# **Heterodimeric *ent*-Kauranoids** from *Isodon tenuifolius*

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Jian-Xin Pu[*,†] and Han-Dong Sun[†]

## Supporting Information List

### Characterization Data of New Compounds



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[†] Kunming Institute of Botany, Chinese Academy of Sciences.

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**For compound 1:**

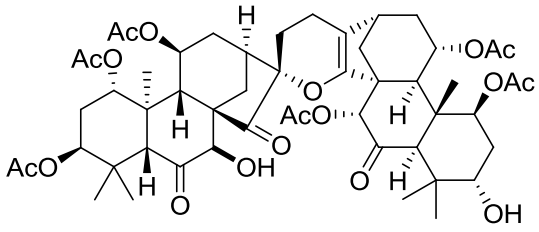



Figure 1. $^{1}$H NMR spectrum of bistenuifolin A (**1**)

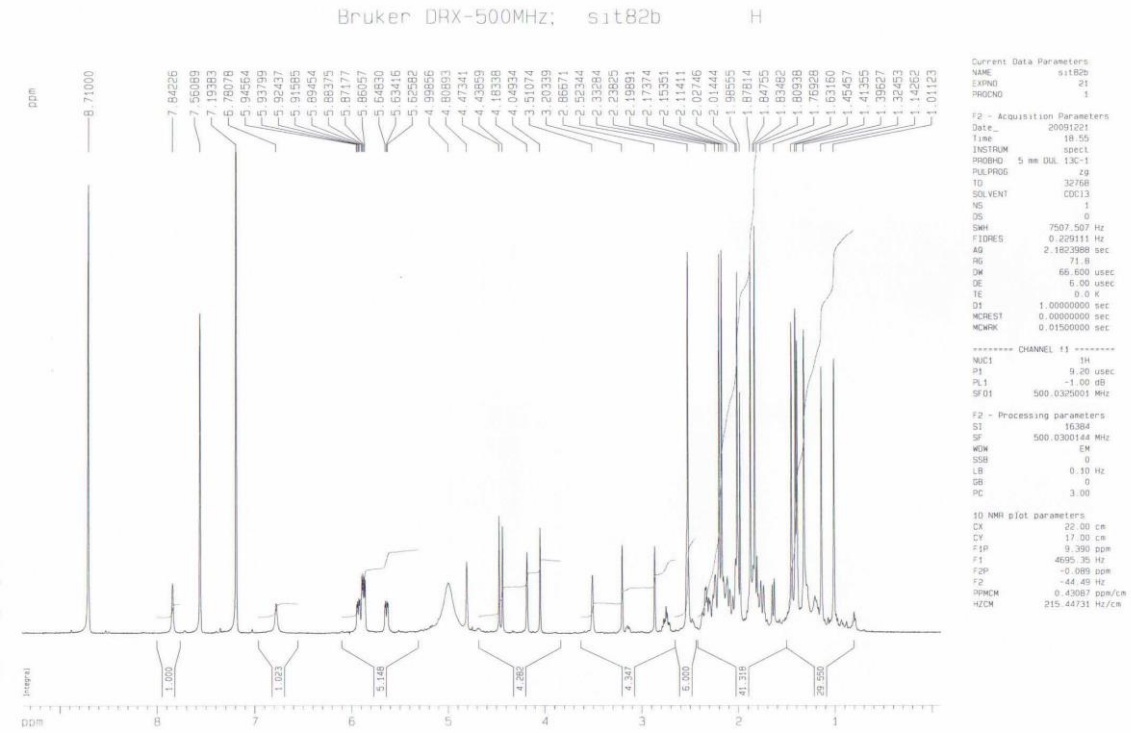


Figure 2. $^{13}$C NMR spectrum of bistenuifolin A (**1**)

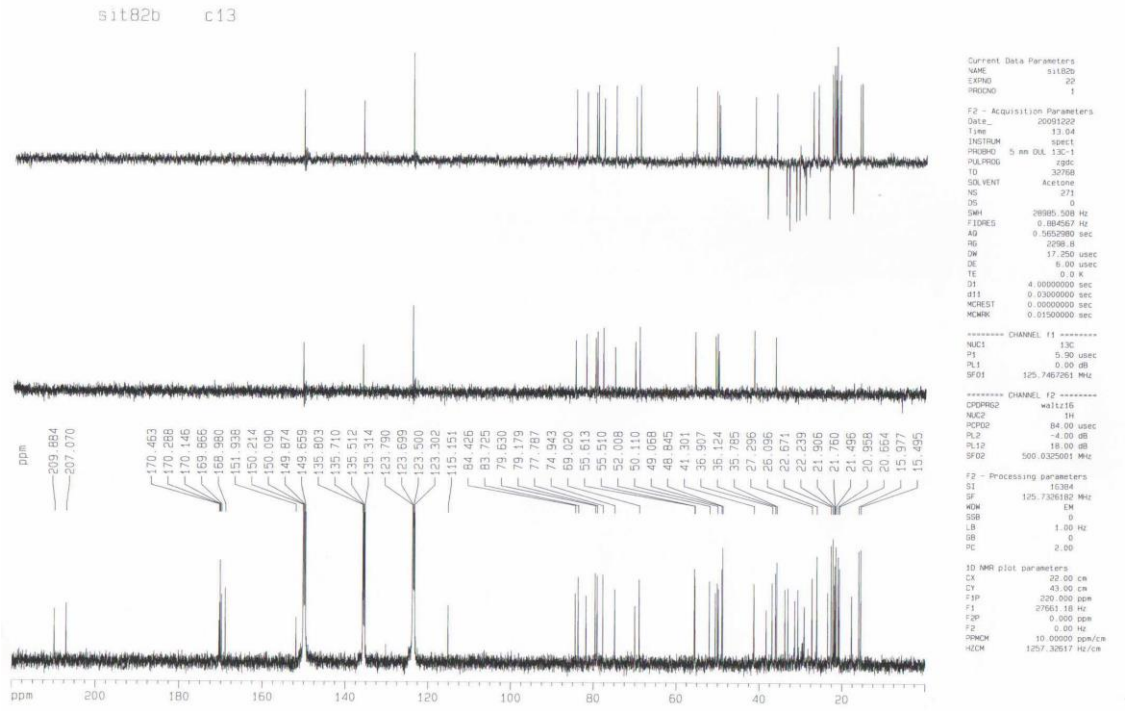



Figure 3. HSQC spectrum of bistenuifolin A (**1**)

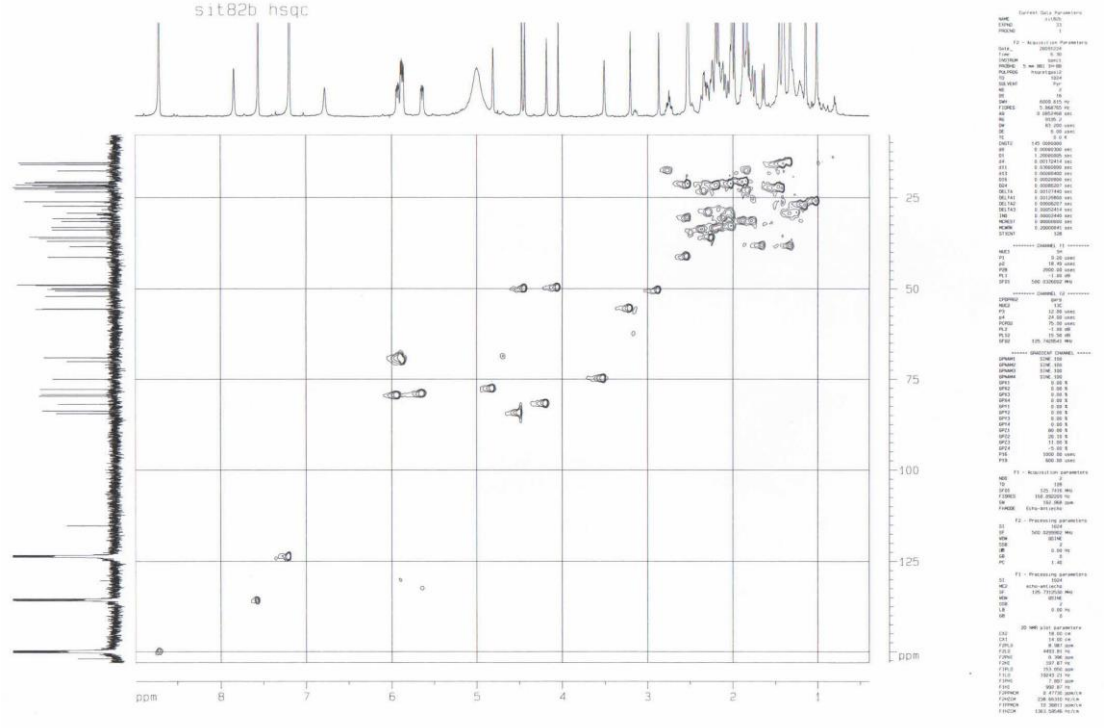


Figure 4. HMBC spectrum of bistenuifolin A (**1**)

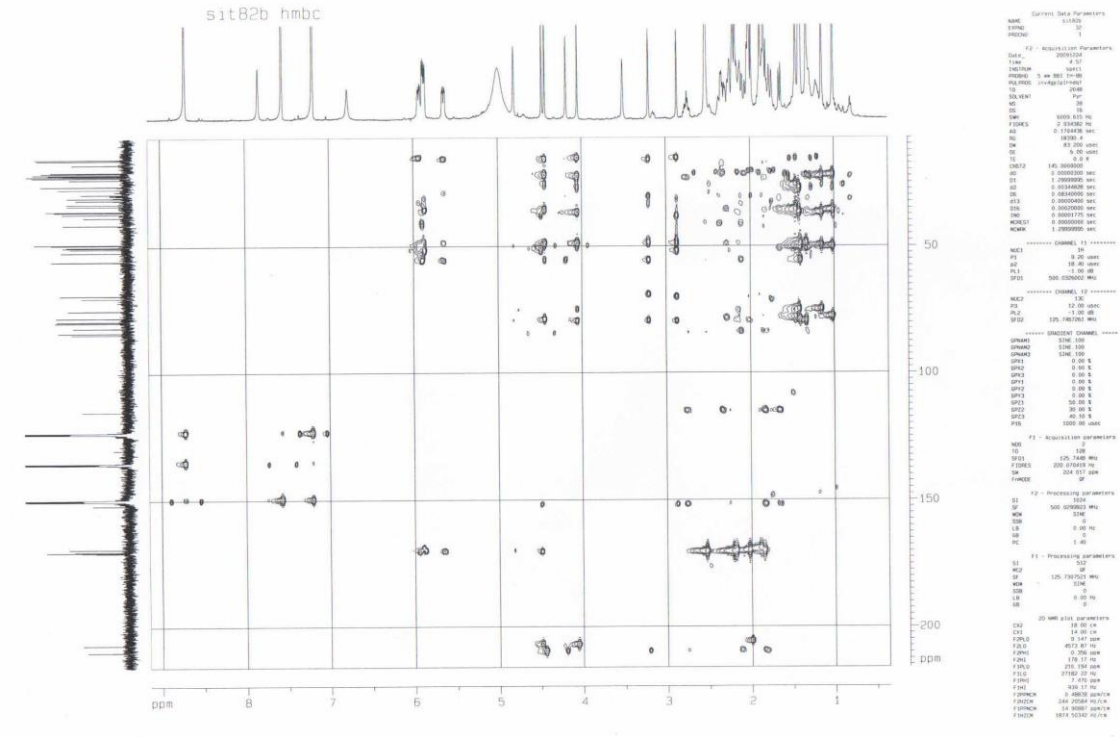



Figure 5. COSY spectrum of bistenuifolin A (**1**)

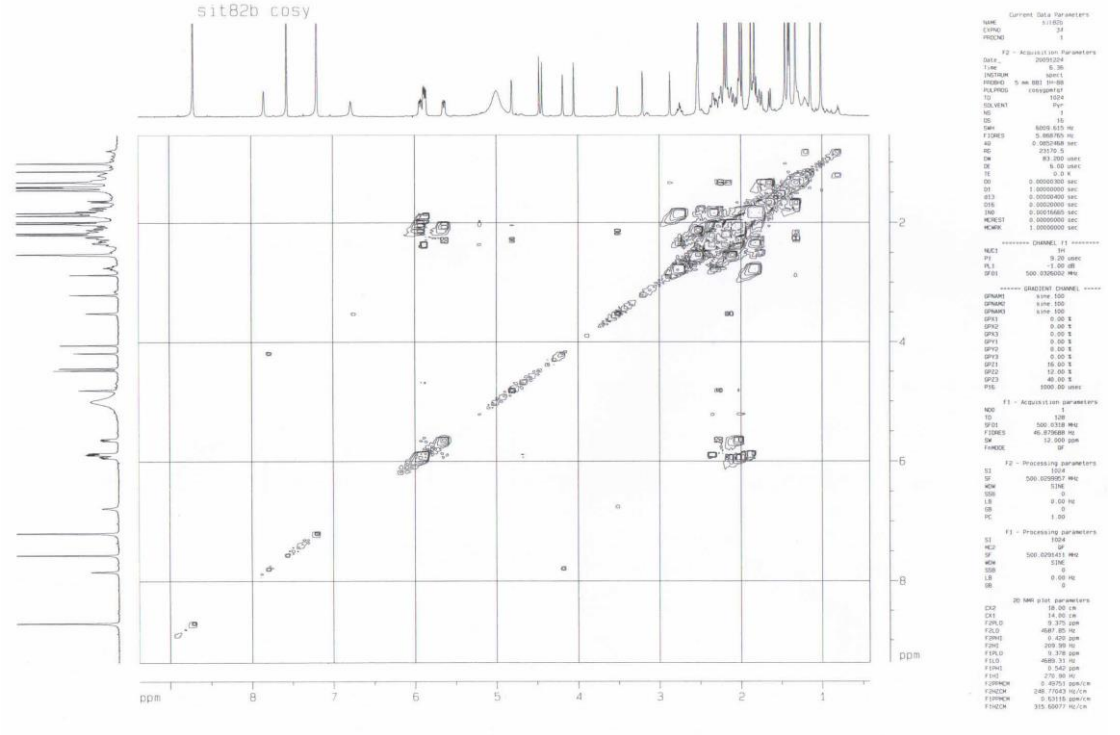


Figure 6. ROESY spectrum of bistenuifolin A (**1**)

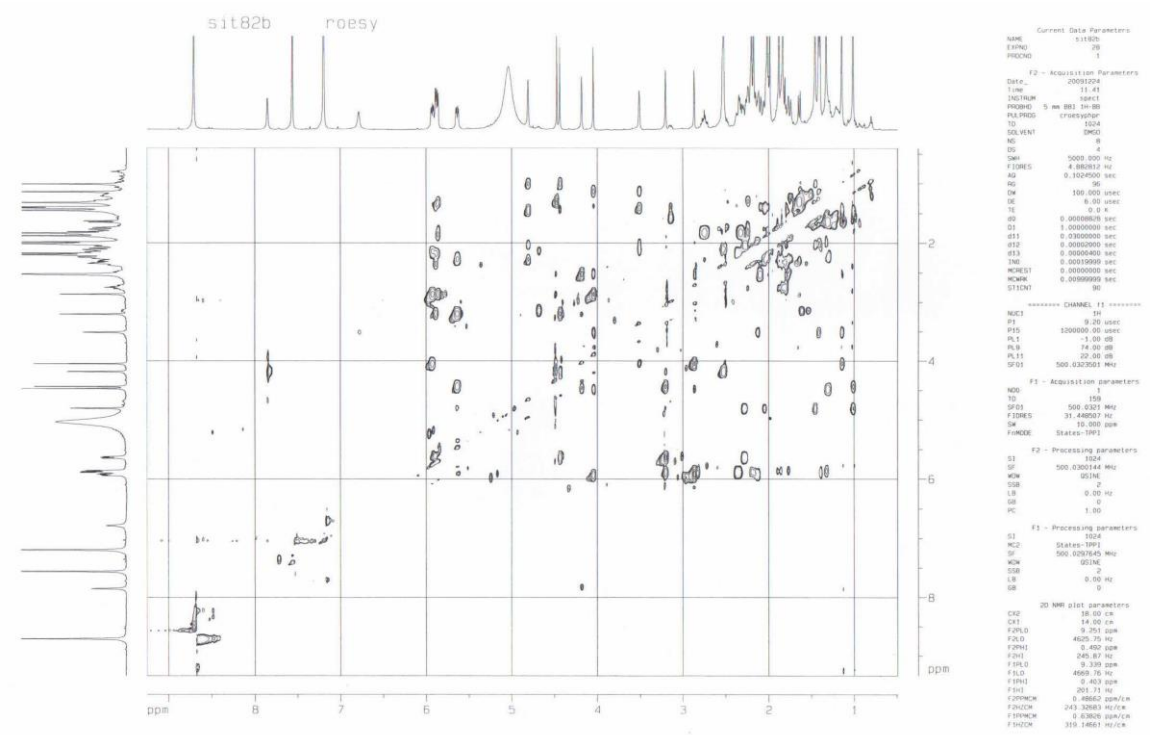
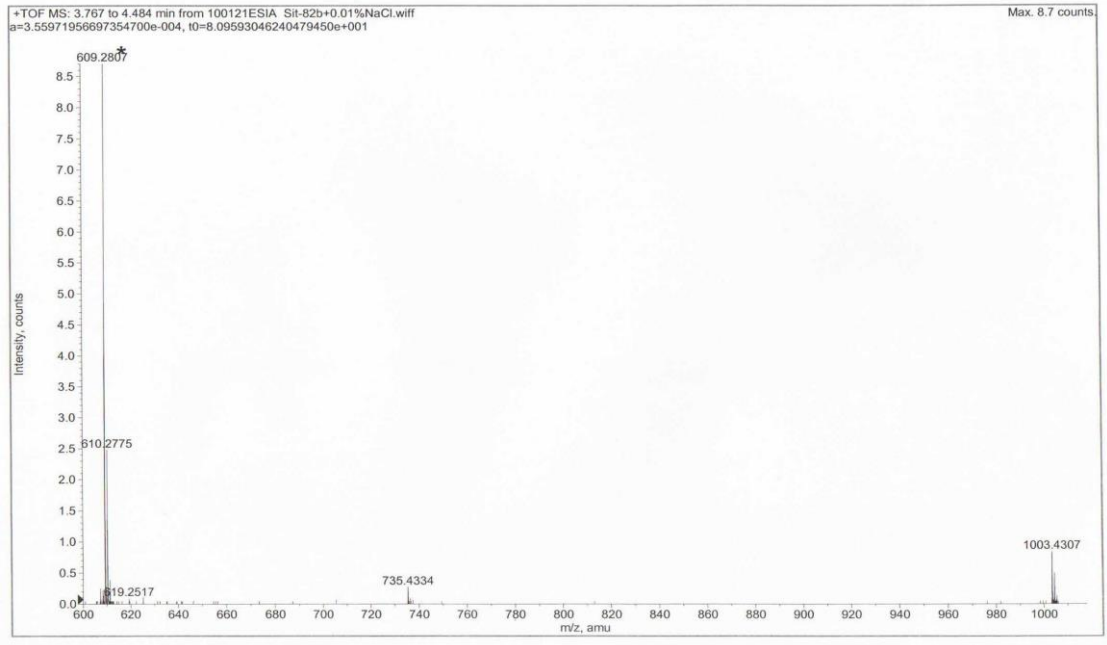
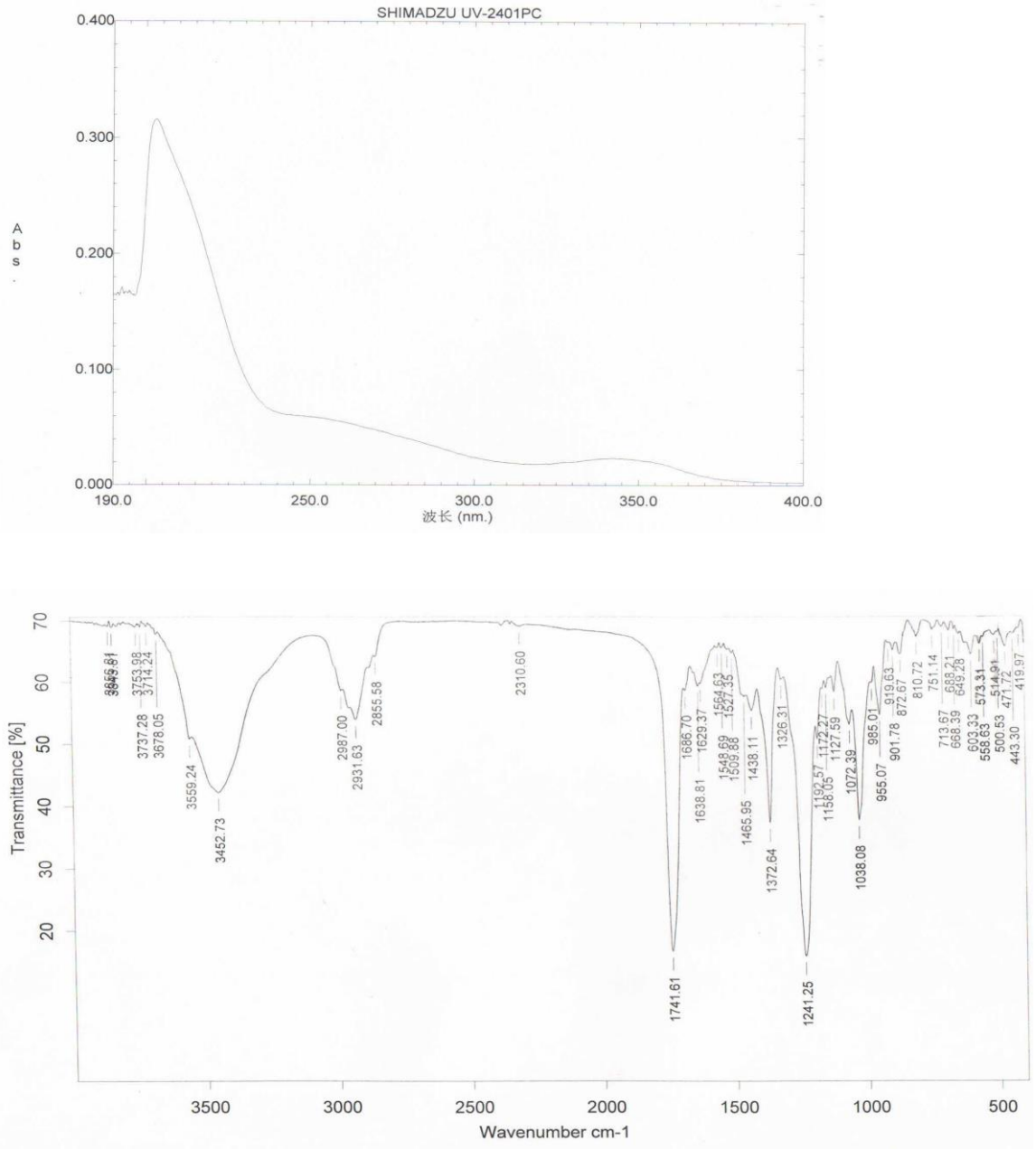



Figure 7. HRESIMS spectrum of bistenuifolin A (**1**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C52 H68 O18 Na | 1003.4303 | 0.3640 | 0.3628 | 18.5 |

Figure 8. UV and IR spectra of bistenuifolin A (**1**)



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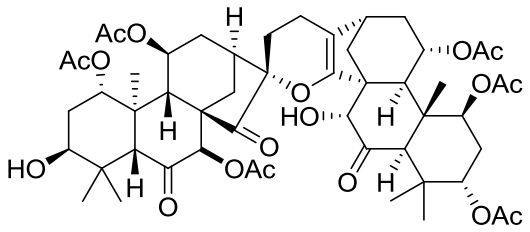



Figure 9. $^{1}$H NMR spectrum of bistenuifolin B (**2**)

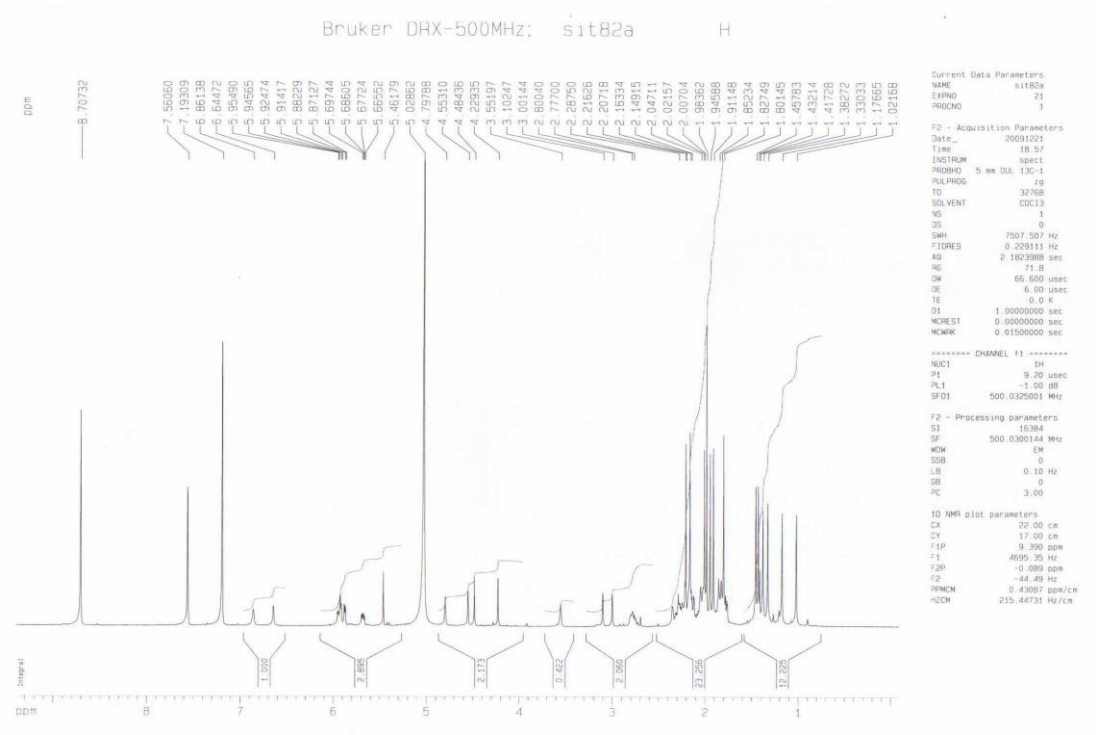


Figure 10. $^{13}$C NMR spectrum of bistenuifolin B (**2**)

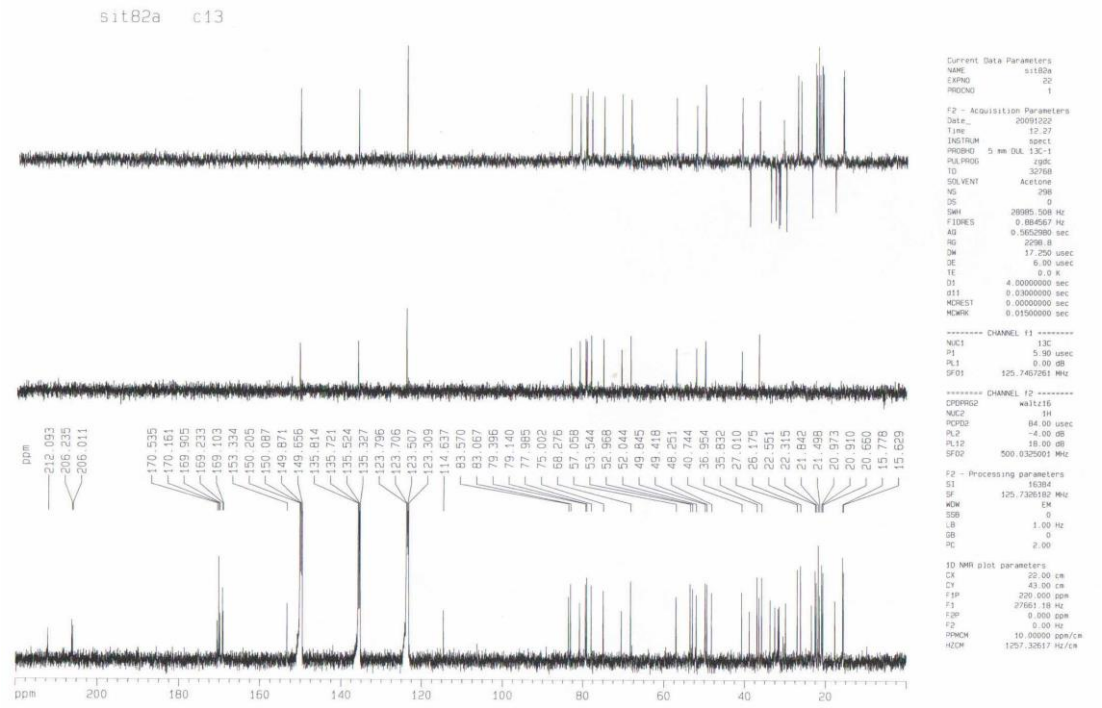



Figure 11. HSQC spectrum of bistenuifolin B (**2**)

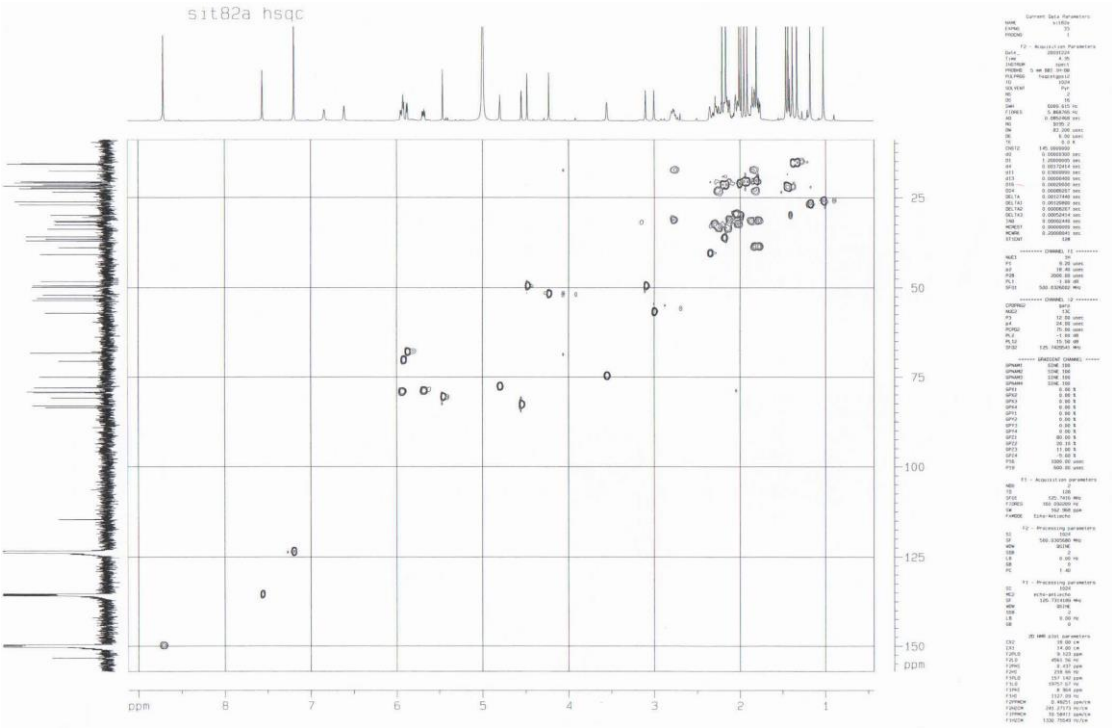


Figure 12. HMBC spectrum of bistenuifolin B (**2**)

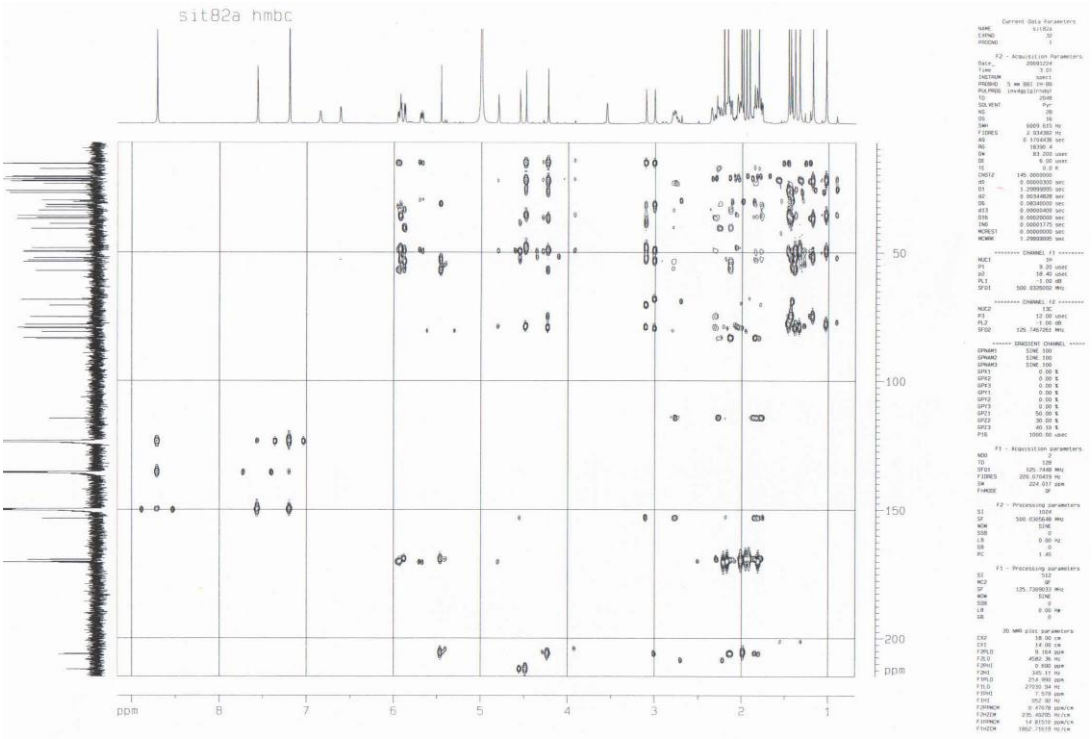



Figure 13. COSY spectrum of bistenuifolin B (**2**)

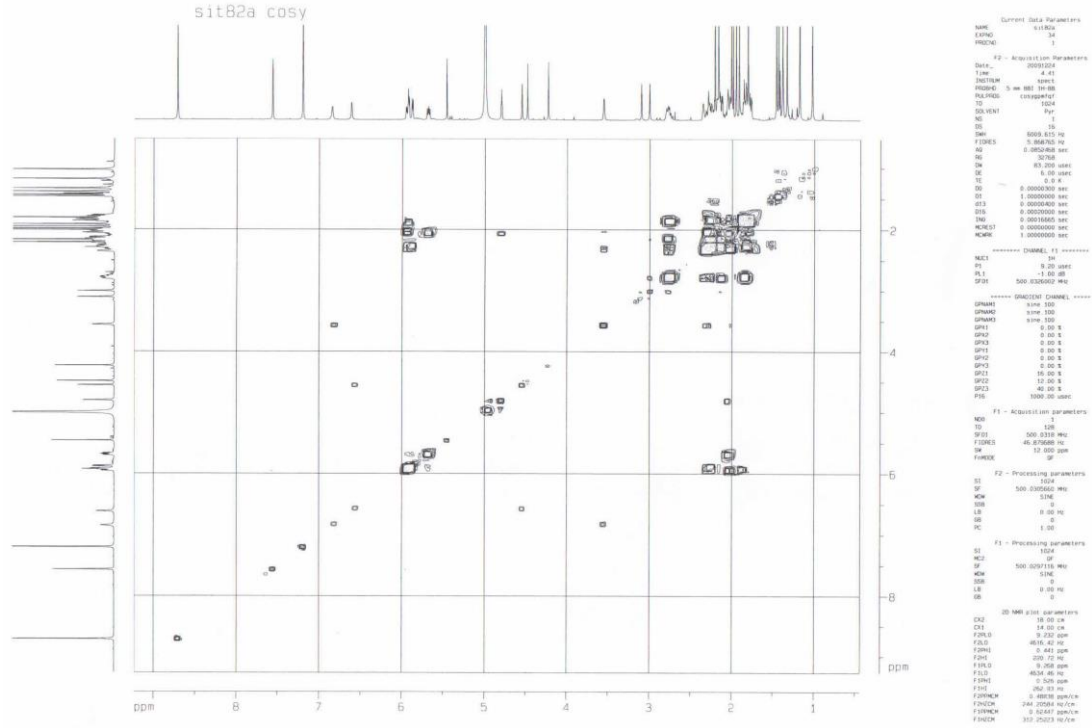


Figure 14. ROESY spectrum of bistenuifolin B (**2**)

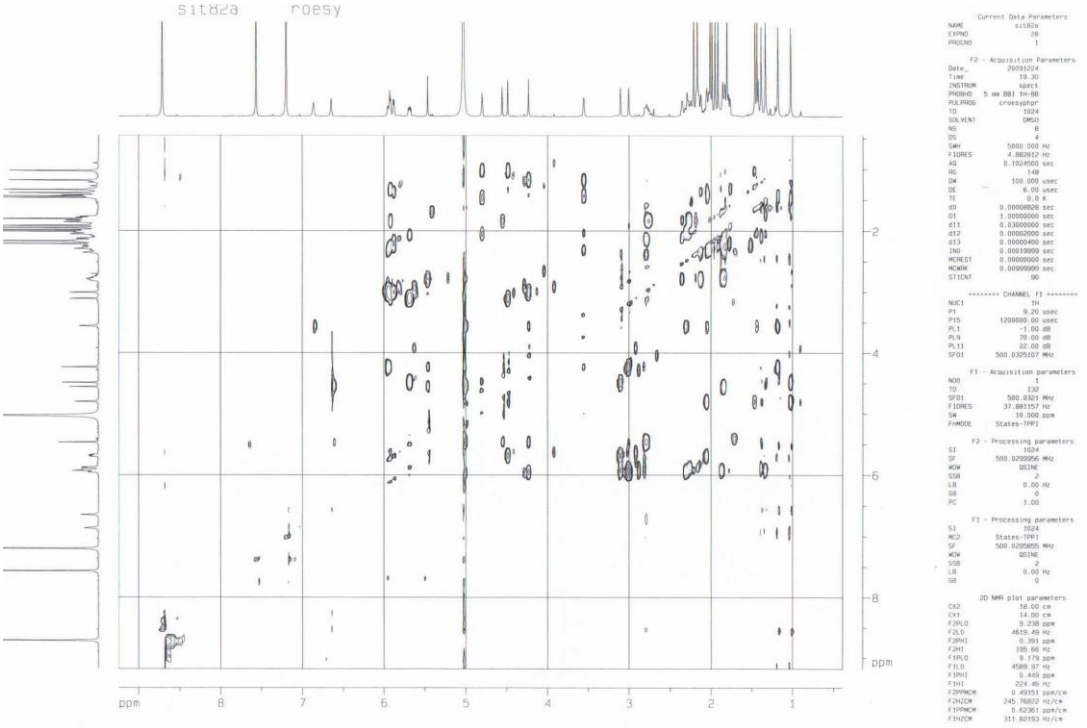
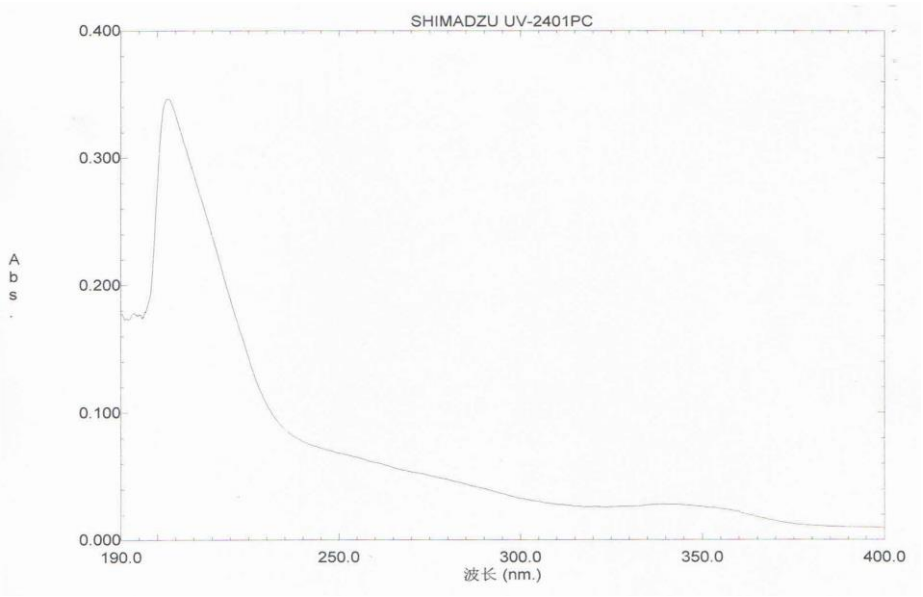
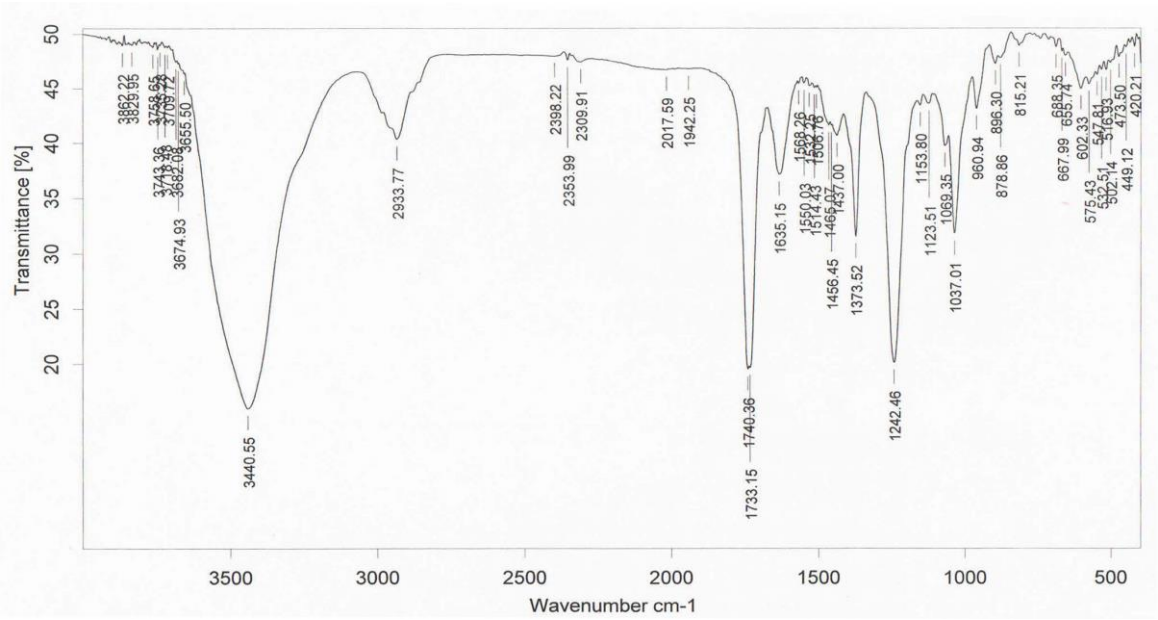



Figure 15. HRESIMS spectrum of bistenuifolin B (**2**)


| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C52 H68 O18 Na | 1003.4303 | 2.9640 | 2.9539 | 18.5 |

Figure 16. UV and IR spectra of bistenuifolin B (**2**)



**For compound 3:**

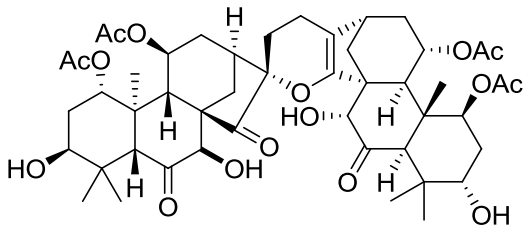



Figure 17. $^{1}$H NMR spectrum of bistenuifolin C (**3**)

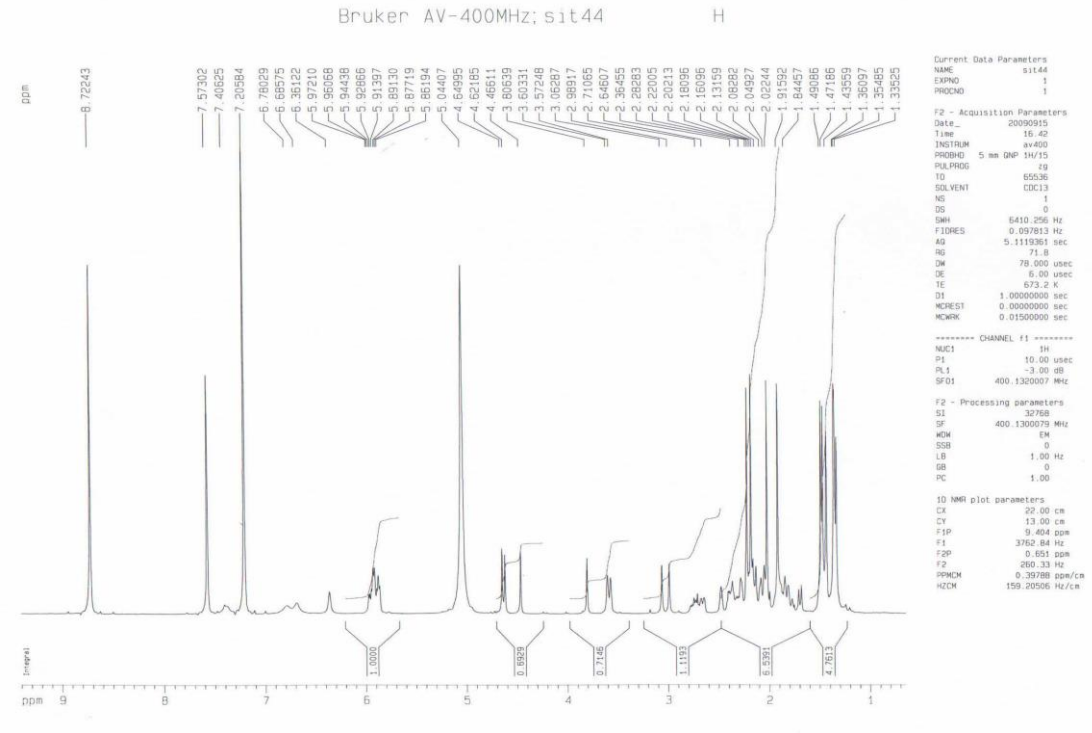


Figure 18. $^{13}$C NMR spectrum of bistenuifolin C (**3**)

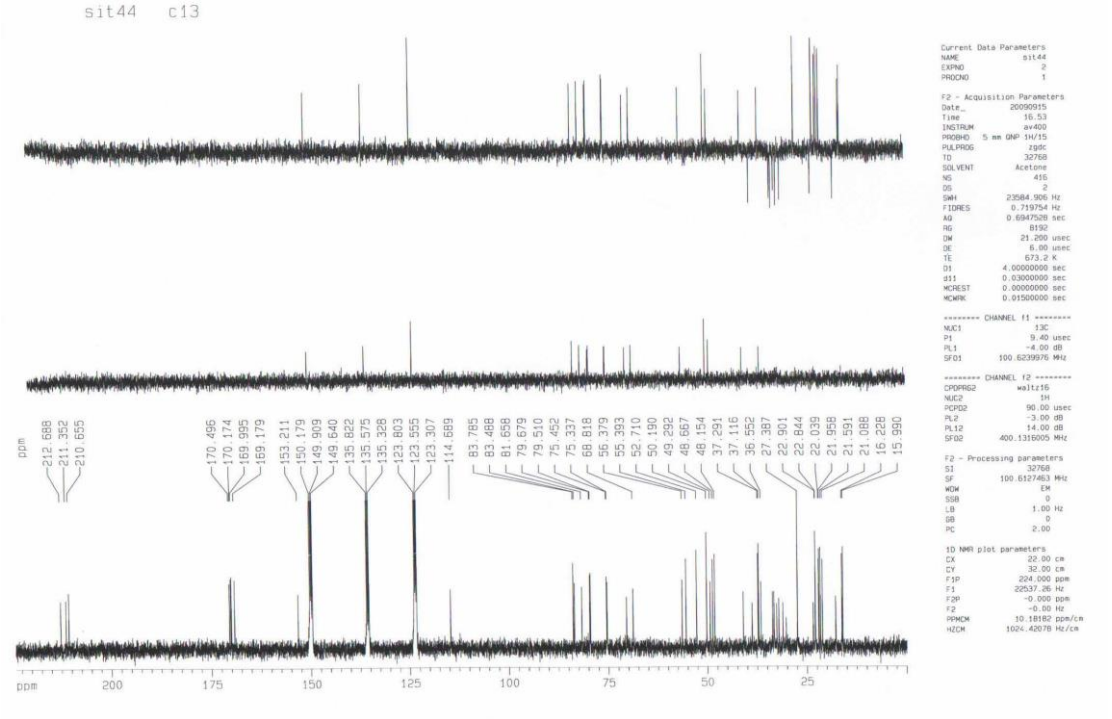



Figure 19. HSQC spectrum of bistenuifolin C (**3**)

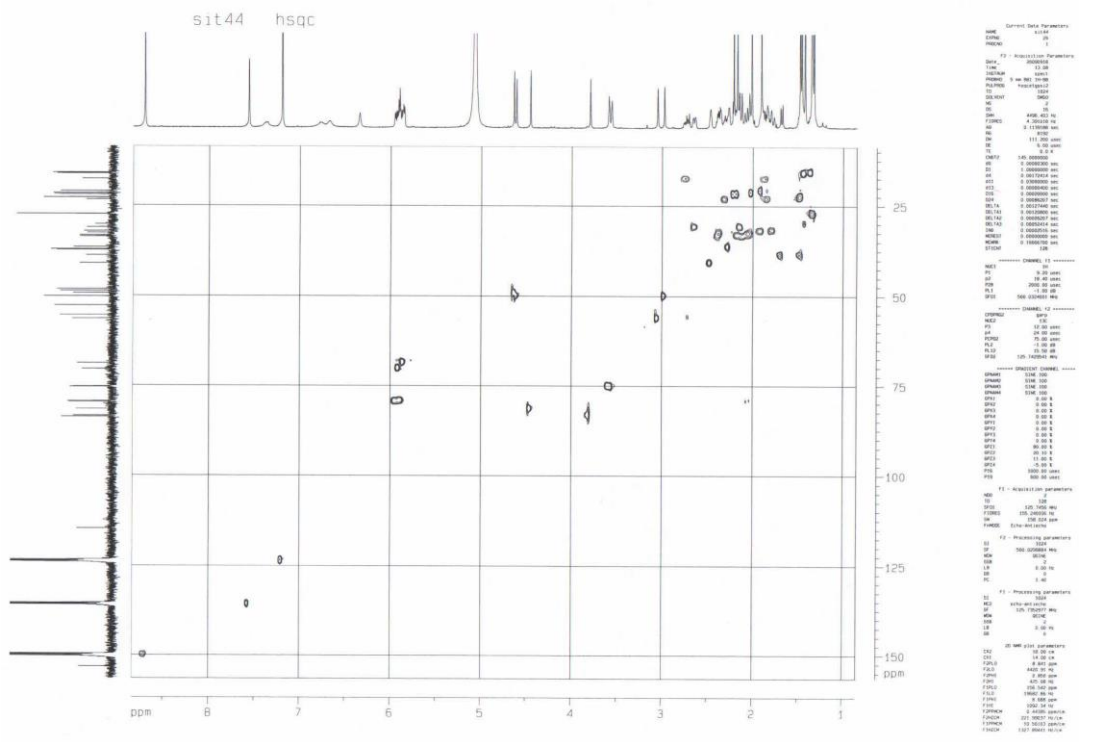


Figure 20. HMBC spectrum of bistenuifolin C (**3**)

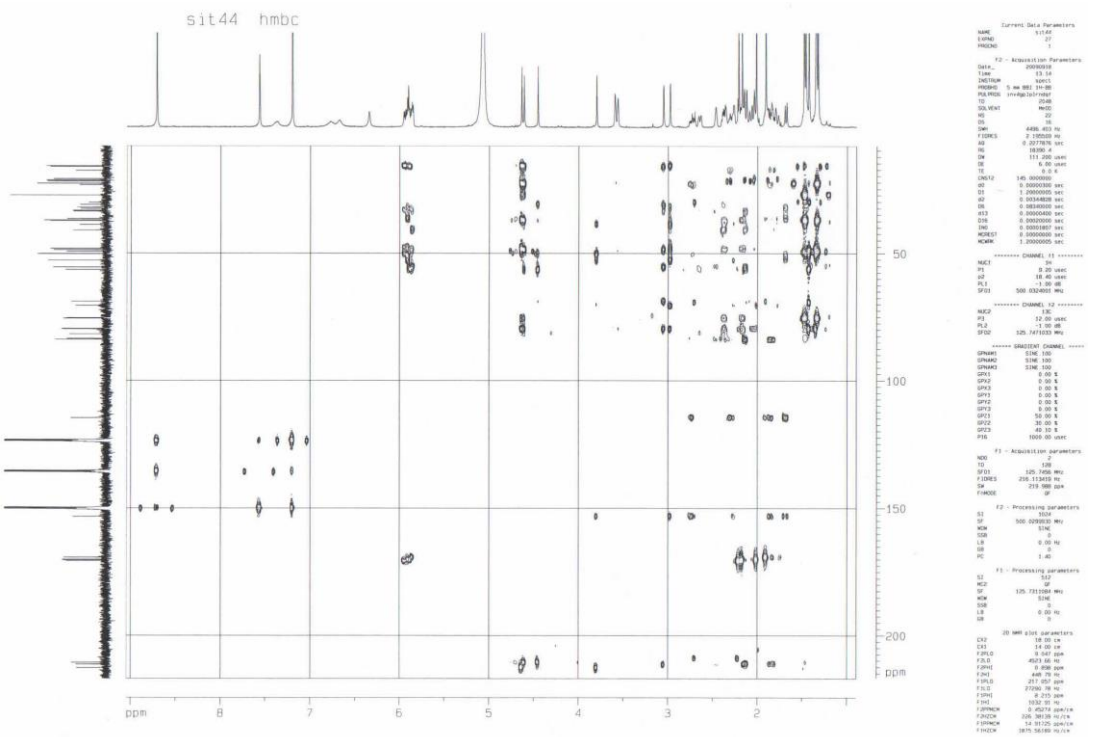



Figure 21. COSY spectrum of bistenuifolin C (**3**)

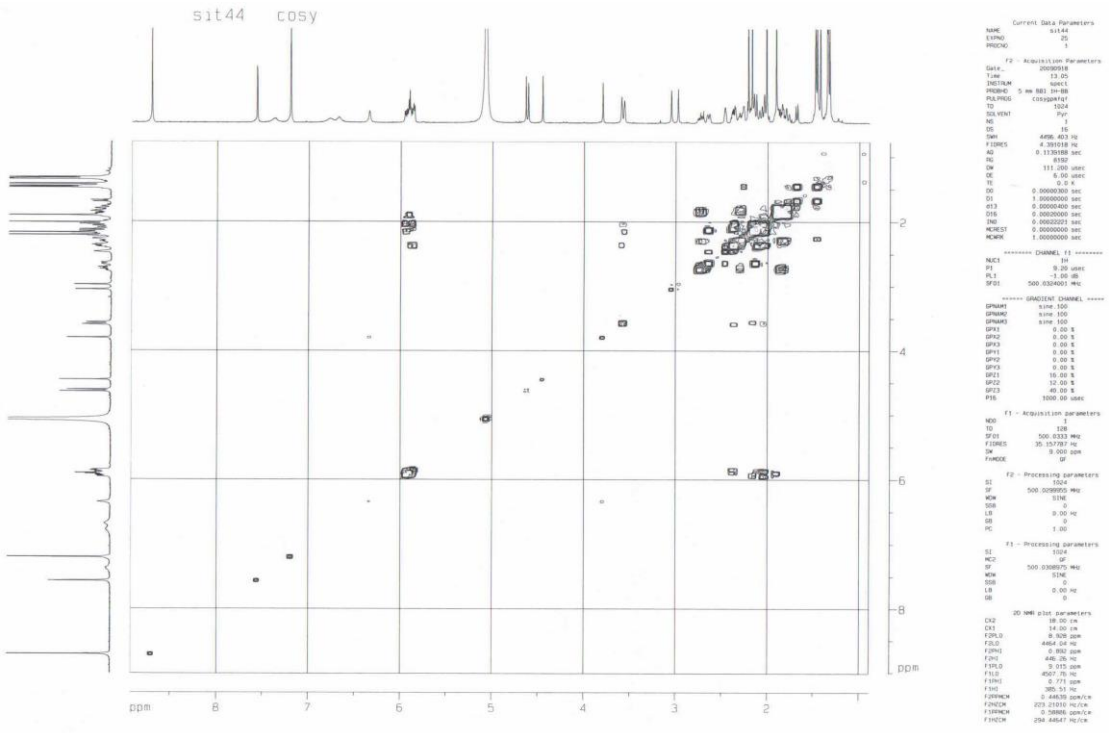


Figure 22. ROESY spectrum of bistenuifolin C (**3**)

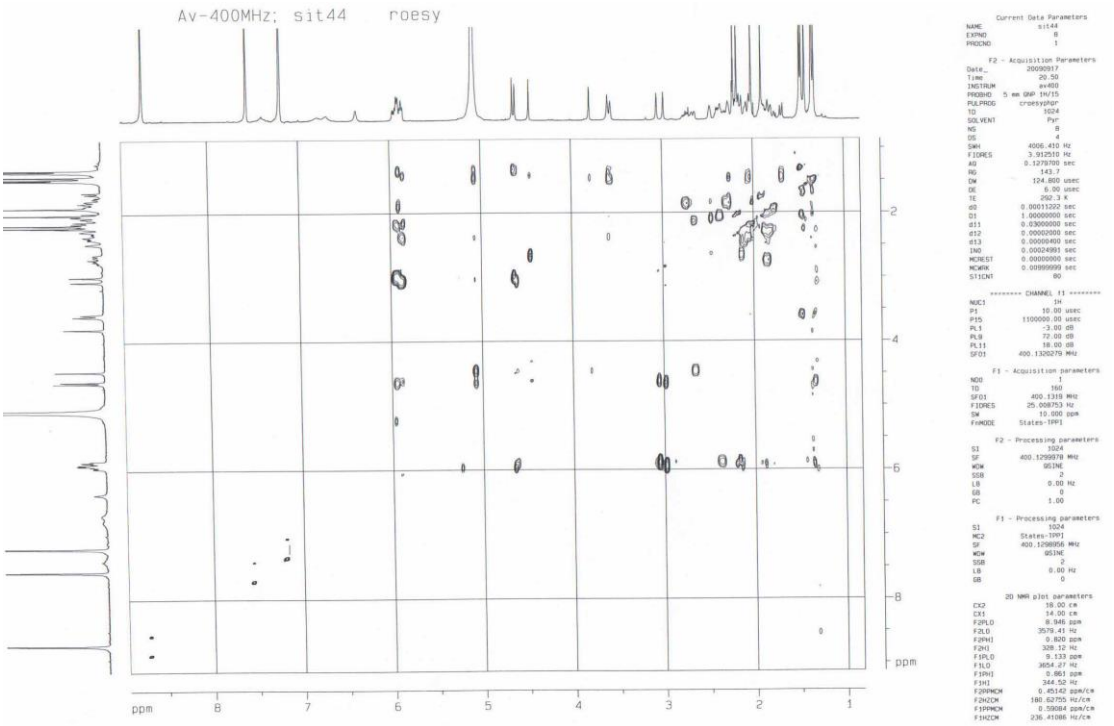
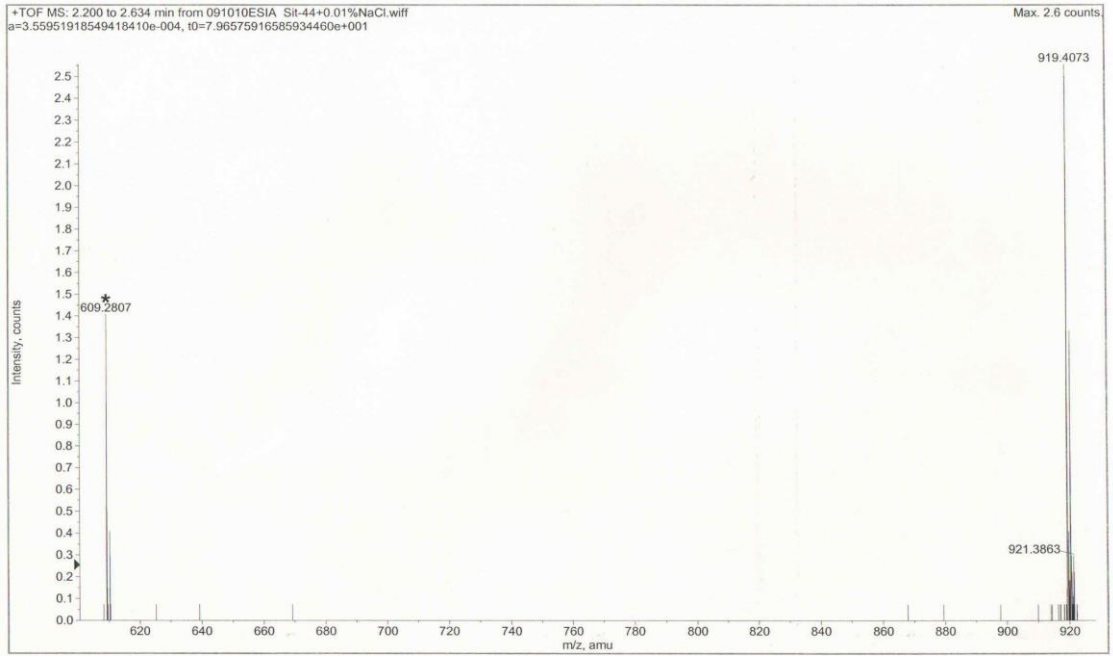
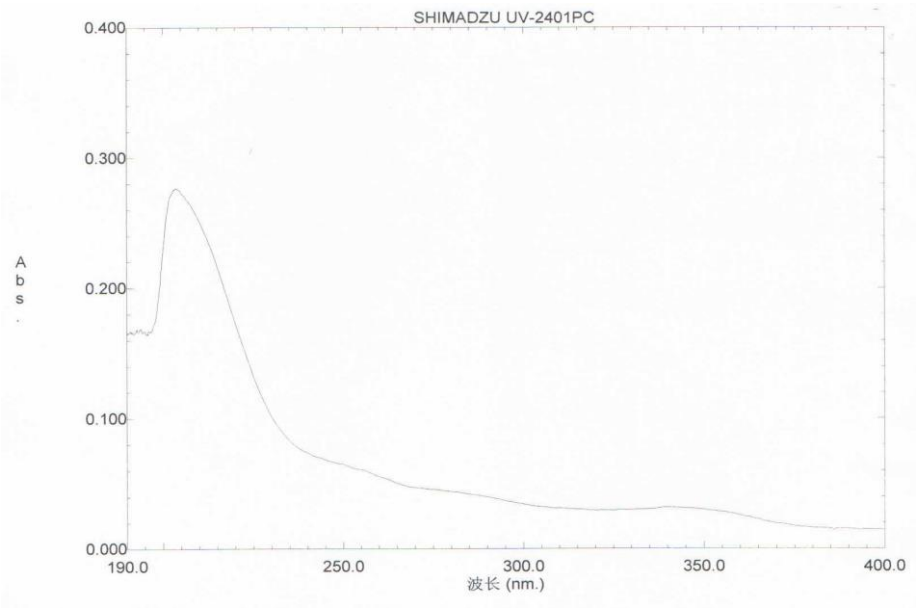


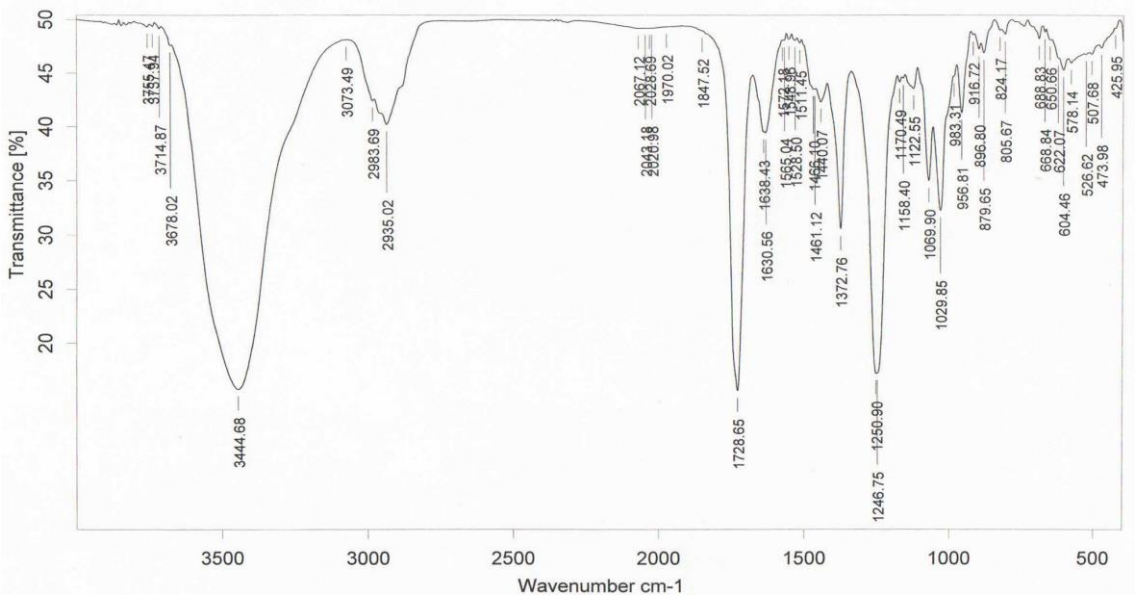

Figure 23. HRESIMS spectrum of bistenuifolin C (**3**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C48 H64 O16 Na | 919.4092 | -1.9065 | -2.0736 | 16.5 |

Figure 24. UV and IR spectra of bistenuifolin C (**3**)



**For compound 4:**

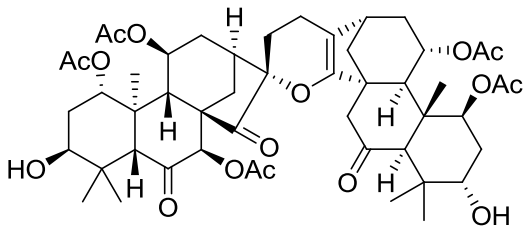



Figure 25. $^{1}$H NMR spectrum of bistenuifolin D (**4**)

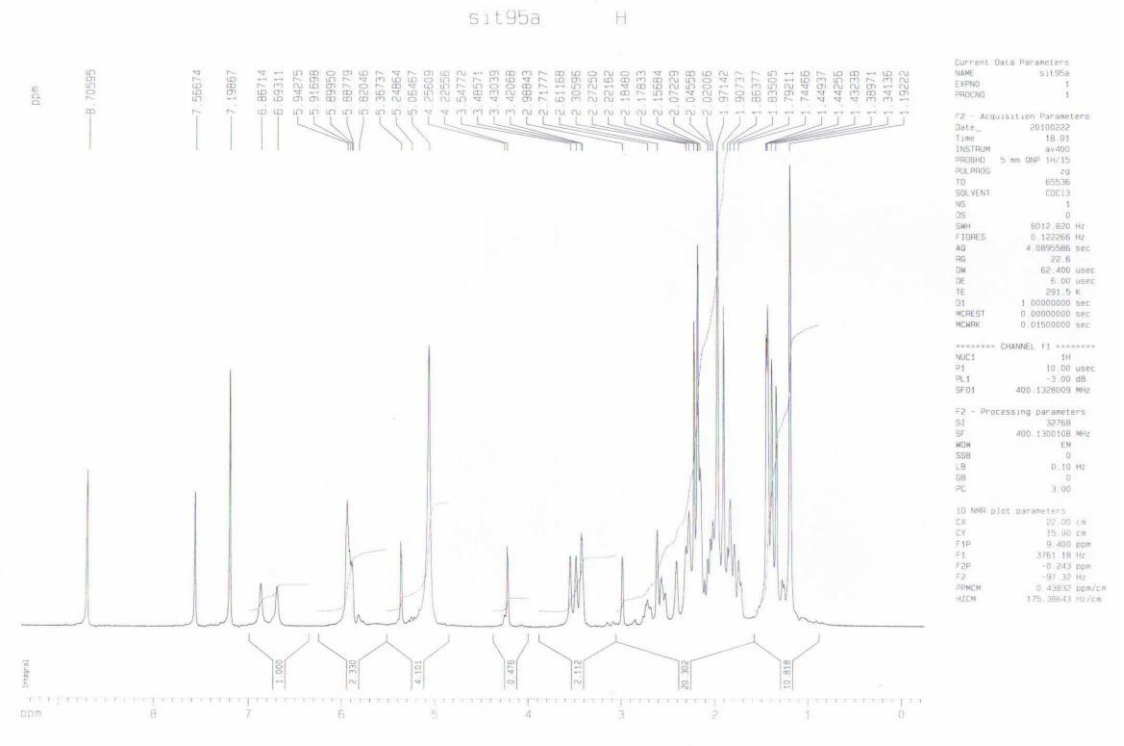


Figure 26. $^{13}$C NMR spectrum of bistenuifolin D (**4**)

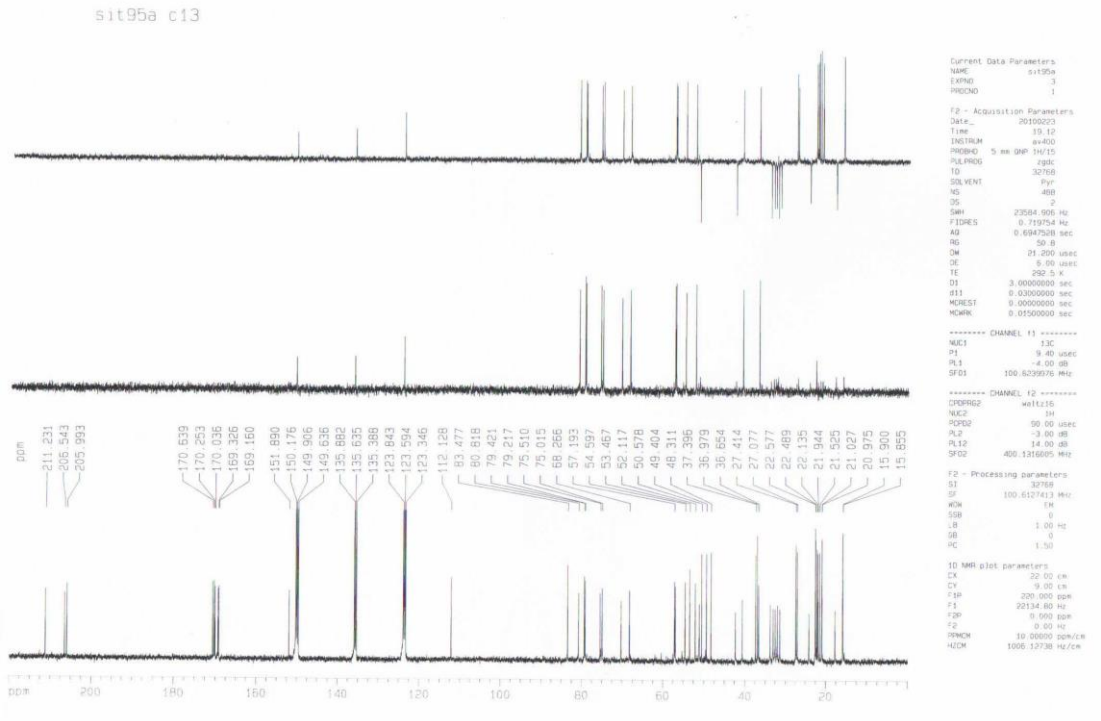



Figure 27. HSQC spectrum of bistenuifolin D (**4**)

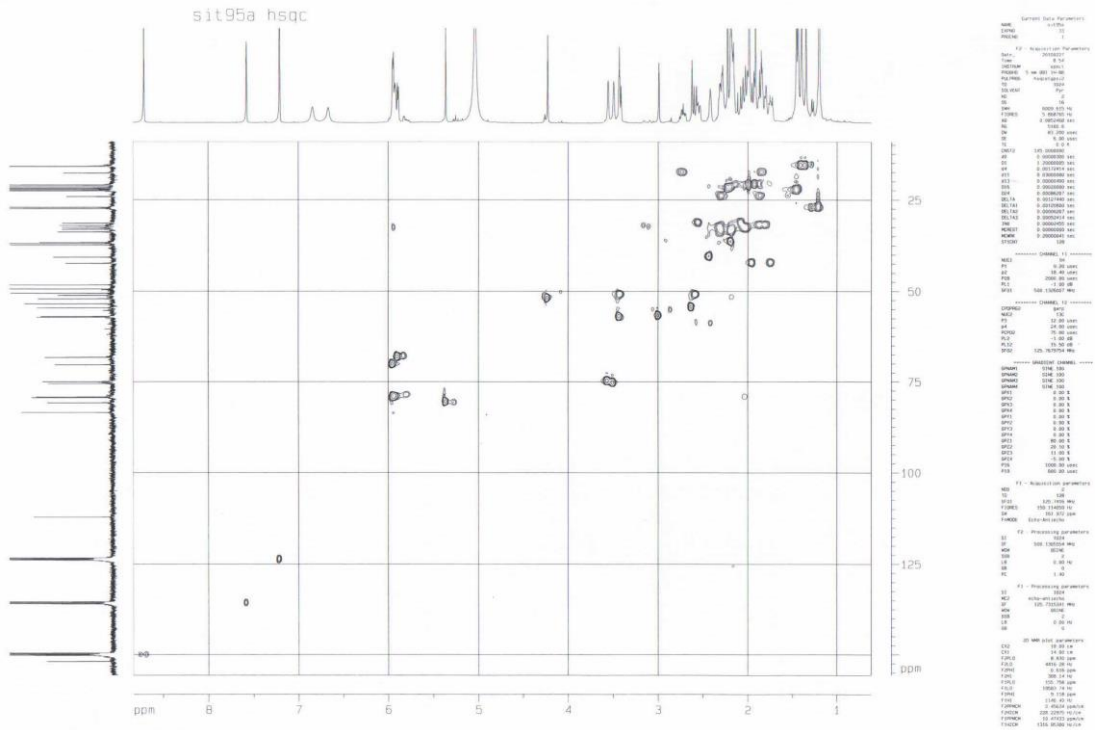


Figure 28. HMBC spectrum of bistenuifolin D (**4**)

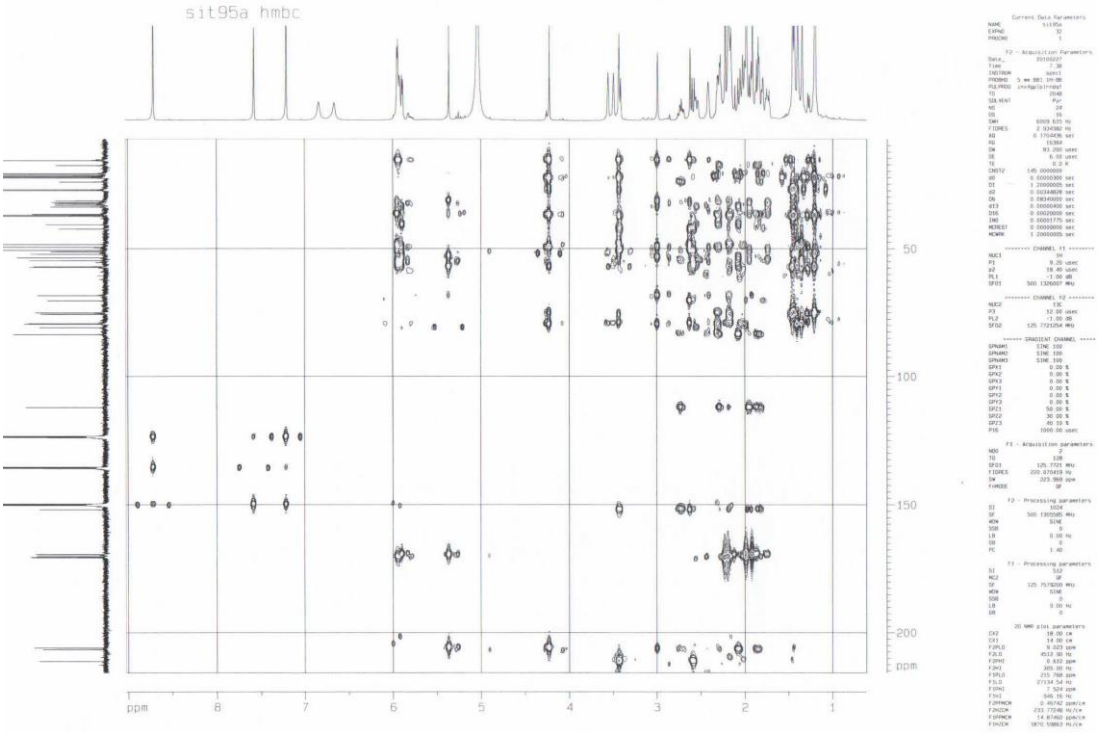



Figure 29. COSY spectrum of bistenuifolin D (**4**)

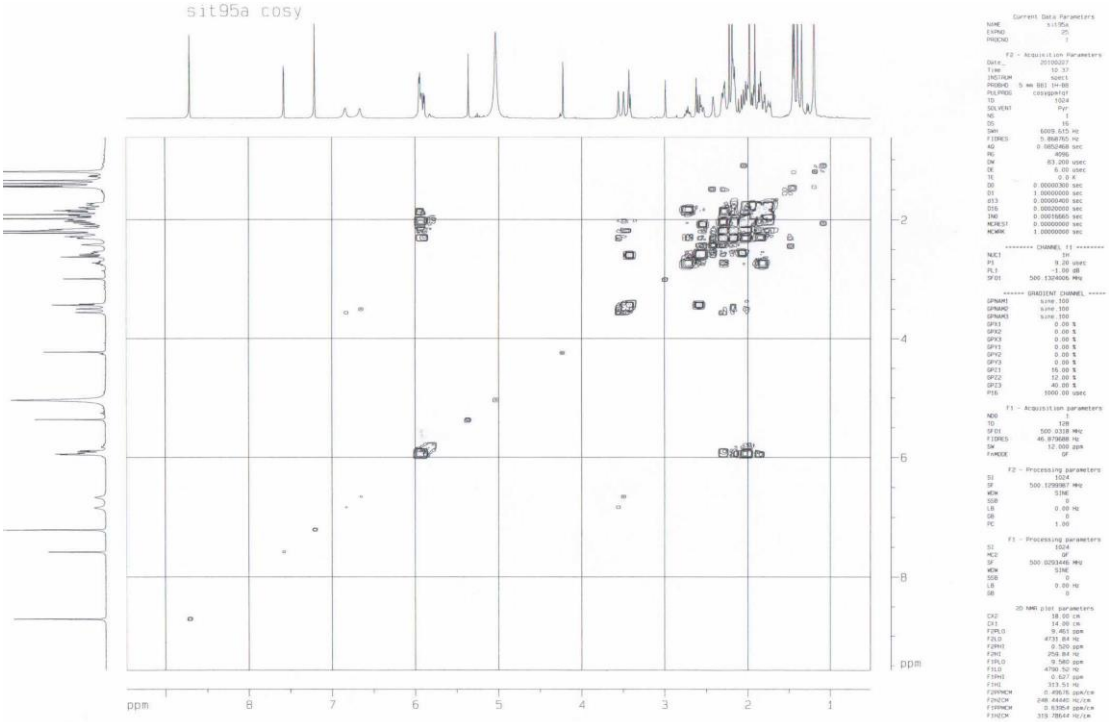


Figure 30. ROESY spectrum of bistenuifolin D (**4**)

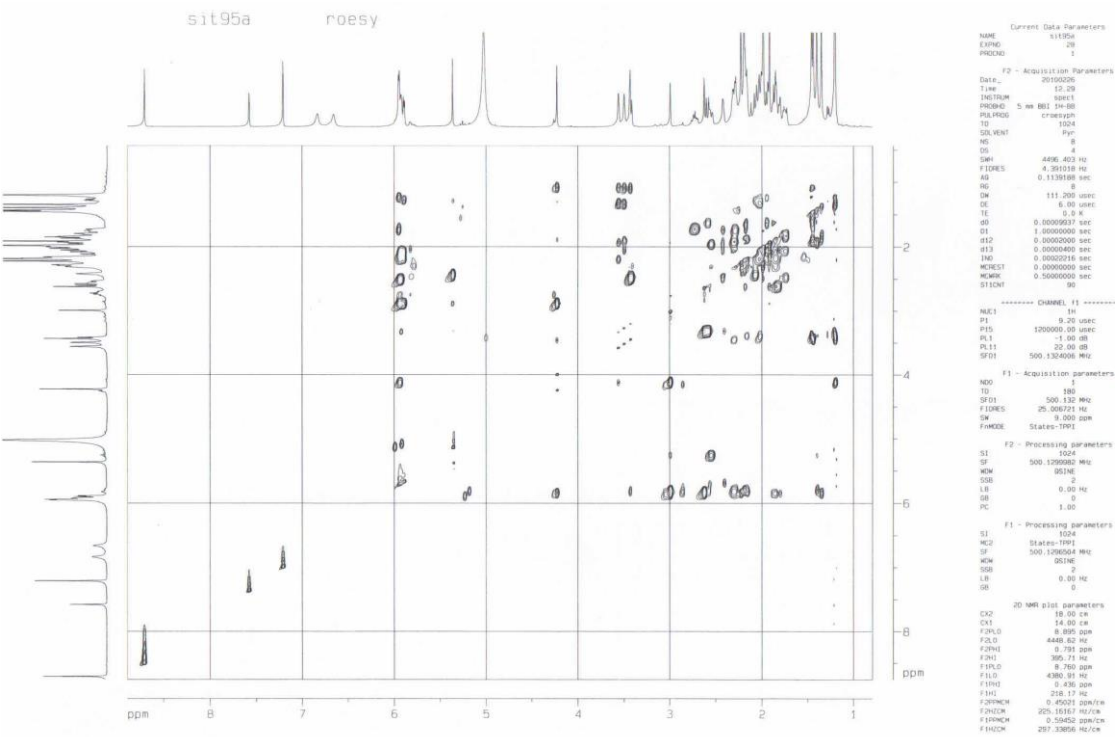
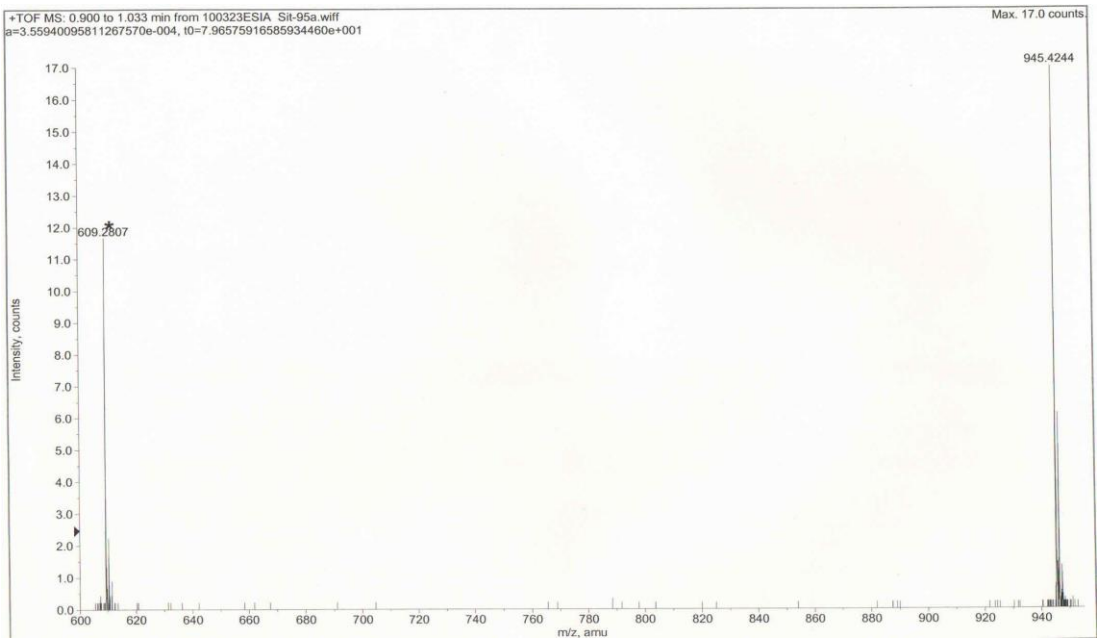
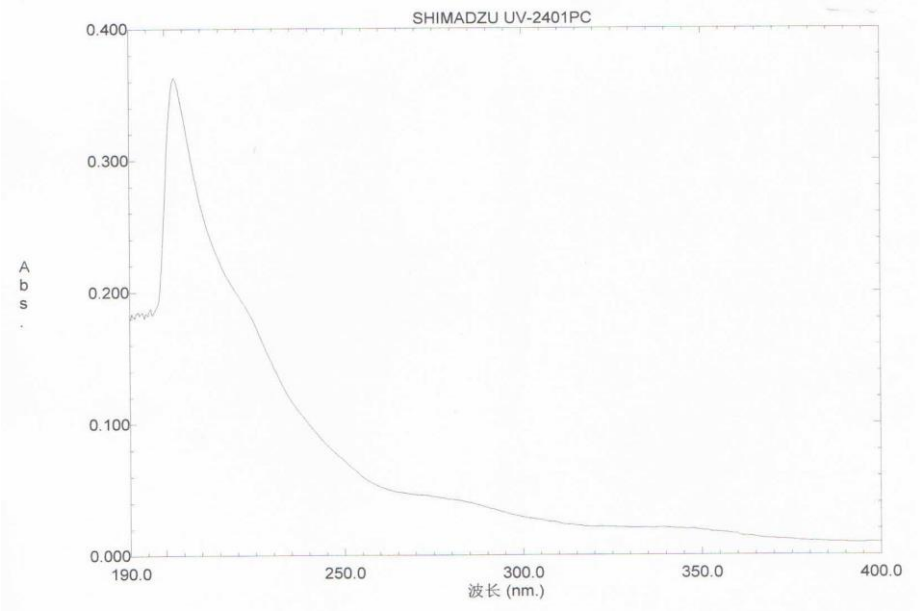


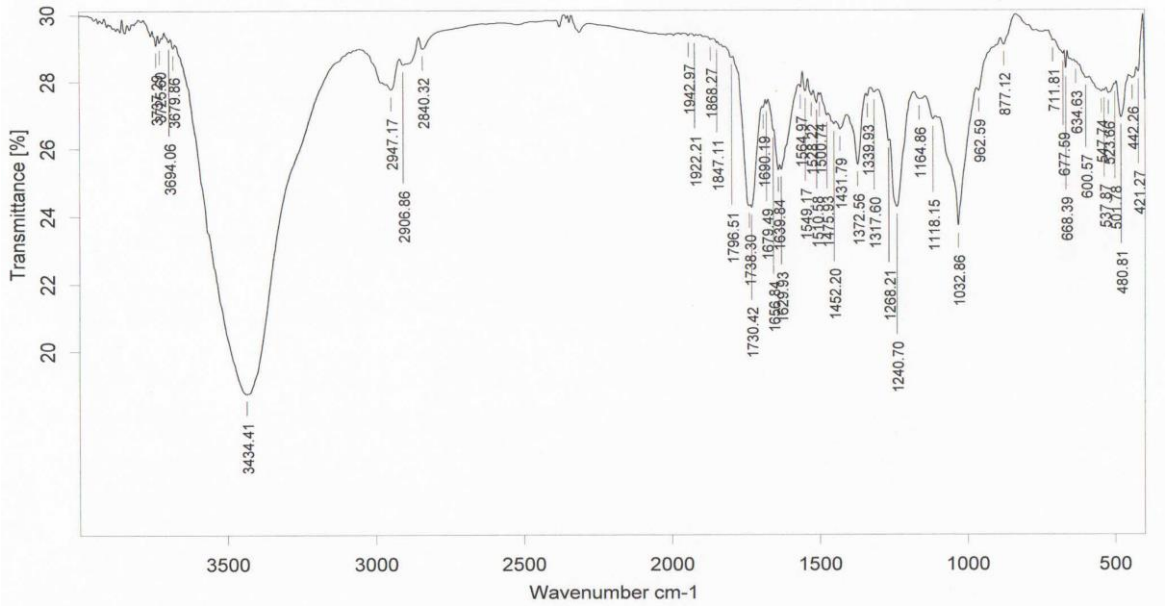

Figure 31. HRESIMS spectrum of bistenuifolin D (**4**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C50 H66 O16 Na | 945.4248 | -0.4565 | -0.4829 | 17.5 |

Figure 32. UV and IR spectra of bistenuifolin D (**4**)



**For compound 5:**

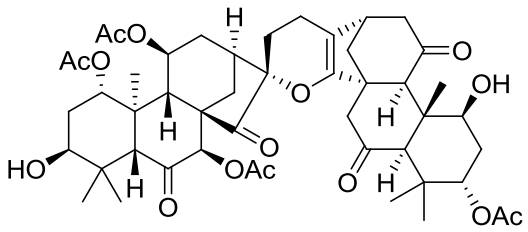



Figure 33. $^{1}$H NMR spectrum of bistenuifolin E (**5**)

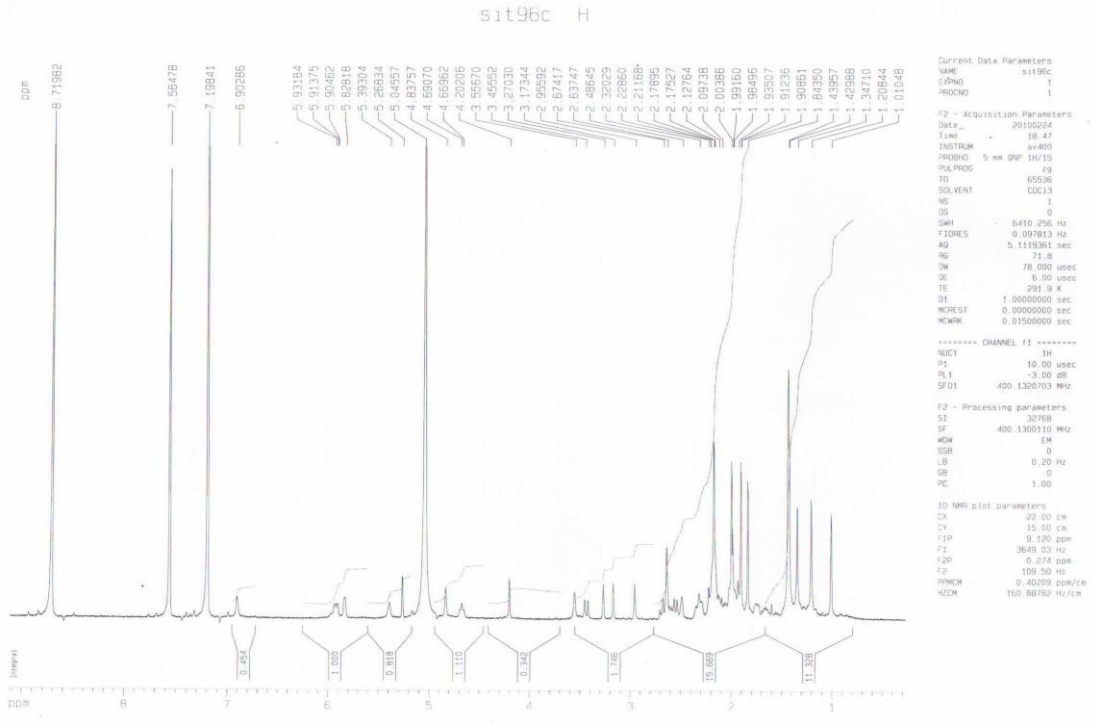


Figure 34. $^{13}$C NMR spectrum of bistenuifolin E (**5**)

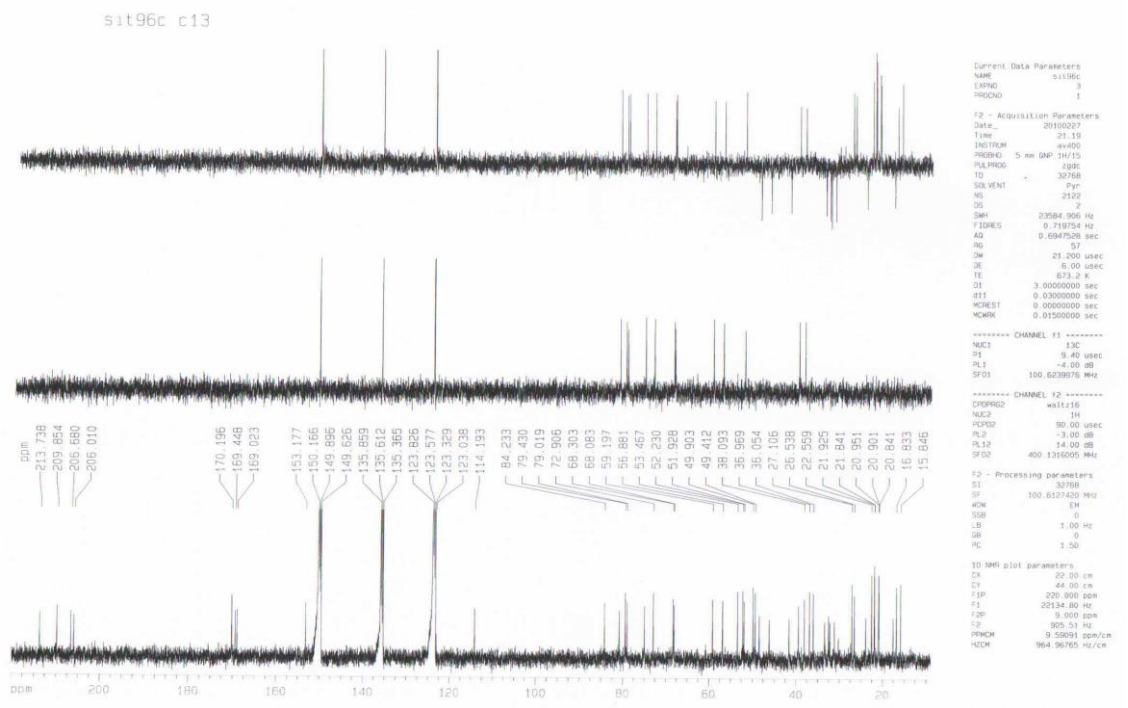



Figure 35. HSQC spectrum of bistenuifolin E (**5**)

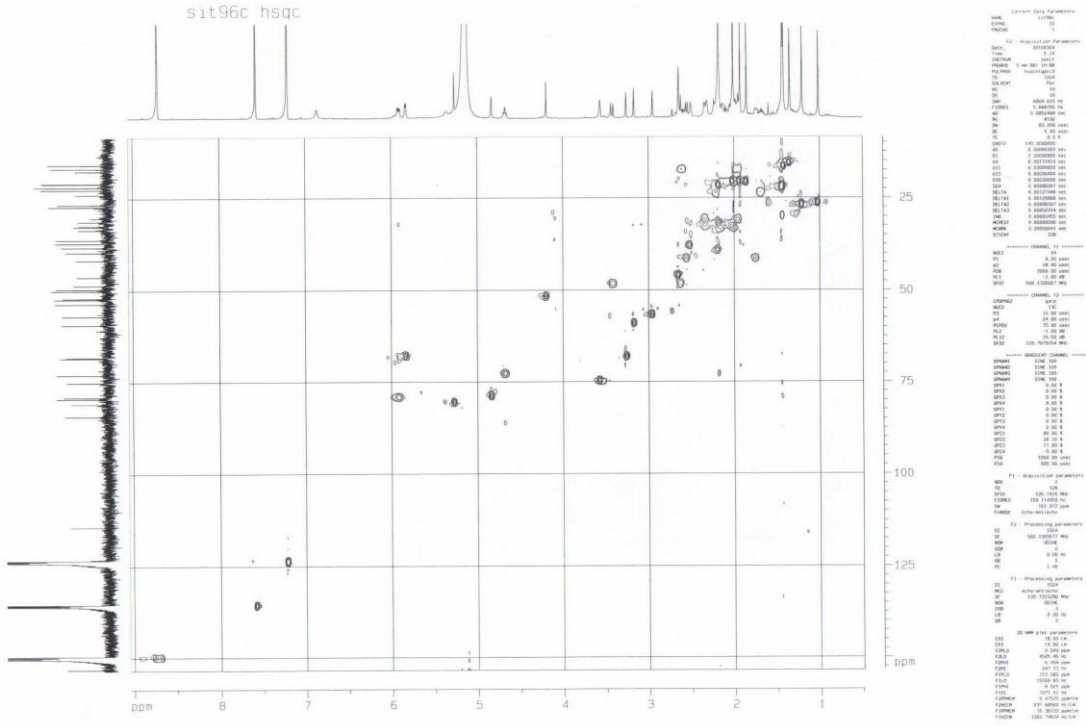


Figure 36. HMBC spectrum of bistenuifolin E (**5**)

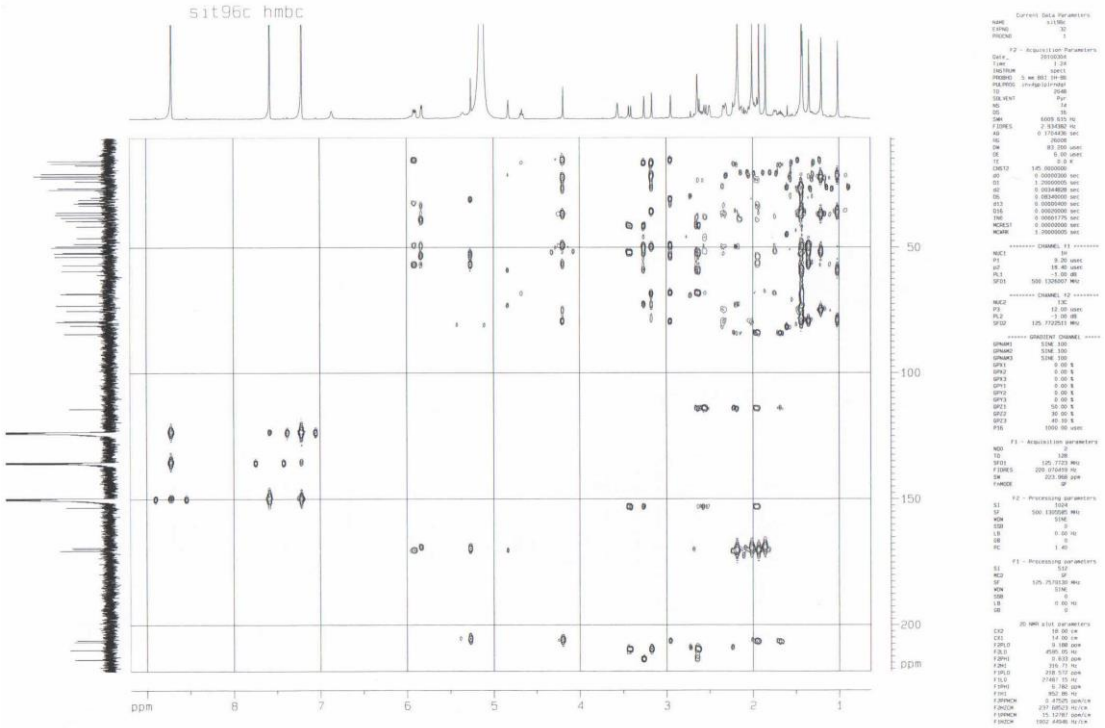



Figure 37. COSY spectrum of bistenuifolin E (**5**)

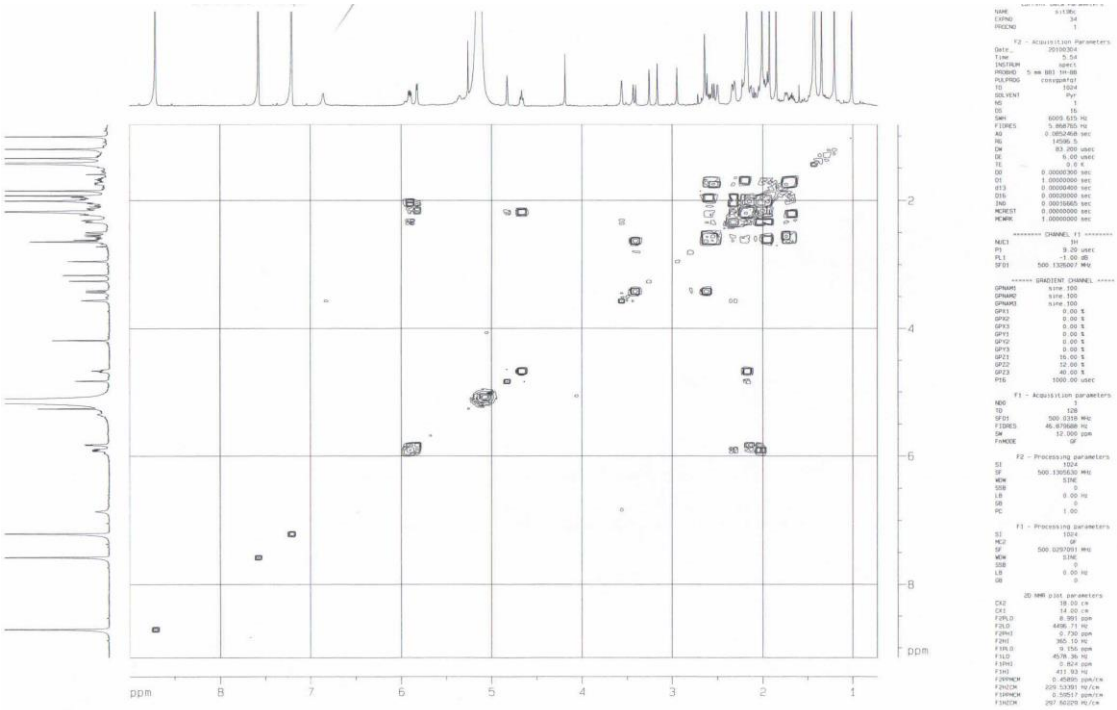


Figure 38. ROESY spectrum of bistenuifolin E (**5**)

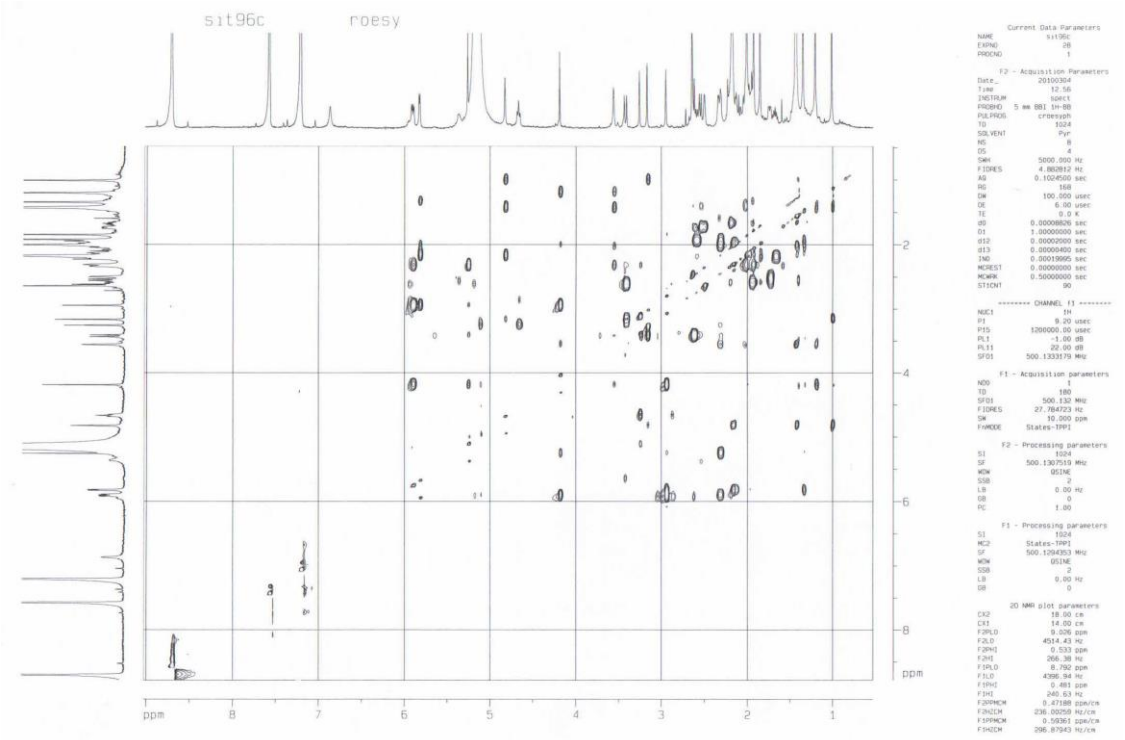
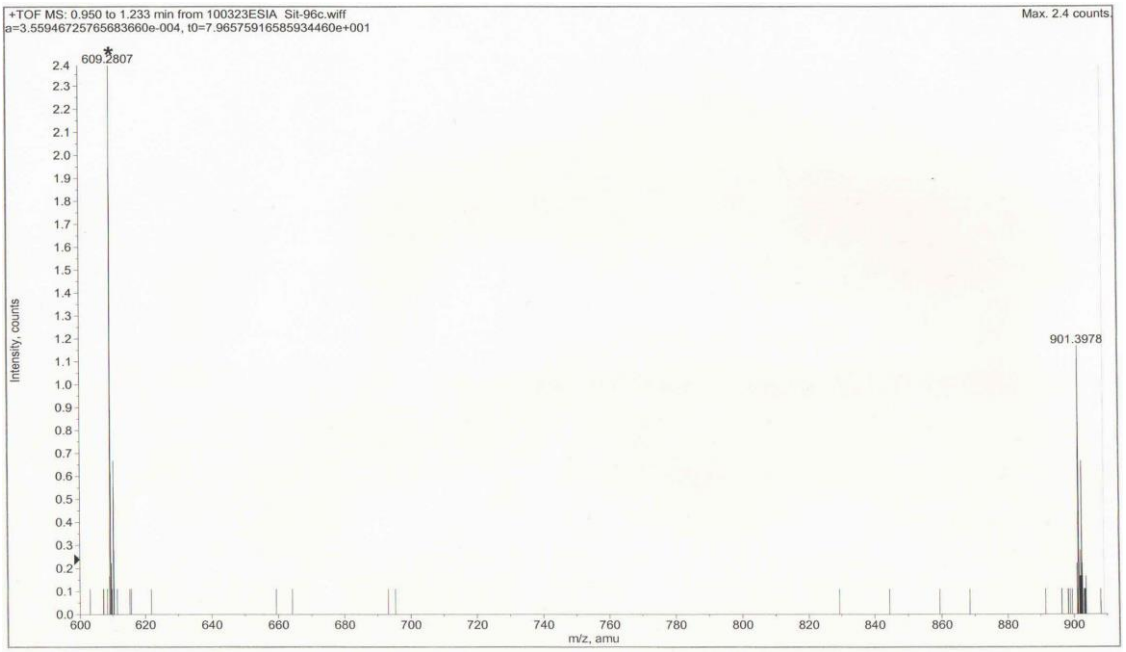
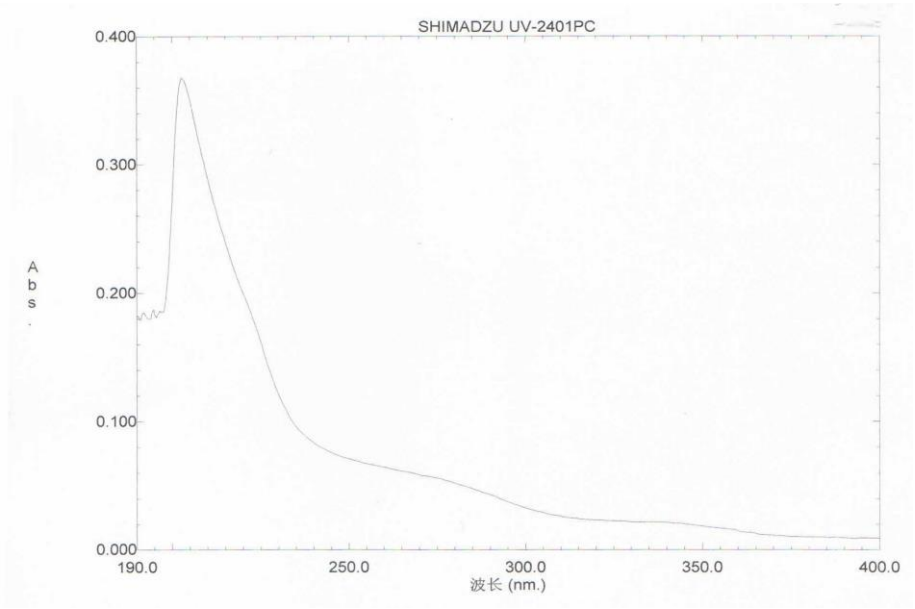


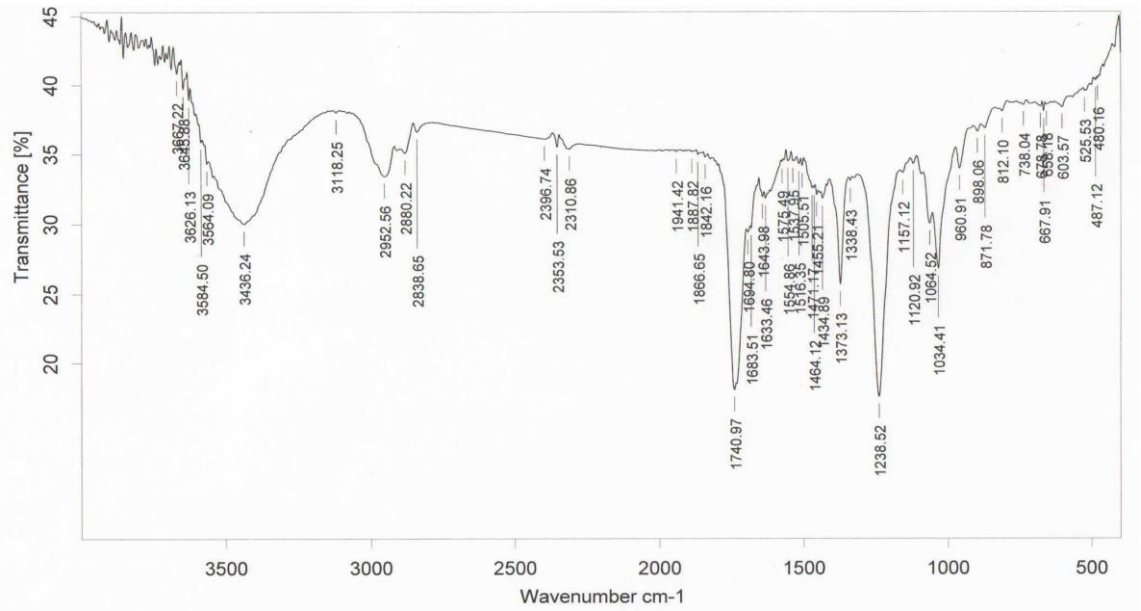

Figure 39. HRESIMS spectrum of bistenuifolin E (**5**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C48 H62 O15 Na | 901.3986 | -0.8417 | -0.9338 | 17.5 |

Figure 40. UV and IR spectra of bistenuifolin E (**5**)



**For compound 6:**

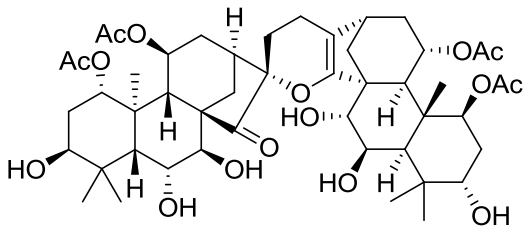



Figure 41. $^{1}$H NMR spectrum of bistenuifolin F (**6**)

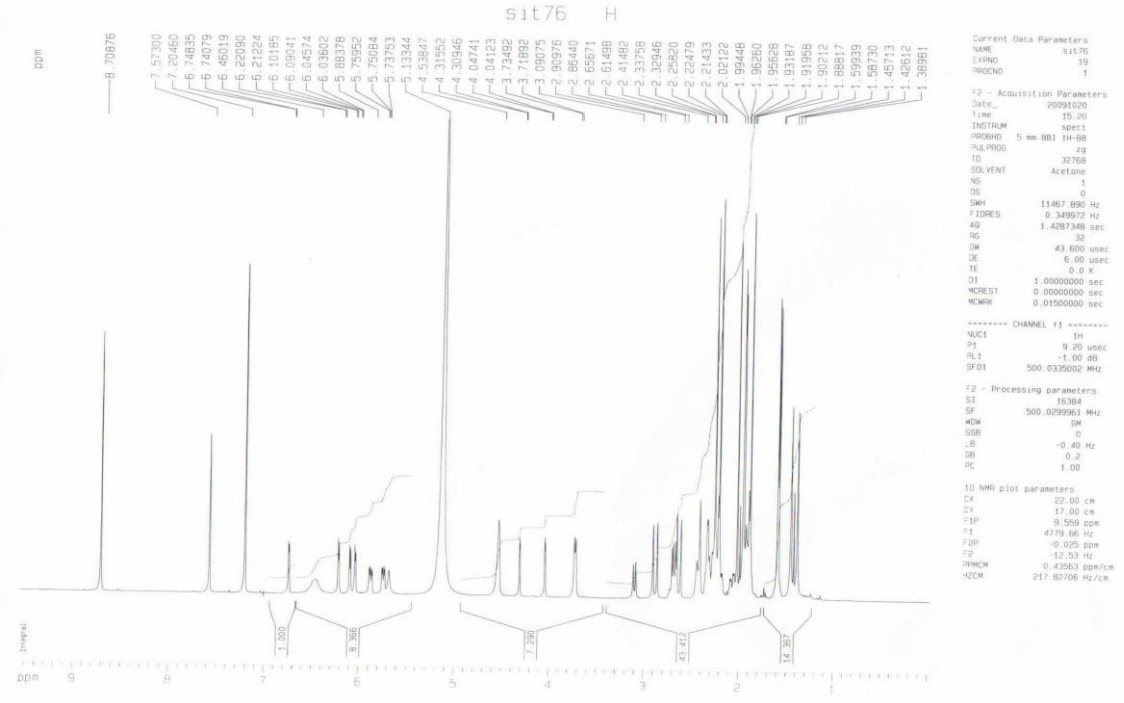


Figure 42. $^{13}$C NMR spectrum of bistenuifolin F (**6**)

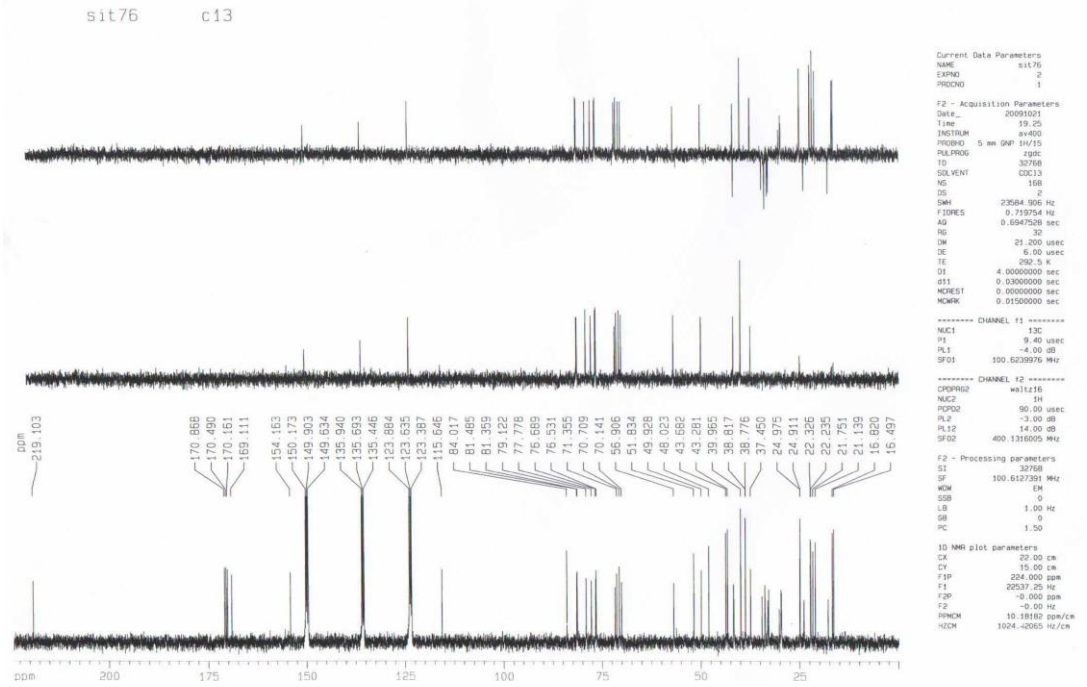



Figure 43. HSQC spectrum of bistenuifolin F (**6**)

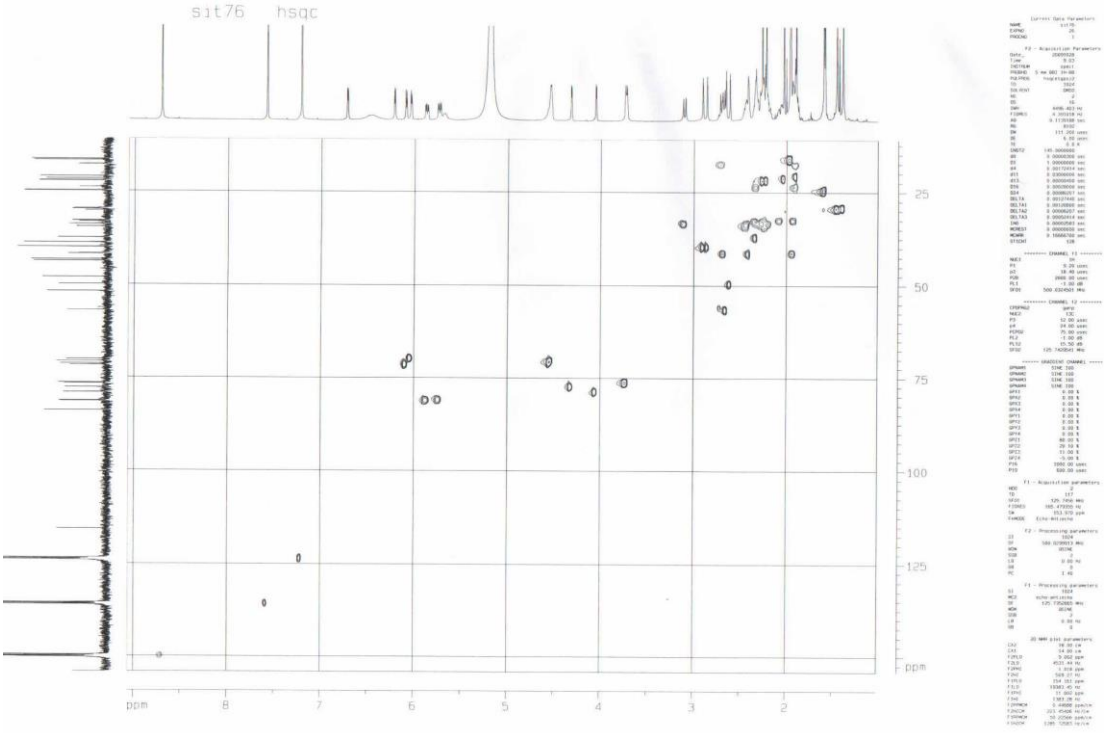


Figure 44. HMBC spectrum of bistenuifolin F (**6**)

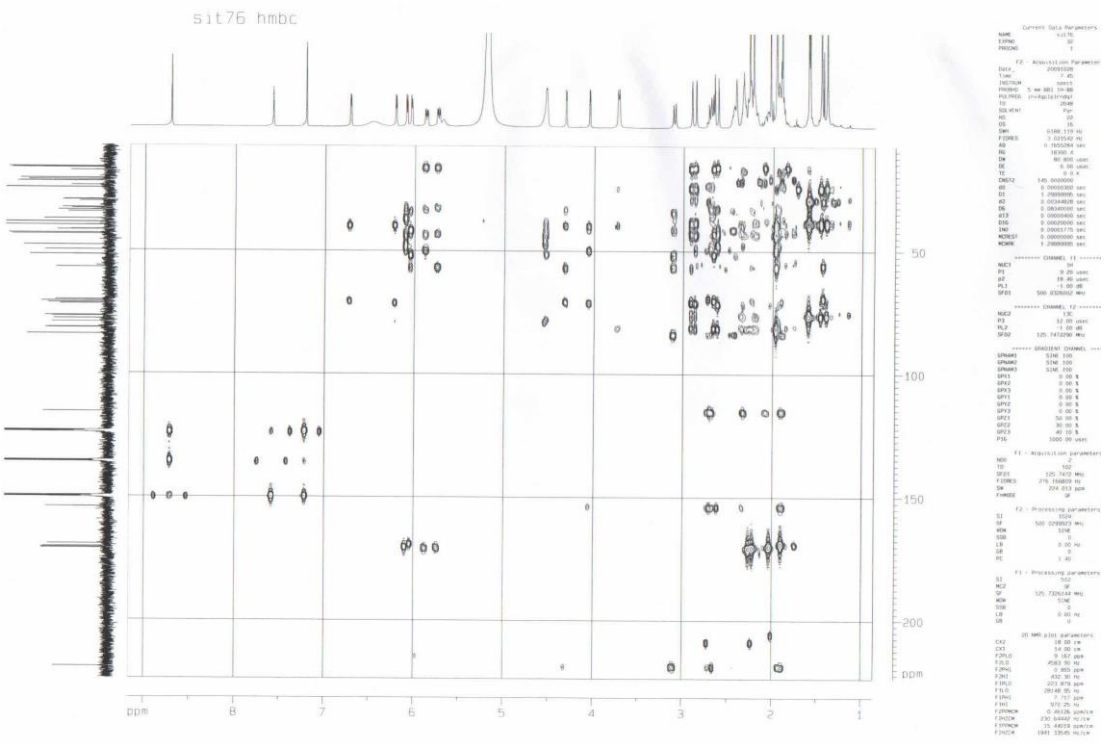



Figure 45. COSY spectrum of bistenuifolin F (**6**)

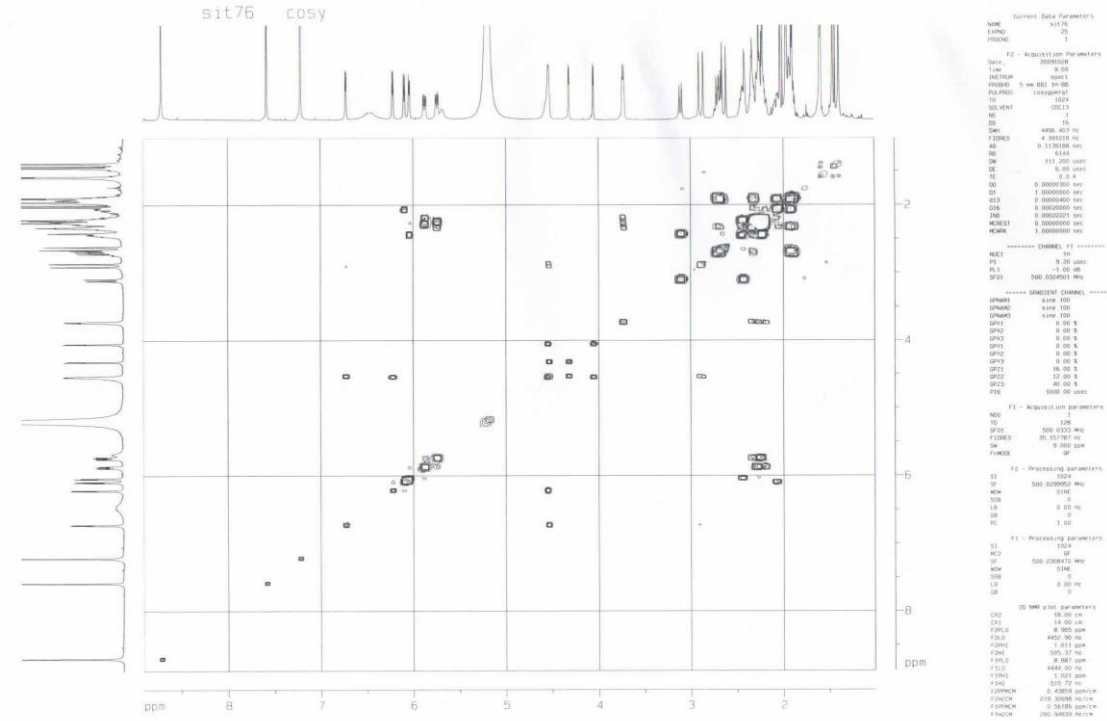


Figure 46. ROESY spectrum of bistenuifolin F (**6**)

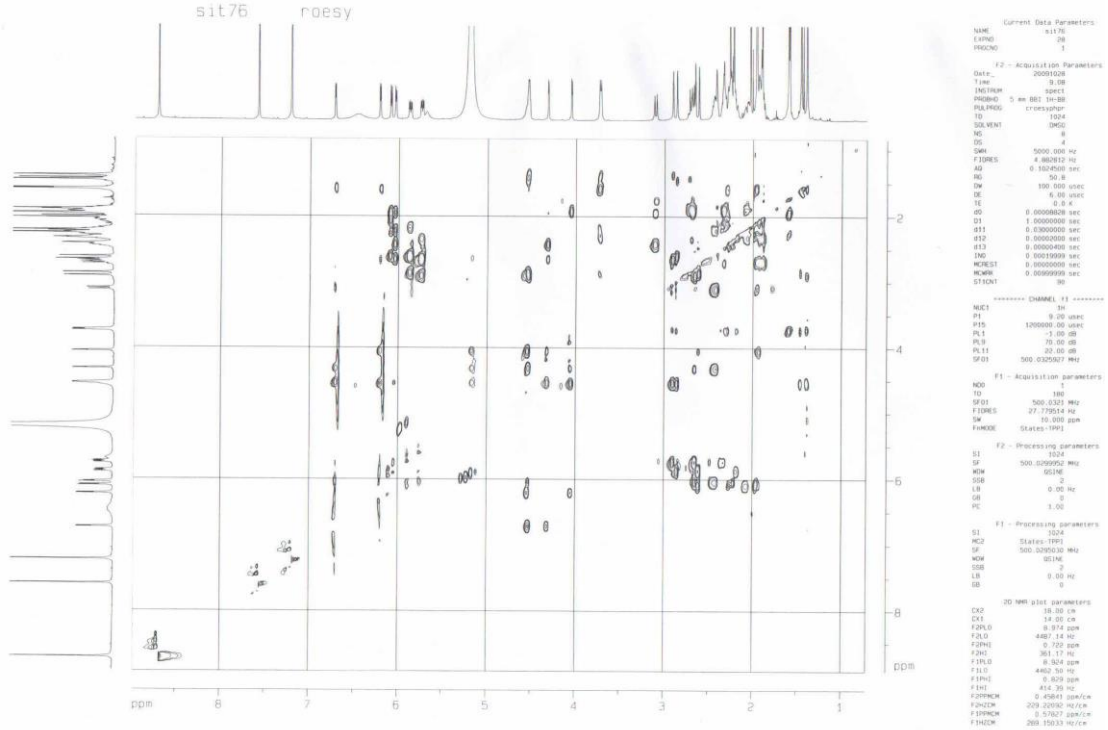
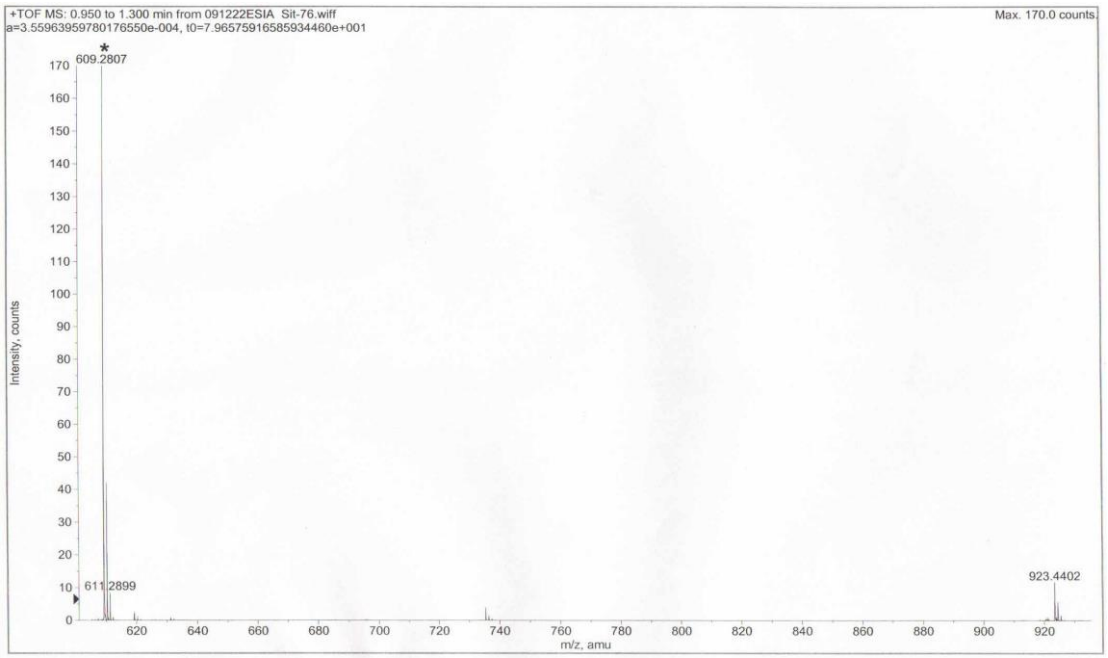
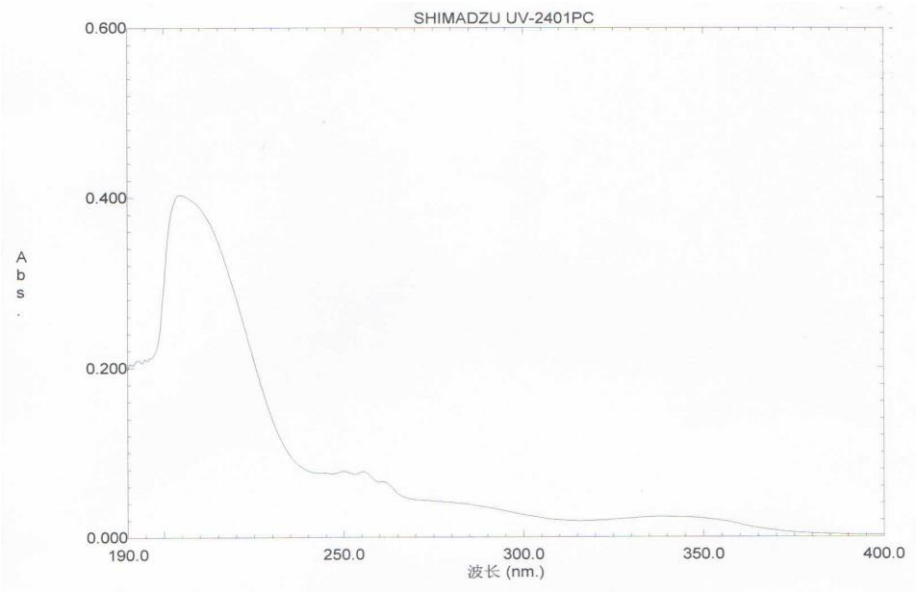


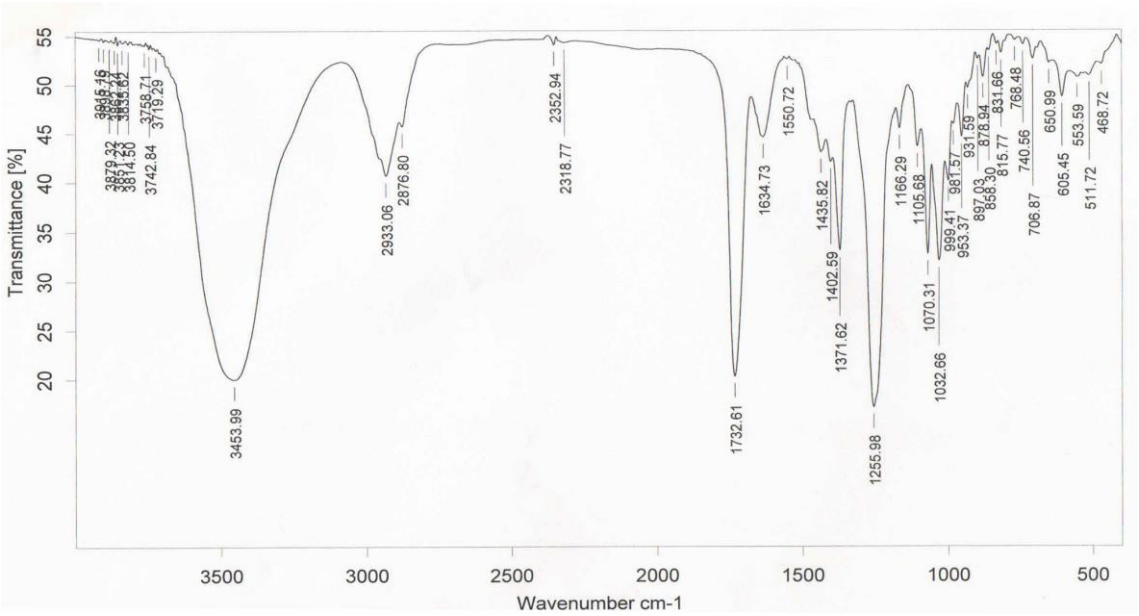

Figure 47. HRESIMS spectrum of bistenuifolin F (**6**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C48 H68 O16 Na | 923.4405 | -0.3066 | -0.3320 | 14.5 |

Figure 48. UV and IR spectra of bistenuifolin F (**6**)



**For compound 7:**

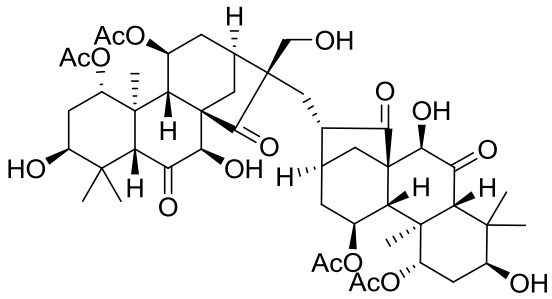



Figure 49. $^{1}$H NMR spectrum of bistenuifolin G (**7**)

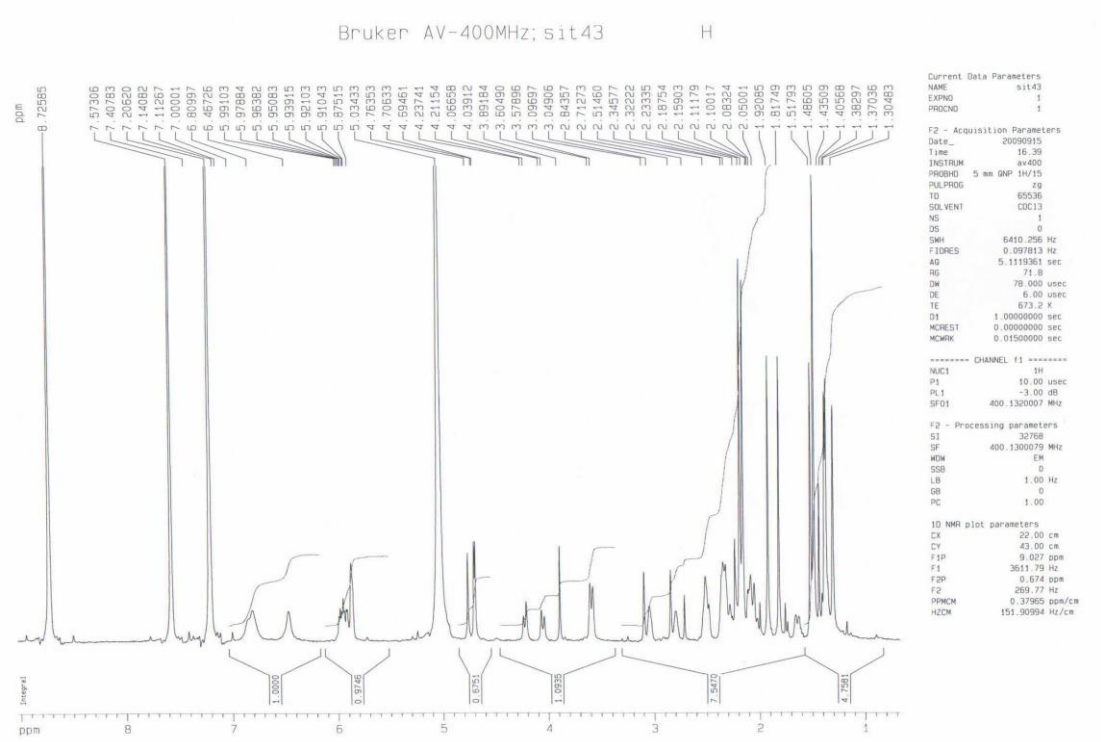


Figure 50. $^{13}$C NMR spectrum of bistenuifolin G (**7**)

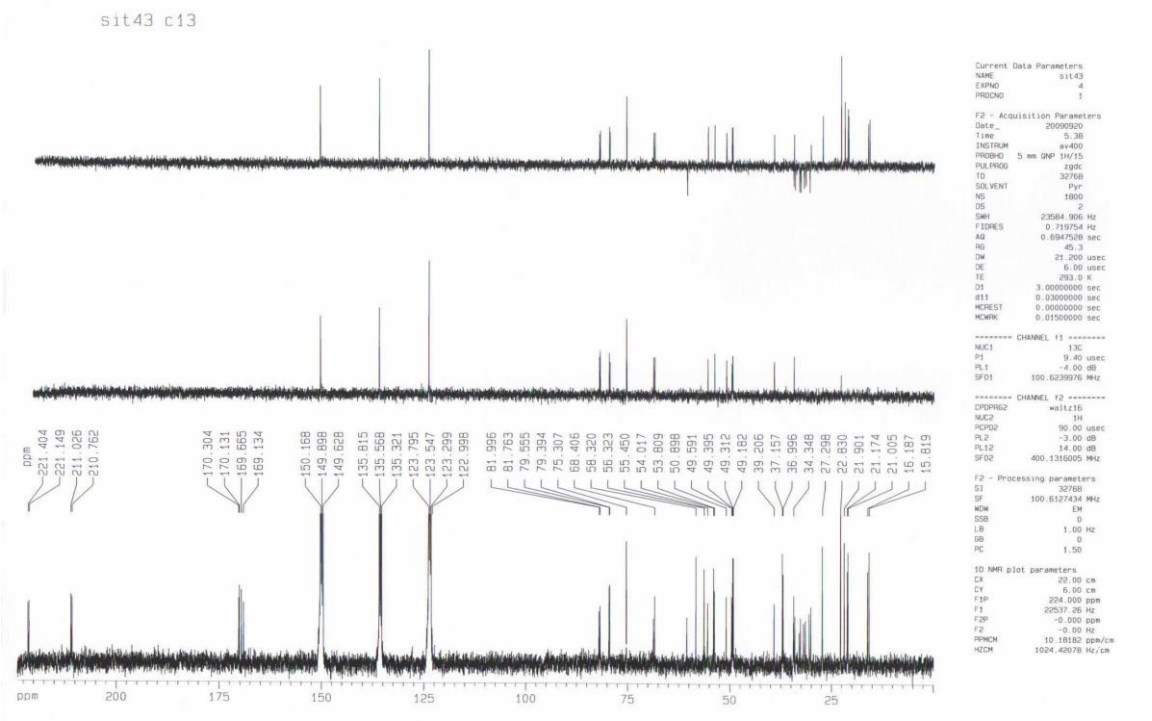



Figure 51. HSQC spectrum of bistenuifolin G (**7**)

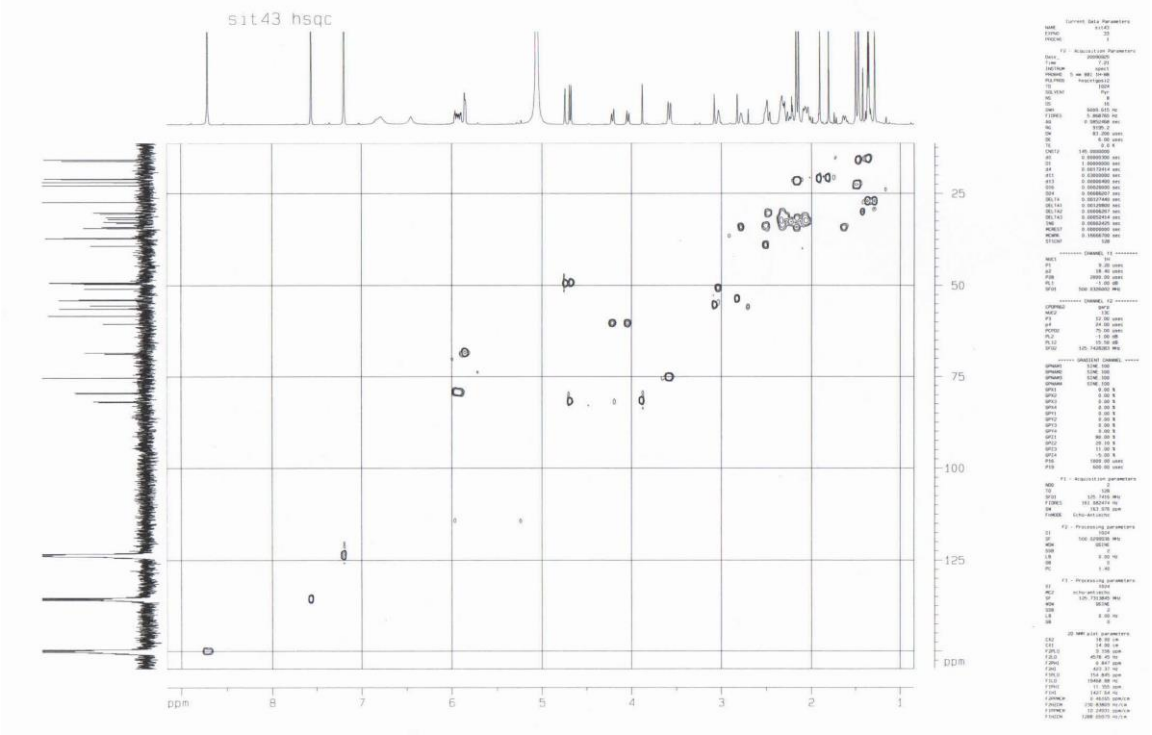


Figure 52. HMBC spectrum of bistenuifolin G (**7**)

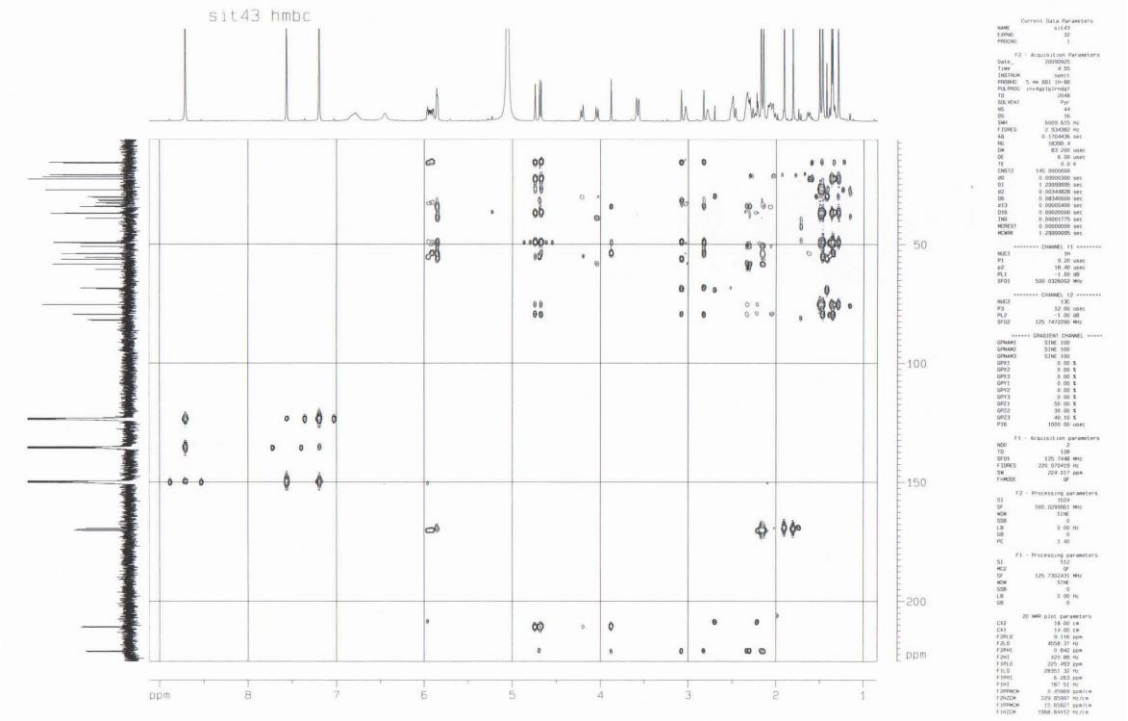



Figure 53. COSY spectrum of bistenuifolin G (**7**)

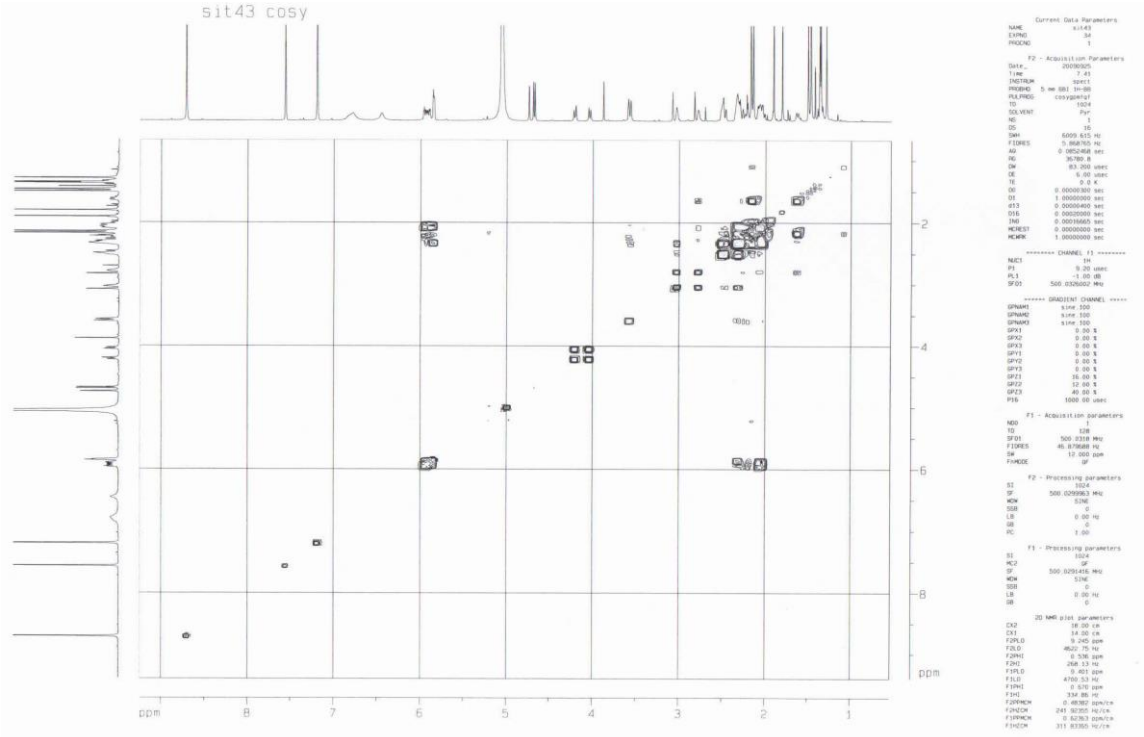


Figure 54. ROESY spectrum of bistenuifolin G (**7**)

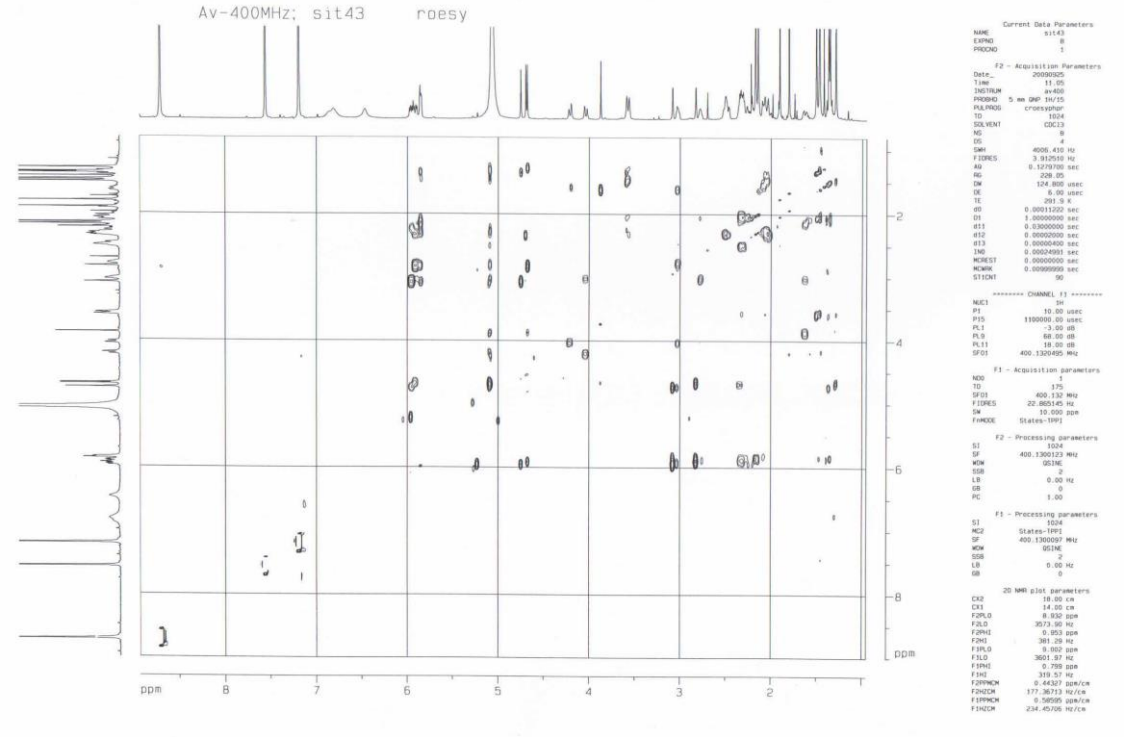
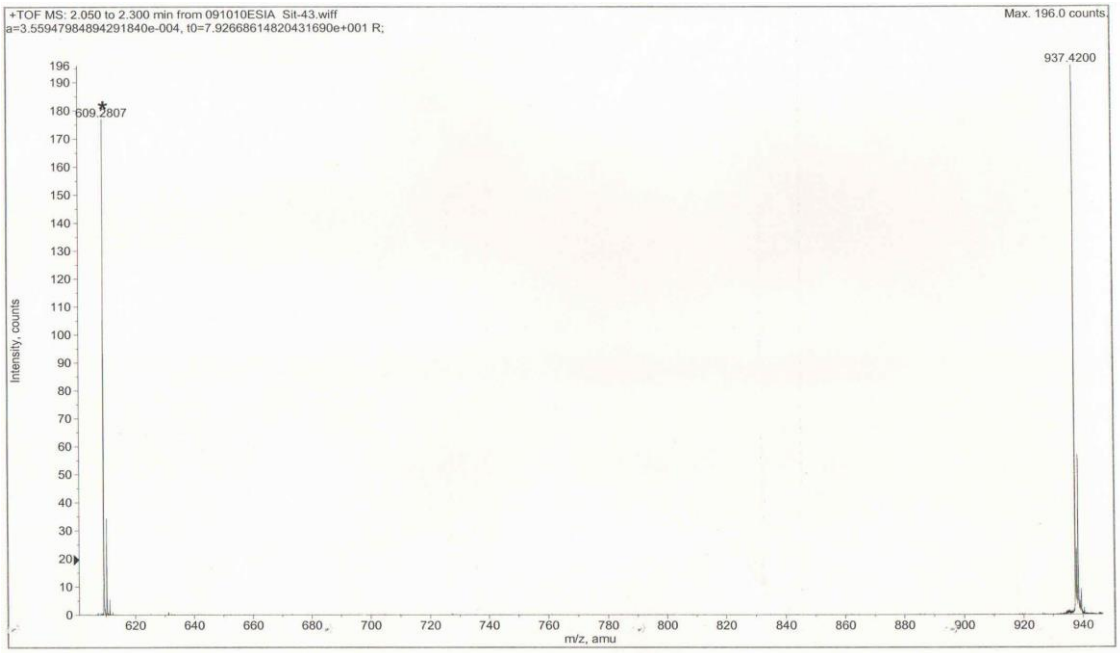
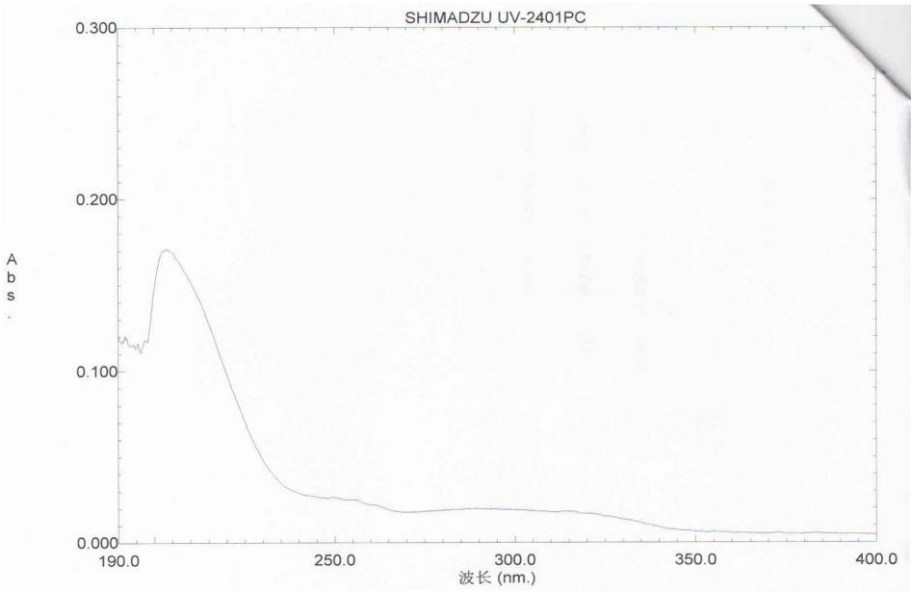


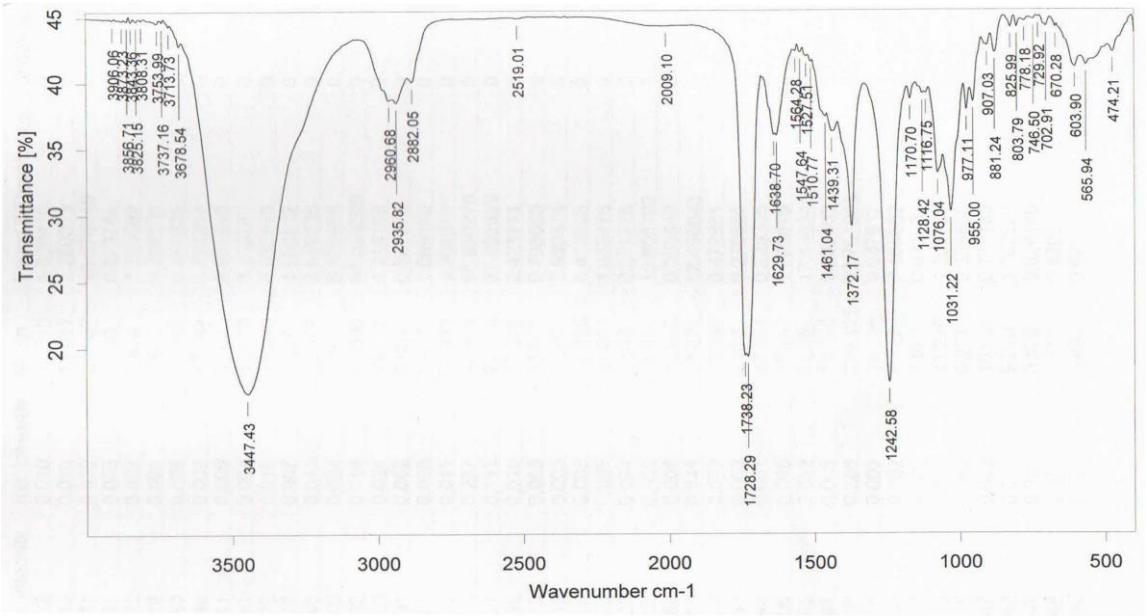

Figure 55. HRESIMS spectrum of bistenuifolin G (**7**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C48 H66 O17 Na | 937.4197 | 0.2287 | 0.2440 | 15.5 |

Figure 56. UV and IR spectra of bistenuifolin G (**7**)



**For compound 8:**

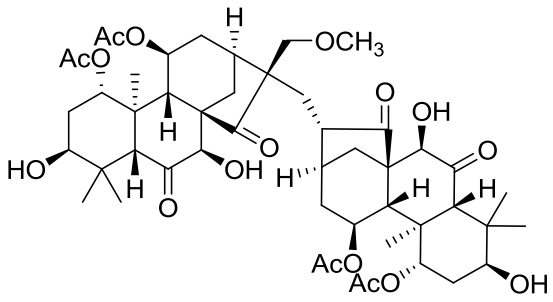



Figure 57. $^{1}$H NMR spectrum of bistenuifolin H (**8**)

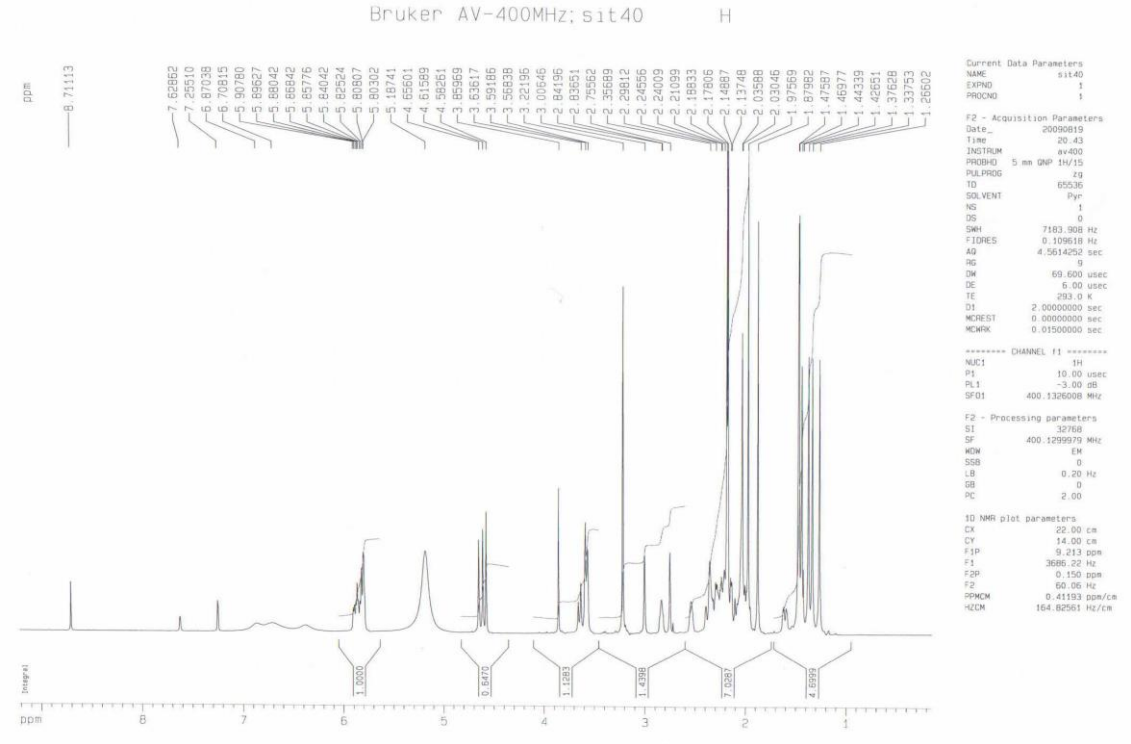


Figure 58. $^{13}$C NMR spectrum of bistenuifolin H (**8**)

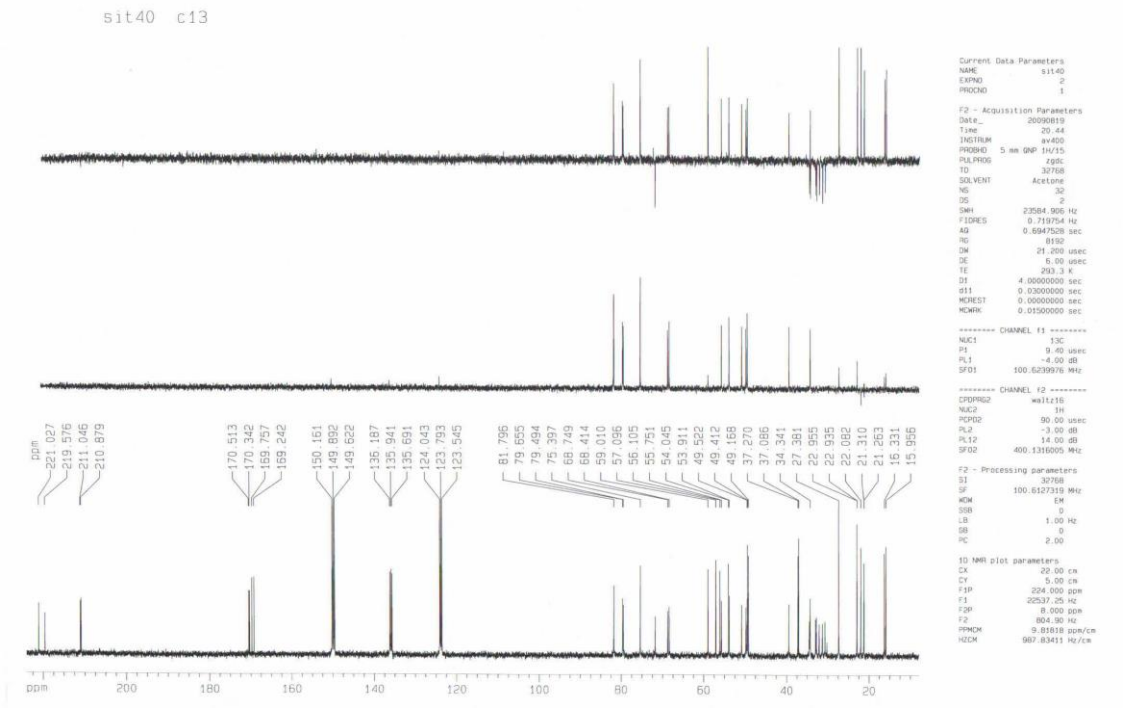



Figure 59. HSQC spectrum of bistenuifolin H (**8**)

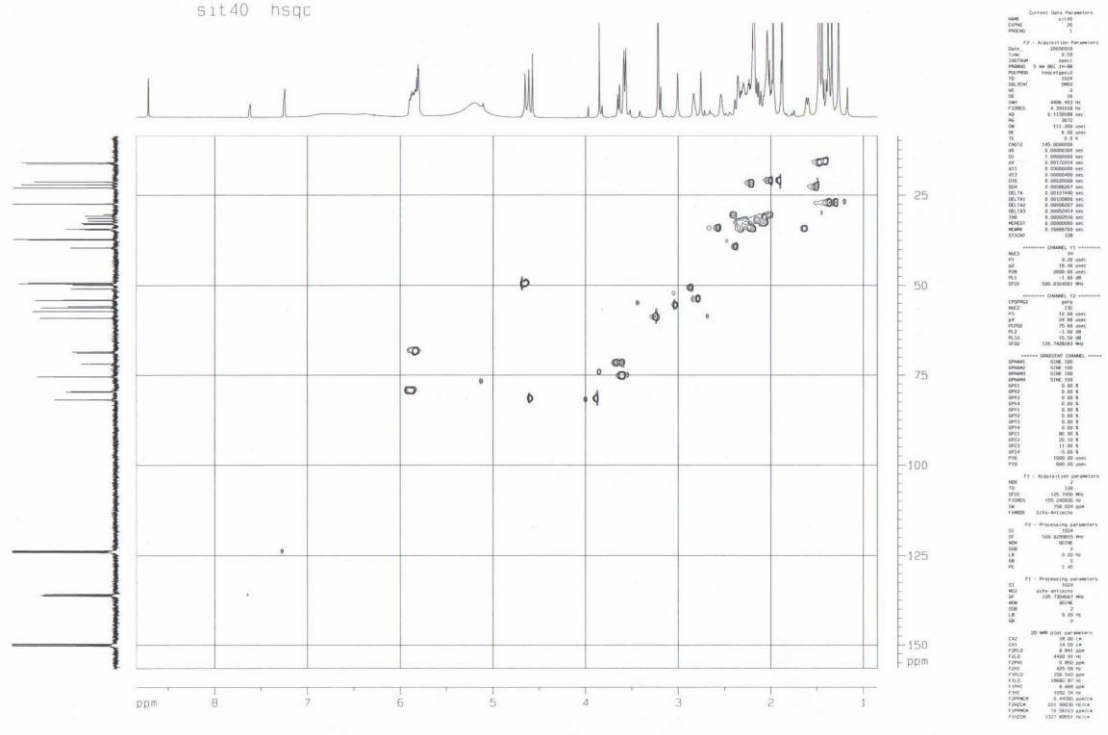


Figure 60. HMBC spectrum of bistenuifolin H (**8**)

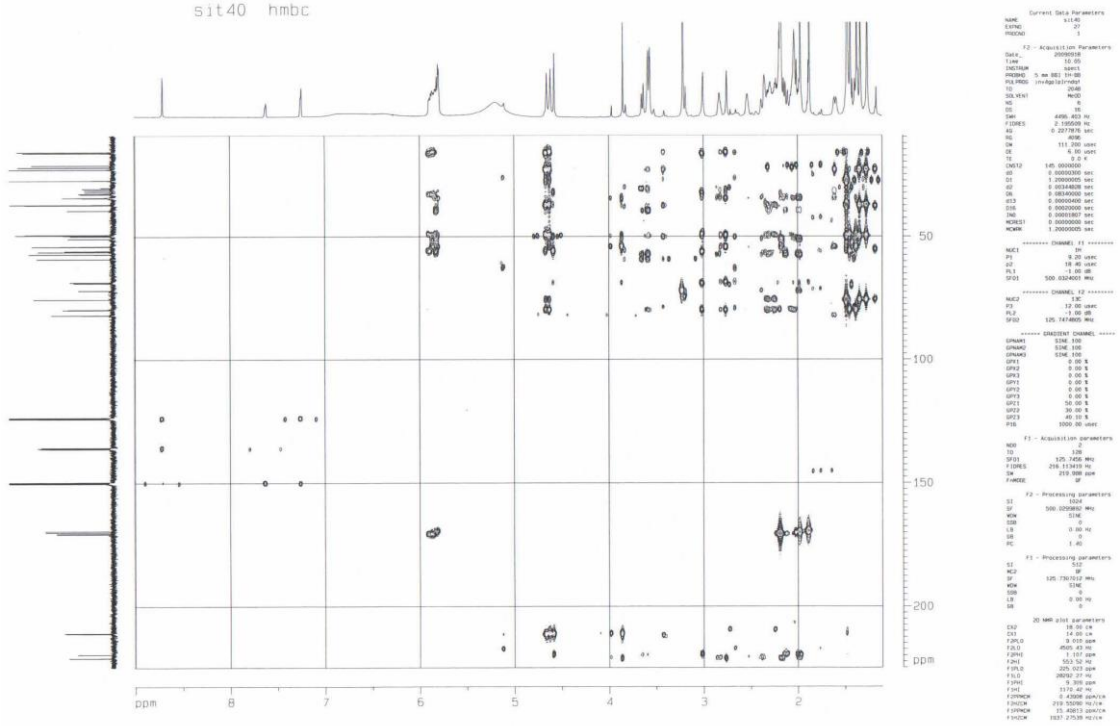



Figure 61. COSY spectrum of bistenuifolin H (**8**)

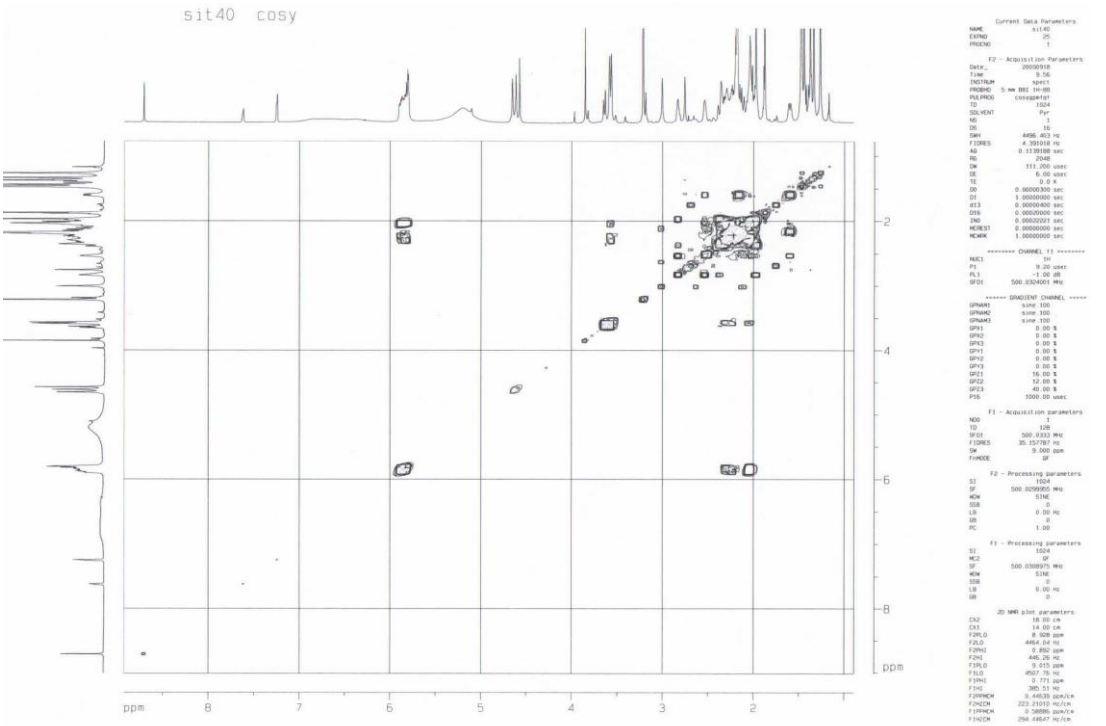


Figure 62. ROESY spectrum of bistenuifolin H (**8**)

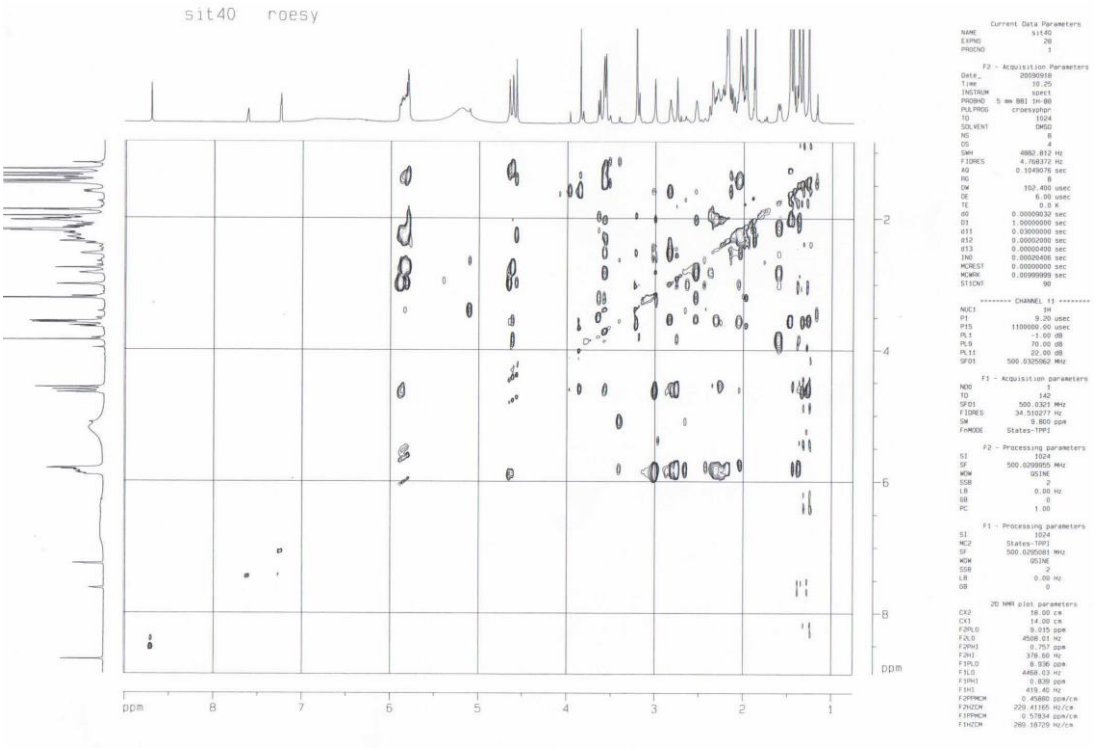
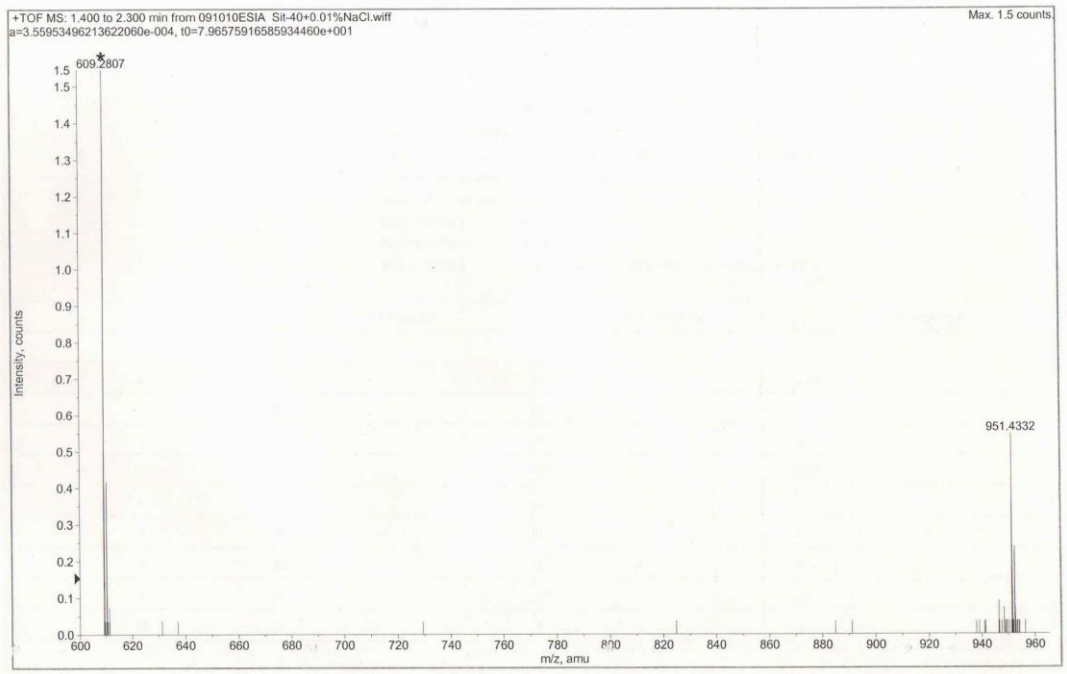
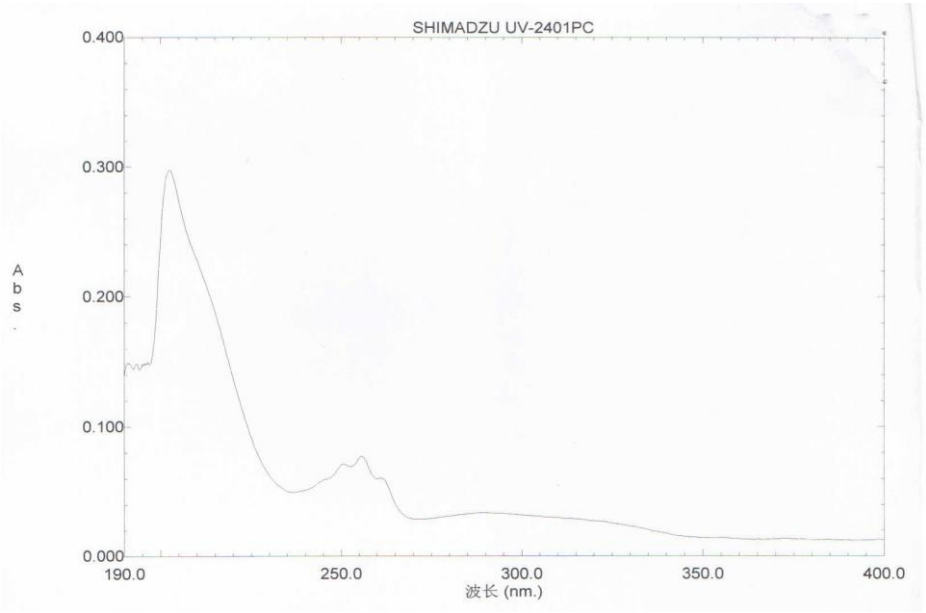


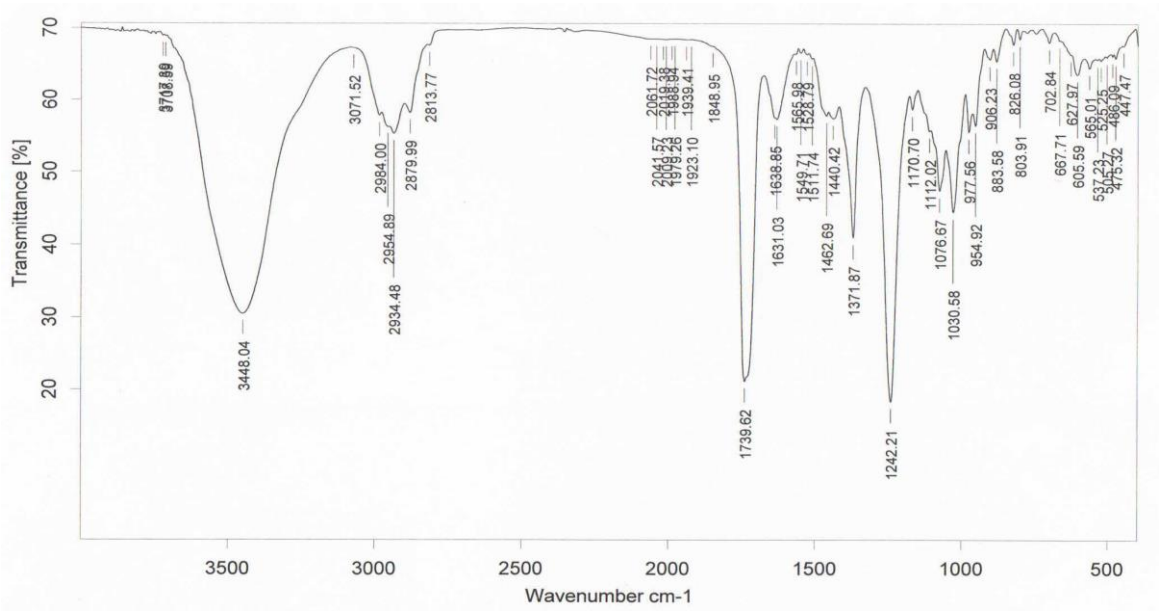

Figure 63. HRESIMS spectrum of bistenuifolin H (**8**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C49 H68 O17 Na | 951.4354 | -2.2212 | -2.3346 | 15.5 |

Figure 64. UV and IR spectra of bistenuifolin H (**8**)



**For compound 9:**

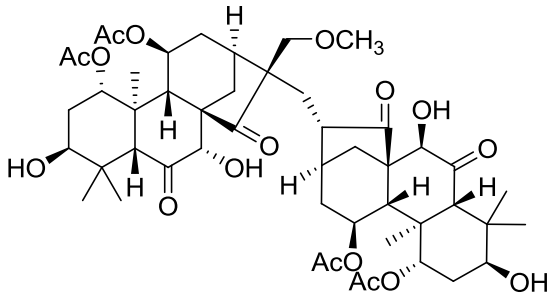



Figure 65. $^{1}$H NMR spectrum of bistenuifolin I (**9**)

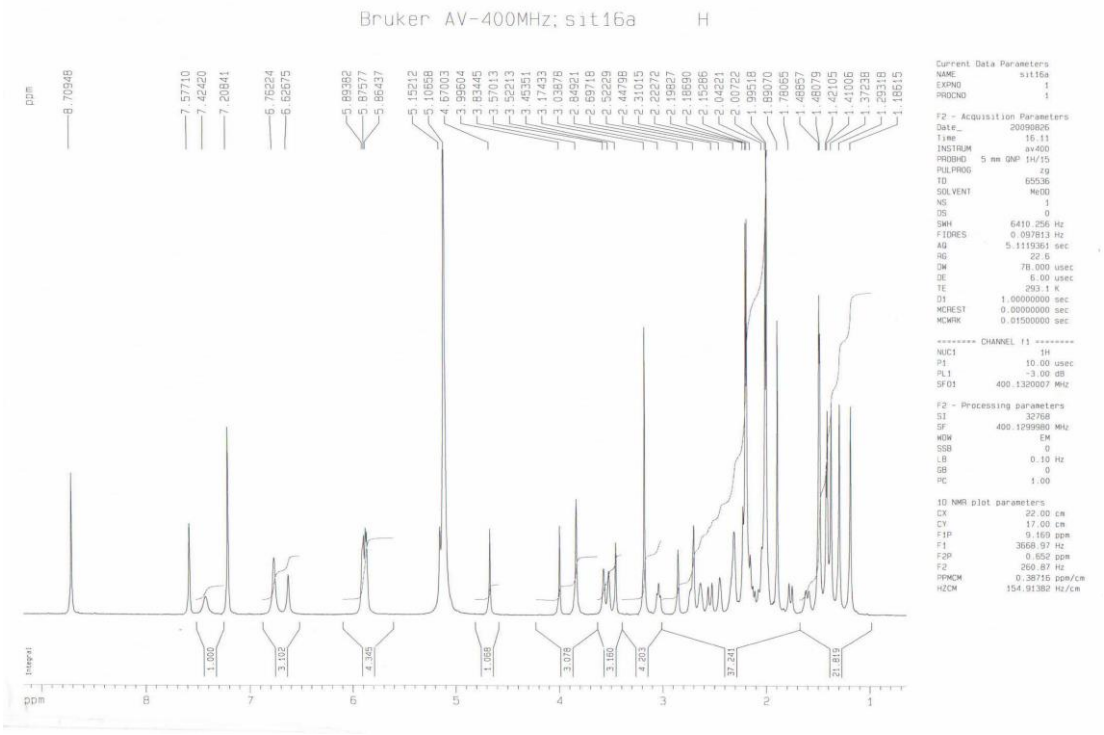


Figure 66. $^{13}$C NMR spectrum of bistenuifolin I (**9**)

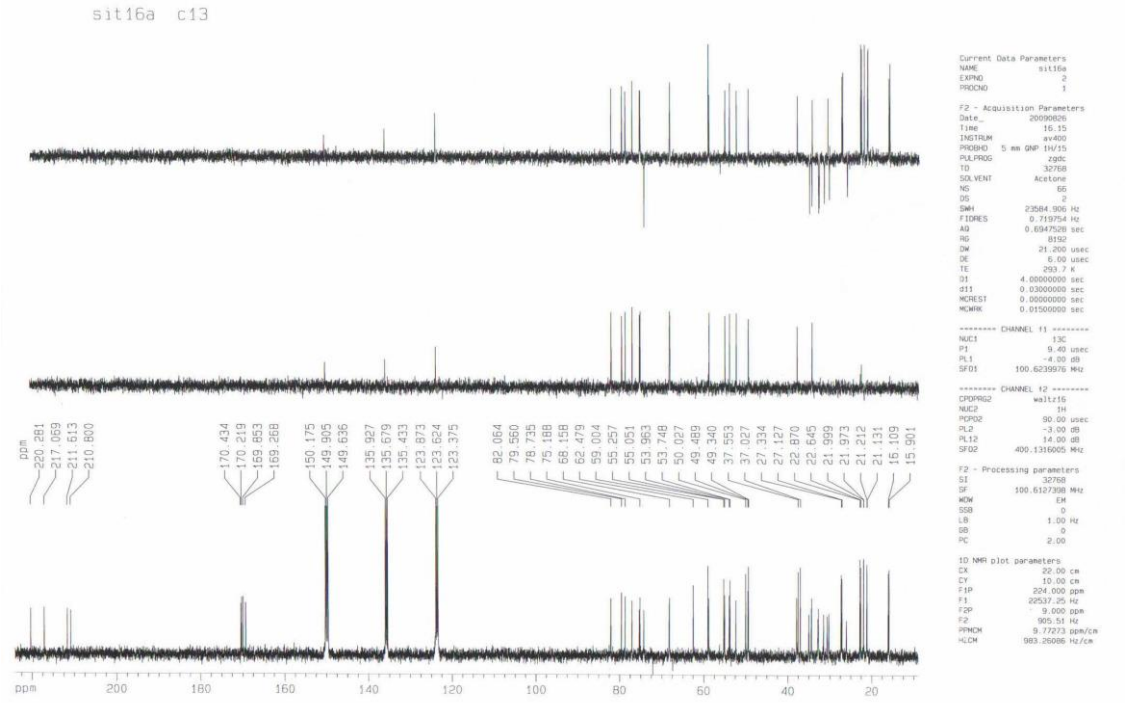



Figure 67. HSQC spectrum of bistenuifolin I (**9**)

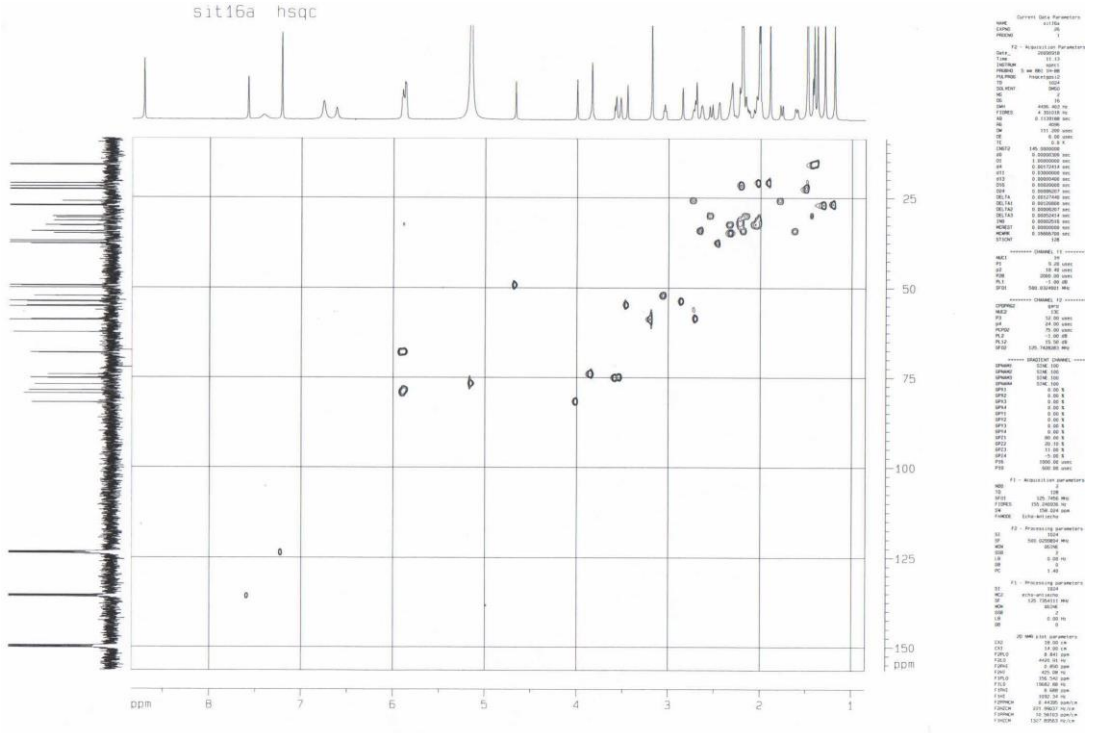


Figure 68. HMBC spectrum of bistenuifolin I (**9**)

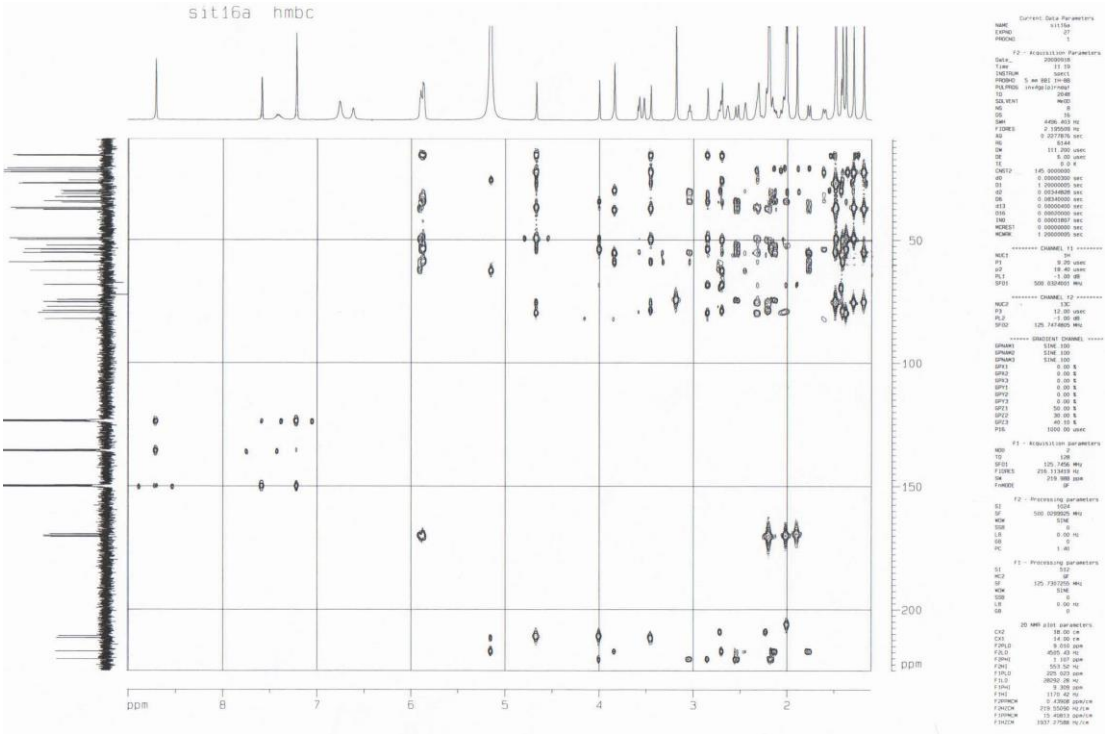



Figure 69. COSY spectrum of bistenuifolin I (**9**)

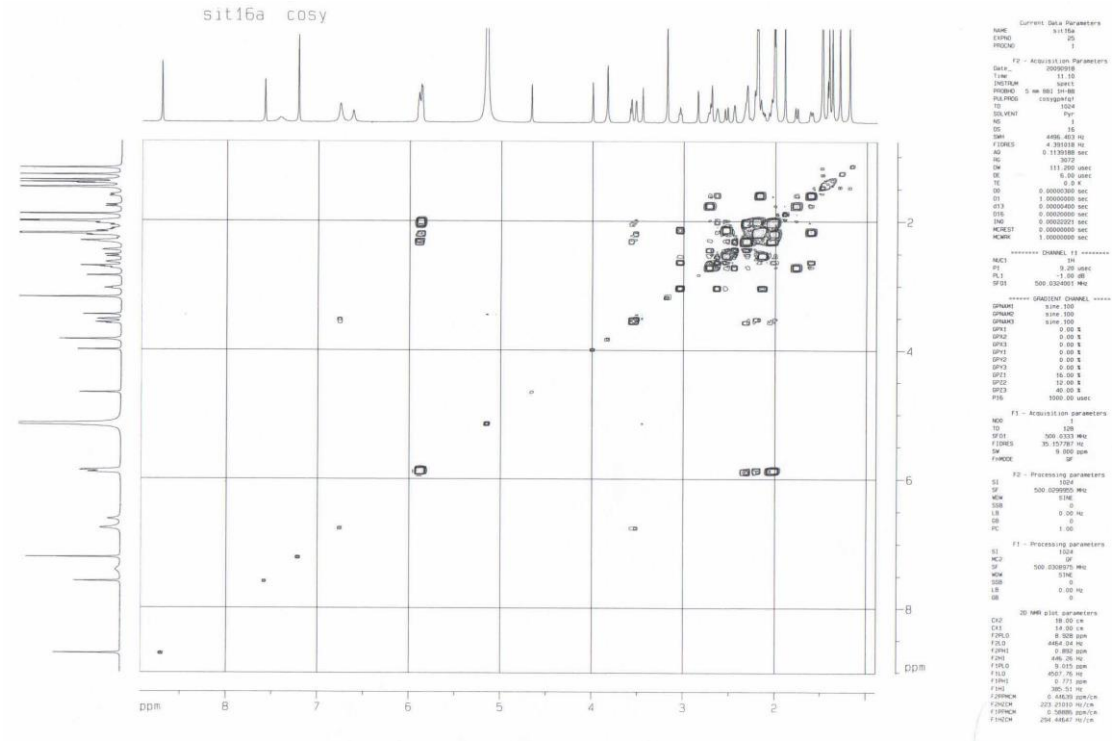


Figure 70. ROESY spectrum of bistenuifolin I (**9**)

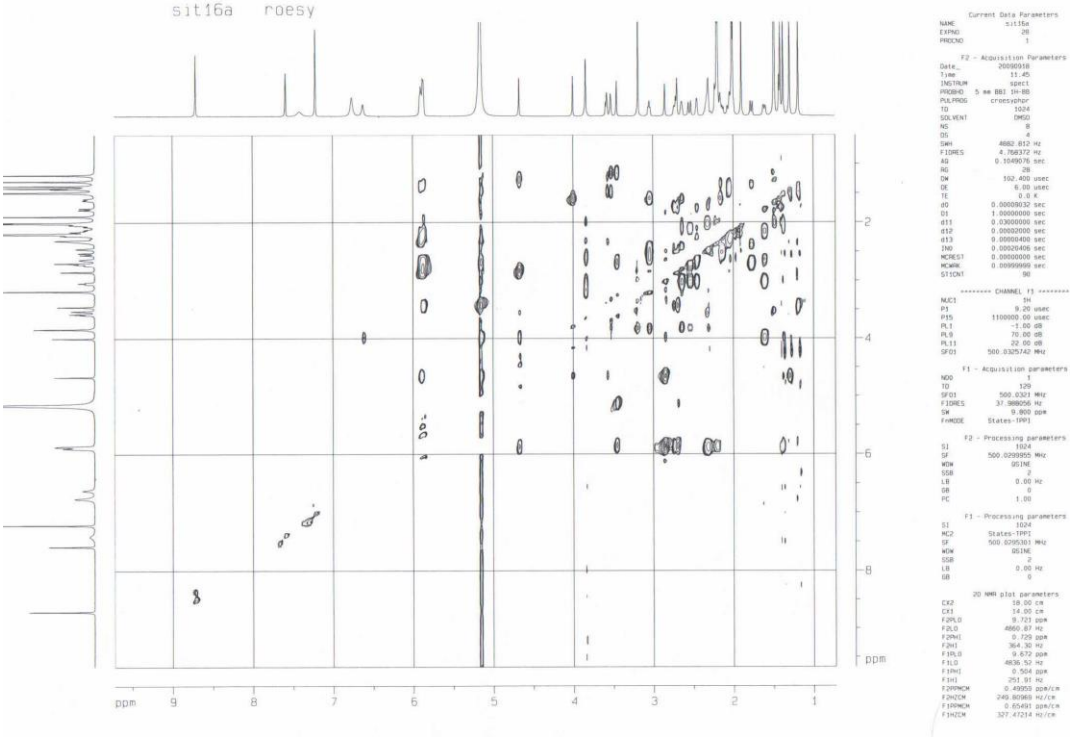
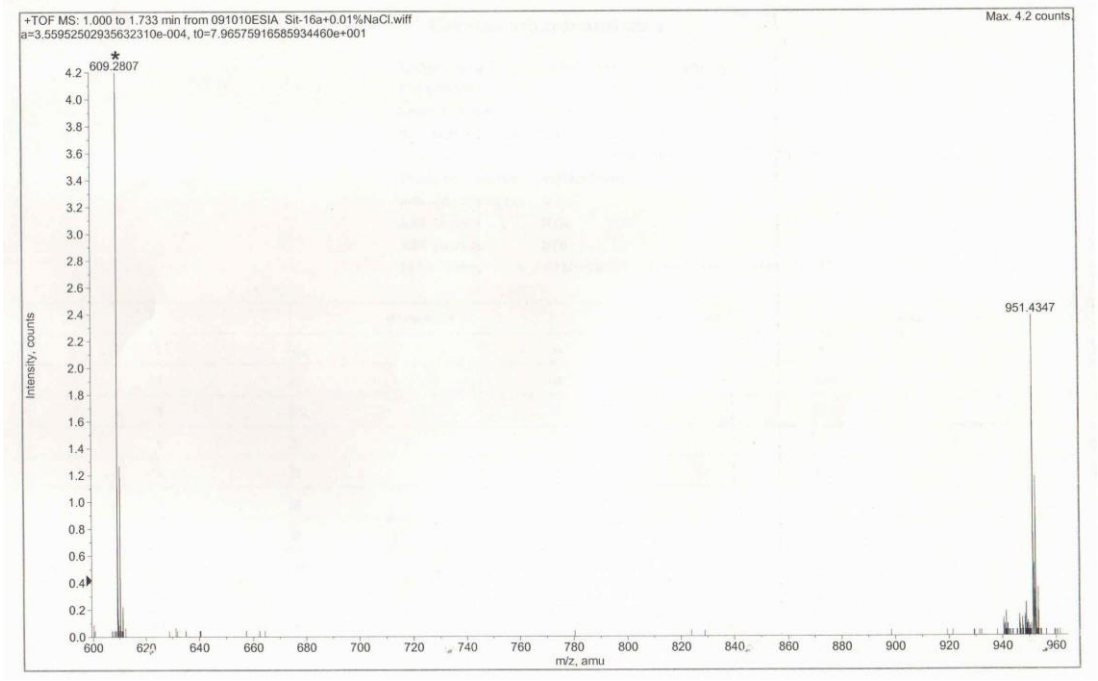
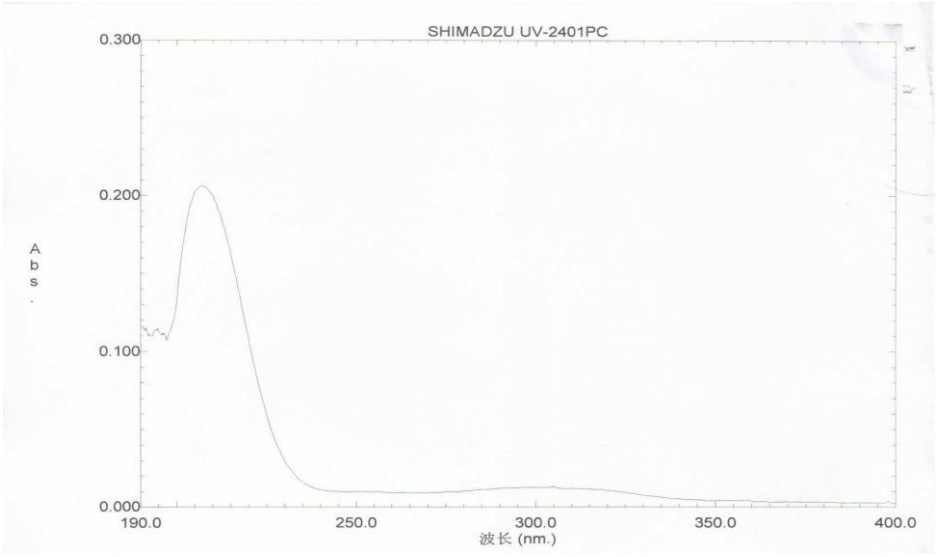


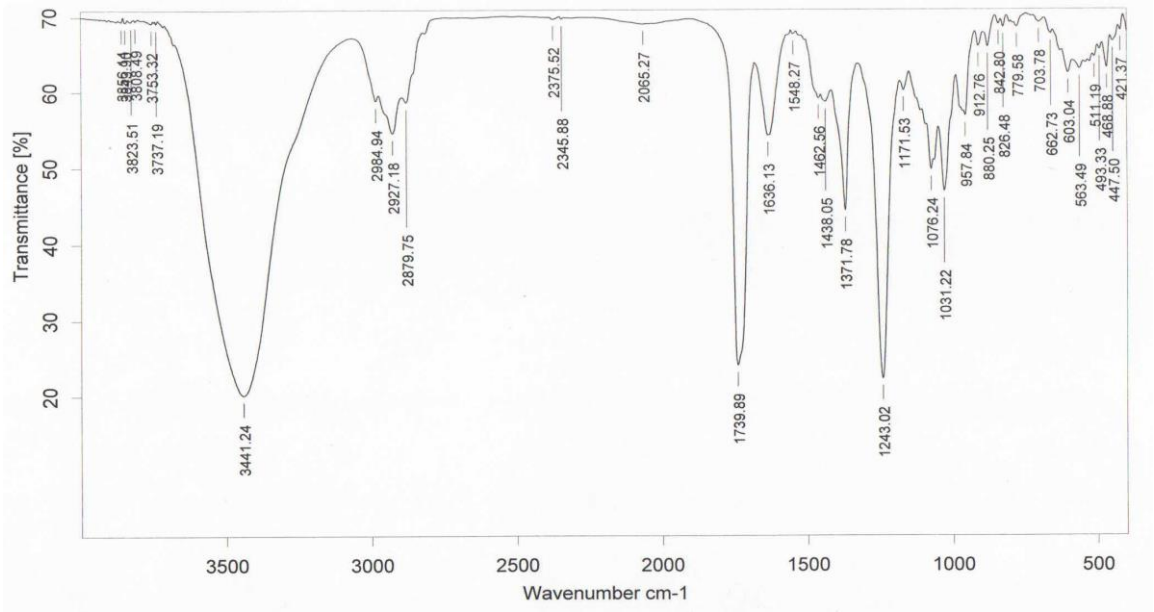

Figure 71. HRESIMS spectrum of bistenuifolin I (**9**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C49 H68 O17 Na | 951.4354 | -0.7212 | -0.7581 | 15.5 |

Figure 72. UV and IR spectra of bistenuifolin I (**9**)



**For compound 10:**

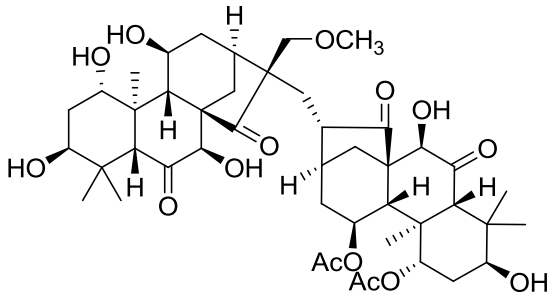



Figure 73. $^{1}$H NMR spectrum of bistenuifolin J (**10**)

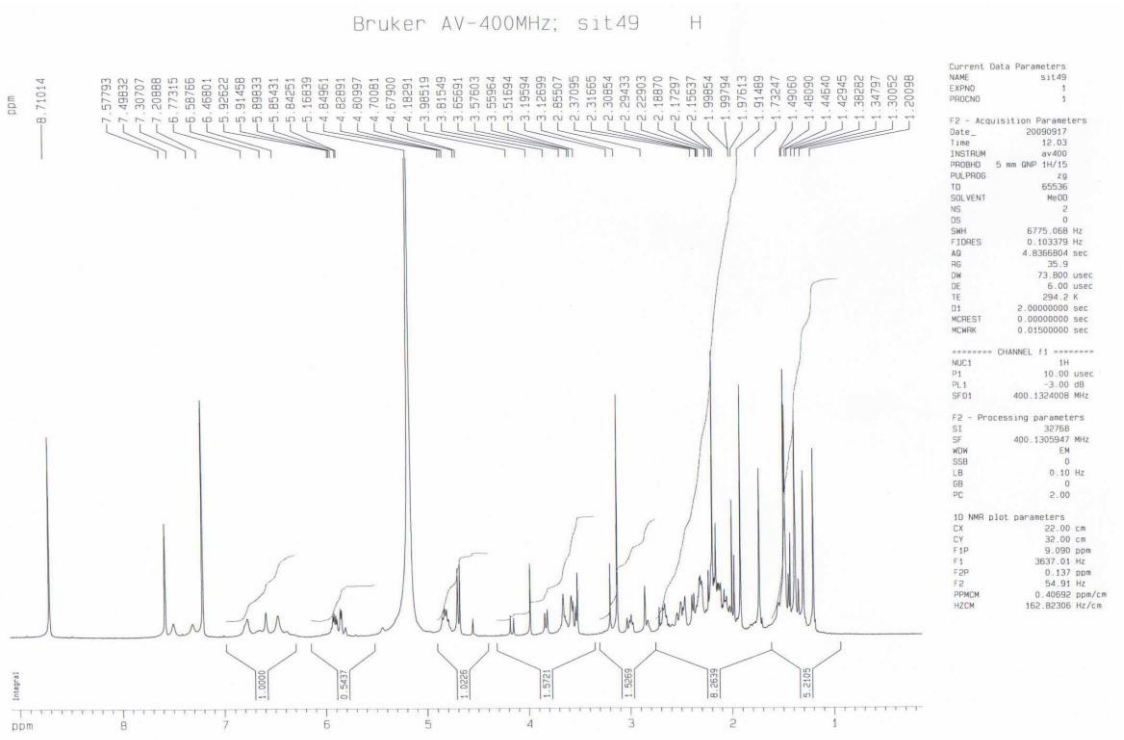


Figure 74. $^{13}$C NMR spectrum of bistenuifolin J (**10**)

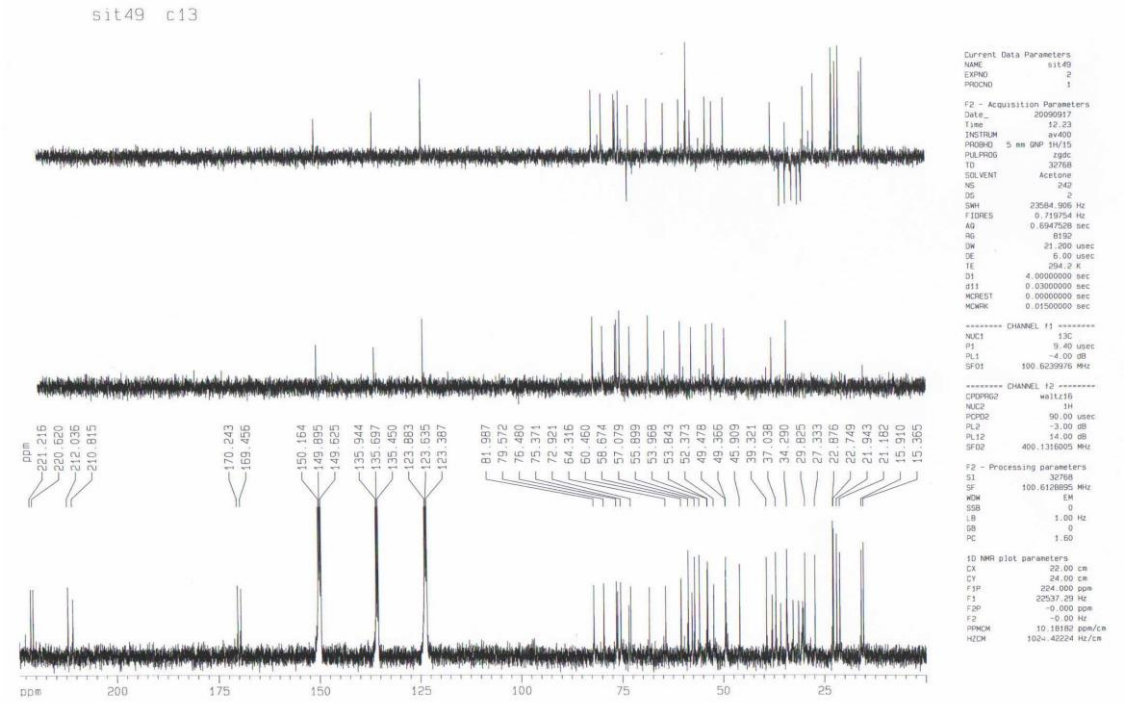



Figure 75. HSQC spectrum of bistenuifolin J (**10**)

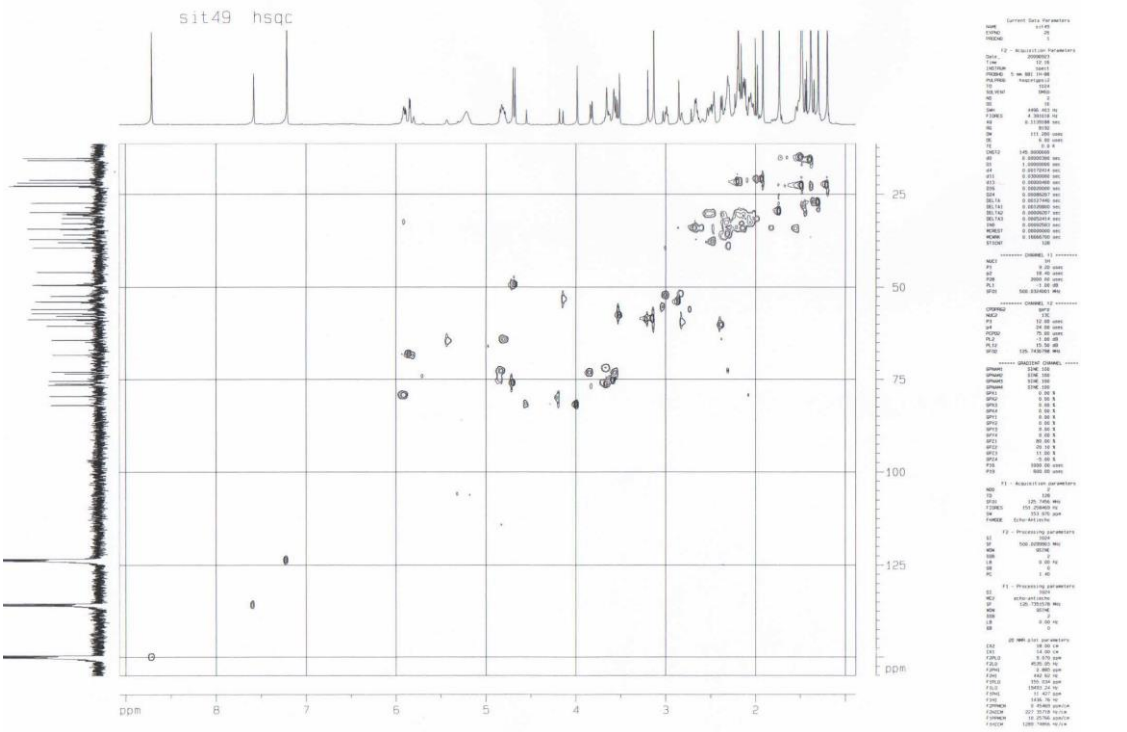


Figure 76. HMBC spectrum of bistenuifolin J (**10**)

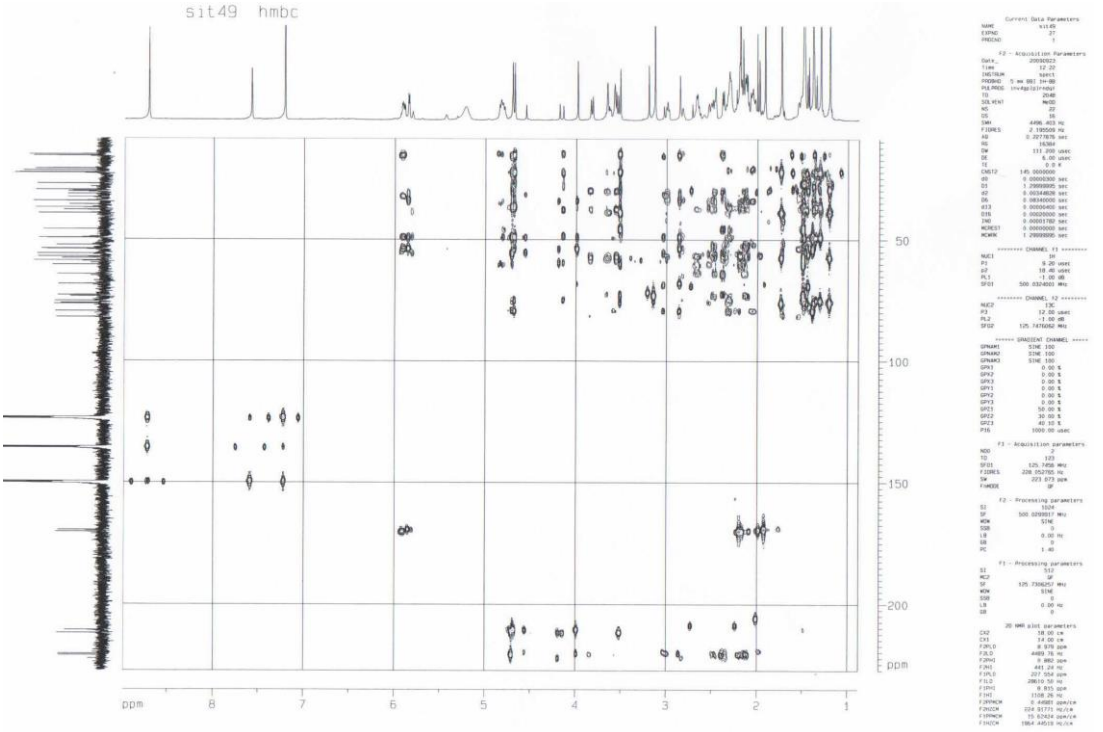



Figure 77. COSY spectrum of bistenuifolin J (**10**)

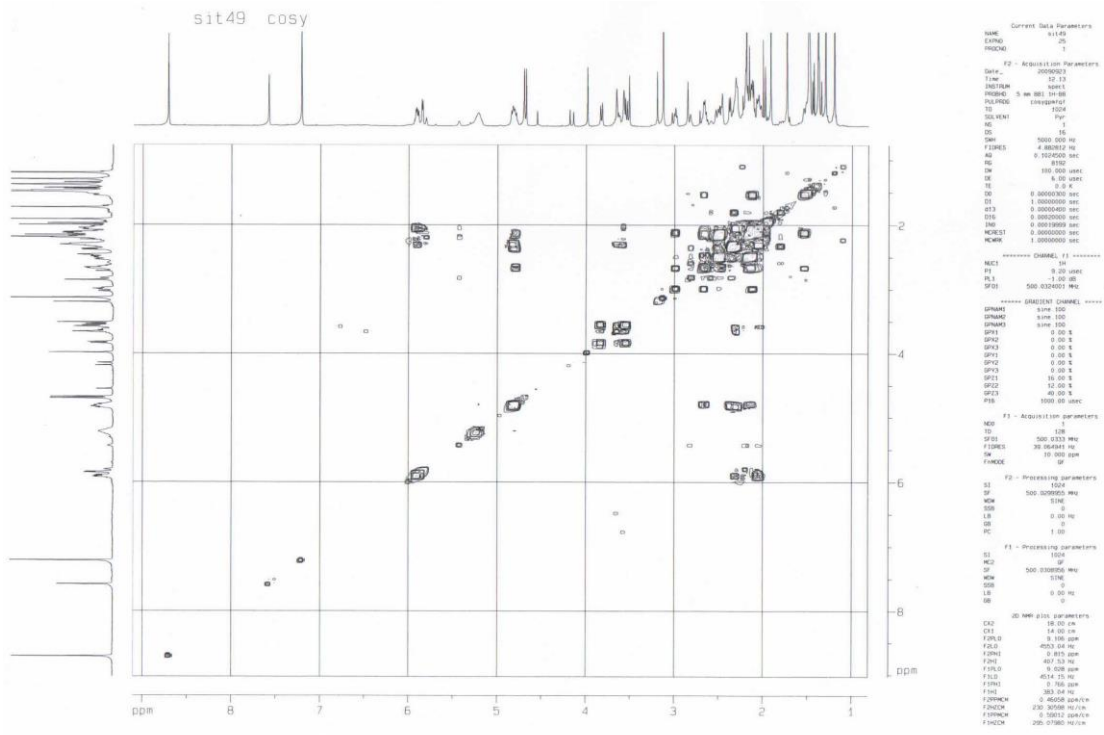


Figure 78. ROESY spectrum of bistenuifolin J (**10**)

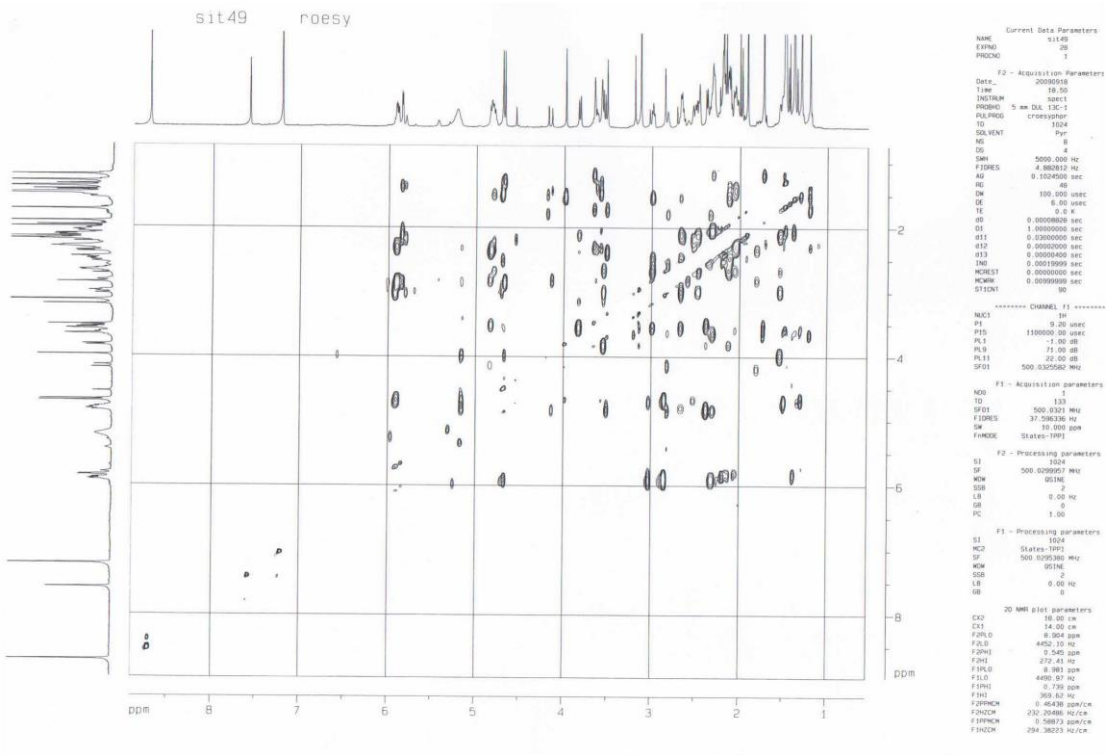
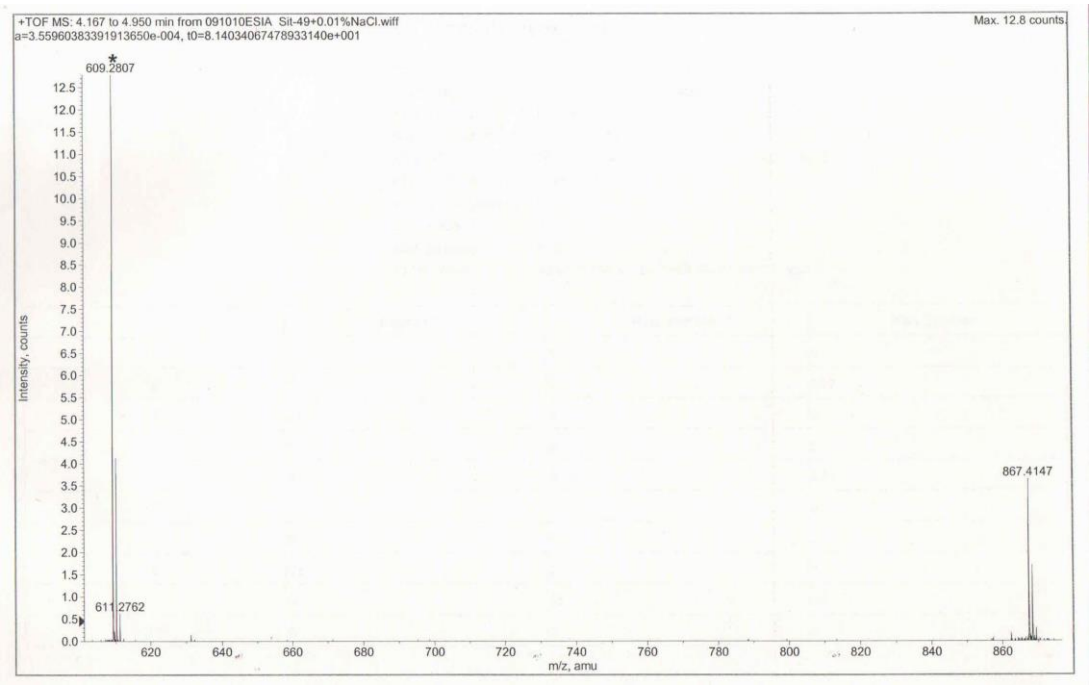
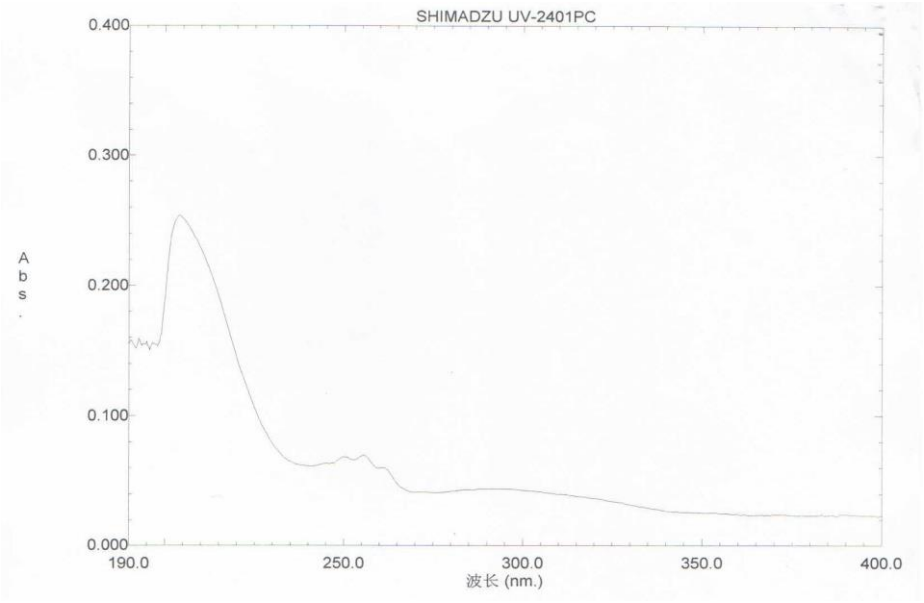


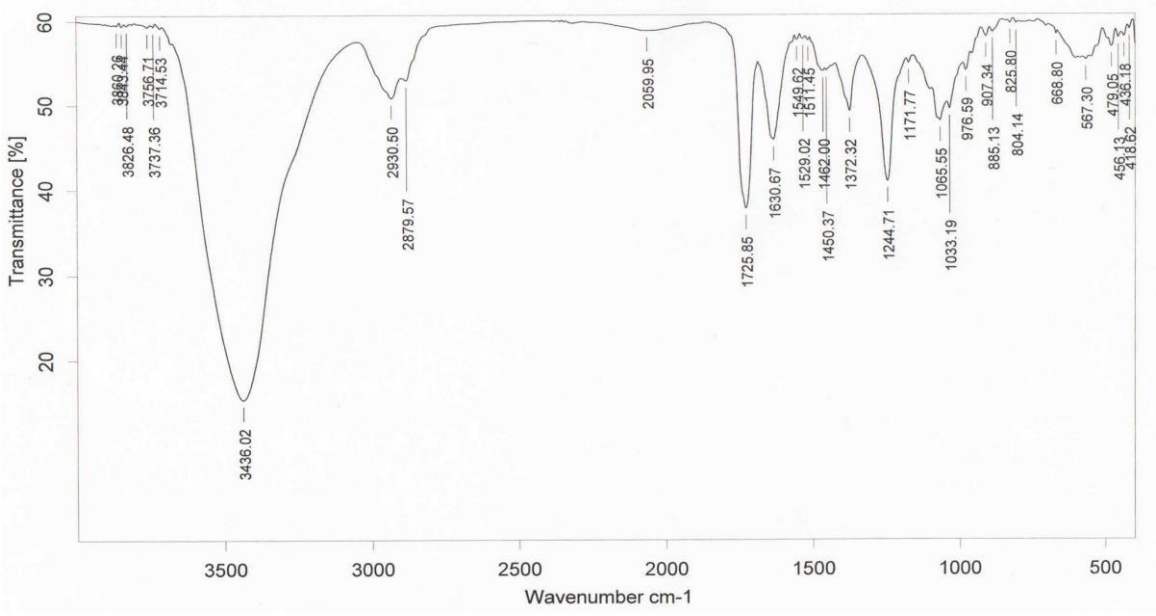

Figure 79. HRESIMS spectrum of bistenuifolin J (**10**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C45 H64 O15 Na | 867.4142 | 0.4081 | 0.4705 | 13.5 |

Figure 80. UV and IR spectra of bistenuifolin J (**10**)



**For compound 11:**

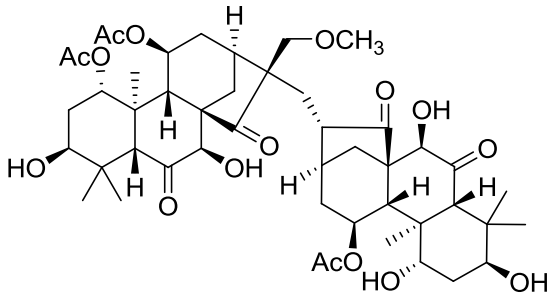



Figure 81. $^{1}$H NMR spectrum of bistenuifolin K (**11**)

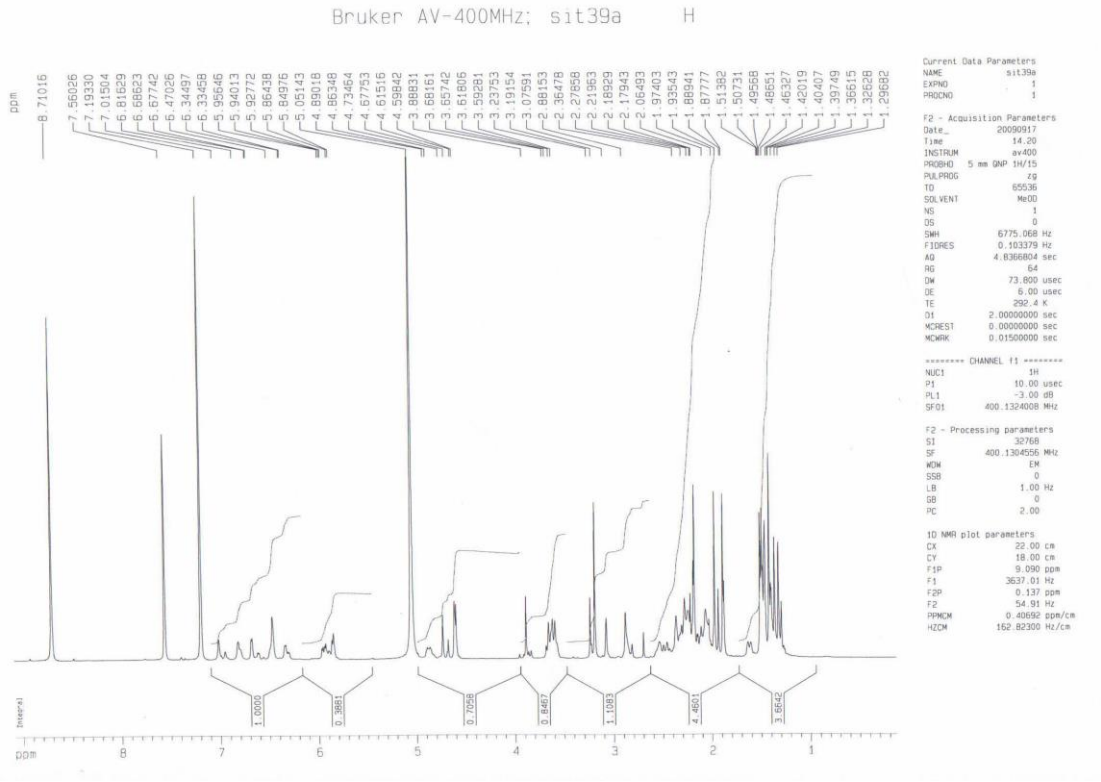


Figure 82. $^{13}$C NMR spectrum of bistenuifolin K (**11**)

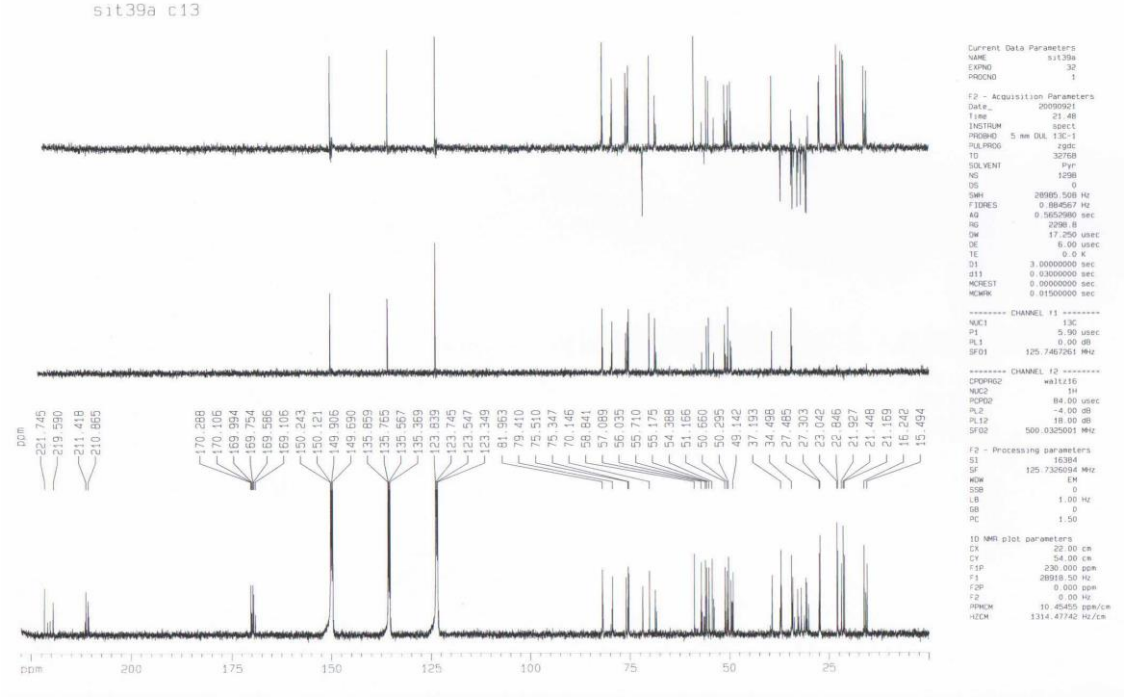



Figure 83. HSQC spectrum of bistenuifolin K (**11**)

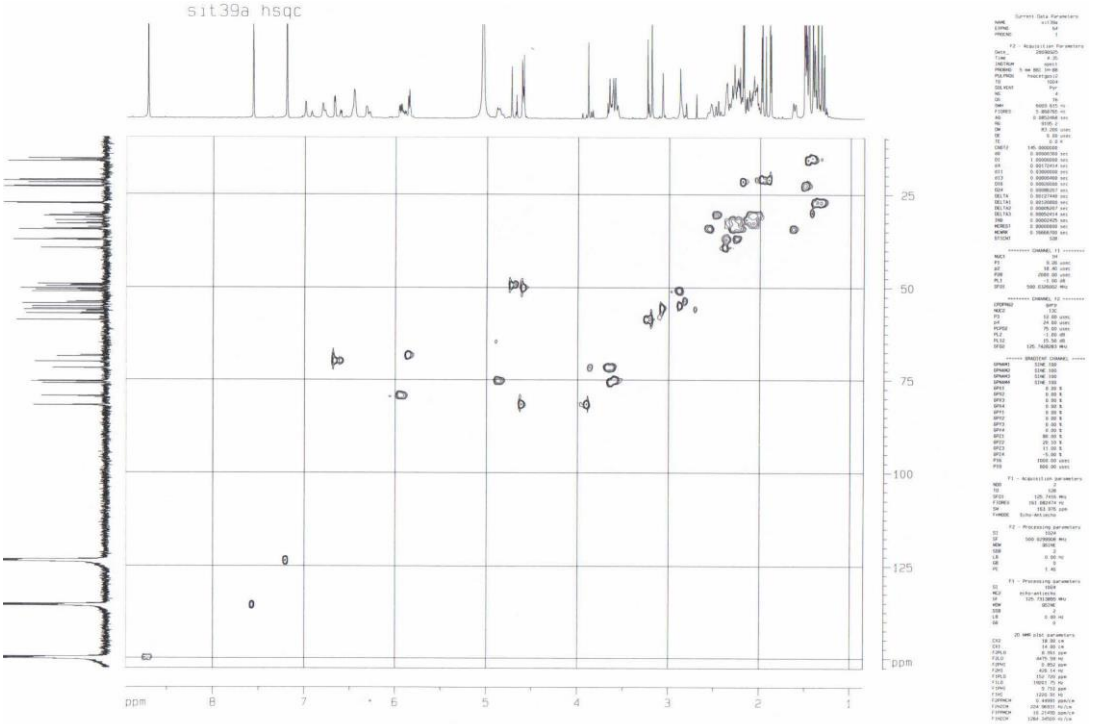


Figure 84. HMBC spectrum of bistenuifolin K (**11**)

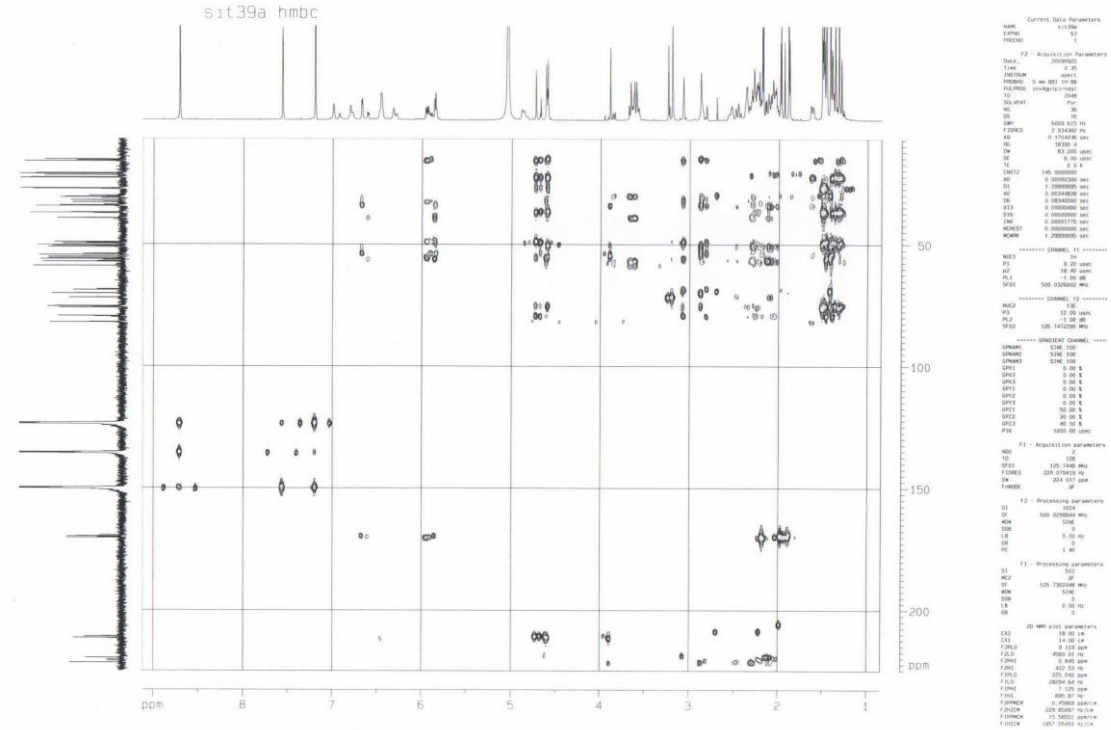



Figure 85. COSY spectrum of bistenuifolin K (**11**)

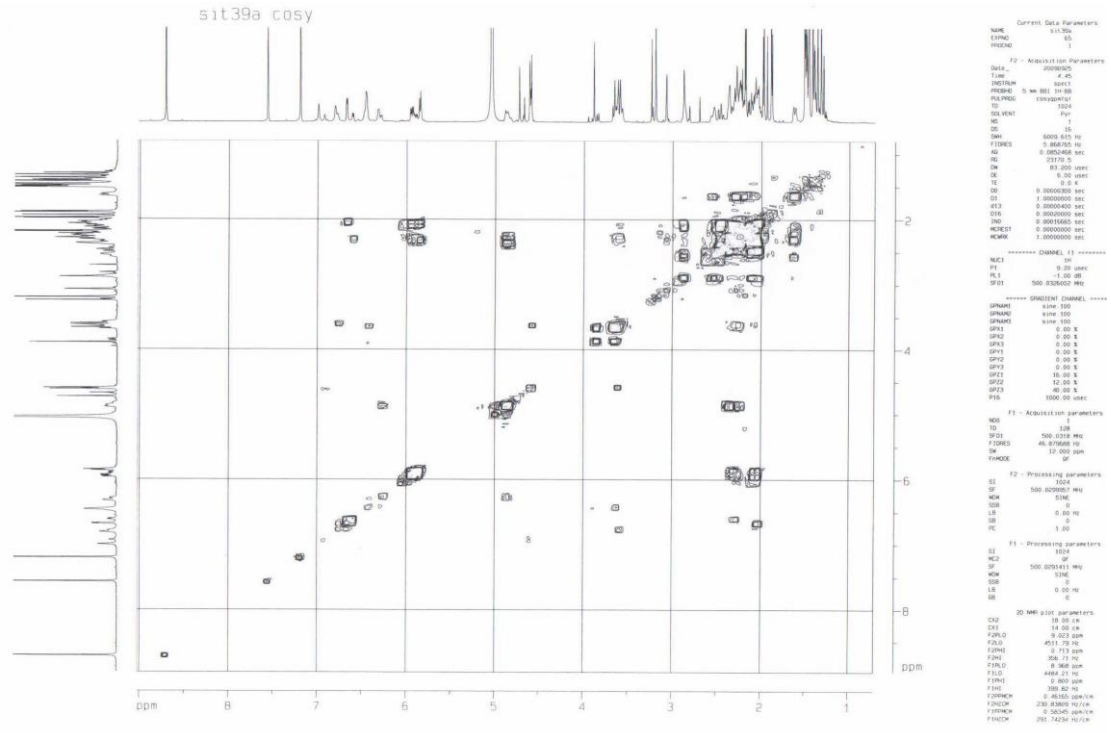


Figure 86. ROESY spectrum of bistenuifolin K (**11**)

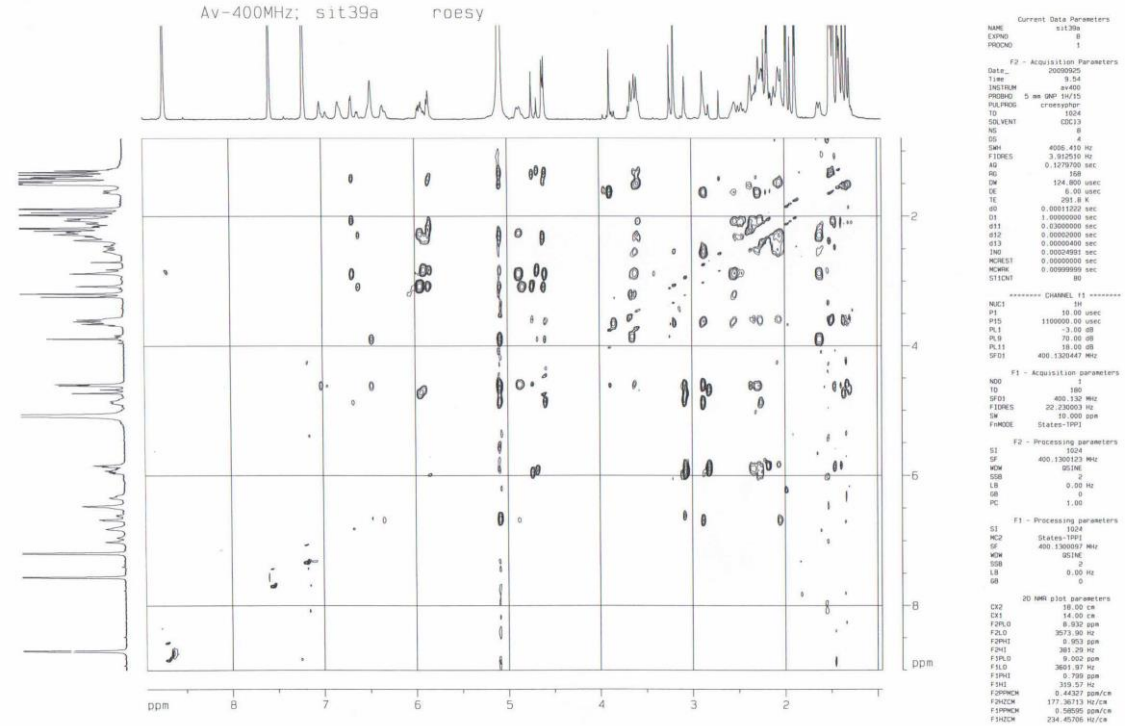
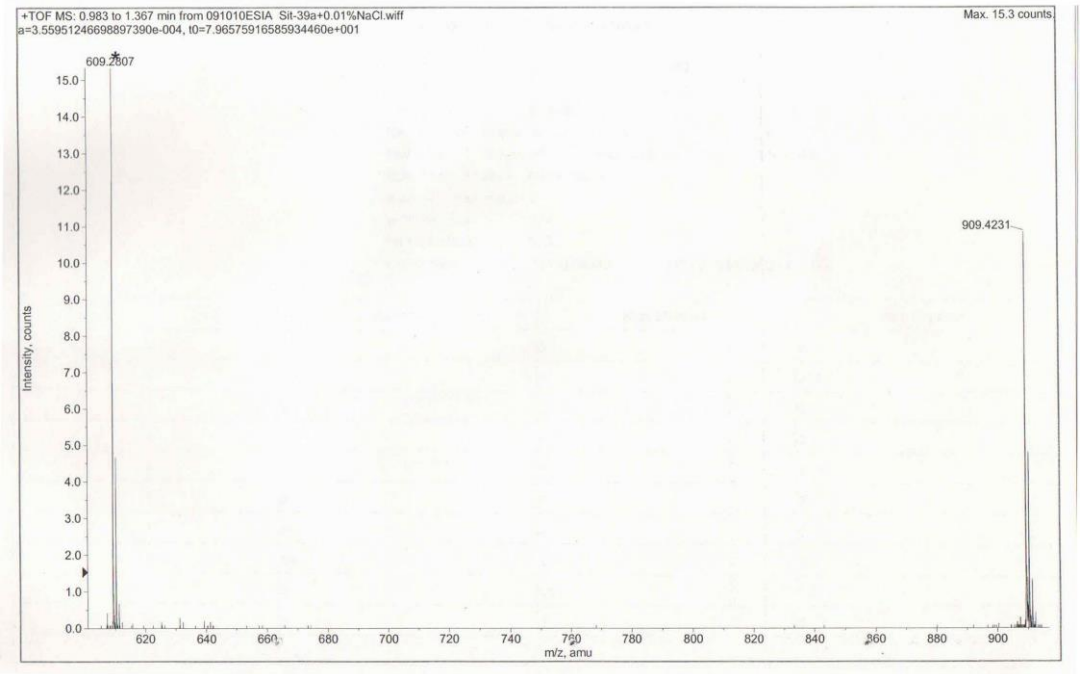
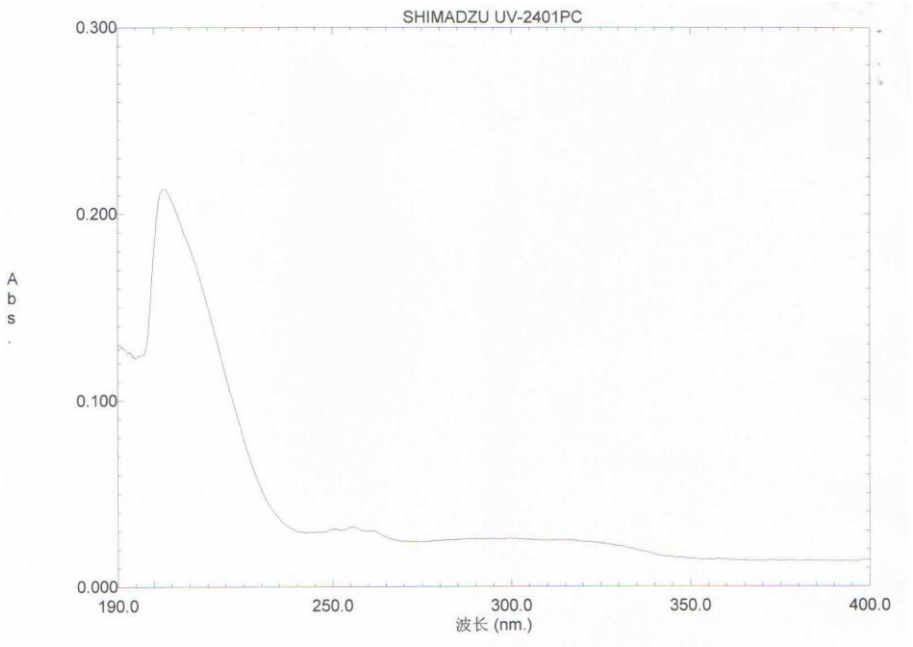


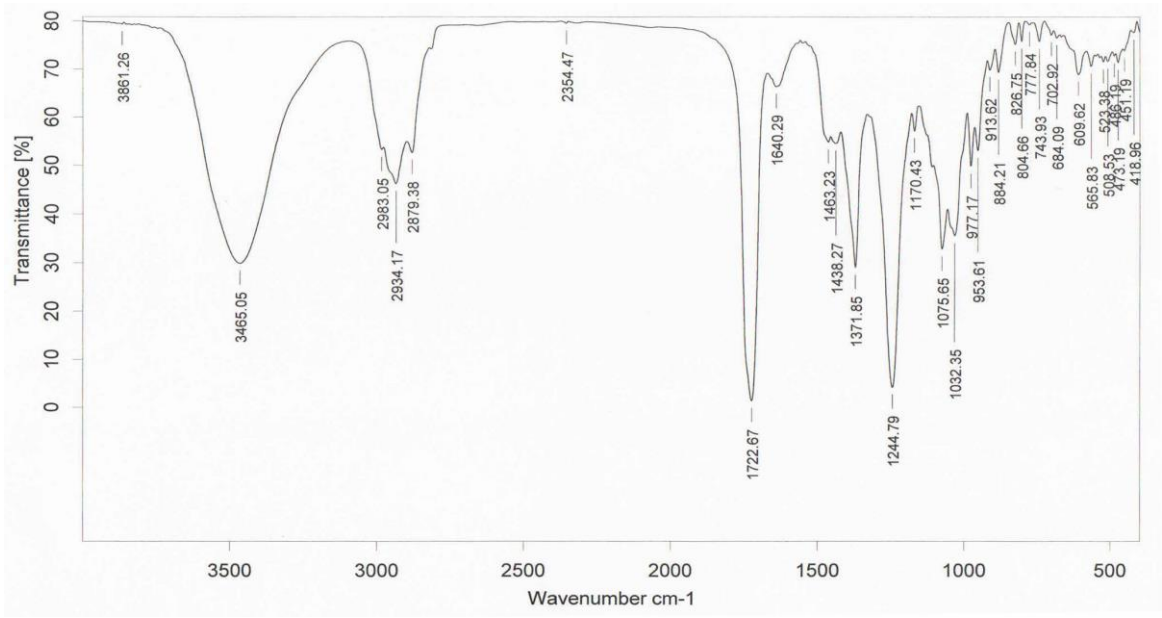

Figure 87. HRESIMS spectrum of bistenuifolin K (**11**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C47 H66 O16 Na | 909.4248 | -1.7565 | -1.9315 | 14.5 |

Figure 88. UV and IR spectra of bistenuifolin K (**11**)



For compound 12:

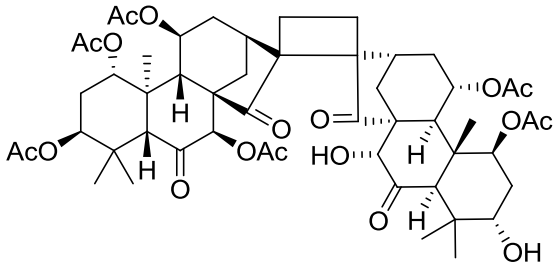



Figure 89. $^{1}$H NMR spectrum of bistenuifolin L (**12**)

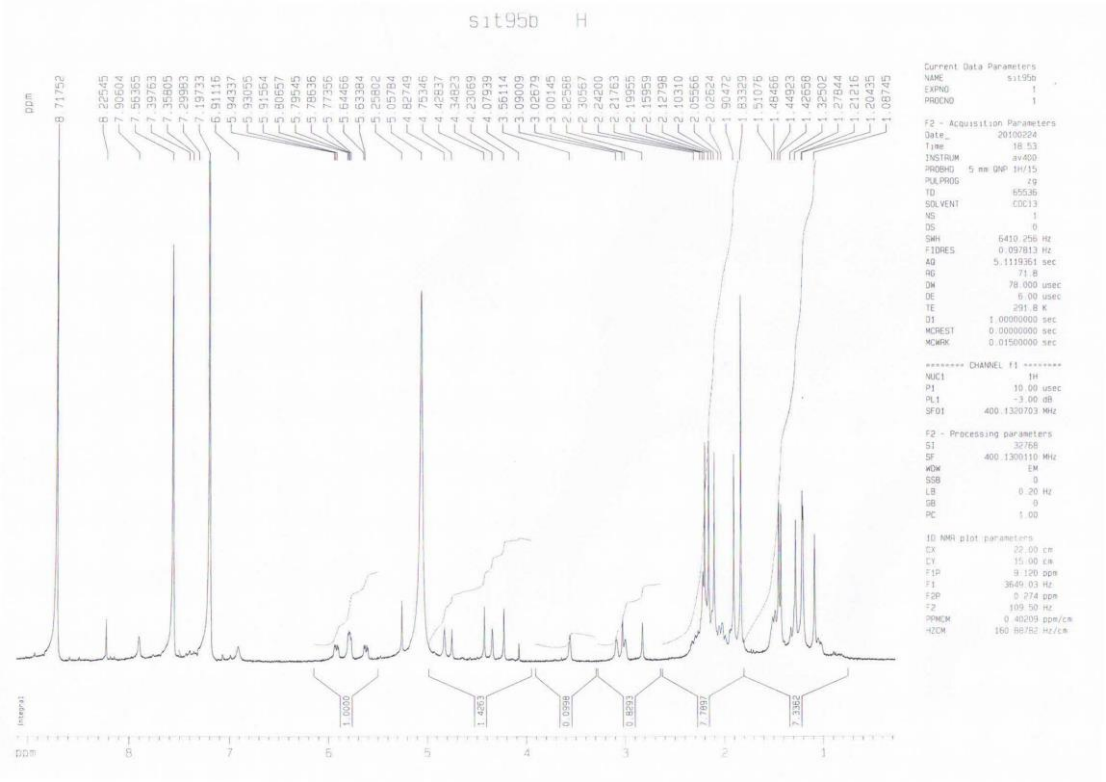


Figure 90. $^{13}$C NMR spectrum of bistenuifolin L (**12**)

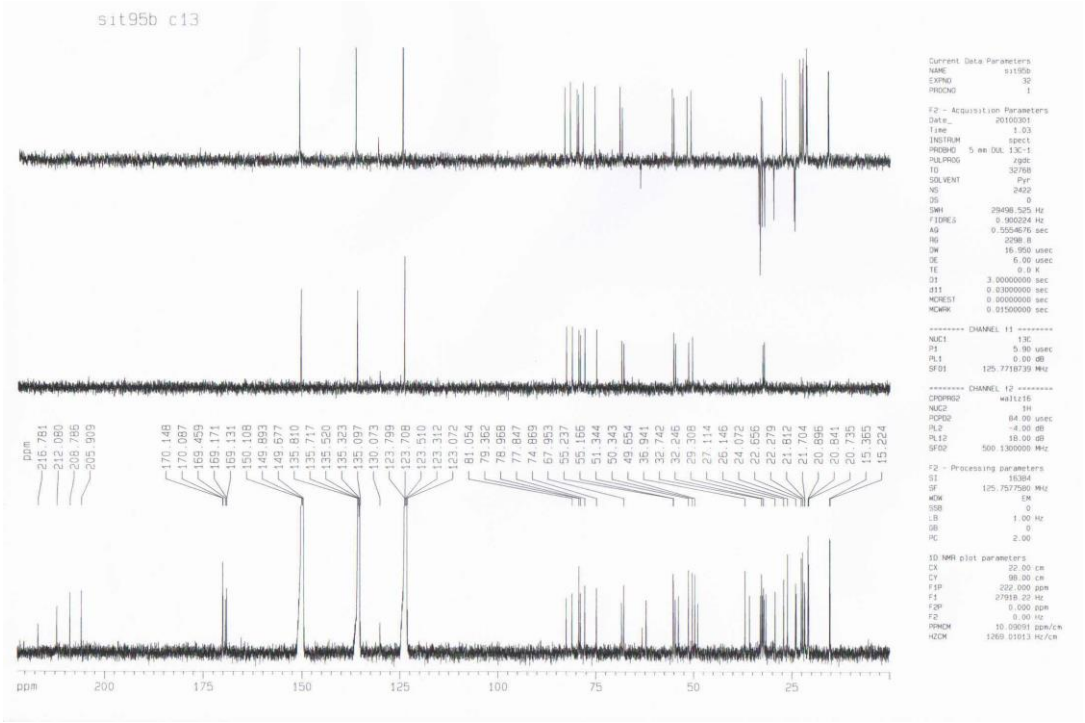



Figure 91. HSQC spectrum of bistenuifolin L (**12**)

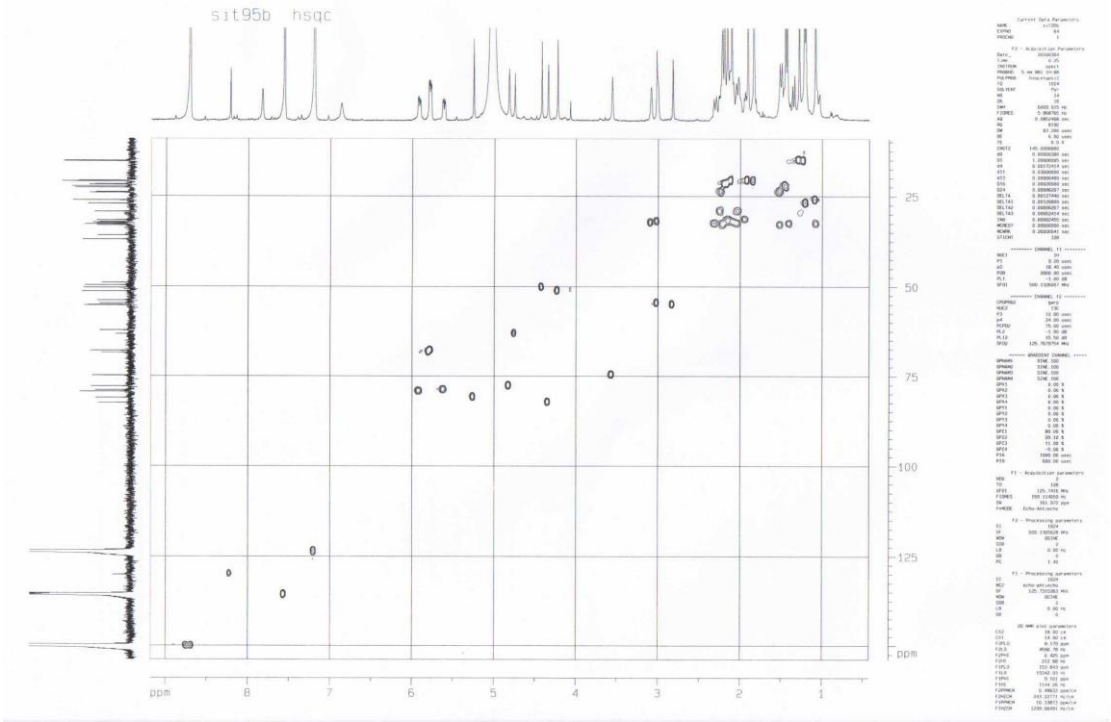


Figure 92. HMBC spectrum of bistenuifolin L (**12**)

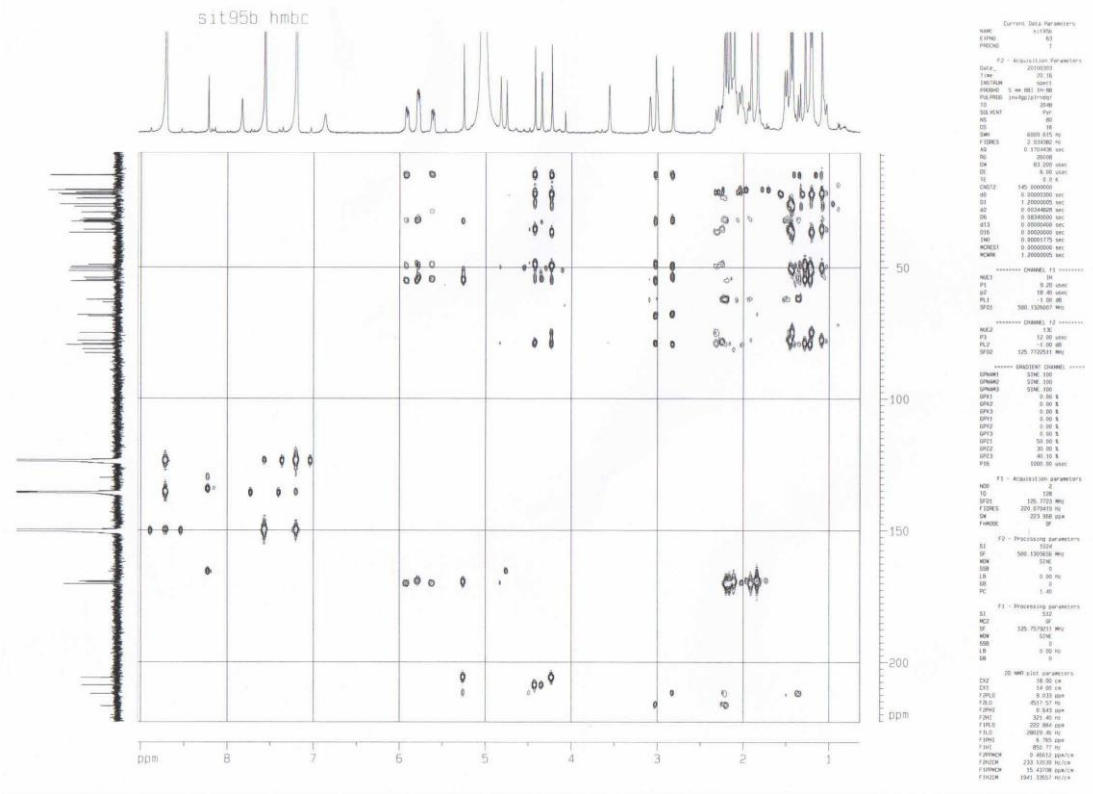



Figure 93. COSY spectrum of bistenuifolin L (**12**)

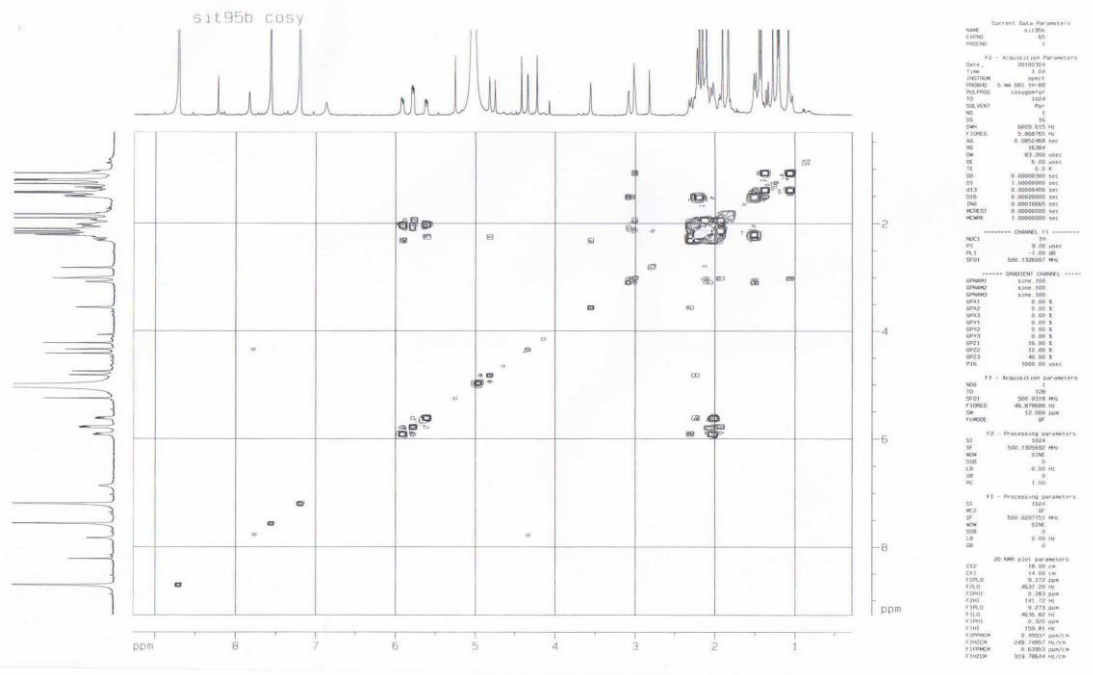


Figure 94. ROESY spectrum of bistenuifolin L (**12**)

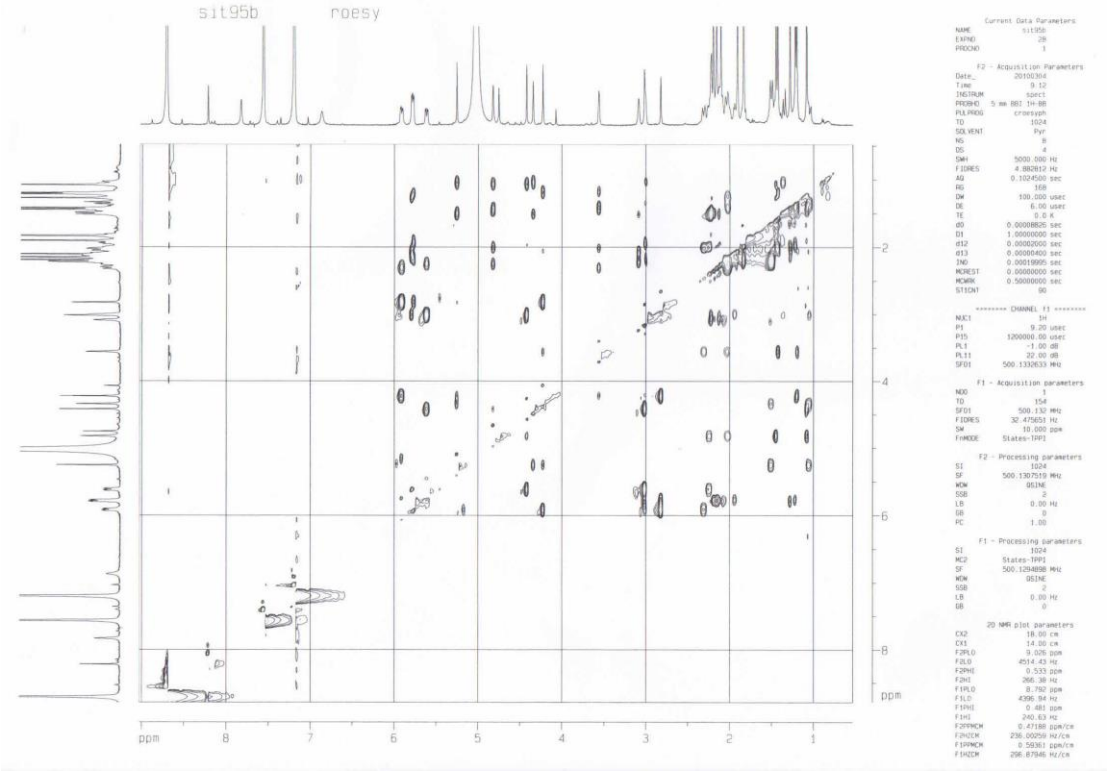
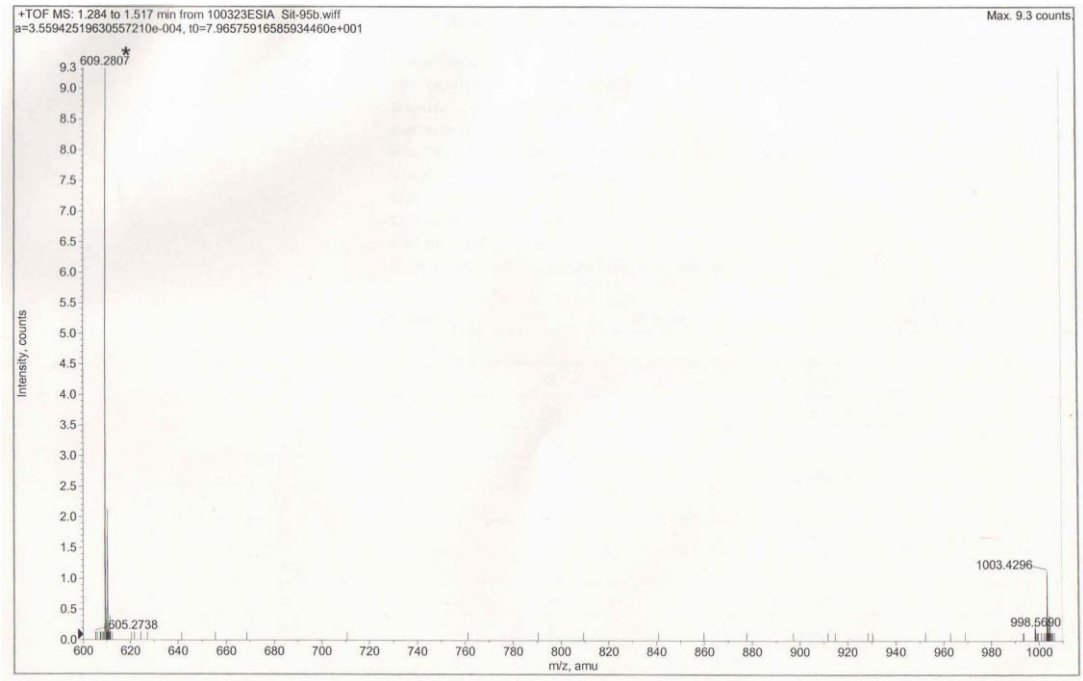
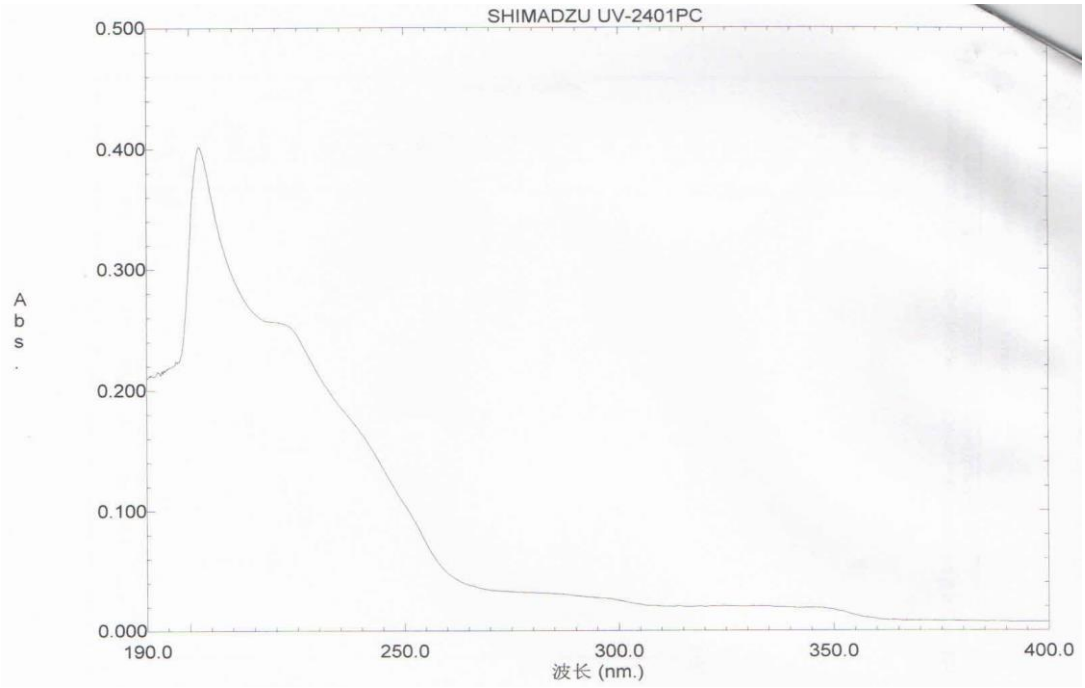


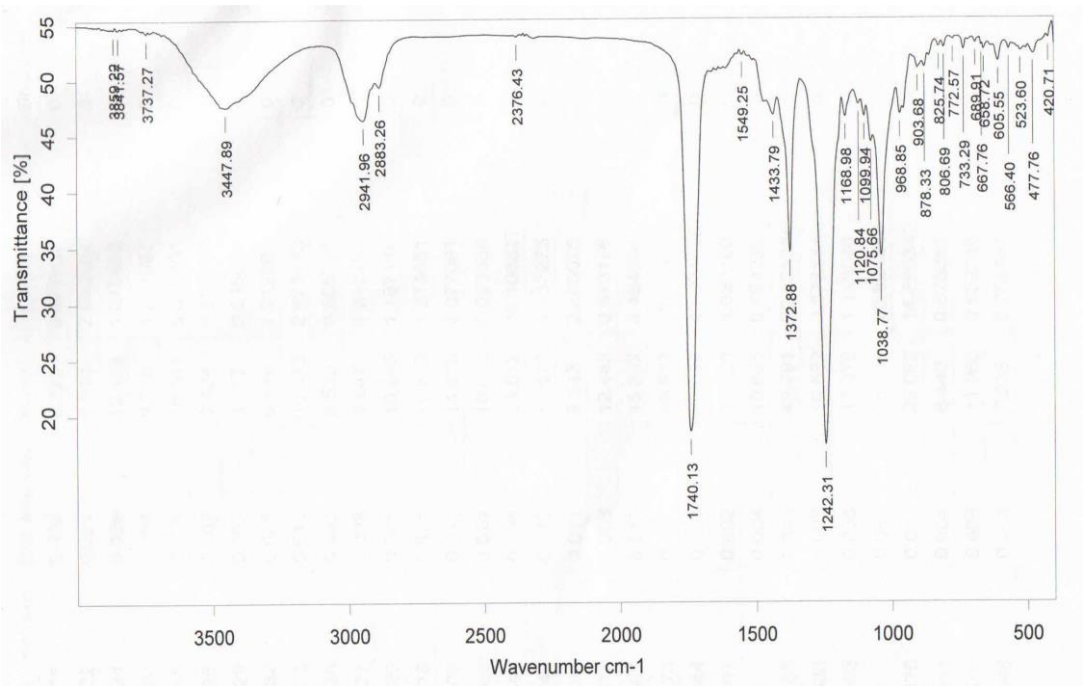

Figure 95. HRESIMS spectrum of bistenuifolin L (**12**)




| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C52 H68 O18 Na | 1003.4303 | -0.7359 | -0.7334 | 18.5 |

Figure 96. UV and IR spectra of bistenuifolin L (**12**)



**For compound 13:**

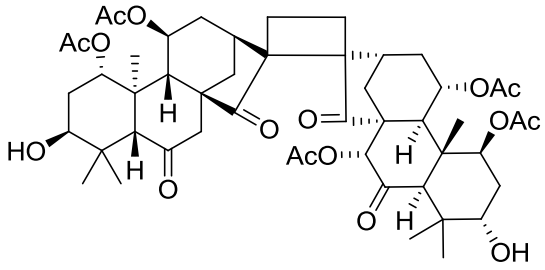



Figure 97. $^{1}$H NMR spectrum of bistenuifolin M (**13**)

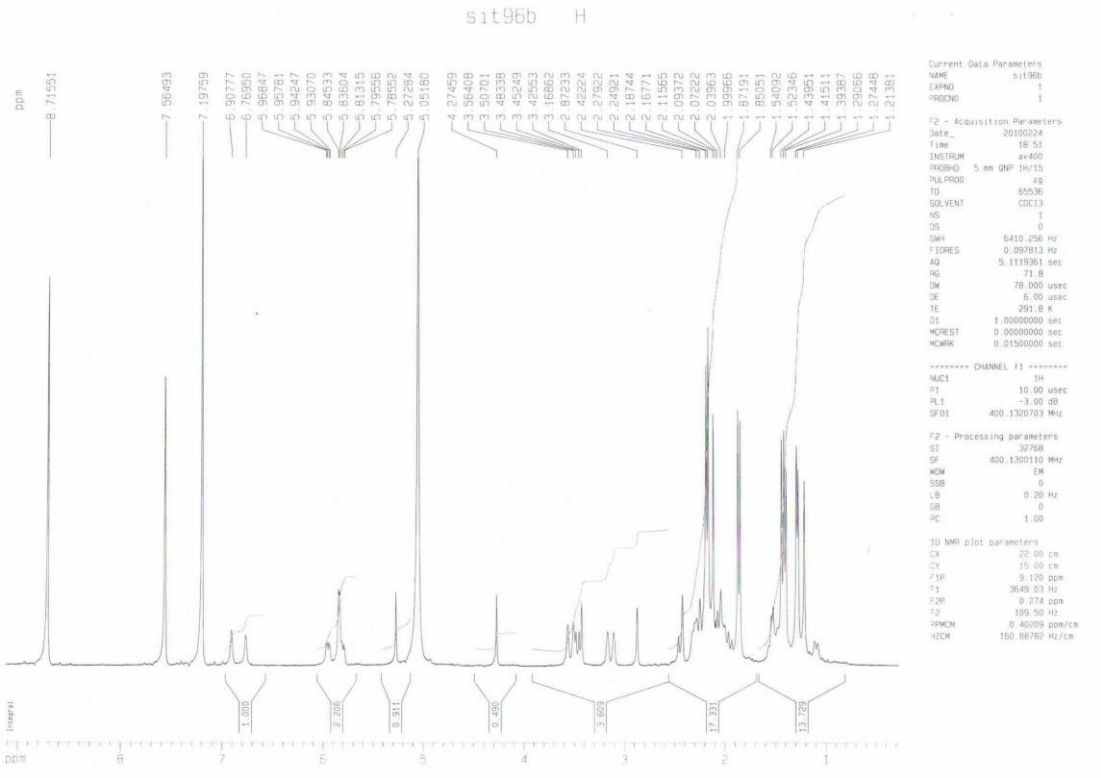


Figure 98. $^{13}$C NMR spectrum of bistenuifolin M (**13**)

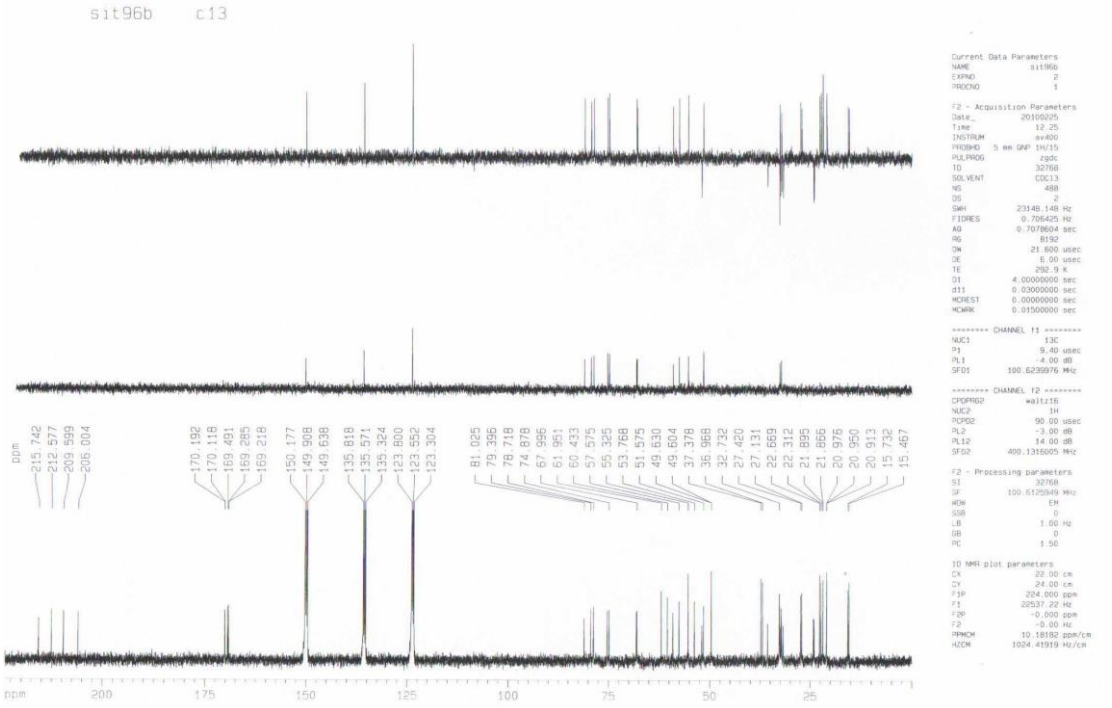



Figure 99. HSQC spectrum of bistenuifolin M (**13**)

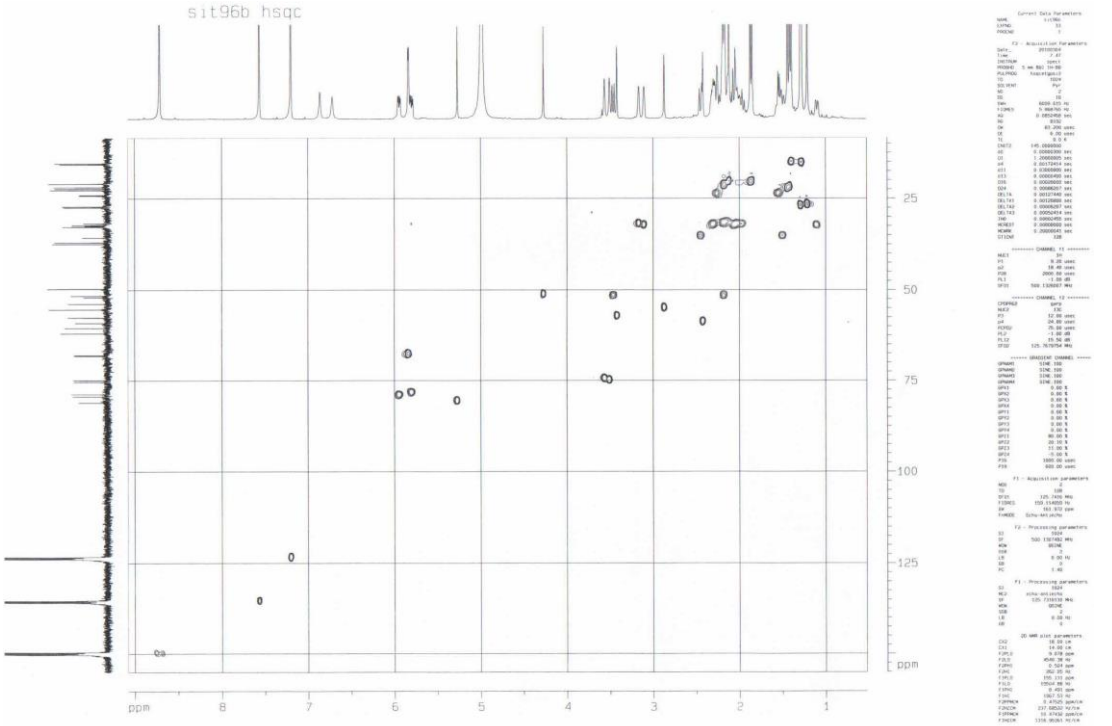


Figure 100. HMBC spectrum of bistenuifolin M (**13**)

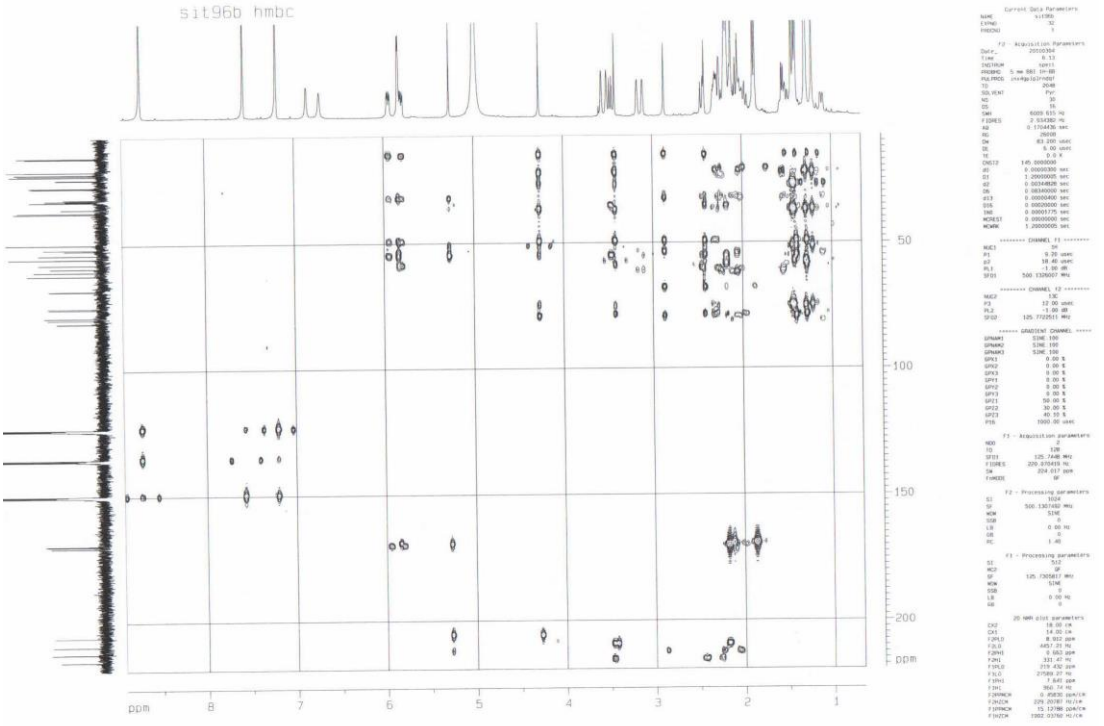



Figure 101. COSY spectrum of bistenuifolin M (**13**)

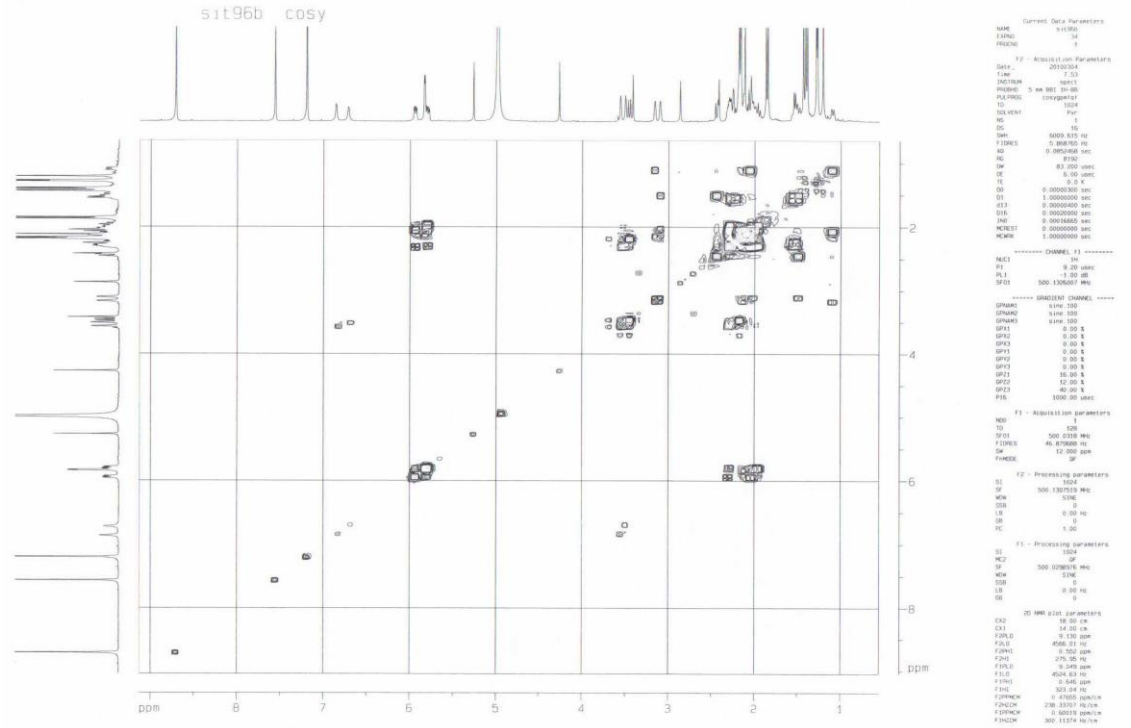


Figure 102. ROESY spectrum of bistenuifolin M (**13**)

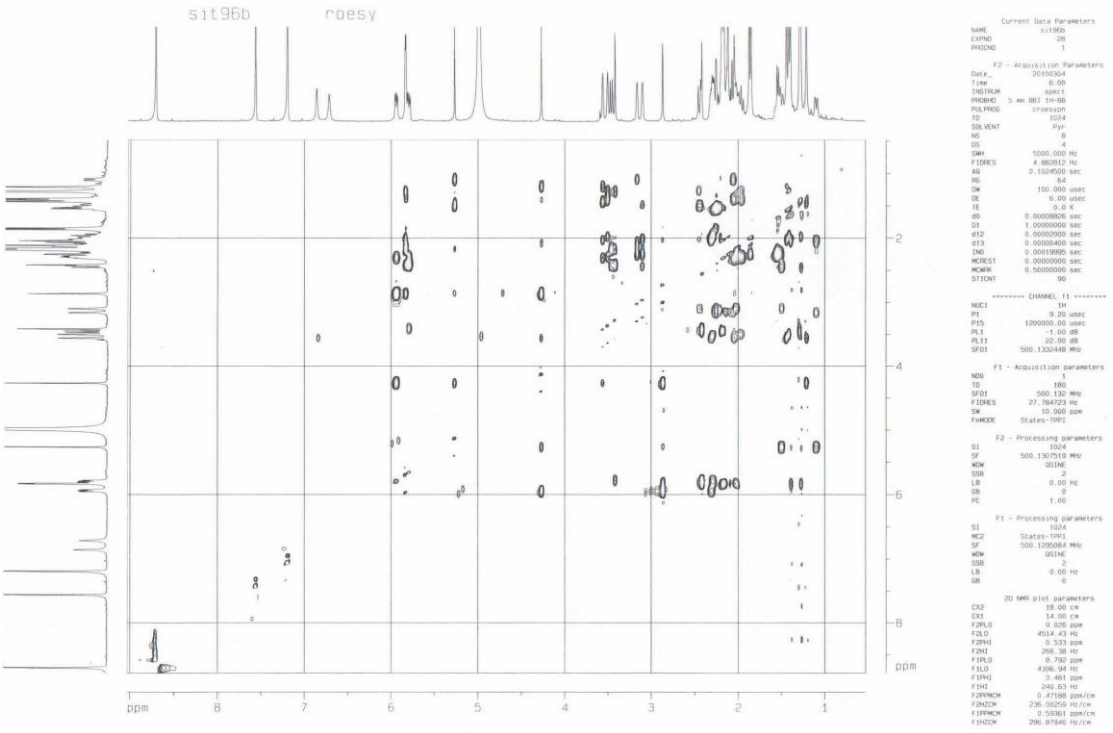
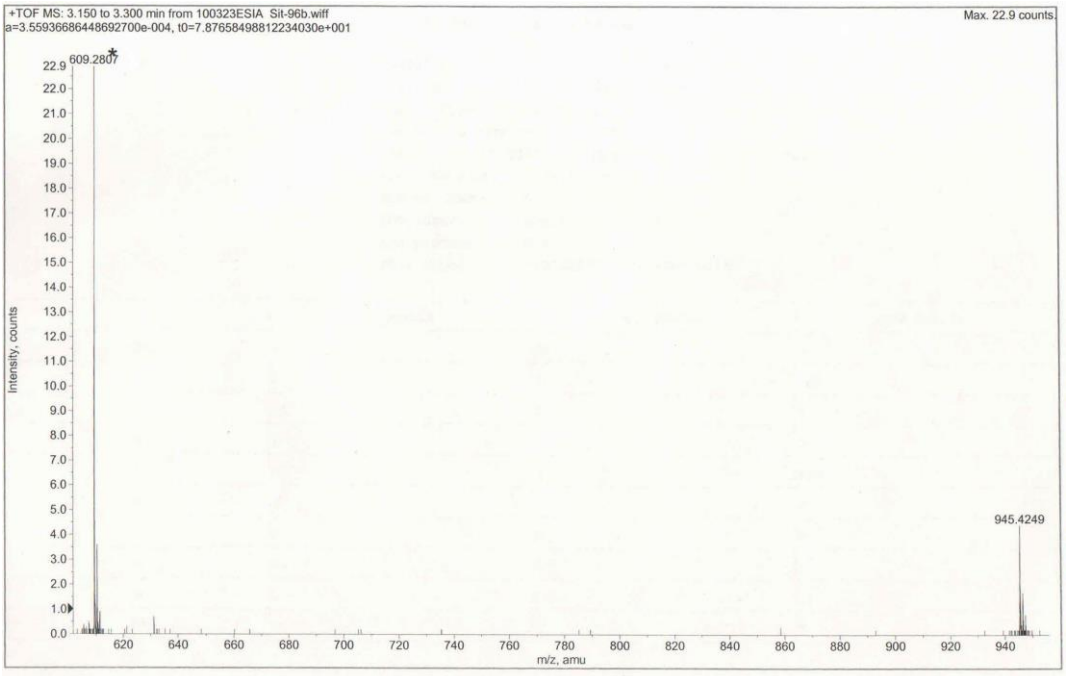
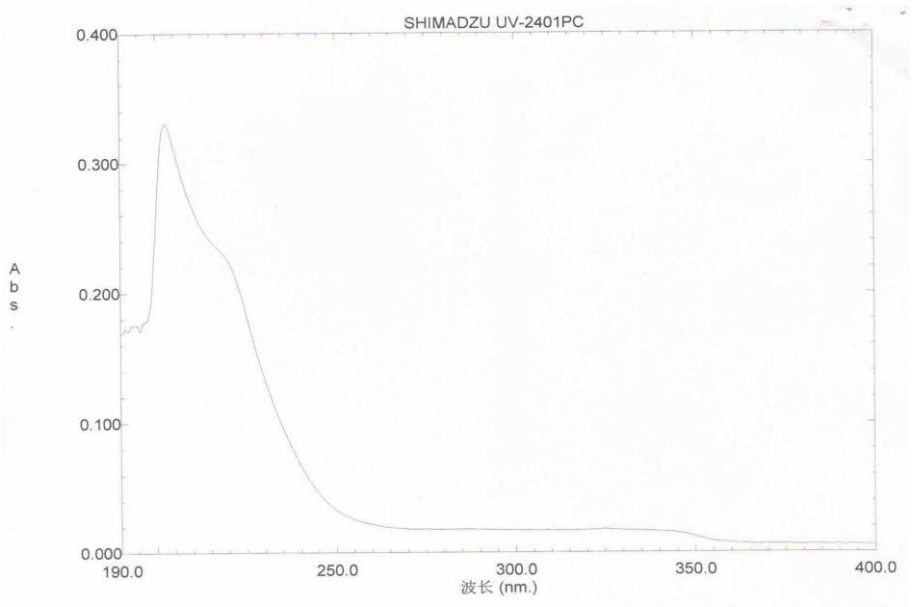


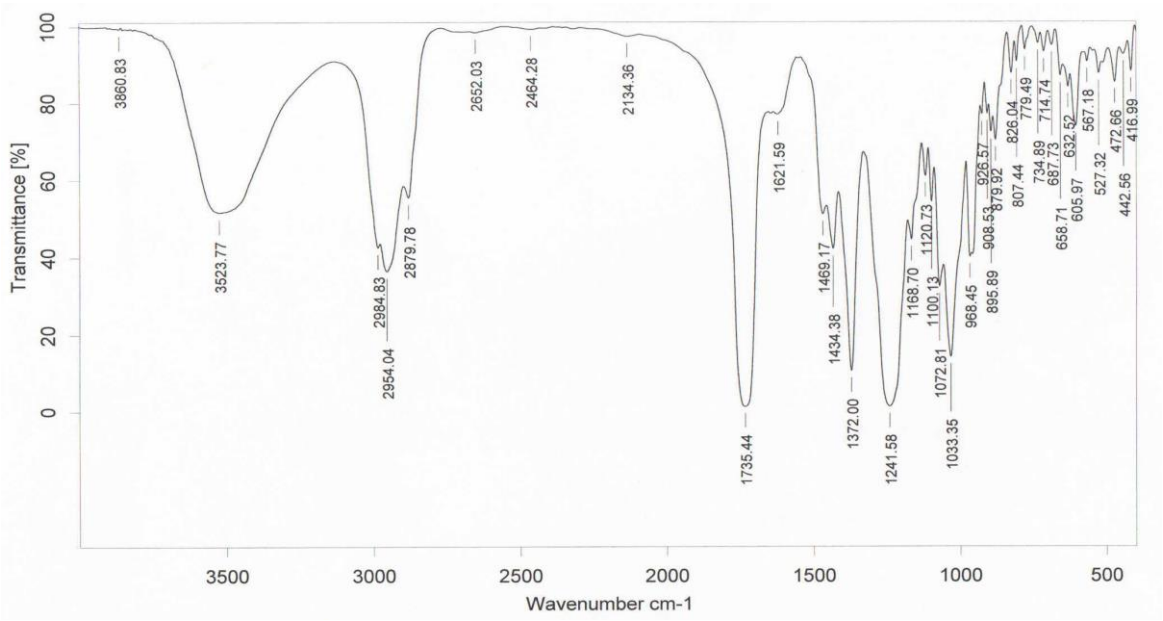

Figure 103. HRESIMS spectrum of bistenuifolin M (**13**)



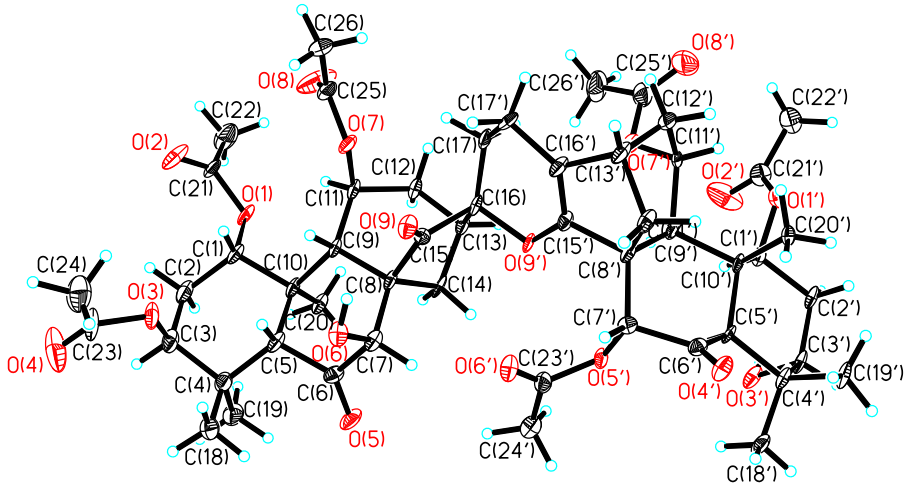

| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C50 H66 O16 Na | 945.4248 | 0.0434 | 0.0459 | 17.5 |

Figure 104. UV and IR spectra of bistenuifolin M (**13**)



**X-ray data of compound 1**




ORTEP Plot of compound **1**

**Table 1.** Atomic coordinates (x$10^4$) and equivalent isotropic displacement parameters (Å$^2$ x $10^3$) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| O(18) | 2309(2) | 5172(2) | 7046(1) | 25(1) |
| O(7) | 2602(2) | 11919(2) | 6936(1) | 25(1) |
| O(1) | 5663(2) | 7197(2) | 5578(1) | 21(1) |
| O(18') | 3002(2) | -197(2) | 8014(1) | 25(1) |
| O(1') | -581(2) | 1458(2) | 9411(1) | 20(1) |
| O(7') | 2459(2) | 6605(2) | 8299(1) | 20(1) |
| C(18) | 1219(2) | 5774(3) | 6601(1) | 24(1) |
| C(4) | 1600(2) | 6502(3) | 5925(1) | 20(1) |
| C(5) | 2527(2) | 7929(3) | 6092(1) | 20(1) |
| C(10) | 3447(2) | 8283(3) | 5533(1) | 19(1) |
| C(9) | 4482(2) | 9292(3) | 5913(1) | 19(1) |
| C(11) | 5696(2) | 8611(3) | 5917(1) | 18(1) |
| C(12) | 6797(2) | 9273(3) | 6298(1) | 20(1) |
| C(13) | 6598(2) | 10594(3) | 6708(1) | 21(1) |
| C(15) | 7766(2) | 11281(3) | 7178(1) | 25(1) |
| C(16) | 8276(4) | 10062(4) | 7729(2) | 45(1) |
| C(19) | 284(2) | 6900(3) | 5497(1) | 28(1) |

| | | | | |
|---|---|---|---|---|
| C(8) | 4252(2) | 10534(3) | 6341(1) | 20(1) |
| C(7) | 2826(2) | 10972(3) | 6356(1) | 21(1) |
| C(6) | 1892(2) | 9490(3) | 6290(1) | 22(1) |
| C(14) | 5341(2) | 11206(3) | 6736(1) | 21(1) |
| C(1) | 4277(2) | 6816(3) | 5355(1) | 20(1) |
| C(2) | 3834(2) | 5309(3) | 5690(1) | 21(1) |
| C(3) | 2327(2) | 5230(3) | 5533(1) | 21(1) |
| C(17) | 8866(3) | 11868(4) | 6783(2) | 36(1) |
| C(20) | 2773(2) | 9047(3) | 4873(1) | 23(1) |
| C(18') | 4026(2) | 399(3) | 8500(1) | 22(1) |
| C(4') | 3552(2) | 1033(3) | 9169(1) | 19(1) |
| C(5') | 2575(2) | 2413(3) | 9002(1) | 17(1) |
| C(10') | 1607(2) | 2648(3) | 9547(1) | 17(1) |
| C(9') | 572(2) | 3671(3) | 9170(1) | 17(1) |
| C(11') | -626(2) | 2926(3) | 9114(1) | 17(1) |
| C(12') | -1725(2) | 3607(3) | 8740(1) | 18(1) |
| C(13') | -1545(2) | 5036(3) | 8400(1) | 19(1) |
| C(15') | -2700(2) | 5892(3) | 7988(1) | 24(1) |
| C(17') | -4043(2) | 5382(4) | 8169(1) | 30(1) |
| C(3') | 2831(2) | -323(3) | 9518(1) | 20(1) |
| C(2') | 1330(2) | -316(3) | 9330(1) | 20(1) |
| C(1') | 805(2) | 1124(3) | 9670(1) | 19(1) |
| C(16') | -2652(3) | 5740(3) | 7208(1) | 29(1) |
| C(14') | -292(2) | 5702(3) | 8407(1) | 19(1) |
| C(8') | 790(2) | 4997(3) | 8786(1) | 18(1) |
| C(20') | 2209(2) | 3338(3) | 10240(1) | 20(1) |
| C(6') | 3157(2) | 4030(3) | 8820(1) | 19(1) |
| C(7') | 2214(2) | 5493(3) | 8817(1) | 18(1) |
| C(19') | 4804(2) | 1492(3) | 9636(1) | 24(1) |

**Table 2.** Bond lengths [Å] and angles [ °] for compound **1**.

| | |
|---|---|
| O(18)-C(18) | 1.428(3) |
| O(18)-H(18) | 0.8400 |
| O(7)-C(7) | 1.427(3) |
| O(7)-H(7) | 0.8400 |
| O(1)-C(11) | 1.364(3) |
| O(1)-C(1) | 1.475(3) |
| O(18')-C(18') | 1.424(3) |
| O(18')-H(18') | 0.8400 |
| O(1')-C(11') | 1.367(3) |
| O(1')-C(1') | 1.481(3) |
| O(7')-C(7') | 1.424(3) |
| O(7')-H(7') | 0.8400 |
| C(18)-C(4) | 1.547(3) |
| C(18)-H(18A) | 0.9900 |
| C(18)-H(18B) | 0.9900 |
| C(4)-C(19) | 1.542(3) |
| C(4)-C(5) | 1.546(3) |
| C(4)-C(3) | 1.559(3) |
| C(5)-C(6) | 1.539(3) |
| C(5)-C(10) | 1.554(3) |
| C(5)-H(5) | 1.0000 |
| C(10)-C(9) | 1.491(3) |
| C(10)-C(20) | 1.534(3) |
| C(10)-C(1) | 1.565(3) |
| C(9)-C(11) | 1.372(3) |
| C(9)-C(8) | 1.378(3) |
| C(11)-C(12) | 1.396(3) |
| C(12)-C(13) | 1.403(4) |
| C(12)-H(12) | 0.9500 |
| C(13)-C(14) | 1.397(3) |
| C(13)-C(15) | 1.536(3) |
| C(15)-C(17) | 1.522(4) |
| C(15)-C(16) | 1.537(4) |
| C(15)-H(15) | 1.0000 |
| C(16)-H(16A) | 0.9800 |
| C(16)-H(16B) | 0.9800 |
| C(16)-H(16C) | 0.9800 |
| C(19)-H(19A) | 0.9800 |
| C(19)-H(19B) | 0.9800 |
| C(19)-H(19C) | 0.9800 |
| C(8)-C(14) | 1.403(3) |
| C(8)-C(7) | 1.514(3) |

| | |
|---|---|
| C(7)-C(6) | 1.572(3) |
| C(7)-H(7A) | 1.0000 |
| C(6)-H(6A) | 0.9900 |
| C(6)-H(6B) | 0.9900 |
| C(14)-H(14) | 0.9500 |
| C(1)-C(2) | 1.525(3) |
| C(1)-H(1) | 1.0000 |
| C(2)-C(3) | 1.544(3) |
| C(2)-H(2A) | 0.9900 |
| C(2)-H(2B) | 0.9900 |
| C(3)-H(3A) | 0.9900 |
| C(3)-H(3B) | 0.9900 |
| C(17)-H(17A) | 0.9800 |
| C(17)-H(17B) | 0.9800 |
| C(17)-H(17C) | 0.9800 |
| C(20)-H(20A) | 0.9800 |
| C(20)-H(20B) | 0.9800 |
| C(20)-H(20C) | 0.9800 |
| C(18')-C(4') | 1.543(3) |
| C(18')-H(18C) | 0.9900 |
| C(18')-H(18D) | 0.9900 |
| C(4')-C(19') | 1.537(3) |
| C(4')-C(5') | 1.547(3) |
| C(4')-C(3') | 1.562(3) |
| C(5')-C(6') | 1.548(3) |
| C(5')-C(10') | 1.552(3) |
| C(5')-H(5') | 1.0000 |
| C(10')-C(9') | 1.496(3) |
| C(10')-C(20') | 1.537(3) |
| C(10')-C(1') | 1.561(3) |
| C(9')-C(11') | 1.374(3) |
| C(9')-C(8') | 1.380(3) |
| C(11')-C(12') | 1.395(3) |
| C(12')-C(13') | 1.400(4) |
| C(12')-H(12') | 0.9500 |
| C(13')-C(14') | 1.402(3) |
| C(13')-C(15') | 1.535(3) |
| C(15')-C(17') | 1.523(3) |
| C(15')-C(16') | 1.536(4) |
| C(15')-H(15') | 1.0000 |
| C(17')-H(17D) | 0.9800 |
| C(17')-H(17E) | 0.9800 |
| C(17')-H(17F) | 0.9800 |
| C(3')-C(2') | 1.542(3) |

| | |
|---|---|
| C(3')-H(3'1) | 0.9900 |
| C(3')-H(3'2) | 0.9900 |
| C(2')-C(1') | 1.514(3) |
| C(2')-H(2'1) | 0.9900 |
| C(2')-H(2'2) | 0.9900 |
| C(1')-H(1') | 1.0000 |
| C(16')-H(16D) | 0.9800 |
| C(16')-H(16E) | 0.9800 |
| C(16')-H(16F) | 0.9800 |
| C(14')-C(8') | 1.396(3) |
| C(14')-H(14') | 0.9500 |
| C(8')-C(7') | 1.515(3) |
| C(20')-H(20D) | 0.9800 |
| C(20')-H(20E) | 0.9800 |
| C(20')-H(20F) | 0.9800 |
| C(6')-C(7') | 1.569(3) |
| C(6')-H(6'1) | 0.9900 |
| C(6')-H(6'2) | 0.9900 |
| C(7')-H(7'1) | 1.0000 |
| C(19')-H(19D) | 0.9800 |
| C(19')-H(19E) | 0.9800 |
| C(19')-H(19F) | 0.9800 |

| | |
|---|---|
| C(18)-O(18)-H(18) | 109.5 |
| C(7)-O(7)-H(7) | 109.5 |
| C(11)-O(1)-C(1) | 107.65(17) |
| C(18')-O(18')-H(18') | 109.5 |
| C(11')-O(1')-C(1') | 107.57(17) |
| C(7')-O(7')-H(7') | 109.5 |
| O(18)-C(18)-C(4) | 113.80(18) |
| O(18)-C(18)-H(18A) | 108.8 |
| C(4)-C(18)-H(18A) | 108.8 |
| O(18)-C(18)-H(18B) | 108.8 |
| C(4)-C(18)-H(18B) | 108.8 |
| H(18A)-C(18)-H(18B) | 107.7 |
| C(19)-C(4)-C(5) | 115.1(2) |
| C(19)-C(4)-C(18) | 104.92(19) |
| C(5)-C(4)-C(18) | 109.78(19) |
| C(19)-C(4)-C(3) | 108.81(19) |
| C(5)-C(4)-C(3) | 108.87(18) |
| C(18)-C(4)-C(3) | 109.2(2) |
| C(6)-C(5)-C(4) | 116.92(19) |
| C(6)-C(5)-C(10) | 108.71(19) |
| C(4)-C(5)-C(10) | 114.2(2) |

| | |
|---|---|
| C(6)-C(5)-H(5) | 105.3 |
| C(4)-C(5)-H(5) | 105.3 |
| C(10)-C(5)-H(5) | 105.3 |
| C(9)-C(10)-C(20) | 113.8(2) |
| C(9)-C(10)-C(5) | 102.49(19) |
| C(20)-C(10)-C(5) | 114.82(19) |
| C(9)-C(10)-C(1) | 100.86(18) |
| C(20)-C(10)-C(1) | 110.5(2) |
| C(5)-C(10)-C(1) | 113.3(2) |
| C(11)-C(9)-C(8) | 122.4(2) |
| C(11)-C(9)-C(10) | 110.9(2) |
| C(8)-C(9)-C(10) | 125.0(2) |
| O(1)-C(11)-C(9) | 113.1(2) |
| O(1)-C(11)-C(12) | 125.6(2) |
| C(9)-C(11)-C(12) | 120.9(2) |
| C(11)-C(12)-C(13) | 117.4(2) |
| C(11)-C(12)-H(12) | 121.3 |
| C(13)-C(12)-H(12) | 121.3 |
| C(14)-C(13)-C(12) | 120.8(2) |
| C(14)-C(13)-C(15) | 119.9(2) |
| C(12)-C(13)-C(15) | 119.1(2) |
| C(17)-C(15)-C(13) | 113.2(2) |
| C(17)-C(15)-C(16) | 111.1(3) |
| C(13)-C(15)-C(16) | 110.2(2) |
| C(17)-C(15)-H(15) | 107.4 |
| C(13)-C(15)-H(15) | 107.4 |
| C(16)-C(15)-H(15) | 107.4 |
| C(15)-C(16)-H(16A) | 109.5 |
| C(15)-C(16)-H(16B) | 109.5 |
| H(16A)-C(16)-H(16B) | 109.5 |
| C(15)-C(16)-H(16C) | 109.5 |
| H(16A)-C(16)-H(16C) | 109.5 |
| H(16B)-C(16)-H(16C) | 109.5 |
| C(4)-C(19)-H(19A) | 109.5 |
| C(4)-C(19)-H(19B) | 109.5 |
| H(19A)-C(19)-H(19B) | 109.5 |
| C(4)-C(19)-H(19C) | 109.5 |
| H(19A)-C(19)-H(19C) | 109.5 |
| H(19B)-C(19)-H(19C) | 109.5 |
| C(9)-C(8)-C(14) | 117.3(2) |
| C(9)-C(8)-C(7) | 115.6(2) |
| C(14)-C(8)-C(7) | 127.0(2) |
| O(7)-C(7)-C(8) | 113.4(2) |
| O(7)-C(7)-C(6) | 111.05(18) |

| | |
|---|---|
| C(8)-C(7)-C(6) | 112.7(2) |
| O(7)-C(7)-H(7A) | 106.4 |
| C(8)-C(7)-H(7A) | 106.4 |
| C(6)-C(7)-H(7A) | 106.4 |
| C(5)-C(6)-C(7) | 115.53(18) |
| C(5)-C(6)-H(6A) | 108.4 |
| C(7)-C(6)-H(6A) | 108.4 |
| C(5)-C(6)-H(6B) | 108.4 |
| C(7)-C(6)-H(6B) | 108.4 |
| H(6A)-C(6)-H(6B) | 107.5 |
| C(13)-C(14)-C(8) | 120.7(2) |
| C(13)-C(14)-H(14) | 119.6 |
| C(8)-C(14)-H(14) | 119.6 |
| O(1)-C(1)-C(2) | 112.36(19) |
| O(1)-C(1)-C(10) | 107.04(19) |
| C(2)-C(1)-C(10) | 111.56(18) |
| O(1)-C(1)-H(1) | 108.6 |
| C(2)-C(1)-H(1) | 108.6 |
| C(10)-C(1)-H(1) | 108.6 |
| C(1)-C(2)-C(3) | 106.99(19) |
| C(1)-C(2)-H(2A) | 110.3 |
| C(3)-C(2)-H(2A) | 110.3 |
| C(1)-C(2)-H(2B) | 110.3 |
| C(3)-C(2)-H(2B) | 110.3 |
| H(2A)-C(2)-H(2B) | 108.6 |
| C(2)-C(3)-C(4) | 113.42(19) |
| C(2)-C(3)-H(3A) | 108.9 |
| C(4)-C(3)-H(3A) | 108.9 |
| C(2)-C(3)-H(3B) | 108.9 |
| C(4)-C(3)-H(3B) | 108.9 |
| H(3A)-C(3)-H(3B) | 107.7 |
| C(15)-C(17)-H(17A) | 109.5 |
| C(15)-C(17)-H(17B) | 109.5 |
| H(17A)-C(17)-H(17B) | 109.5 |
| C(15)-C(17)-H(17C) | 109.5 |
| H(17A)-C(17)-H(17C) | 109.5 |
| H(17B)-C(17)-H(17C) | 109.5 |
| C(10)-C(20)-H(20A) | 109.5 |
| C(10)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(10)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| O(18')-C(18')-C(4') | 113.95(18) |

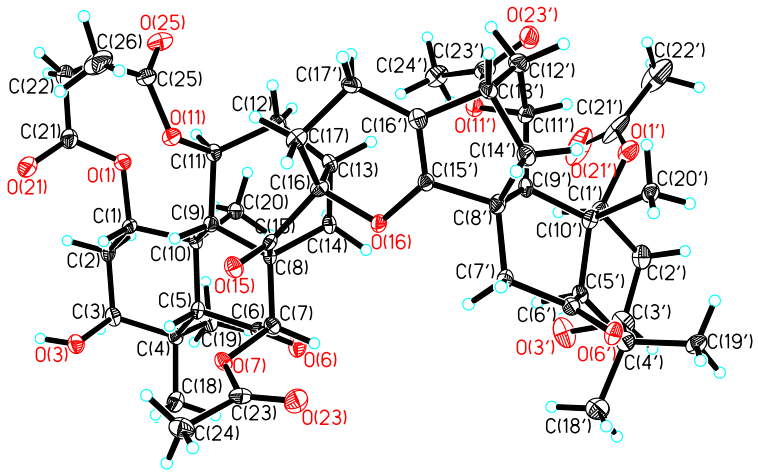
| | |
|---|---|
| O(18')-C(18')-H(18C) | 108.8 |
| C(4')-C(18')-H(18C) | 108.8 |
| O(18')-C(18')-H(18D) | 108.8 |
| C(4')-C(18')-H(18D) | 108.8 |
| H(18C)-C(18')-H(18D) | 107.7 |
| C(19')-C(4')-C(18') | 105.41(18) |
| C(19')-C(4')-C(5') | 114.4(2) |
| C(18')-C(4')-C(5') | 109.97(19) |
| C(19')-C(4')-C(3') | 109.39(19) |
| C(18')-C(4')-C(3') | 109.1(2) |
| C(5')-C(4')-C(3') | 108.44(17) |
| C(4')-C(5')-C(6') | 117.11(18) |
| C(4')-C(5')-C(10') | 113.67(19) |
| C(6')-C(5')-C(10') | 109.80(19) |
| C(4')-C(5')-H(5') | 105.0 |
| C(6')-C(5')-H(5') | 105.0 |
| C(10')-C(5')-H(5') | 105.0 |
| C(9')-C(10')-C(20') | 113.9(2) |
| C(9')-C(10')-C(5') | 102.17(18) |
| C(20')-C(10')-C(5') | 115.45(19) |
| C(9')-C(10')-C(1') | 101.19(18) |
| C(20')-C(10')-C(1') | 110.04(19) |
| C(5')-C(10')-C(1') | 113.01(19) |
| C(11')-C(9')-C(8') | 121.8(2) |
| C(11')-C(9')-C(10') | 110.7(2) |
| C(8')-C(9')-C(10') | 125.8(2) |
| O(1')-C(11')-C(9') | 113.3(2) |
| O(1')-C(11')-C(12') | 125.6(2) |
| C(9')-C(11')-C(12') | 121.0(2) |
| C(11')-C(12')-C(13') | 117.4(2) |
| C(11')-C(12')-H(12') | 121.3 |
| C(13')-C(12')-H(12') | 121.3 |
| C(12')-C(13')-C(14') | 120.8(2) |
| C(12')-C(13')-C(15') | 121.2(2) |
| C(14')-C(13')-C(15') | 118.0(2) |
| C(17')-C(15')-C(13') | 114.3(2) |
| C(17')-C(15')-C(16') | 109.9(2) |
| C(13')-C(15')-C(16') | 111.63(19) |
| C(17')-C(15')-H(15') | 106.9 |
| C(13')-C(15')-H(15') | 106.9 |
| C(16')-C(15')-H(15') | 106.9 |
| C(15')-C(17')-H(17D) | 109.5 |
| C(15')-C(17')-H(17E) | 109.5 |
| H(17D)-C(17')-H(17E) | 109.5 |

| | |
|---|---|
| C(15')-C(17')-H(17F) | 109.5 |
| H(17D)-C(17')-H(17F) | 109.5 |
| H(17E)-C(17')-H(17F) | 109.5 |
| C(2')-C(3')-C(4') | 113.82(19) |
| C(2')-C(3')-H(3'1) | 108.8 |
| C(4')-C(3')-H(3'1) | 108.8 |
| C(2')-C(3')-H(3'2) | 108.8 |
| C(4')-C(3')-H(3'2) | 108.8 |
| H(3'1)-C(3')-H(3'2) | 107.7 |
| C(1')-C(2')-C(3') | 107.12(19) |
| C(1')-C(2')-H(2'1) | 110.3 |
| C(3')-C(2')-H(2'1) | 110.3 |
| C(1')-C(2')-H(2'2) | 110.3 |
| C(3')-C(2')-H(2'2) | 110.3 |
| H(2'1)-C(2')-H(2'2) | 108.5 |
| O(1')-C(1')-C(2') | 112.31(19) |
| O(1')-C(1')-C(10') | 107.08(19) |
| C(2')-C(1')-C(10') | 111.95(18) |
| O(1')-C(1')-H(1') | 108.5 |
| C(2')-C(1')-H(1') | 108.5 |
| C(10')-C(1')-H(1') | 108.5 |
| C(15')-C(16')-H(16D) | 109.5 |
| C(15')-C(16')-H(16E) | 109.5 |
| H(16D)-C(16')-H(16E) | 109.5 |
| C(15')-C(16')-H(16F) | 109.5 |
| H(16D)-C(16')-H(16F) | 109.5 |
| H(16E)-C(16')-H(16F) | 109.5 |
| C(8')-C(14')-C(13') | 120.4(2) |
| C(8')-C(14')-H(14') | 119.8 |
| C(13')-C(14')-H(14') | 119.8 |
| C(9')-C(8')-C(14') | 117.8(2) |
| C(9')-C(8')-C(7') | 114.8(2) |
| C(14')-C(8')-C(7') | 127.4(2) |
| C(10')-C(20')-H(20D) | 109.5 |
| C(10')-C(20')-H(20E) | 109.5 |
| H(20D)-C(20')-H(20E) | 109.5 |
| C(10')-C(20')-H(20F) | 109.5 |
| H(20D)-C(20')-H(20F) | 109.5 |
| H(20E)-C(20')-H(20F) | 109.5 |
| C(5')-C(6')-C(7') | 116.22(18) |
| C(5')-C(6')-H(6'1) | 108.2 |
| C(7')-C(6')-H(6'1) | 108.2 |
| C(5')-C(6')-H(6'2) | 108.2 |
| C(7')-C(6')-H(6'2) | 108.2 |

| | |
|---|---|
| H(6'1)-C(6')-H(6'2) | 107.4 |
| O(7')-C(7')-C(8') | 113.80(19) |
| O(7')-C(7')-C(6') | 111.26(17) |
| C(8')-C(7')-C(6') | 111.98(19) |
| O(7')-C(7')-H(7'1) | 106.4 |
| C(8')-C(7')-H(7'1) | 106.4 |
| C(6')-C(7')-H(7'1) | 106.4 |
| C(4')-C(19')-H(19D) | 109.5 |
| C(4')-C(19')-H(19E) | 109.5 |
| H(19D)-C(19')-H(19E) | 109.5 |
| C(4')-C(19')-H(19F) | 109.5 |
| H(19D)-C(19')-H(19F) | 109.5 |
| H(19E)-C(19')-H(19F) | 109.5 |

Symmetry transformations used to generate equivalent atoms:

**X-ray data of compound 4**




ORTEP Plot of compound **4**

**Table 3.** Atomic coordinates ( x$10^4$) and equivalent isotropic displacement parameters (Å$^2$ x $10^3$) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| O(17) | 9930(1) | 3221(2) | 7369(1) | 24(1) |
| O(3) | 6493(1) | 6040(2) | 334(1) | 22(1) |
| O(15) | 8711(1) | 7143(2) | 4998(1) | 19(1) |
| O(6) | 6899(1) | 2095(2) | 3601(1) | 20(1) |
| O(7) | 7497(1) | 6771(2) | 3829(1) | 18(1) |
| O(1) | 8074(1) | 2977(2) | 920(1) | 20(1) |
| O(11) | 9223(1) | 4979(2) | 3572(1) | 18(1) |
| O(21) | 8881(1) | 5898(2) | 1887(1) | 25(1) |
| C(23) | 10098(1) | 3298(4) | 8462(1) | 33(1) |
| C(17) | 9357(1) | 4019(3) | 6783(1) | 20(1) |
| C(16) | 9237(1) | 3972(3) | 5635(1) | 16(1) |
| C(15) | 8716(1) | 5318(3) | 4966(1) | 15(1) |
| C(8) | 8206(1) | 3963(3) | 4233(1) | 14(1) |
| C(7) | 7613(1) | 4722(3) | 4158(1) | 15(1) |
| C(6) | 7150(1) | 3376(3) | 3349(1) | 14(1) |
| C(5) | 7094(1) | 3713(3) | 2263(1) | 14(1) |
| C(4) | 6491(1) | 3135(3) | 1356(1) | 17(1) |
| C(3) | 6501(1) | 3883(3) | 342(1) | 19(1) |
| C(13) | 9045(1) | 1889(3) | 5130(1) | 16(1) |
| C(14) | 8382(1) | 1904(3) | 4791(1) | 16(1) |

| | | | | |
|---|---|---|---|---|
| C(9) | 8208(1) | 3961(3) | 3139(1) | 13(1) |
| C(10) | 7670(1) | 2887(3) | 2224(1) | 15(1) |
| C(2) | 7039(1) | 3094(3) | 240(1) | 18(1) |
| C(1) | 7615(1) | 3694(3) | 1161(1) | 15(1) |
| C(19) | 6319(1) | 880(3) | 1244(1) | 23(1) |
| C(18) | 6014(1) | 4328(3) | 1516(1) | 21(1) |
| C(20) | 7715(1) | 566(3) | 2266(1) | 18(1) |
| C(11) | 8823(1) | 3217(3) | 3284(1) | 16(1) |
| C(21) | 9216(1) | 6141(3) | 2802(1) | 19(1) |
| C(22) | 9667(1) | 7798(3) | 3180(2) | 24(1) |
| C(12) | 9132(1) | 1648(3) | 4139(1) | 18(1) |

**Table 4.** Bond lengths [Å] and angles [ °] for compound **4**.

| | |
|---|---|
| O(17)-C(17) | 1.423(2) |
| O(17)-C(23) | 1.426(2) |
| O(3)-C(3) | 1.424(2) |
| O(3)-H(3) | 0.8400 |
| O(15)-C(15) | 1.206(2) |
| O(6)-C(6) | 1.207(2) |
| O(7)-C(7) | 1.419(2) |
| O(7)-H(7) | 0.8400 |
| O(1)-C(1) | 1.4342(19) |
| O(1)-H(1) | 0.8400 |
| O(11)-C(21) | 1.336(2) |
| O(11)-C(11) | 1.478(2) |
| O(21)-C(21) | 1.214(2) |
| C(23)-H(23A) | 0.9800 |
| C(23)-H(23B) | 0.9800 |
| C(23)-H(23C) | 0.9800 |
| C(17)-C(16) | 1.531(2) |
| C(17)-H(17A) | 0.9900 |
| C(17)-H(17B) | 0.9900 |
| C(16)-C(15) | 1.528(2) |
| C(16)-C(13) | 1.529(2) |
| C(16)-H(16) | 1.0000 |
| C(15)-C(8) | 1.542(2) |
| C(8)-C(14) | 1.539(2) |
| C(8)-C(7) | 1.544(2) |
| C(8)-C(9) | 1.566(2) |
| C(7)-C(6) | 1.519(2) |
| C(7)-H(7A) | 1.0000 |
| C(6)-C(5) | 1.511(2) |
| C(5)-C(4) | 1.555(2) |
| C(5)-C(10) | 1.584(2) |
| C(5)-H(5) | 1.0000 |
| C(4)-C(19) | 1.540(3) |
| C(4)-C(3) | 1.541(2) |
| C(4)-C(18) | 1.545(2) |
| C(3)-C(2) | 1.529(2) |
| C(3)-H(3A) | 1.0000 |
| C(13)-C(14) | 1.533(2) |
| C(13)-C(12) | 1.533(2) |
| C(13)-H(13) | 1.0000 |
| C(14)-H(14A) | 0.9900 |

| | |
|---|---|
| C(14)-H(14B) | 0.9900 |
| C(9)-C(11) | 1.561(2) |
| C(9)-C(10) | 1.582(2) |
| C(9)-H(9) | 1.0000 |
| C(10)-C(20) | 1.536(2) |
| C(10)-C(1) | 1.557(2) |
| C(2)-C(1) | 1.526(2) |
| C(2)-H(2A) | 0.9900 |
| C(2)-H(2B) | 0.9900 |
| C(1)-H(1A) | 1.0000 |
| C(19)-H(19A) | 0.9800 |
| C(19)-H(19B) | 0.9800 |
| C(19)-H(19C) | 0.9800 |
| C(18)-H(18A) | 0.9800 |
| C(18)-H(18B) | 0.9800 |
| C(18)-H(18C) | 0.9800 |
| C(20)-H(20A) | 0.9800 |
| C(20)-H(20B) | 0.9800 |
| C(20)-H(20C) | 0.9800 |
| C(11)-C(12) | 1.528(2) |
| C(11)-H(11) | 1.0000 |
| C(21)-C(22) | 1.502(3) |
| C(22)-H(22A) | 0.9800 |
| C(22)-H(22B) | 0.9800 |
| C(22)-H(22C) | 0.9800 |
| C(12)-H(12A) | 0.9900 |
| C(12)-H(12B) | 0.9900 |

| | |
|---|---|
| C(17)-O(17)-C(23) | 111.36(14) |
| C(3)-O(3)-H(3) | 109.5 |
| C(7)-O(7)-H(7) | 109.5 |
| C(1)-O(1)-H(1) | 109.5 |
| C(21)-O(11)-C(11) | 117.68(13) |
| O(17)-C(23)-H(23A) | 109.5 |
| O(17)-C(23)-H(23B) | 109.5 |
| H(23A)-C(23)-H(23B) | 109.5 |
| O(17)-C(23)-H(23C) | 109.5 |
| H(23A)-C(23)-H(23C) | 109.5 |
| H(23B)-C(23)-H(23C) | 109.5 |
| O(17)-C(17)-C(16) | 106.90(13) |
| O(17)-C(17)-H(17A) | 110.3 |
| C(16)-C(17)-H(17A) | 110.3 |
| O(17)-C(17)-H(17B) | 110.3 |
| C(16)-C(17)-H(17B) | 110.3 |

| | |
|---|---|
| H(17A)-C(17)-H(17B) | 108.6 |
| C(15)-C(16)-C(13) | 102.78(13) |
| C(15)-C(16)-C(17) | 111.47(13) |
| C(13)-C(16)-C(17) | 113.30(14) |
| C(15)-C(16)-H(16) | 109.7 |
| C(13)-C(16)-H(16) | 109.7 |
| C(17)-C(16)-H(16) | 109.7 |
| O(15)-C(15)-C(16) | 125.32(15) |
| O(15)-C(15)-C(8) | 125.81(15) |
| C(16)-C(15)-C(8) | 108.86(14) |
| C(14)-C(8)-C(15) | 101.25(13) |
| C(14)-C(8)-C(7) | 112.03(13) |
| C(15)-C(8)-C(7) | 111.15(13) |
| C(14)-C(8)-C(9) | 112.77(13) |
| C(15)-C(8)-C(9) | 107.74(12) |
| C(7)-C(8)-C(9) | 111.39(13) |
| O(7)-C(7)-C(6) | 109.16(13) |
| O(7)-C(7)-C(8) | 112.67(13) |
| C(6)-C(7)-C(8) | 105.47(13) |
| O(7)-C(7)-H(7A) | 109.8 |
| C(6)-C(7)-H(7A) | 109.8 |
| C(8)-C(7)-H(7A) | 109.8 |
| O(6)-C(6)-C(5) | 125.96(16) |
| O(6)-C(6)-C(7) | 121.15(15) |
| C(5)-C(6)-C(7) | 112.66(13) |
| C(6)-C(5)-C(4) | 115.55(13) |
| C(6)-C(5)-C(10) | 108.36(12) |
| C(4)-C(5)-C(10) | 118.14(13) |
| C(6)-C(5)-H(5) | 104.4 |
| C(4)-C(5)-H(5) | 104.4 |
| C(10)-C(5)-H(5) | 104.4 |
| C(19)-C(4)-C(3) | 109.52(15) |
| C(19)-C(4)-C(18) | 107.67(14) |
| C(3)-C(4)-C(18) | 108.38(15) |
| C(19)-C(4)-C(5) | 116.95(15) |
| C(3)-C(4)-C(5) | 106.60(13) |
| C(18)-C(4)-C(5) | 107.47(14) |
| O(3)-C(3)-C(2) | 110.44(15) |
| O(3)-C(3)-C(4) | 108.80(15) |
| C(2)-C(3)-C(4) | 111.52(14) |
| O(3)-C(3)-H(3A) | 108.7 |
| C(2)-C(3)-H(3A) | 108.7 |
| C(4)-C(3)-H(3A) | 108.7 |
| C(16)-C(13)-C(14) | 102.63(14) |

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|---|---|
| C(16)-C(13)-C(12) | 112.57(14) |
| C(14)-C(13)-C(12) | 107.13(13) |
| C(16)-C(13)-H(13) | 111.4 |
| C(14)-C(13)-H(13) | 111.4 |
| C(12)-C(13)-H(13) | 111.4 |
| C(13)-C(14)-C(8) | 101.42(13) |
| C(13)-C(14)-H(14A) | 111.5 |
| C(8)-C(14)-H(14A) | 111.5 |
| C(13)-C(14)-H(14B) | 111.5 |
| C(8)-C(14)-H(14B) | 111.5 |
| H(14A)-C(14)-H(14B) | 109.3 |
| C(11)-C(9)-C(8) | 108.27(12) |
| C(11)-C(9)-C(10) | 114.67(13) |
| C(8)-C(9)-C(10) | 116.17(12) |
| C(11)-C(9)-H(9) | 105.6 |
| C(8)-C(9)-H(9) | 105.6 |
| C(10)-C(9)-H(9) | 105.6 |
| C(20)-C(10)-C(1) | 110.56(14) |
| C(20)-C(10)-C(9) | 113.13(14) |
| C(1)-C(10)-C(9) | 108.90(13) |
| C(20)-C(10)-C(5) | 113.40(14) |
| C(1)-C(10)-C(5) | 103.32(12) |
| C(9)-C(10)-C(5) | 106.98(12) |
| C(1)-C(2)-C(3) | 112.74(14) |
| C(1)-C(2)-H(2A) | 109.0 |
| C(3)-C(2)-H(2A) | 109.0 |
| C(1)-C(2)-H(2B) | 109.0 |
| C(3)-C(2)-H(2B) | 109.0 |
| H(2A)-C(2)-H(2B) | 107.8 |
| O(1)-C(1)-C(2) | 106.16(13) |
| O(1)-C(1)-C(10) | 112.98(13) |
| C(2)-C(1)-C(10) | 112.99(14) |
| O(1)-C(1)-H(1A) | 108.2 |
| C(2)-C(1)-H(1A) | 108.2 |
| C(10)-C(1)-H(1A) | 108.2 |
| C(4)-C(19)-H(19A) | 109.5 |
| C(4)-C(19)-H(19B) | 109.5 |
| H(19A)-C(19)-H(19B) | 109.5 |
| C(4)-C(19)-H(19C) | 109.5 |
| H(19A)-C(19)-H(19C) | 109.5 |
| H(19B)-C(19)-H(19C) | 109.5 |
| C(4)-C(18)-H(18A) | 109.5 |
| C(4)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |

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|---|---|
| C(4)-C(18)-H(18C) | 109.5 |
| H(18A)-C(18)-H(18C) | 109.5 |
| H(18B)-C(18)-H(18C) | 109.5 |
| C(10)-C(20)-H(20A) | 109.5 |
| C(10)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(10)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| O(11)-C(11)-C(12) | 105.29(13) |
| O(11)-C(11)-C(9) | 108.21(13) |
| C(12)-C(11)-C(9) | 116.70(13) |
| O(11)-C(11)-H(11) | 108.8 |
| C(12)-C(11)-H(11) | 108.8 |
| C(9)-C(11)-H(11) | 108.8 |
| O(21)-C(21)-O(11) | 124.03(17) |
| O(21)-C(21)-C(22) | 122.95(17) |
| O(11)-C(21)-C(22) | 113.02(15) |
| C(21)-C(22)-H(22A) | 109.5 |
| C(21)-C(22)-H(22B) | 109.5 |
| H(22A)-C(22)-H(22B) | 109.5 |
| C(21)-C(22)-H(22C) | 109.5 |
| H(22A)-C(22)-H(22C) | 109.5 |
| H(22B)-C(22)-H(22C) | 109.5 |
| C(11)-C(12)-C(13) | 115.82(14) |
| C(11)-C(12)-H(12A) | 108.3 |
| C(13)-C(12)-H(12A) | 108.3 |
| C(11)-C(12)-H(12B) | 108.3 |
| C(13)-C(12)-H(12B) | 108.3 |
| H(12A)-C(12)-H(12B) | 107.4 |

Symmetry transformations used to generate equivalent atoms: