

Supplementary Materials

Bioactive Compounds from *Euphorbia usambarica* Pax. with HIV-1 Latency Reversal Activity

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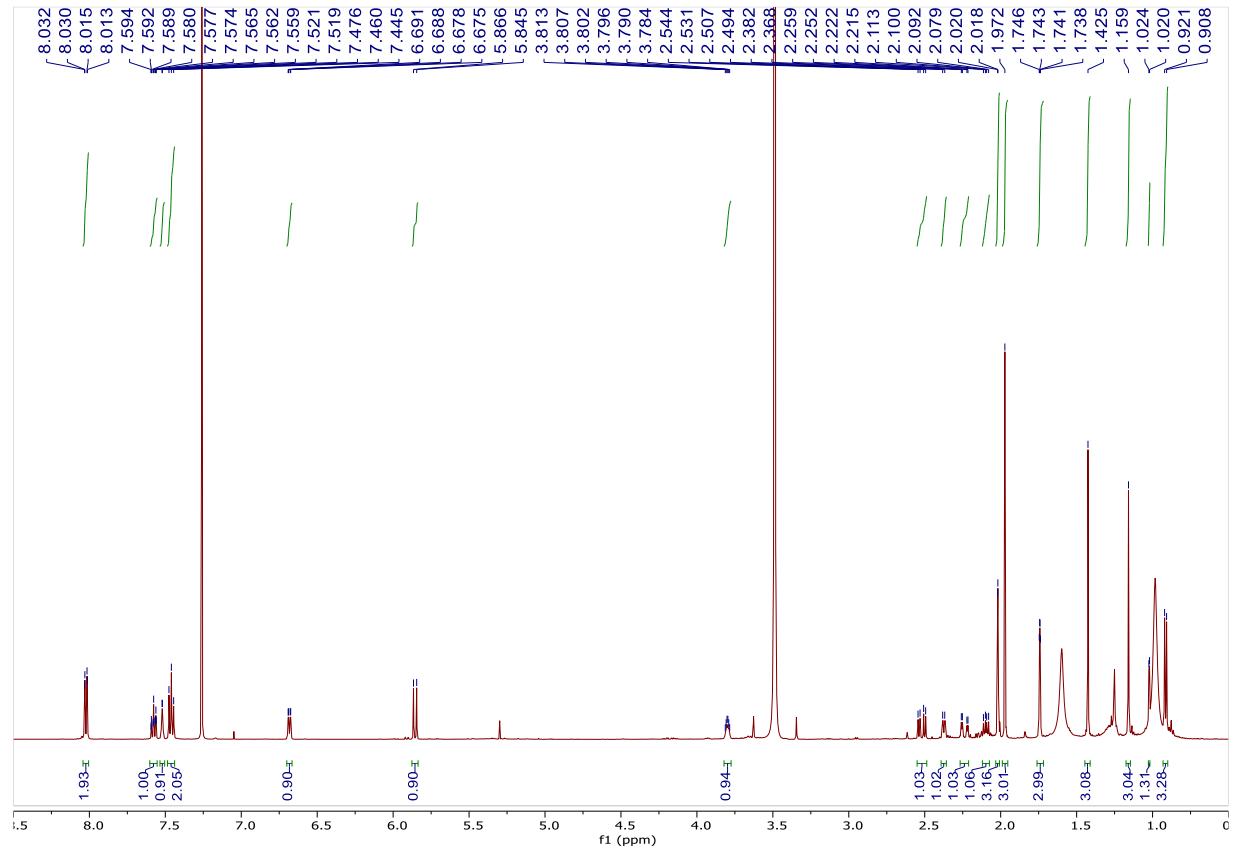


Figure S1. The ^1H -NMR spectrum of euphordraculoate C (1) (500 MHz, CDCl_3).

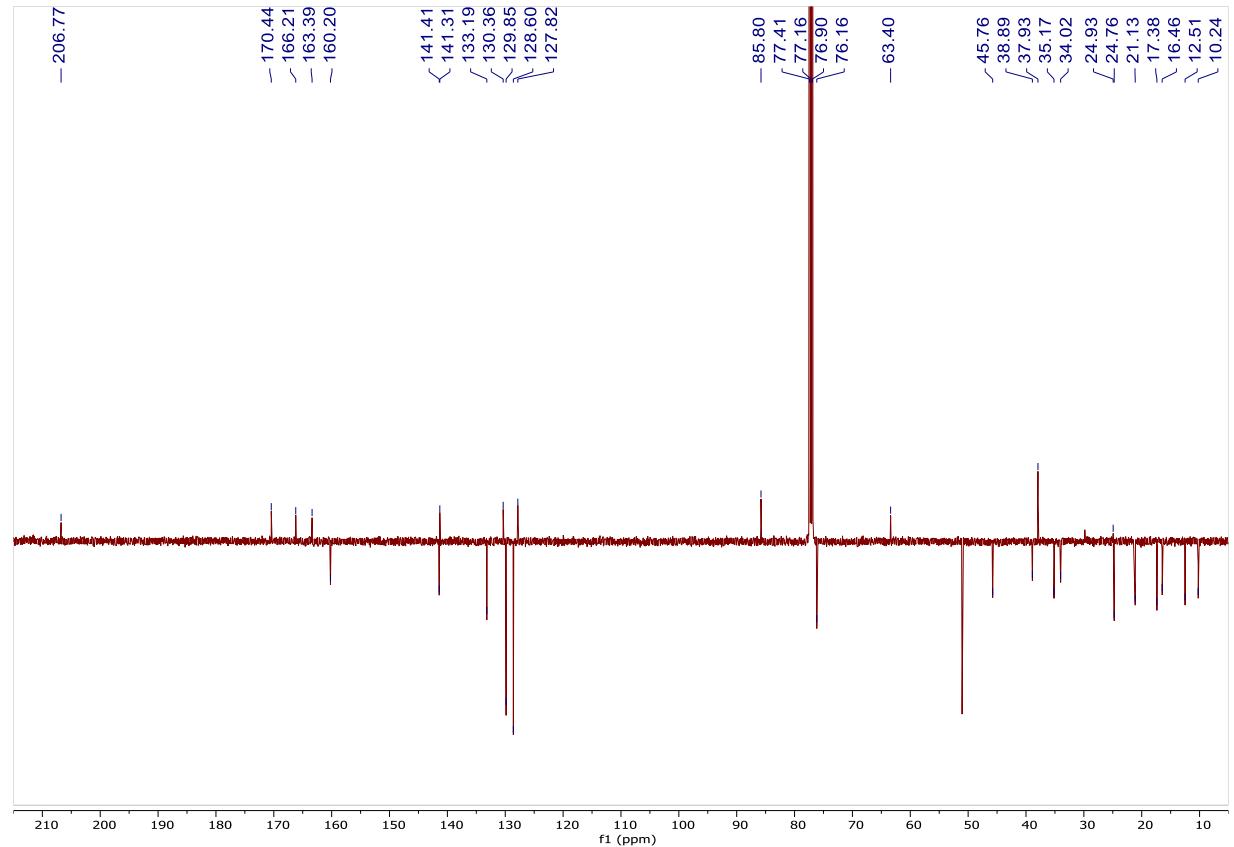


Figure S2. The ^{13}C -JMOD spectrum of euphordraculoate C (1) (125 MHz, CDCl_3).

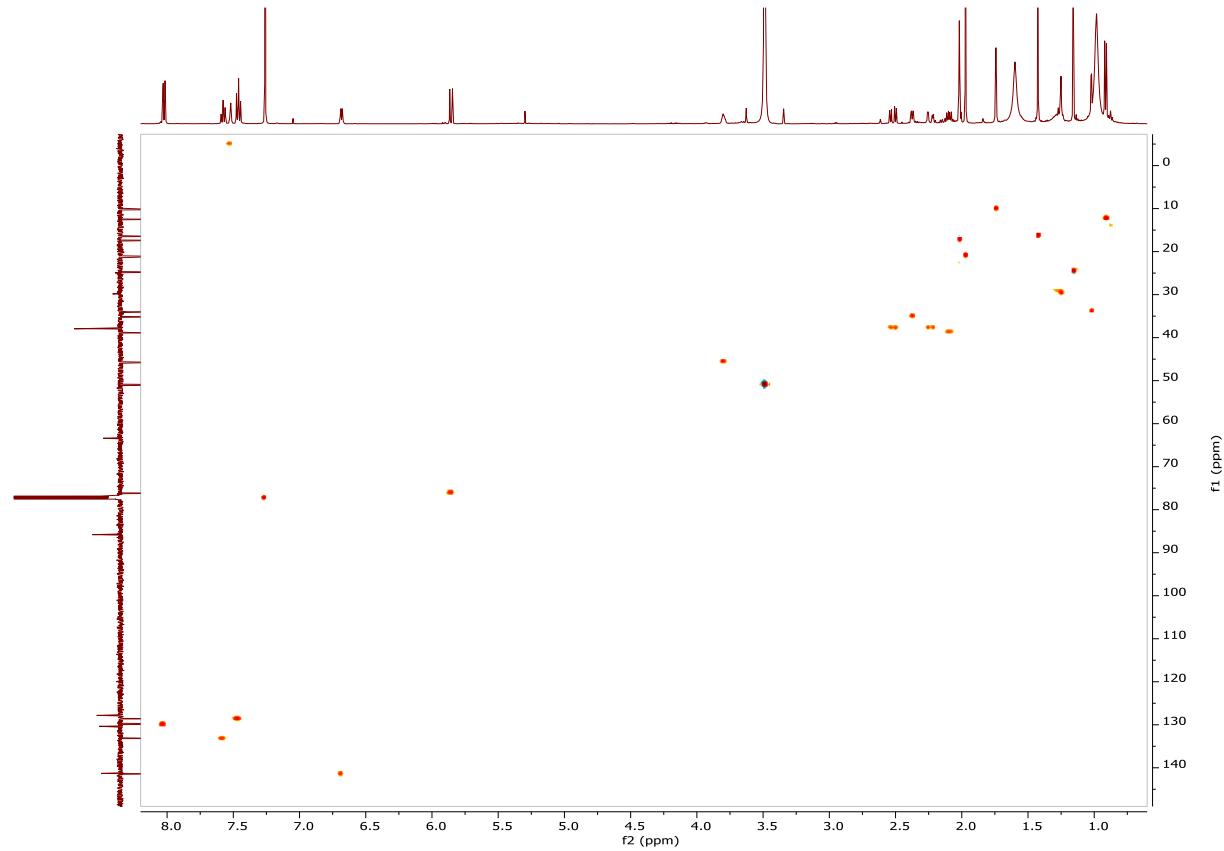


Figure S3. The HSQC spectrum of euphordraculoate C (**1**).

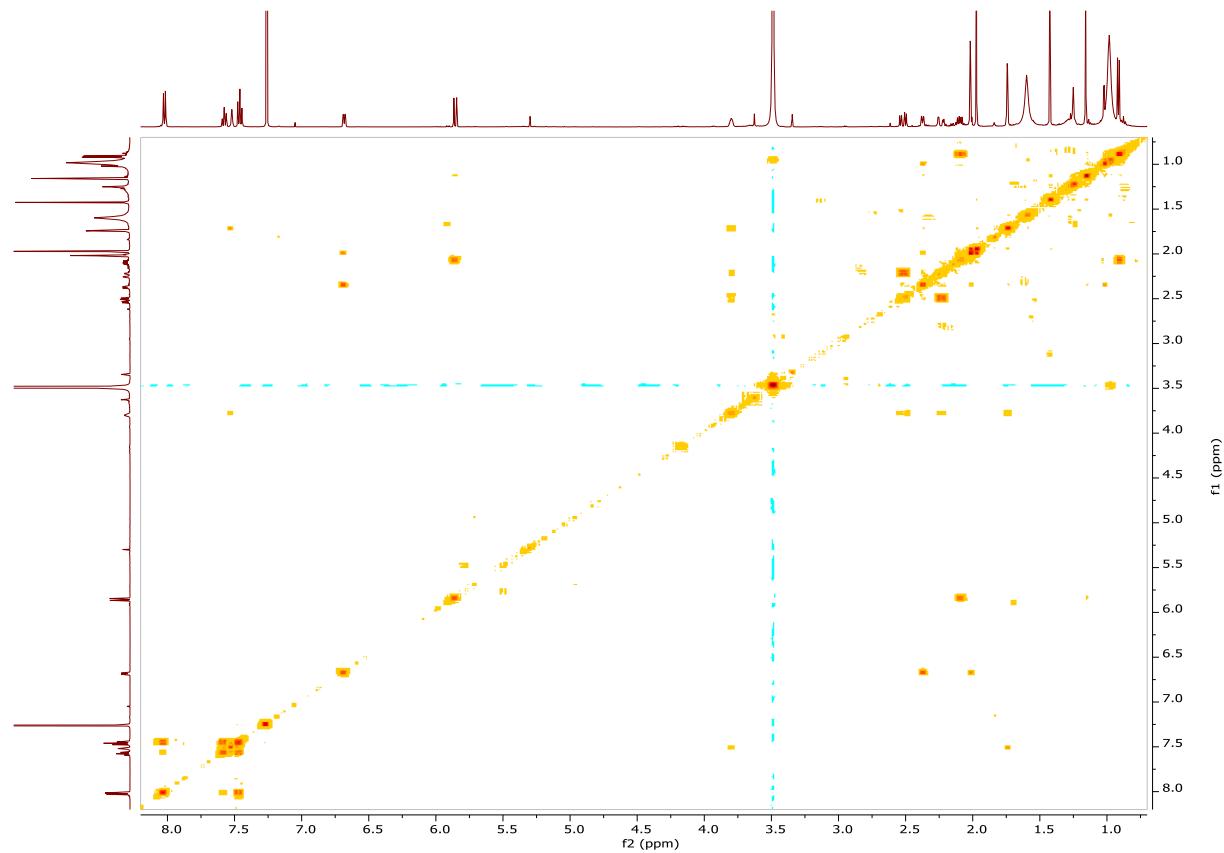


Figure S4. The ¹H-¹H COSY spectrum of euphordraculoate C (**1**).

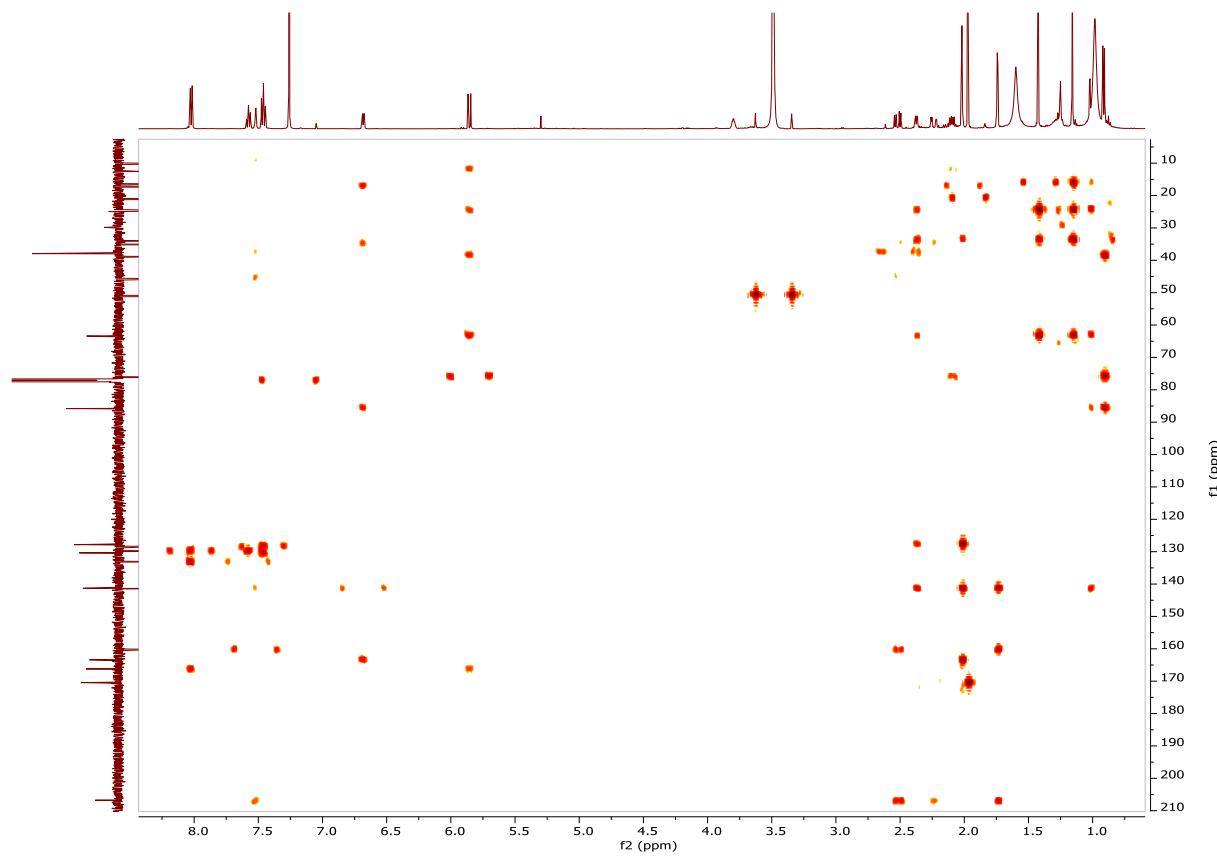


Figure S5. The HMBC spectrum of euphordraculoate C (**1**).

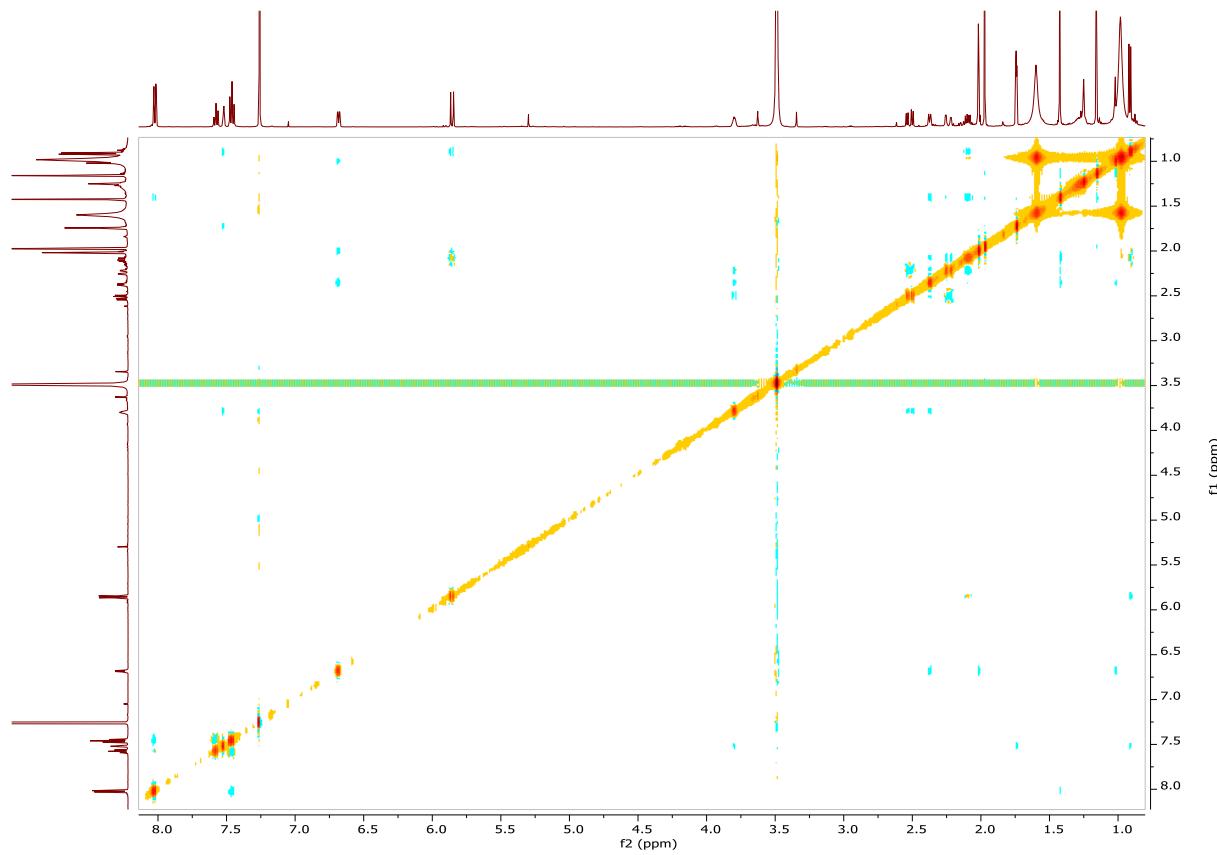


Figure S6. The NOESY spectrum of euphordraculoate C (**1**).

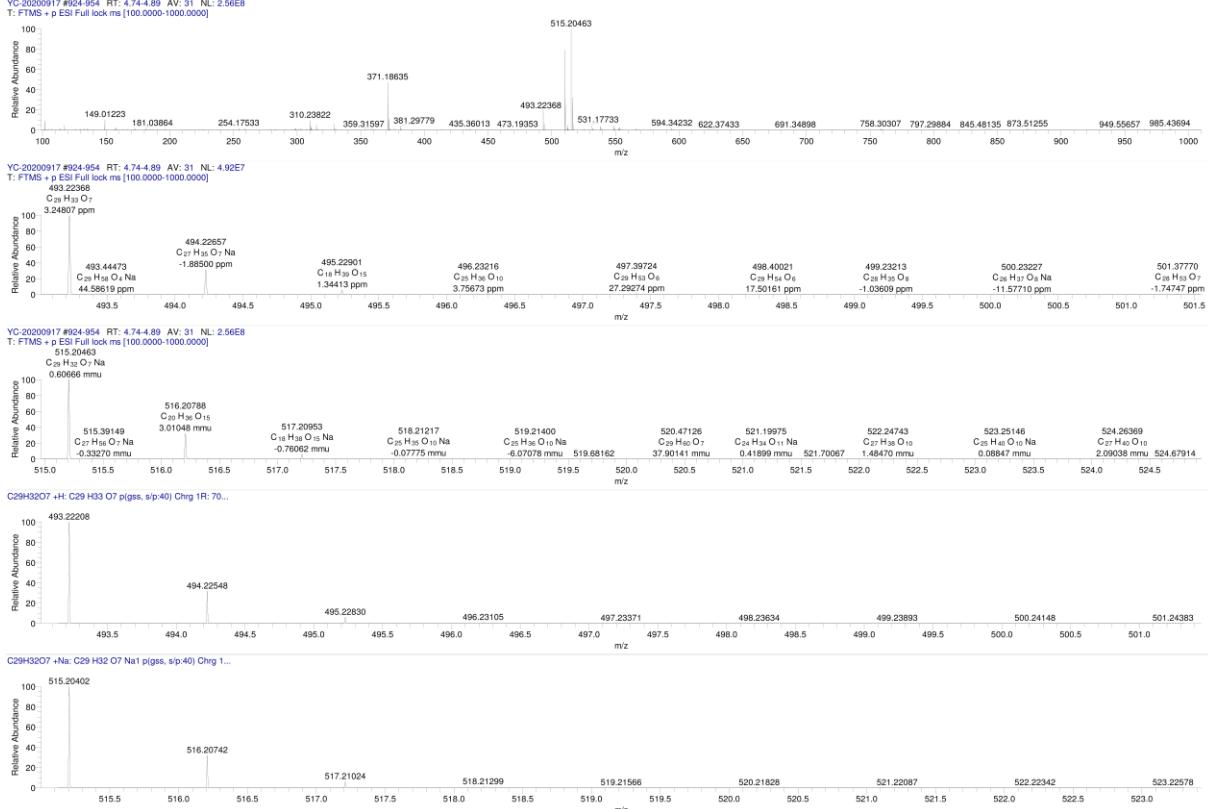


Figure S7. The HR-ESIMS spectra of euphordraculoate C (1).

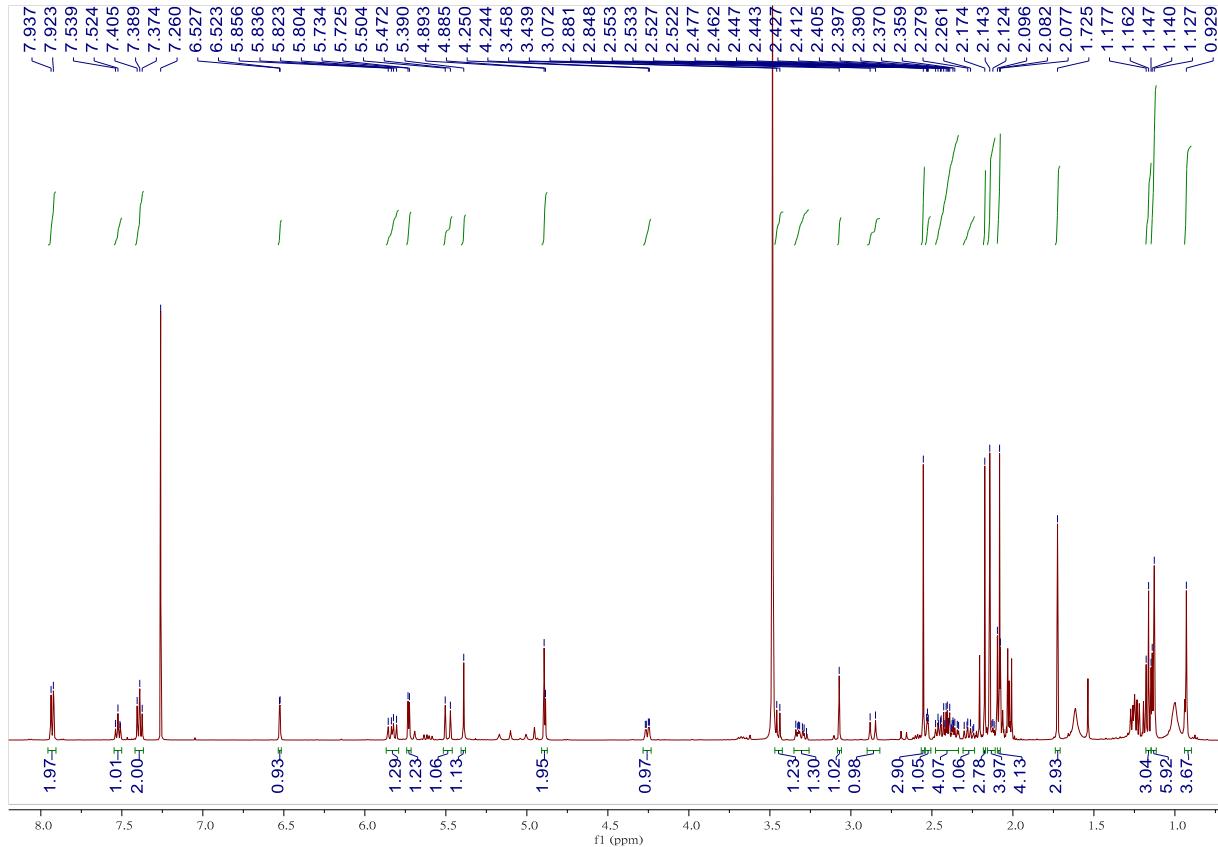


Figure S8. The ^1H -NMR spectrum of usambariphane A (**2**) (500 MHz, CDCl_3).

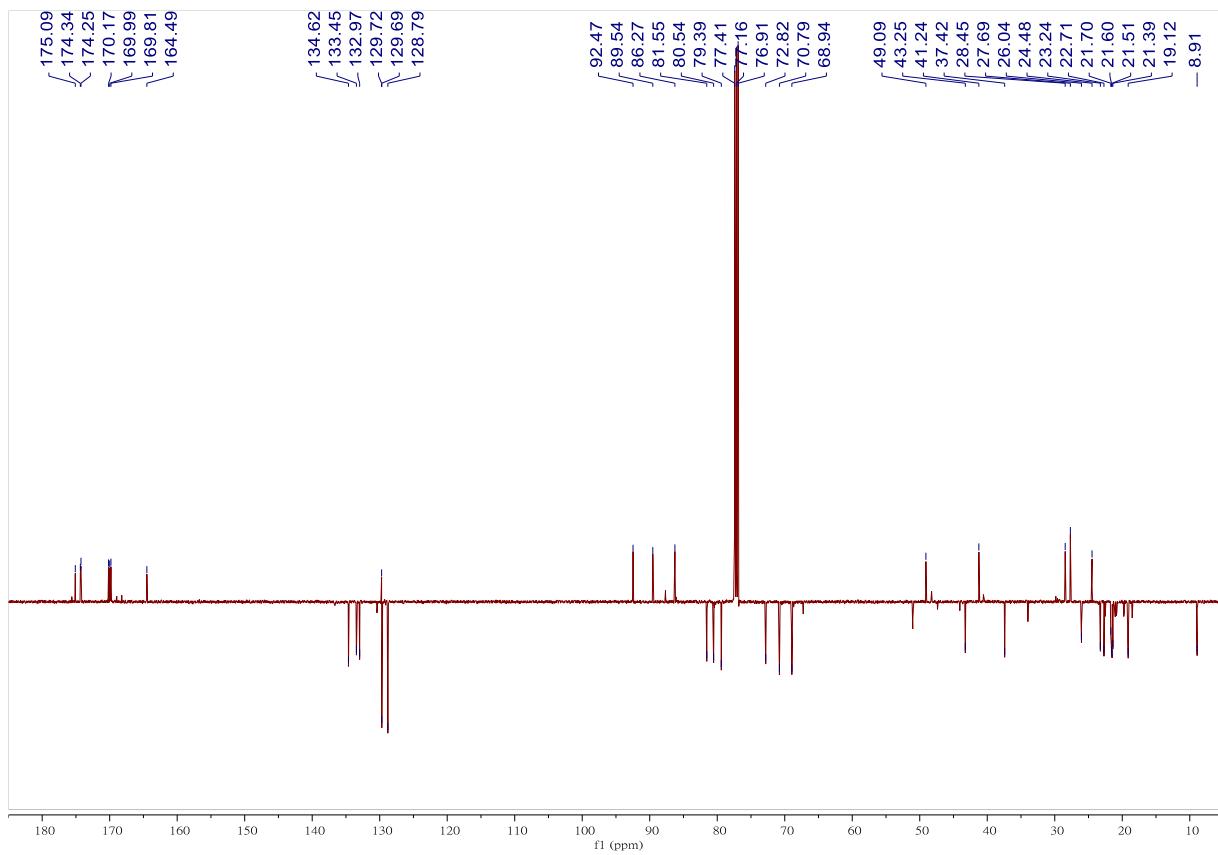


Figure S9. The ^{13}C -JMOD spectrum of usambariphane A (**2**) (125 MHz, CDCl_3).

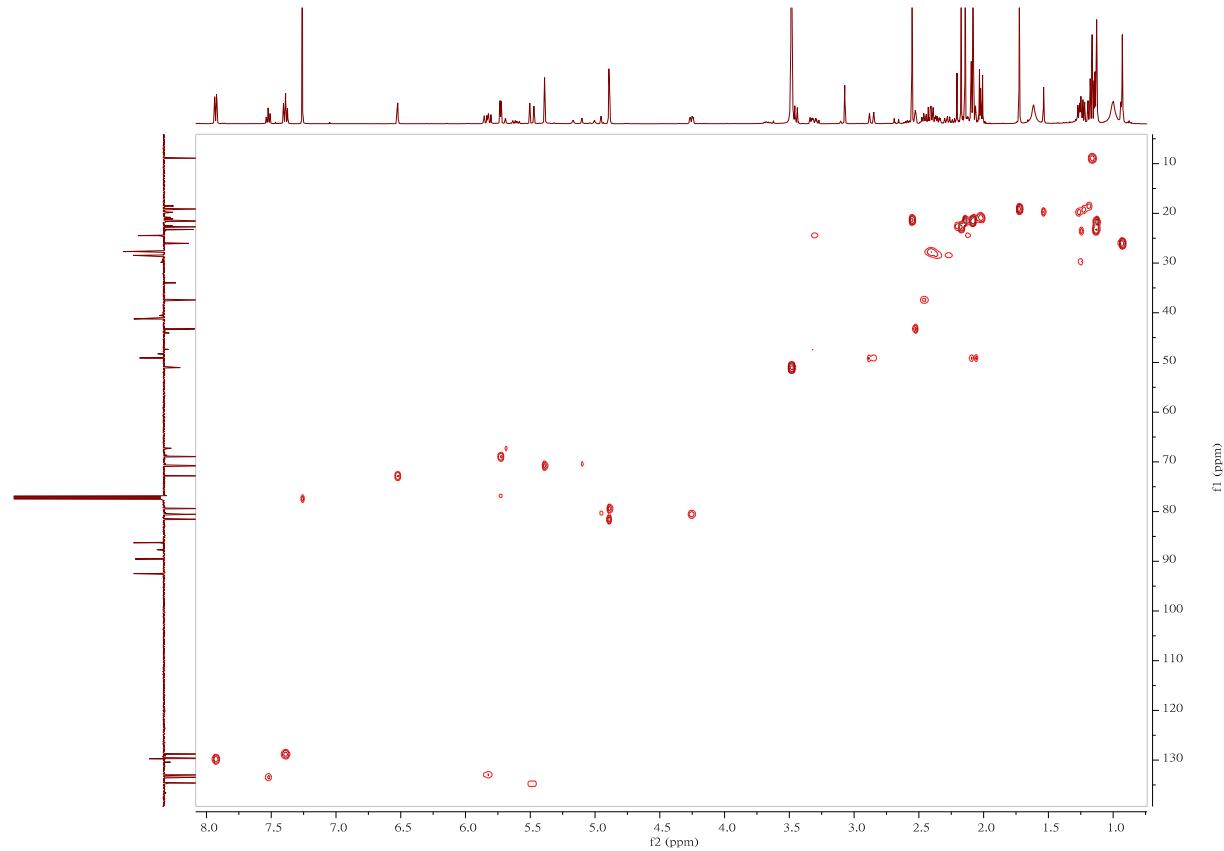


Figure S10. The HSQC spectrum of usambariphane A (2).

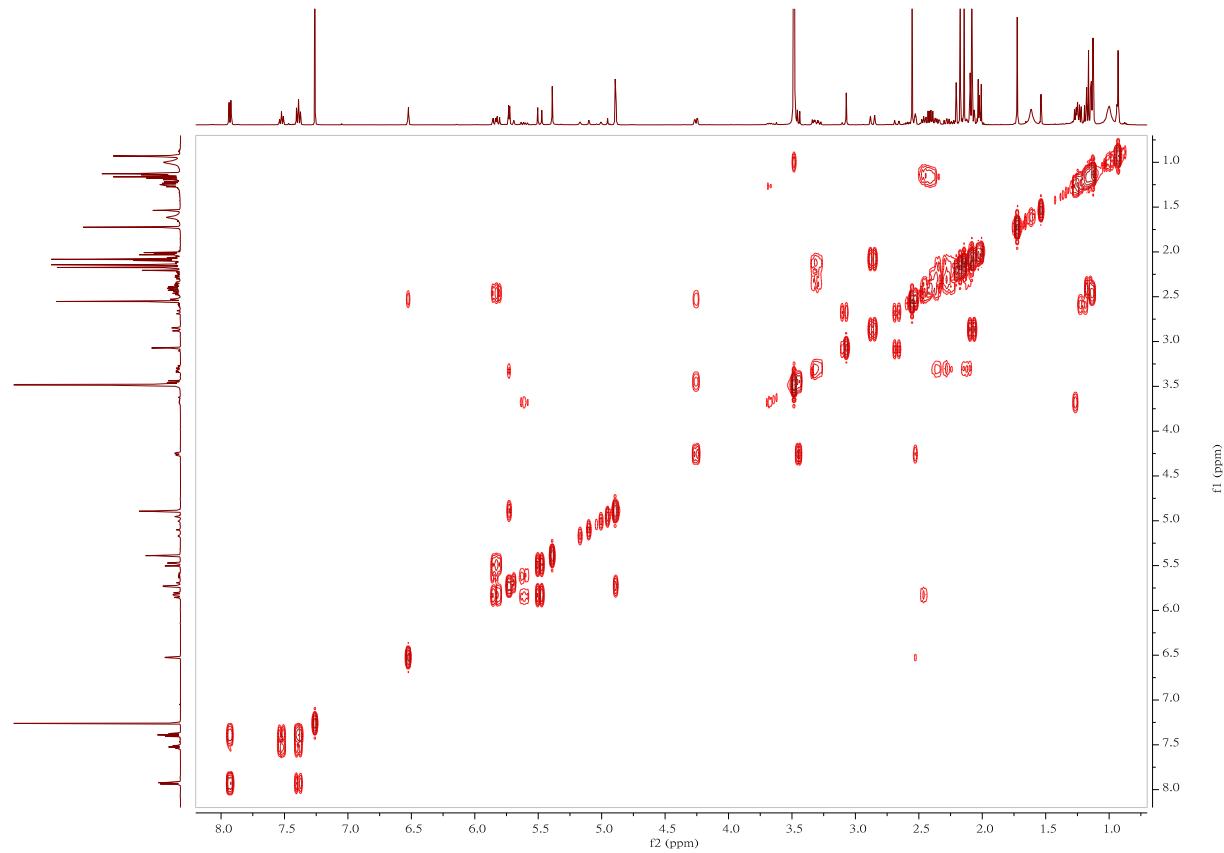


Figure S11. The ^1H - ^1H COSY spectrum of usambariphane A (2).

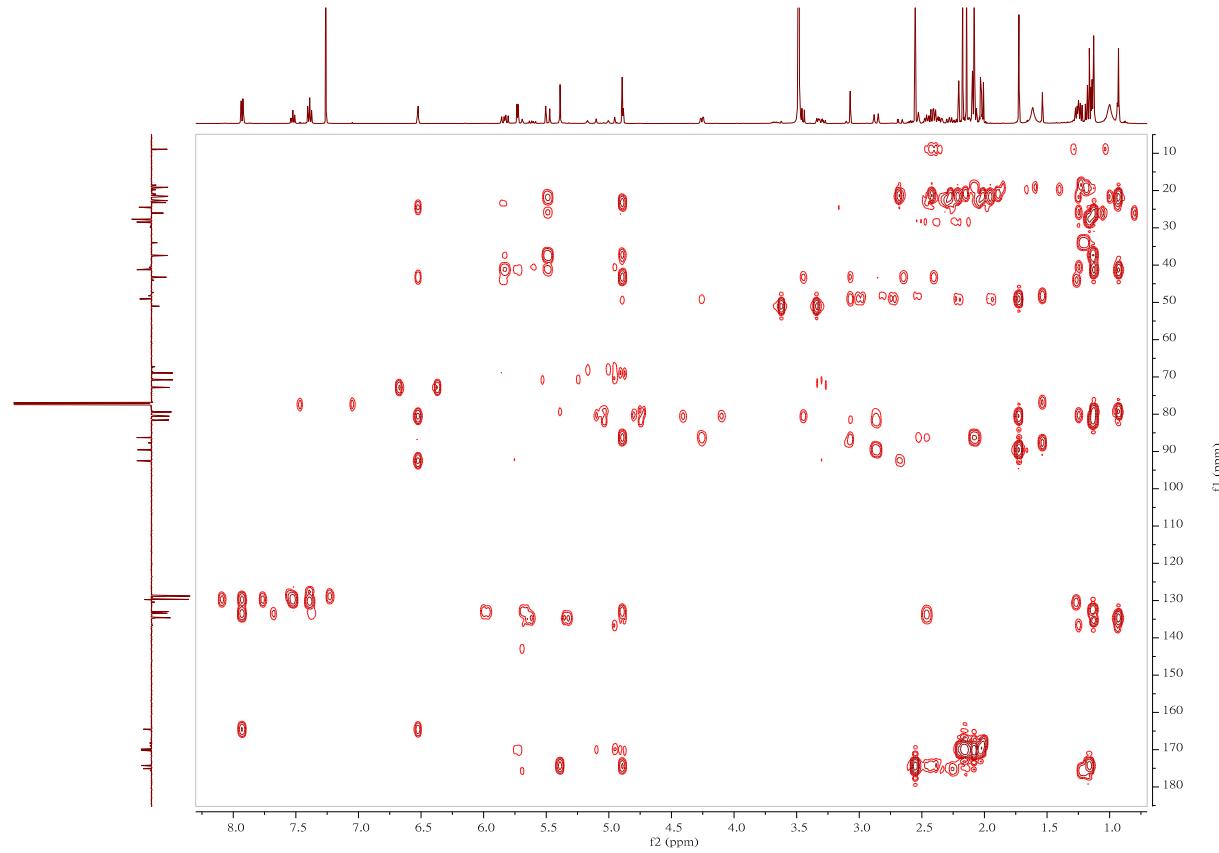


Figure S12. The HMBC spectrum of usambariphane A (2).

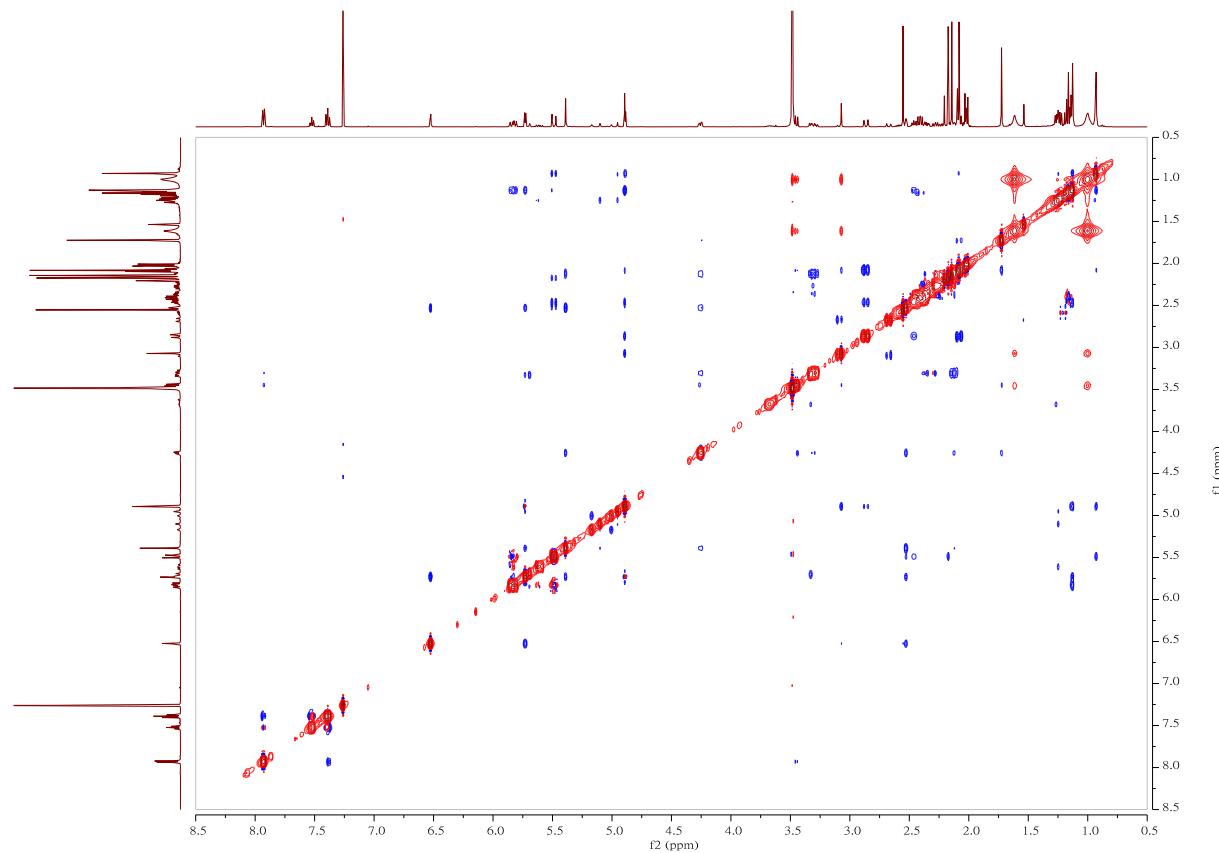


Figure S13. The NOESY spectrum of usambariphane A (2).

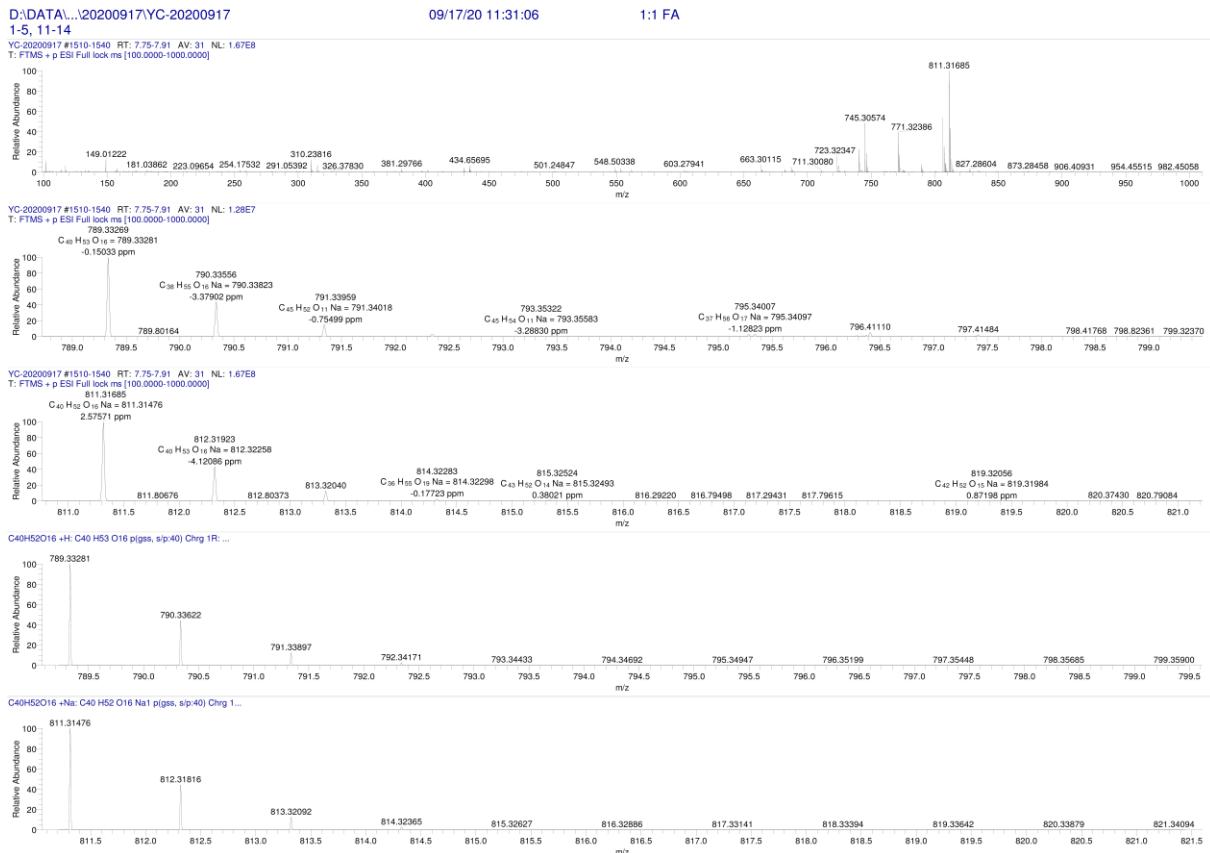


Figure S14. The HR-ESIMS spectra of usambariphane A (**2**).

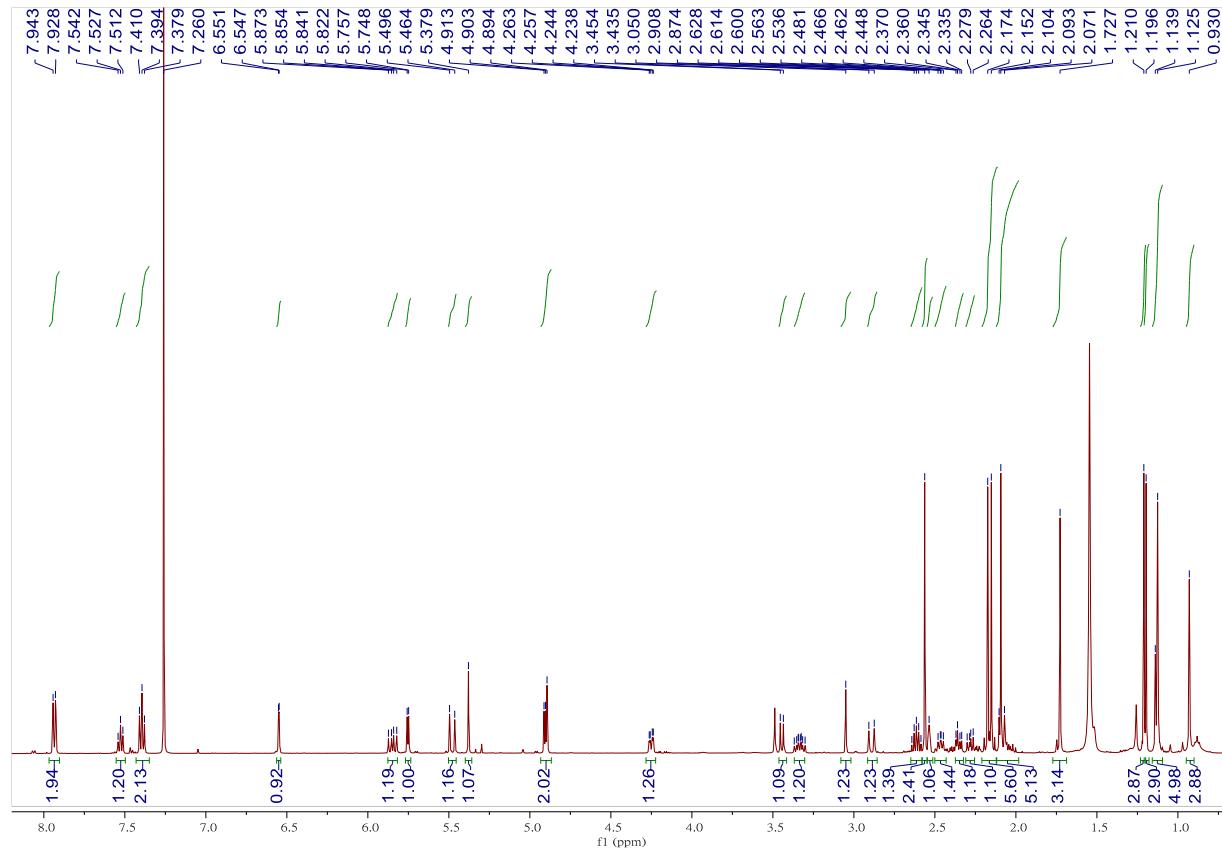


Figure S15. The ^1H -NMR spectrum of usambariphane B (3) (500 MHz, CDCl_3).

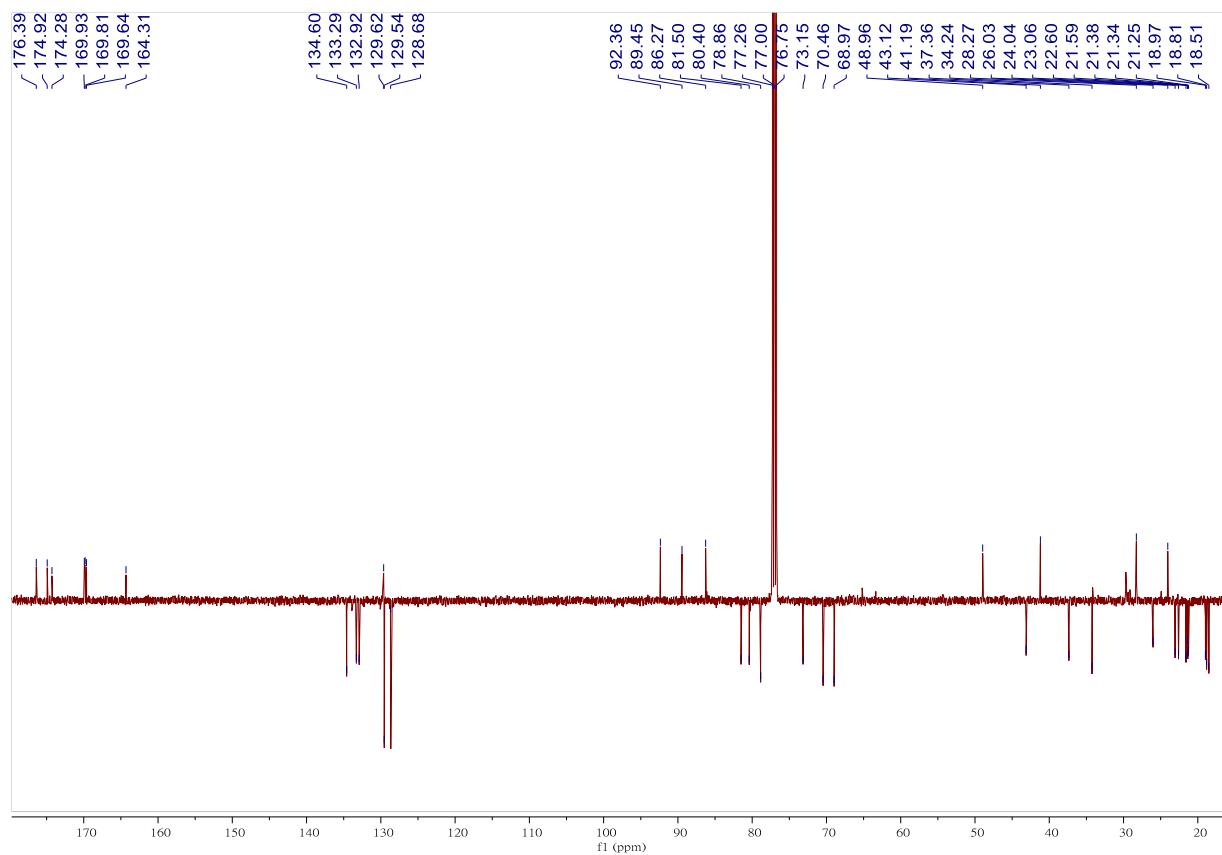


Figure S16. The ^{13}C -JMOD spectrum of usambariphane B (3) (125 MHz, CDCl_3).

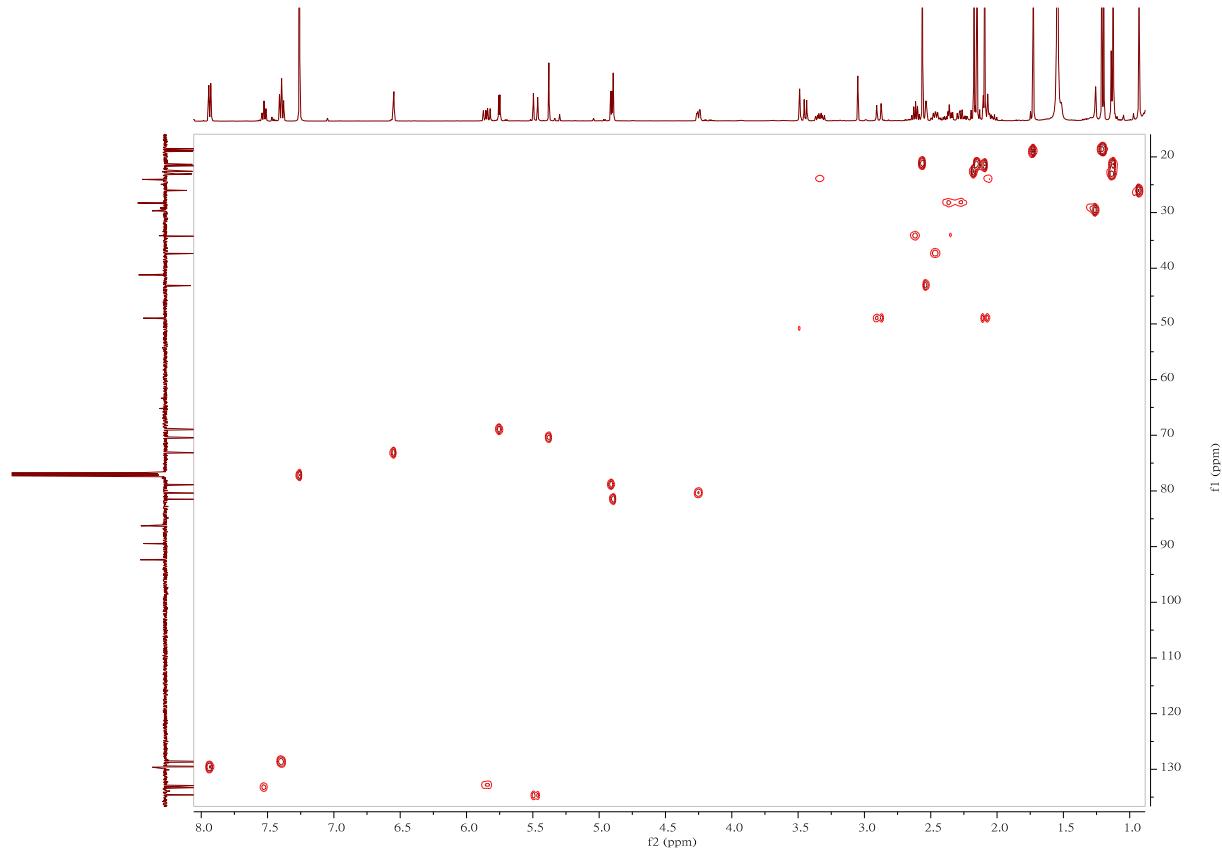


Figure S17. The HSQC spectrum of usambariphane B (3).

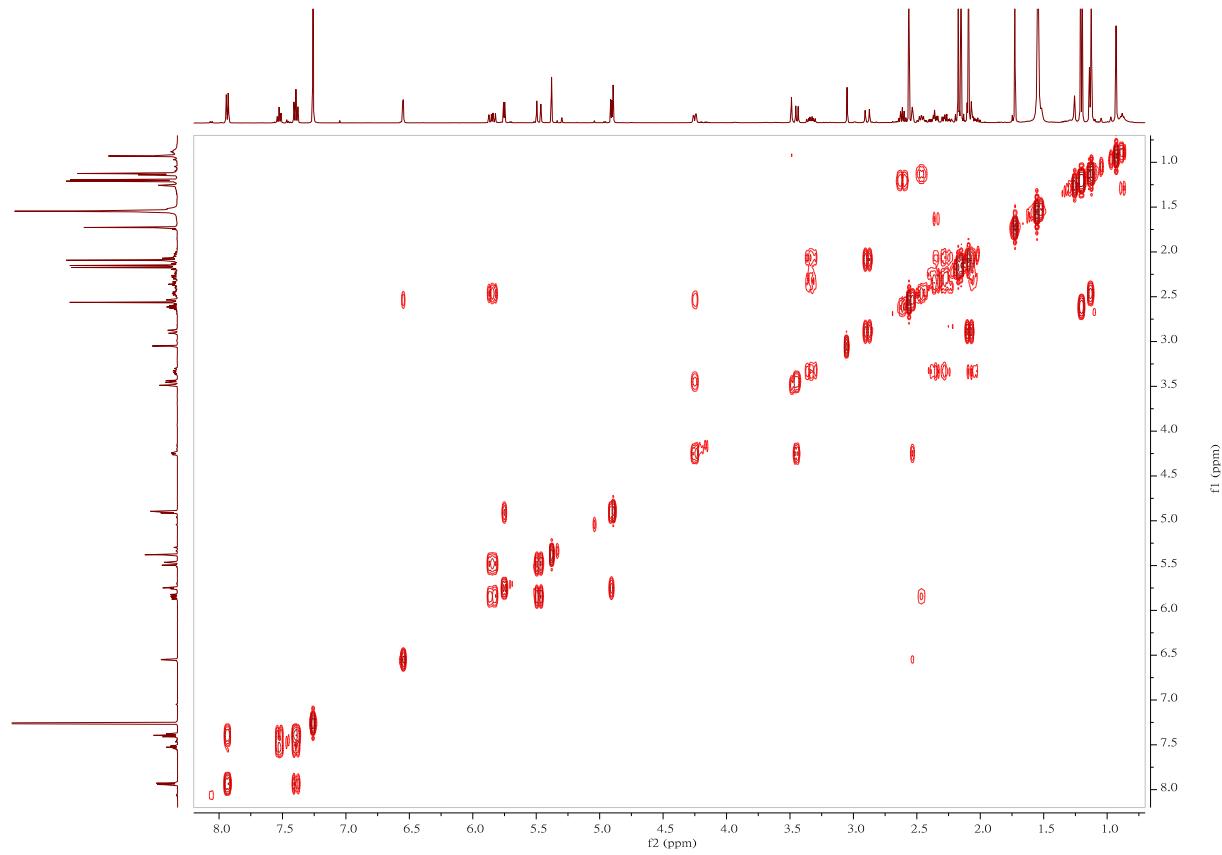


Figure S18. The ^1H - ^1H COSY spectrum of usambariphane B (3).

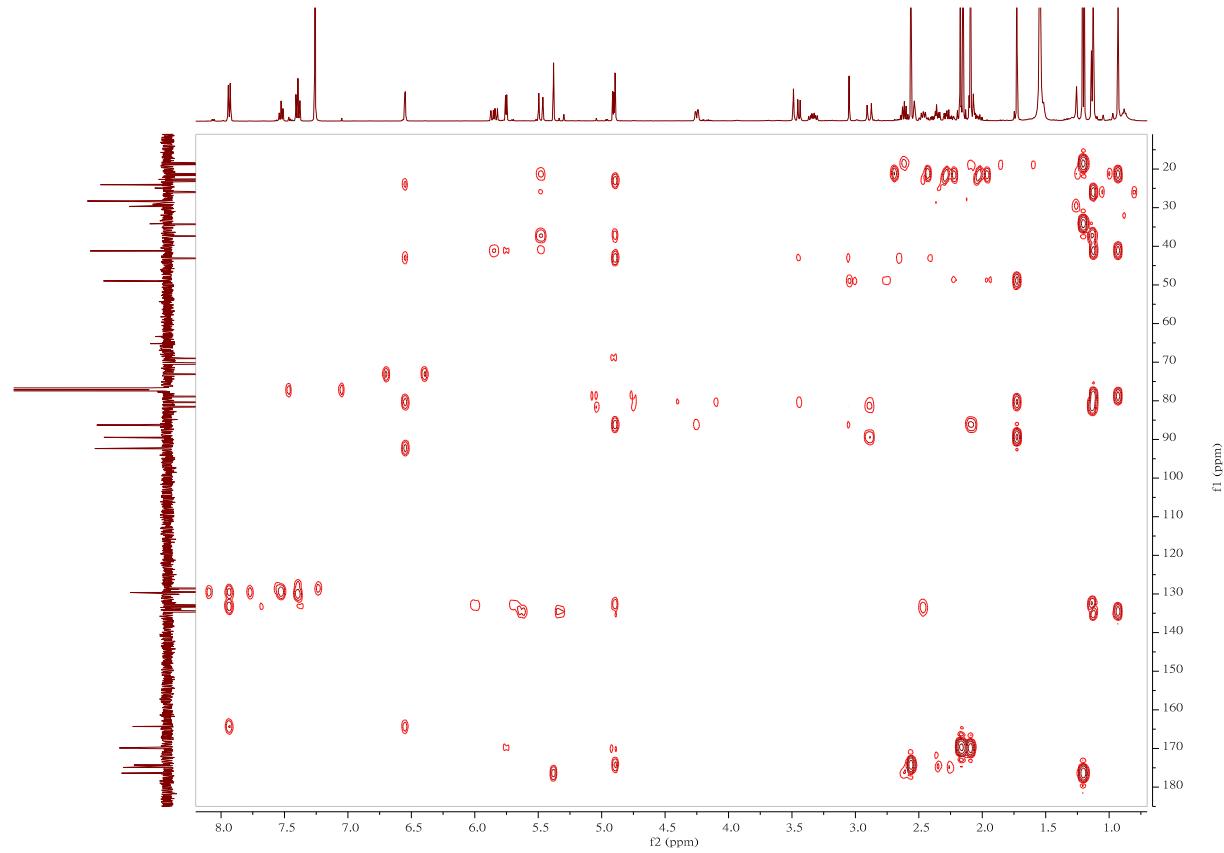


Figure S19. The HMBC spectrum of usambariphane B (3).

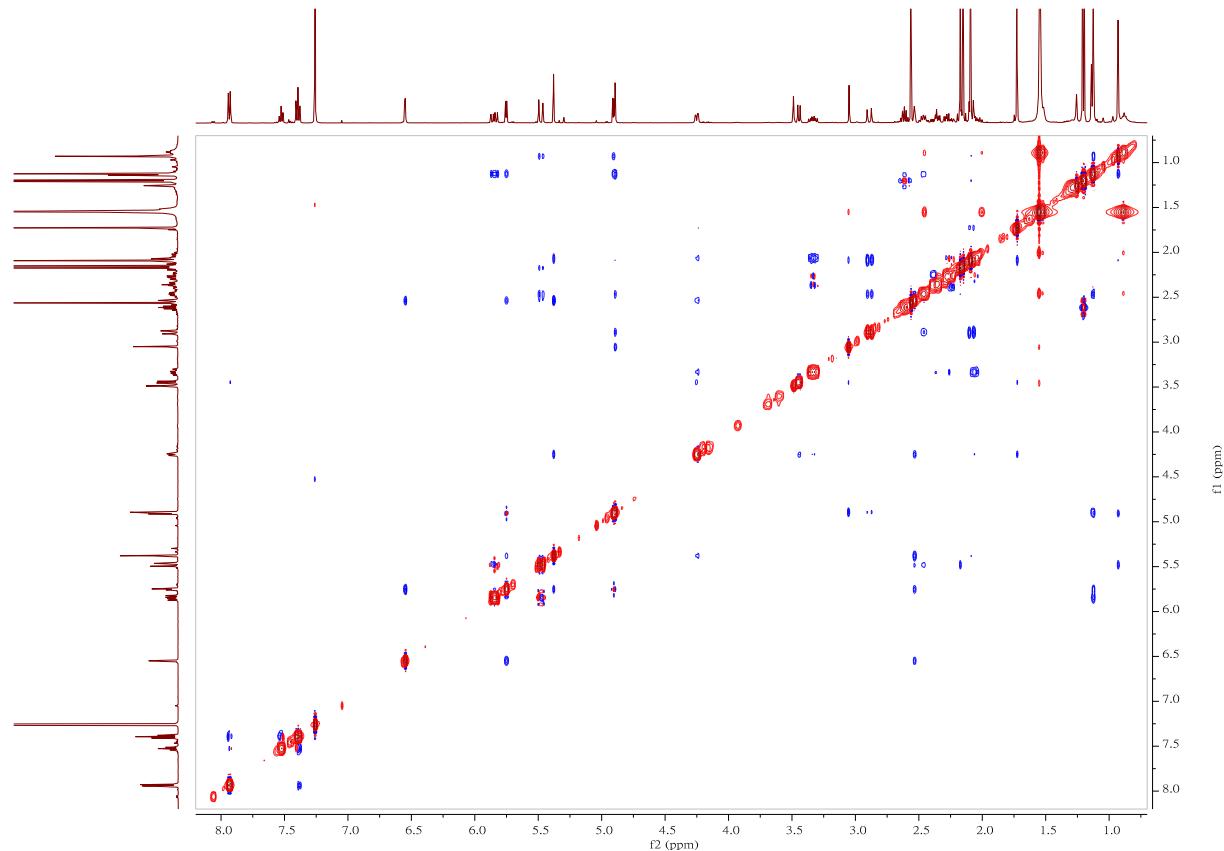
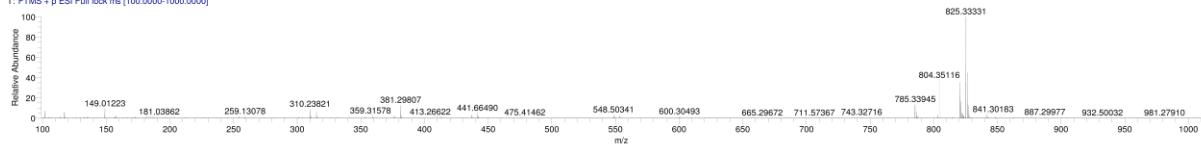
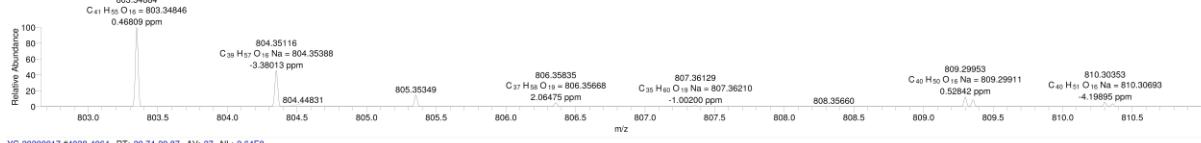


Figure S20. The NOESY spectrum of usambariphane B (3).

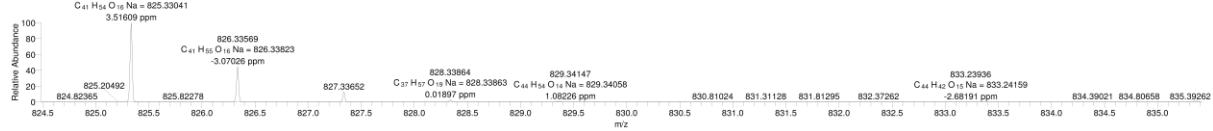
1-5, 11-14
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 T: FTMS + p ESI Full lock ms [100.000-1000.000]



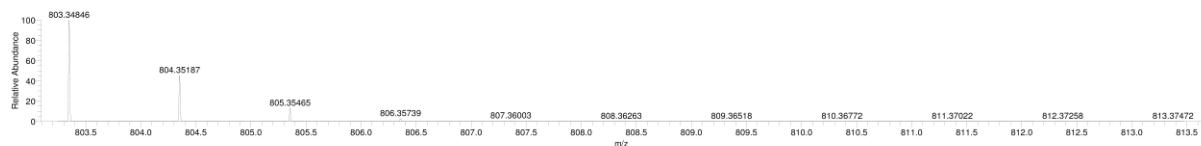
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 $C_{41}H_{55}O_{16}Na = 803.34846$
 0.46809 ppm



YC_20200917 #4038-4064 RT: 20.74-20.87 AV: 27 NL: 2.64E8
 T: FTMS + p ESI Full lock ms [100.000-1000.000]
 825.33331
 $C_{41}H_{55}O_{16}Na = 825.33041$
 3.51609 ppm



C41H54O16 +H: C41 H55 O16 p(gs, s/p:40) Chrg 1R: ...



C41H54O16 +Na: C41 H54 O16 Na1 p(gs, s/p:40) Chrg 1...:

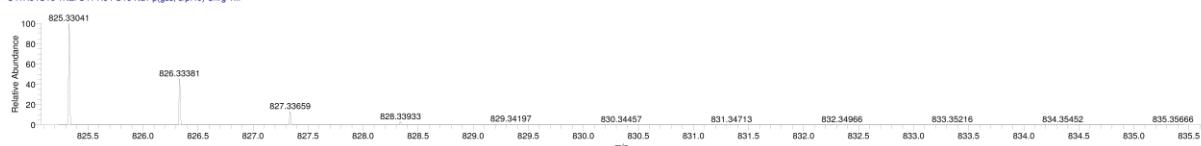


Figure S21. The HR-ESIMS spectra of usambariphane B (3).

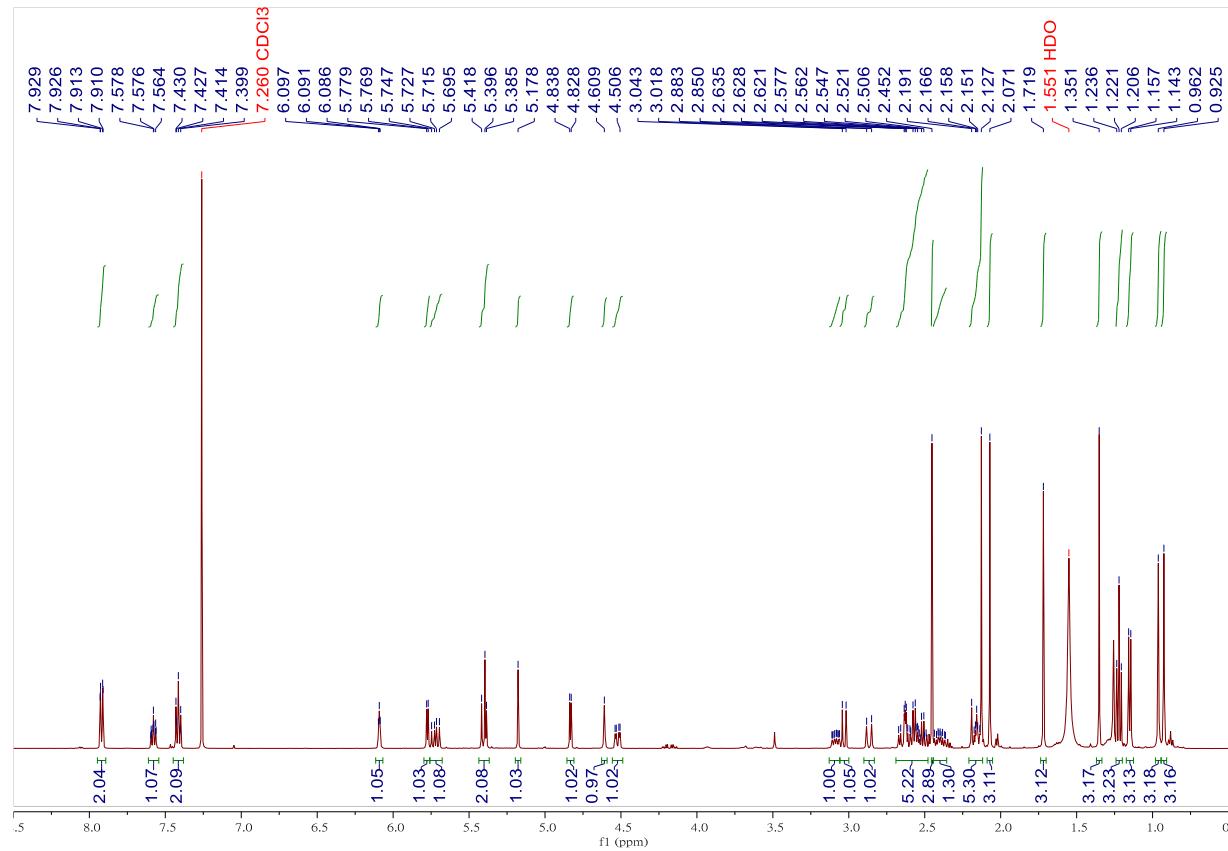


Figure S22. The ^1H -NMR spectrum of usambariphane C (**4**) (500 MHz, CDCl_3).

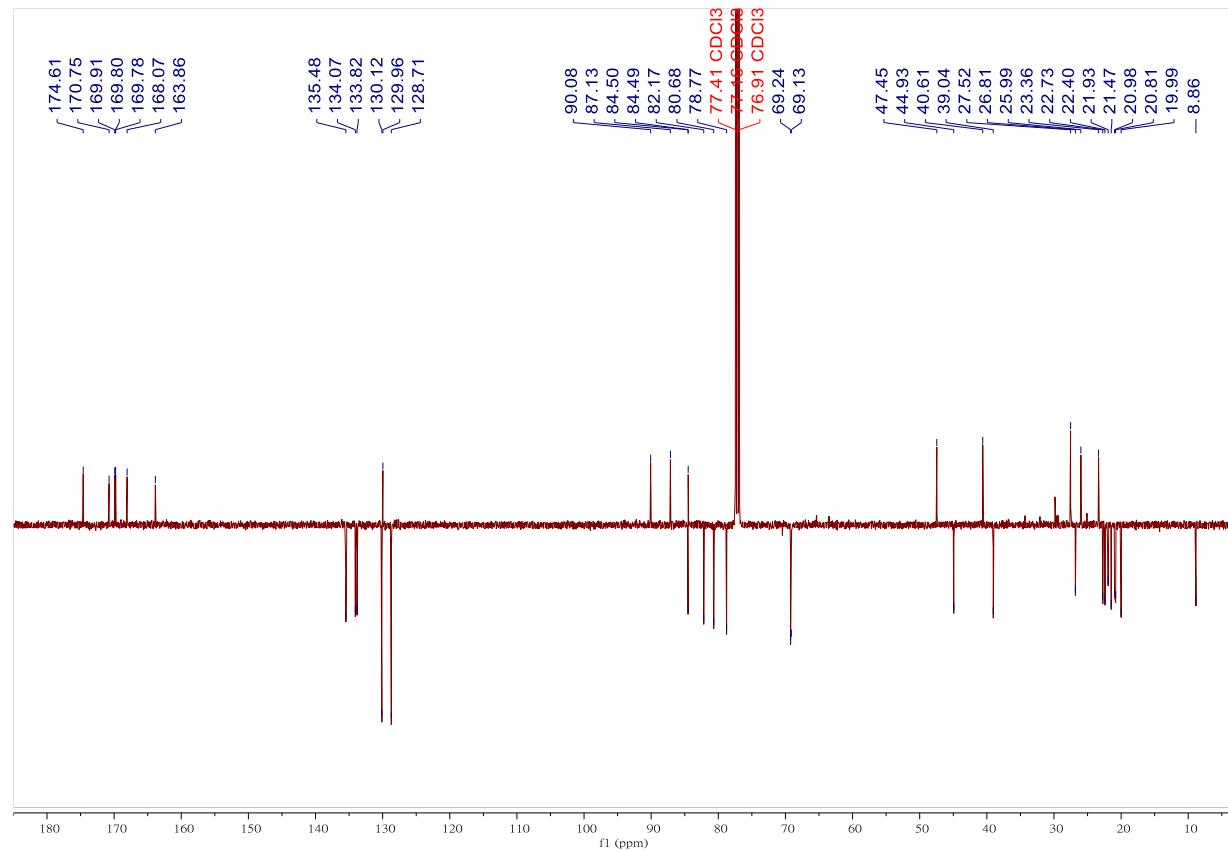


Figure S23. The ^{13}C -JMOD spectrum of usambariphane C (**4**) (125 MHz, CDCl_3).

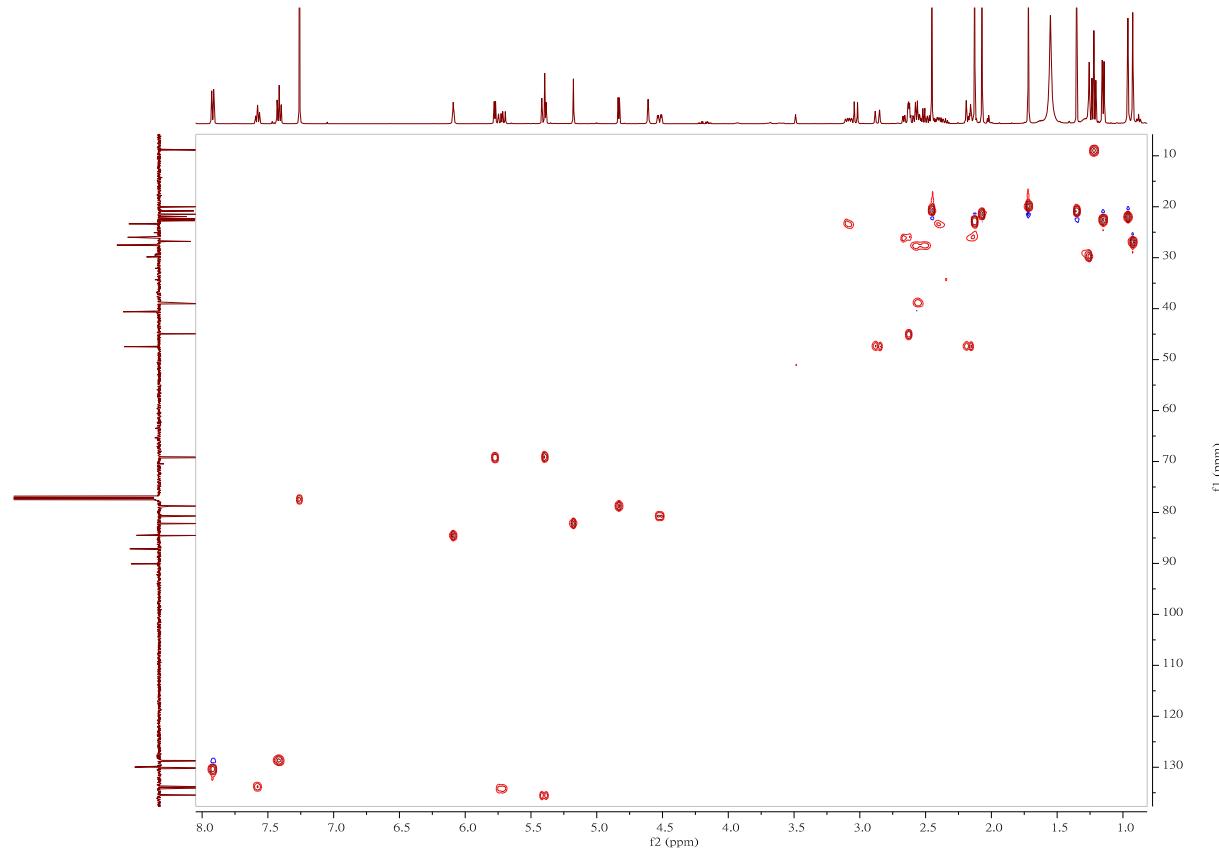


Figure S24. The HSQC spectrum of usambariphane C (4).

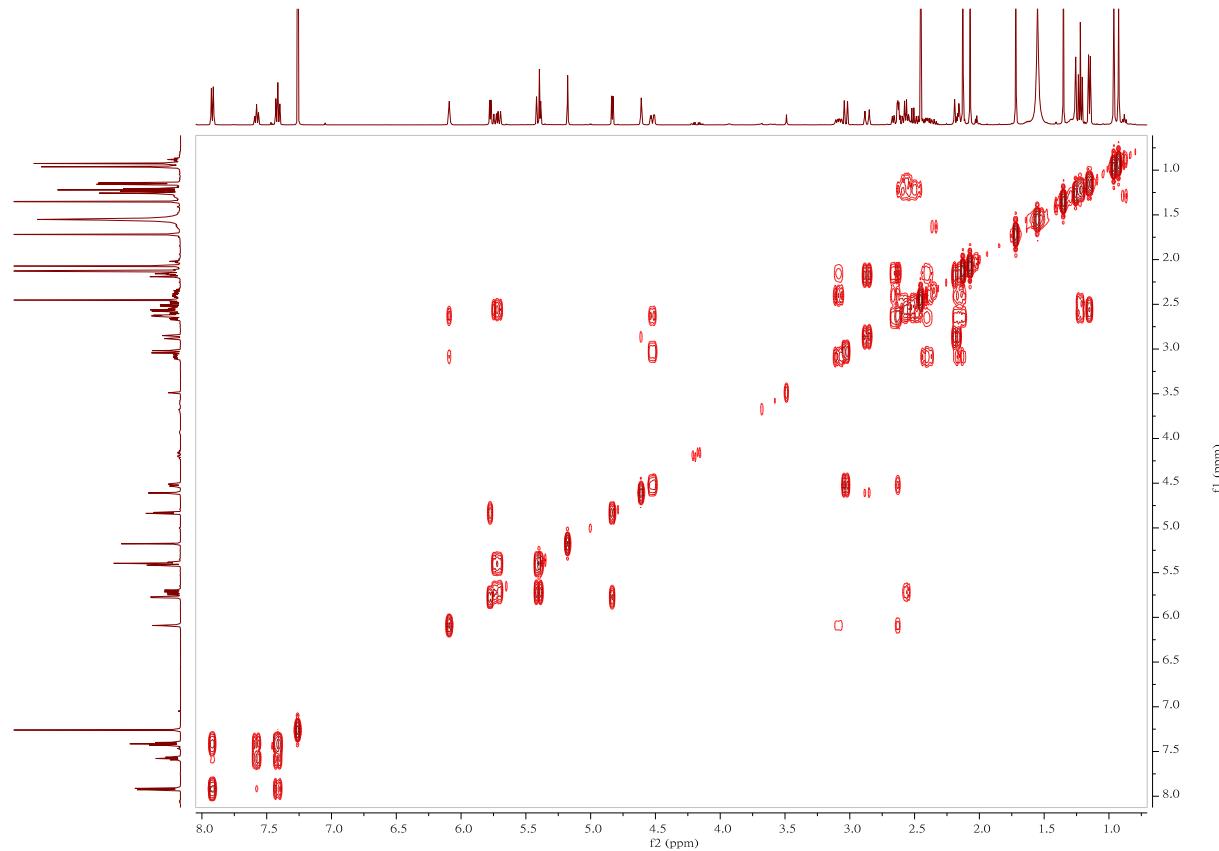


Figure S25. The ¹H-¹H COSY spectrum of usambariphane C (4).

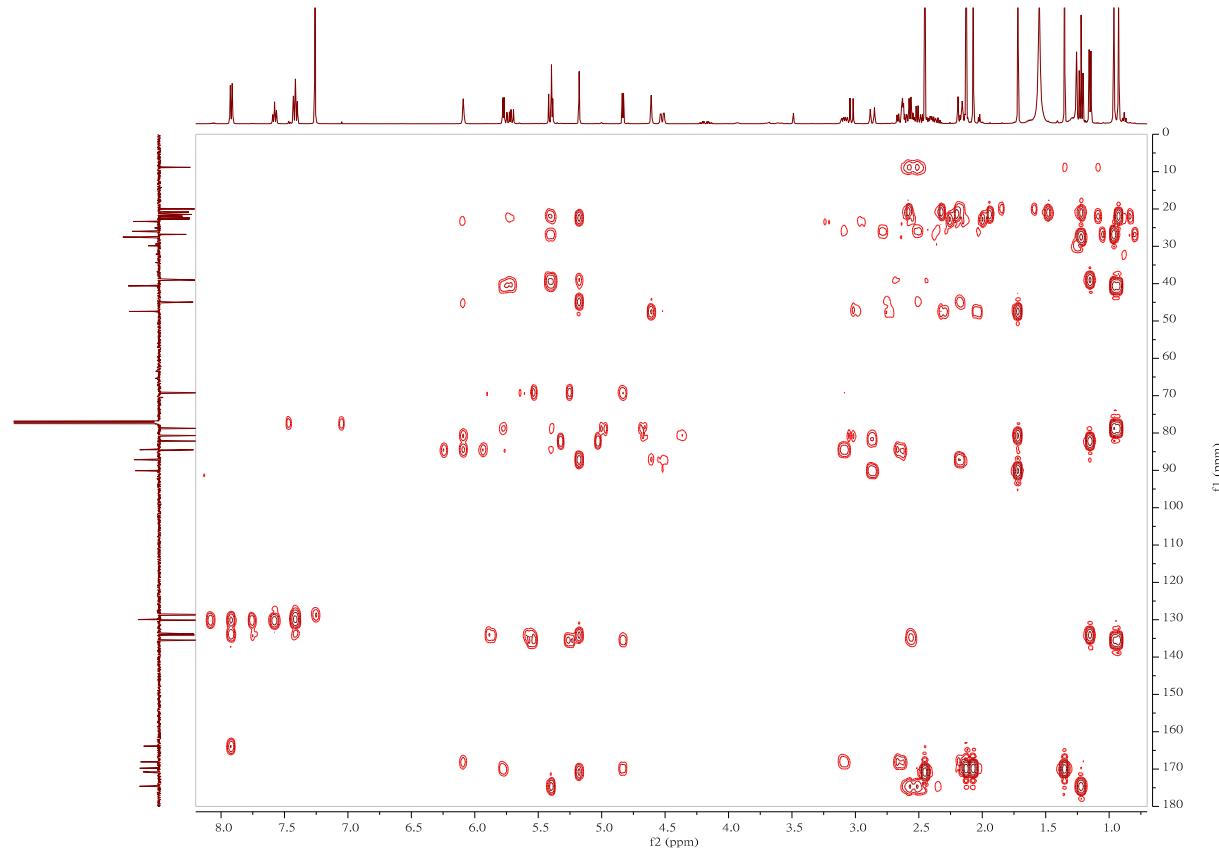


Figure S26. The HMBC spectrum of usambariphane C (4).

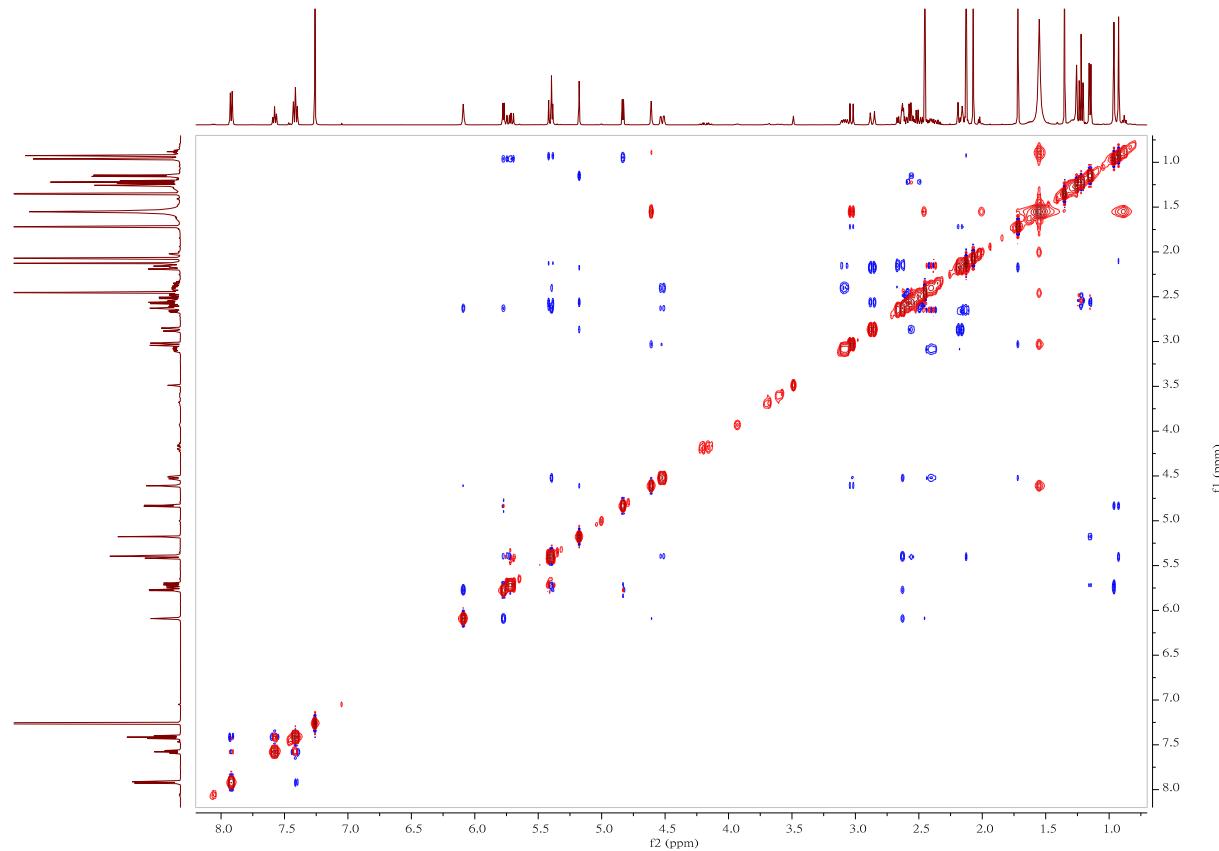


Figure S27. The NOESY spectrum of usambariphane C (4).

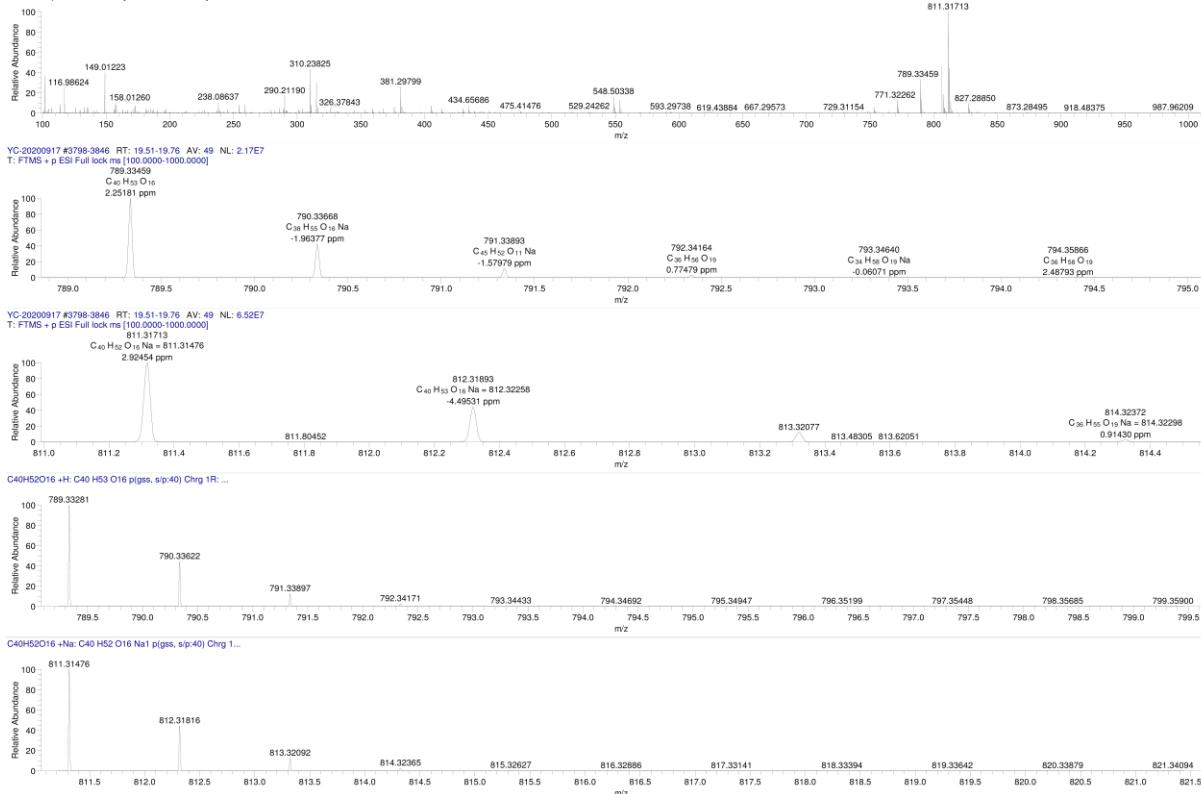


Figure S28. The HR-ESIMS spectra of usambariphane C (**4**).

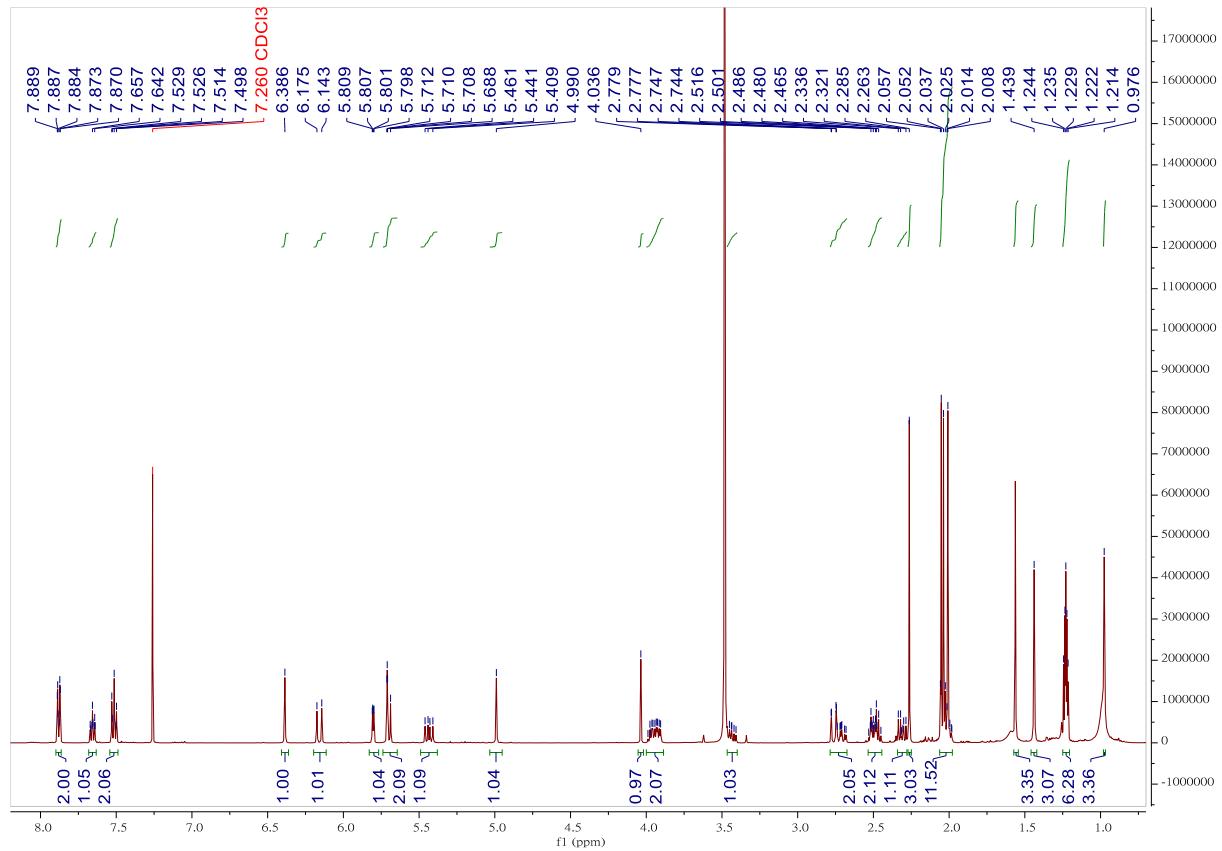


Figure S29. The ^1H -NMR spectrum of usambariphane D (**5**) (500 MHz, CDCl_3).

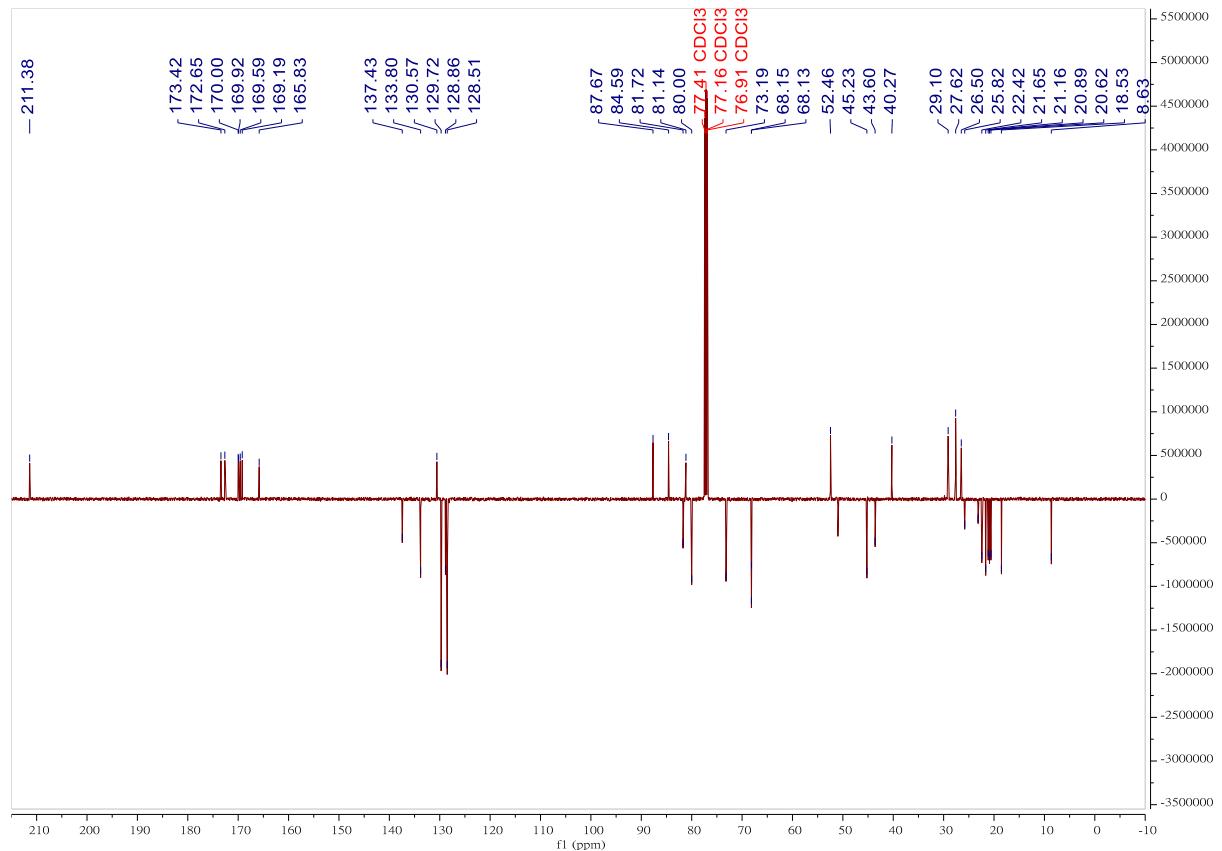


Figure S30. The ^{13}C -JMOD spectrum of usambariphane D (**5**) (125 MHz, CDCl_3).

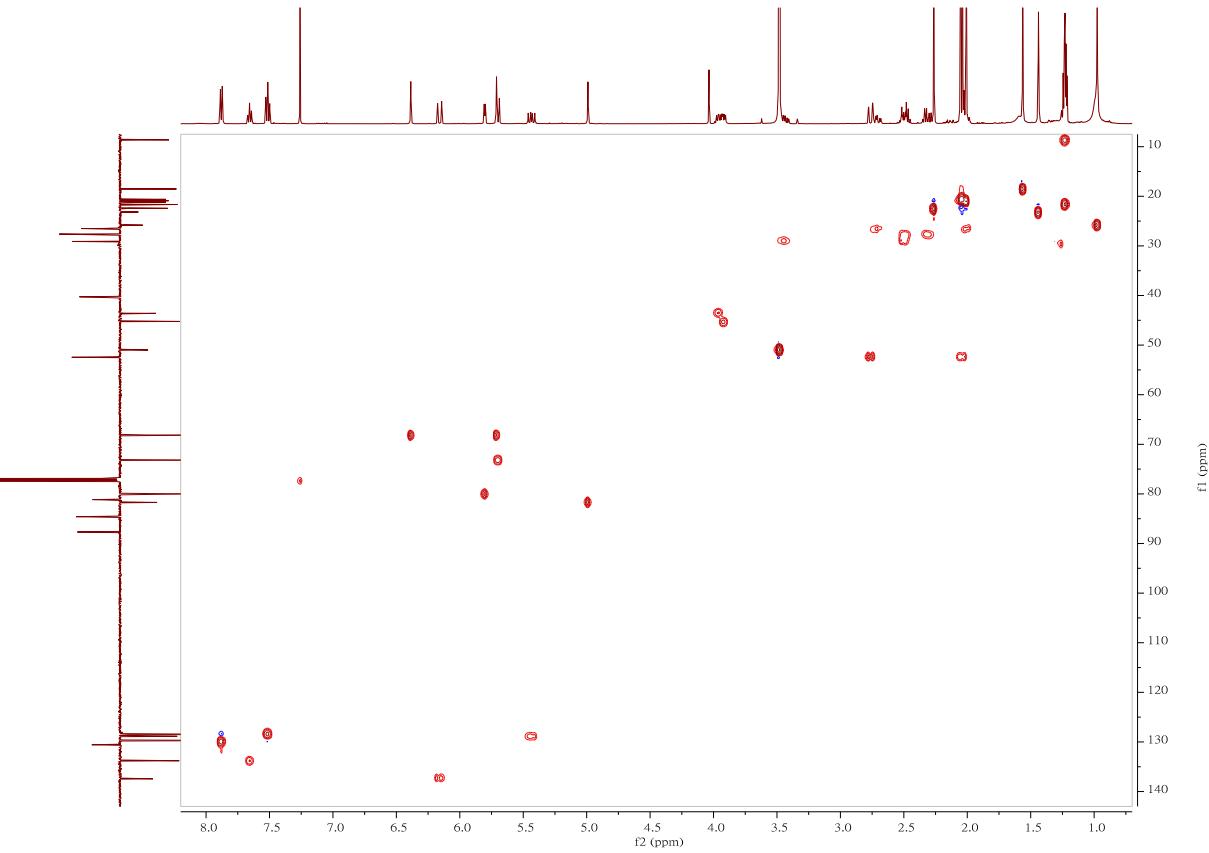


Figure S31. The HSQC spectrum of usambariphane D (5).

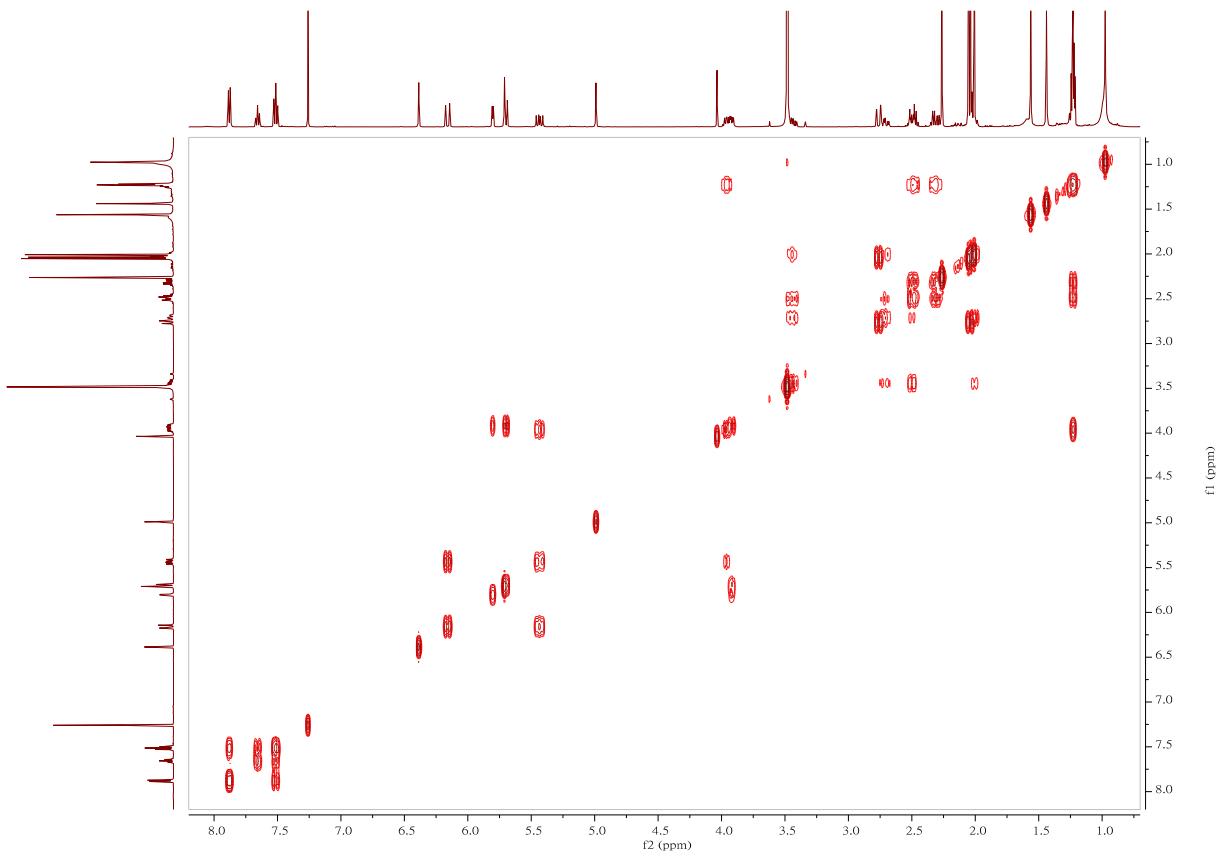


Figure S32. The ^1H - ^1H COSY spectrum of usambariphane D (5).

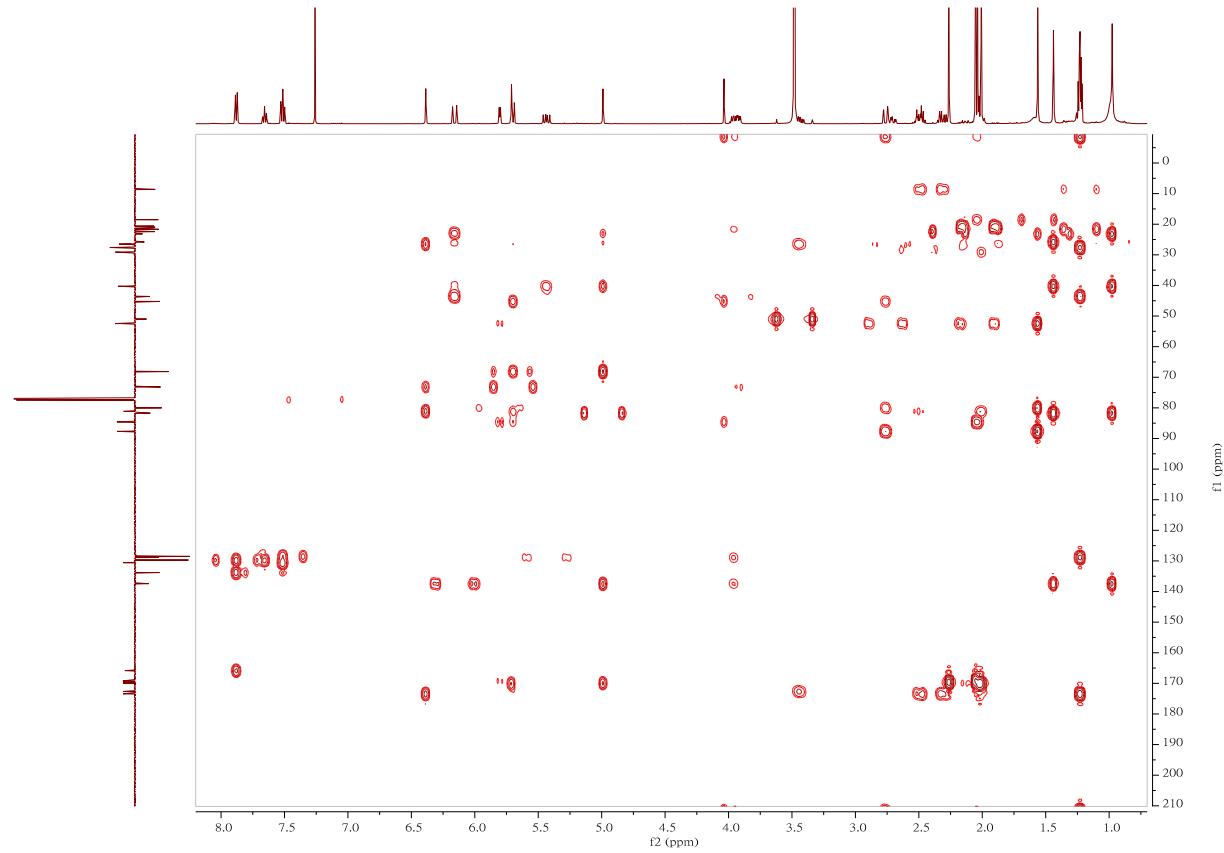


Figure S33. The HMBC spectrum of usambariphane D (5).

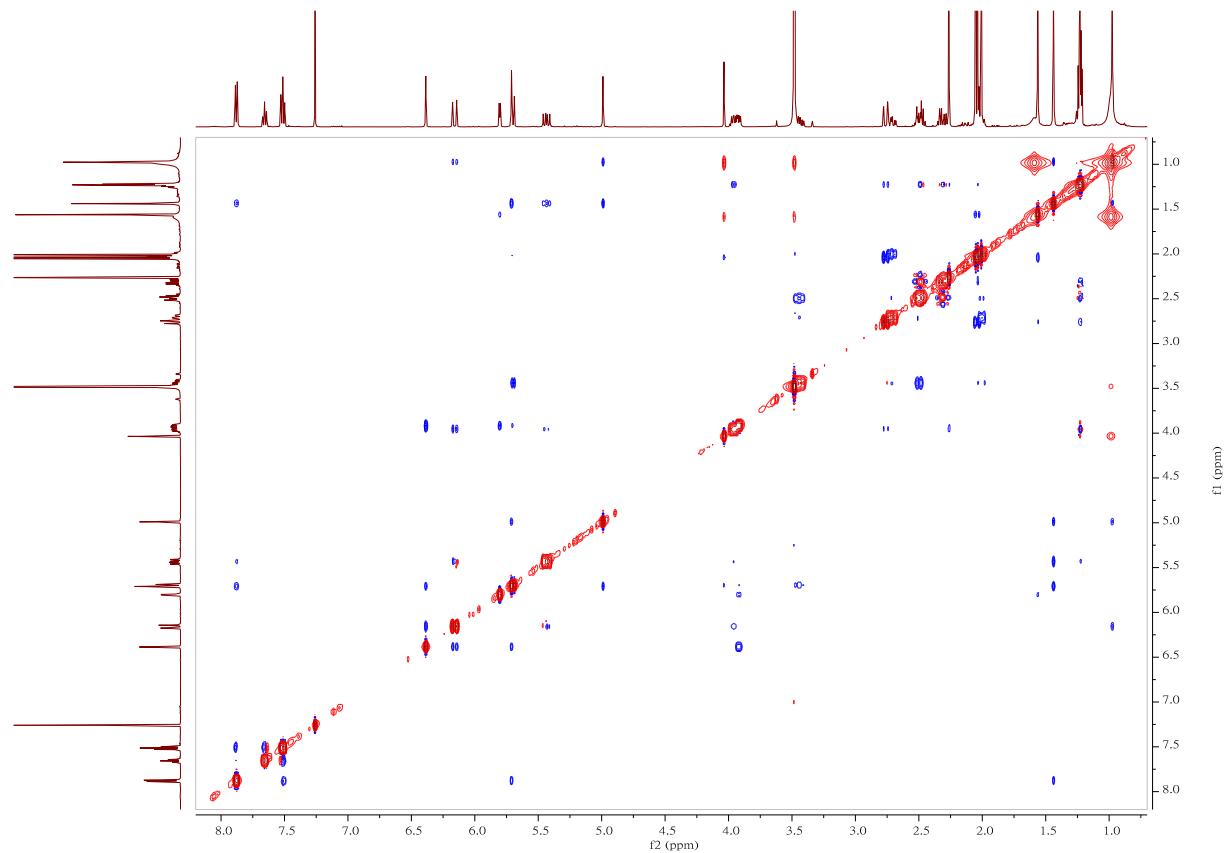
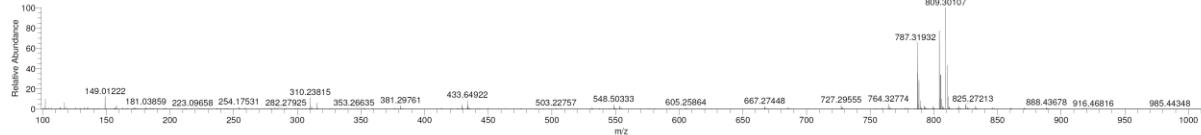


Figure S34. The NOESY spectrum of usambariphane D (5).

1-5, 11-14

YC_20200917 #1743-1769 RT: 8.95-9.08 AV: 25 NL: 1.09E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



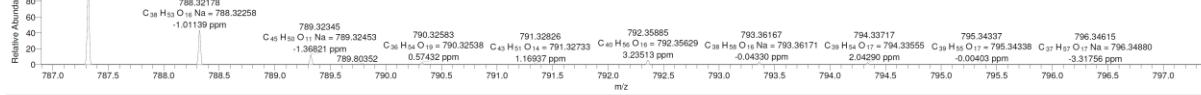
YC_20200917 #1743-1769 RT: 8.95-9.08 AV: 25 NL: 1.09E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

787.31932

 $C_{40}H_{50}O_{10} = 787.31716$

2.74109 ppm



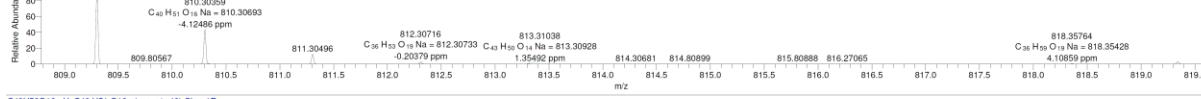
YC_20200917 #1743-1769 RT: 8.95-9.08 AV: 25 NL: 1.09E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

809.30107

 $C_{40}H_{50}O_{10}Na = 809.29911$

2.42864 ppm



C40H50O16 +H: C40H51O16 Na(pgs, s/p=40) Chrg 1R: ...

787.31716

809.29567

788.32057

789.32332

790.32805

791.32868

792.33126

793.33381

794.33634

795.33882

796.34119

797.34335

m/z

Relative Abundance

0 20 40 60 80 100

787.5 788.0 788.5 789.0 789.5 790.0 790.5 791.0 791.5 792.0 792.5 793.0 793.5 794.0 794.5 795.0 795.5 796.0 796.5 797.0

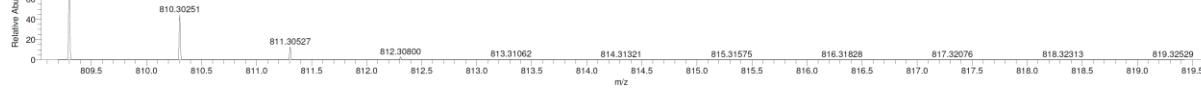


Figure S35. The HR-ESI-MS spectra of usambariphane D (5).

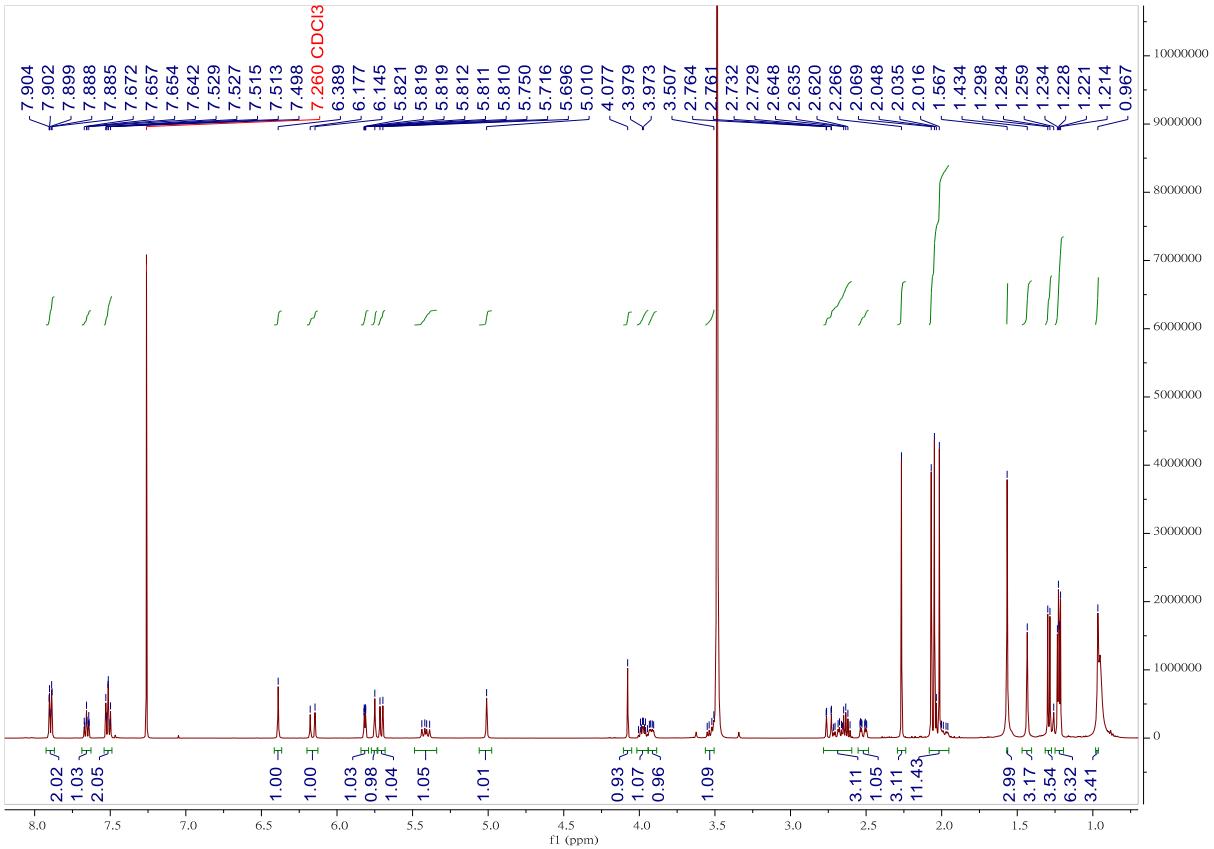


Figure S36. The ^1H -NMR spectrum of usambariphane E (6) (500 MHz, CDCl_3).

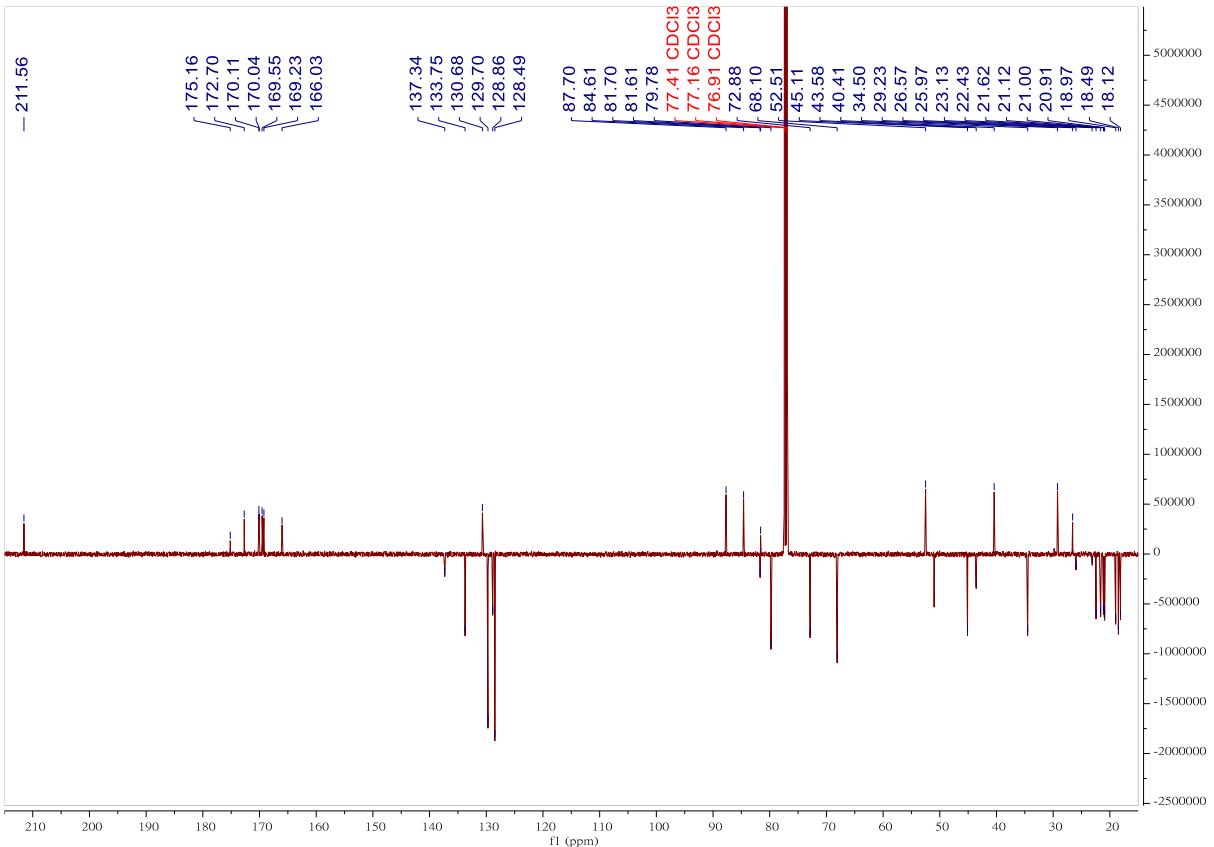


Figure S37. The ^{13}C -JMOD spectrum of usambariphane E (6) (125 MHz, CDCl_3).

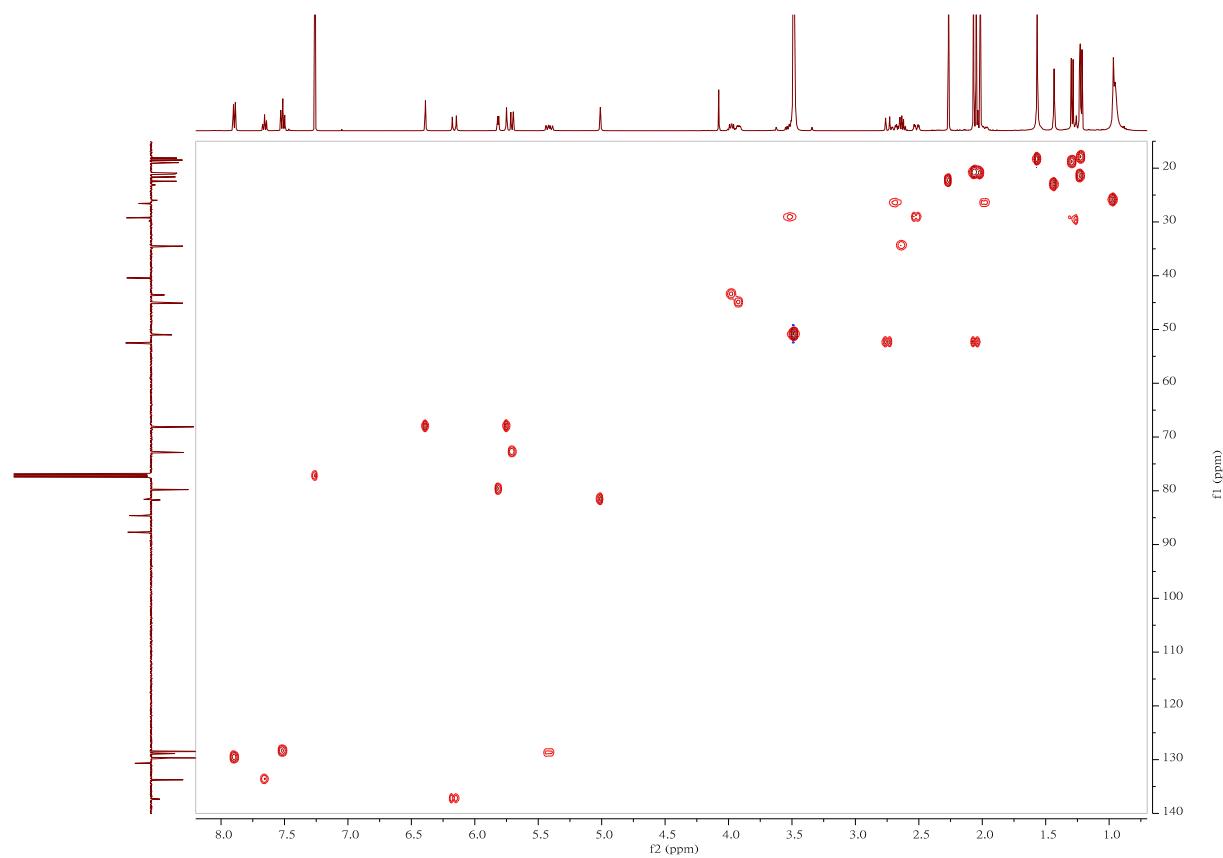


Figure S38. The HSQC spectrum of usambariphane E (6).

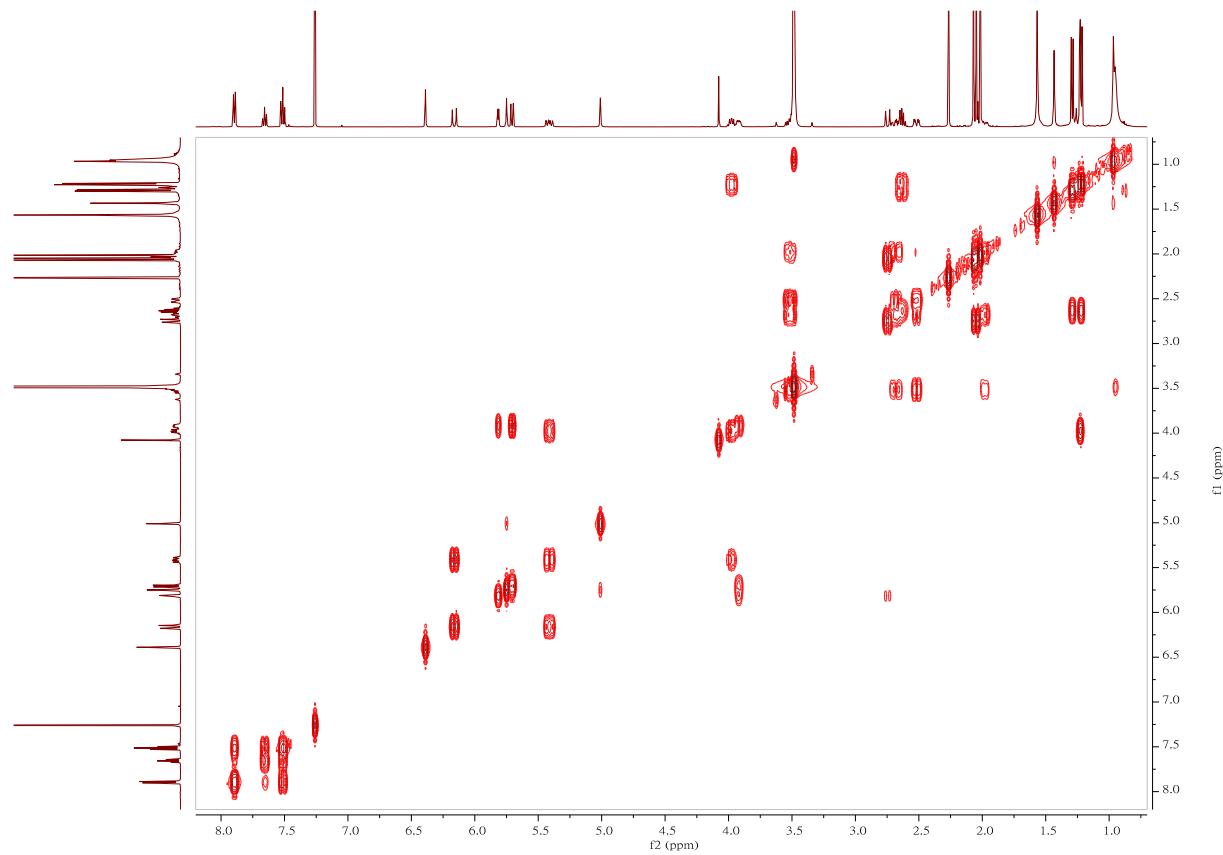


Figure S39. The ^1H - ^1H COSY spectrum of usambariphane E (6).

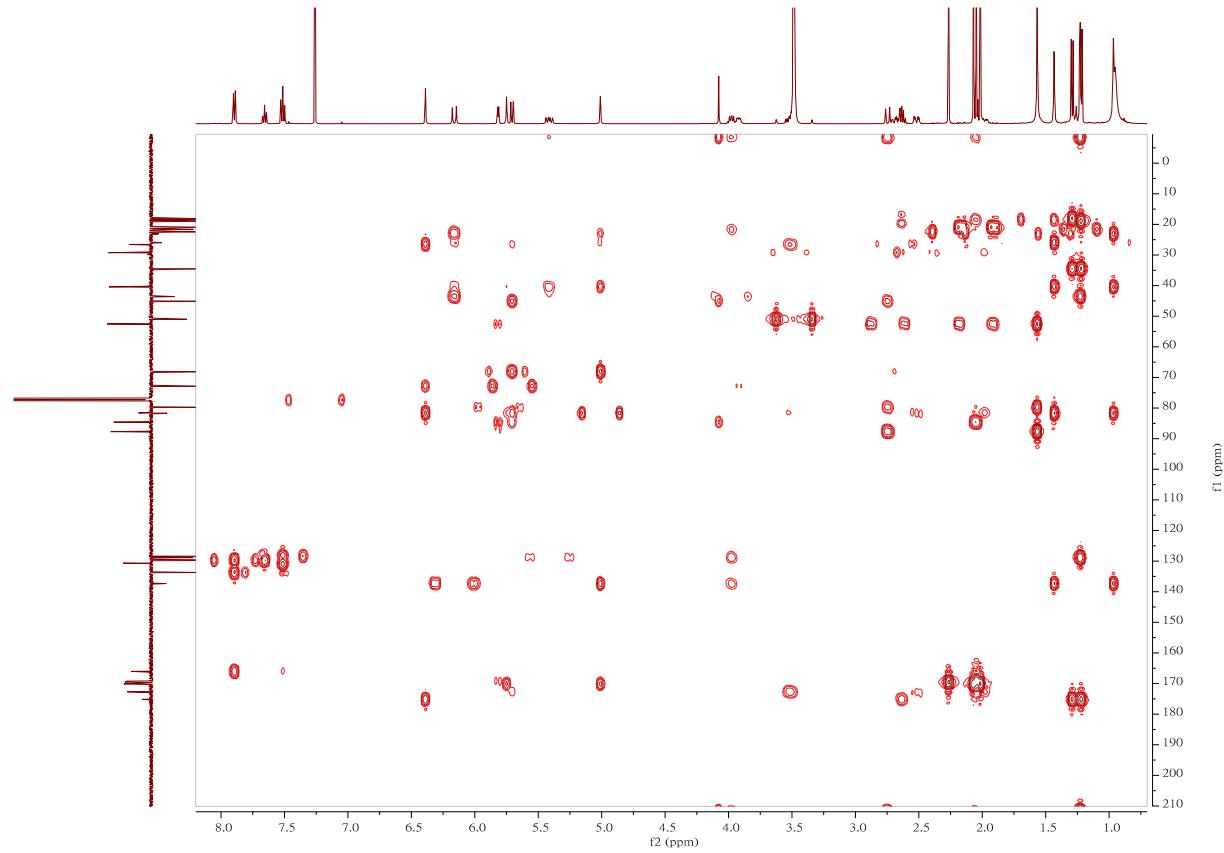


Figure S40. The HMBC spectrum of usambariphane E (6).

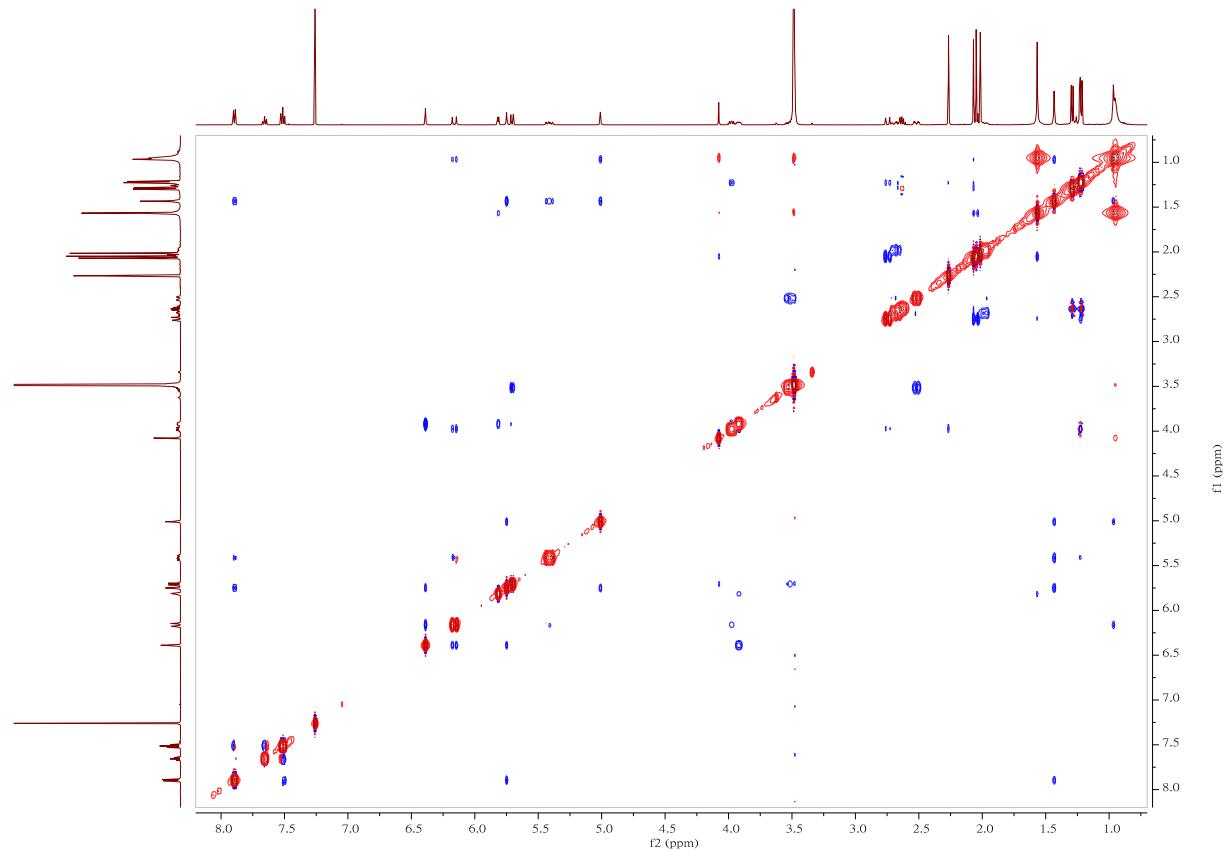
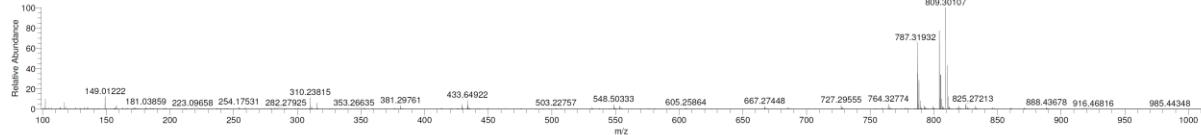


Figure S41. The NOESY spectrum of usambariphane E (6).

1-5, 11-14

YC_20200917 #1743-1769 RT: 8.95-9.08 AV: 25 NL: 1.09E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



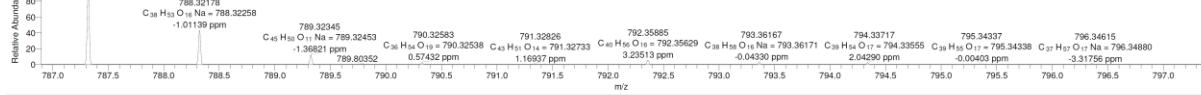
YC_20200917 #1743-1769 RT: 8.95-9.08 AV: 25 NL: 1.09E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

787.31932

C₄₀H₅₀O₁₀ = 787.31716

2.74109 ppm



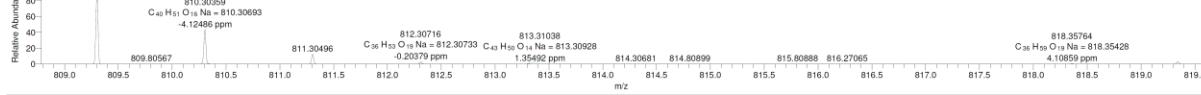
YC_20200917 #1743-1769 RT: 8.95-9.08 AV: 25 NL: 1.09E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

809.30107

C₄₀H₅₀O₁₀ Na+ = 809.29911

2.42864 ppm



C40H50O16 +Na: C40H50O16 Na1 p(gss, s/p=40) Chrg 1R: ...

787.31716

809.30567

788.32057

789.32332

790.32805

791.32868

792.33126

793.33381

794.33634

795.33882

796.34119

797.34335

m/z

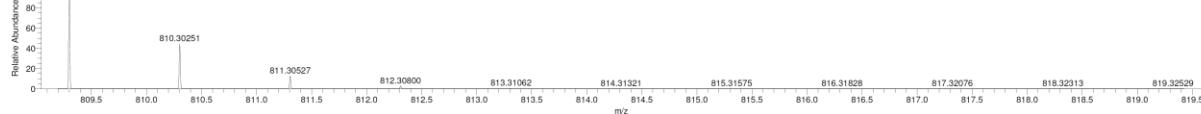


Figure S42. The HR-ESI-MS spectra of usambariphane E (**6**).

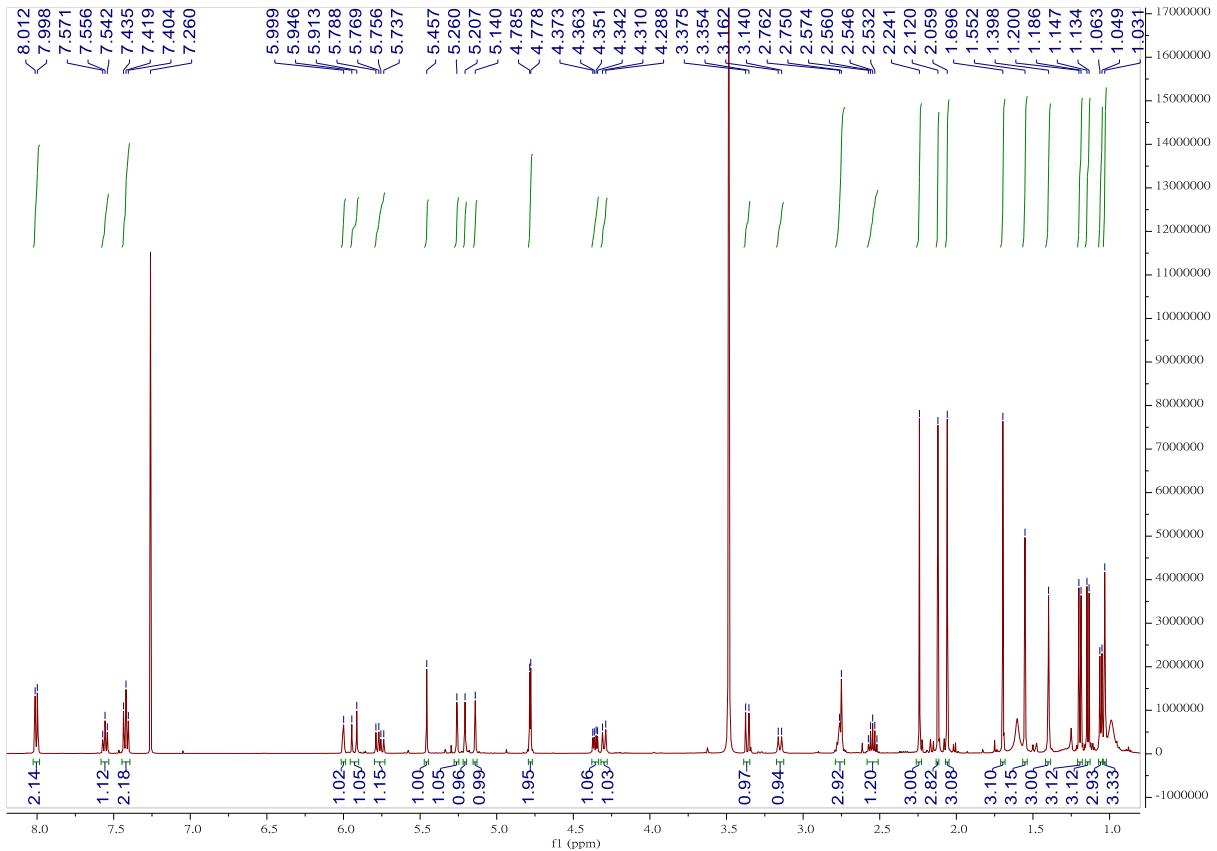


Figure S43. The ¹H-NMR spectrum of usambariphane F (7) (500 MHz, CDCl₃).

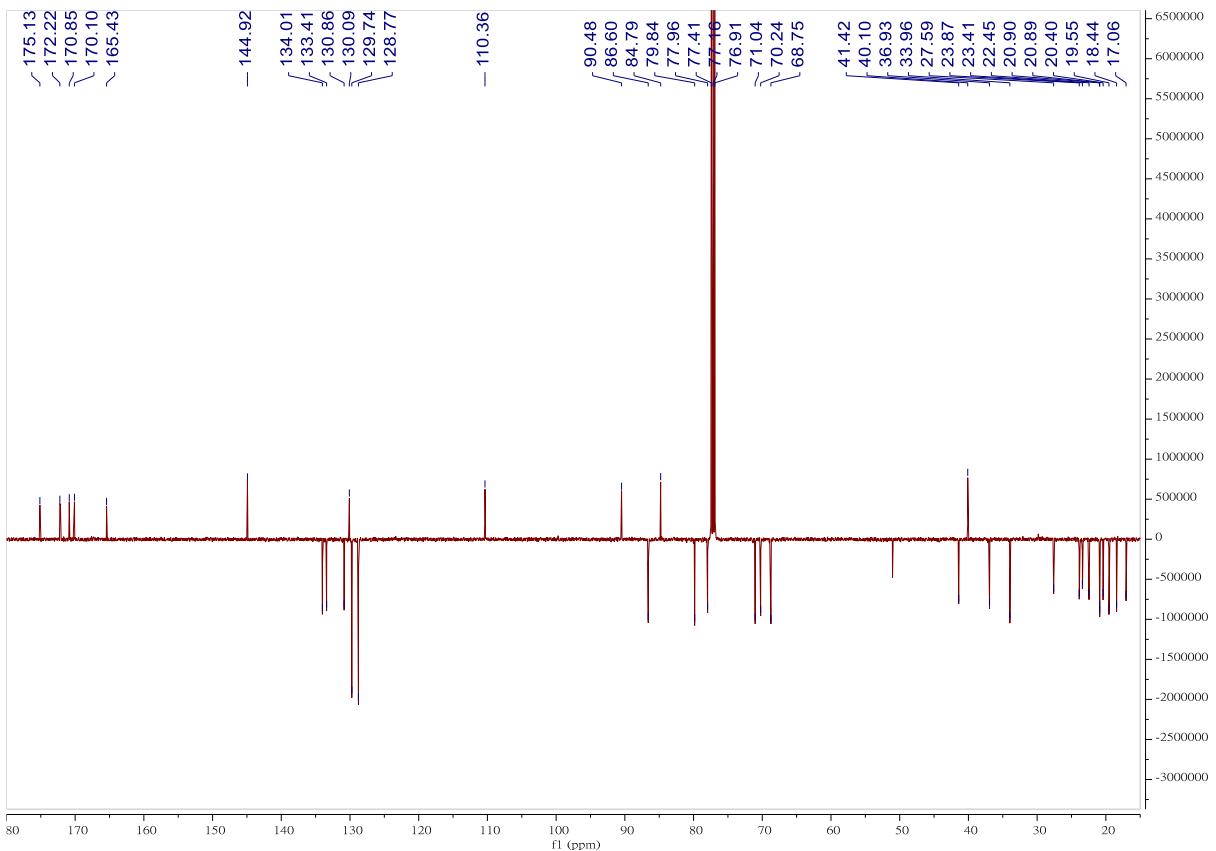


Figure S44. The ¹³C-JMOD spectrum of usambariphane F (7) (125 MHz, CDCl₃).

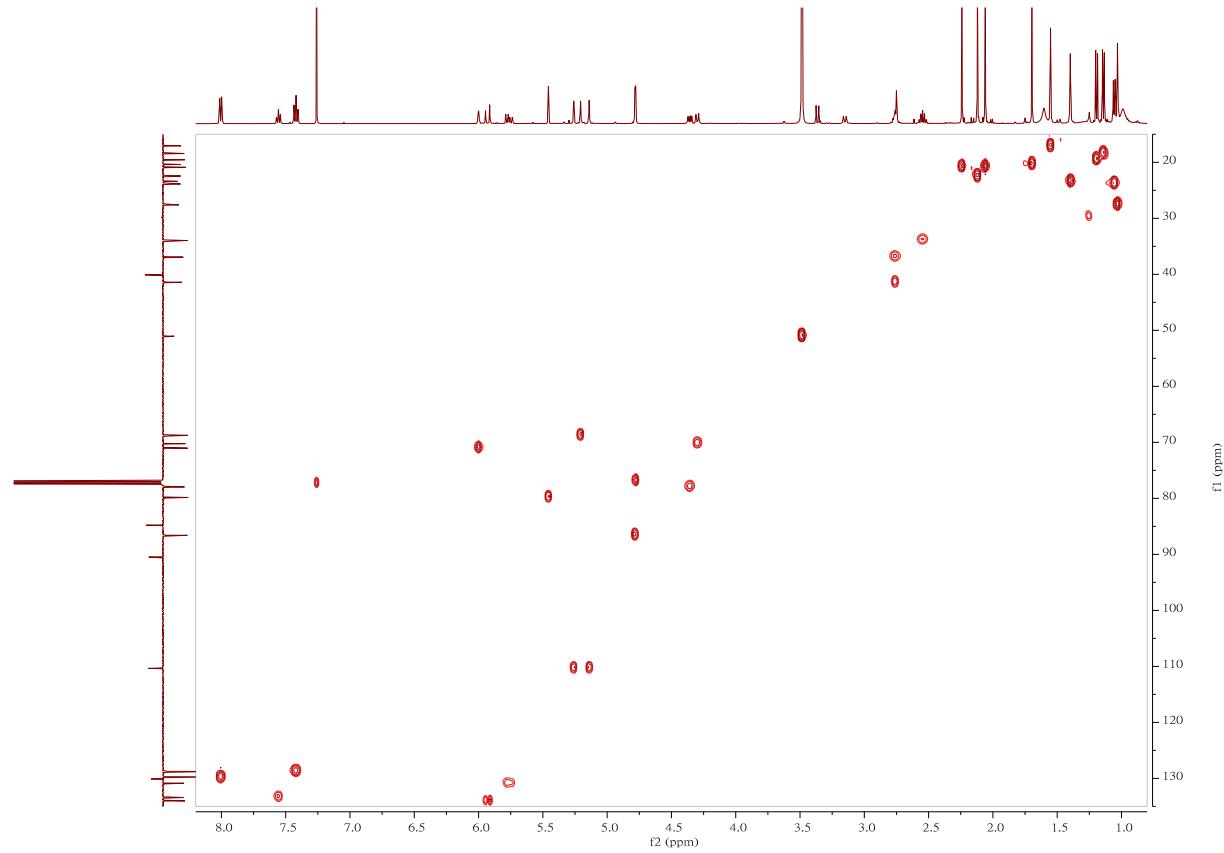


Figure S45. The HSQC spectrum of usambariphane F (7).

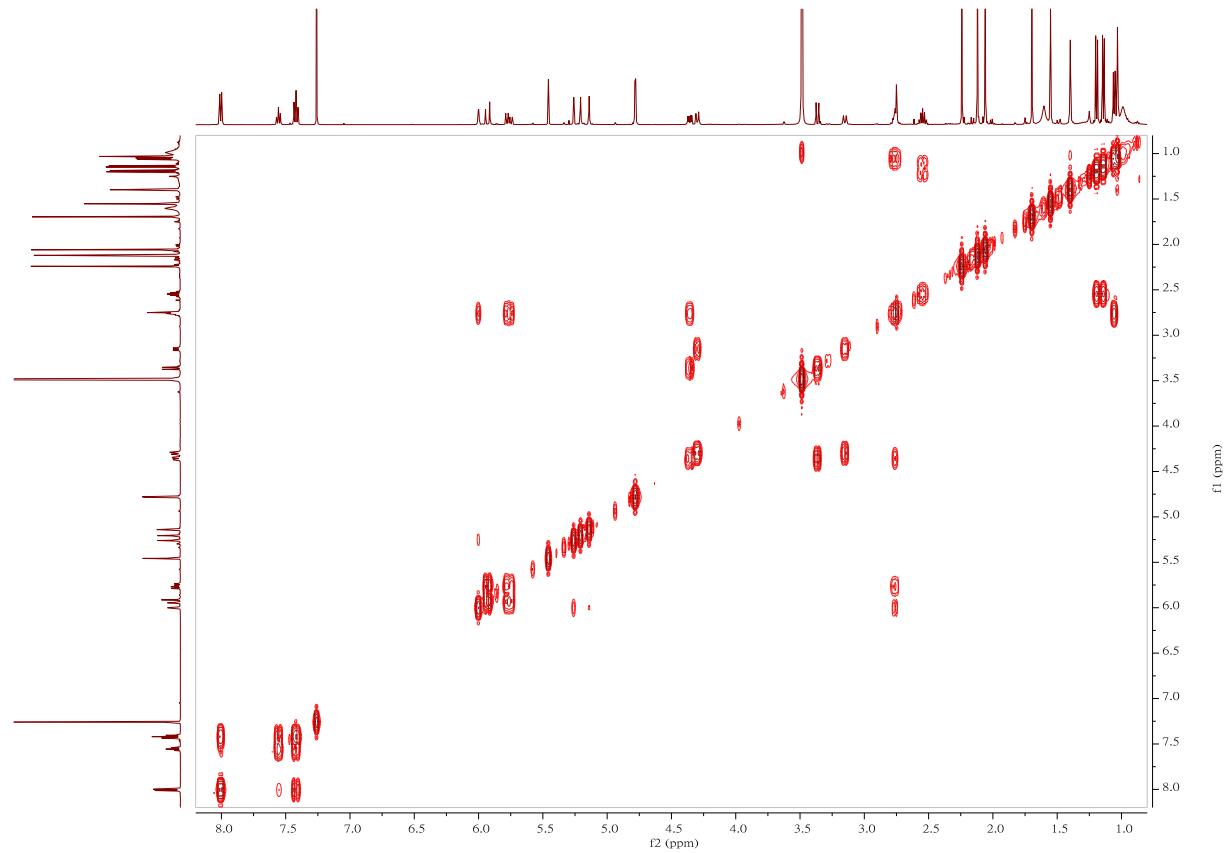


Figure S46. The ¹H-¹H COSY spectrum of usambariphane F (7).

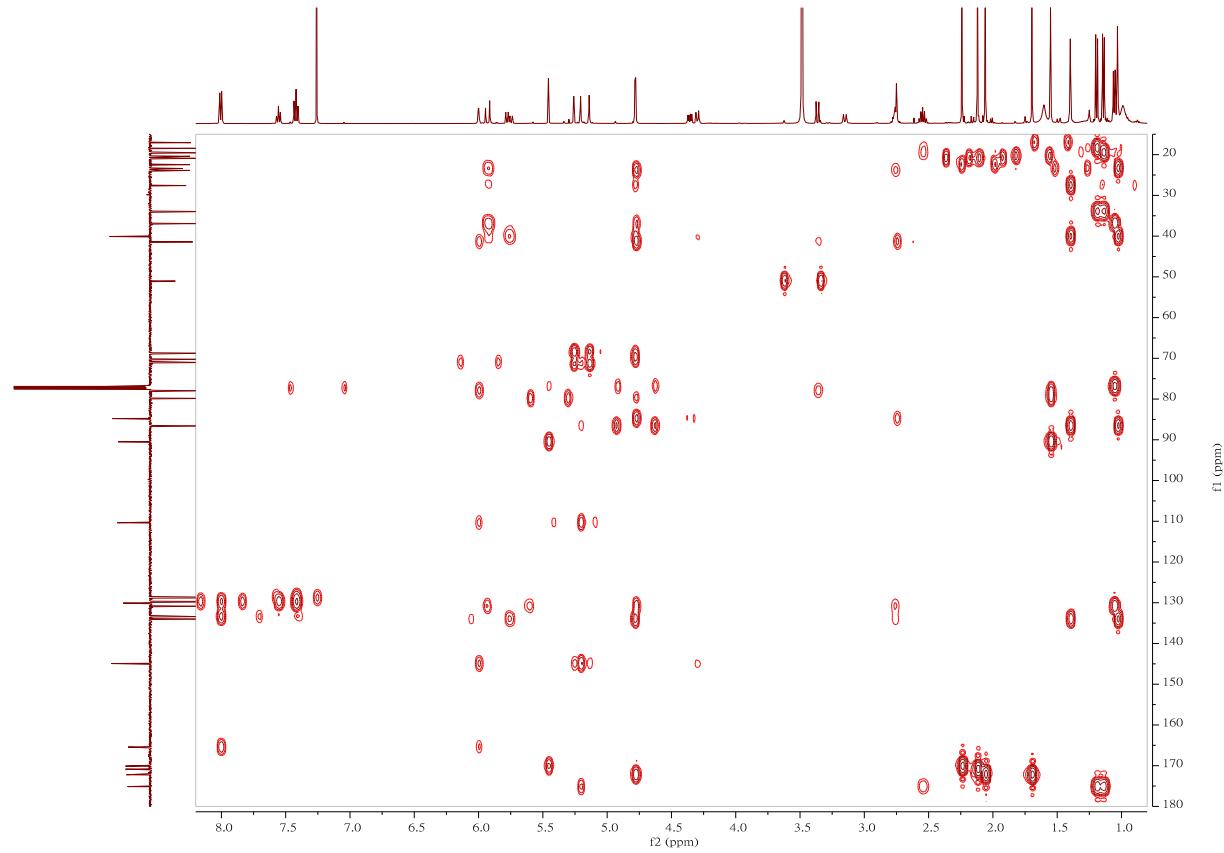


Figure S47. The HMBC spectrum of usambariphane F (7).

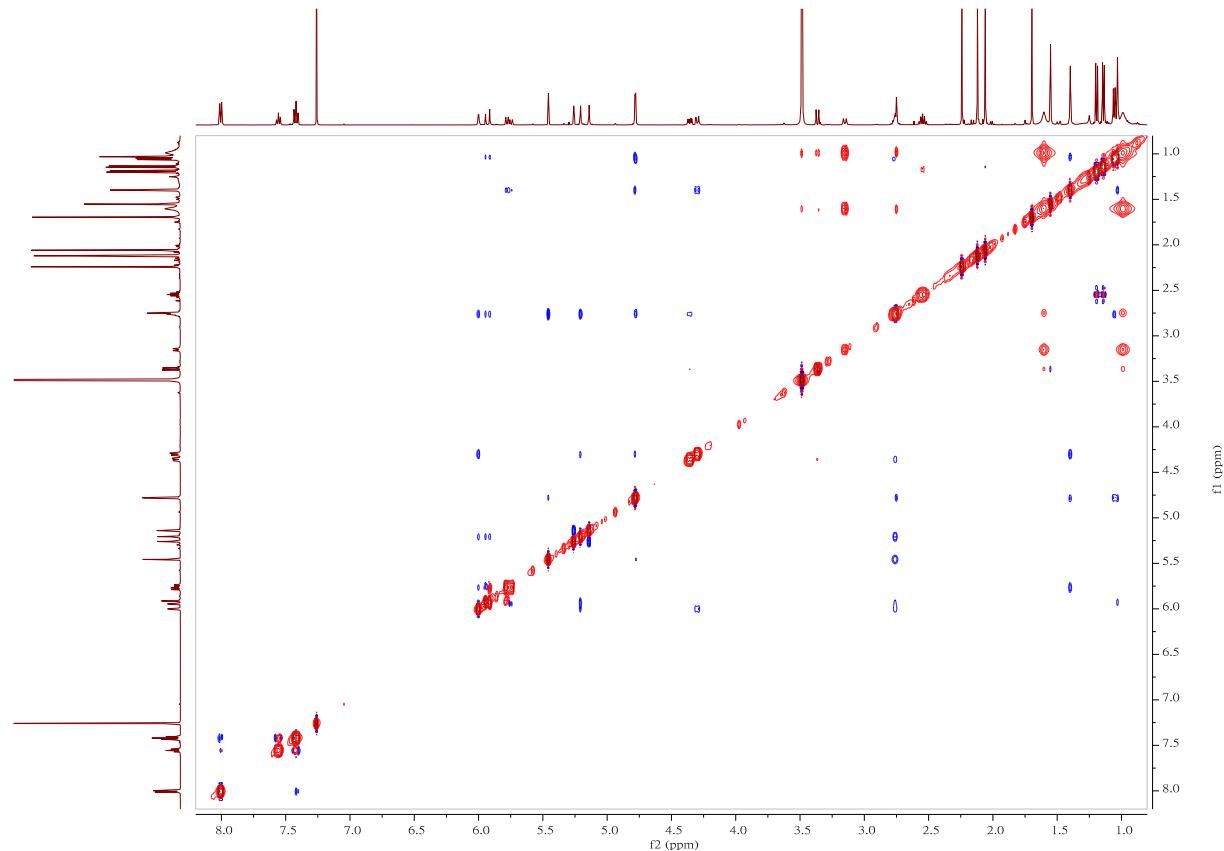
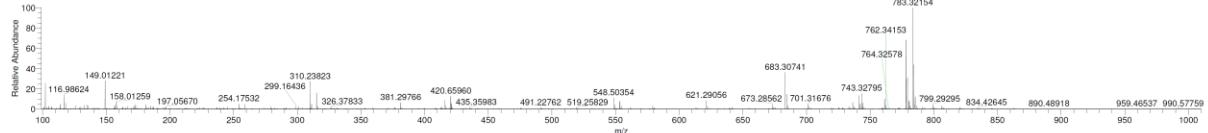


Figure S48. The NOESY spectrum of usambariphane F (7).

1-5, 11-14

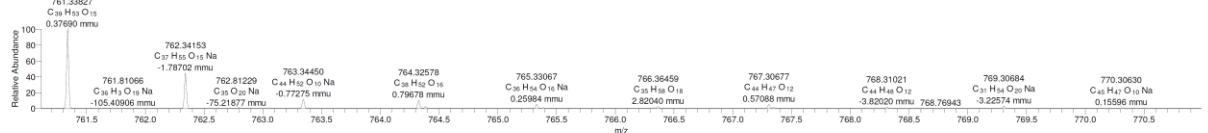
YC-20200917 #1230-1263 RT: 6.31-6.48 AV: 34 NL: 9.05E7

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



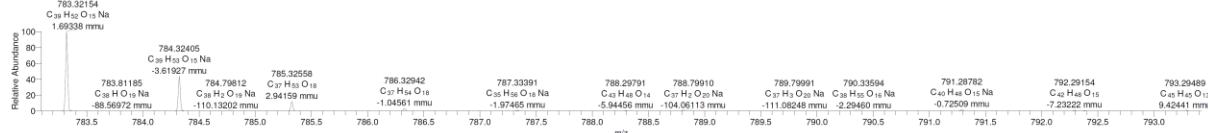
YC-20200917 #1230-1263 RT: 6.31-6.48 AV: 34 NL: 9.19E6

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



YC-20200917 #1230-1263 RT: 6.31-6.48 AV: 34 NL: 9.05E7

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



C39H52O15 +H; C39H53O15 p(gss, s/p=40) Chrg 1R; ...

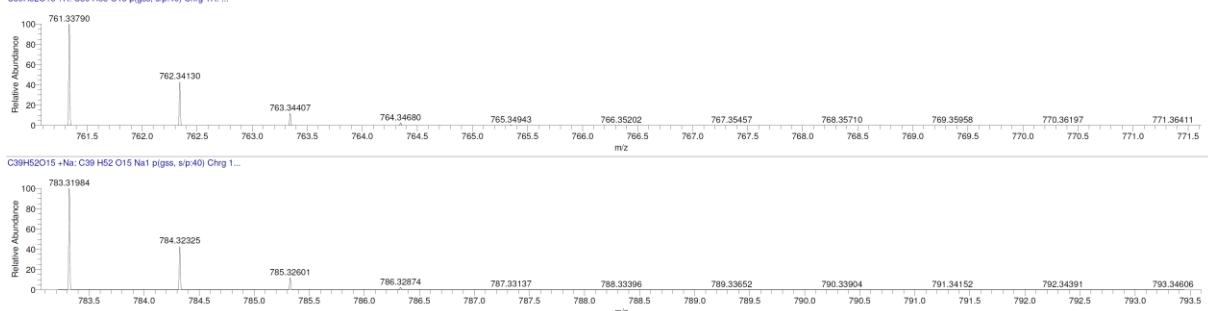


Figure S49. The HR-ESI-MS spectra of usambariphane F (7).

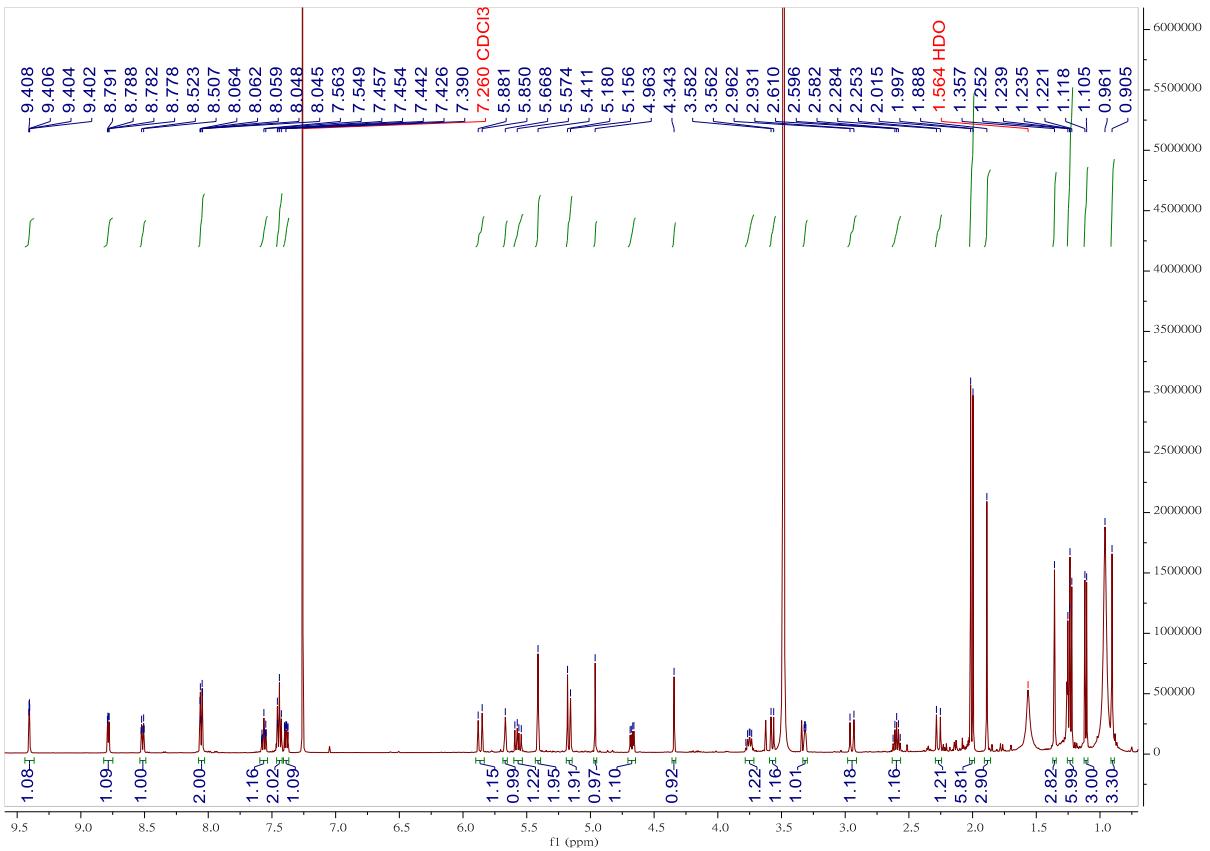


Figure S50. The ^1H -NMR spectrum of usambariphane G (8) (500 MHz, CDCl_3).

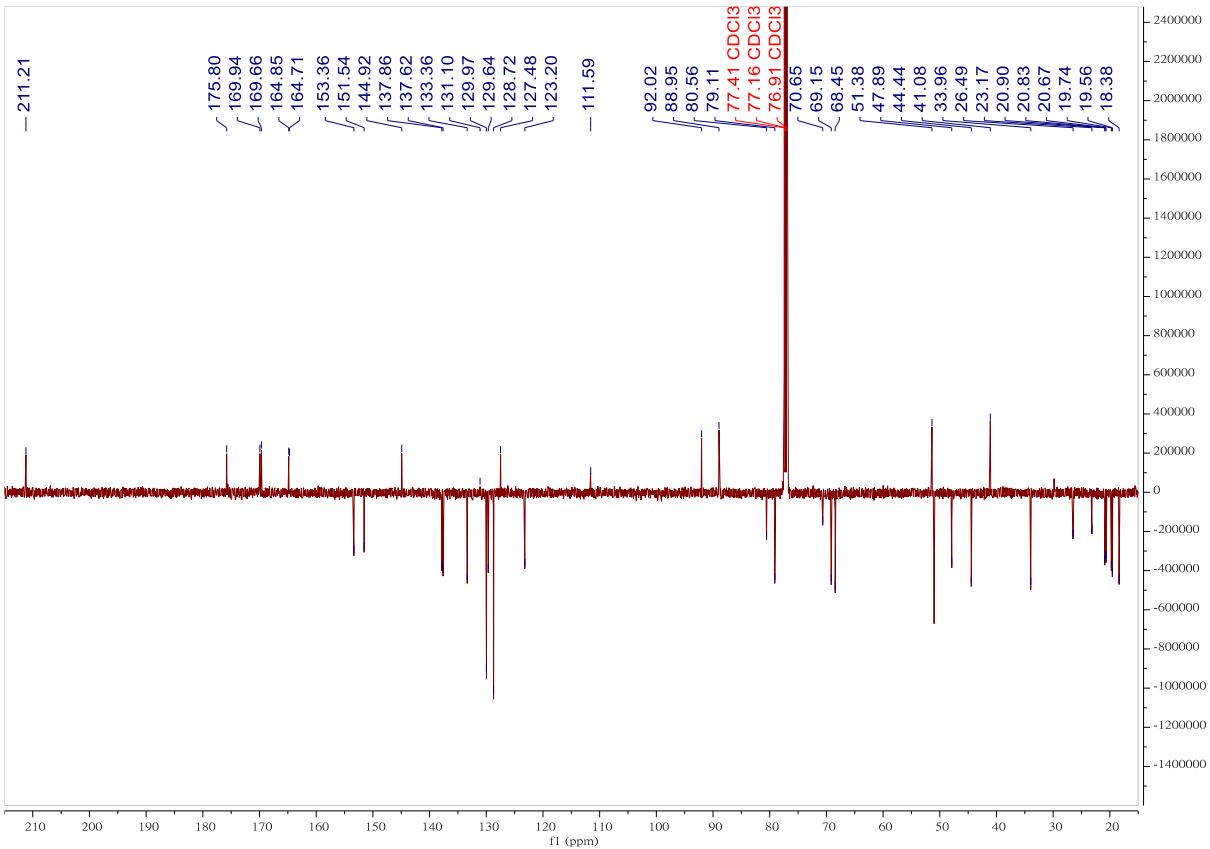


Figure S51. The ^{13}C -JMOD spectrum of usambariphane G (8) (125 MHz, CDCl_3).

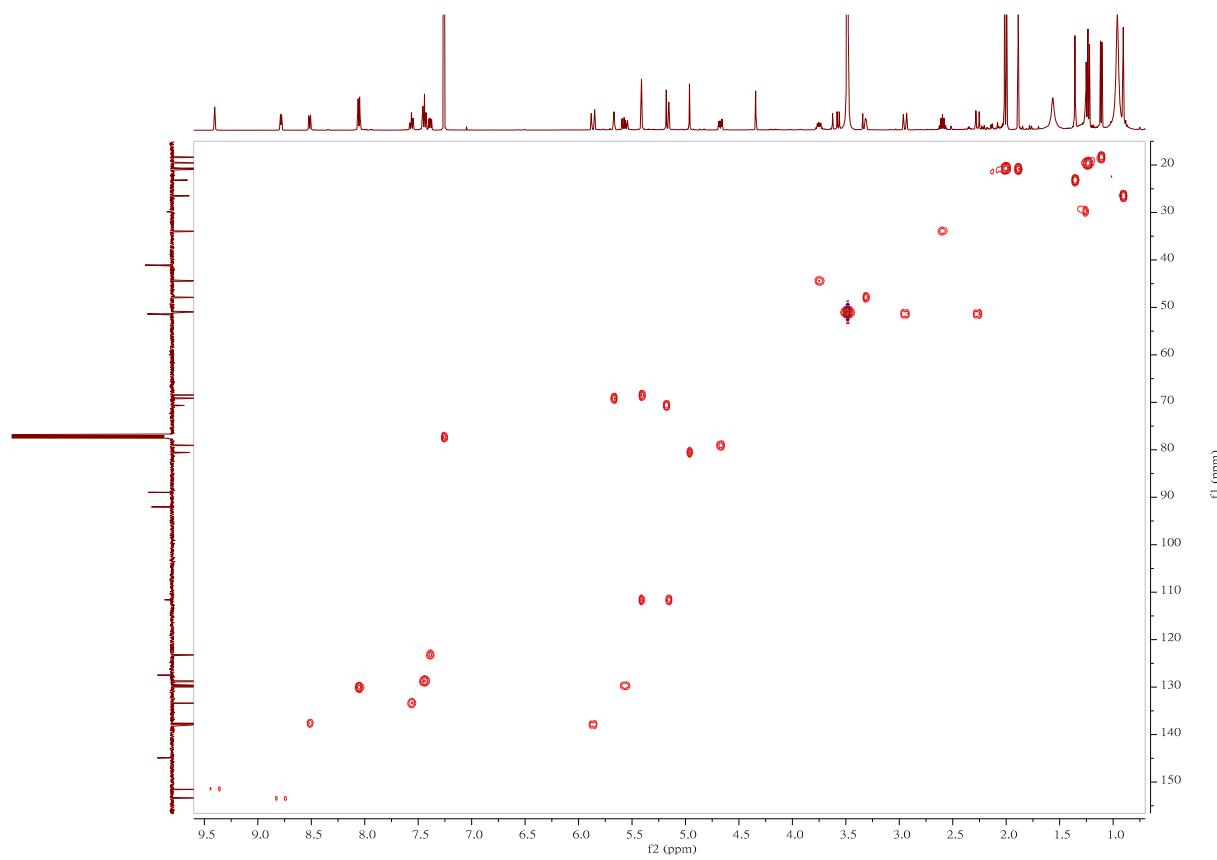


Figure S52. The HSQC spectrum of usambariphane G (8).

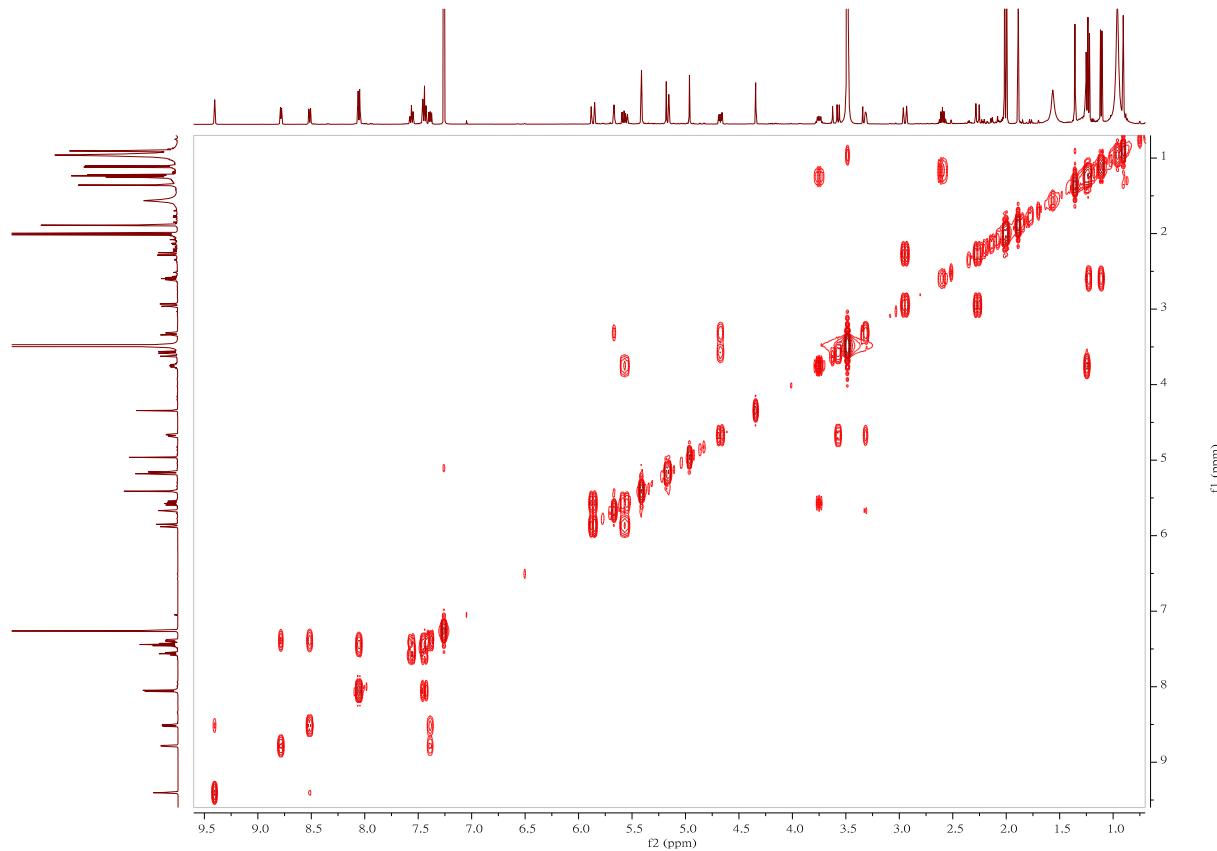


Figure S53. The ¹H-¹H COSY spectrum of usambariphane G (8).

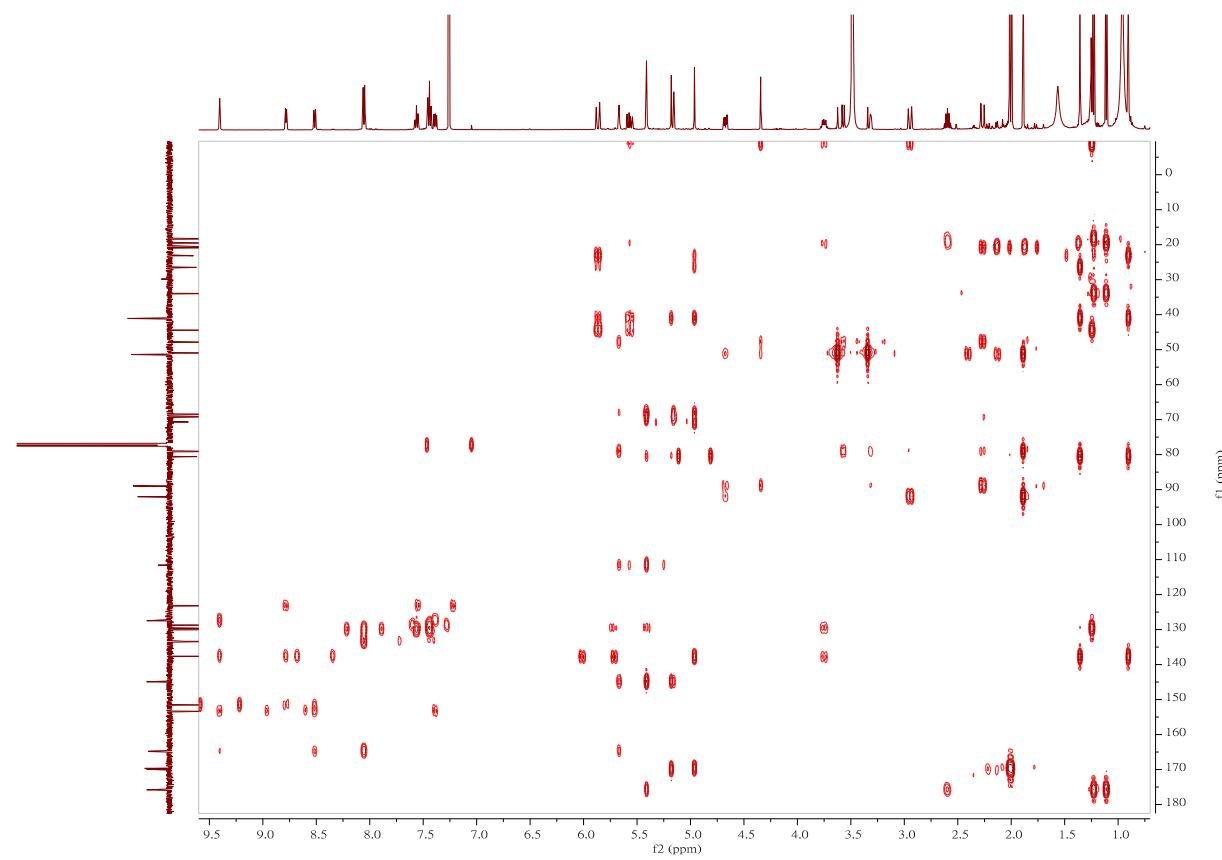


Figure S54. The HMBC spectrum of usambariphane G (8).

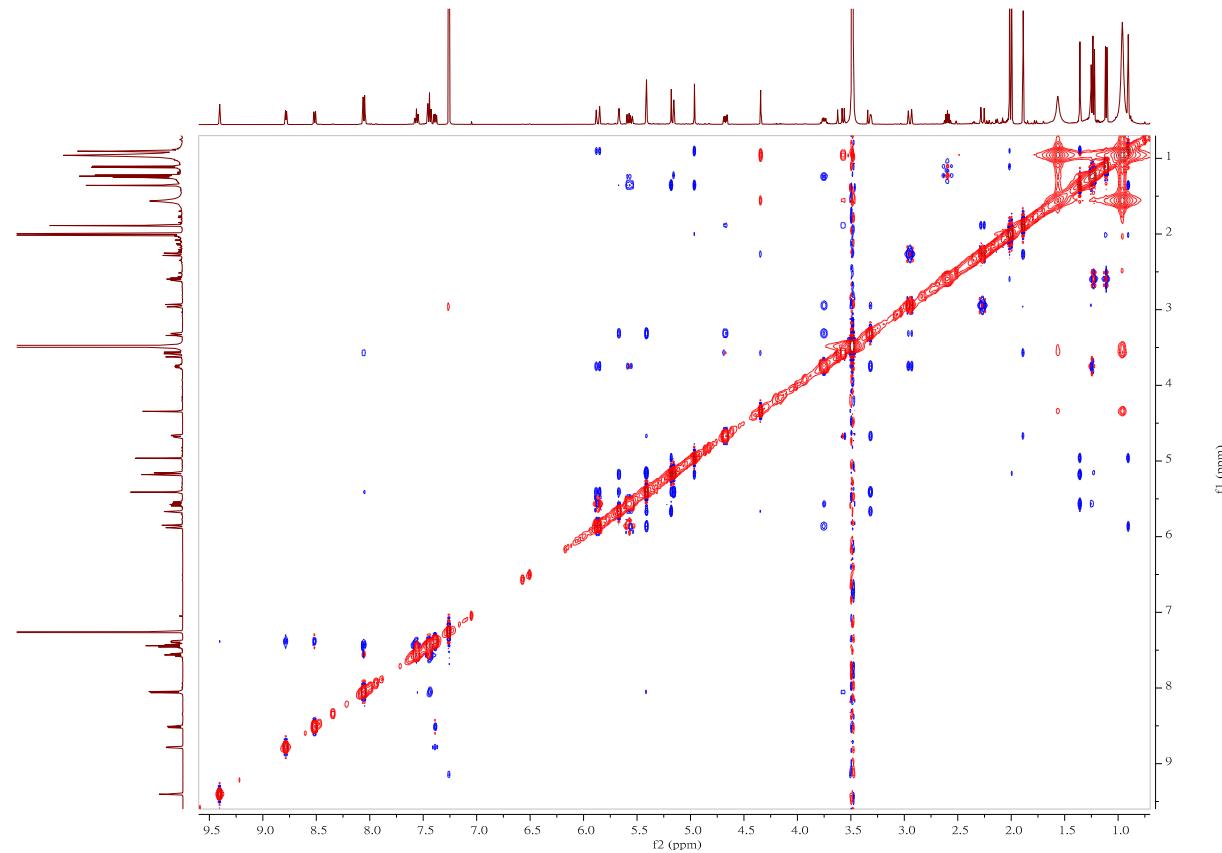
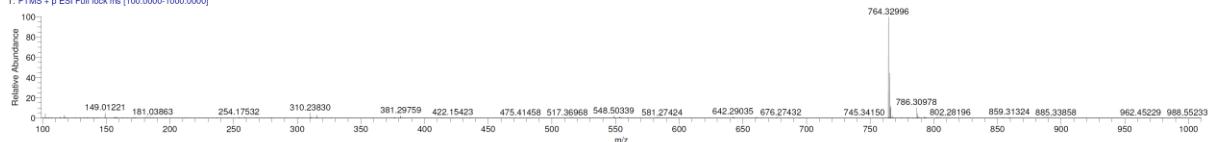
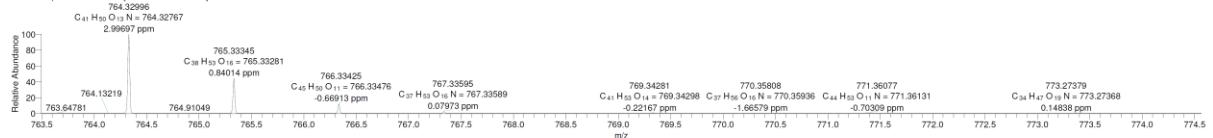


Figure S55. The NOESY spectrum of usambariphane G (8).

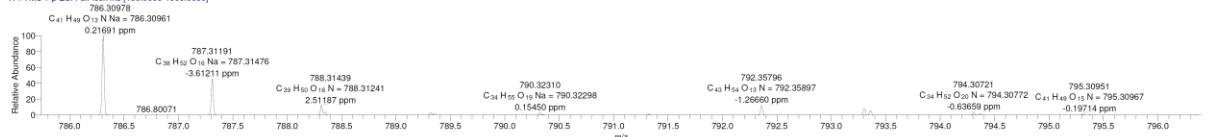
1-5, 11-14
 YC_20200917 #2034-2078 RT: 10.45-10.67 AV: 45 NL: 4.73E8
 T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



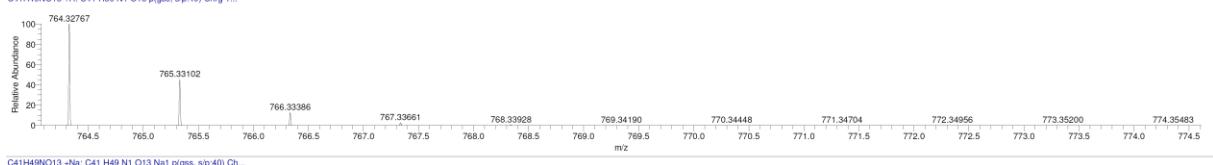
YC_20200917 #2034-2078 RT: 10.45-10.67 AV: 45 NL: 4.73E8
 T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



YC_20200917 #2034-2078 RT: 10.45-10.67 AV: 45 NL: 4.73E8
 T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



C41H49NO13 +H; C41H50N1 O13 p(gss, s/p:40) Chrg 1...



C41H49NO13 +Na; C41H49N1 O13 Na1 p(gss, s/p:40) Ch...

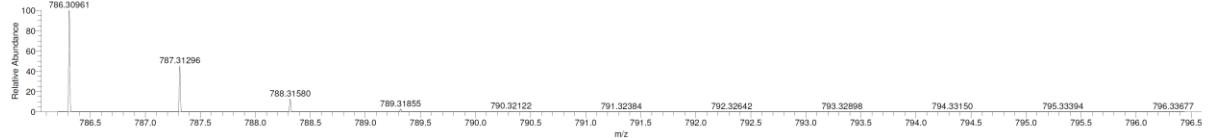


Figure S56. The HR-ESI-MS spectra of usambariphane G (8).

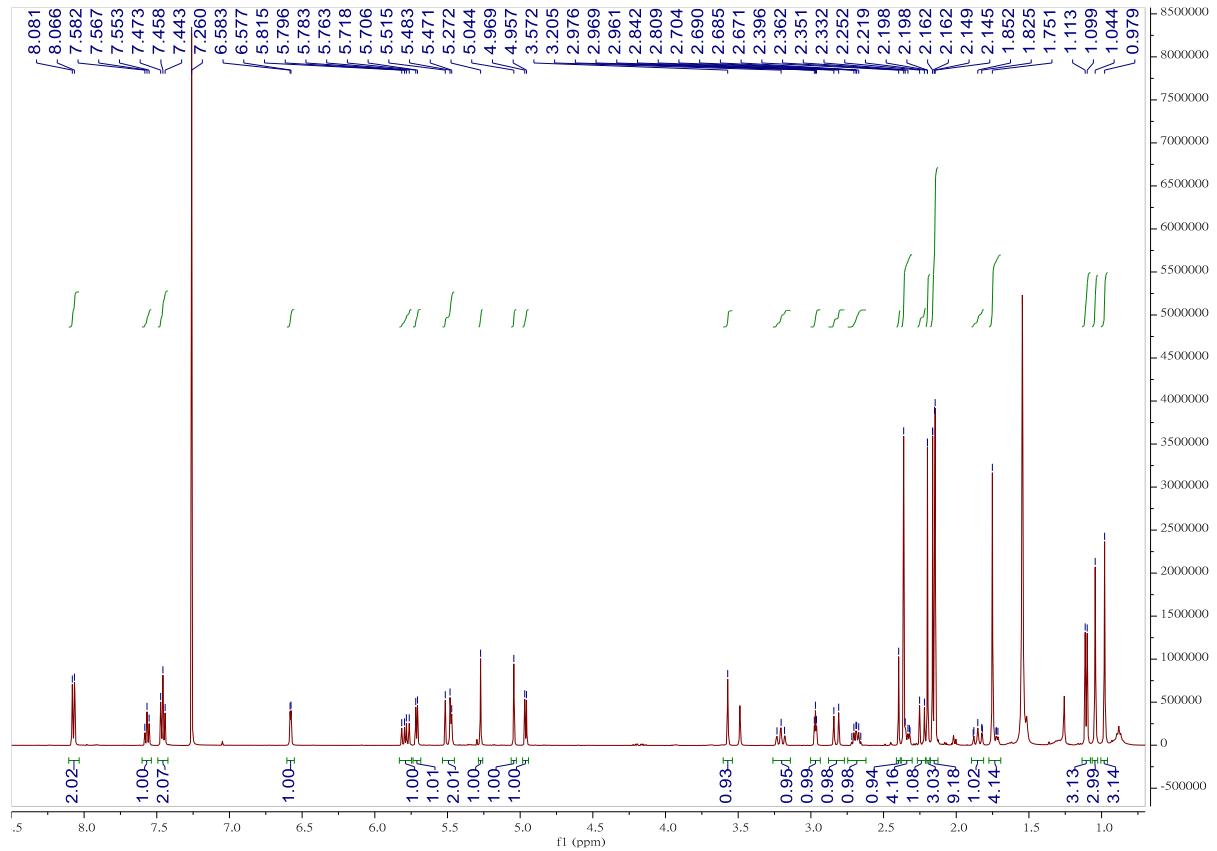


Figure S57. The ^1H -NMR spectrum of isoterracinolide C (9) (500 MHz, CDCl_3).

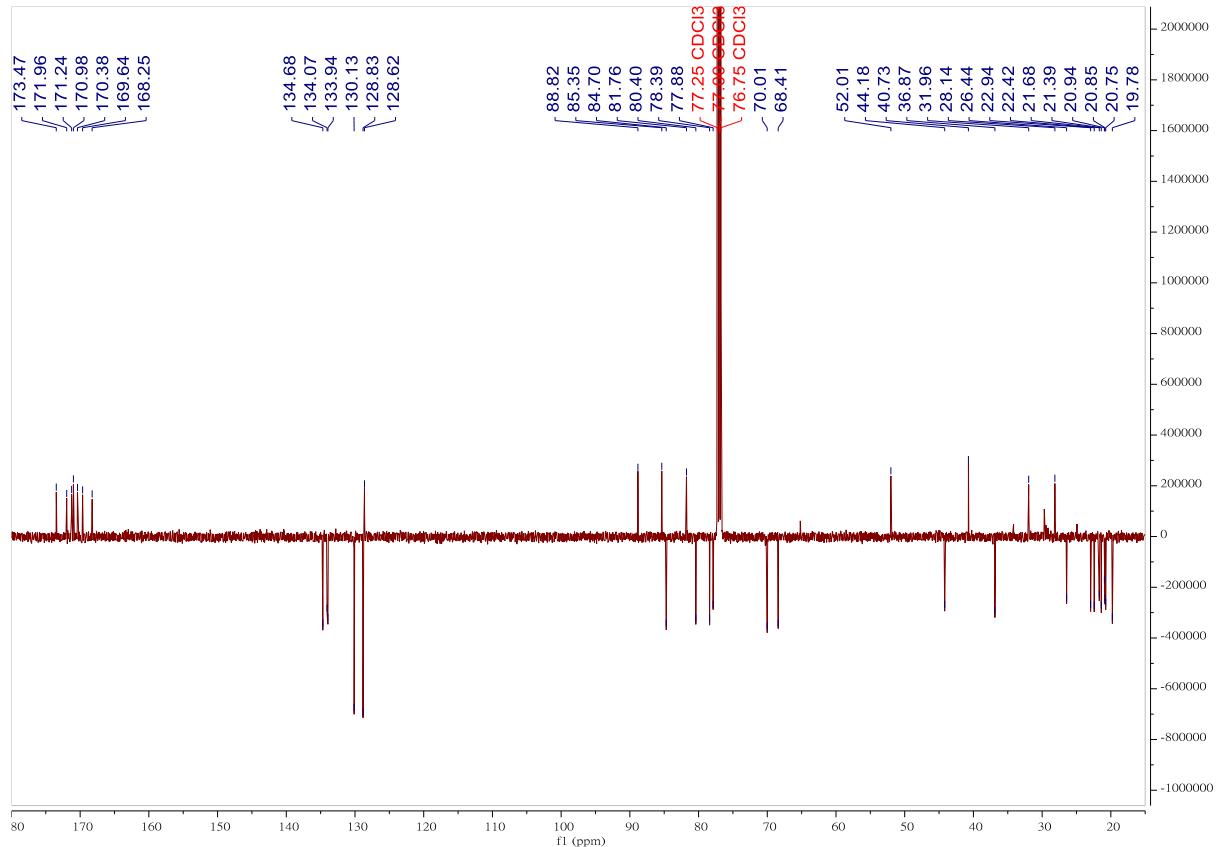


Figure S58. The ^{13}C -JMOD spectrum of isoterracinolide C (9) (500 MHz, CDCl_3).

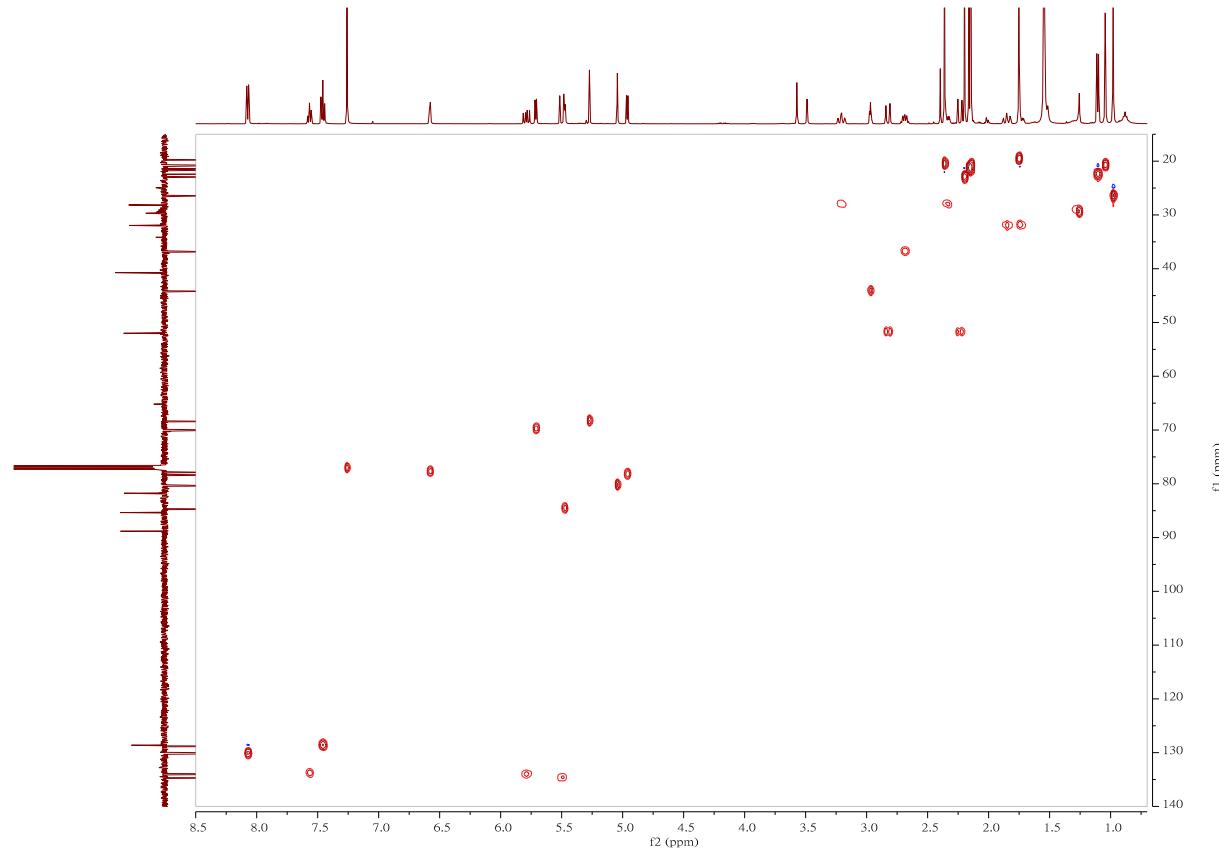


Figure S59. The HSQC spectrum of isoterracinolide C (9).

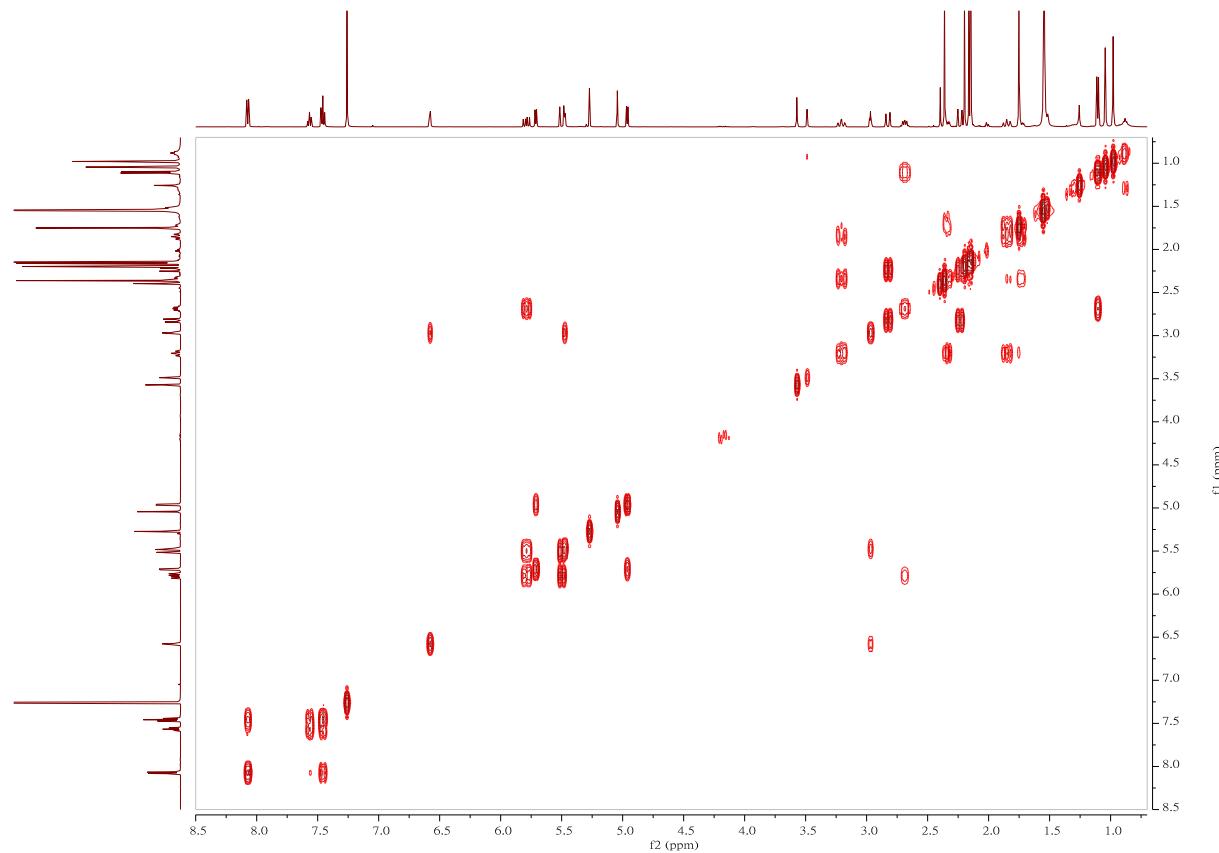


Figure S60. The ^1H - ^1H COSY spectrum of isoterracinolide C (9).

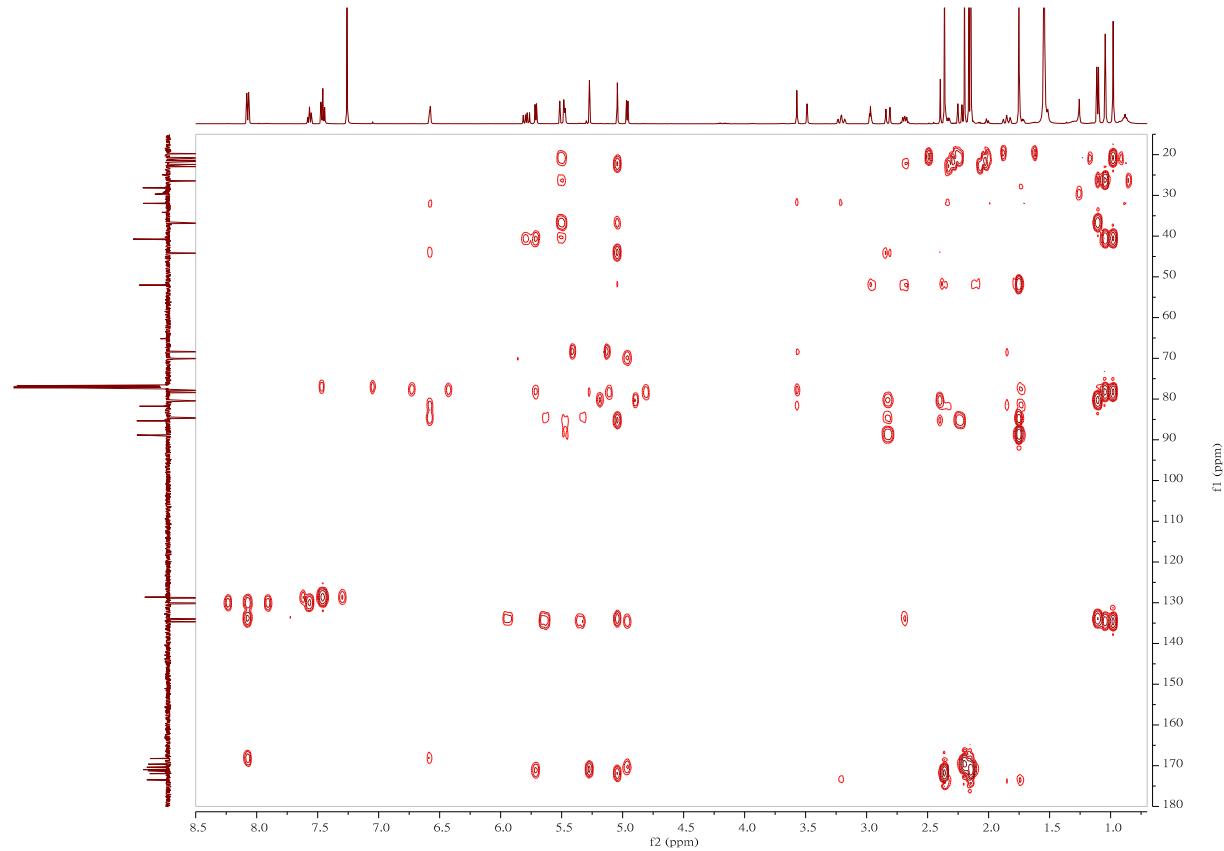


Figure S61. The HMBC spectrum of isoterracinolide C (9).

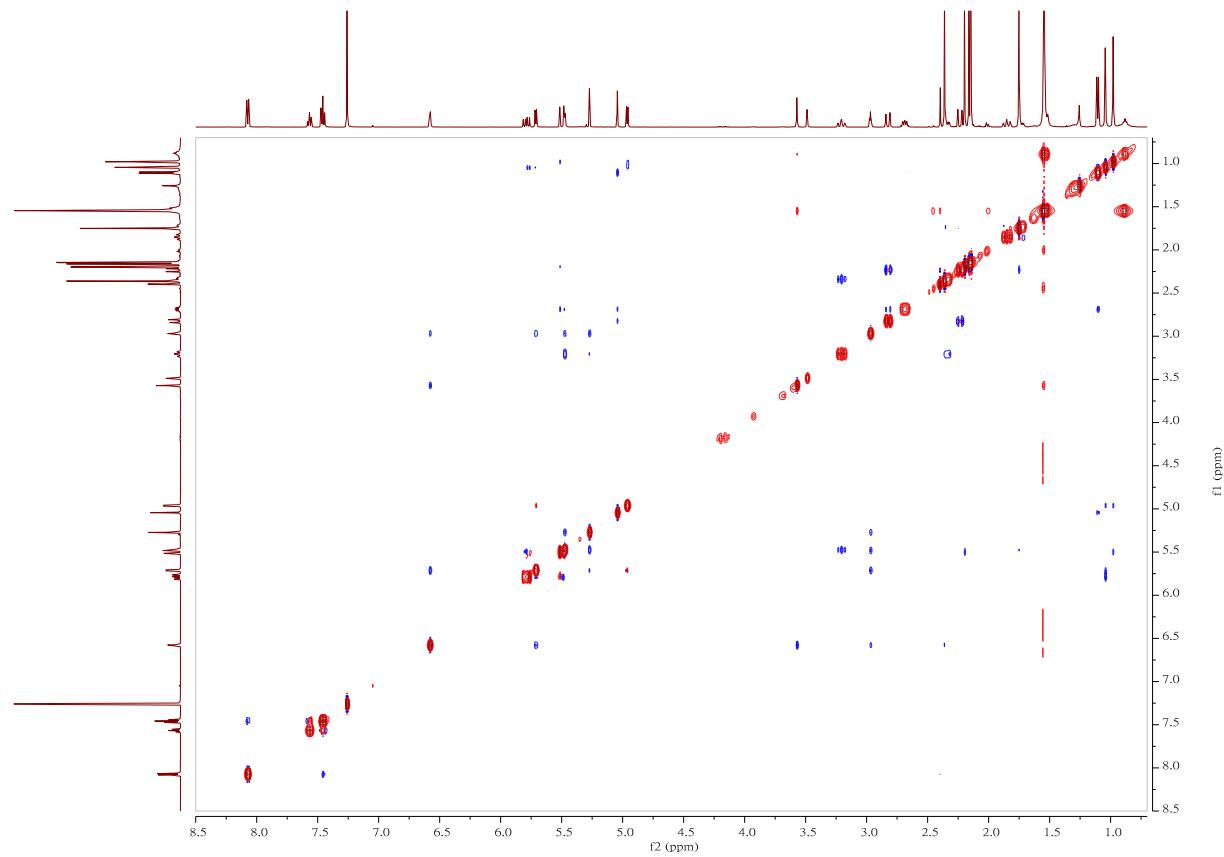
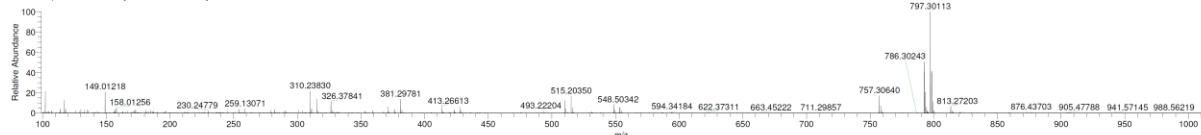


Figure S62. The NOESY spectrum of isoterracinolide C (9).

YC_20200917 #3245-3285 RT: 16.67-16.87 AV: 41 NL: 1.26E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

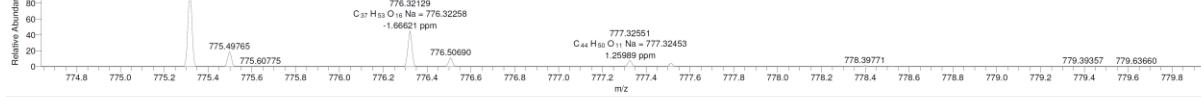


YC_20200917 #3245-3285 RT: 16.67-16.87 AV: 41 NL: 7.04E5

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

775.31721
C₃₉H₅₁O₁₆ Na = 775.31716

0.59565 ppm

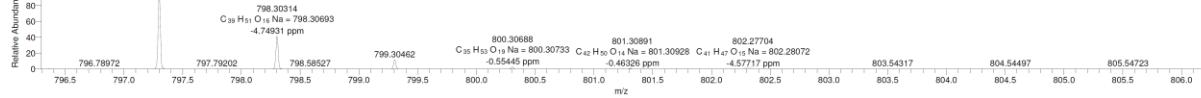


YC_20200917 #3245-3285 RT: 16.67-16.87 AV: 41 NL: 1.26E8

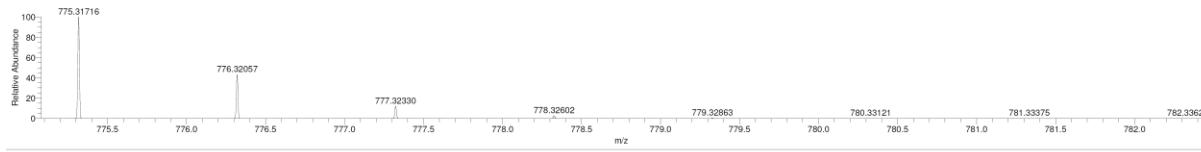
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

797.30113
C₃₉H₅₁O₁₆ Na = 797.29911

2.53207 ppm



C39H50O16 +Na: C39 H50 O16 Na1 (pigg, s/p:40) Chrg 1R: ...



C39H50O16 +Na: C39 H50 O16 Na1 (pigg, s/p:40) Chrg 1...:

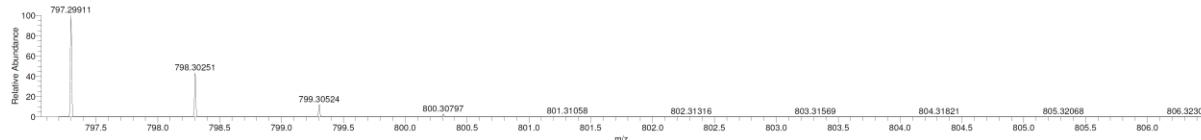


Figure S63. The HR-ESI-MS spectra of isoterracinolide C (9).

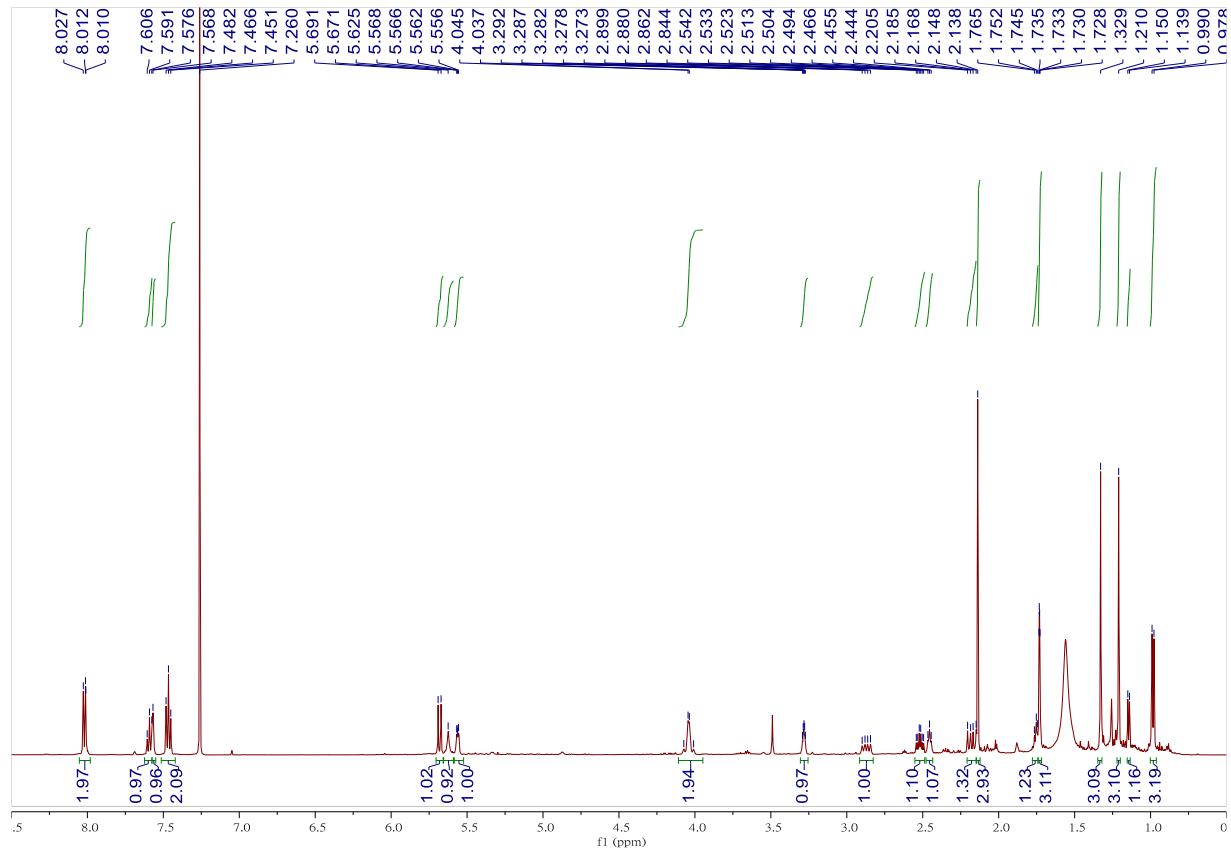


Figure S64. The ^1H -NMR spectrum of 4β -crotignoid K (**14**) (500 MHz, CDCl_3).

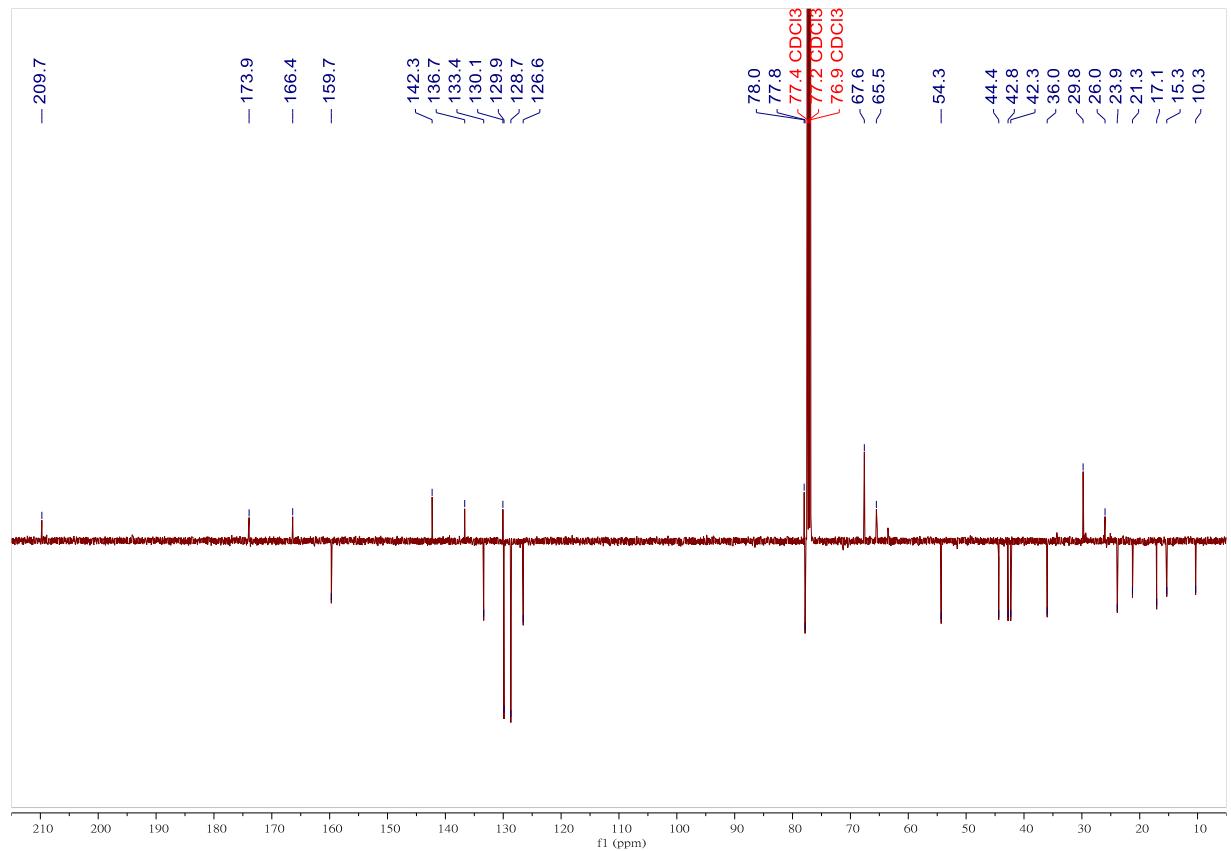


Figure S65. The ^{13}C -JMOD spectrum of 4β -crotignoid K (**14**) (125 MHz, CDCl_3).

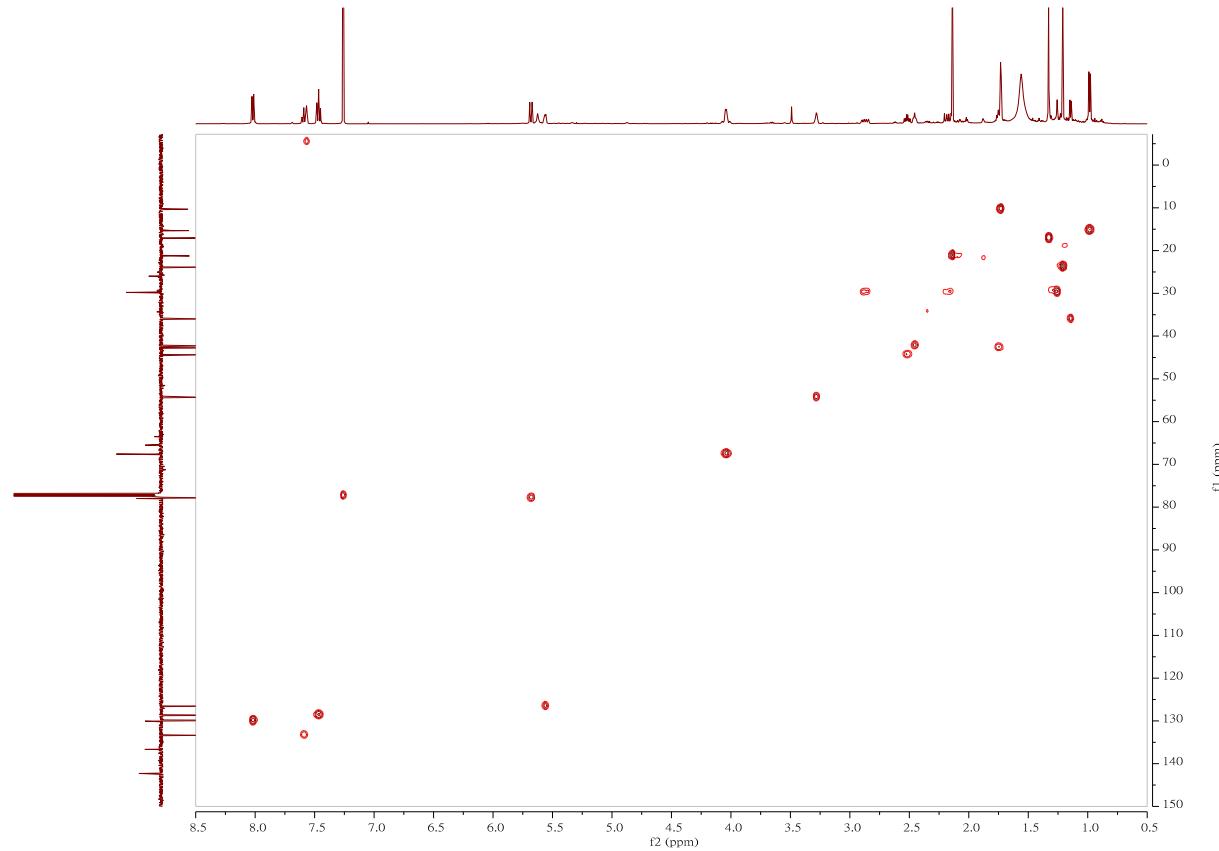


Figure S66. The HSQC spectrum of 4β -crotignoid K (**14**).

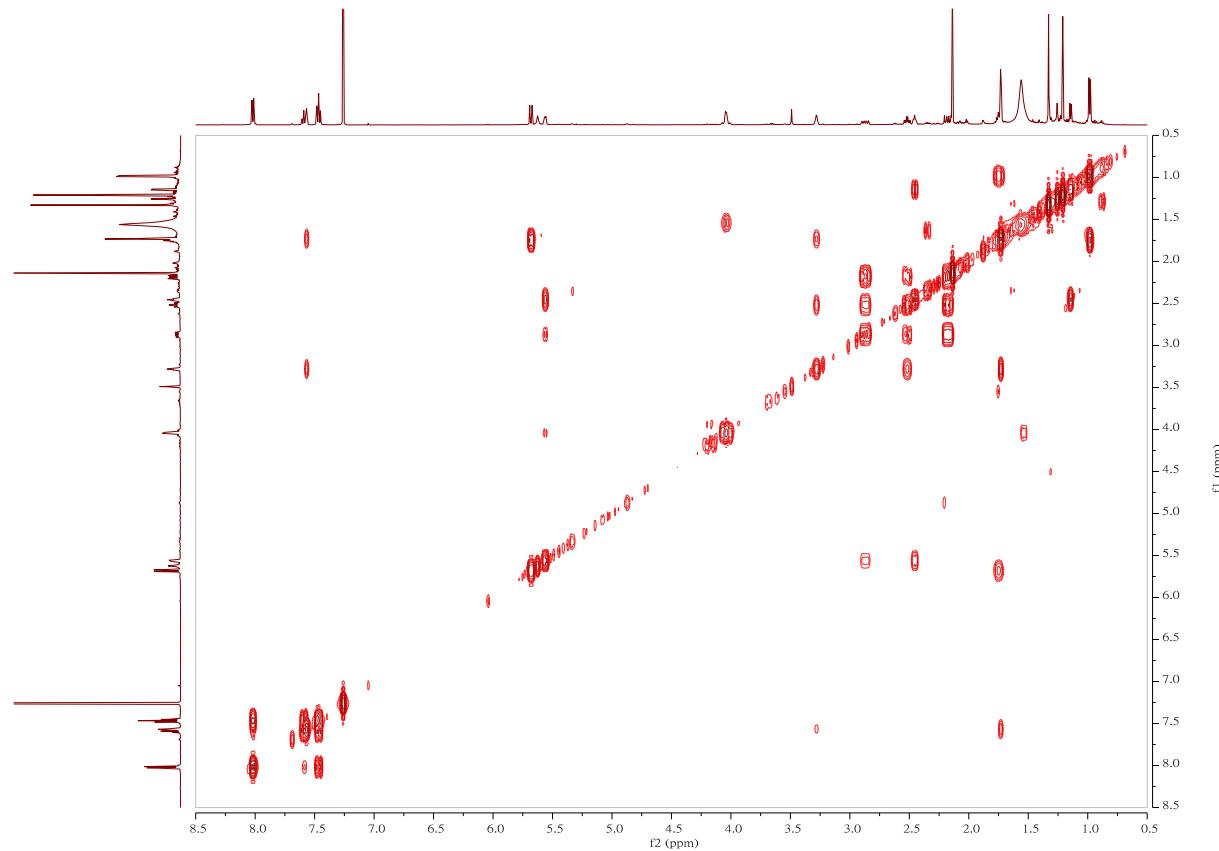


Figure S67. The ^1H - ^1H COSY spectrum of 4β -crotignoid K (**14**).

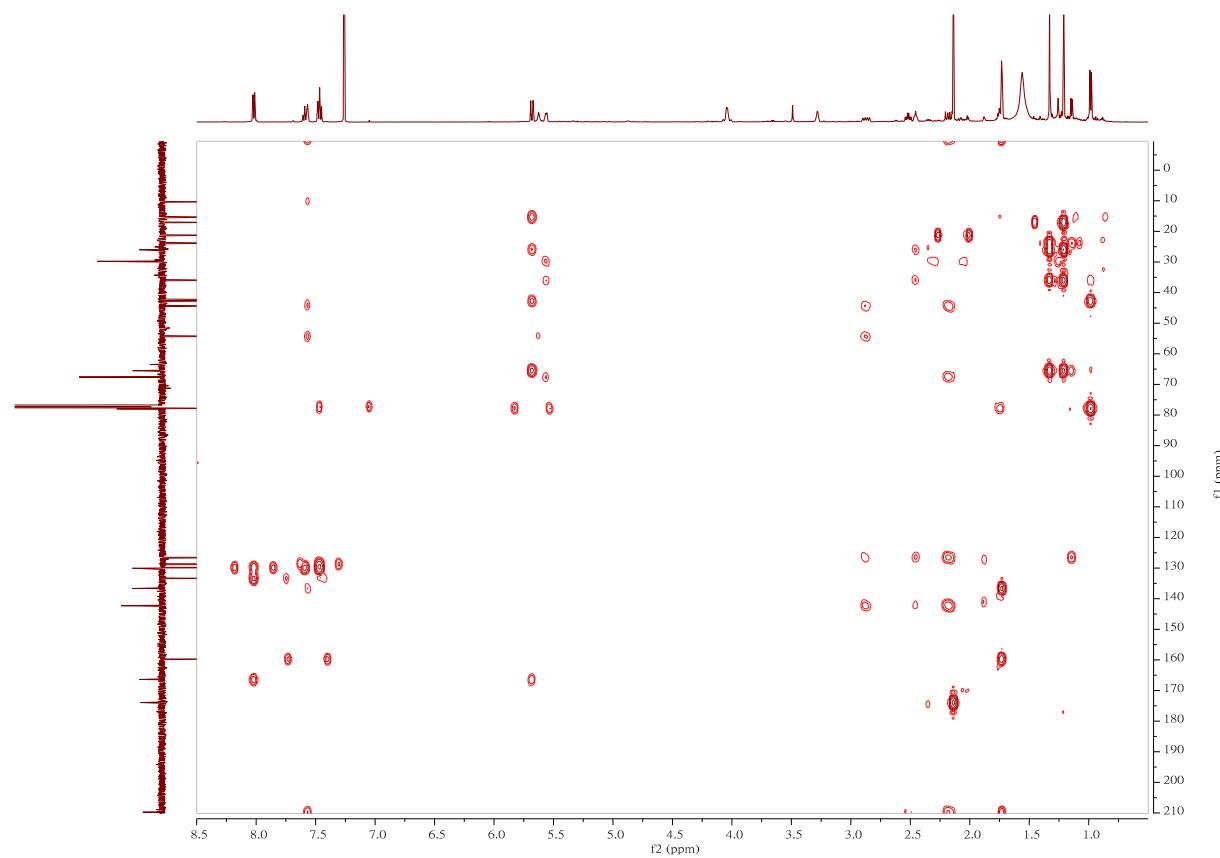


Figure S68. The HMBC spectrum of *4β*-crotignoid K (14).

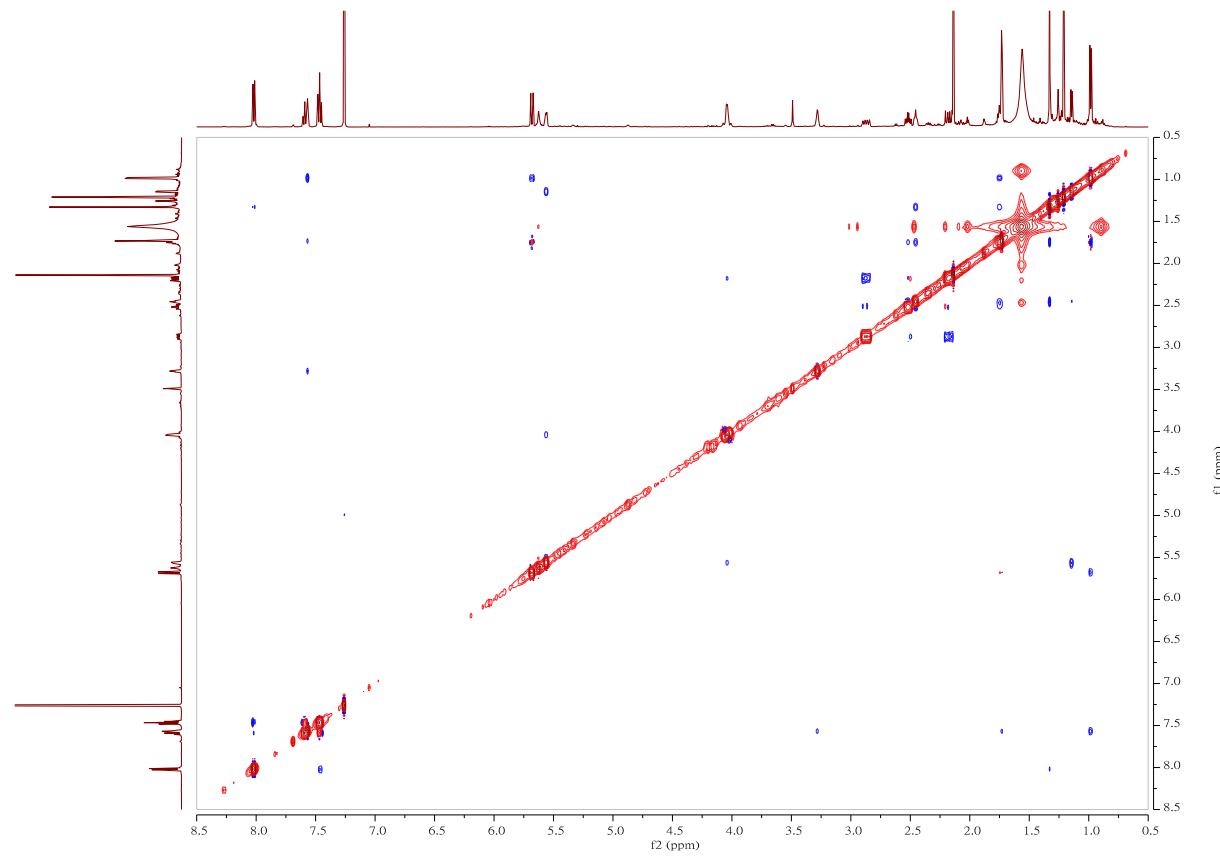
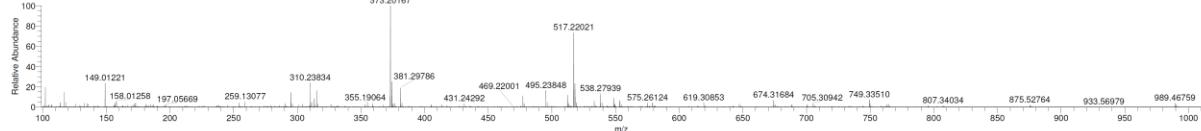


Figure S69. The NOESY spectrum of *4β*-crotignoid K (14).

1-5, 11-14

YC_20200917 #4248-4285 RT: 21.82-22.01 AV: 38 NL: 1.09E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



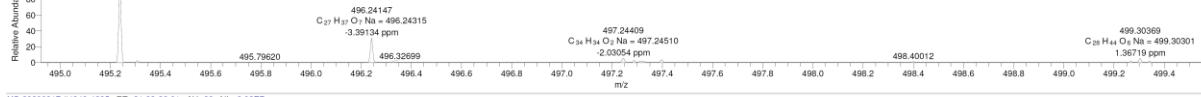
YC_20200917 #4248-4285 RT: 21.82-22.01 AV: 38 NL: 1.78E7

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

495.23848

C₂₉H₃₅O₇ Na = 495.23773

1.51801 ppm



YC_20200917 #4248-4285 RT: 21.82-22.01 AV: 38 NL: 8.03E7

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

517.22021

C₂₉H₃₅O₇ Na = 517.21967

1.50074 ppm

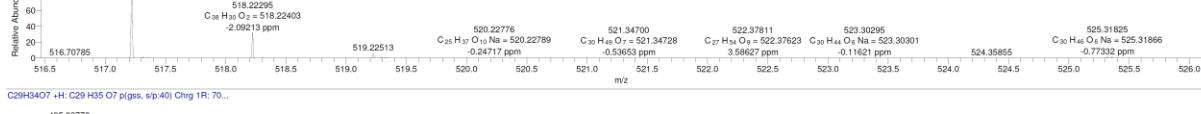
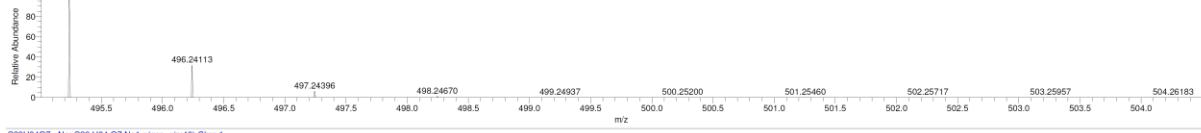
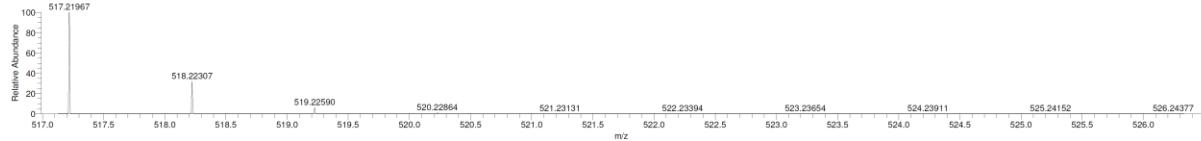
C₂₉H₃₄O₇ +Na: C₂₉H₃₅O₇ Na1 p(gss, s/p:40) Chrg 1R; 70...C₂₉H₃₄O₇ +Na: C₂₉H₃₅O₇ Na1 p(gss, s/p:40) Chrg 1...

Figure S70. The HR-ESI-MS spectra of 4 β -crotignoid K (**14**).

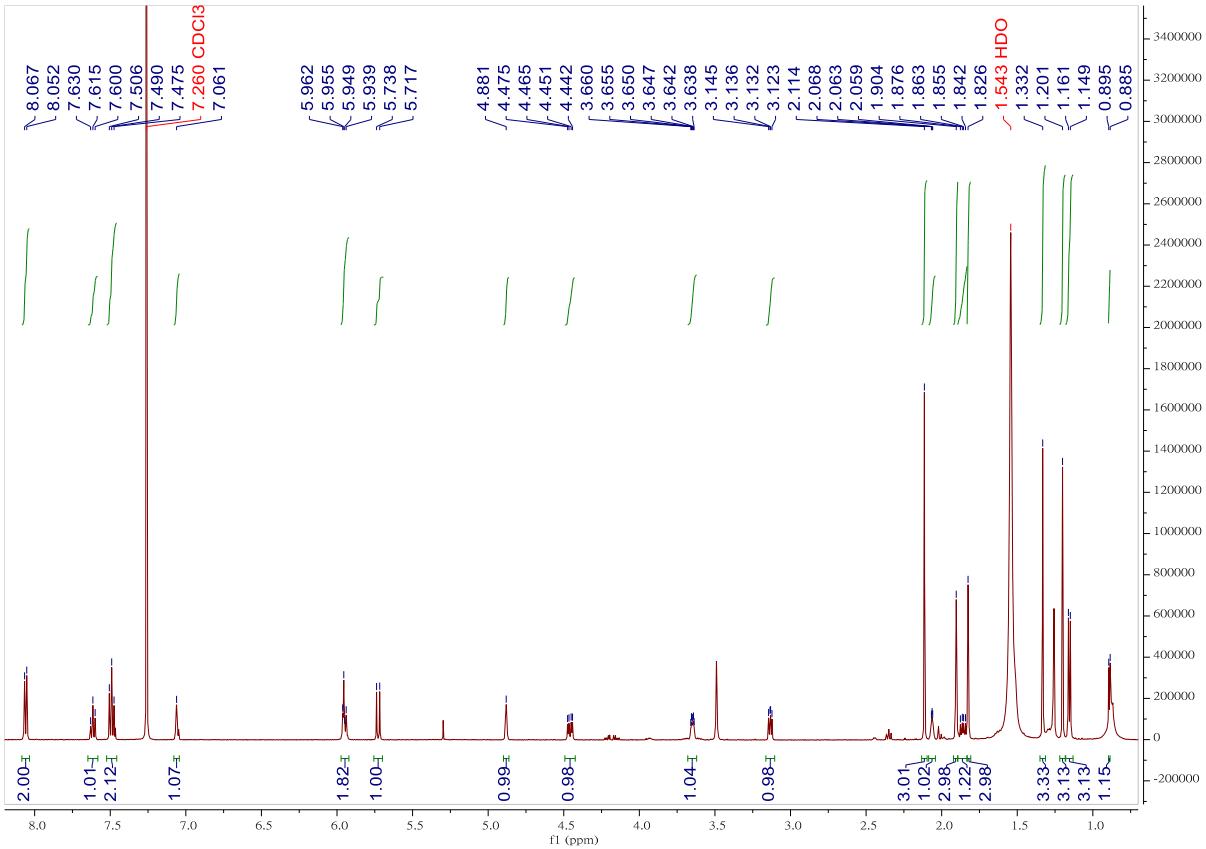


Figure S71. The ^1H -NMR spectrum of euphodendriane B (**15**) (500 MHz, CDCl_3).

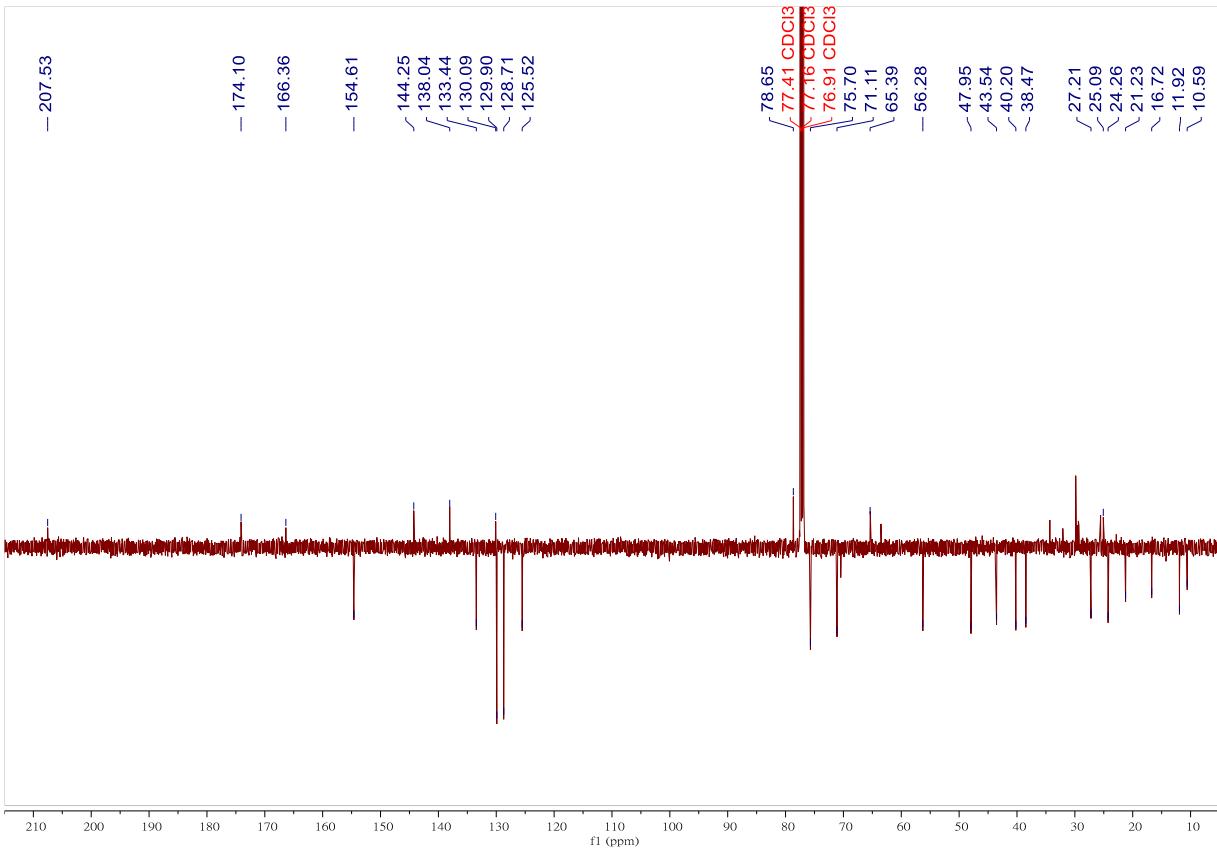


Figure S72. The ^{13}C -JMOD spectrum of euphodendriane B (**15**) (125 MHz, CDCl_3).

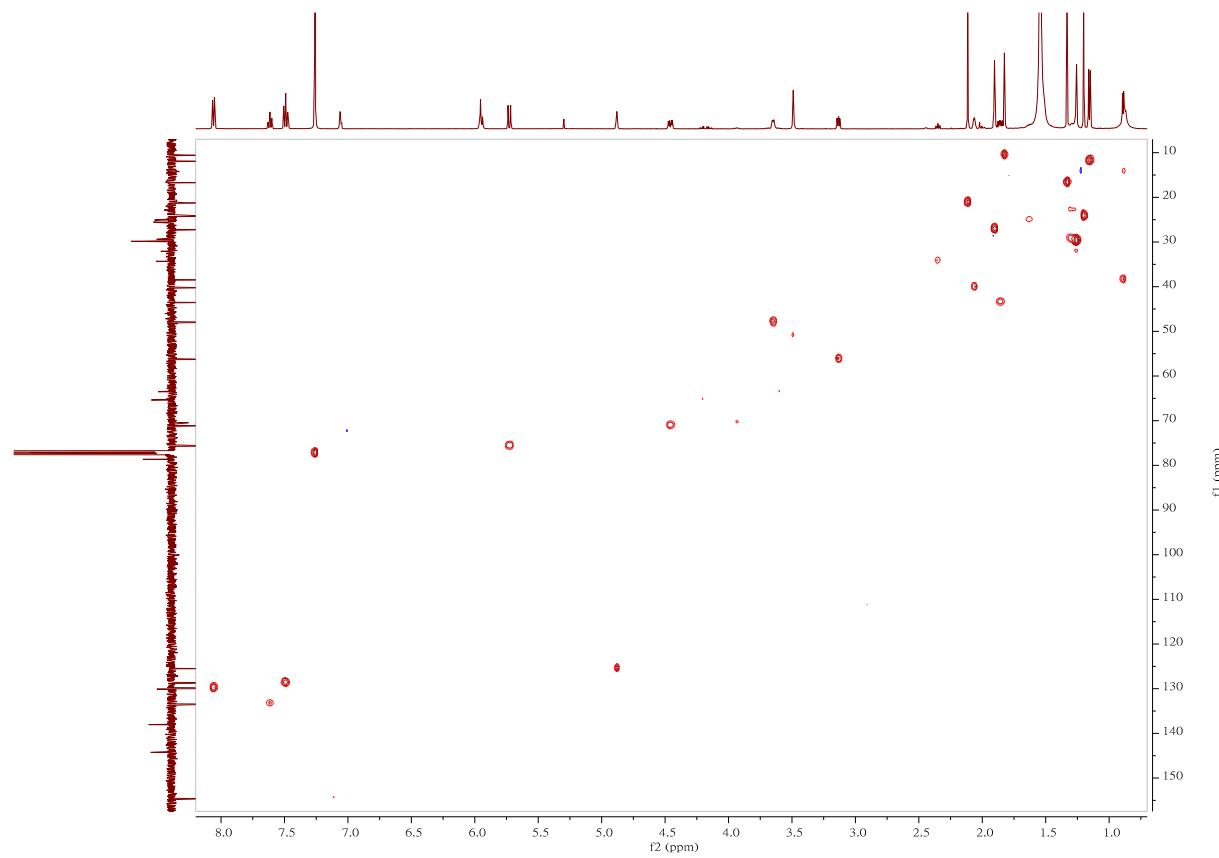


Figure S73. The HSQC spectrum of euphodendriane B (**15**).

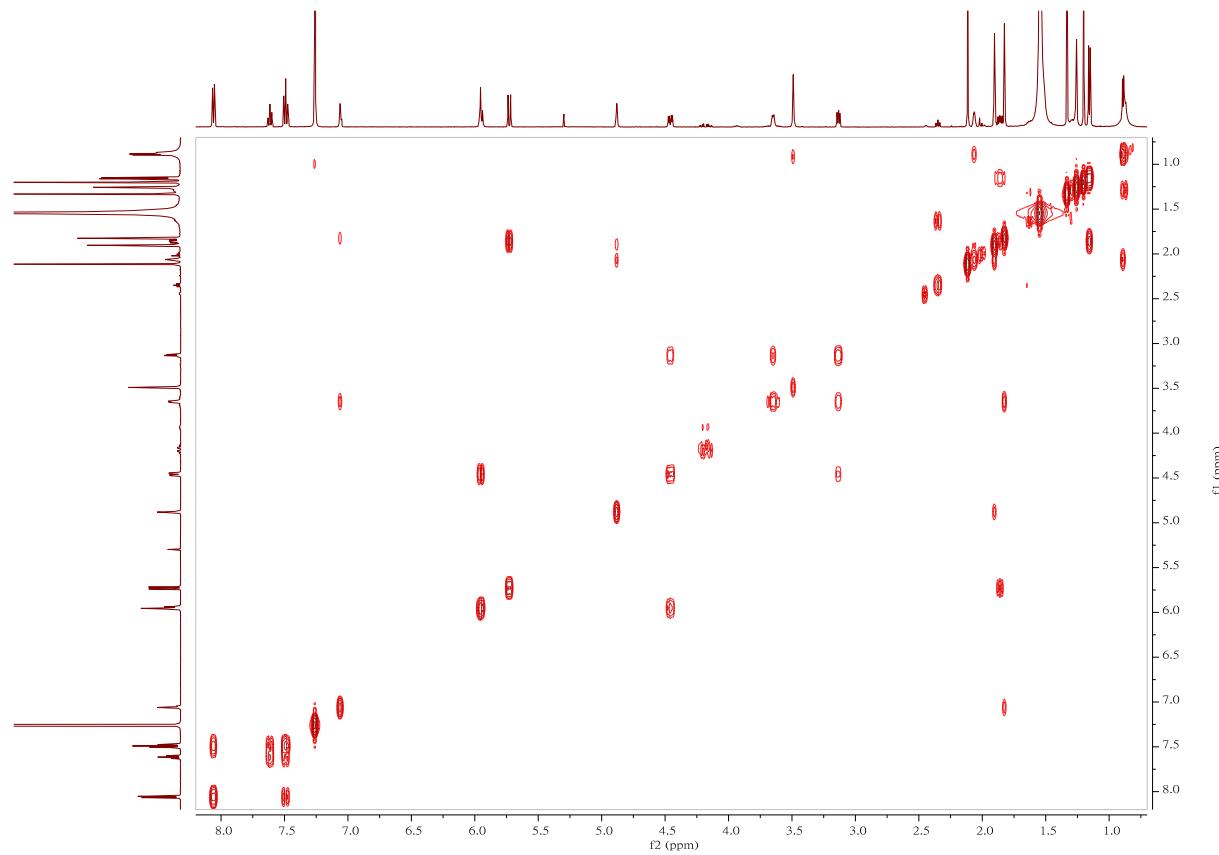


Figure S74. The ^1H - ^1H COSY spectrum of euphodendriane B (**15**).

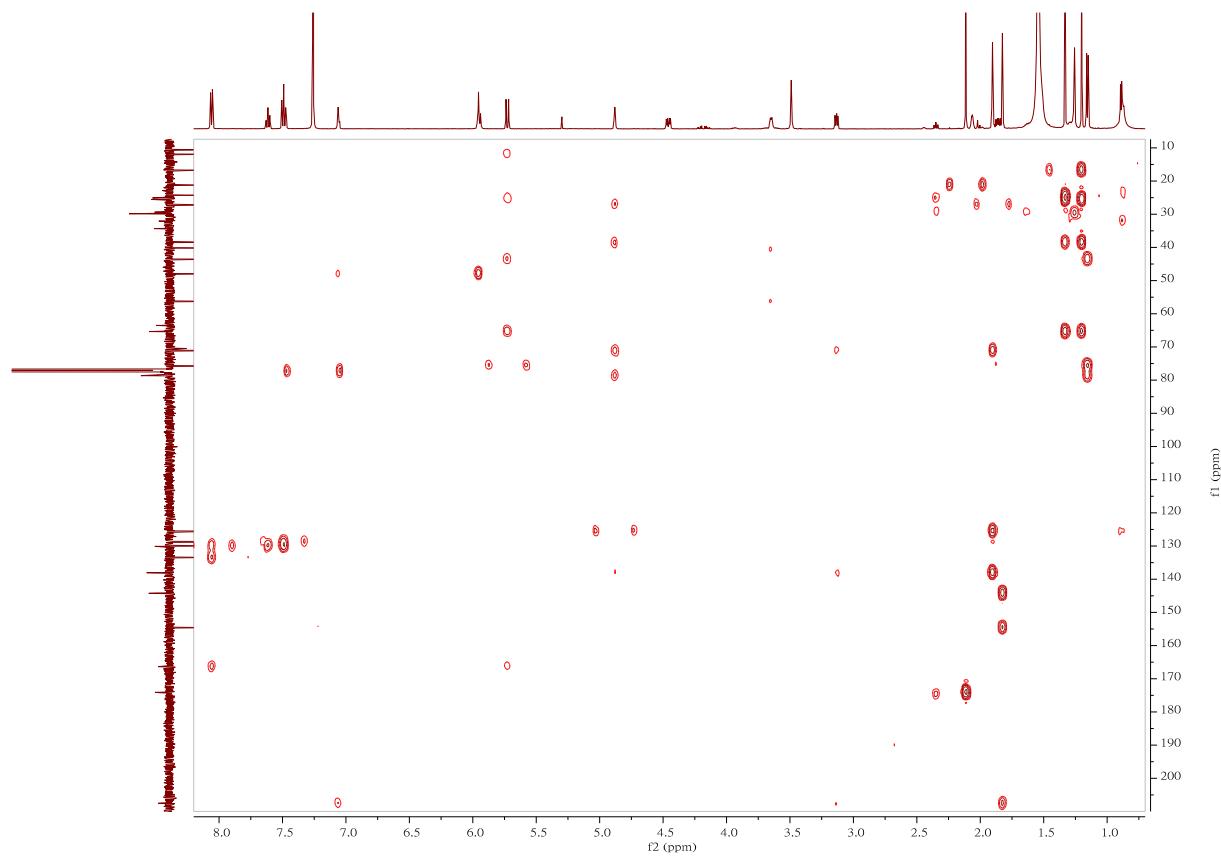


Figure S75. The HMBC spectrum of euphodendriane B (15).

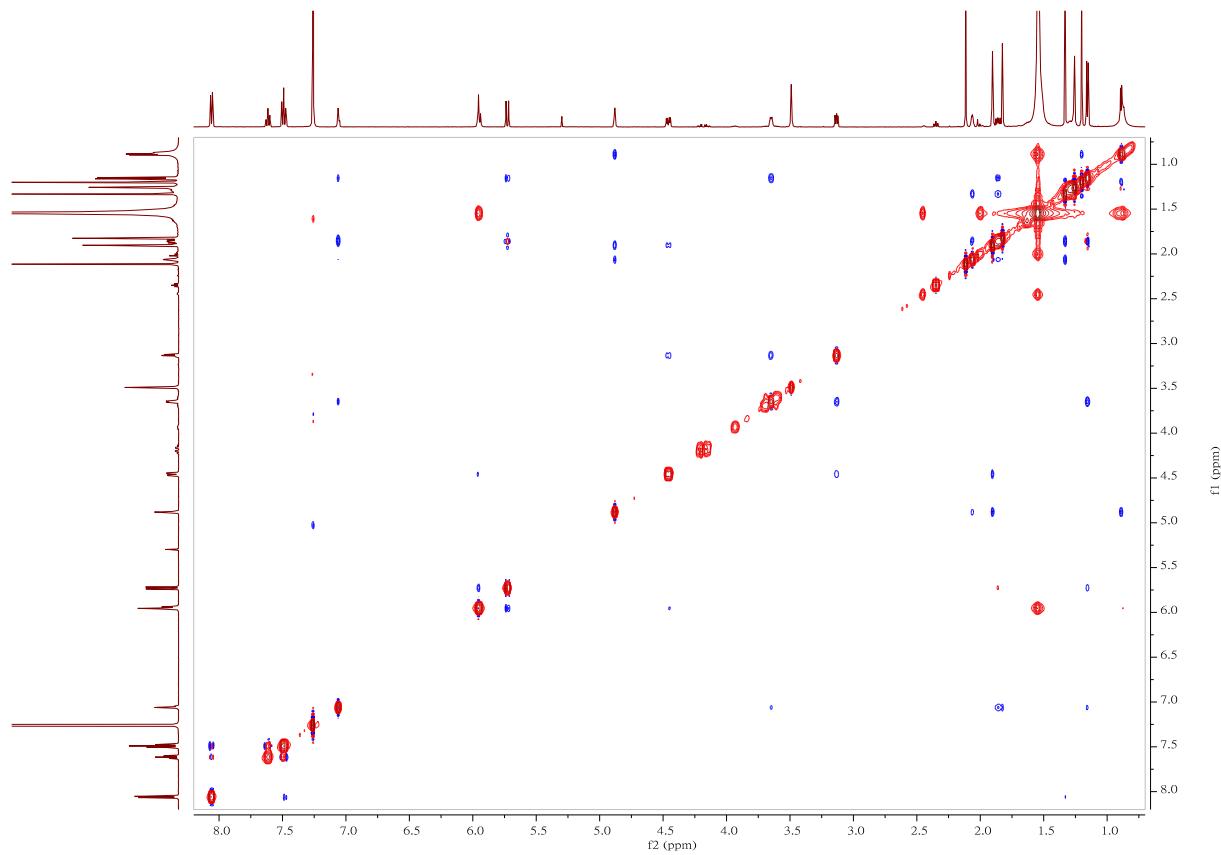
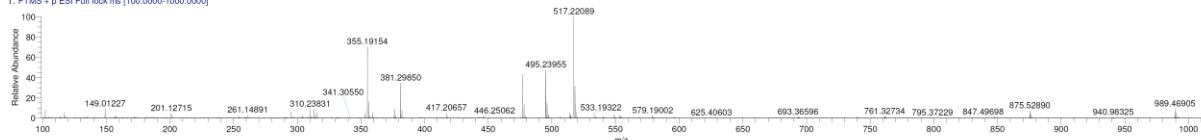
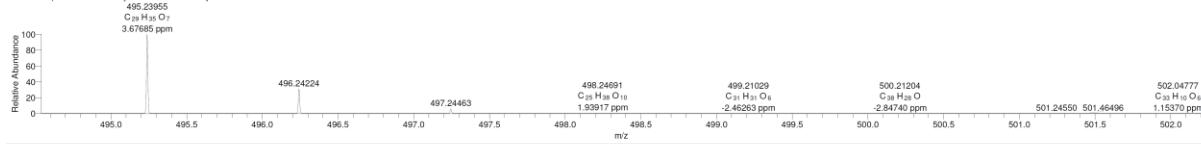


Figure S76. The NOESY spectrum of euphodendriane B (15).

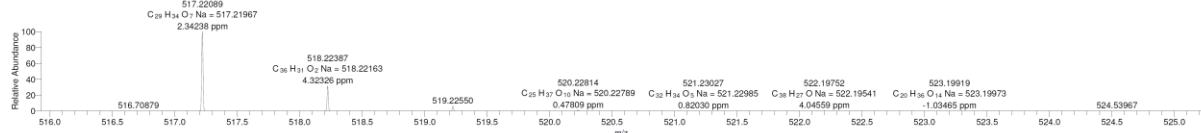
1-5, 11-14
 YC-20200917 #3053-3075 RT: 15.68-15.79 AV: 23 NL: 2.45E8
 T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



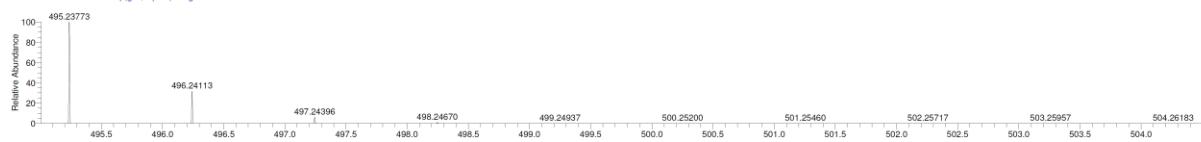
YC-20200917 #3053-3075 RT: 15.68-15.79 AV: 23 NL: 1.17E8
 T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



YC-20200917 #3053-3075 RT: 15.68-15.79 AV: 23 NL: 2.45E8
 T: FTMS + p ESI Full lock ms [100.0000-1000.0000]



C29H34O7 +H: C29 H35 O7 Na1 p(gss, s/p:40) Chrg 1R: 70...



C29H34O7 +Na: C29 H34 O7 Na1 p(gss, s/p:40) Chrg 1...

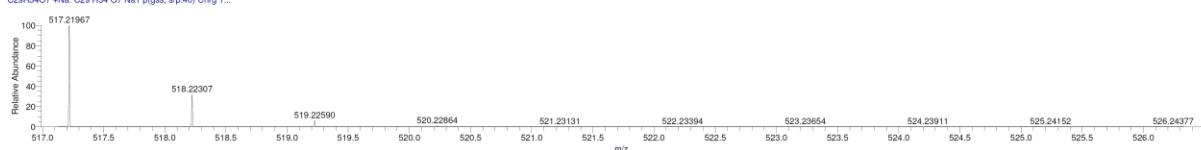


Figure S77. The HR-ESI-MS spectra of eupholodendriane B (**15**).

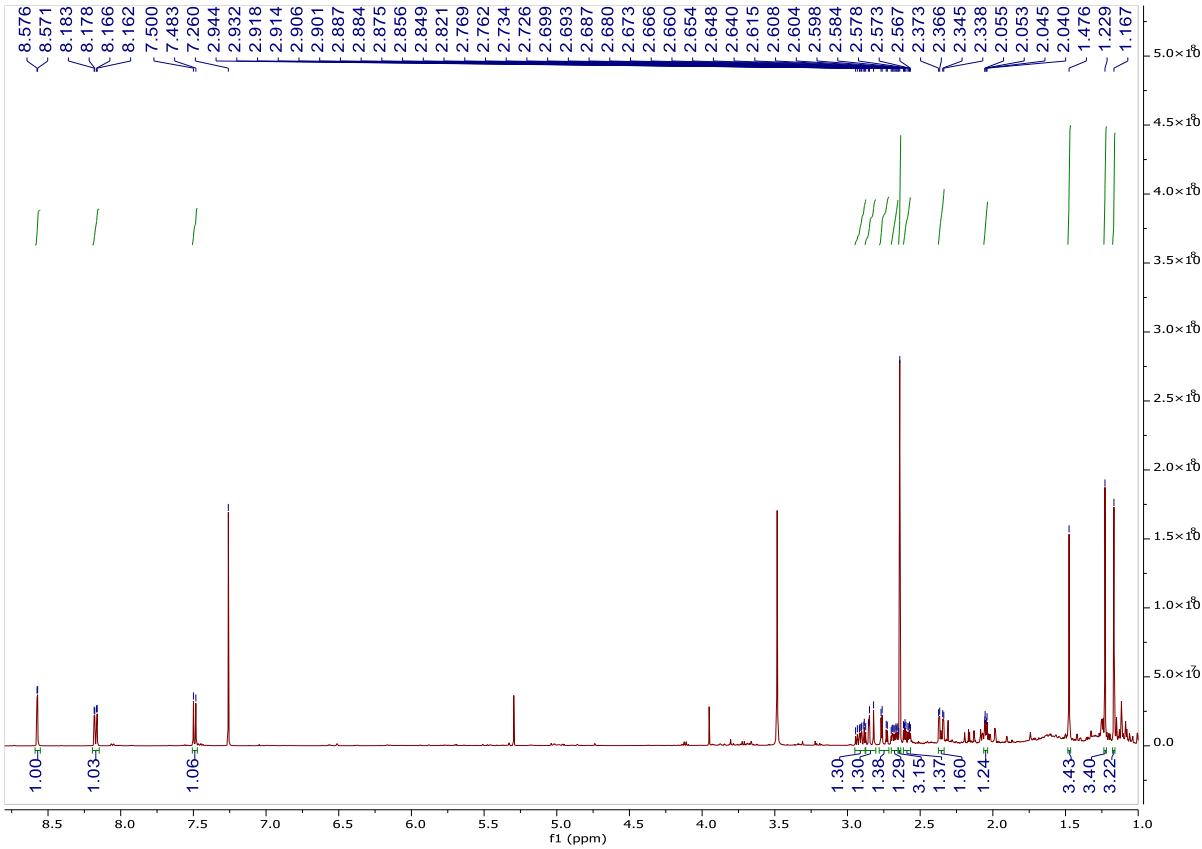


Figure S78. The ^1H -NMR spectrum of 16-nor-abiet-8,11,13-trien-3,7,15-trione (**16**) (500 MHz, CDCl_3).

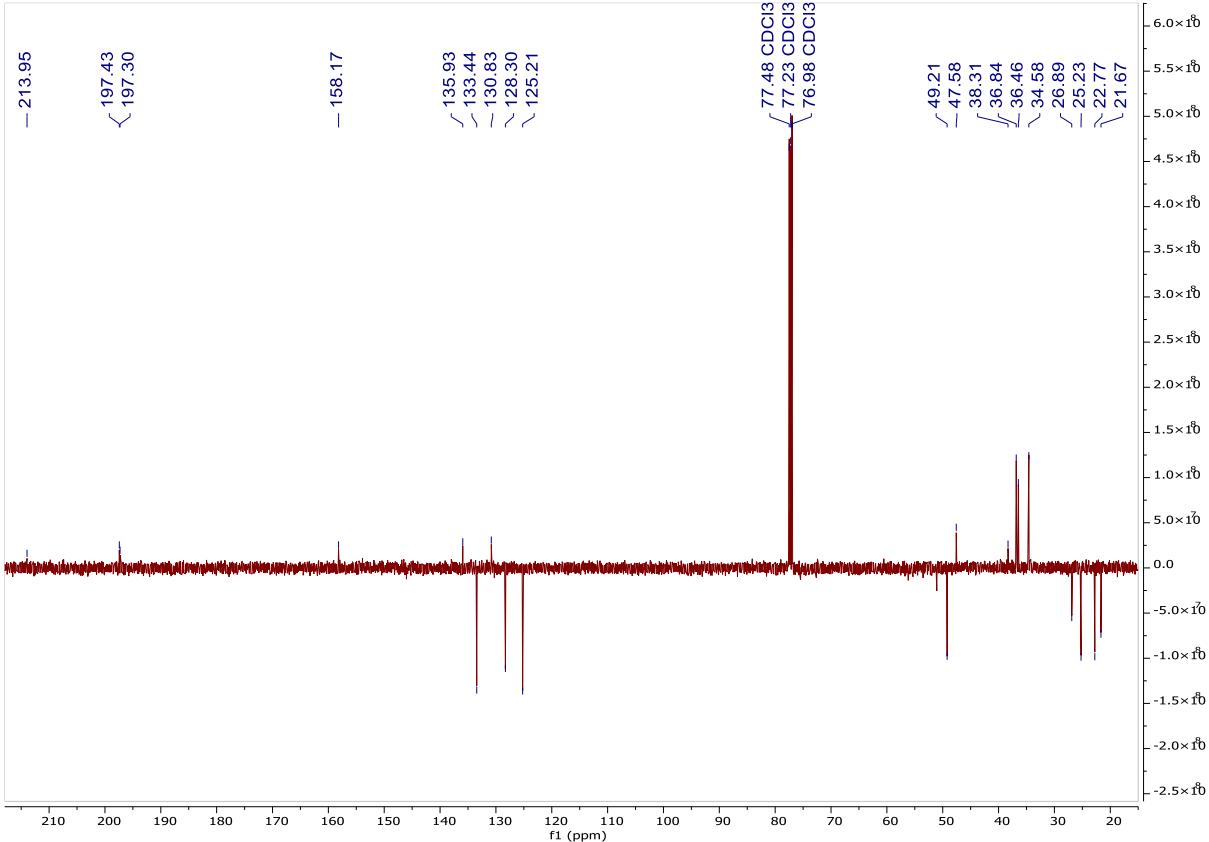


Figure S79. The ^{13}C -JMOD spectrum of 16-nor-abiet-8,11,13-trien-3,7,15-trione (**16**) (125 MHz, CDCl_3).

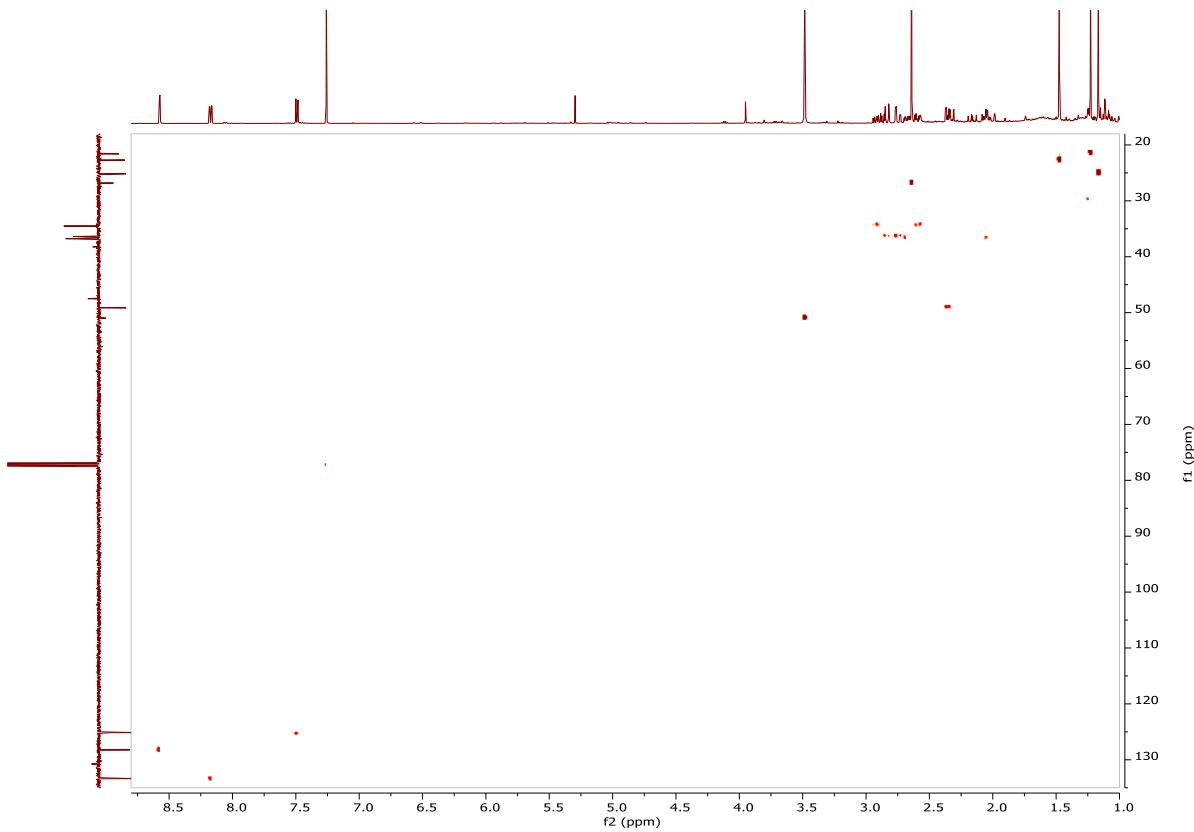


Figure S80. The HSQC spectrum of 16-nor-abiet-8,11,13-trien-3,7,15-trione (**16**).

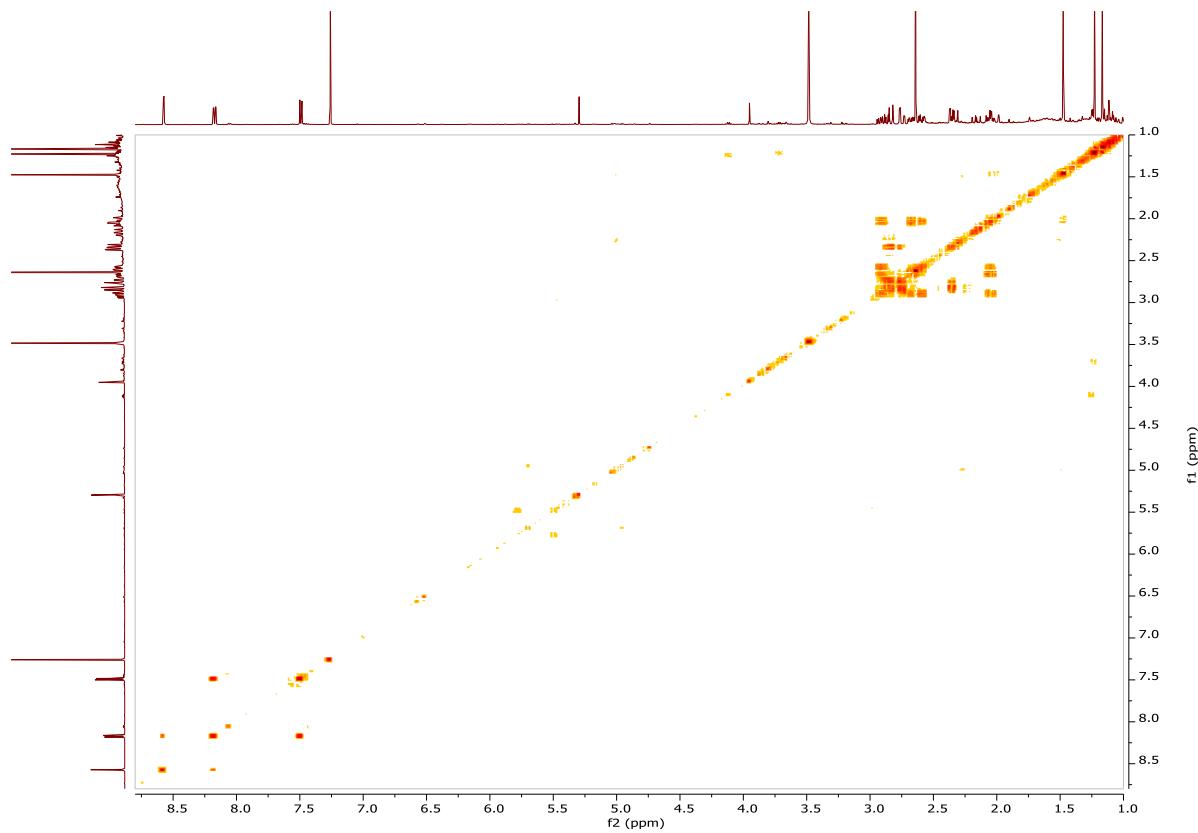


Figure S81. The ¹H-¹H COSY spectrum of 16-nor-abiet-8,11,13-trien-3,7,15-trione (**16**).

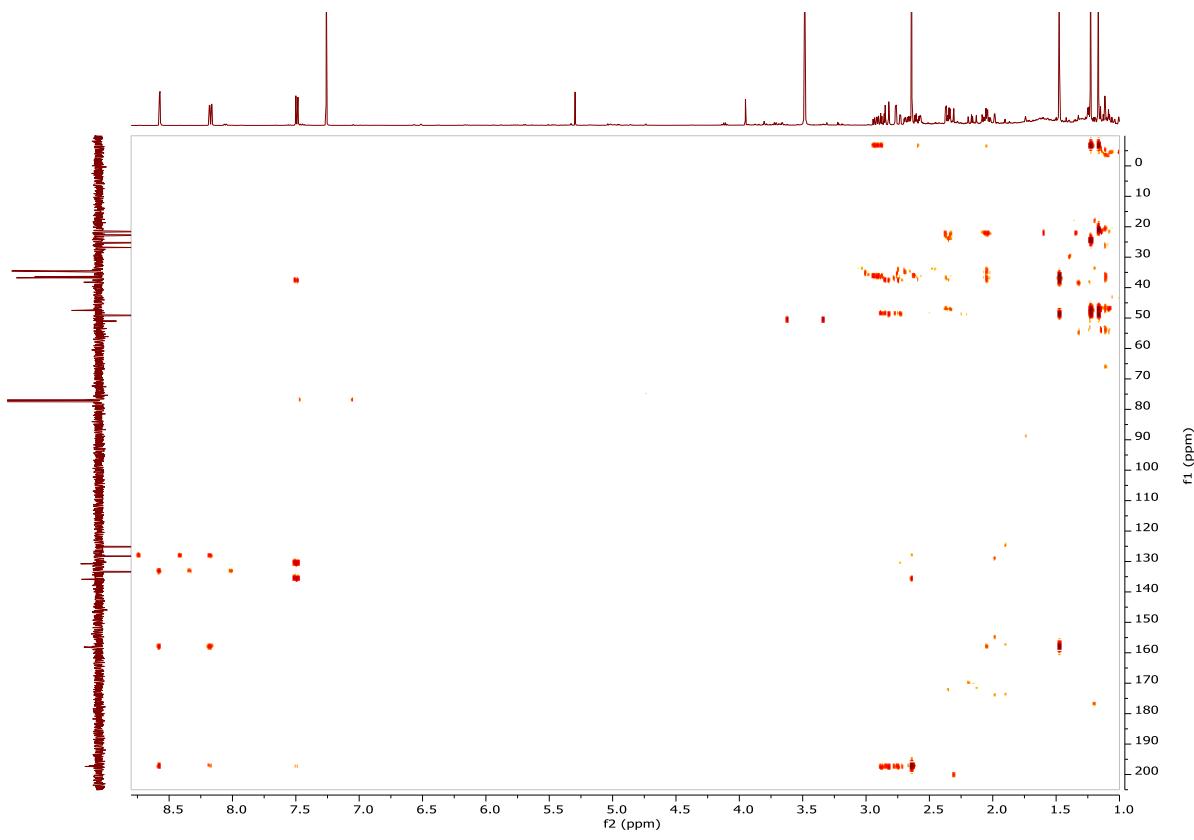


Figure S82. The HMBC spectrum of 16-nor-abiet-8,11,13-trien-3,7,15-trione (**16**).

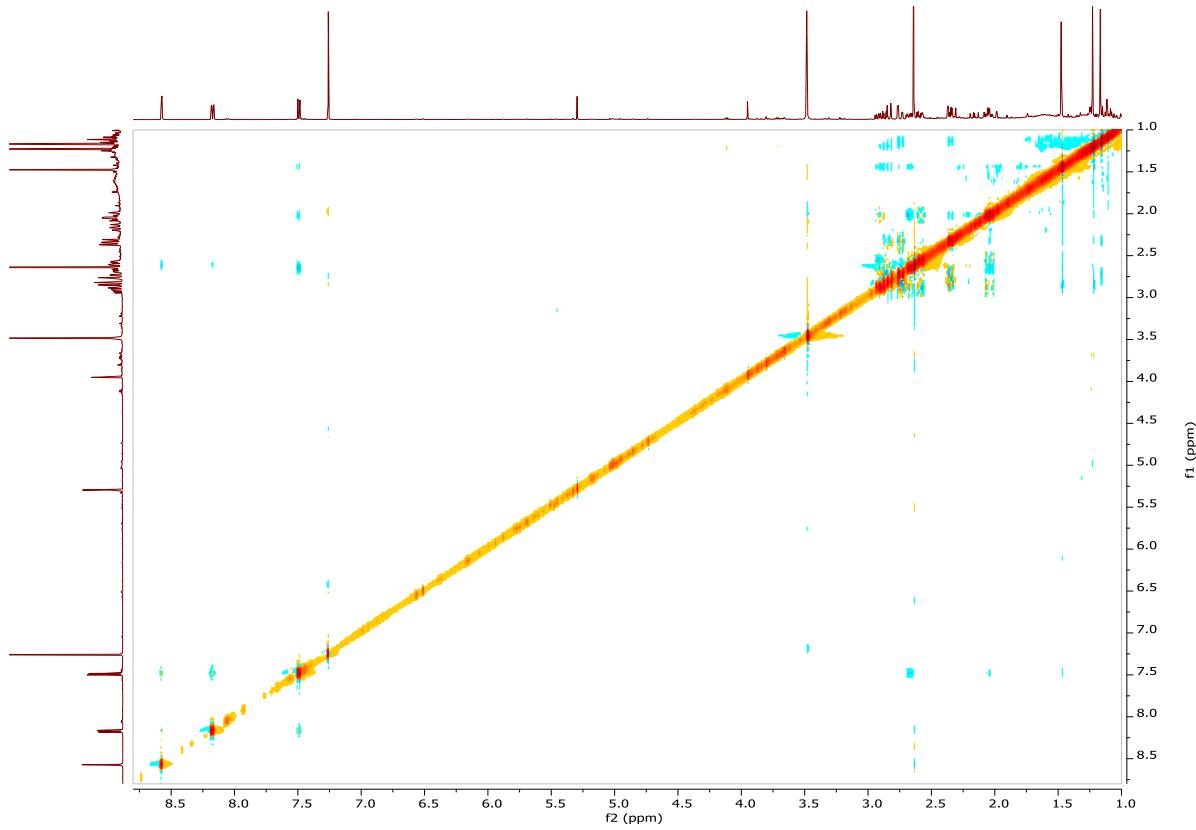


Figure S83. The NOESY spectrum of 16-nor-abiet-8,11,13-trien-3,7,15-trione (**16**).

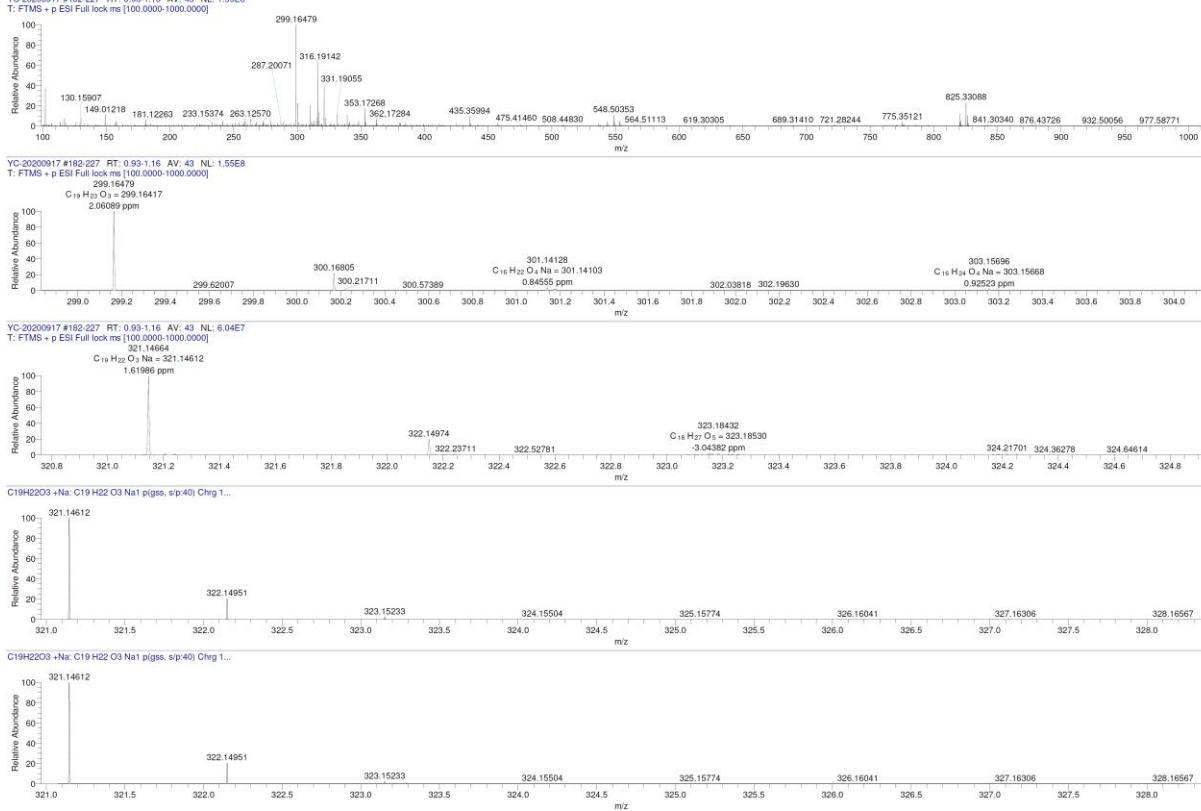


Figure S84. The HR-ESI-MS spectra of 16-nor-abiet-8,11,13-trien-3,7,15-trione (**16**).

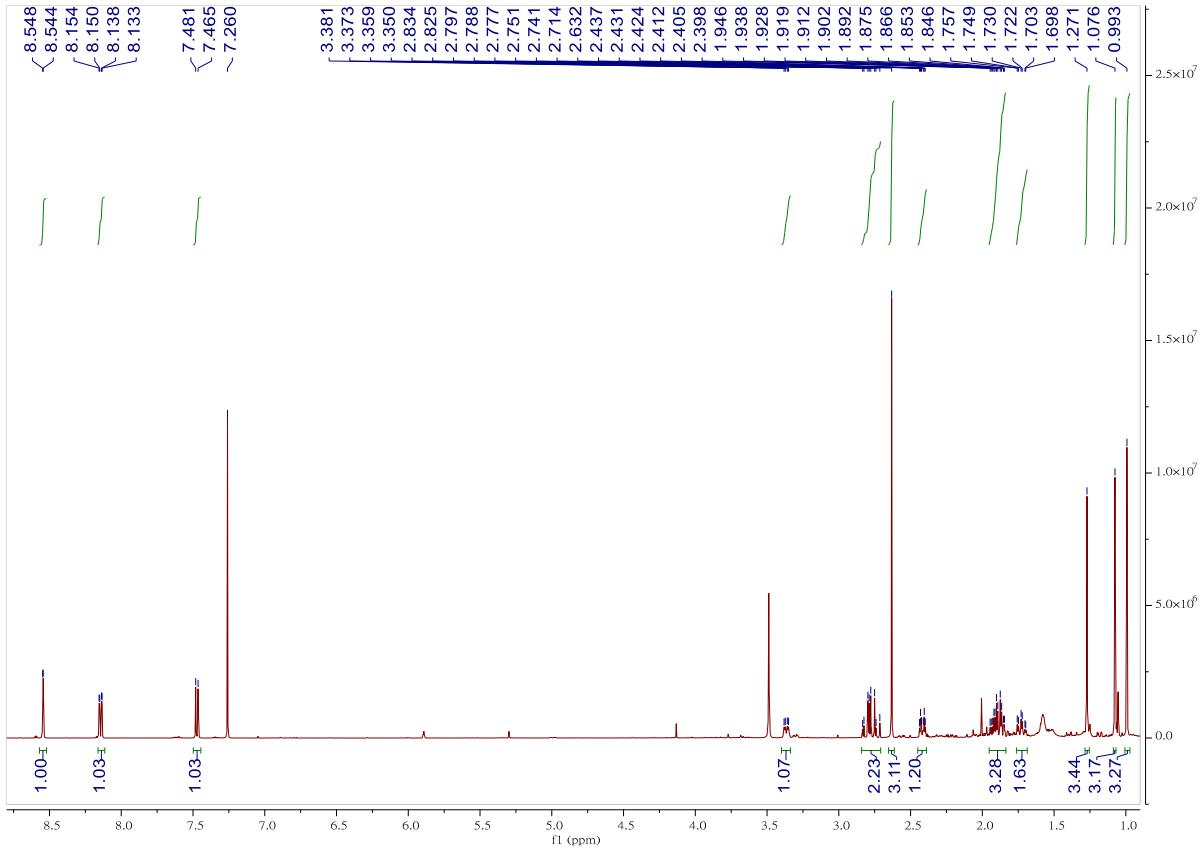


Figure S85. The ^1H -NMR spectrum of 16-nor-3 β -hydroxy-abiet-8,11,13-trien-7,15-dione (**17**) (500 MHz, CDCl_3).

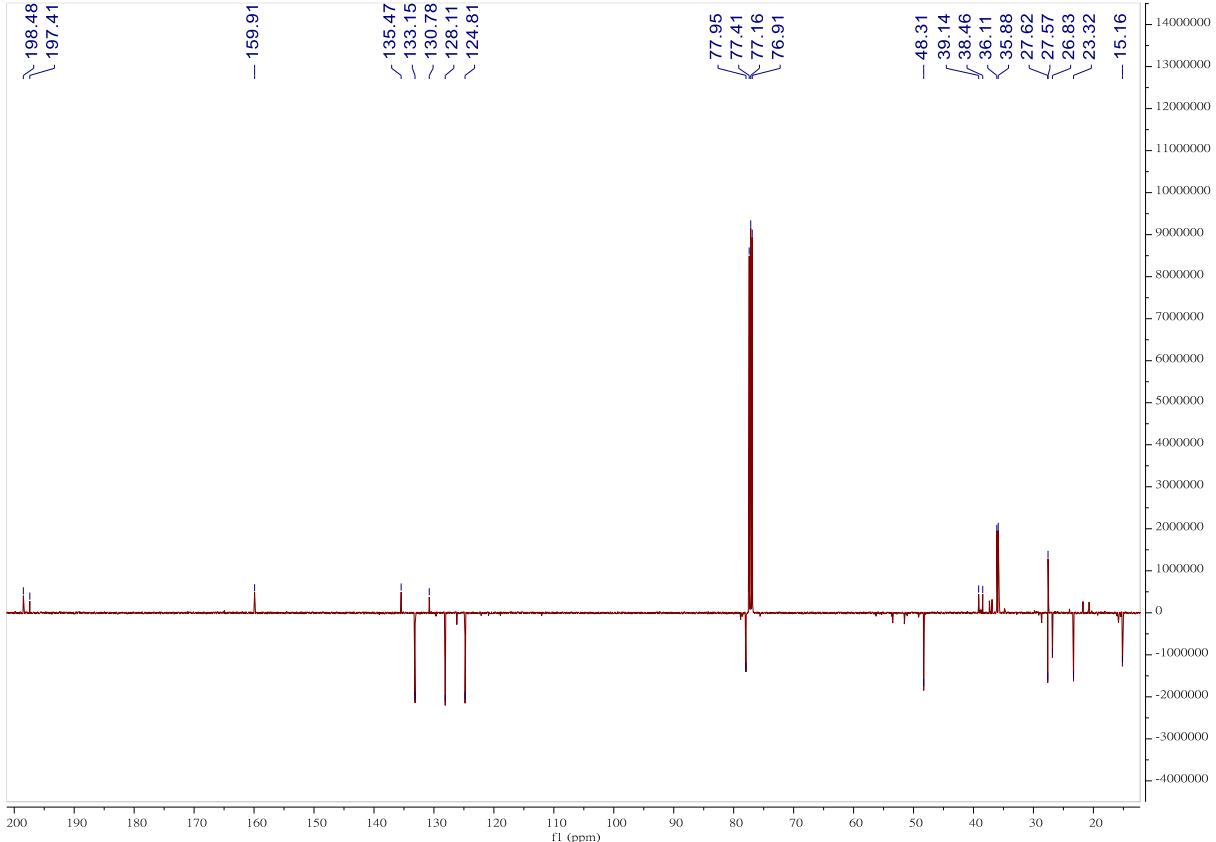


Figure S86. The ^{13}C -JMOD spectrum of 16-nor-3 β -hydroxy-abiet-8,11,13-trien-7,15-dione (**17**) (125 MHz, CDCl_3).

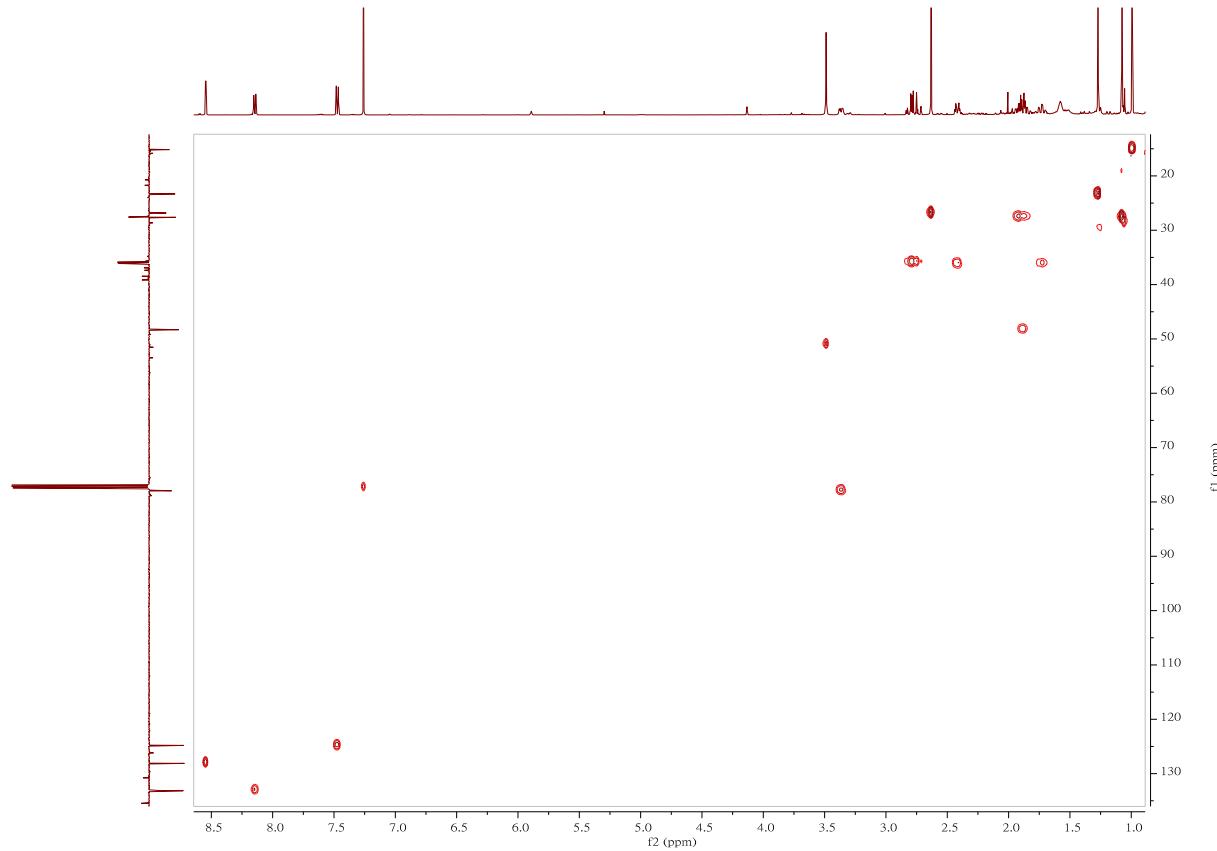


Figure S87. The HSQC spectrum of 16-nor-3 β -hydroxy-abiet-8,11,13-trien-7,15-dione (**17**).

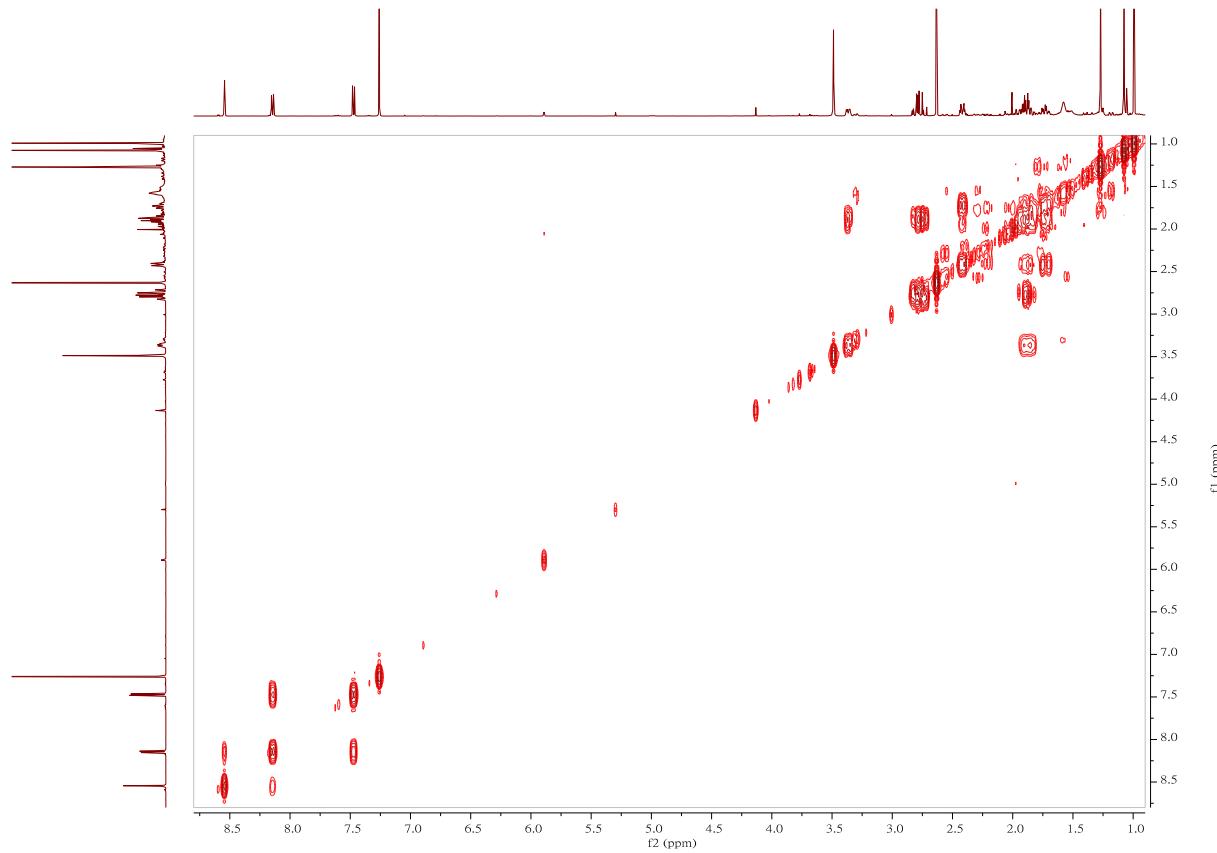


Figure S88. The ^1H - ^1H COSY spectrum of 16-nor-3 β -hydroxy-abiet-8,11,13-trien-7,15-dione (**17**).

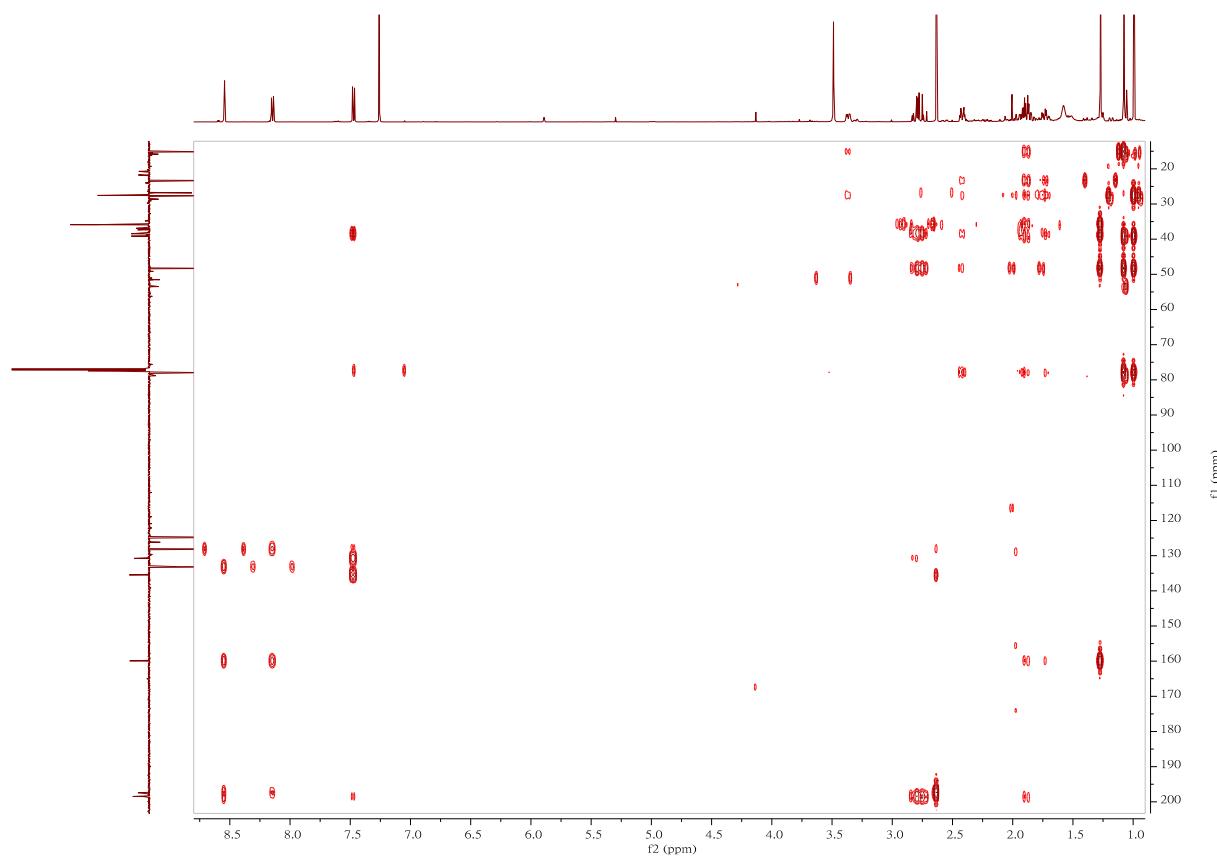


Figure S89. The HMBC spectrum of 16-nor-3 β -hydroxy-abiet-8,11,13-trien-7,15-dione (17).

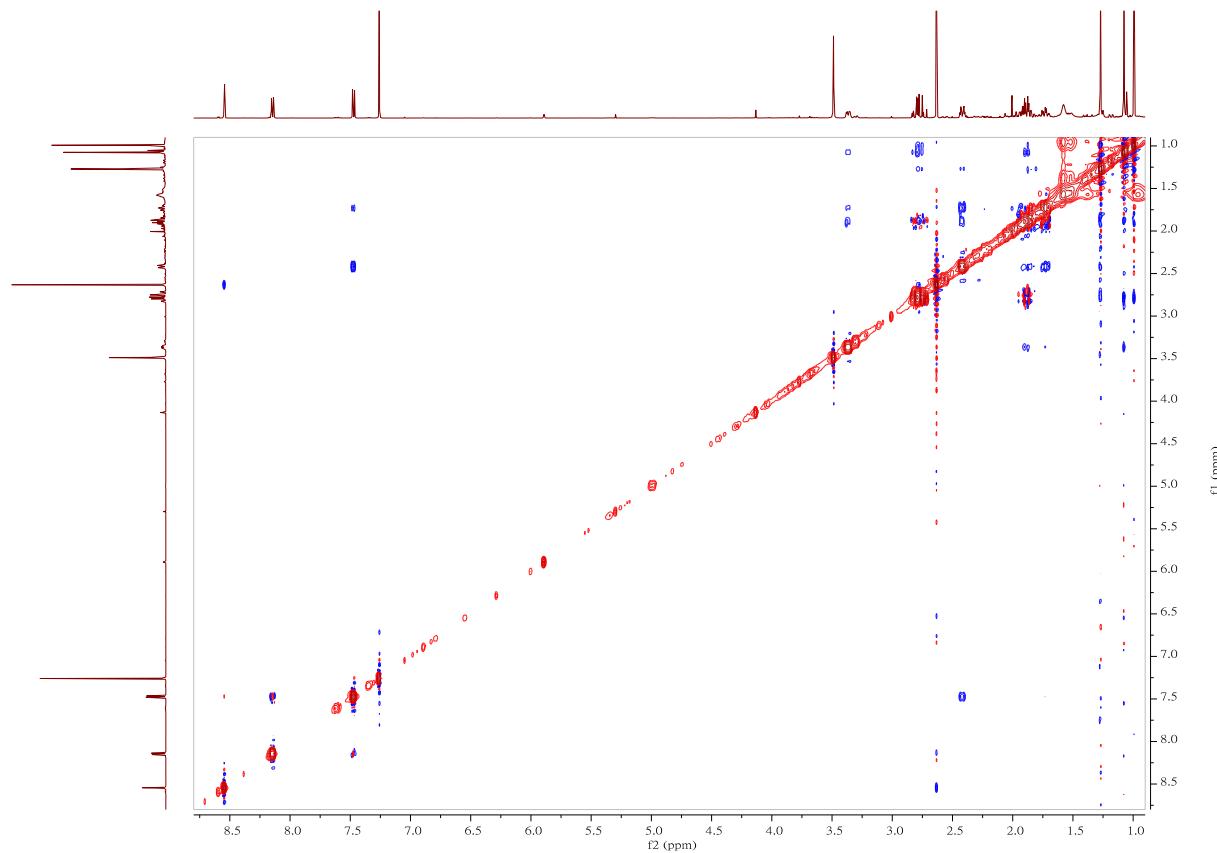
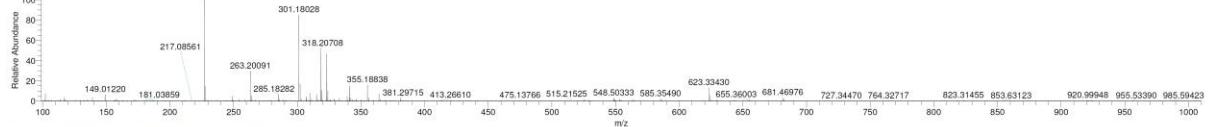


Figure S90. The NOESY spectrum of 16-nor-3 β -hydroxy-abiet-8,11,13-trien-7,15-dione (17).

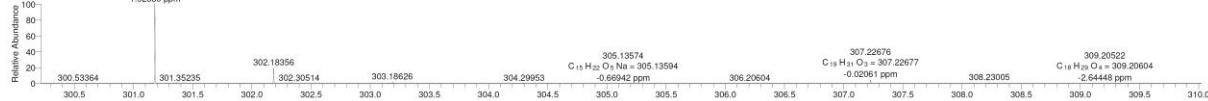


YC_20200917 #2539-2569 RT: 13.04-13.19 AV: 29 NL: 2.90E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

C₁₉H₂₄O₃ = 301.17982

1.52880 ppm



YC_20200917 #2539-2569 RT: 13.04-13.19 AV: 29 NL: 1.59E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

323.16225

C₁₉H₂₄O₃ Na = 323.16177

1.49952 ppm

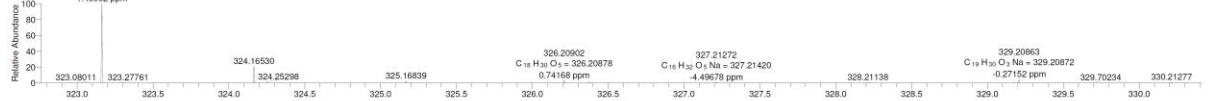
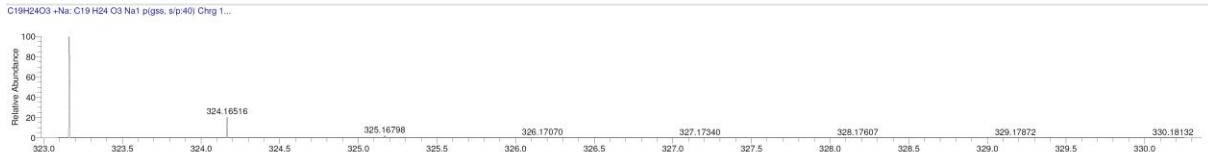
C₁₉H₂₄O₃ +H: C₁₉H₂₅O₃ (gss, s/p:40) Chrg 1R: 70...C₁₉H₂₄O₃ +Na: C₁₉H₂₅O₃ Na (gss, s/p:40) Chrg 1...

Figure S91. The HR-ESI-MS spectra of 16-nor-3 β -hydroxy-abieto-8,11,13-trien-7,15-dione (17).

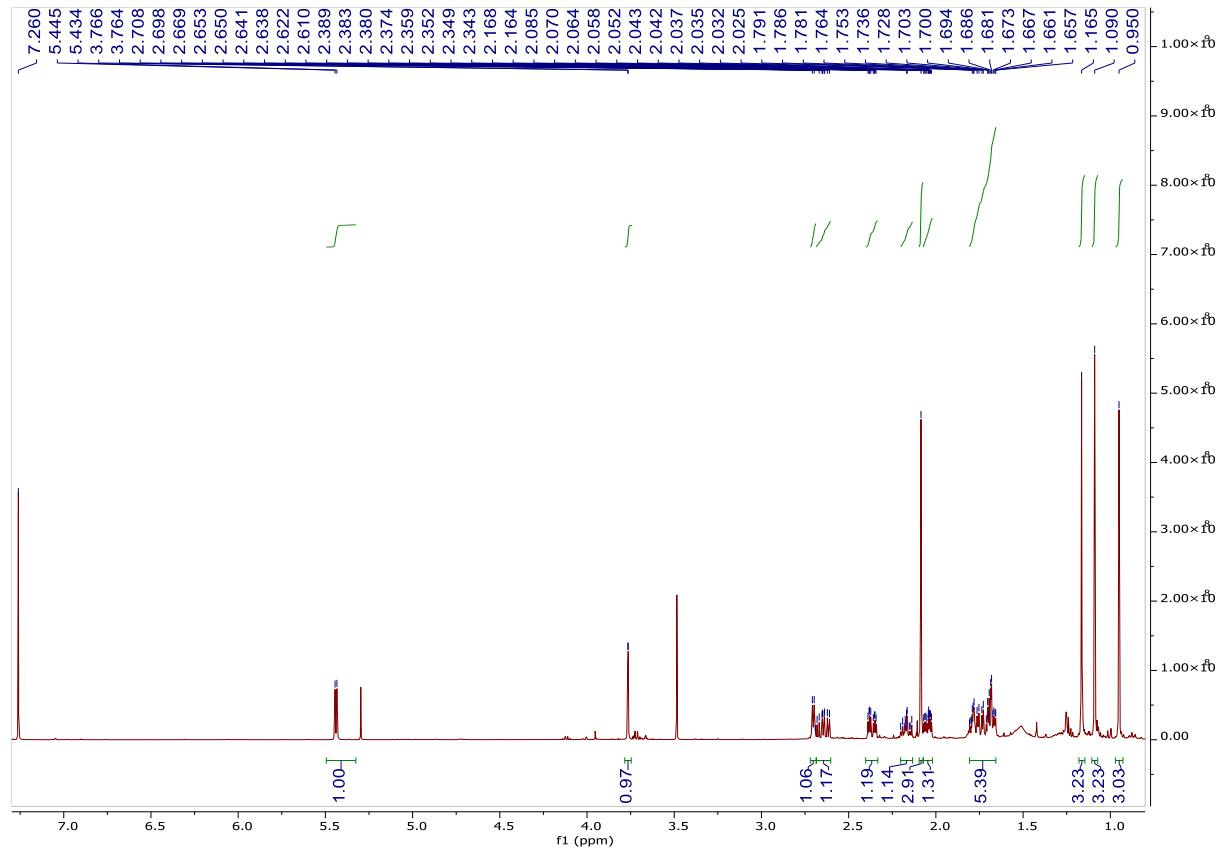


Figure S92. The ¹H-NMR spectrum of *ent*-8 β ,14 β -epoxyabiet-3-one-11,13(15)-dien-16,12-olide (**19**) (500 MHz, CDCl₃).

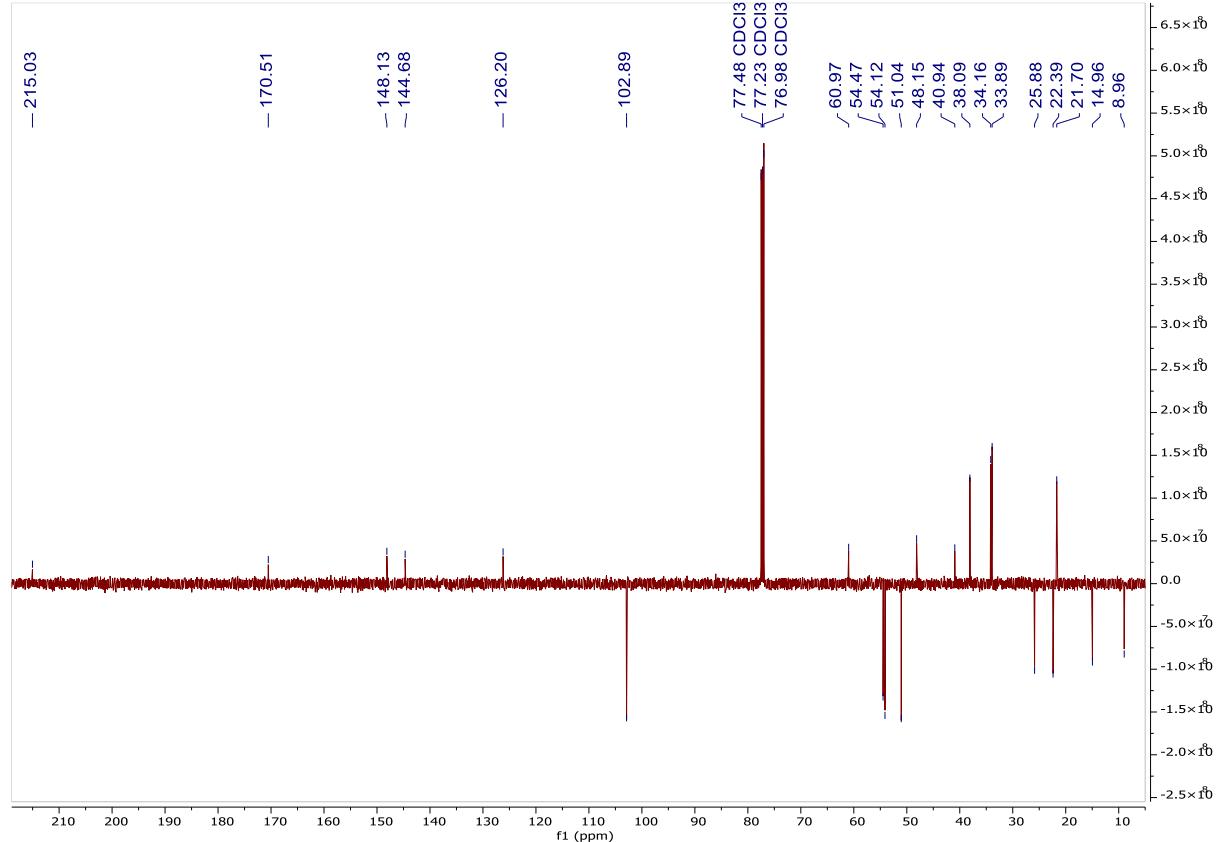


Figure S93. The ¹³C-JMOD spectrum of *ent*-8 β ,14 β -epoxyabiet-3-one-11,13(15)-dien-16,12-olide (**19**) (125 MHz, CDCl₃).

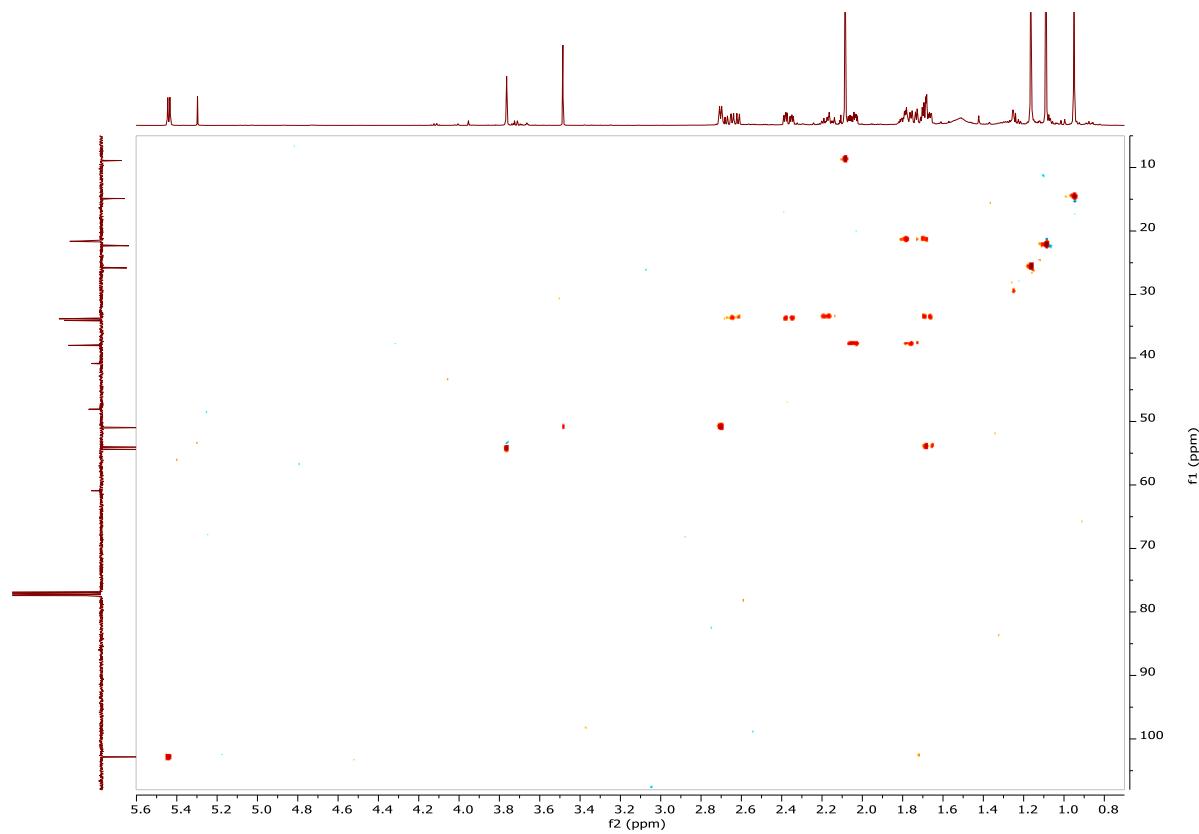


Figure S94. The HSQC spectrum of *ent*-8 β ,14 β -epoxyabiet-3-one-11,13(15)-dien-16,12-olide (**19**).

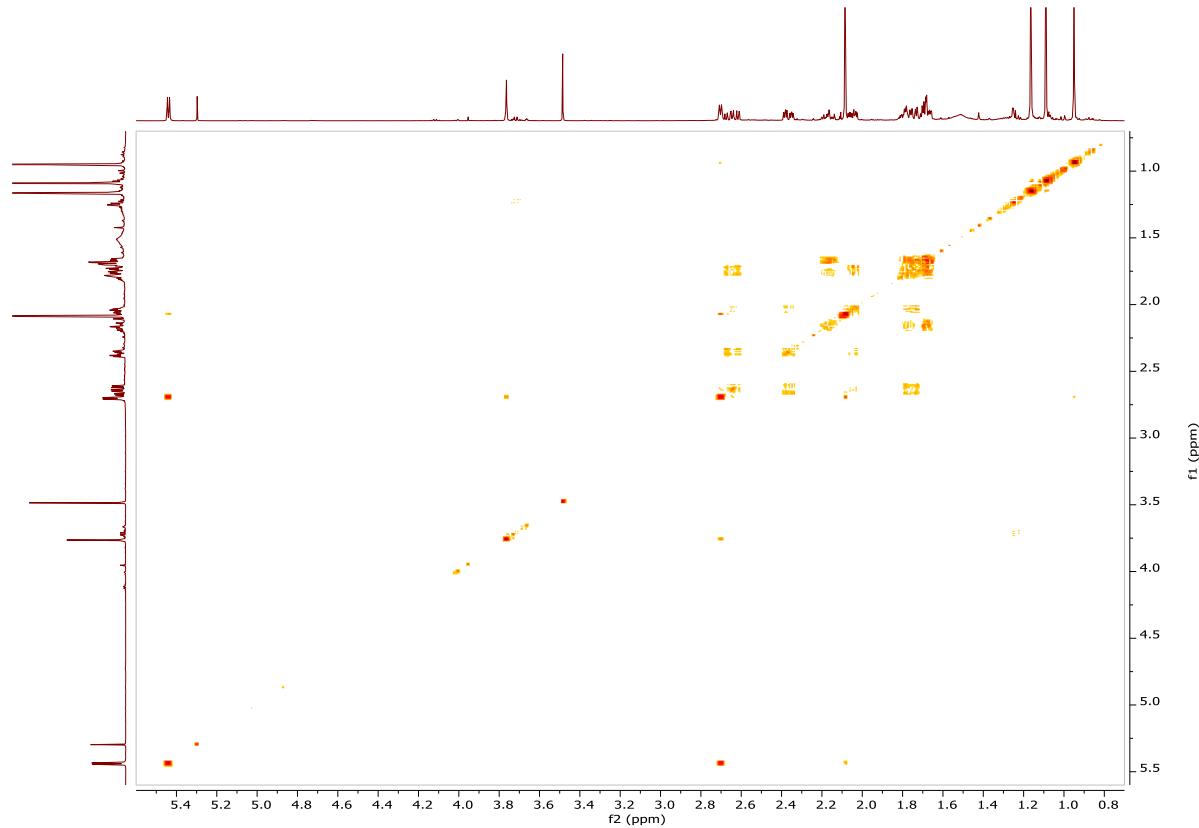


Figure S95. The ^1H - ^1H COSY spectrum of *ent*-8 β ,14 β -epoxyabiet-3-one-11,13(15)-dien-16,12-olide (**19**).

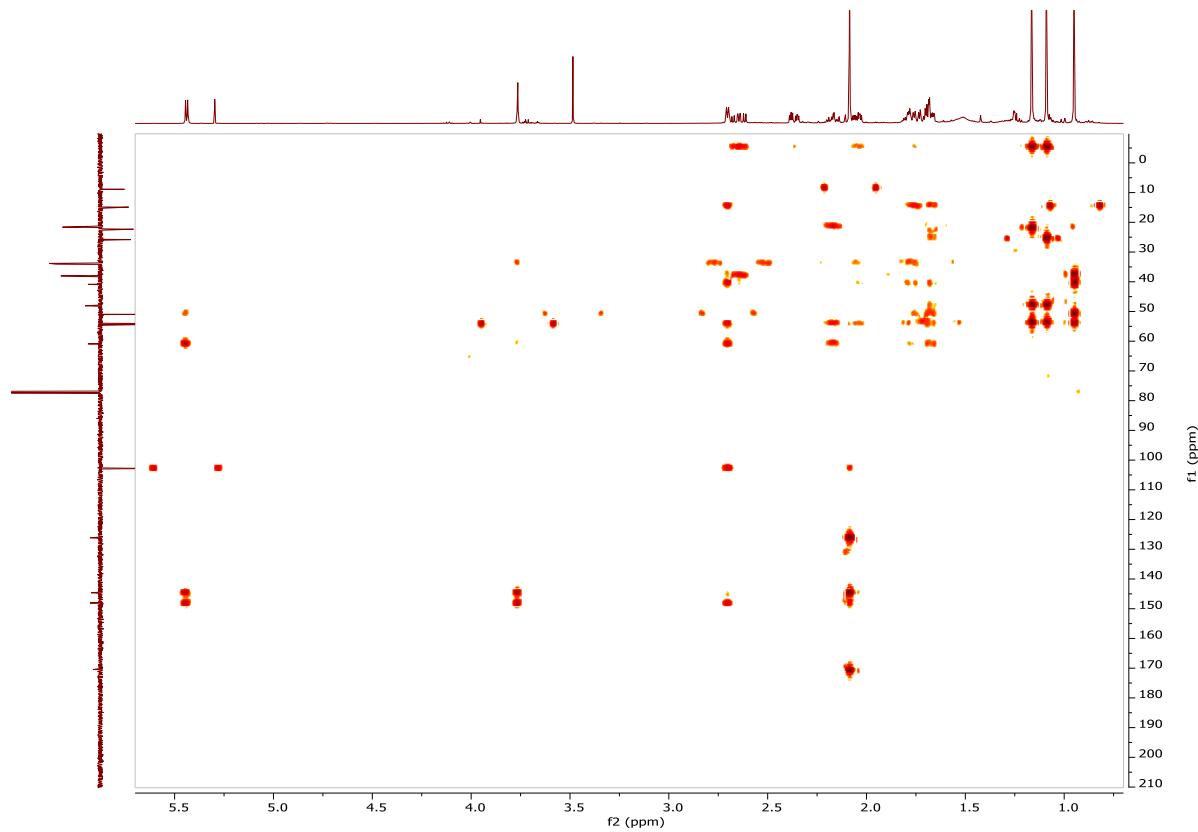


Figure S96. The HMBC spectrum of *ent*-8 β ,14 β -epoxyabieta-3-one-11,13(15)-dien-16,12-olide (**19**).

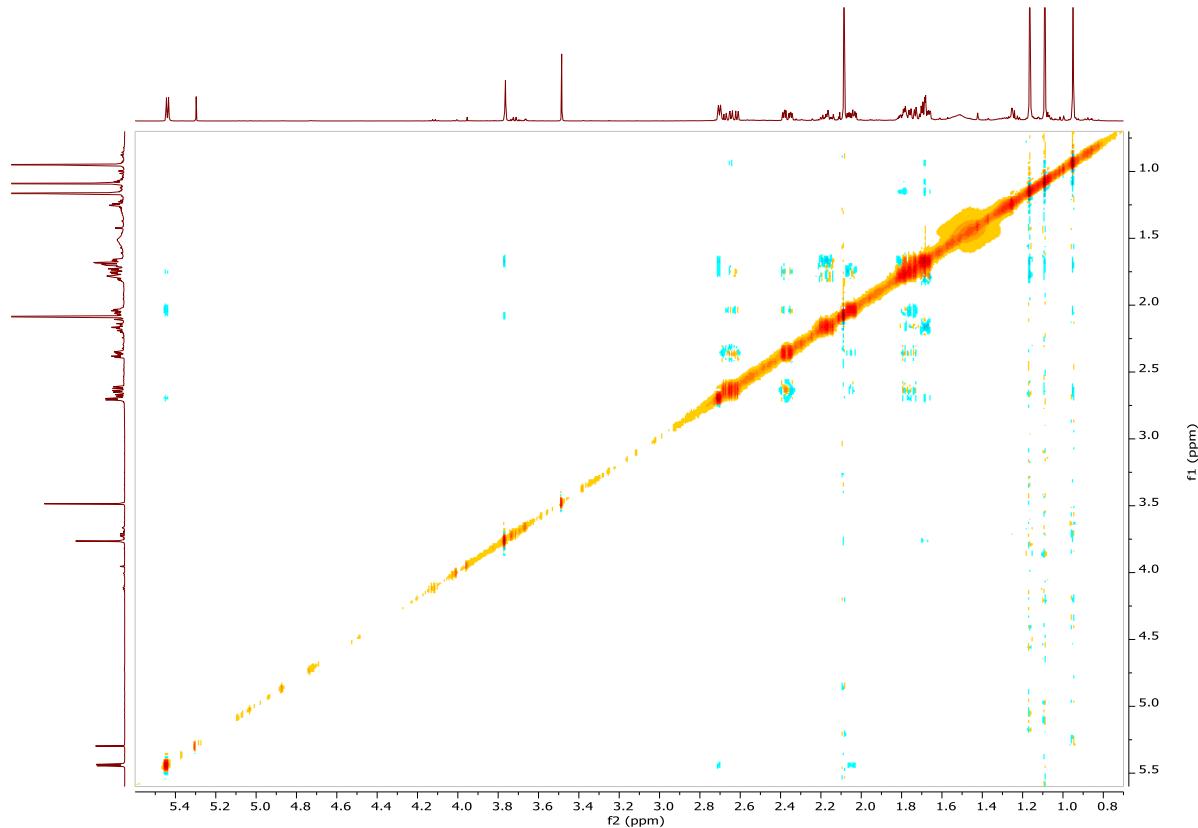


Figure S97. The NOESY spectrum of *ent*-8 β ,14 β -epoxyabieta-3-one-11,13(15)-dien-16,12-olide (**19**).

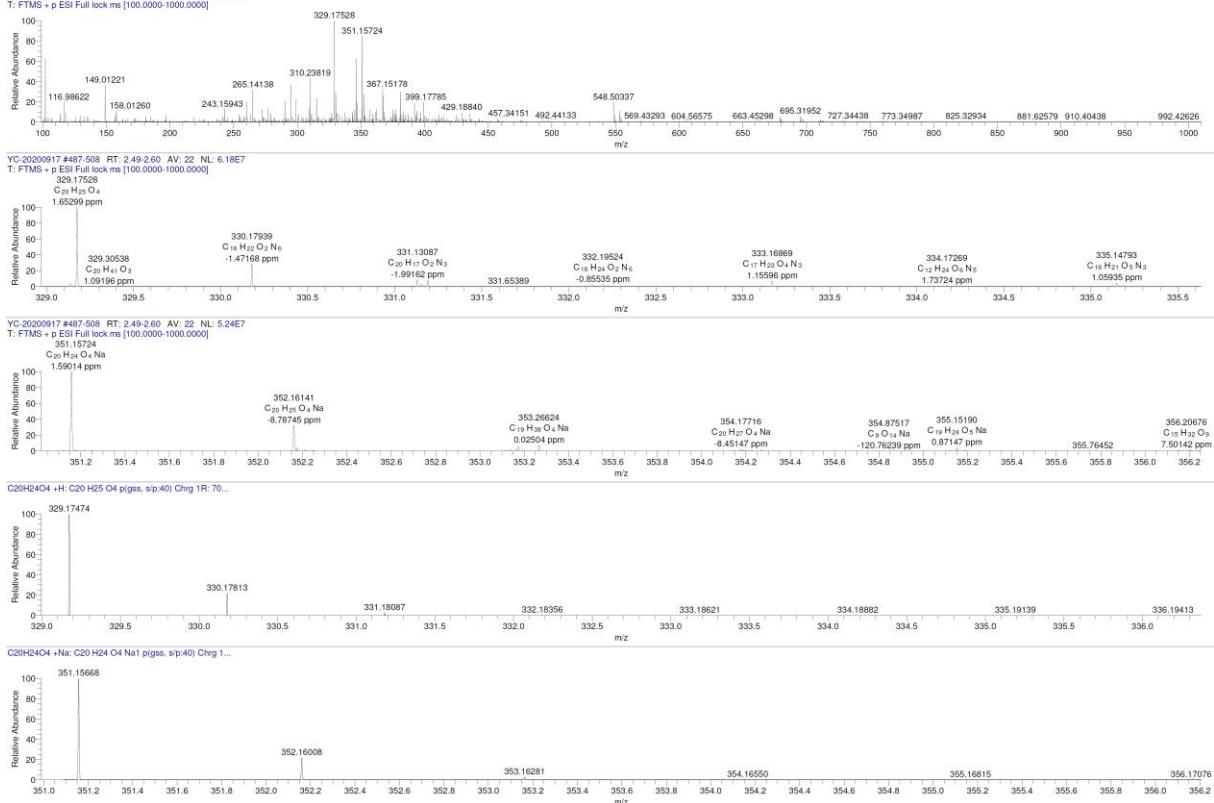


Figure S98. The HR-ESI-MS spectra of *ent*-8 β ,14 β -epoxyabiet-3-one-11,13(15)-dien-16,12-olide (19).

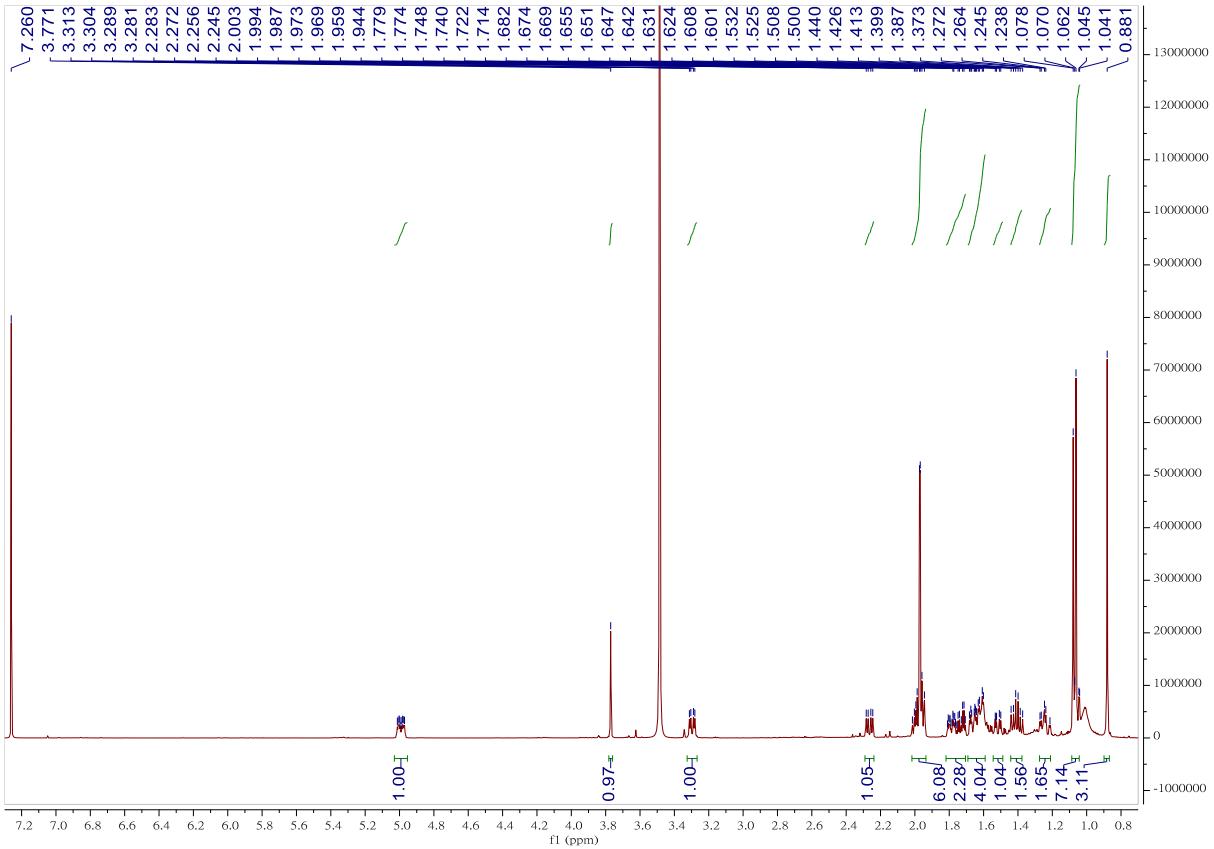


Figure S99. The ¹H-NMR spectrum of *ent*-8 β ,14 β -epoxyabieta-3 α -hydroxy-13(15)-en-16,12-olide (**20**) (500 MHz, CDCl₃).

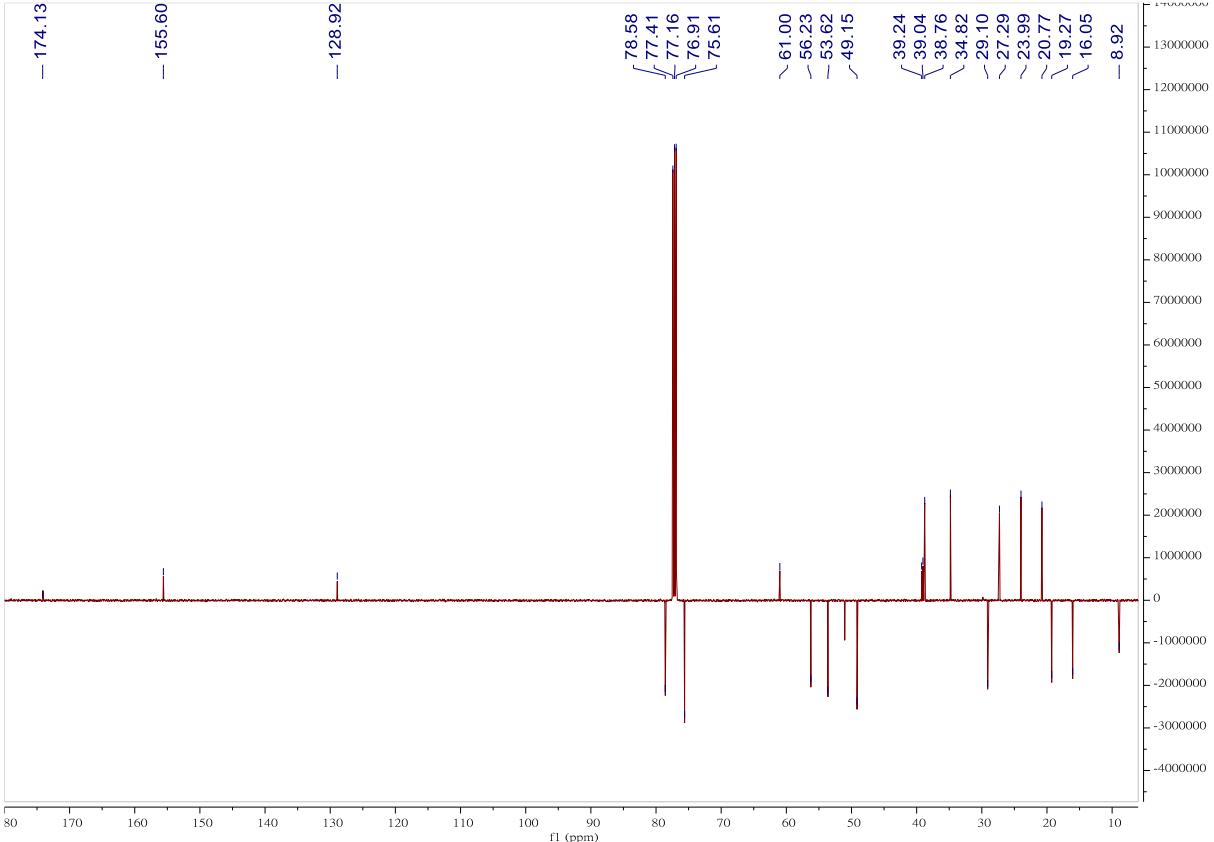


Figure S100. The ¹³C-JMOD spectrum of *ent*-8 β ,14 β -epoxyabieta-3 α -hydroxy-13(15)-en-16,12-olide (**20**) (125 MHz, CDCl₃).

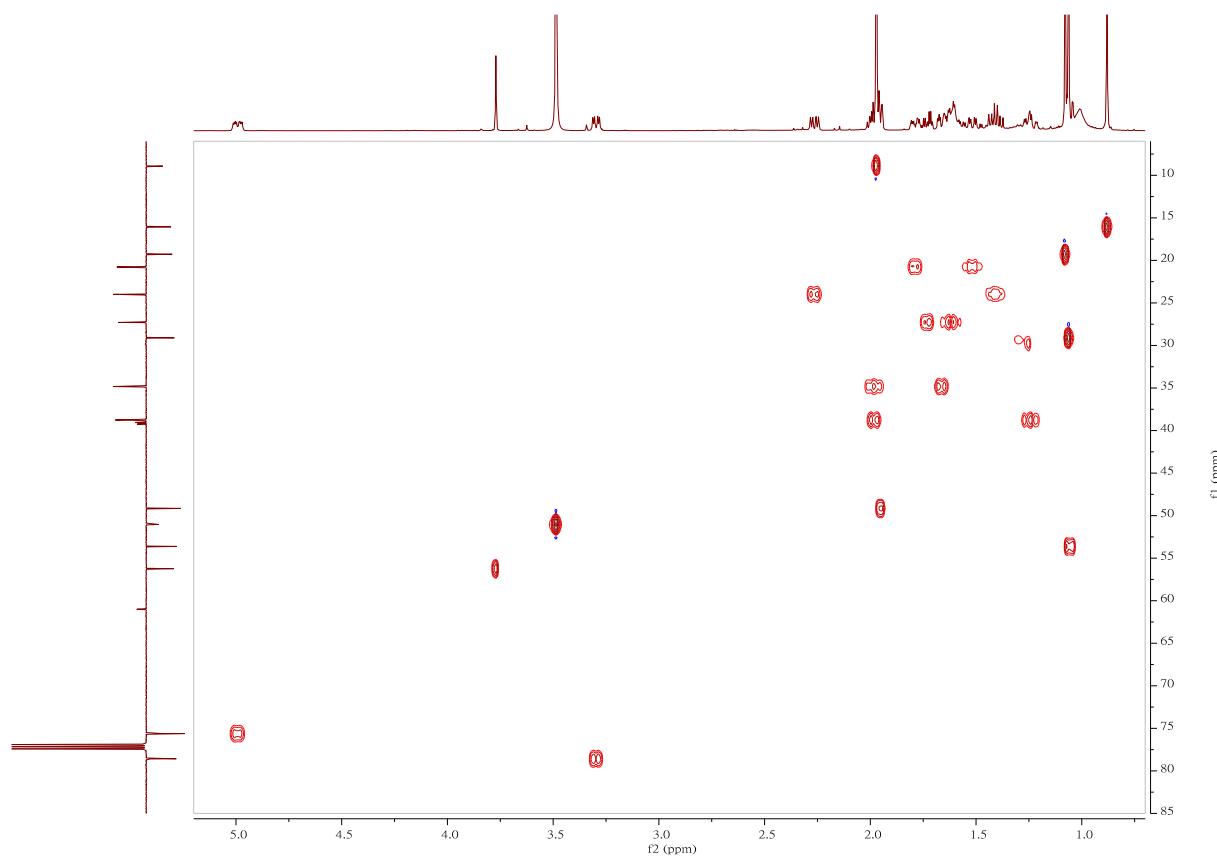


Figure S101. The HSQC spectrum of *ent*-8 β ,14 β -epoxyabieta-3 α -hydroxy-13(15)-en-16,12-olide (20).

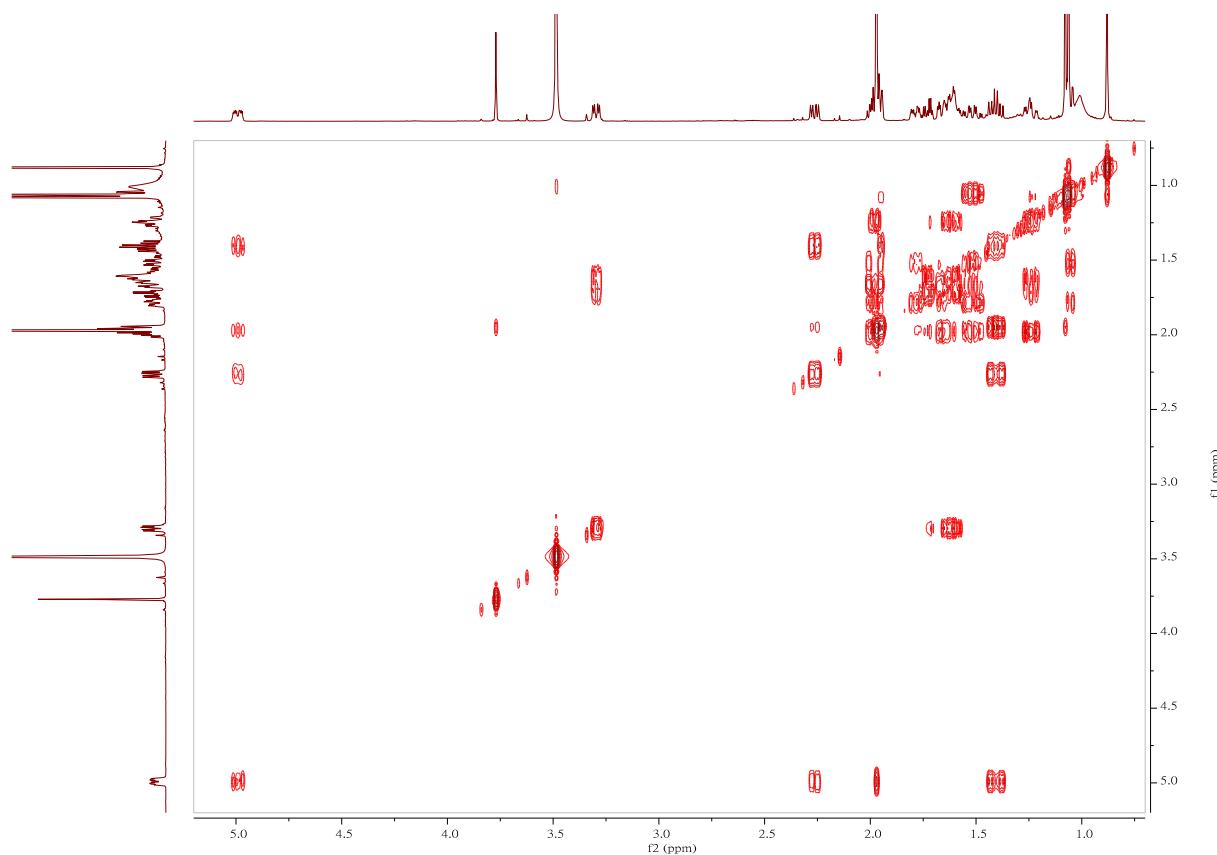


Figure S102. The ¹H-¹H COSY spectrum of *ent*-8 β ,14 β -epoxyabieta-3 α -hydroxy-13(15)-en-16,12-olide (20).

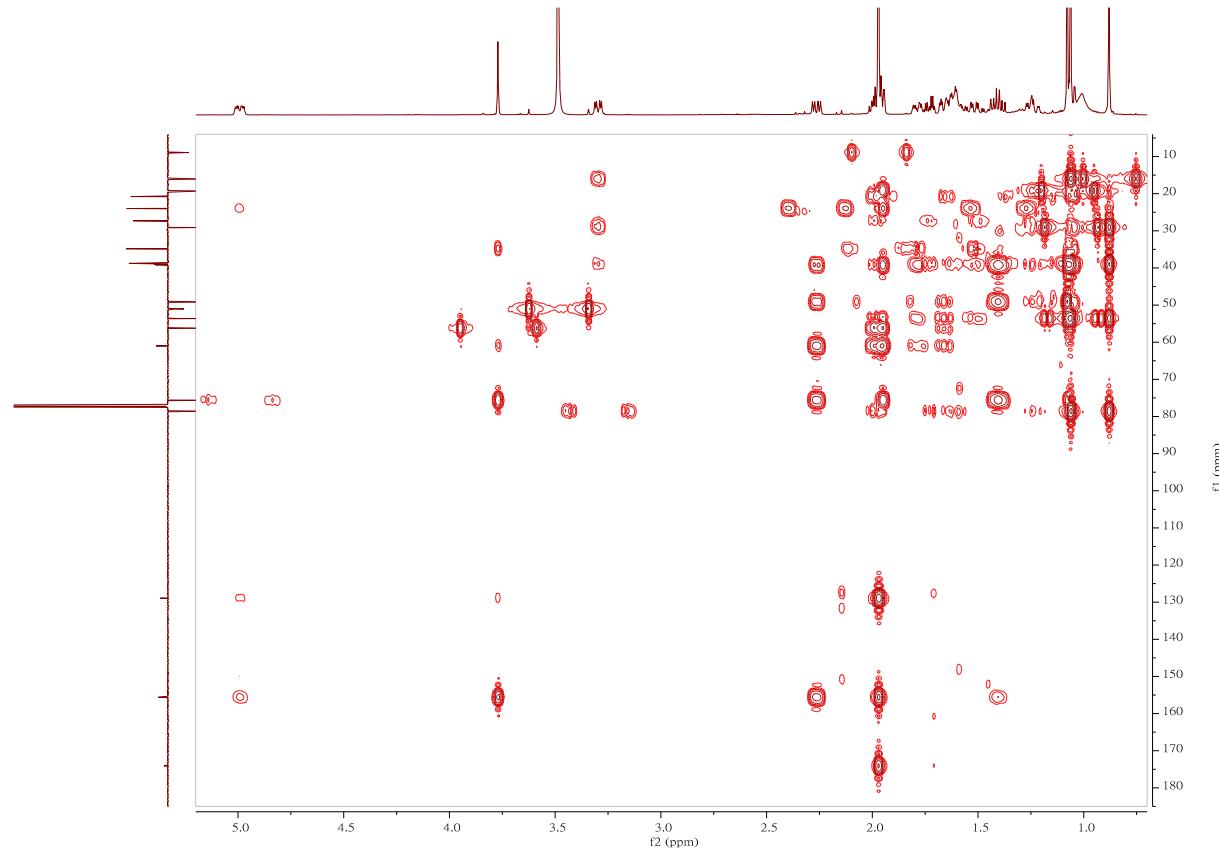


Figure S103. The HMBC spectrum of *ent*-8 β ,14 β -epoxyabieta-3 α -hydroxy-13(15)-en-16,12-olide (20).

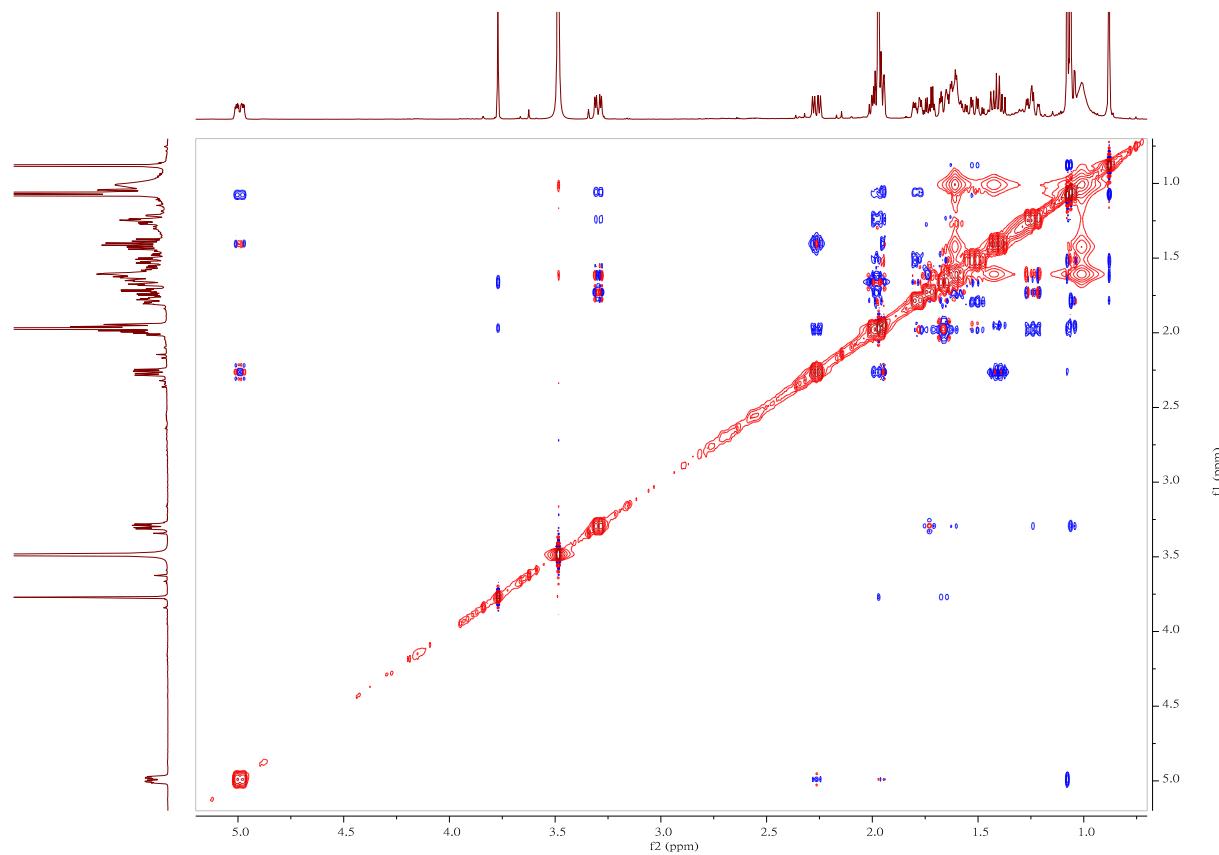


Figure S104. The NOESY spectrum of *ent*-8 β ,14 β -epoxyabieta-3 α -hydroxy-13(15)-en-16,12-olide (20).

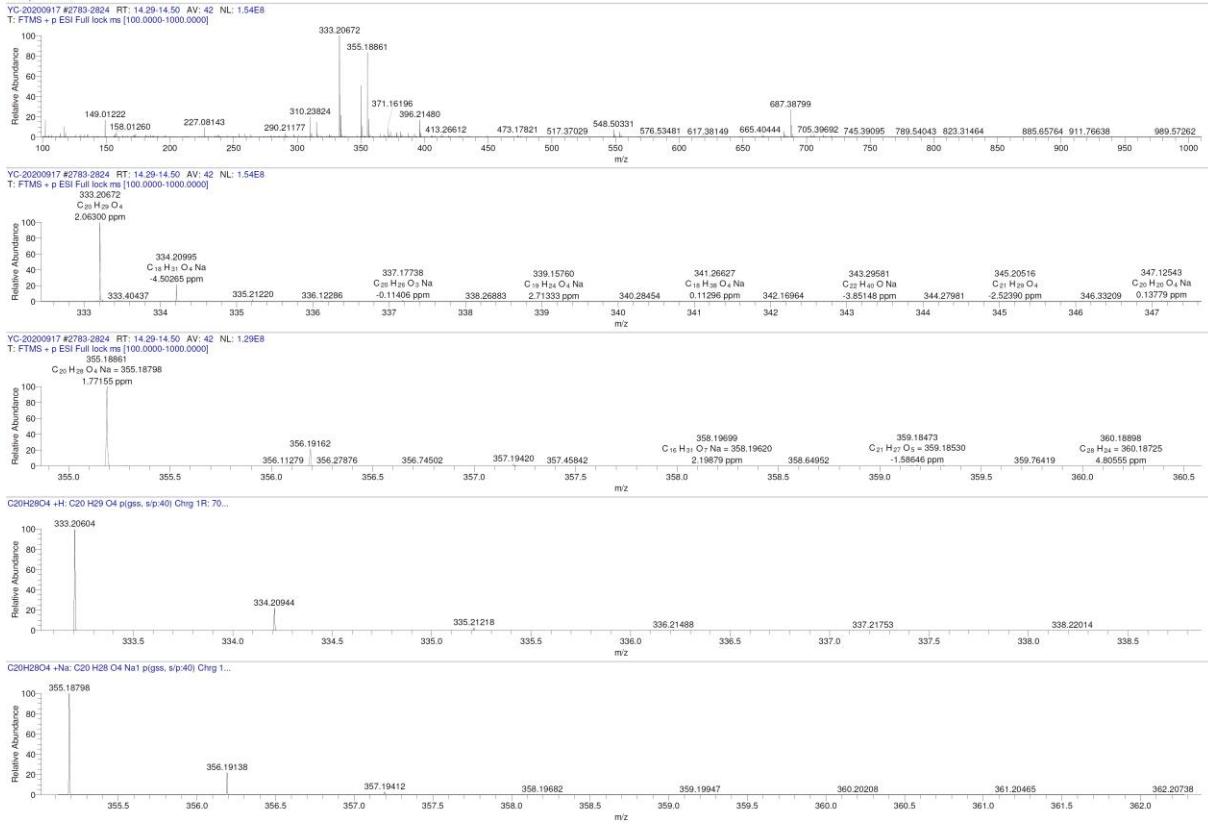


Figure S105. The HR-ESI-MS spectra of *ent*-8 β ,14 β -epoxyabiet-3 α -hydroxy-13(15)-en-16,12-olide (20).

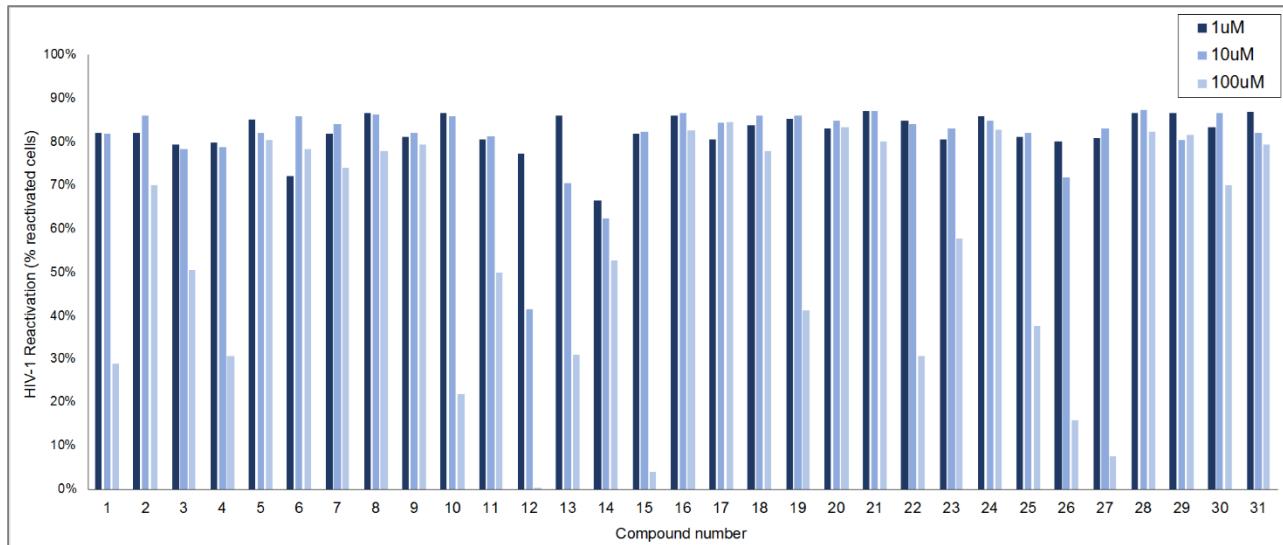


Figure S106. 24 hours cell viability after exposure to the compounds **1–31**.

All compounds were resuspended in DMSO at a concentration of 10 mM, and diluted with PBS and tested with J-lat 10.6 cells at concentrations of 100 μ M, 10 μ M, and 1 μ M. 1% DMSO was used as a control to account for any effect of DMSO in the highest dilution of compounds.