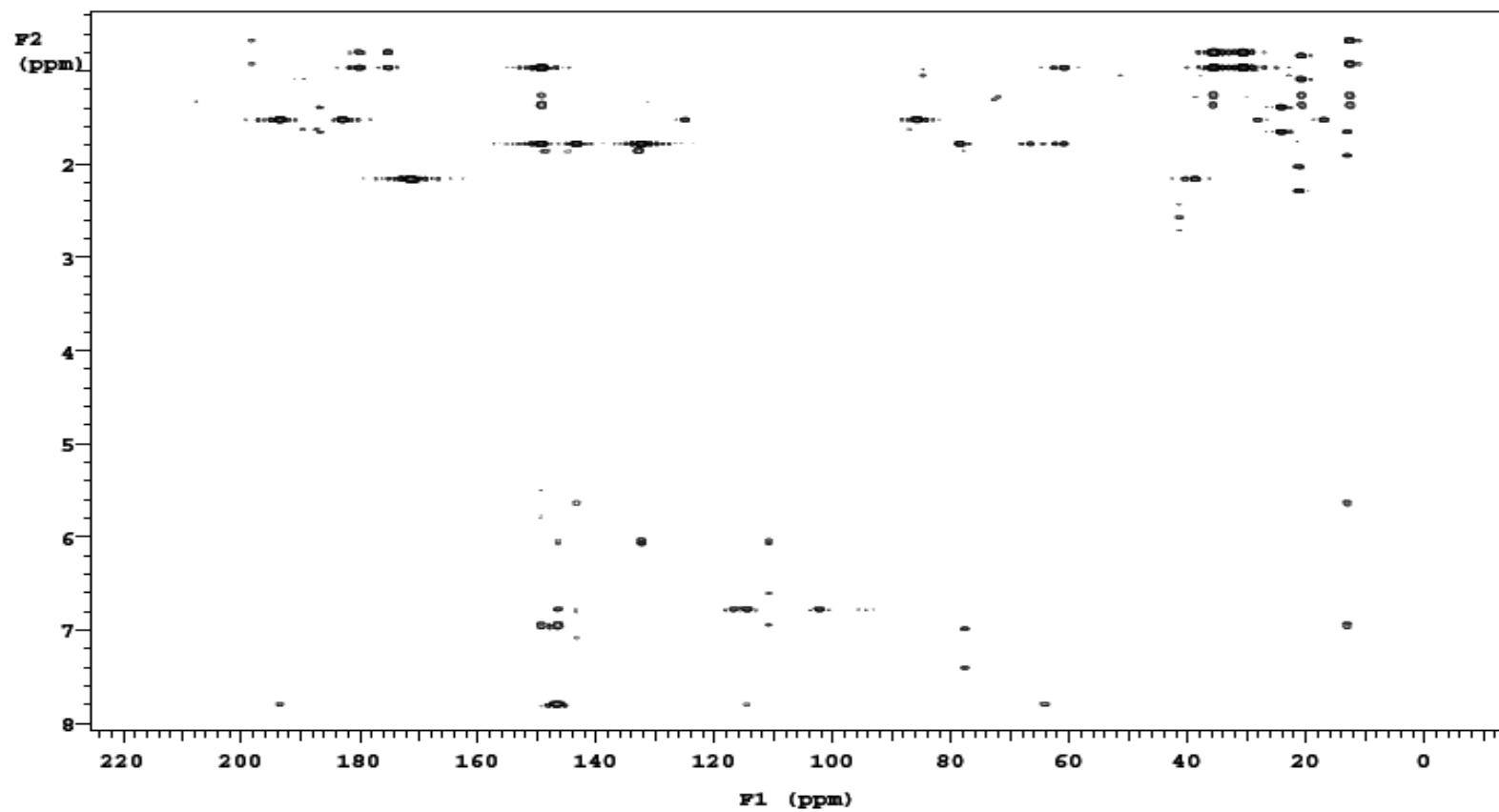


Figure S24. HMBC-NMR (500 MHz, CDCl₃) of sclerotioramine (**6**)

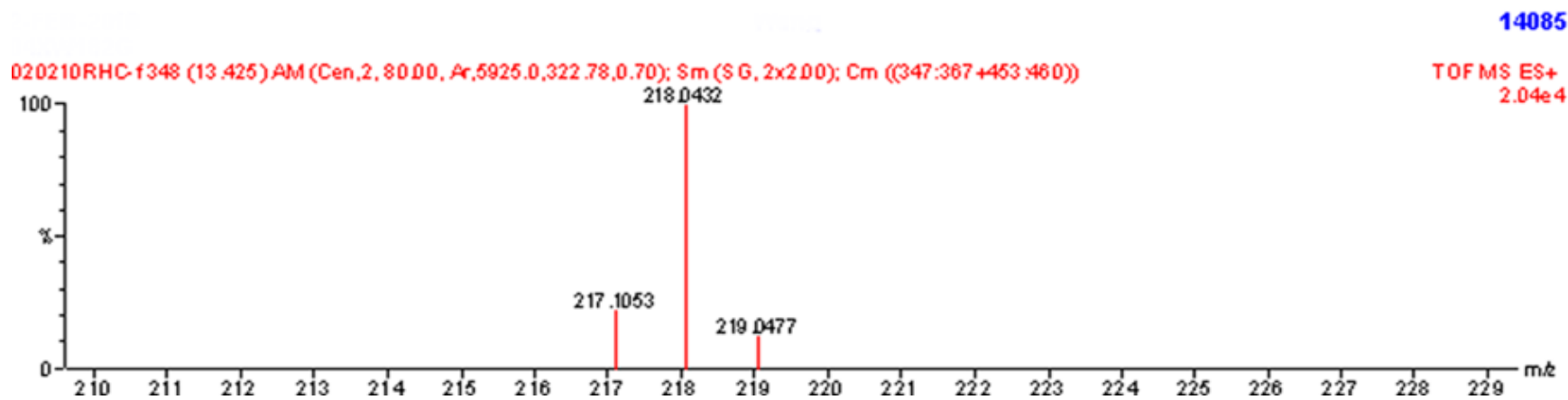


Figure S26. HRESIMS of pencolide (7)

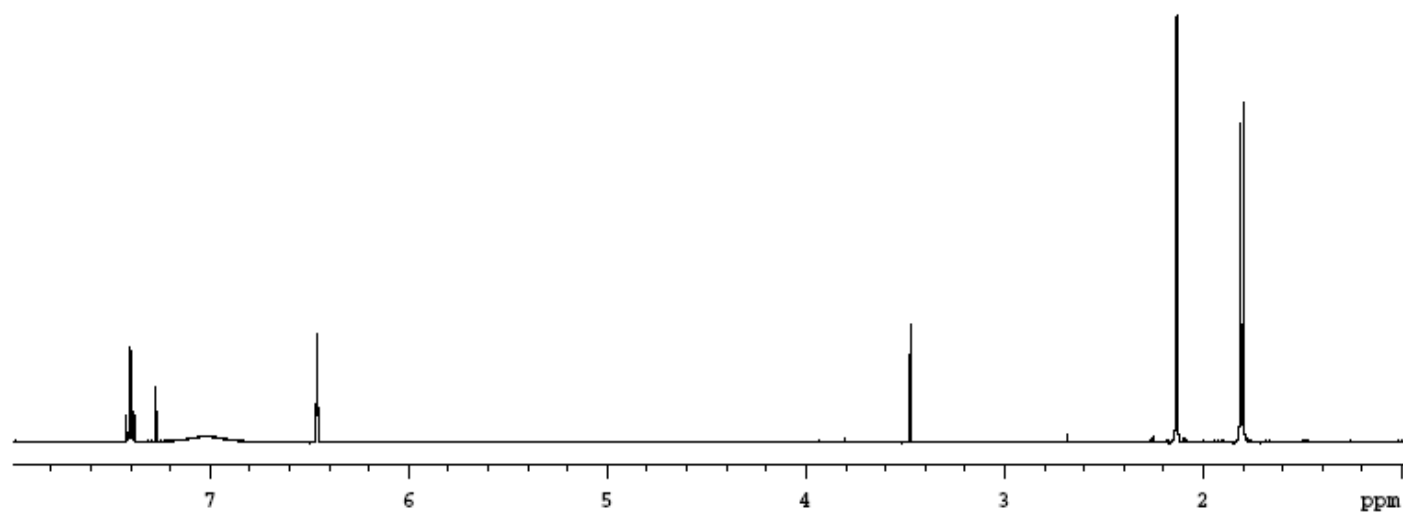


Figure S27. ^1H -NMR (500 MHz, CDCl_3) of pencolide (**7**)

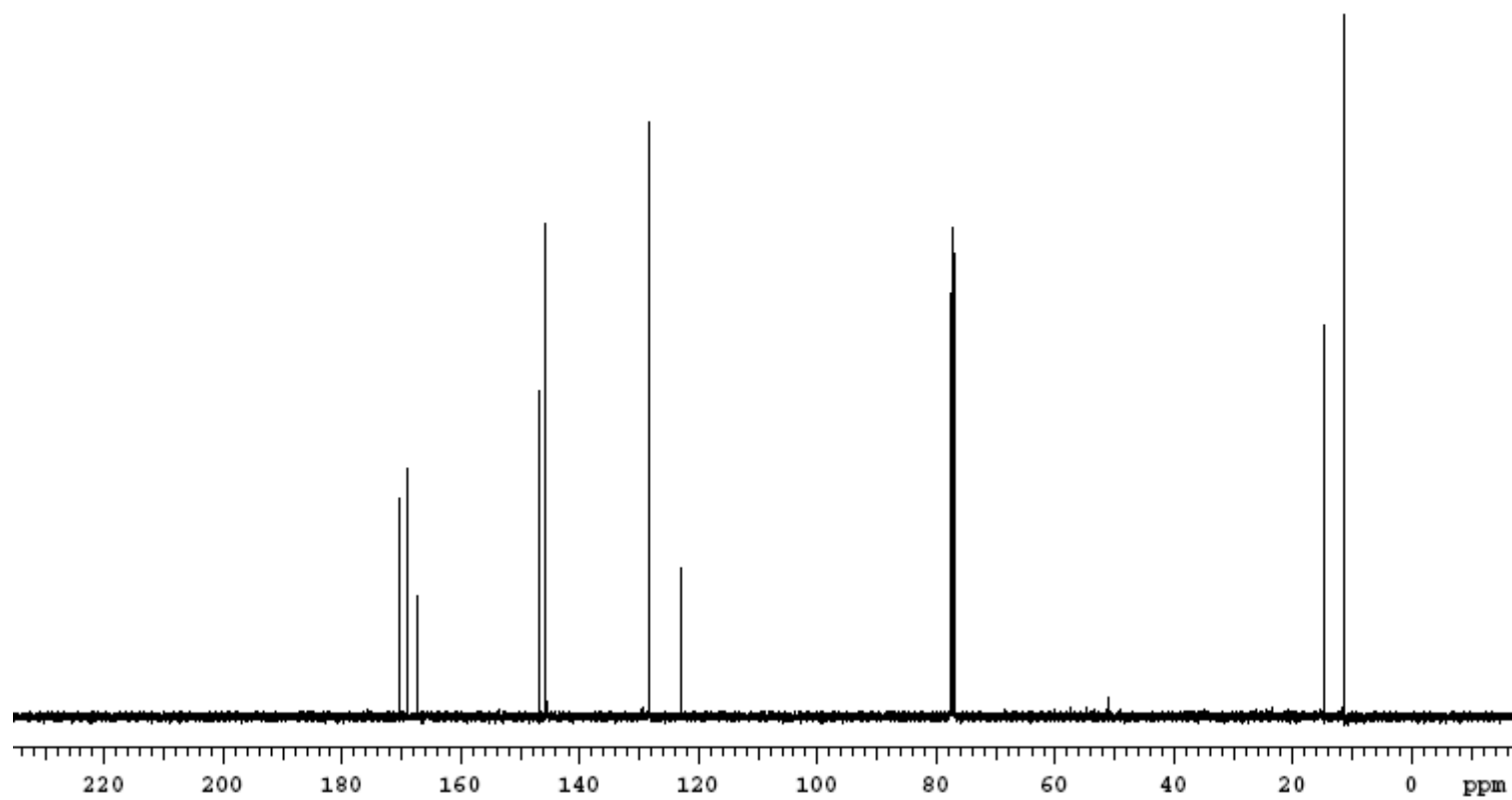


Figure S28. ^{13}C -NMR (125 MHz, CDCl_3) of pencolide (**7**)

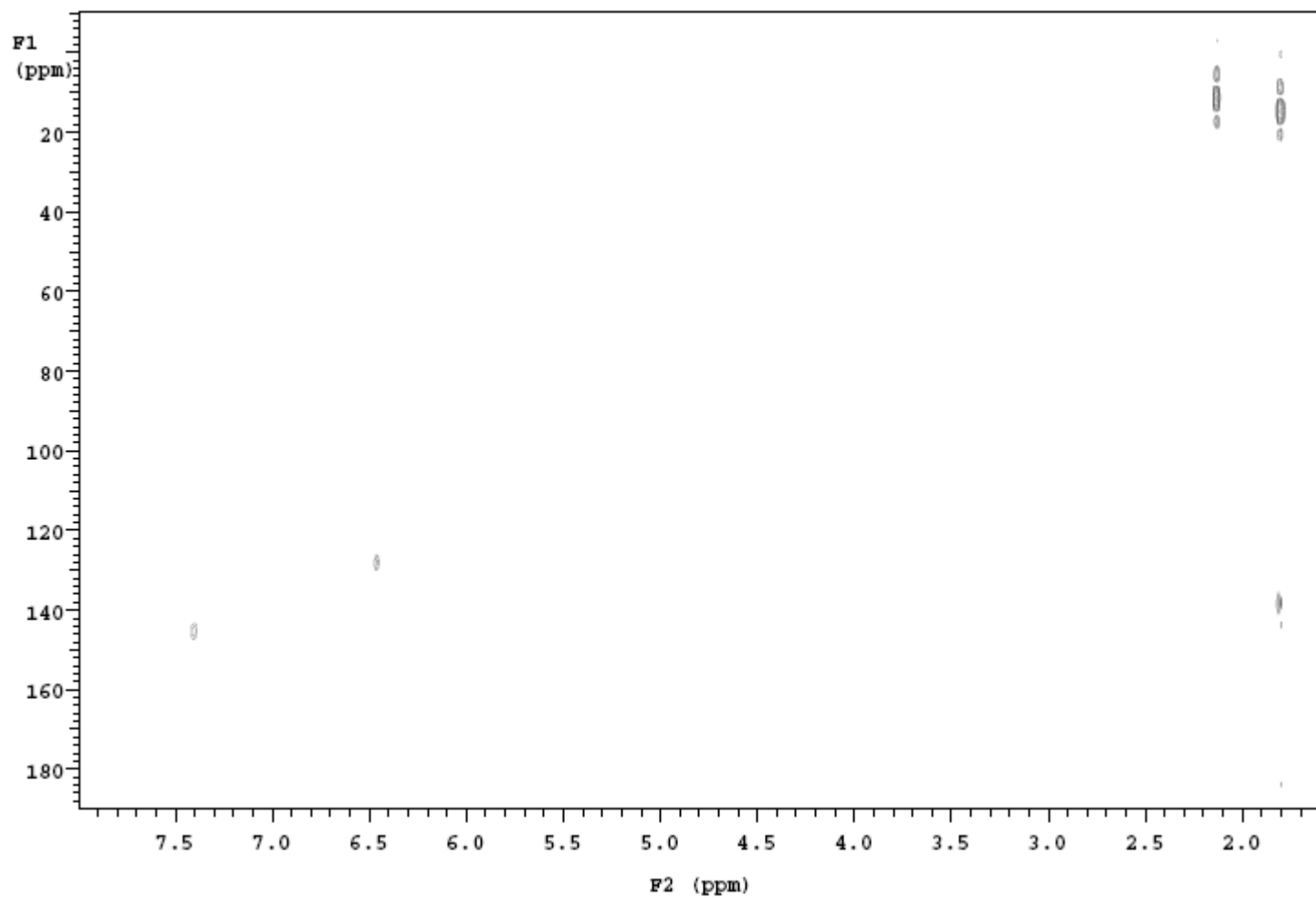


Figure S29. HSQC-NMR (500 MHz, CDCl₃) of pencolide (**7**)

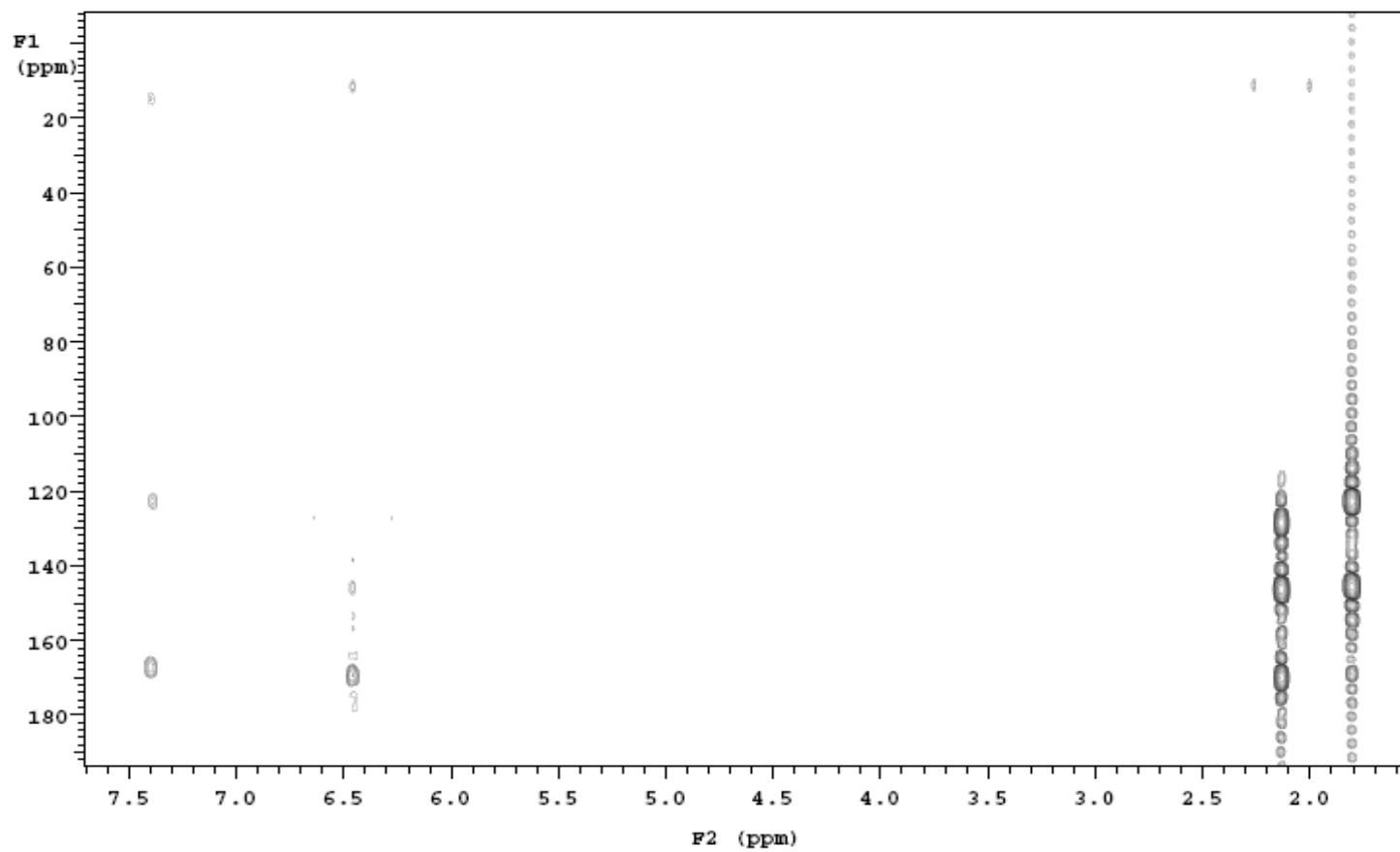


Figure S30. HMBC-NMR (500 MHz, CDCl₃) of pencolide (**7**)

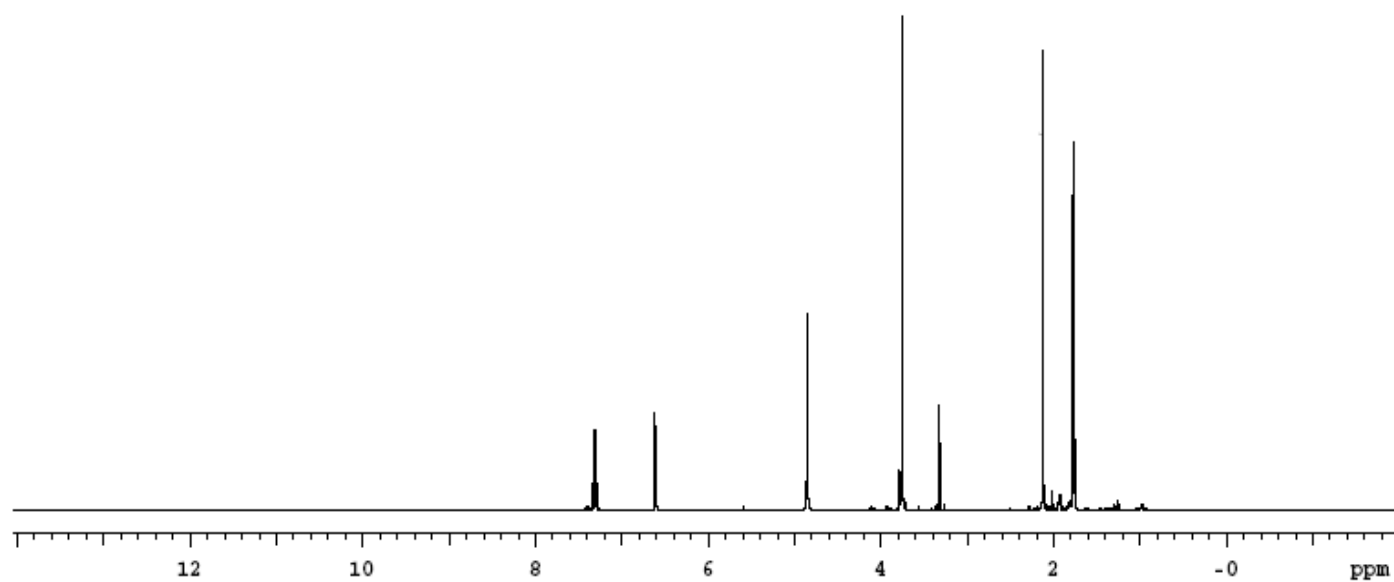


Figure S31. ^1H -NMR (500 MHz, CD_3OD) of pencolide methyl ester (**8**)

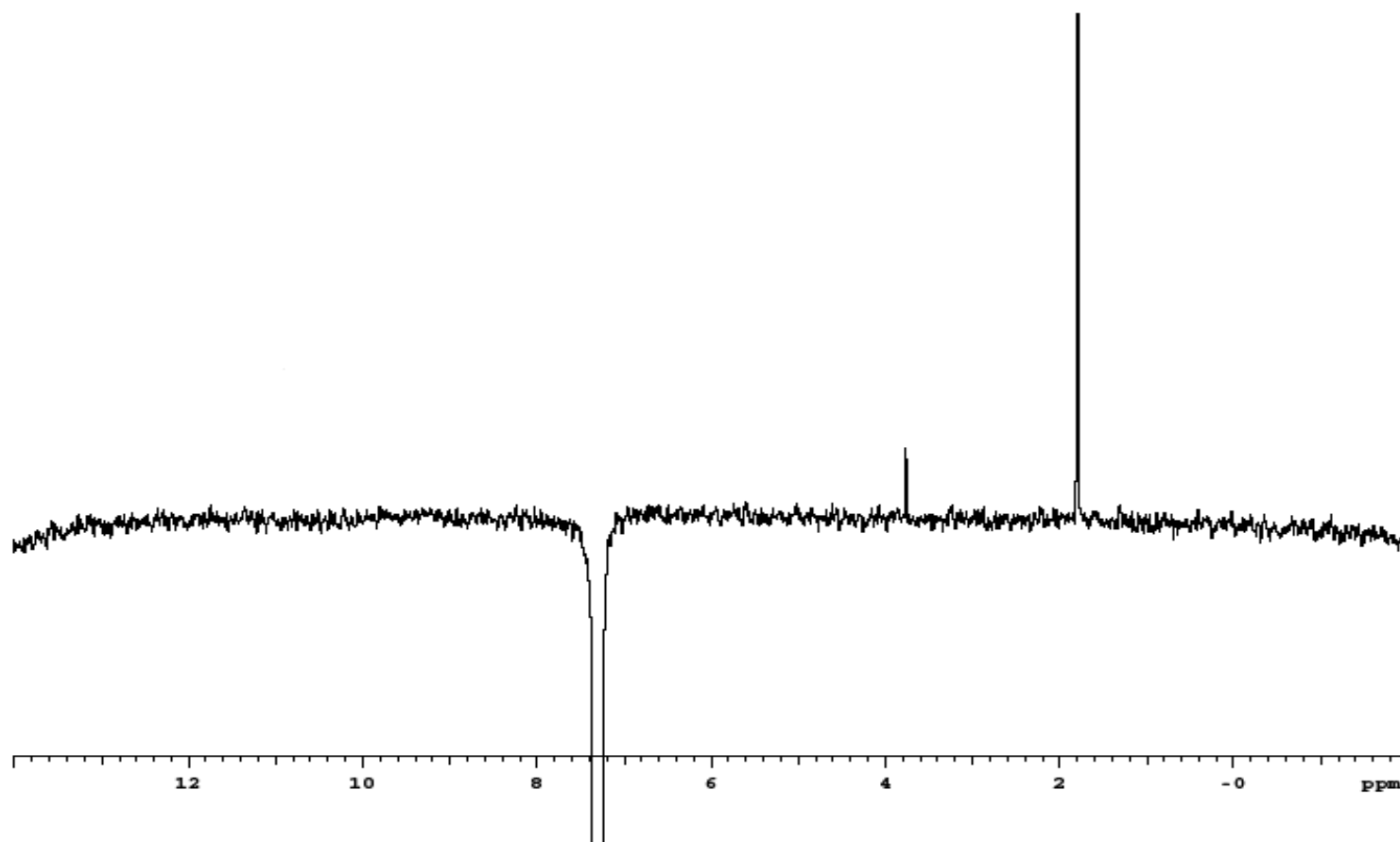


Figure S32. 1D difference NOE-NMR (500 MHz, CDCl_3) of pencolide methyl ester (**8**)