

Supplementary Materials

MS/MS Molecular Networking Unveils the Chemical Diversity of Biscembranoid Derivatives, Neutrophilic Inflammatory Mediators from the Cultured Soft Coral *Sarcophyton trocheliophorum*

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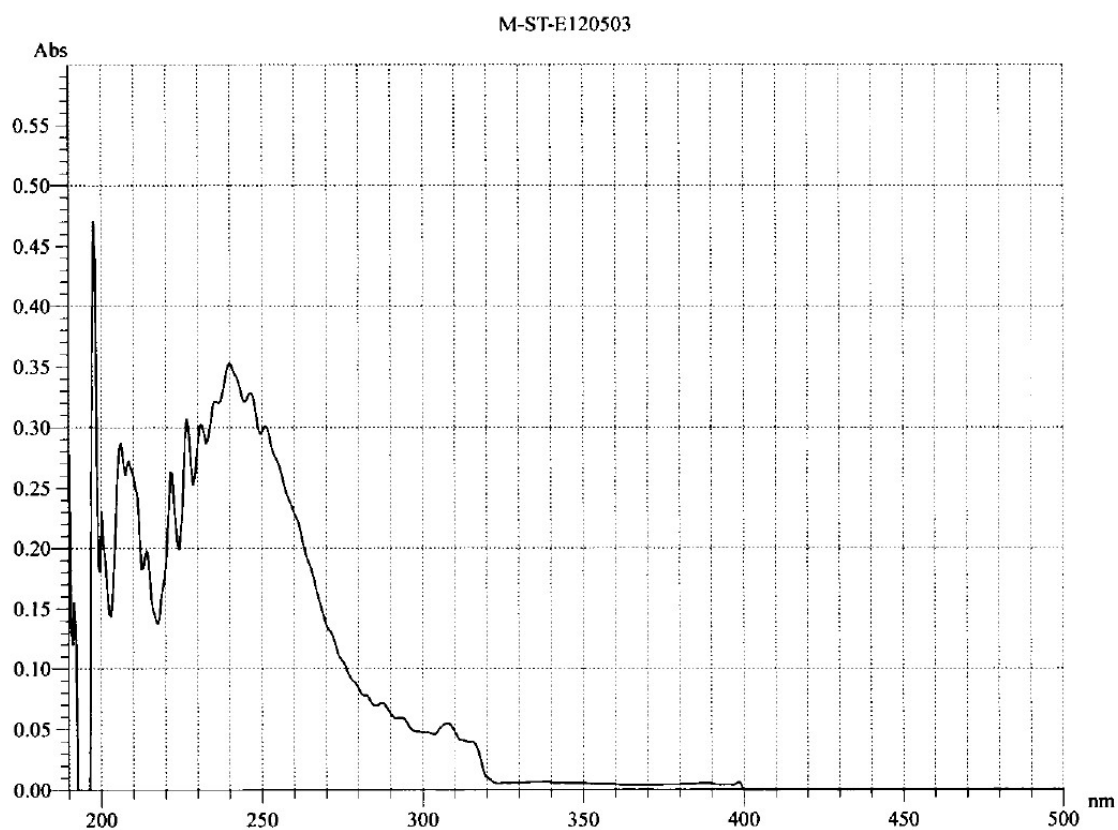
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Sensitivity: 1
Threshold: 0.0100

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1	663.60	663.10	402.10	0.0088	-2.0780	402.10	-0.0211
2	402.10	240.10	228.60	0.3532	14.9237	228.60	0.2529
3	228.60	226.60	224.10	0.3069	1.2972	224.10	0.1990
4	224.10	221.60	217.60	0.2634	1.4044	217.60	0.1375
5	217.60	206.10	203.10	0.2872	3.2287	203.10	0.1436
6	203.10	197.60	194.60	0.4708	0.8882	194.60	-0.4522

Figure S1. UV spectrum of Sarcotrochlide A (1)

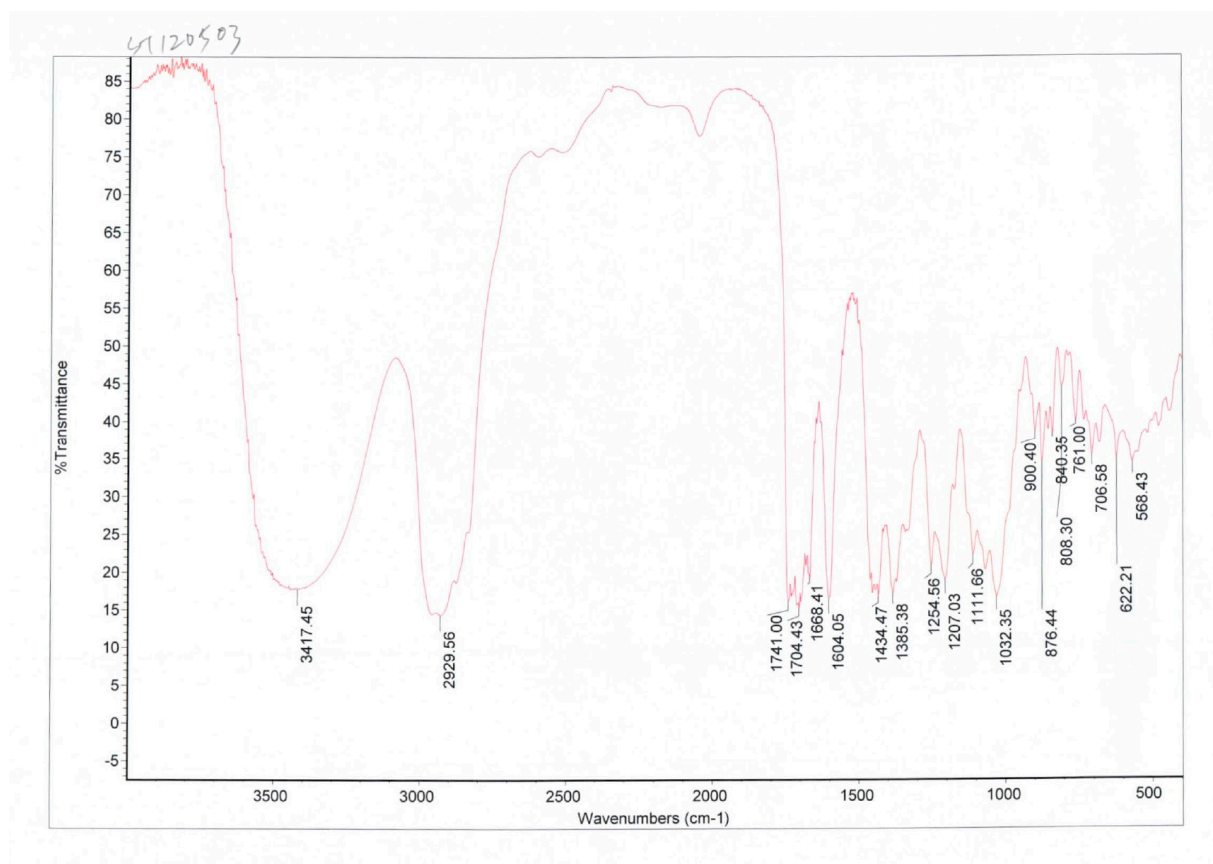


Figure S2. IR spectrum of Sarcotrochlide A (1)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

106 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-50 H: 0-70 O: 0-10 Na: 0-1

20220818_pos_0503 185 (6.329) AM2 (Ar, 18000.0, 556.28, 0.00, LS 3), ABS, Cm (181.186-147.176)

1: TOF MS ES+

7.58e+006

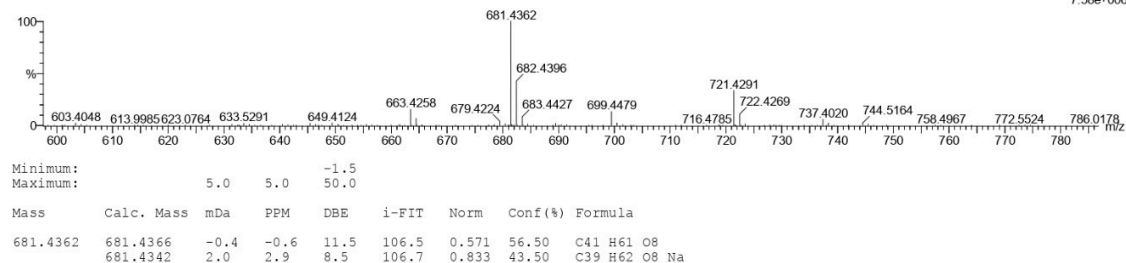


Figure S3. HRESIMS spectrum of Sarcotrochlide A (1)

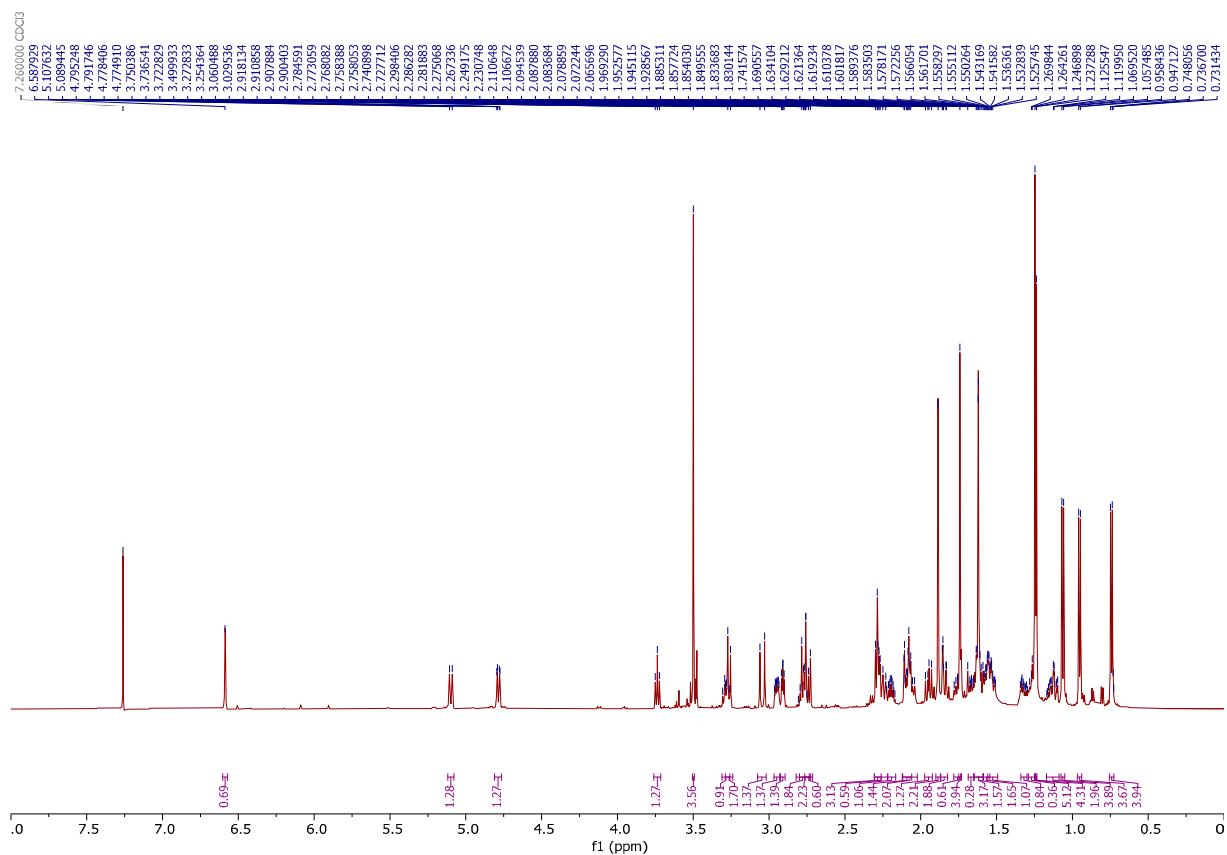


Figure S4. ¹H NMR spectrum of Sarcotrochelande A (1) in CDCl₃ at 600 MHz

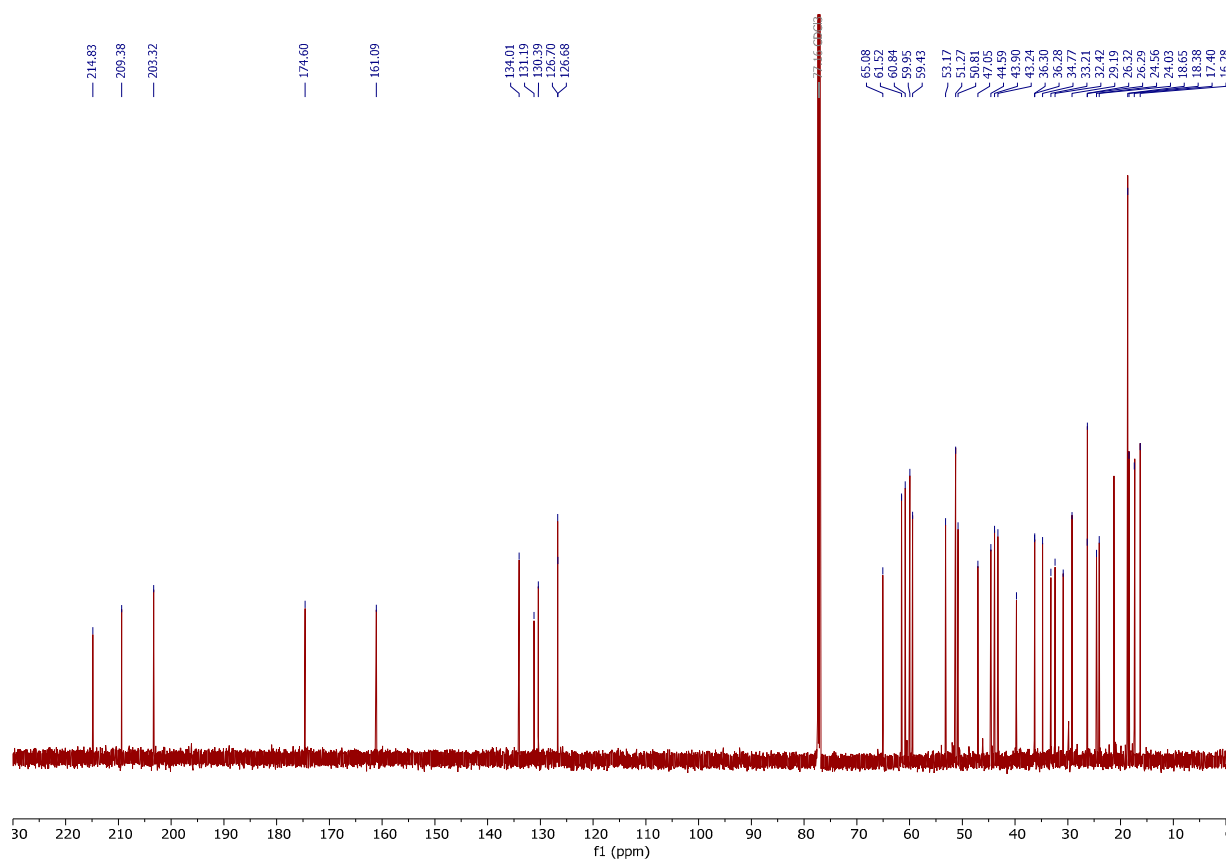


Figure S5. ¹³C NMR spectrum of Sarcotrochelande A (1) in CDCl₃ at 150 MHz

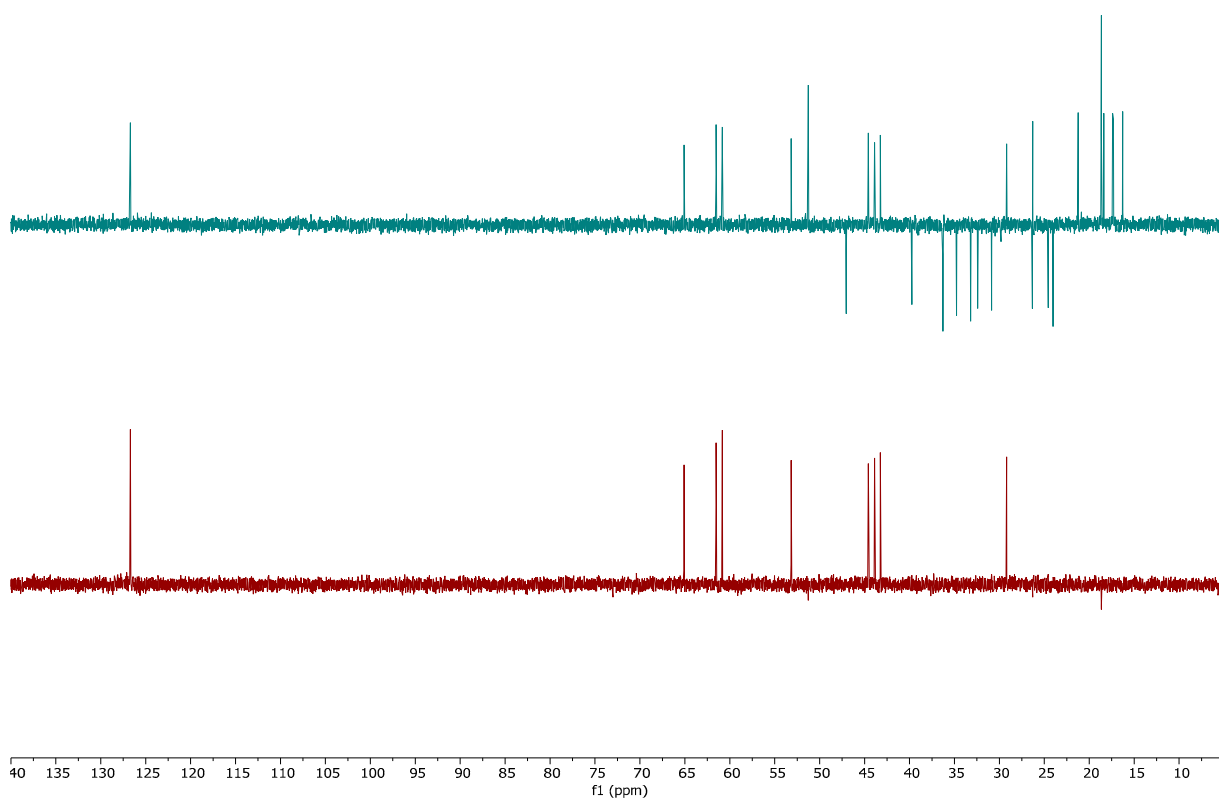


Figure S6. DEPT spectrum of Sarcotrochelande A (**1**) in CDCl₃ at 150 MHz

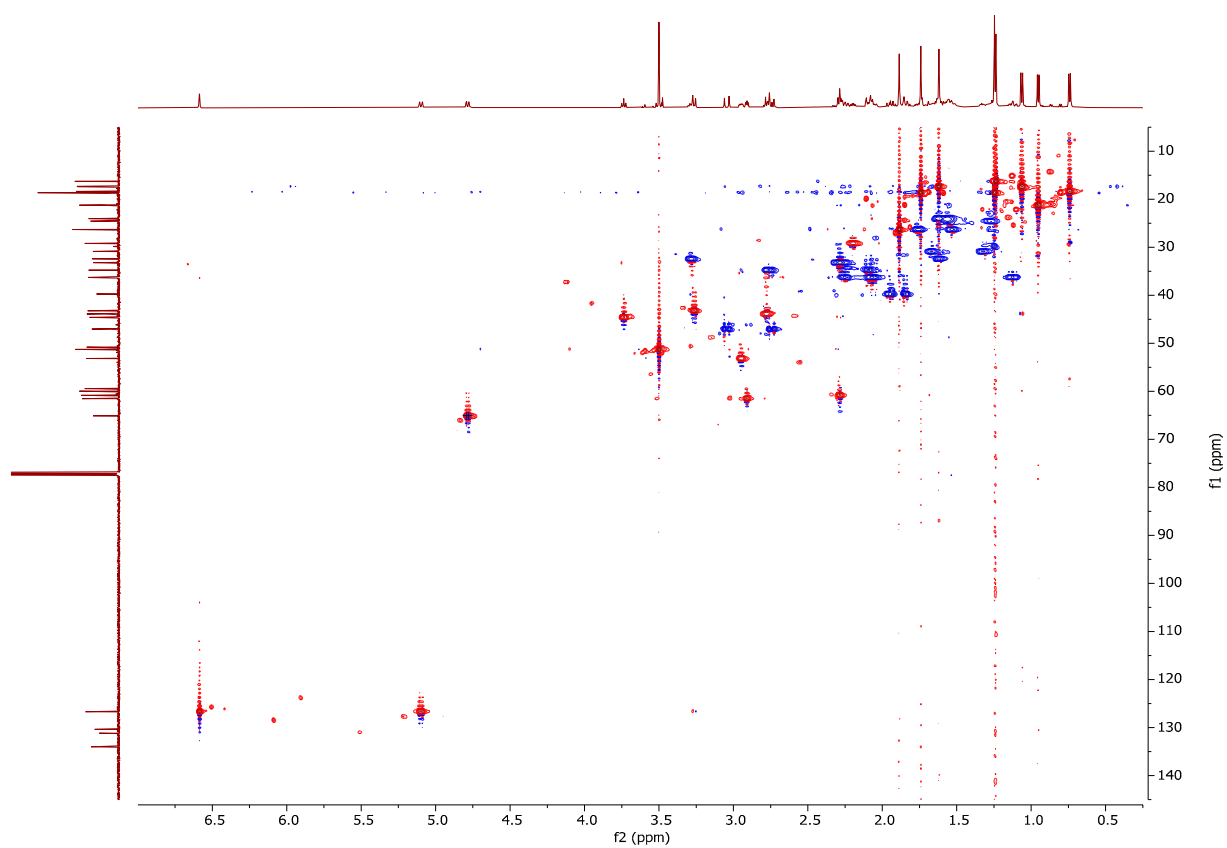


Figure S7. HSQC spectrum of Sarcotrochelande A (**1**) in CDCl₃

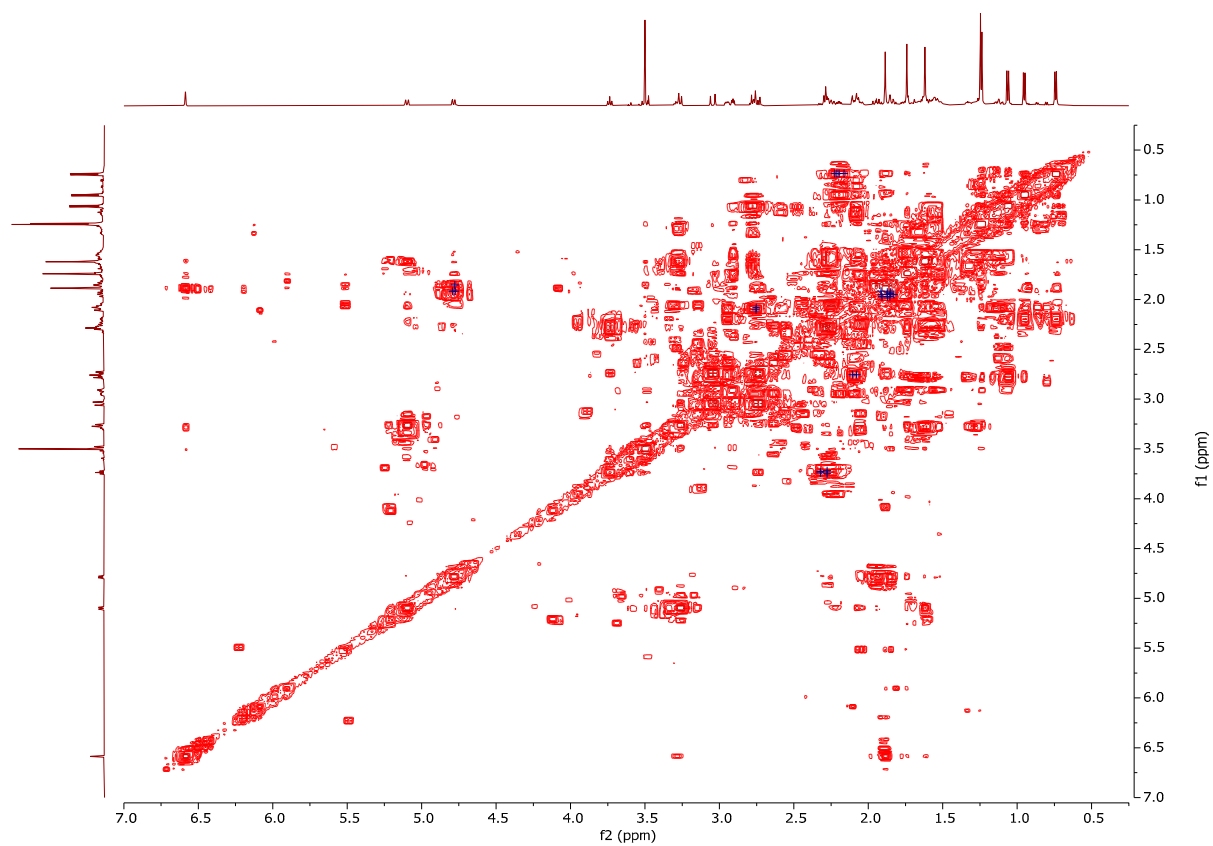


Figure S8. COSY spectrum of Sarcotrochlide A (**1**) in CDCl_3

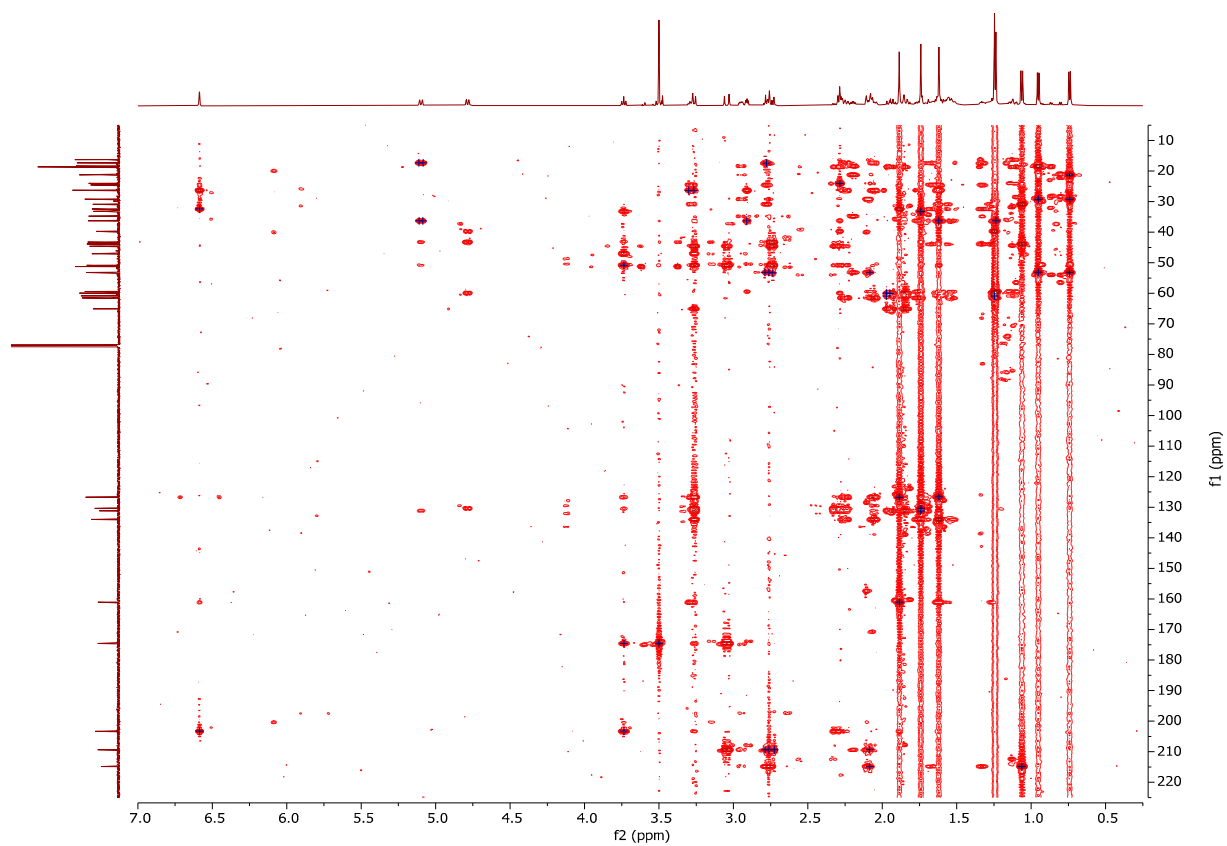


Figure S9. HMBC spectrum of Sarcotrochelide A (**1**) in CDCl_3

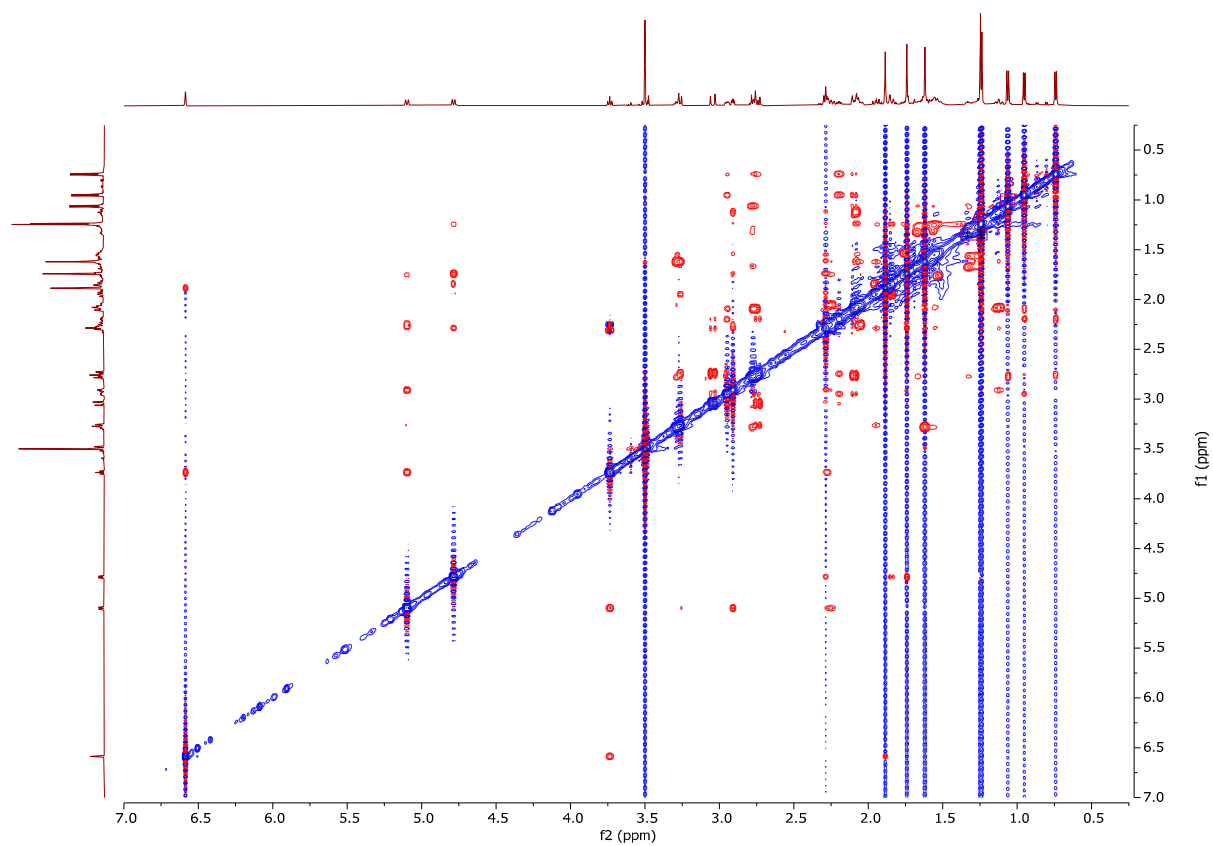
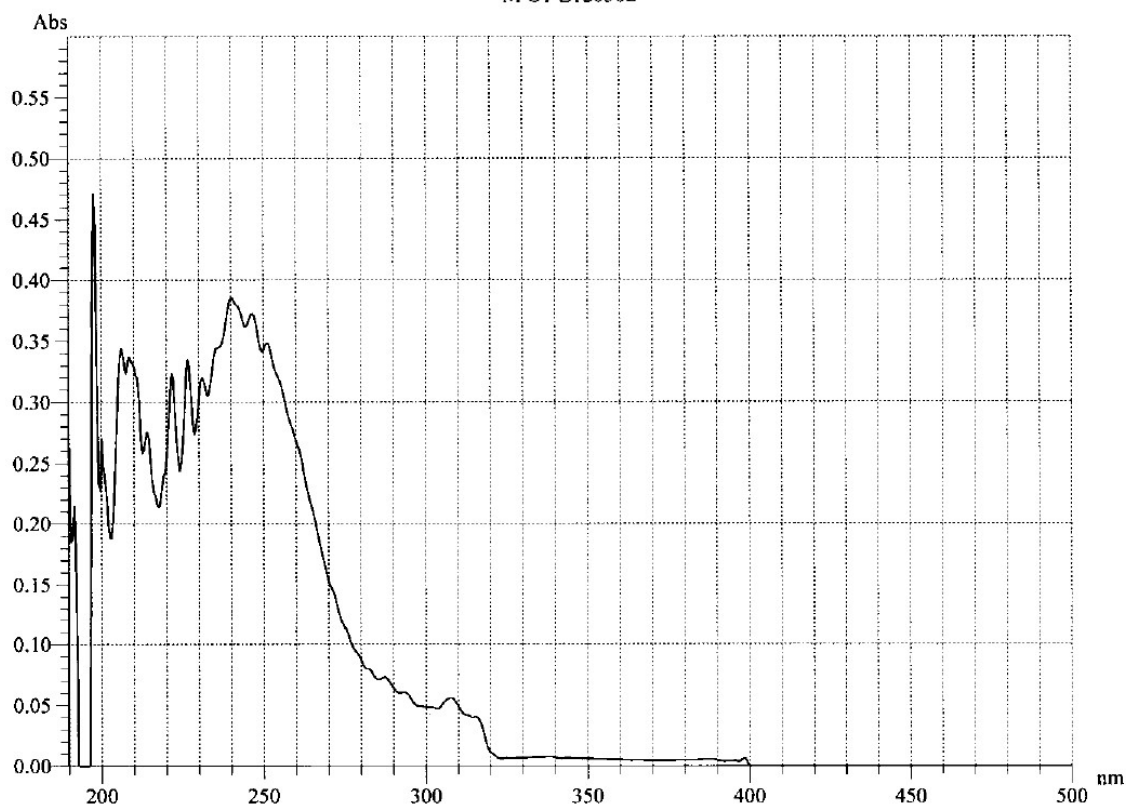


Figure S10. NOESY spectrum of Sarcotrochelande A (**1**) in CDCl_3

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M-ST-E120502



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 File name: M-ST-E120502.UDS
 Run Date: 10:24:00, 09/27/2022
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 Comment:

Peak Integration

Method: Rectangular
 Sensitivity: 1
 Threshold: 0.0100

Peaks

Peak #	Start (nm)	Apex (nm)	End (nm)	Height (Abs)	Area (Abs*nm)	Valley (nm)	Valley (/
1	663.60	663.60	402.10	0.0085	-2.0485	402.10	-0.0211
2	402.10	240.10	228.60	0.3858	16.5096	228.60	0.2734
3	228.60	226.60	224.10	0.3354	1.4531	224.10	0.2436
4	224.10	221.60	217.60	0.3238	1.8416	217.60	0.2130
5	217.60	206.10	203.10	0.3441	4.2360	203.10	0.1884
6	203.10	197.60	194.60	0.4711	1.2803	194.60	-0.3917

Figure S11. UV spectrum of Sarcotrochlide B (2)

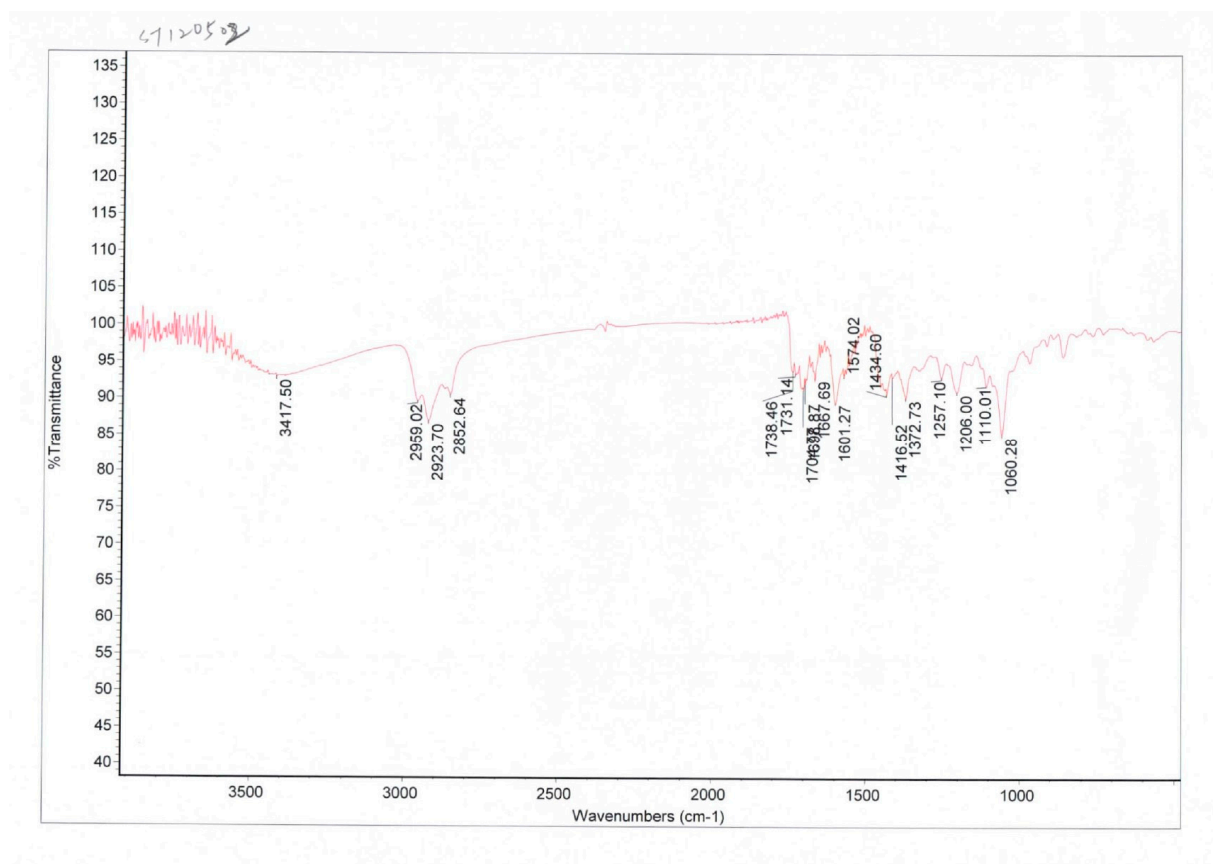


Figure S12. IR spectrum of Sarcotrochelite B (2)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

90 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-50 H: 0-70 O: 0-10 Na: 0-1

20220818_pos_0502 175 (6.302)AM2 (Ar,18000.0,556.28,0.00,LS 3), ABS, Cm (175.176-157.172)

1: TOF MS ES+

3.29e+006

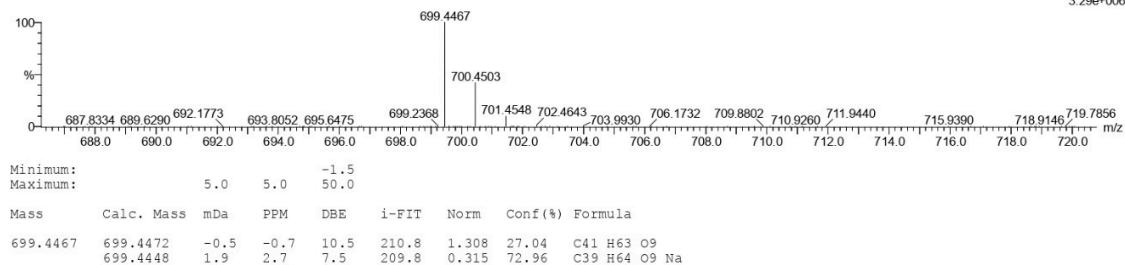


Figure S13. HRESIMS spectrum of Sarcotrochelite B (2)

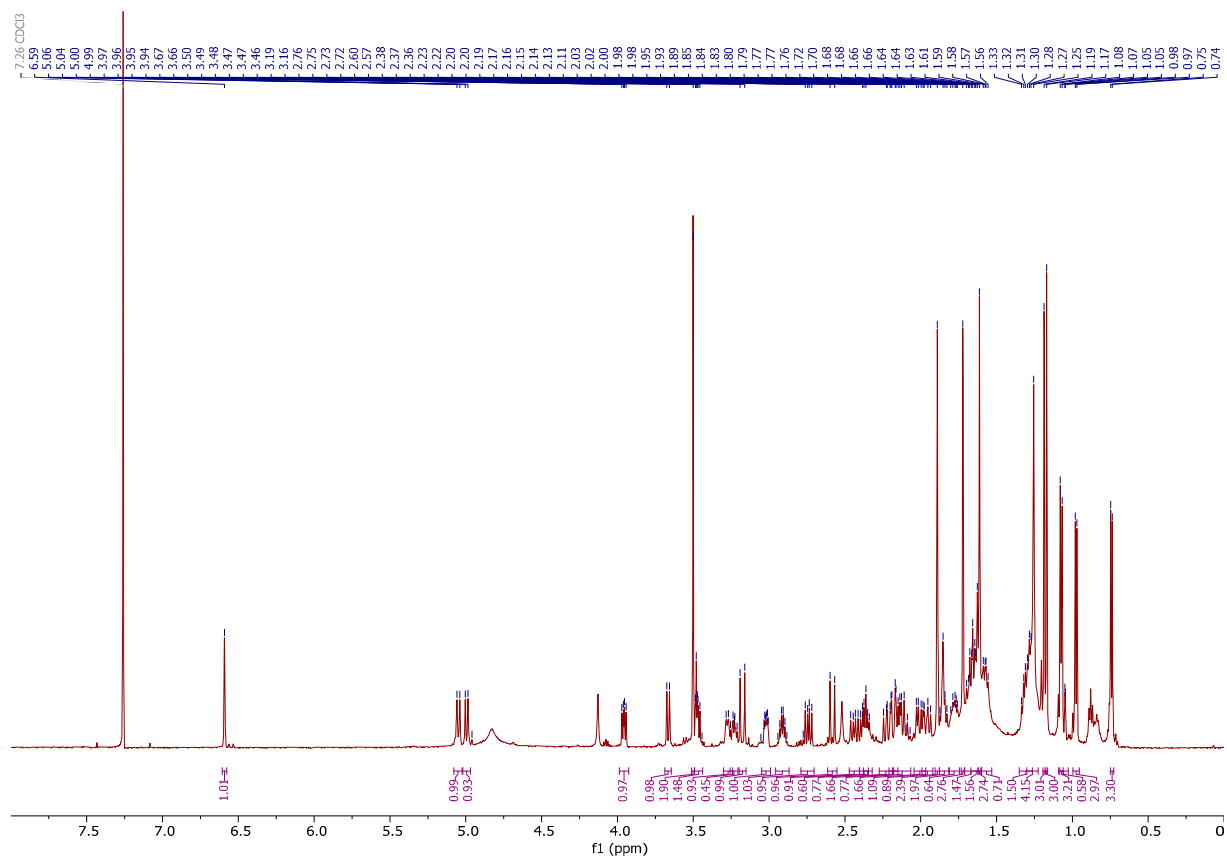


Figure S14. ¹H NMR spectrum of Sarcotrochelde B (**2**) in CDCl₃ at 600 MHz

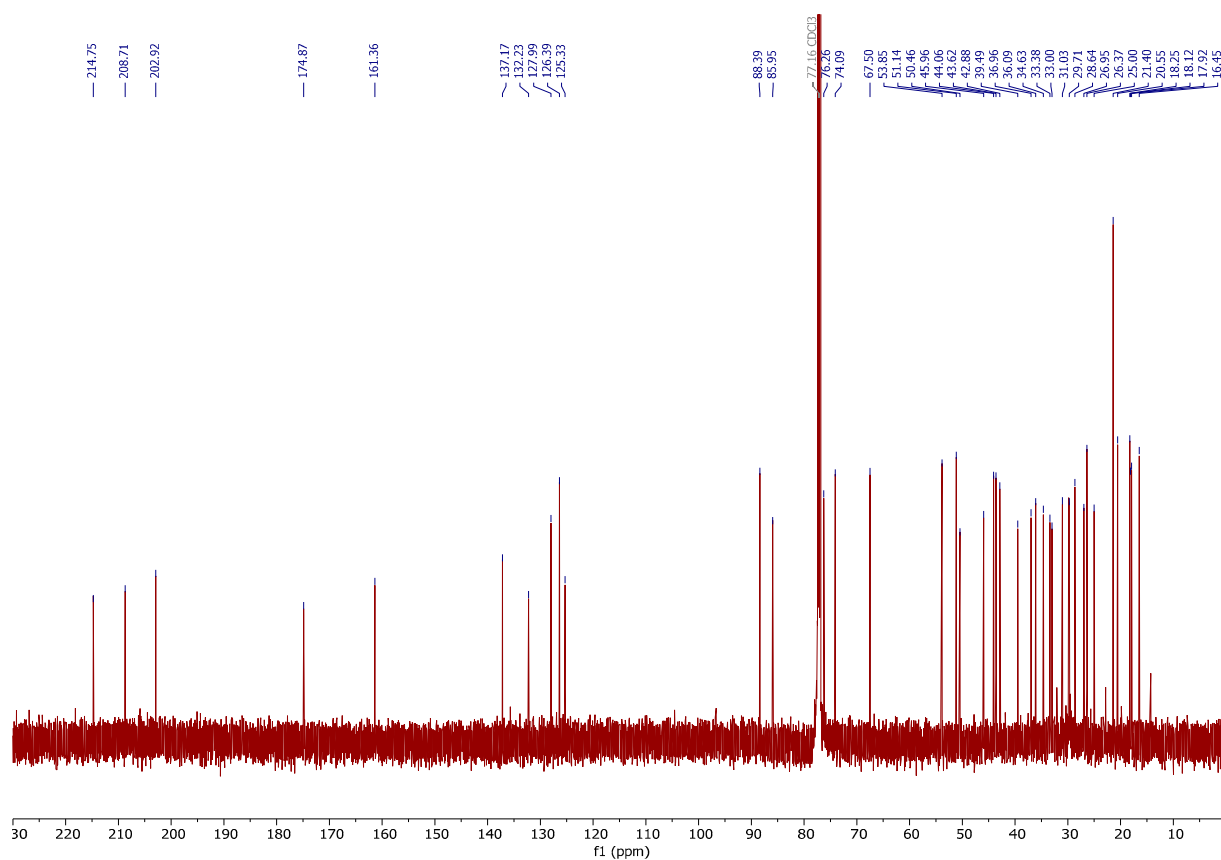


Figure S15. ^{13}C NMR spectrum of Sarcotrochelide B (**2**) in CDCl_3 at 150 MHz

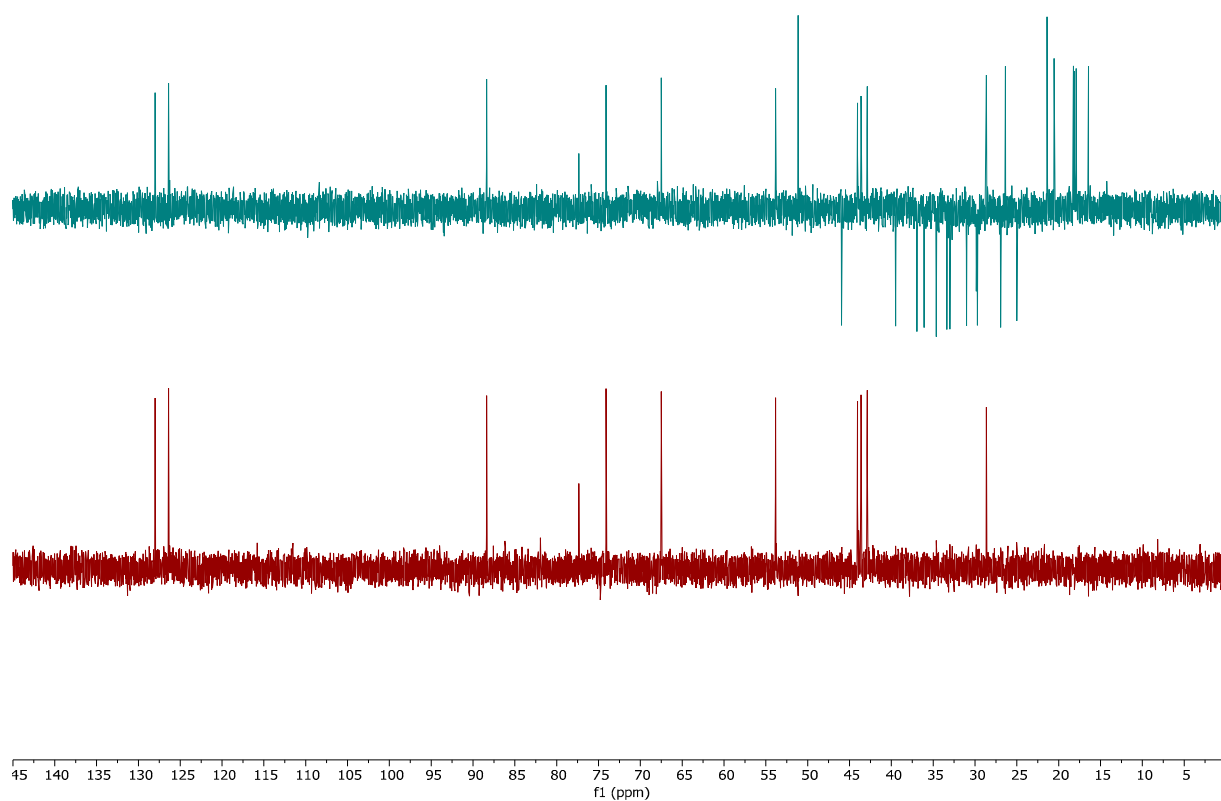


Figure S16. DEPT spectrum of Sarcotrochelande B (**2**) in CDCl_3 at 150 MHz

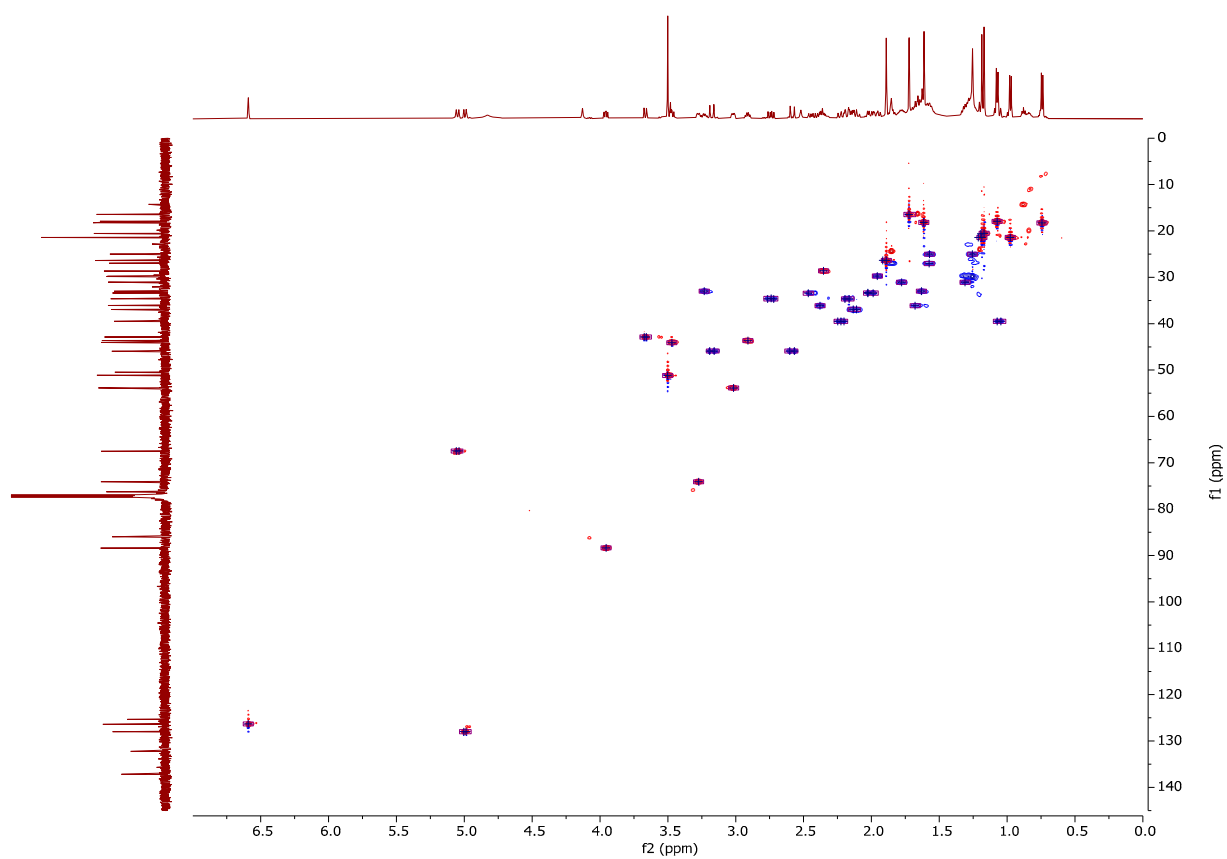


Figure S17. HSQC spectrum of Sarcotrochelande B (**2**) in CDCl_3

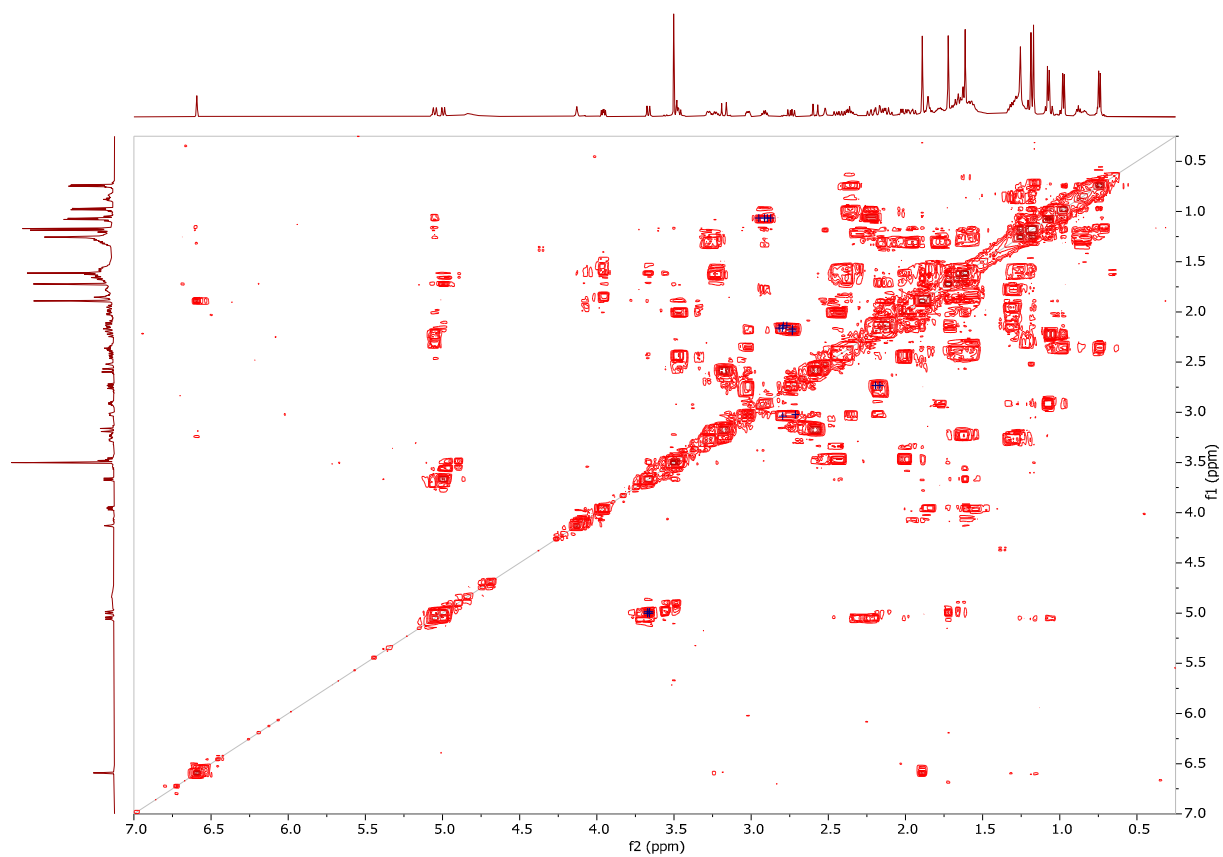


Figure S18. COSY spectrum of Sarcotrochelide B (**2**) in CDCl_3

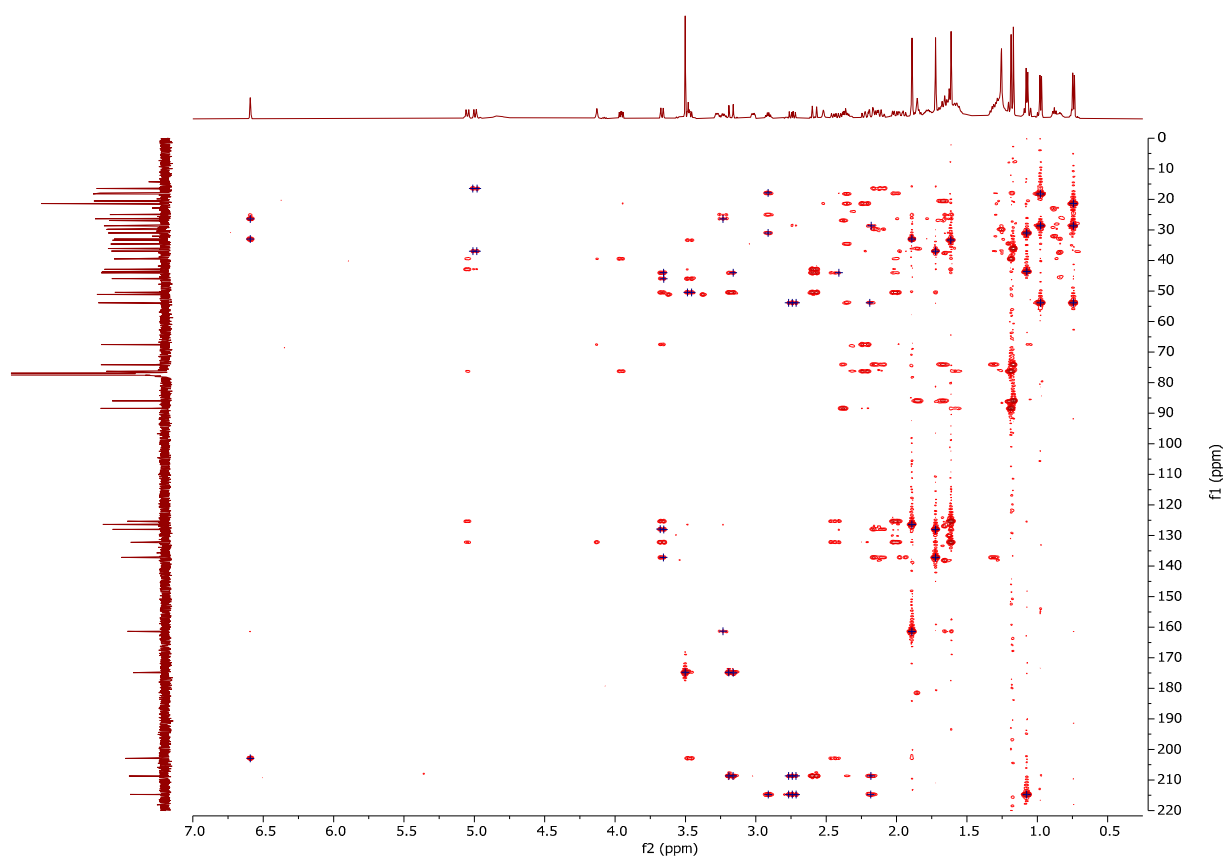


Figure S19. HMBC spectrum of Sarcotrochelande B (**2**) in CDCl_3

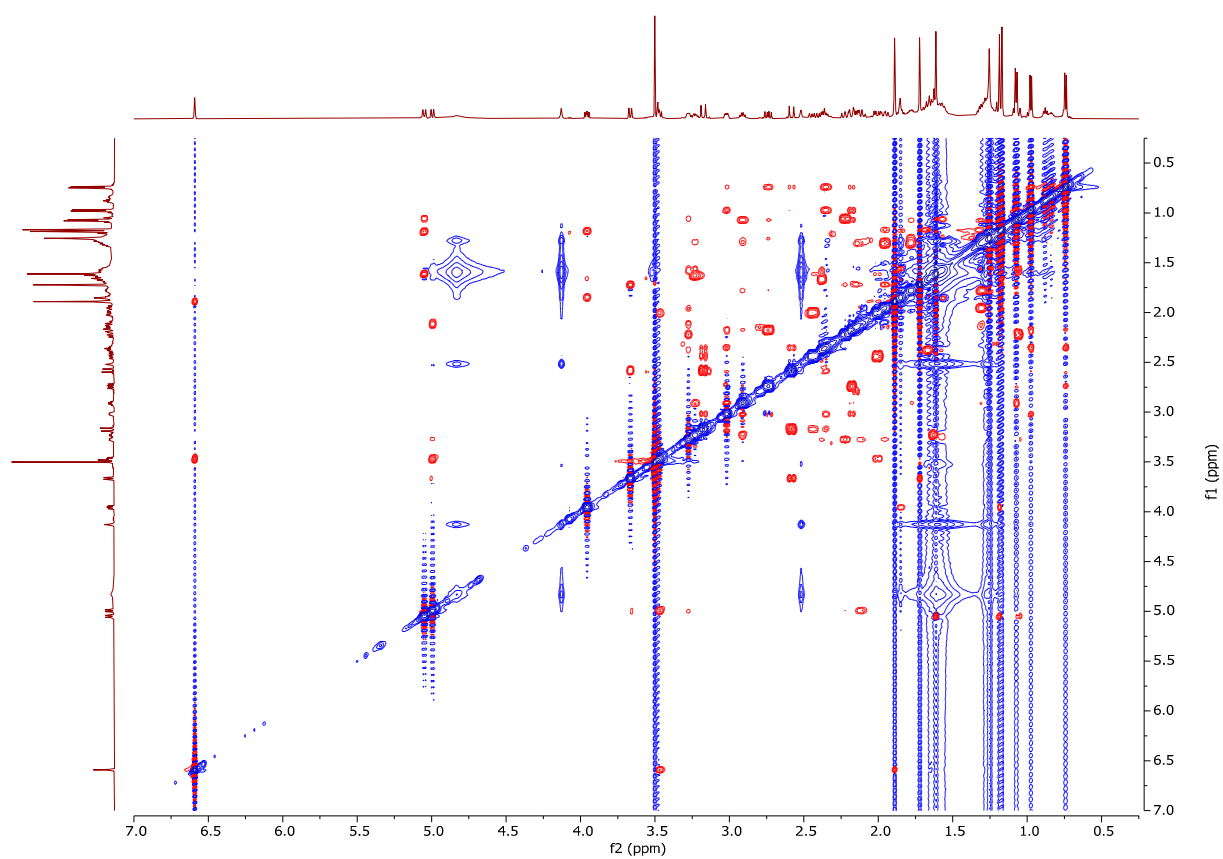


Figure S20. NOESY spectrum of Sarcotrochelide B (**2**) in CDCl_3

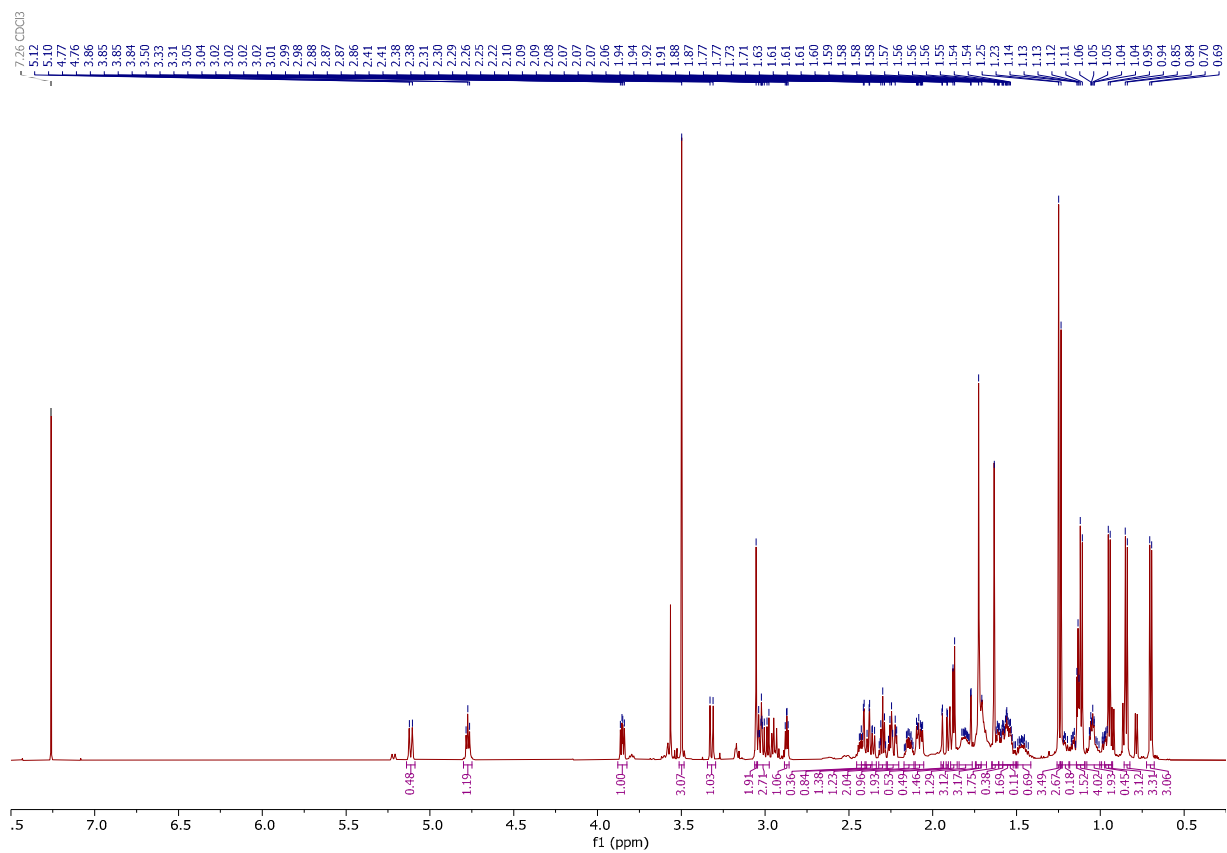


Figure S21. ¹H NMR spectrum of Ximaolide A (3) in CDCl₃ at 600 MHz

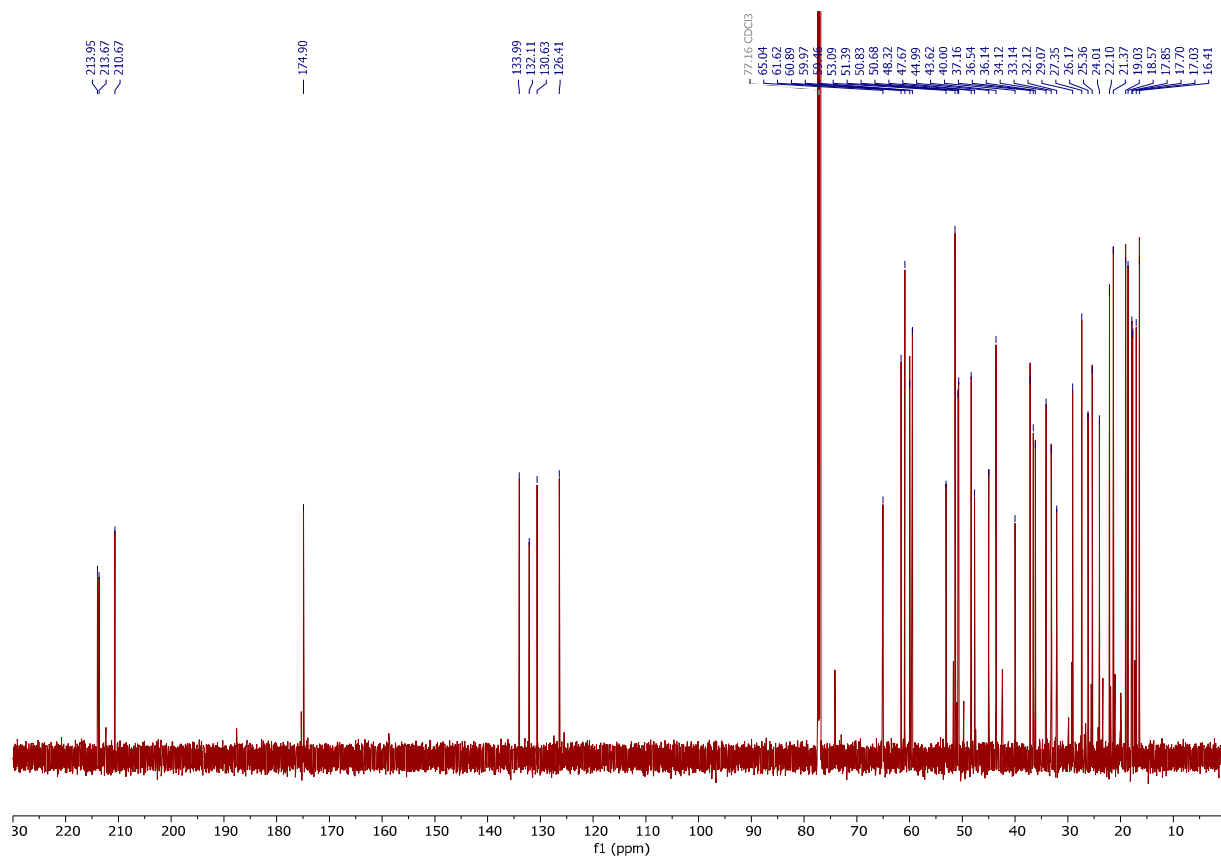


Figure S22. ¹³C NMR spectrum of Ximaolide A (3) in CDCl₃ at 150 MHz

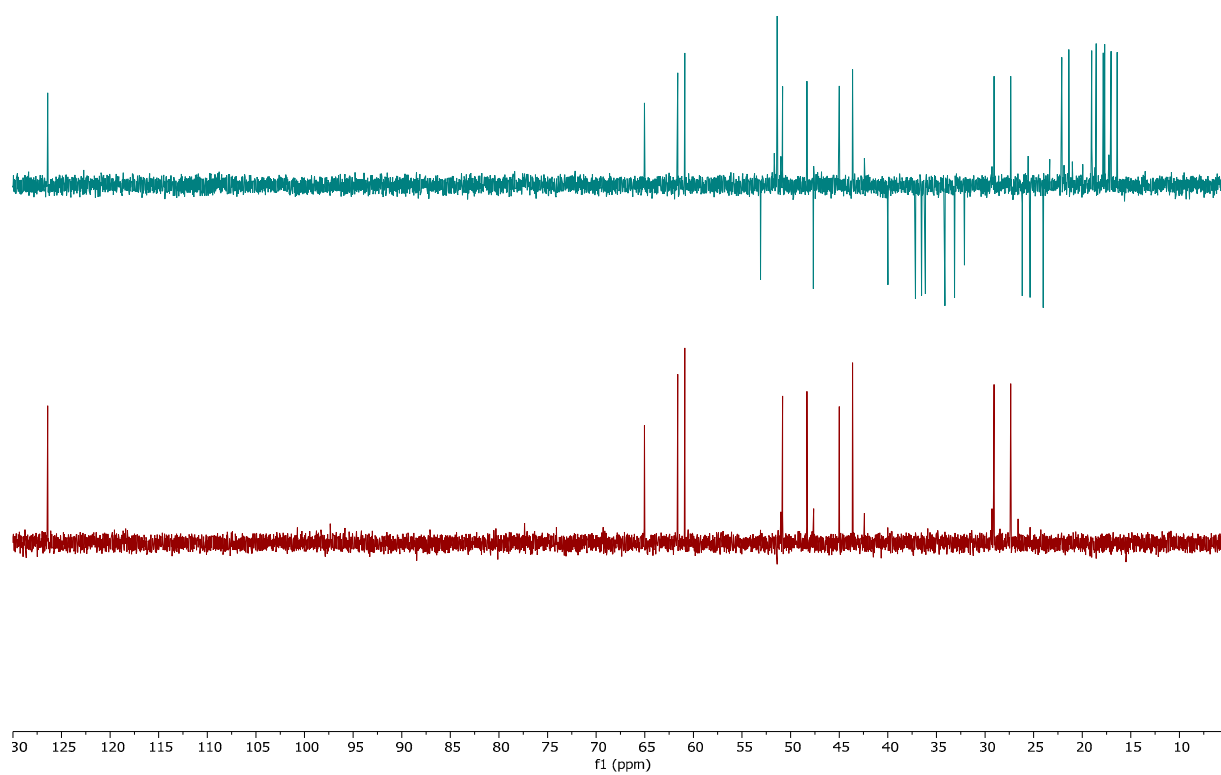


Figure S23. DEPT spectrum of Ximaolide A (**3**) in CDCl_3 at 150 MHz

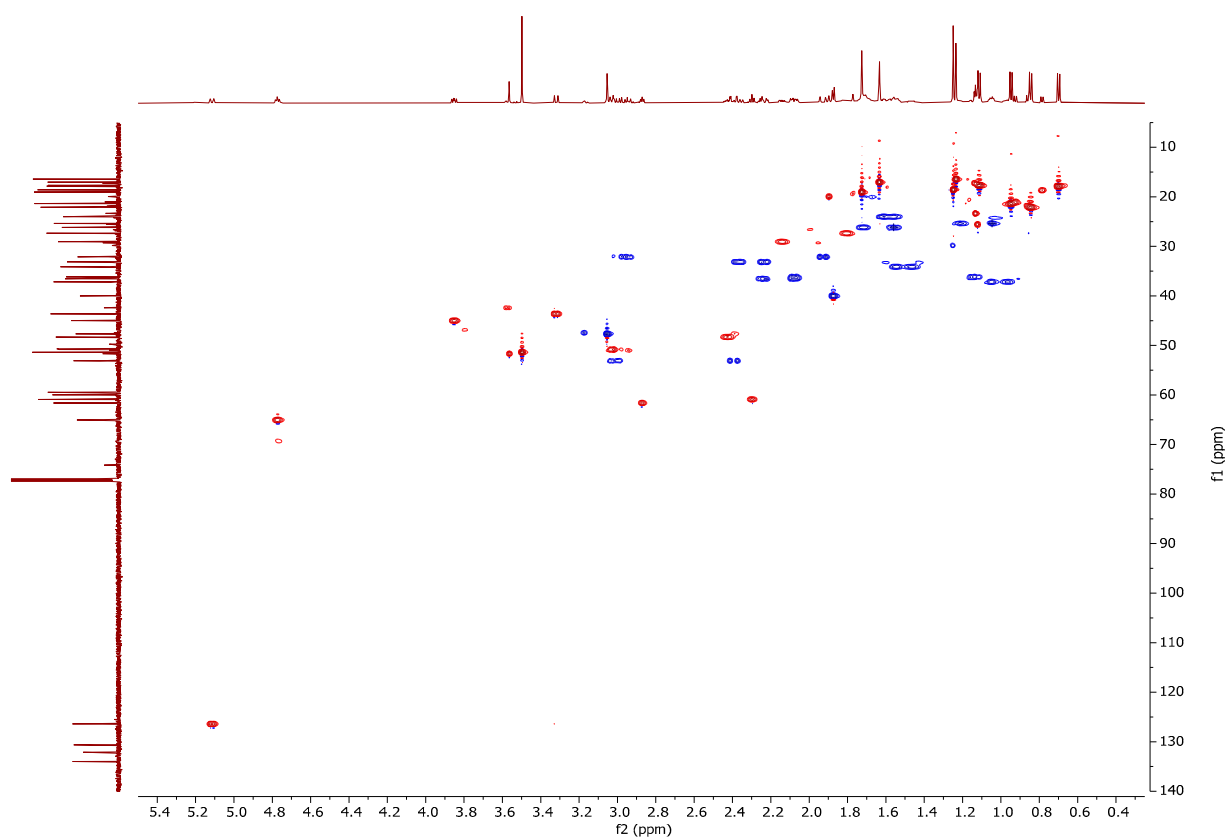


Figure S24. HSQC spectrum of Ximaolide A (3) in CDCl₃

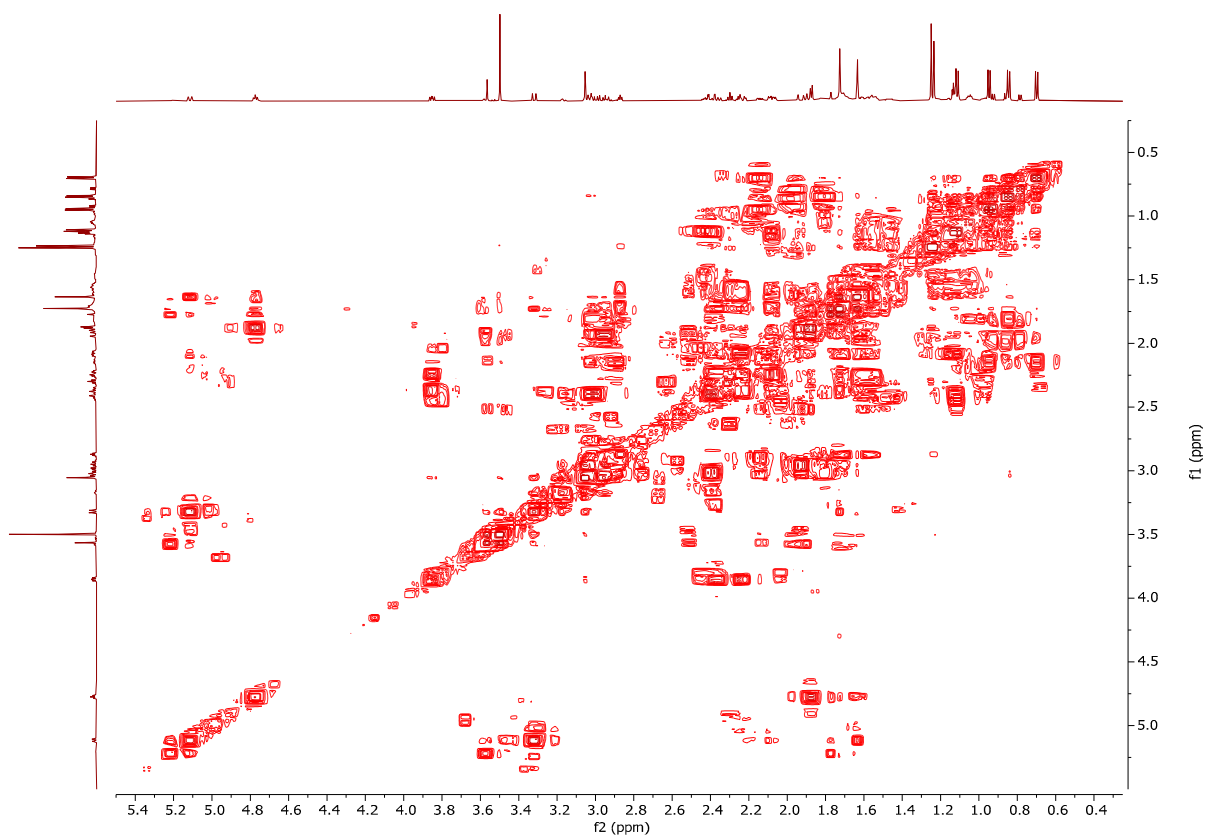


Figure S25. COSY spectrum of Ximaolide A (**3**) in CDCl₃

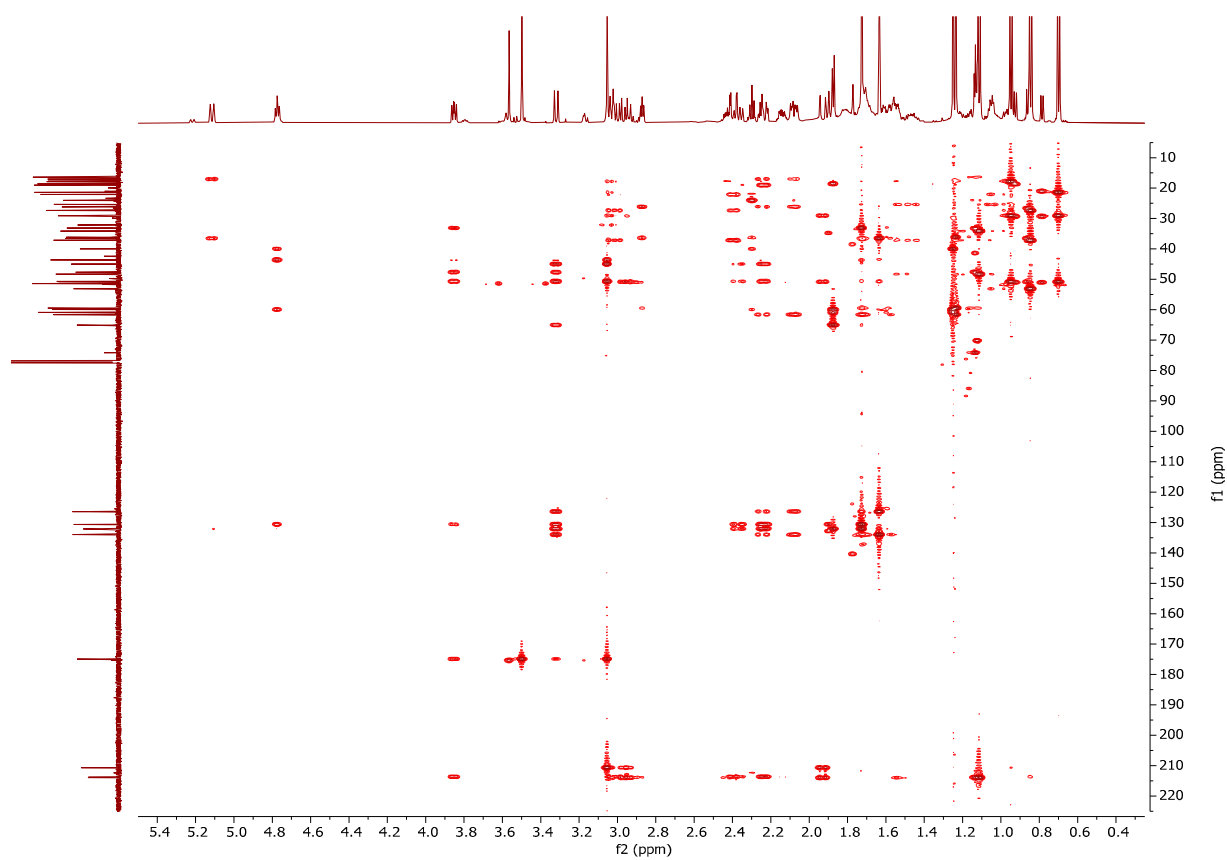


Figure S26. HMBC spectrum of Ximaolide A (**3**) in CDCl₃

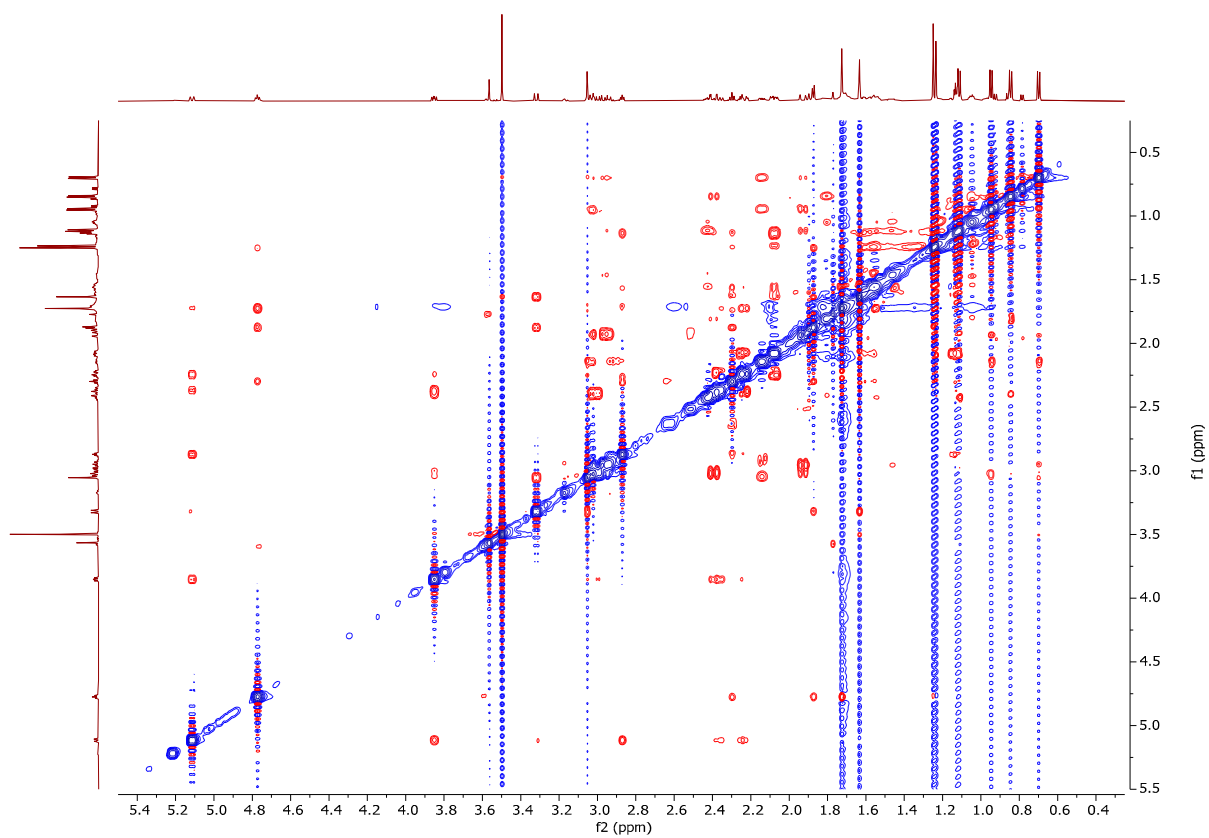


Figure S27. NOESY spectrum of Ximaolide A (**3**) in CDCl₃

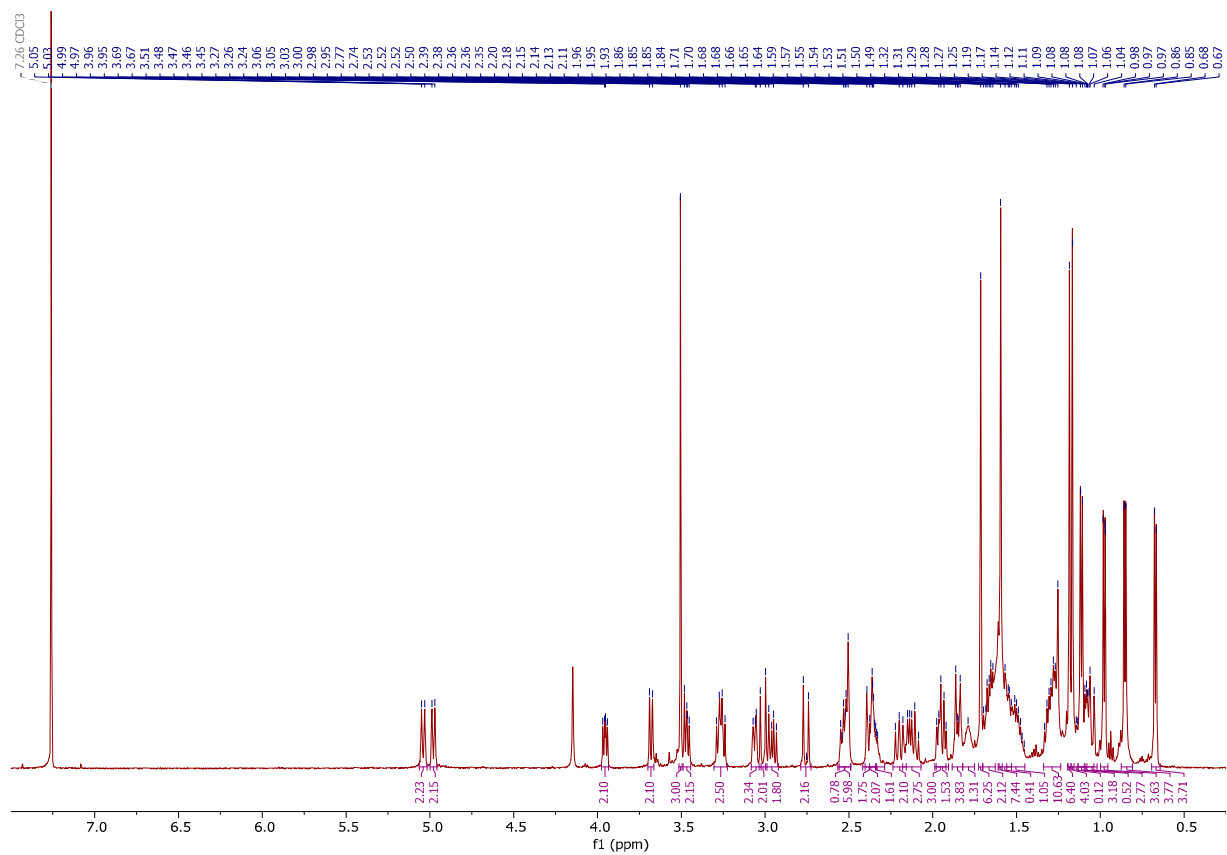


Figure S28. ¹H NMR spectrum of Methyl tortuoate D (4) in CDCl₃ at 600 MHz

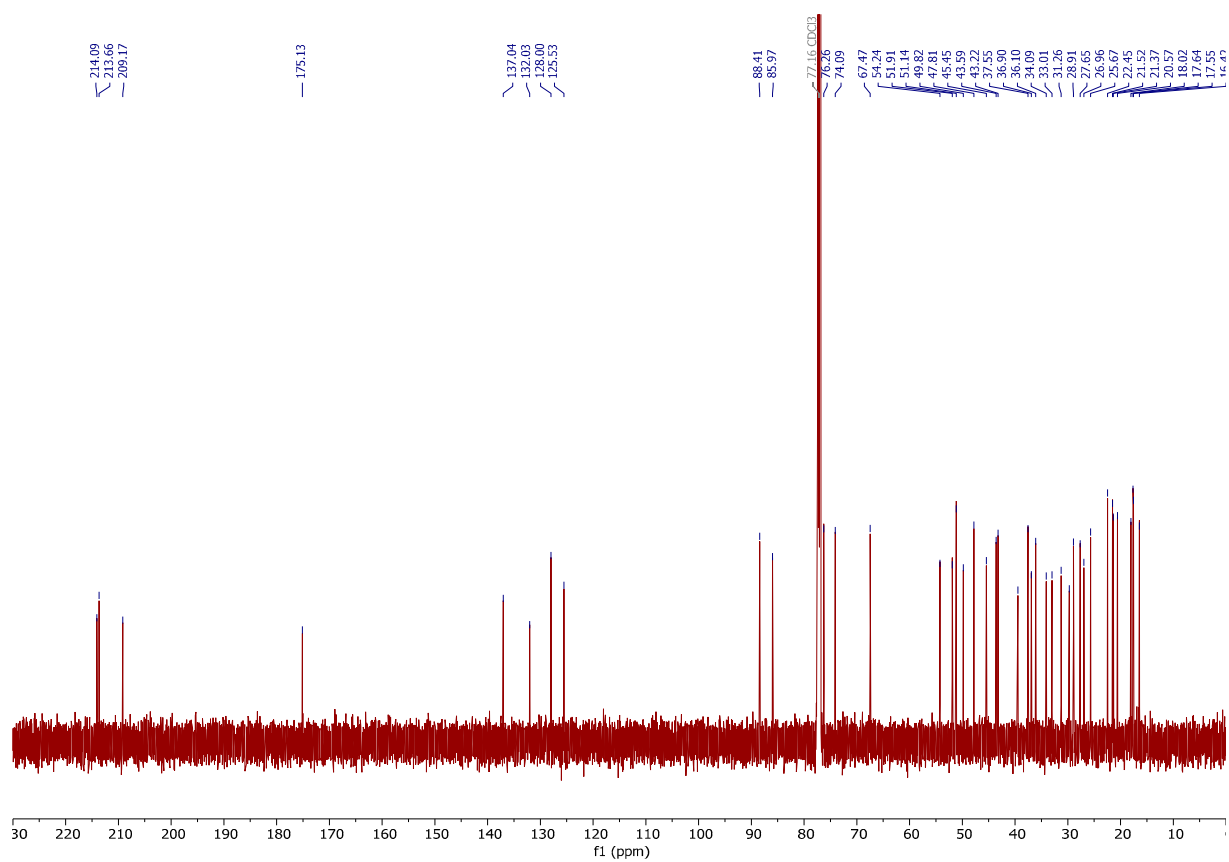


Figure S29. ¹³C NMR spectrum of Methyl tortuoate D (4) in CDCl₃ at 150 MHz

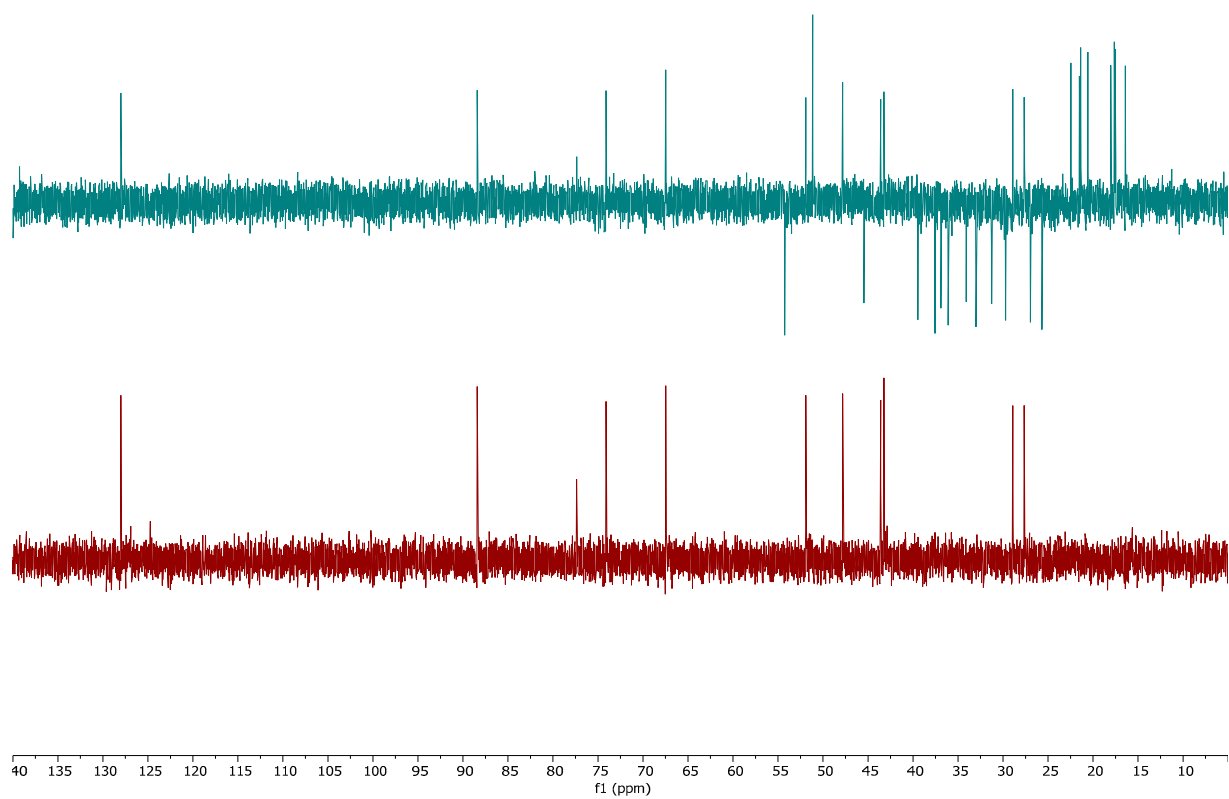


Figure S30. DEPT spectrum of Methyl tortuoate D (**4**) in CDCl₃ at 150 MHz

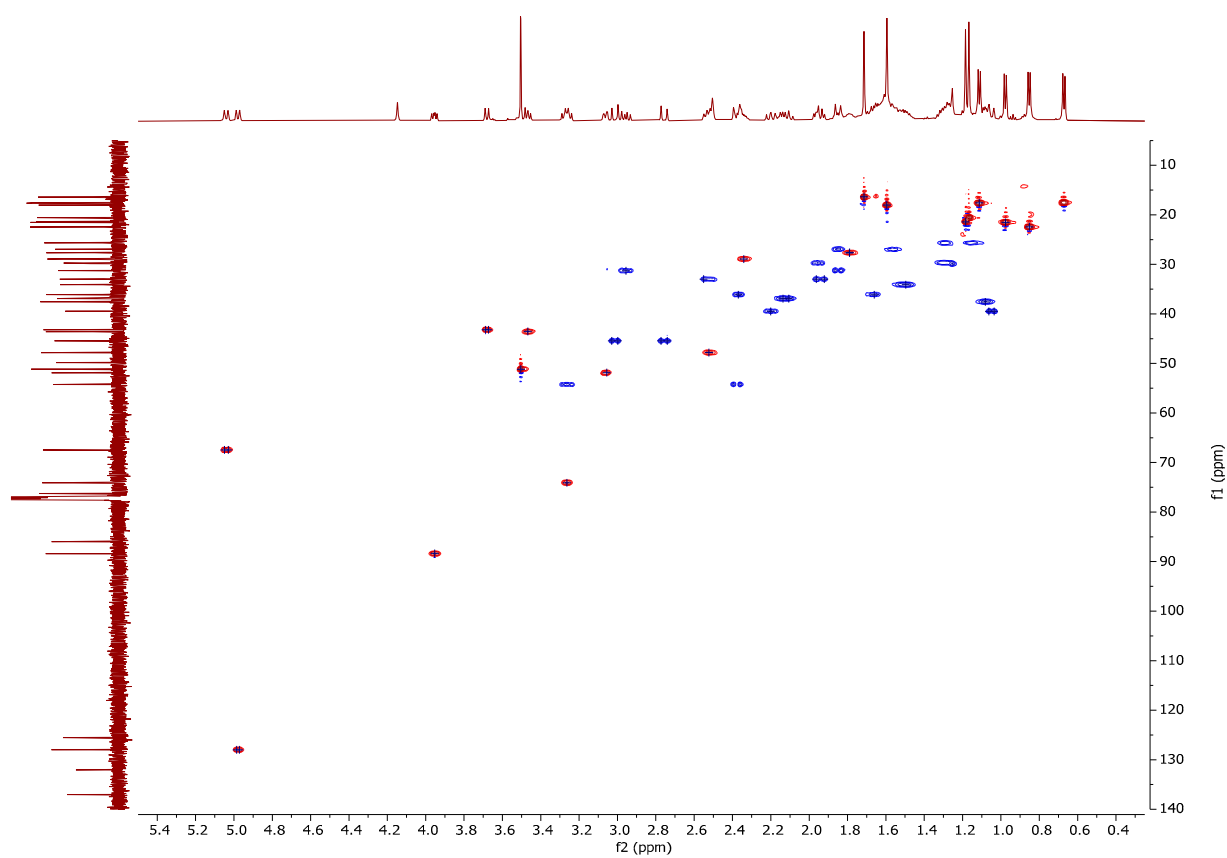


Figure S31. HSQC spectrum of Methyl tortuoate D (**4**) in CDCl_3

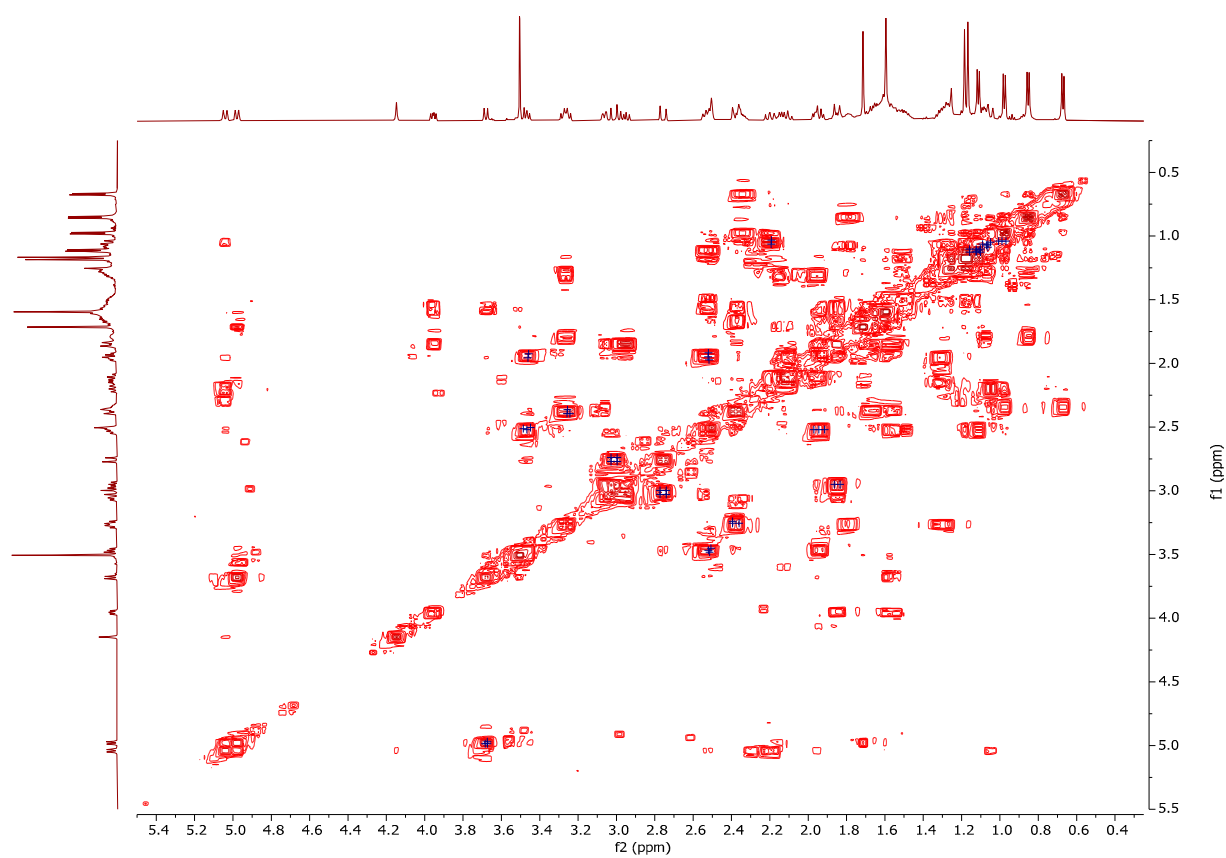


Figure S32. COSY spectrum of Methyl tortuoate D (**4**) in CDCl_3

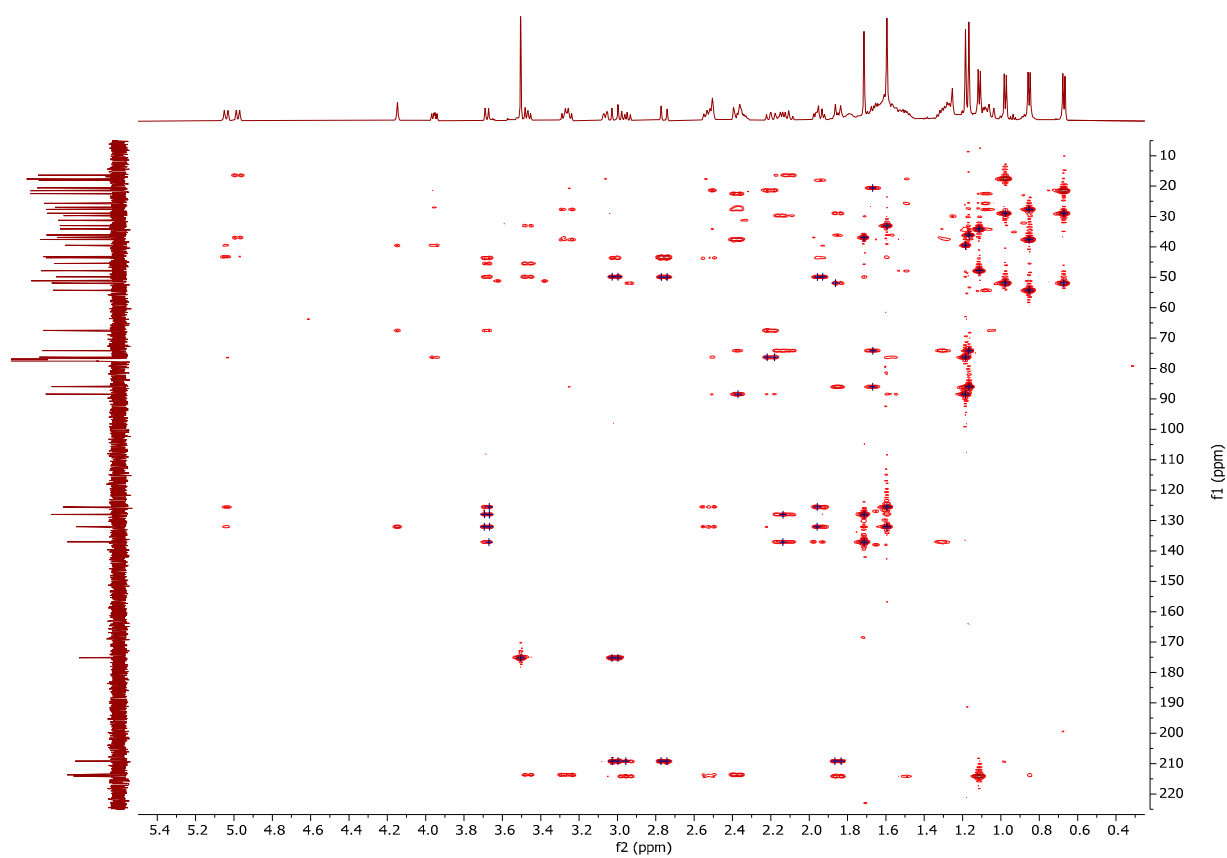


Figure S33. HMBC spectrum of Methyl tortuoate D (**4**) in CDCl_3

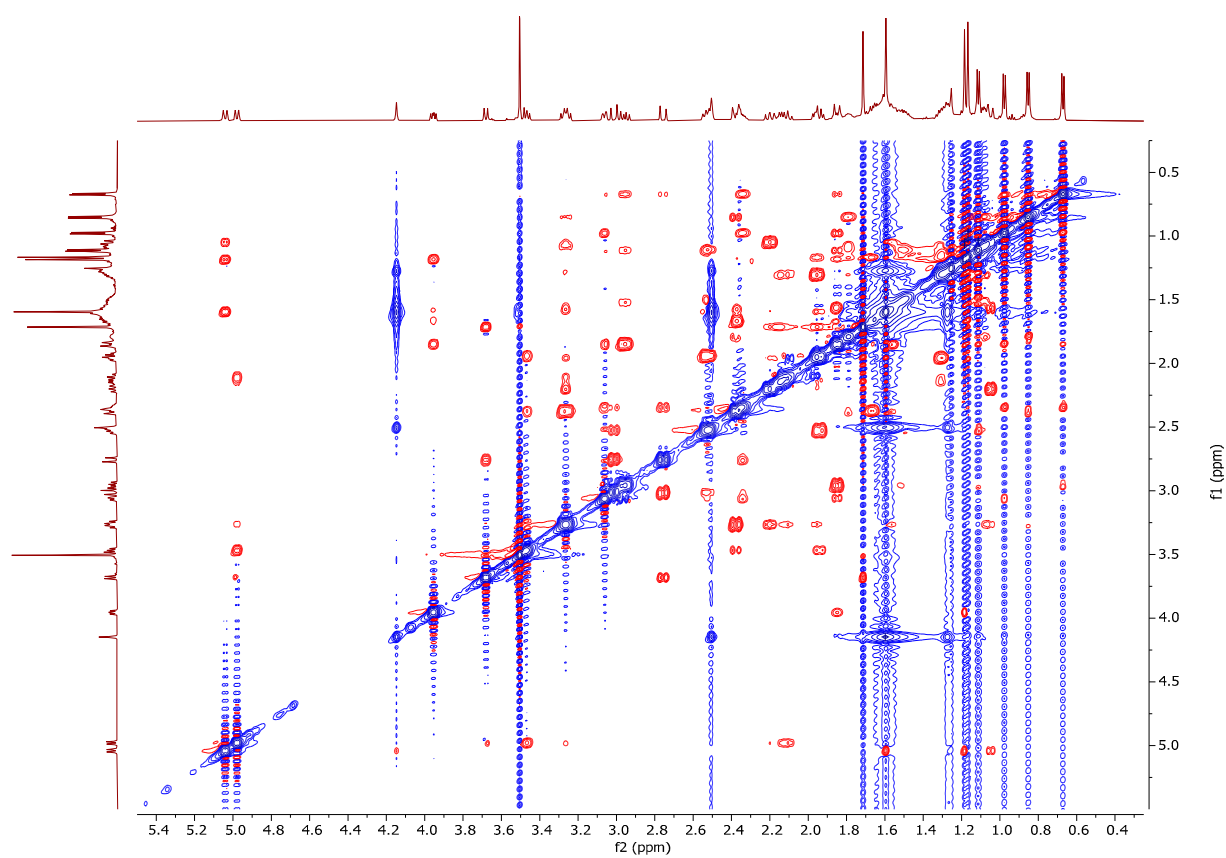


Figure S34. NOESY spectrum of Methyl tortuoate D (**4**) in CDCl₃

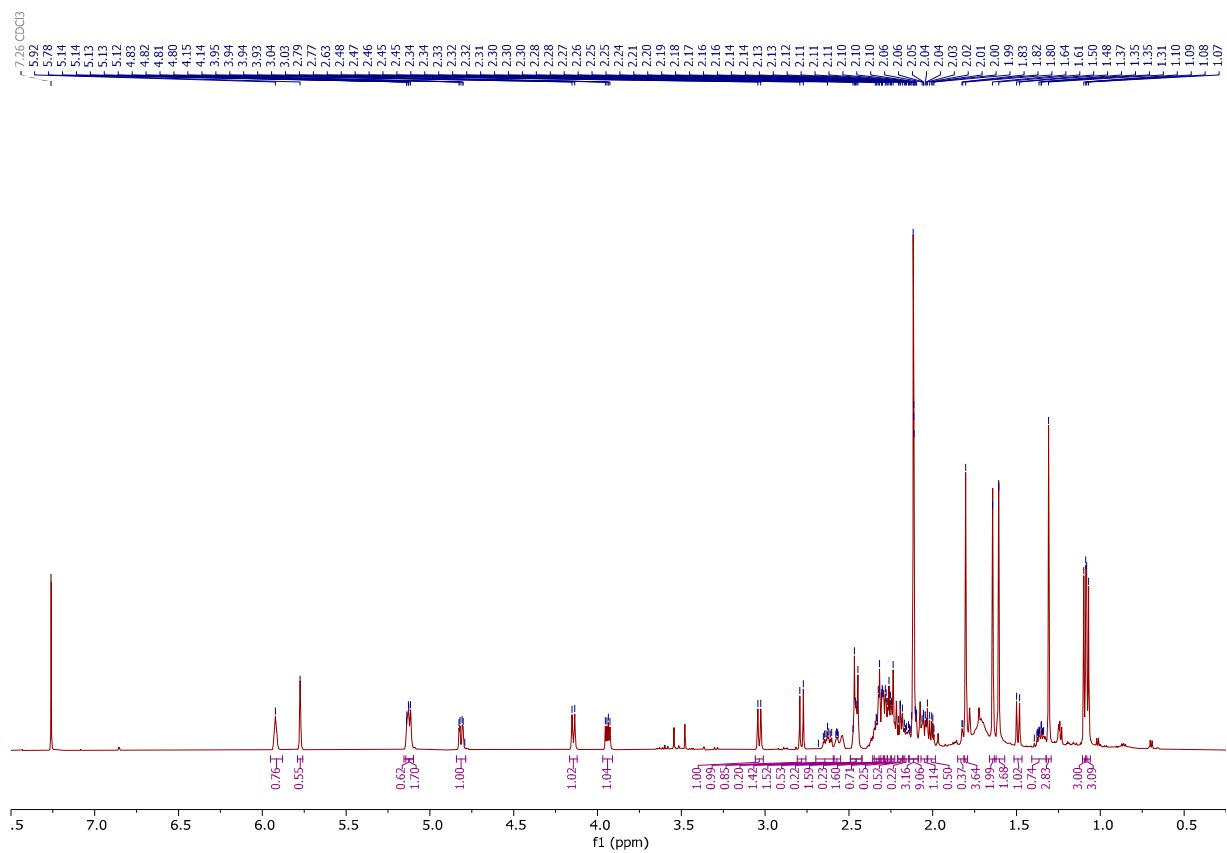


Figure S35. ¹H NMR spectrum of Glaucumolide A (5) in CDCl₃ at 600 MHz

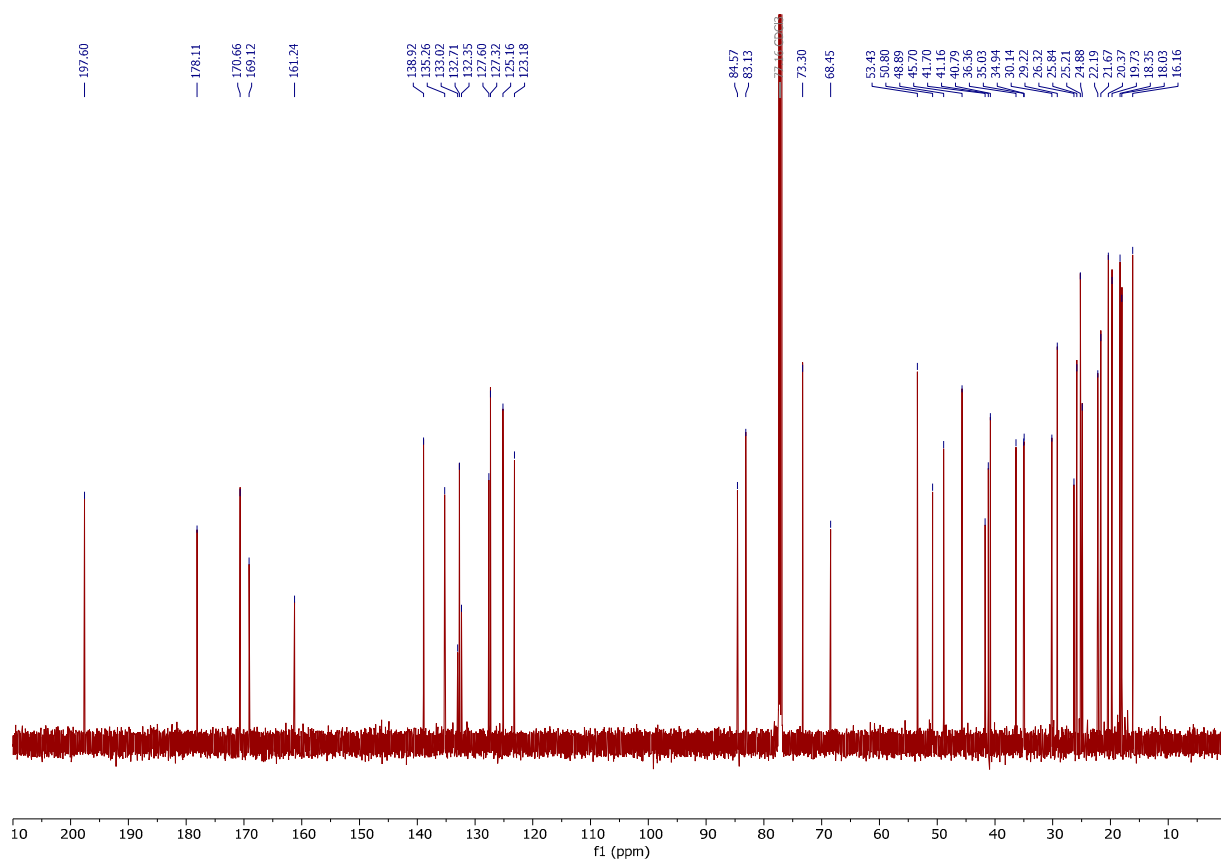


Figure S36. ¹³C NMR spectrum of Glaucumolide A (5) in CDCl₃ at 150 MHz

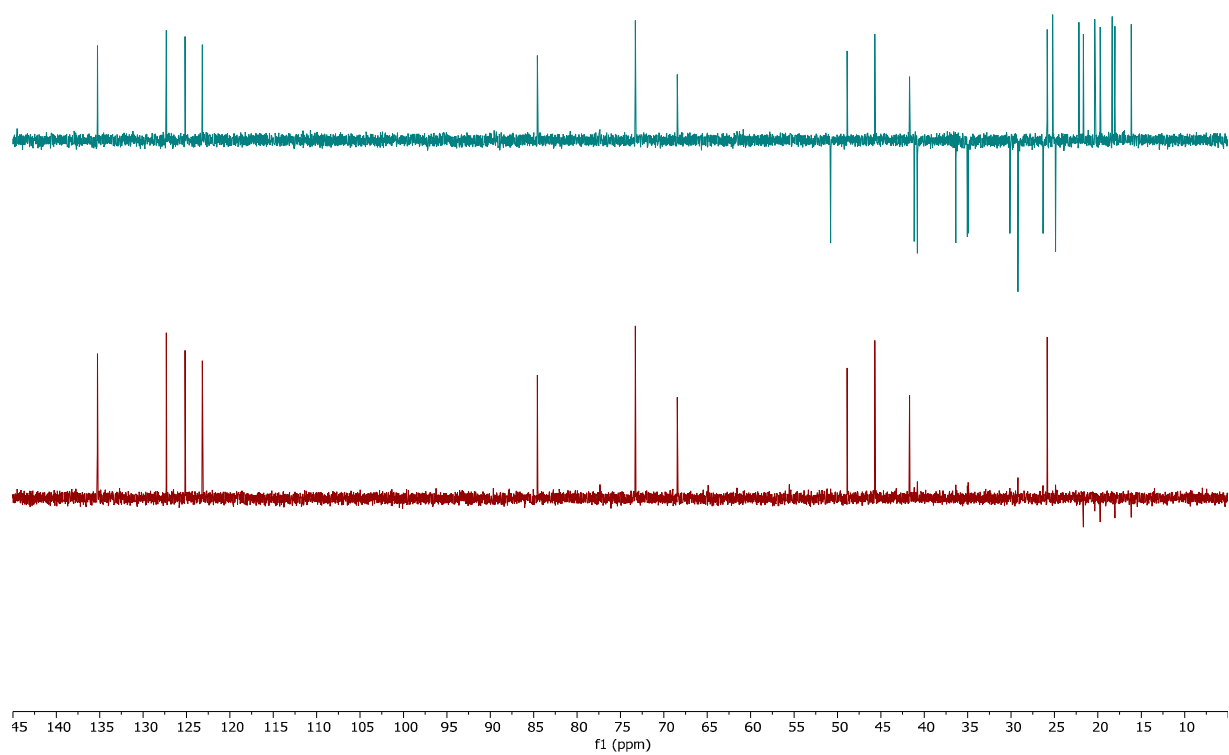


Figure S37. DEPT spectrum of Glaucumolide A (**5**) in CDCl_3 at 150 MHz



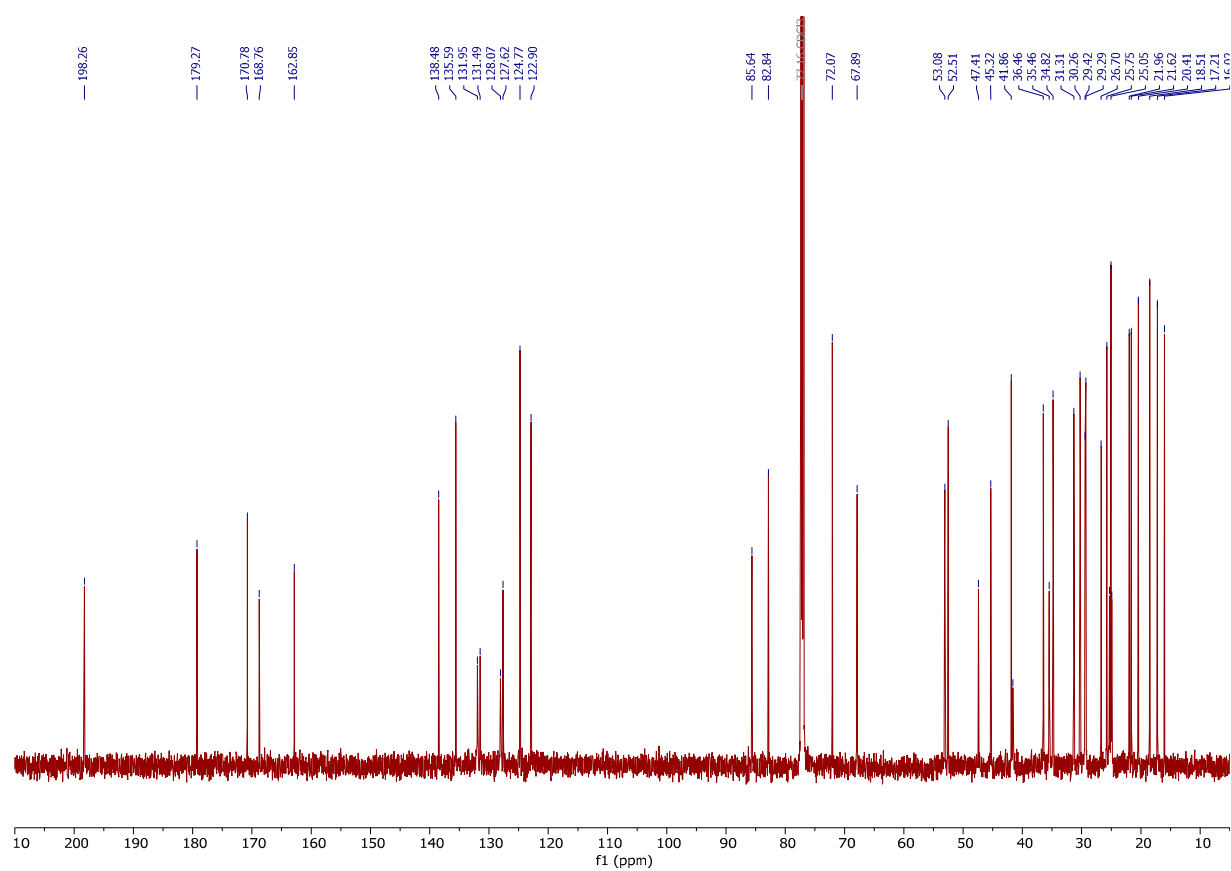


Figure S39. ¹³C NMR spectrum of Glaucumolide B (6) in CDCl₃ at 150 MHz

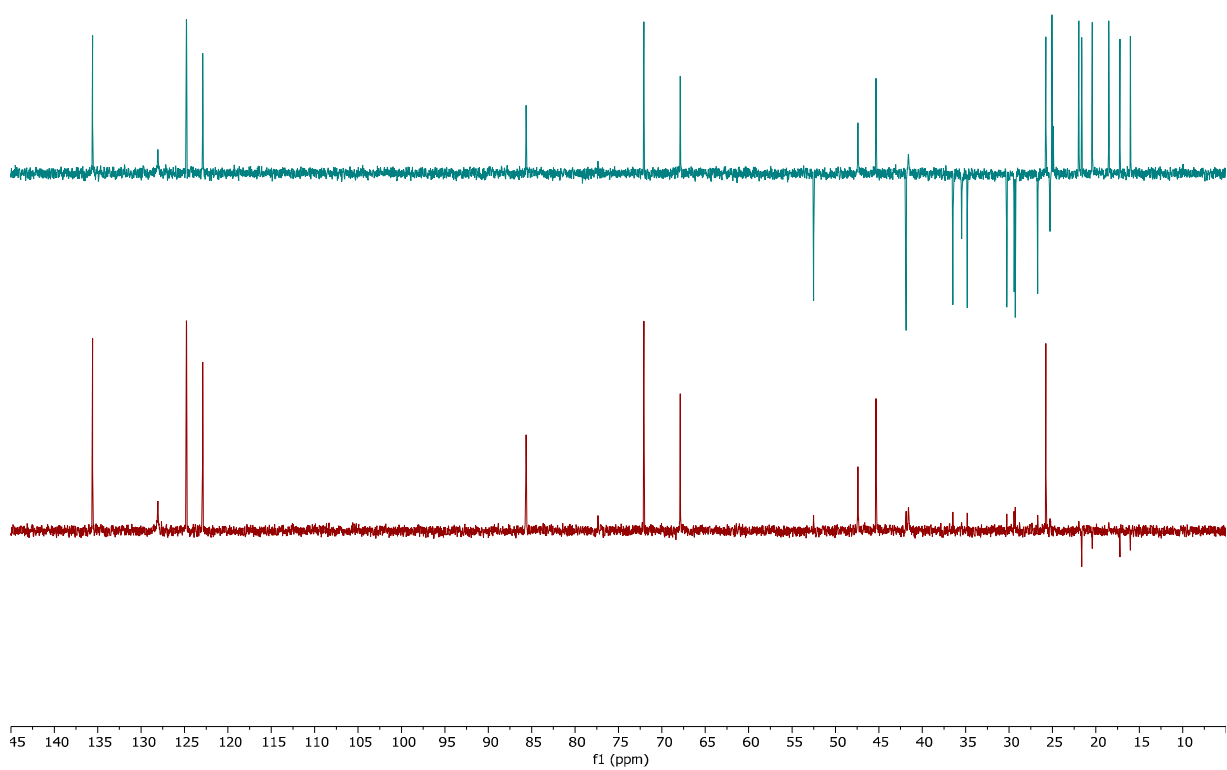


Figure S40. DEPT spectrum of Glaucumolide B (6) in CDCl₃ at 150 MHz

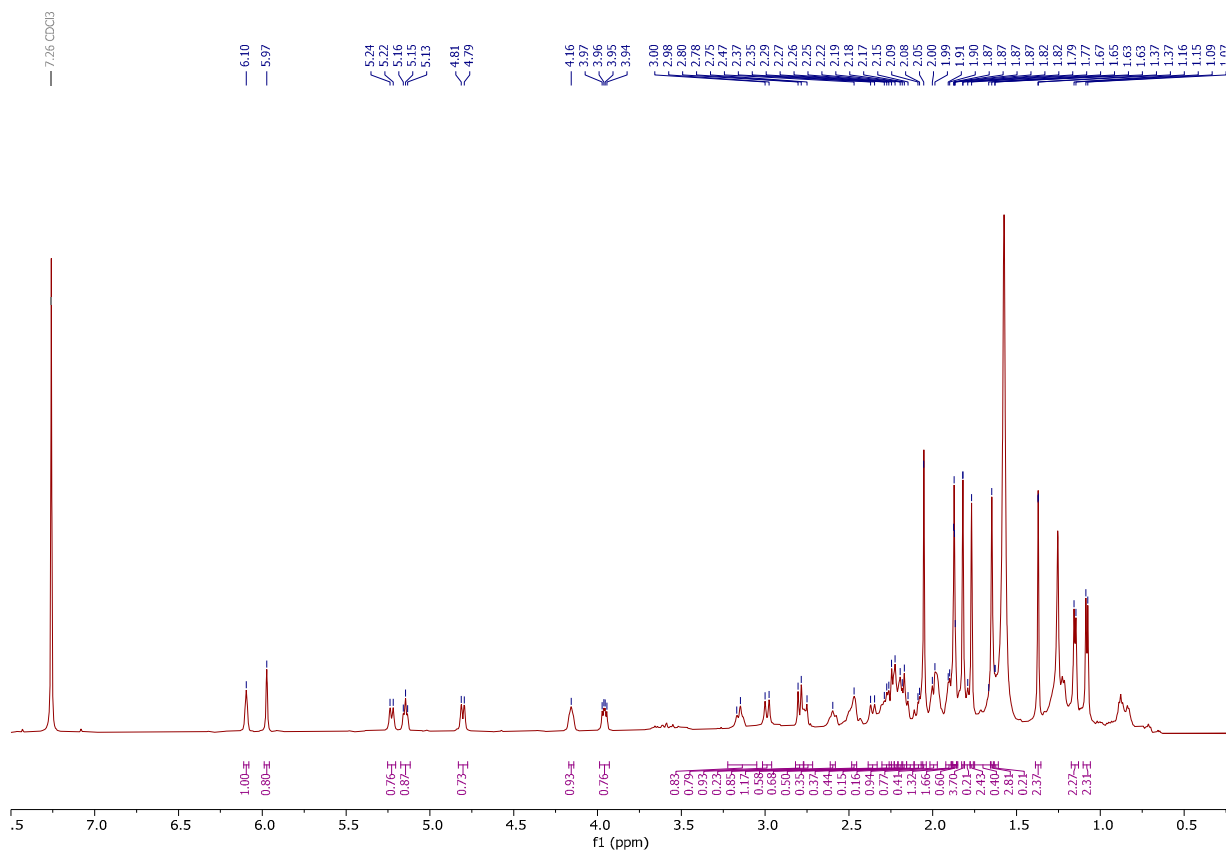


Figure S41. ¹H NMR spectrum of Bistochelide A (**7**) in CDCl₃ at 600 MHz

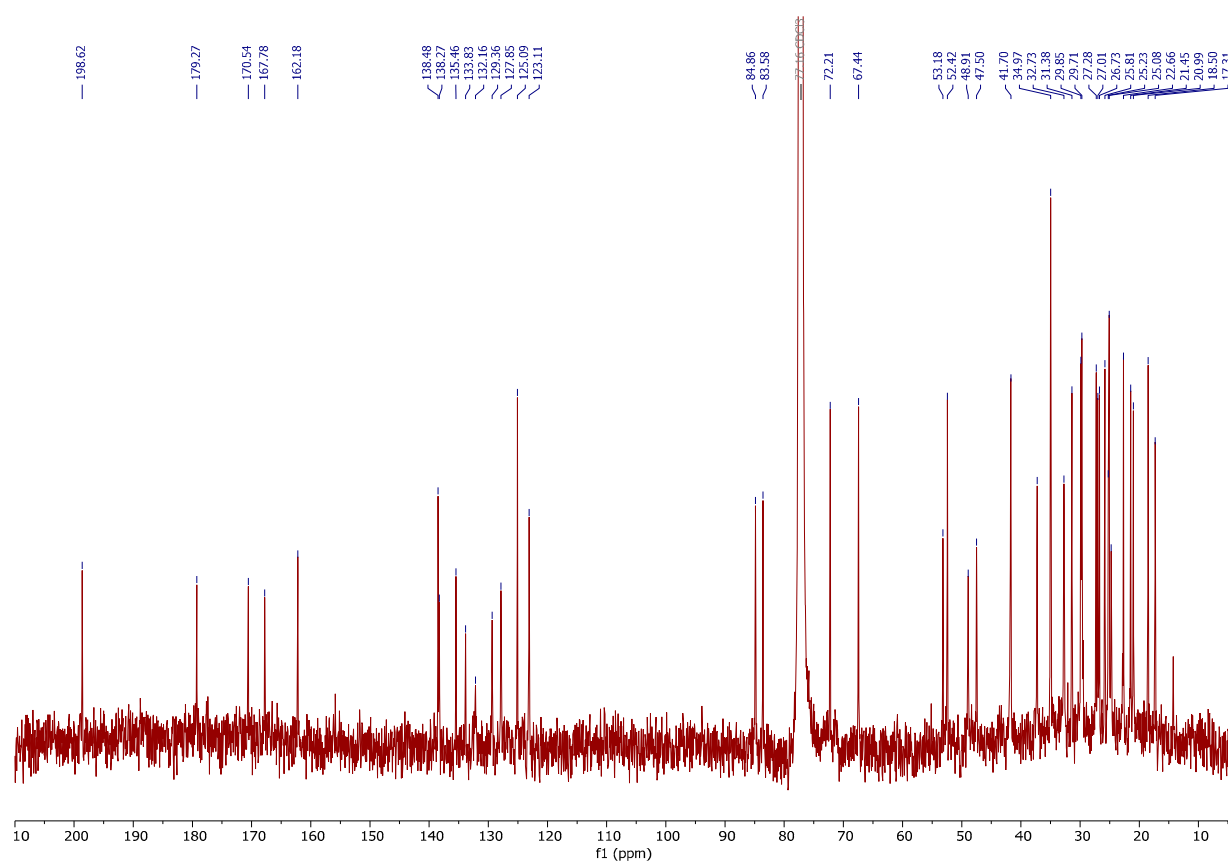


Figure S42. ¹³C NMR spectrum of Bistochelide A (7) in CDCl₃ at 150 MHz

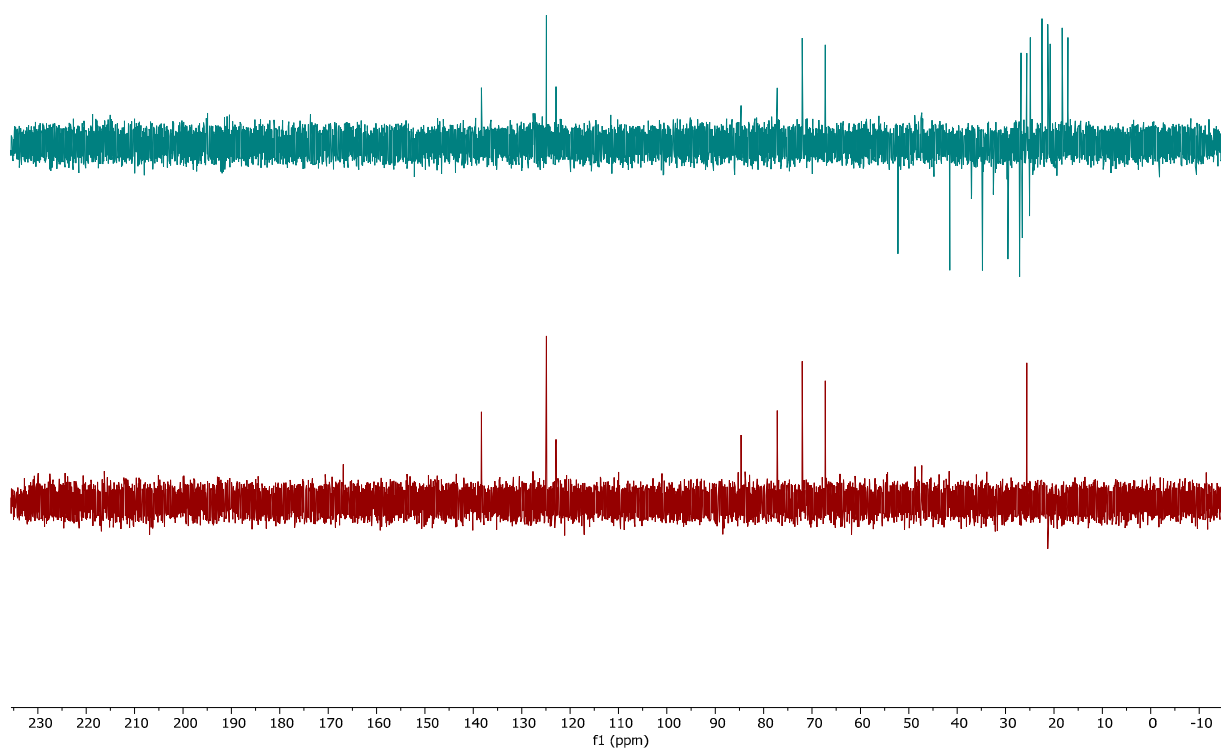


Figure S43. DEPT spectrum of Bistochelide A (7) in CDCl_3 at 150 MHz

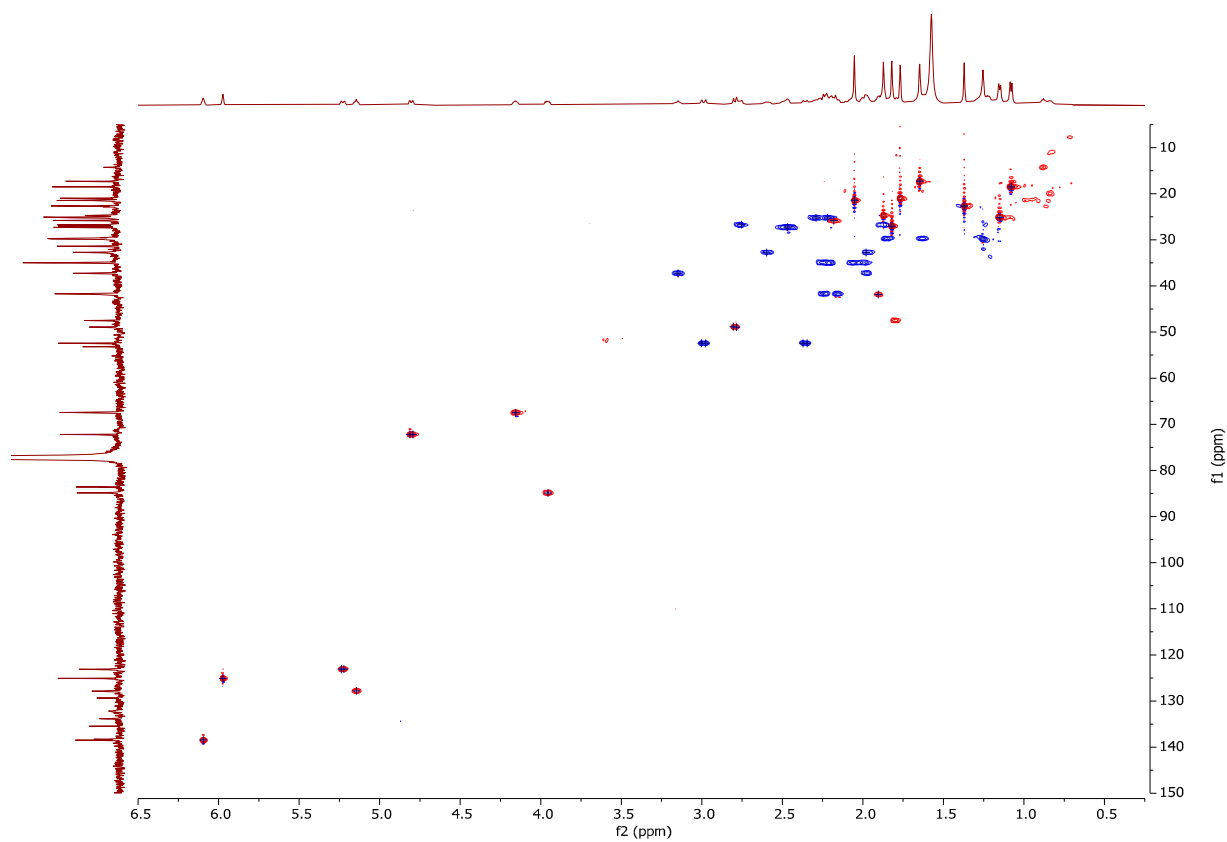


Figure S44. HSQC spectrum of Bistochelide A (**7**) in CDCl₃

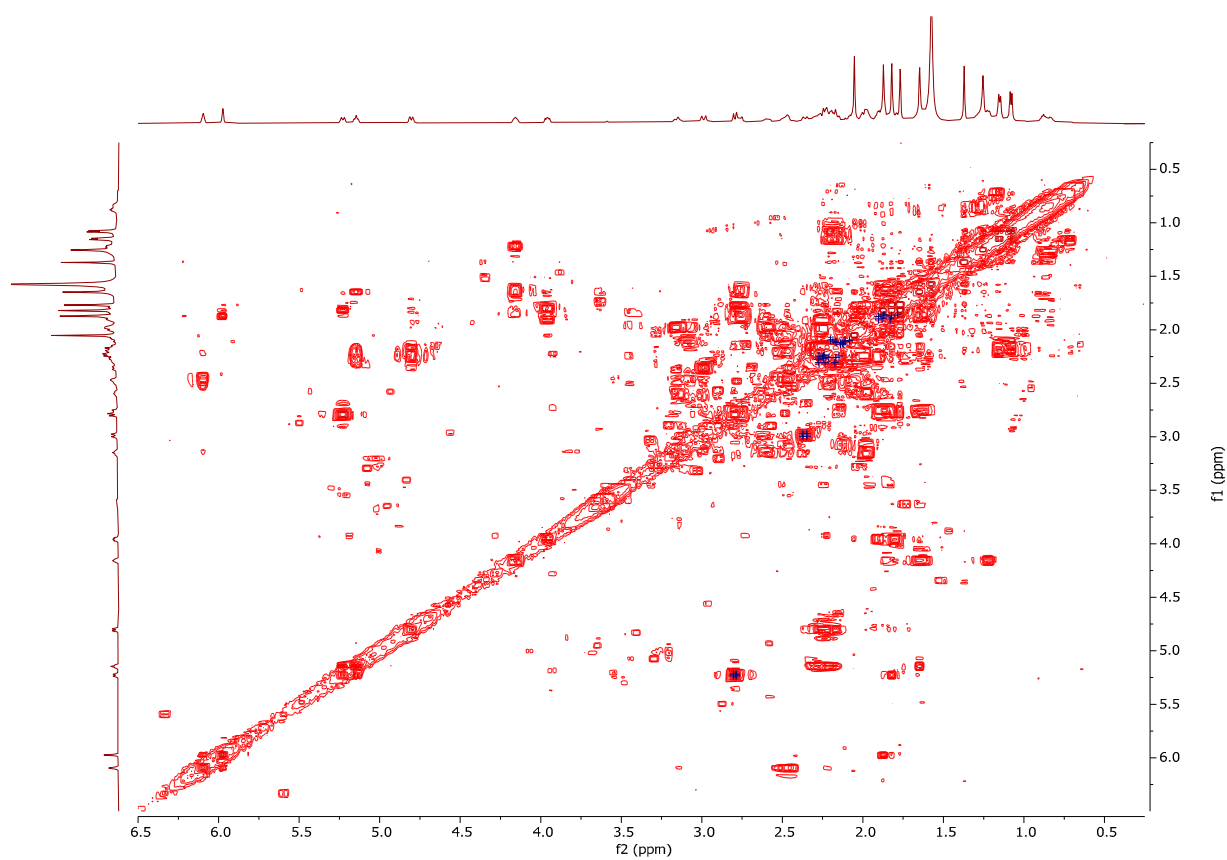


Figure S45. COSY spectrum of Bistochelide A (**7**) in CDCl₃

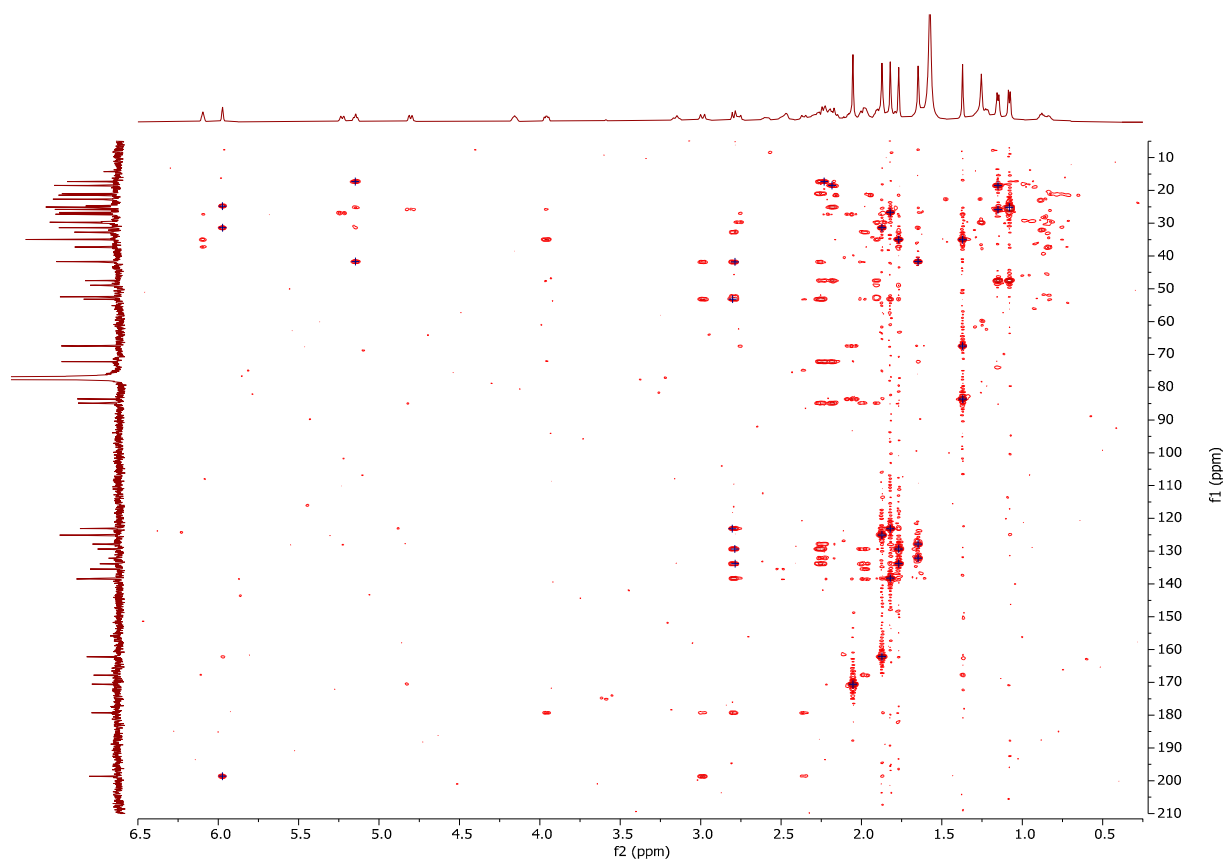


Figure S46. HMBC spectrum of Bistochelide A (**7**) in CDCl₃

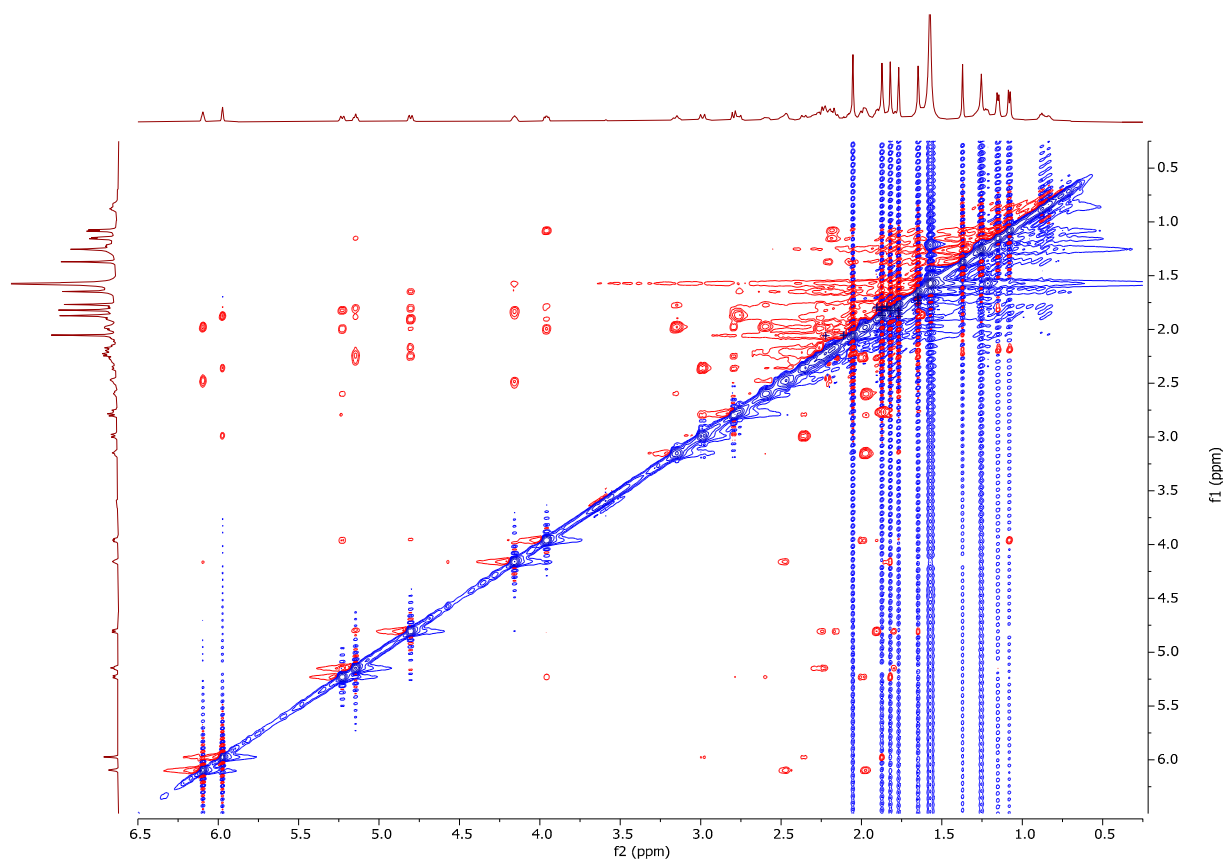


Figure S47. NOESY spectrum of Bistochelide A (**7**) in CDCl₃

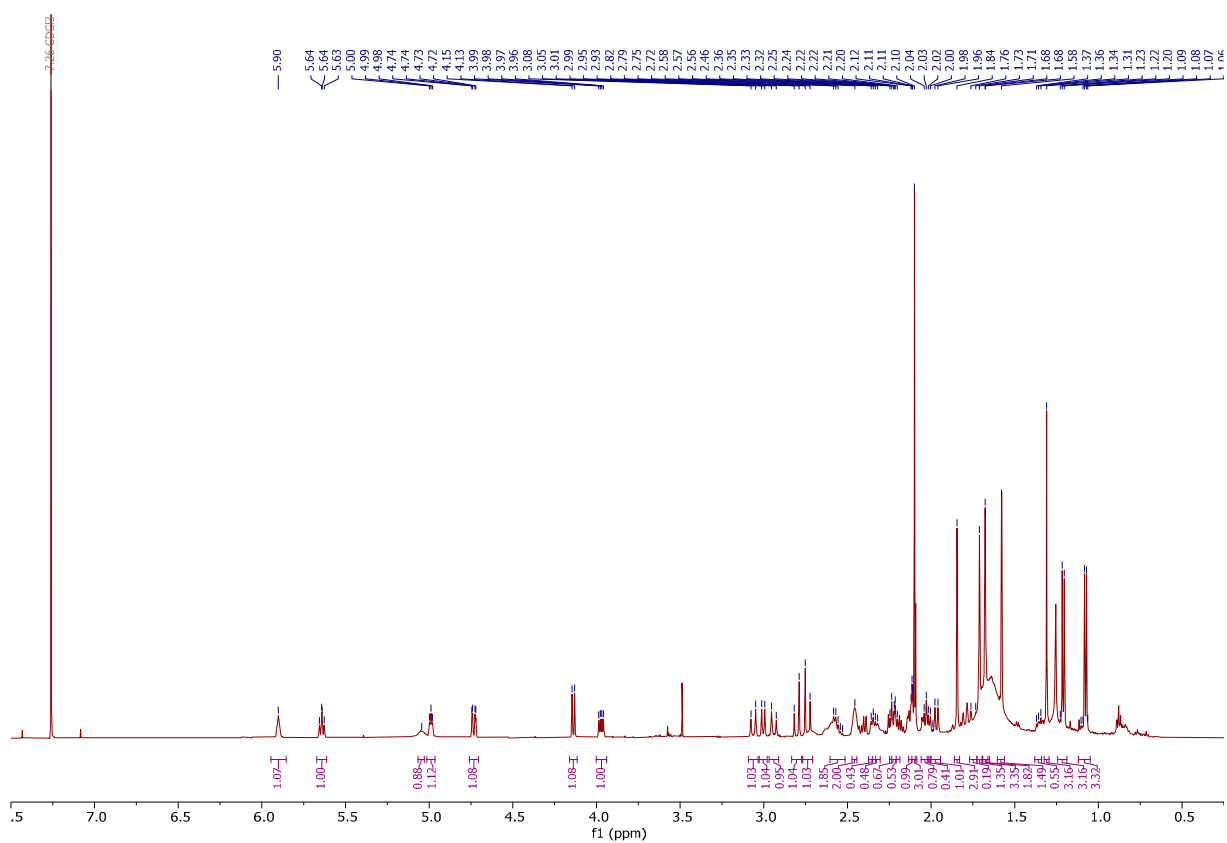


Figure S48. ^1H NMR spectrum of Bistochelide B (**8**) in CDCl_3 at 600 MHz

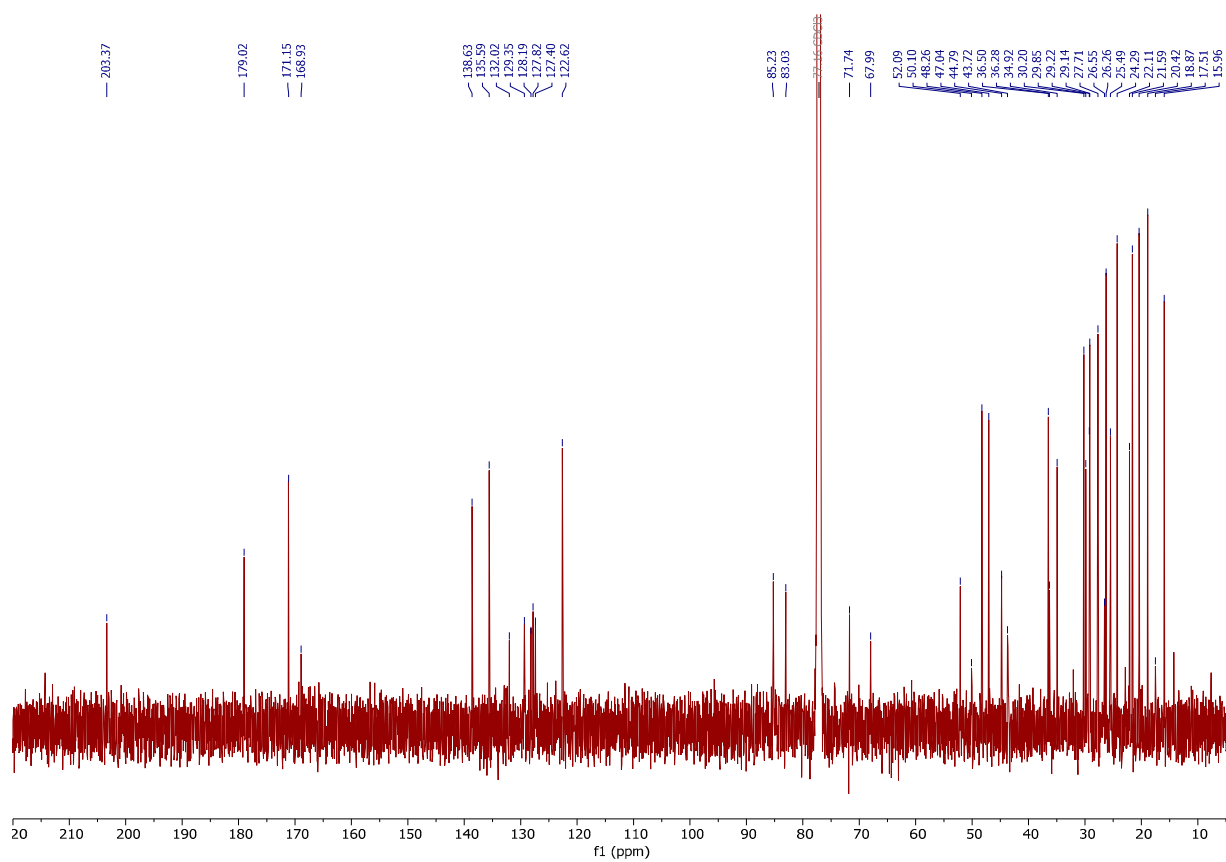


Figure S49. ¹³C NMR spectrum of Bistochelide B (8) in CDCl₃ at 150 MHz

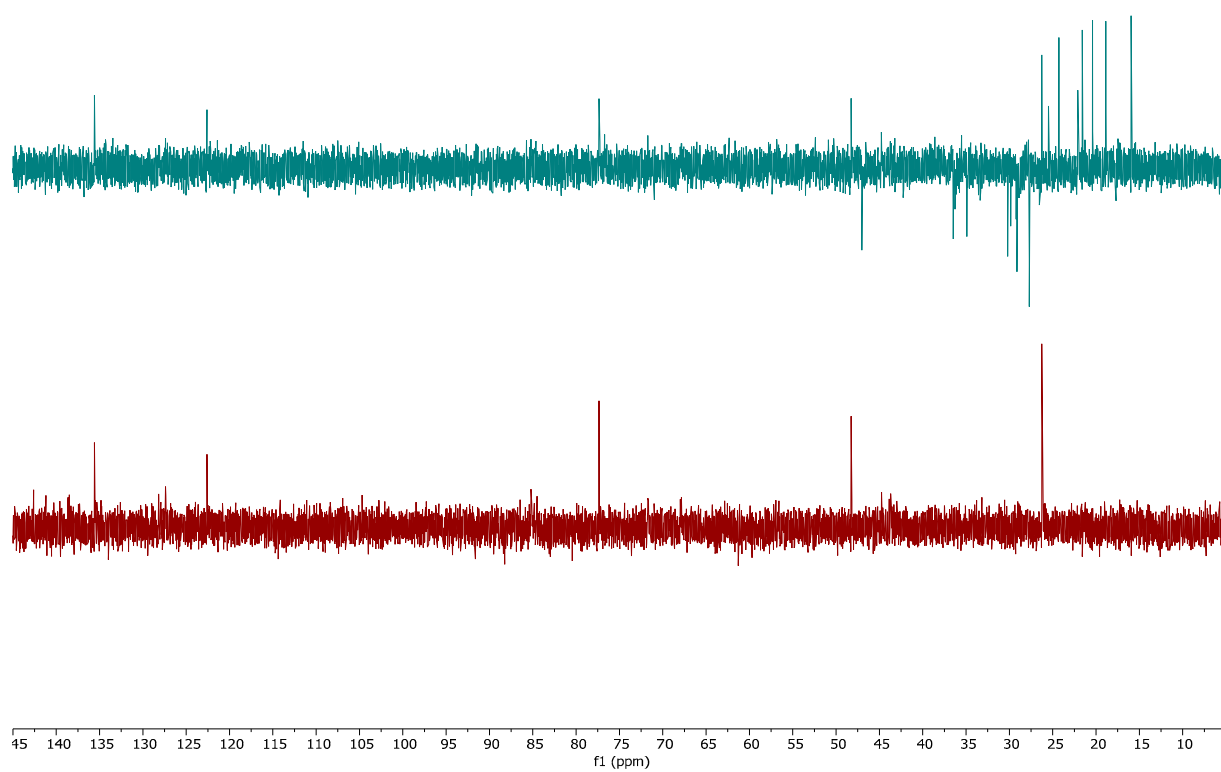


Figure S50. DEPT spectrum of Bistochelide B (**8**) in CDCl_3 at 150 MHz

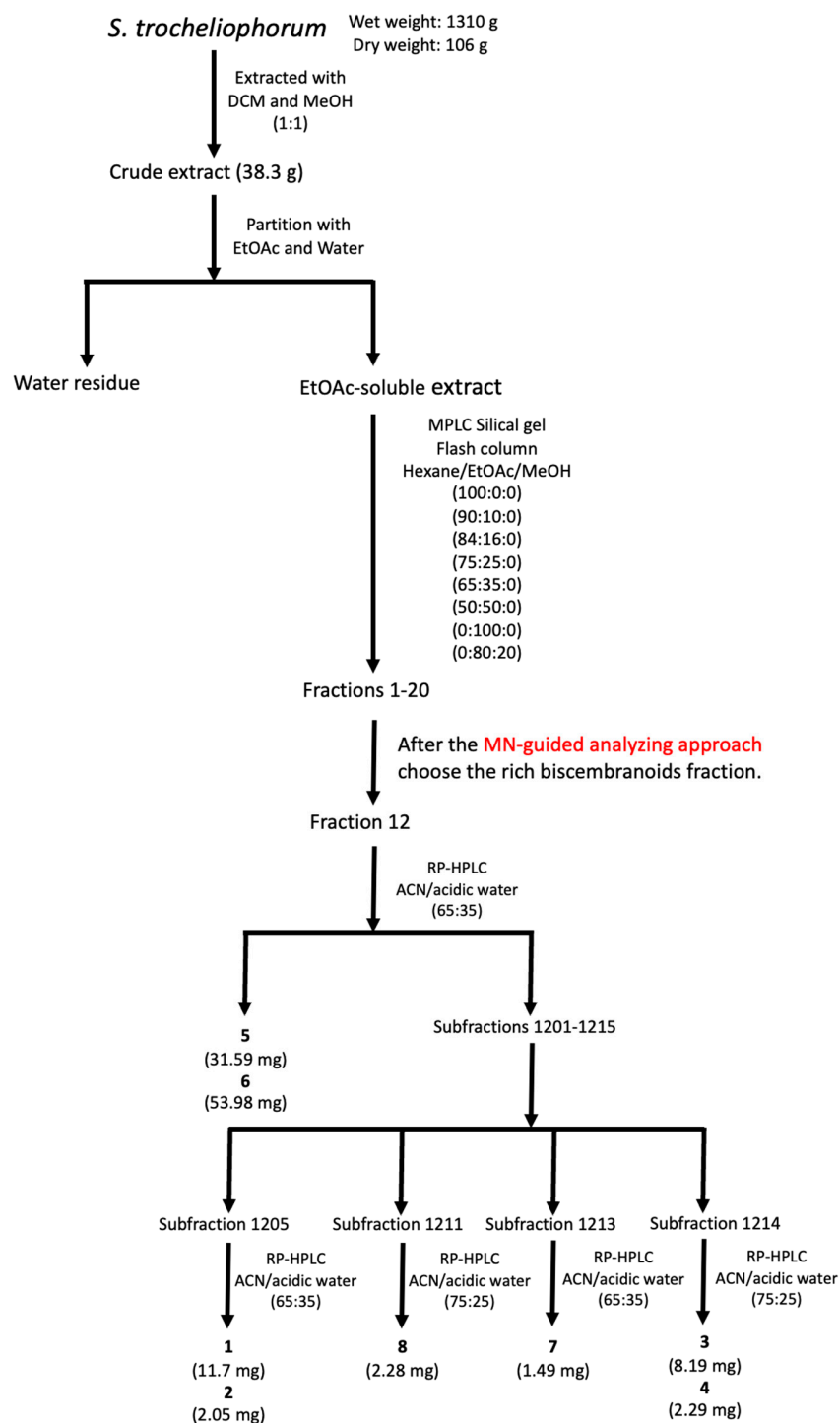


Figure S51. The process of isolation from soft coral *Sarcophyton trocheliophorum*

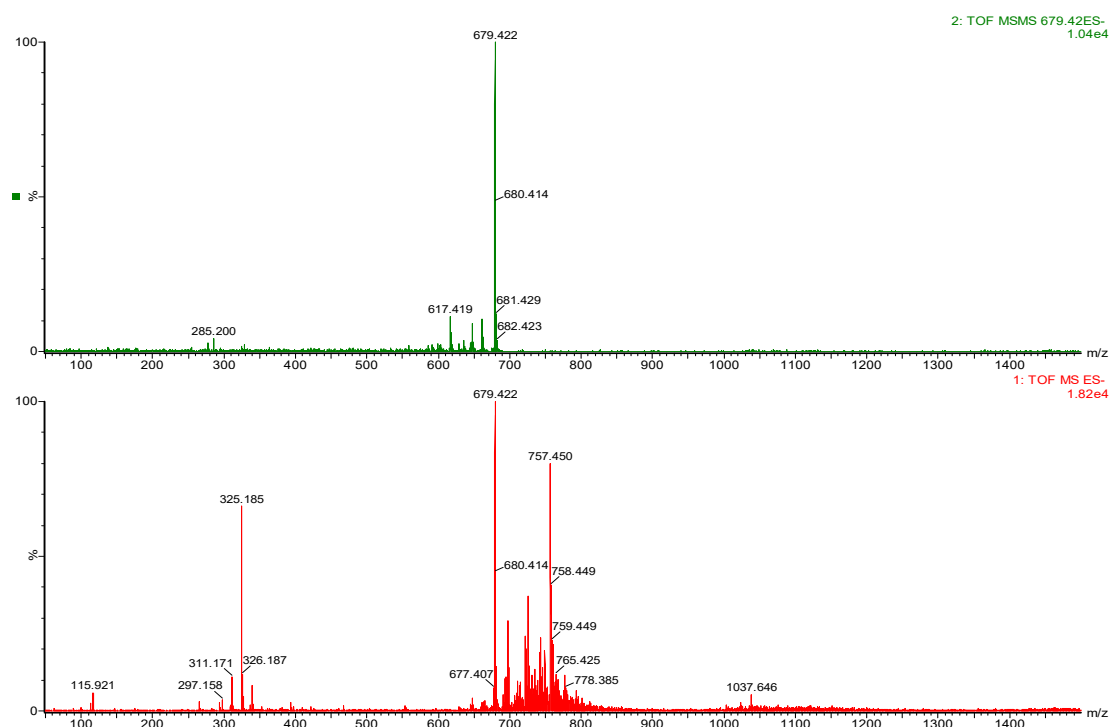


Figure S52. The LC-MS/MS fragment in negative mode of (1)

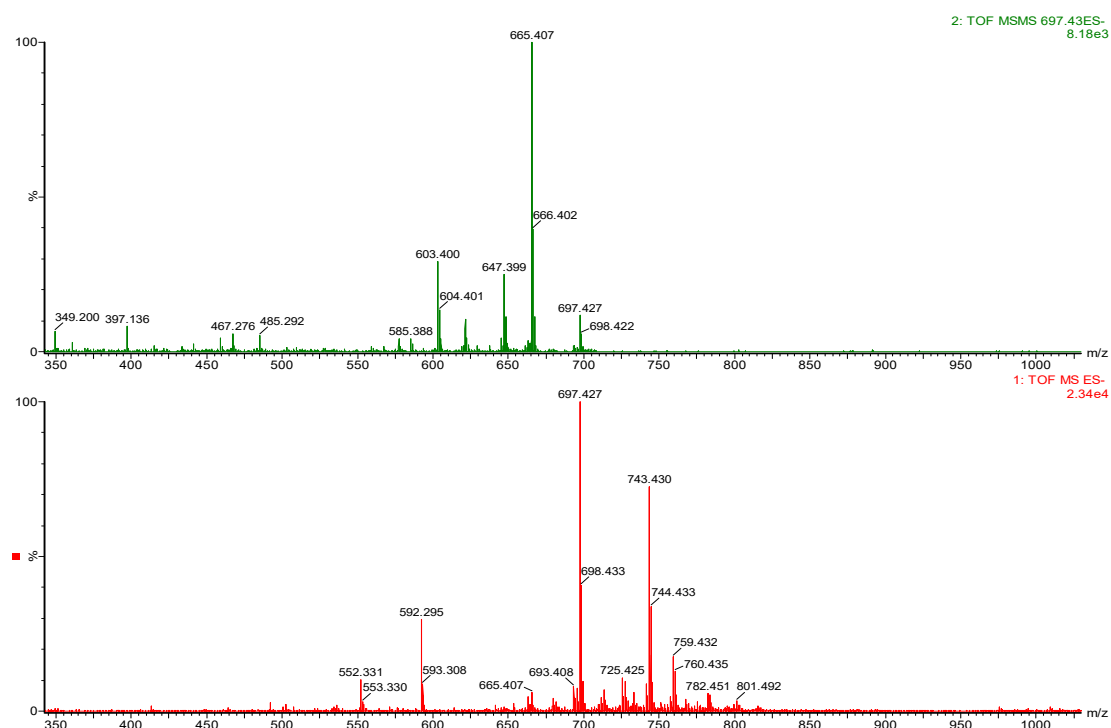


Figure S53. The LC-MS/MS fragment in negative mode of (2)