

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

► ¹H NMR, ¹³C NMR, DEPT, HSQC, HMBC, COSY, ROESY, HRESIMS, UV, and IR spectra of compounds 1-13

► X-ray data of compound 1

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

Table 2. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for compound 1

► X-ray data of compound 4

Table 3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 4. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

Table 4. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for compound 4

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[‡] University of the Chinese Academy of Sciences.

For compound 1:

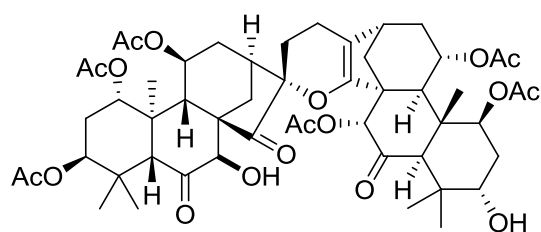


Figure 1. ^1H NMR spectrum of bistenuifolin A (1)

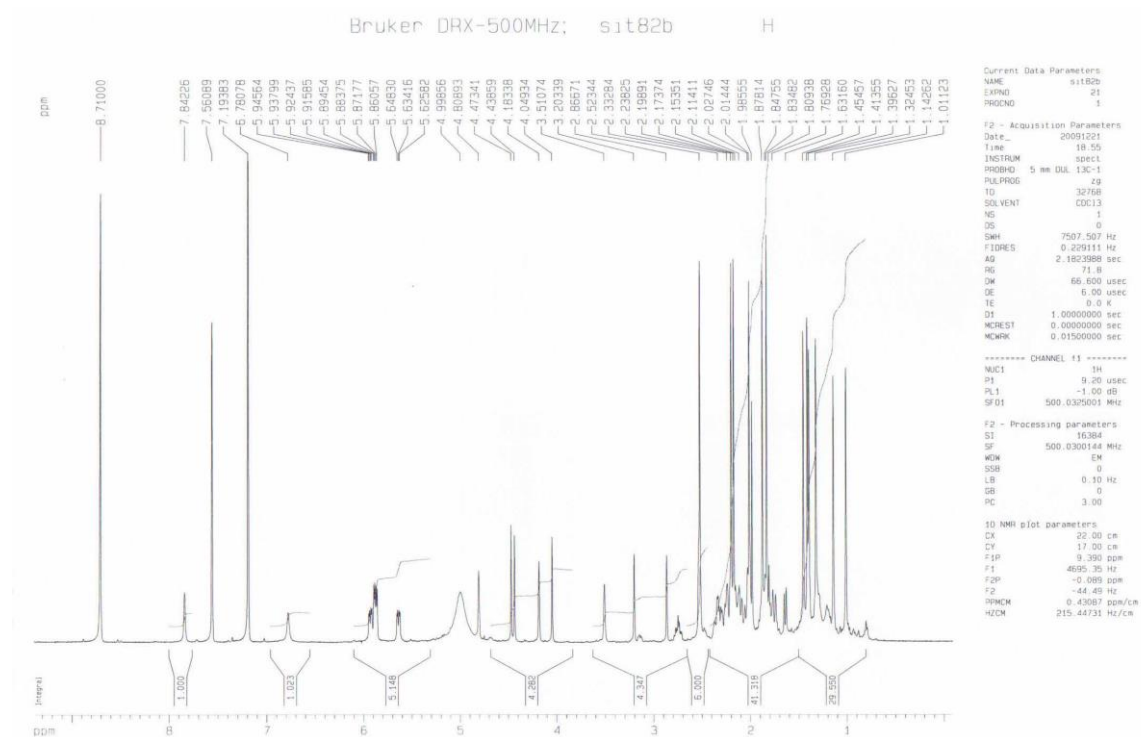


Figure 2. ^{13}C NMR spectrum of bistenuifolin A (1)

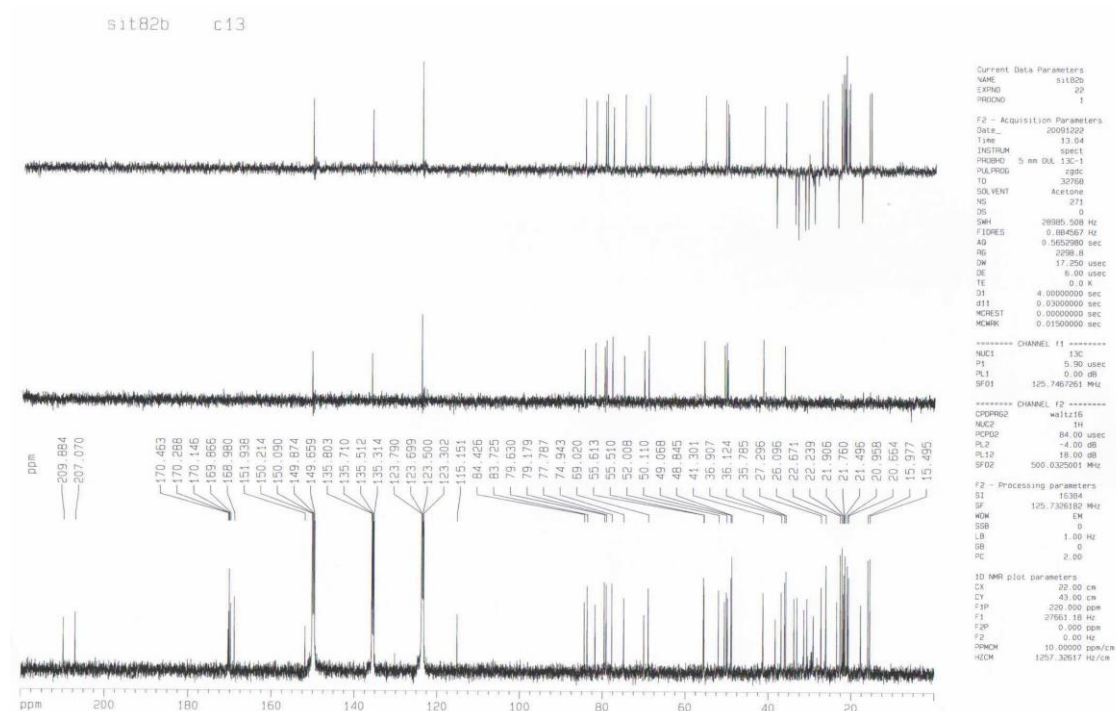


Figure 3. HSQC spectrum of bistenuifolin A (1)

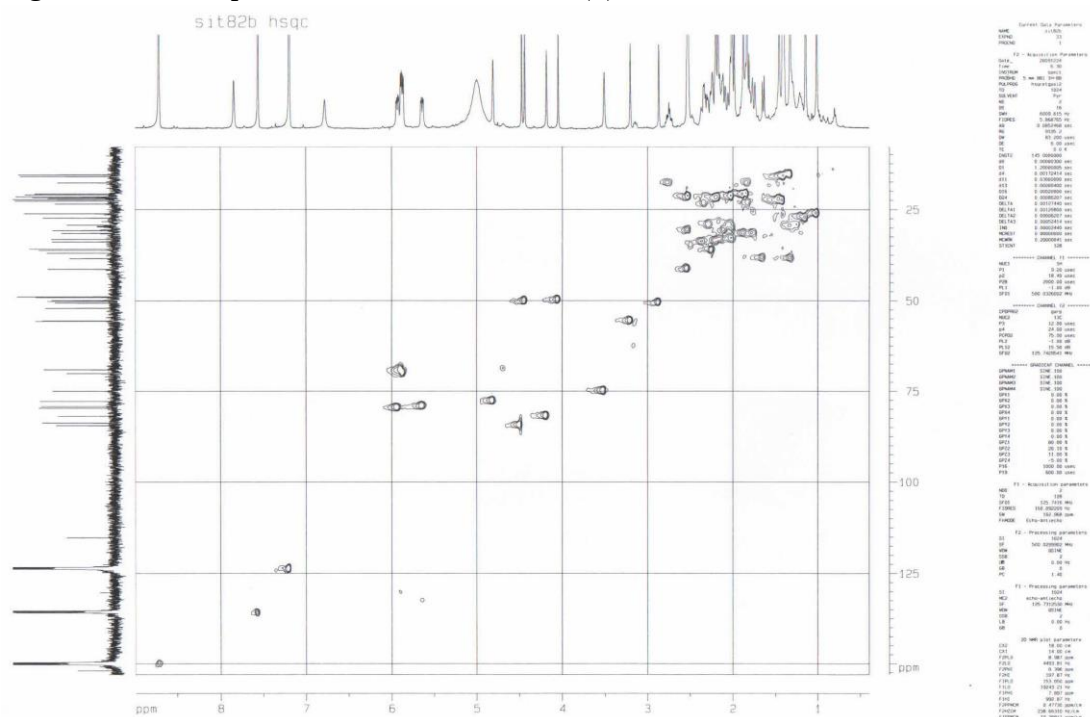


Figure 4. HMBC spectrum of bistenuifolin A (1)

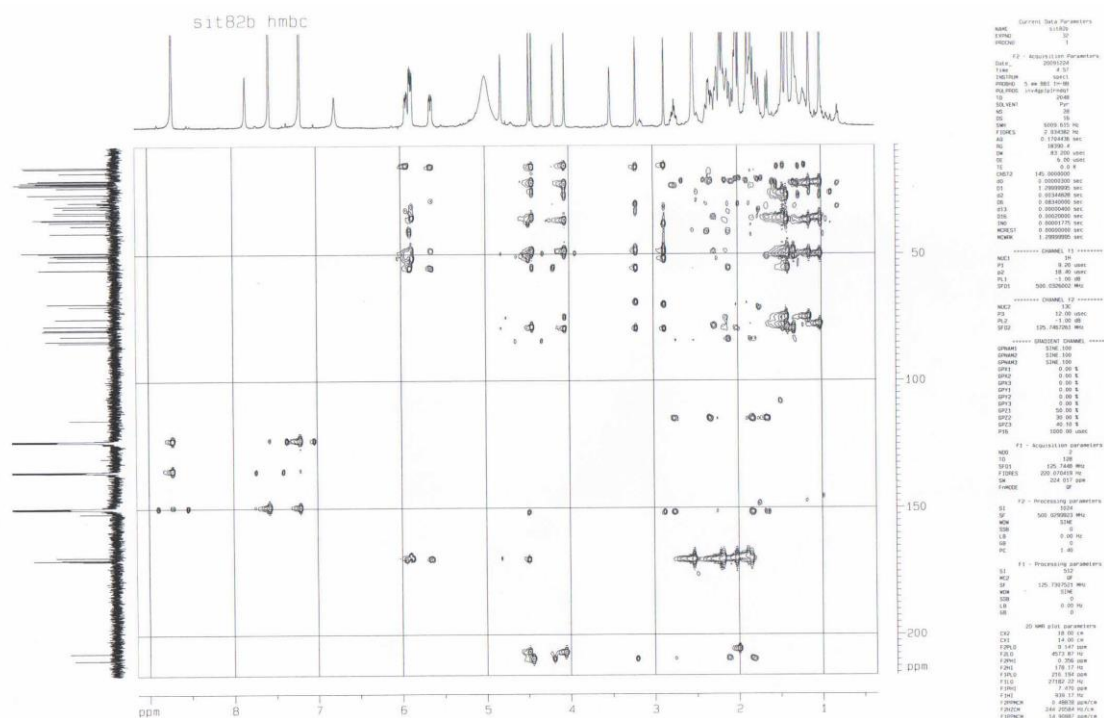


Figure 5. COSY spectrum of bistenuifolin A (1)

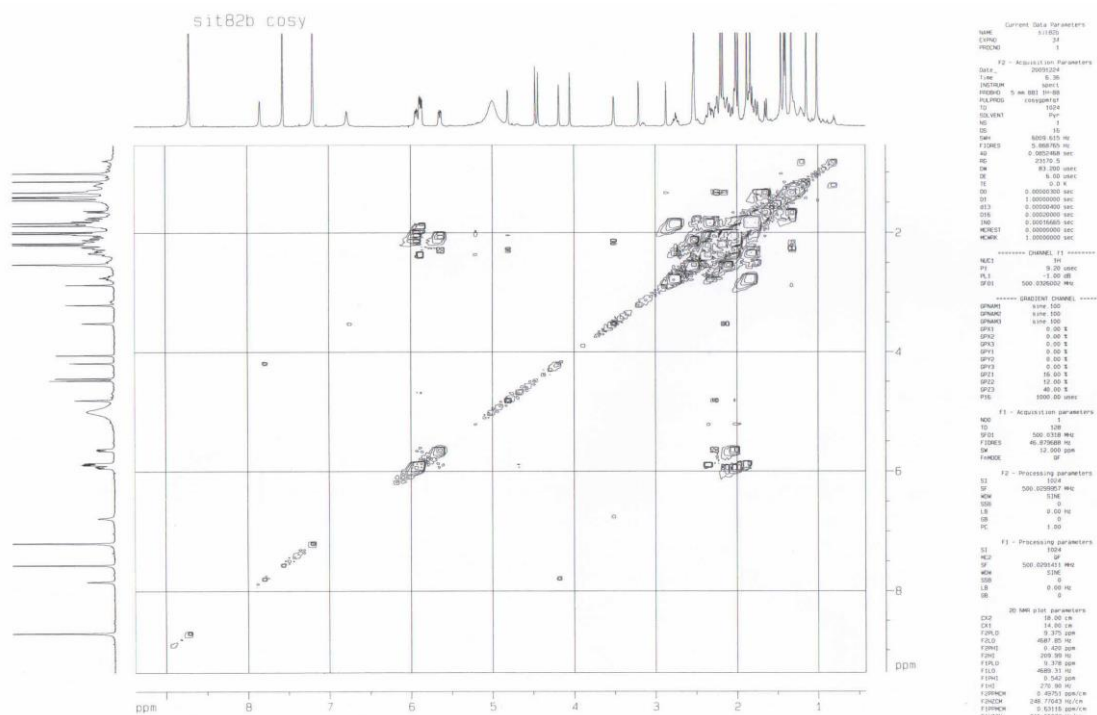


Figure 6. ROESY spectrum of bistenuifolin A (1)

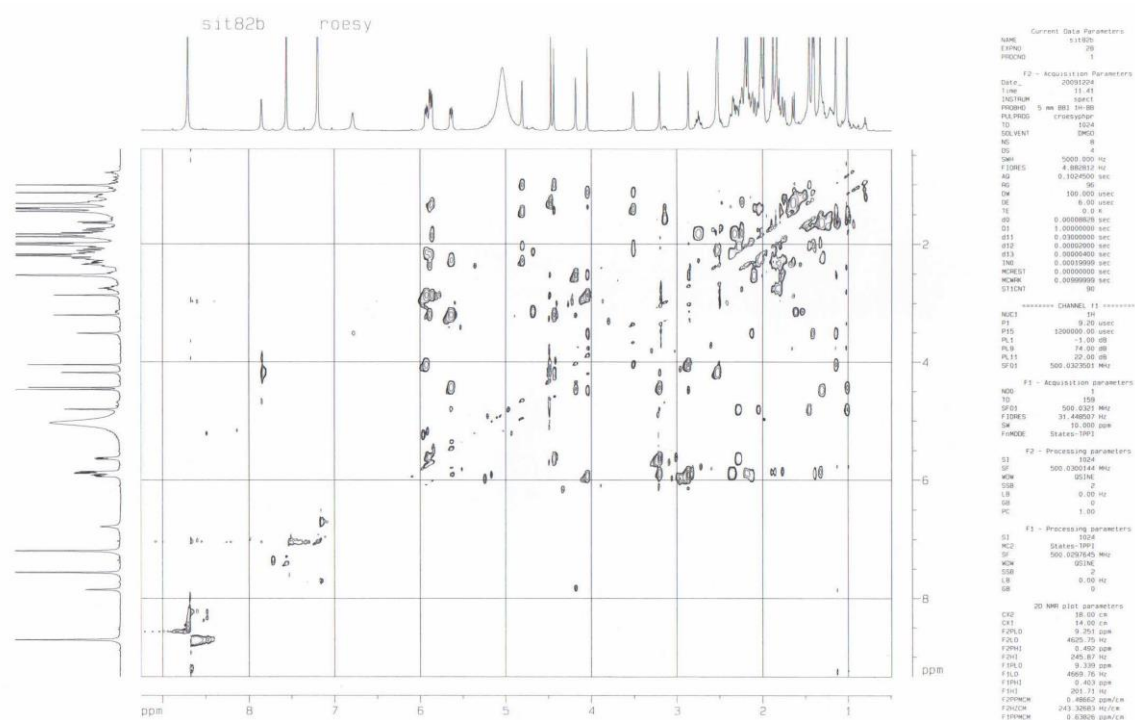
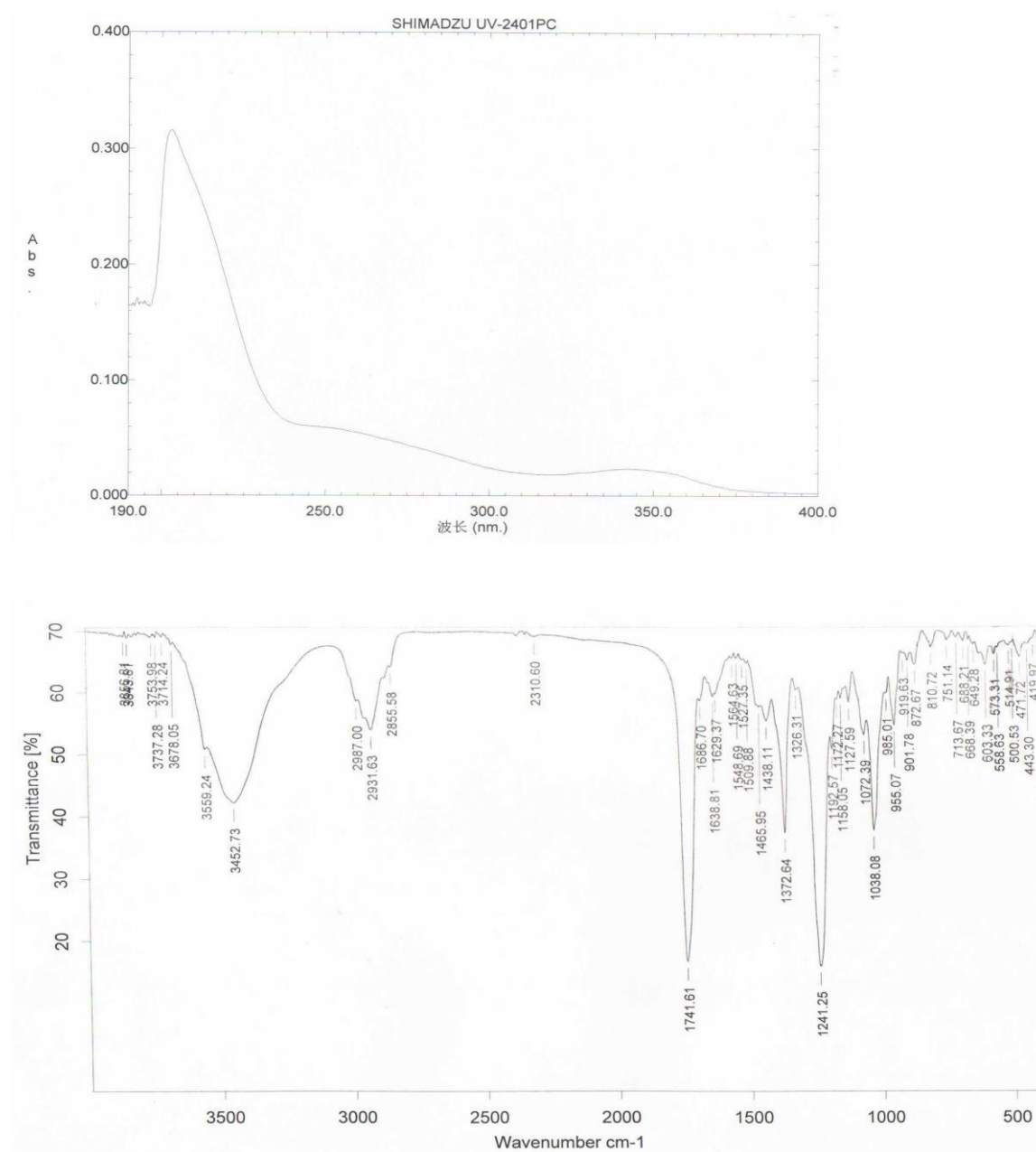


Figure 7. HRESIMS spectrum of bistenuifolin A (1)



	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**)



For compound 2:

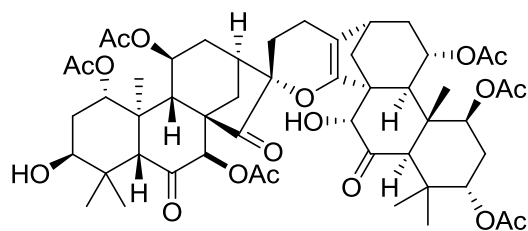


Figure 9. ^1H NMR spectrum of bistenuifolin B (2)

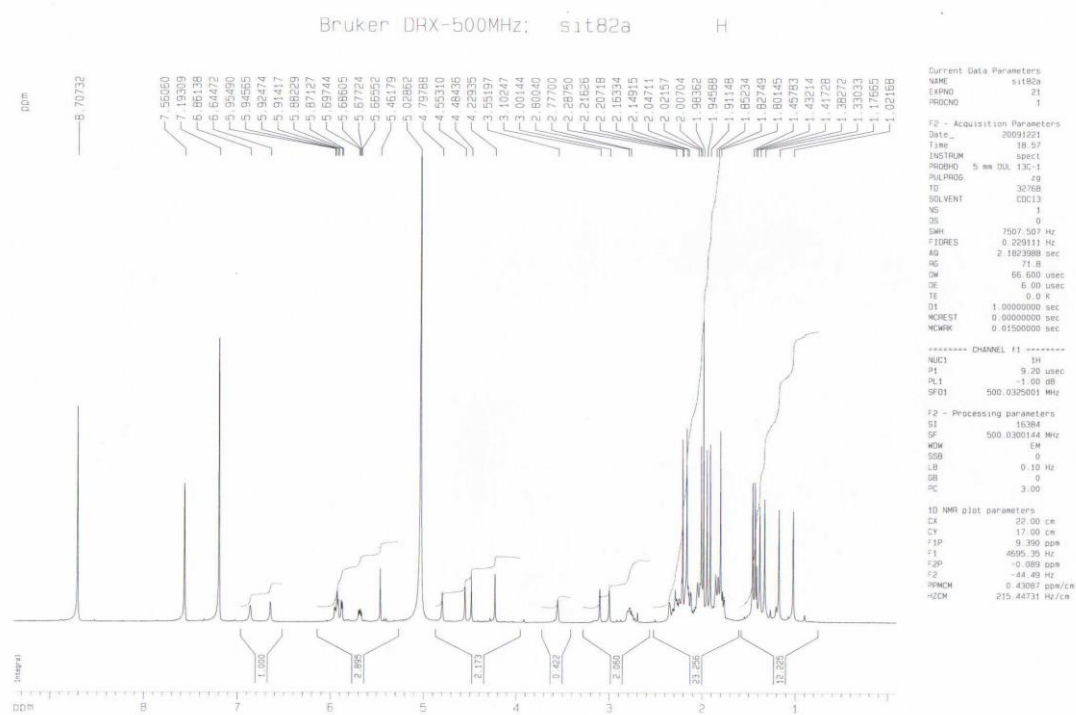


Figure 10. ^{13}C NMR spectrum of bistenuifolin B (2)

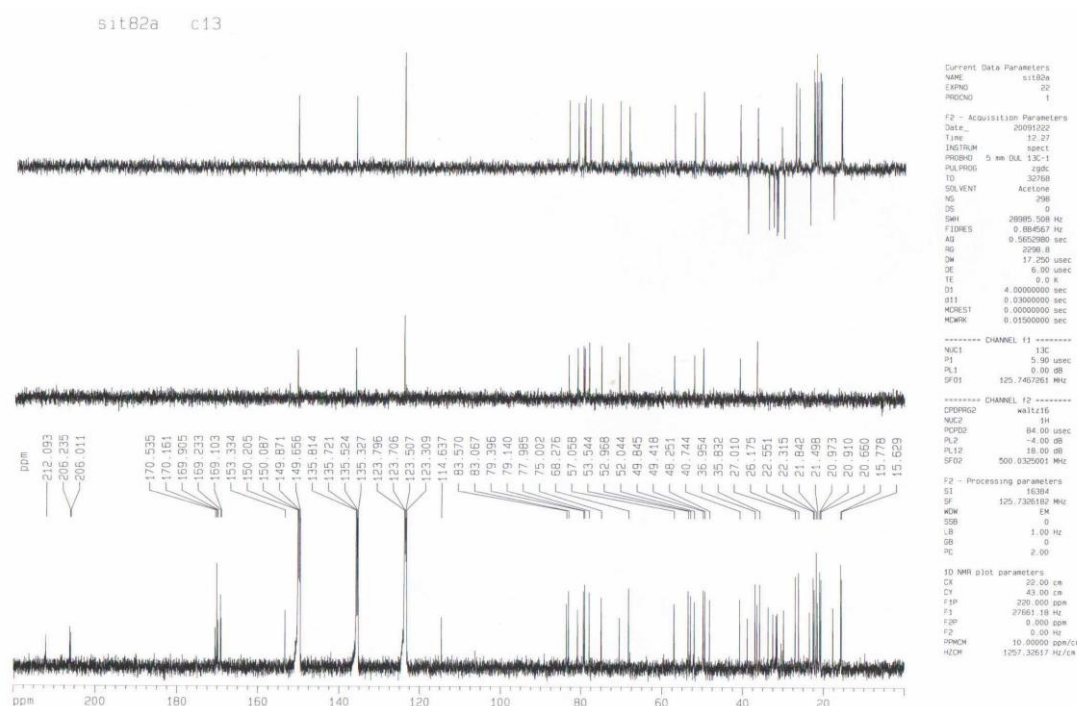
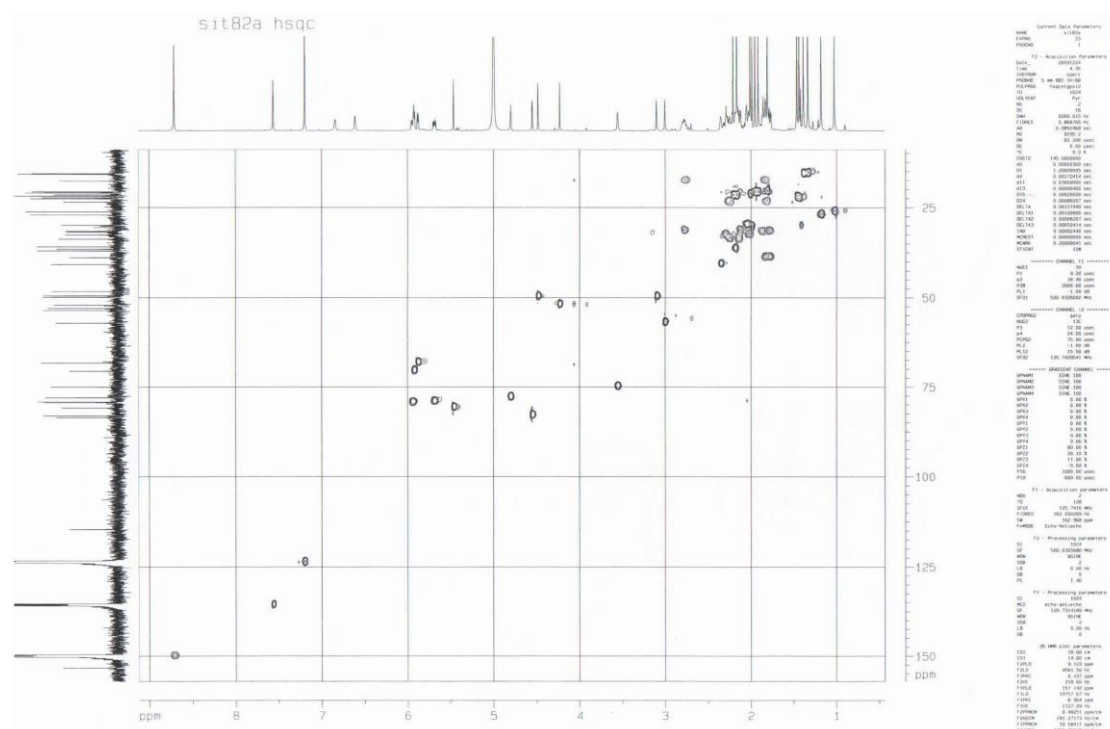


Figure 11. HSQC spectrum of bistenuifolin B (2)



sit82a hmbc

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 PROCNO: 1
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 PULPROG: zgpg30
 TD: 65536
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 RG: 512
 DWDW: 0.00
 FIDRES: 0.000500
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 SFO: 101.254
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PROCNO: 1

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DS: 4
SW: 8885.815 Hz
FIDRES: 0.000450 Hz
AQ: 0.002464 sec
RG: 3274
IN: 83.100 umm
DE: 0.000000 Hz
TE: 300.2 K
D0: 0.00000000 sec
D1: 0.00000000 sec
d13: 0.00000000 sec
d15: 0.00000000 sec
D6: 0.00000000 sec
DELTA: 0.00000000 sec
PCPD1: 0.00000000 sec
PCPD2: 0.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 9.20 umm
PL1: 0.00 dB
SFO1: 500.1326000 MHz

===== GRABFID CHANNEL =====
CPDPRG1: xpmc 100
CPDPRG2: xpmc 100
CPDPRG3: xpmc 100
SP1: 0.00 Hz
SP2: 0.00 Hz
SP3: 0.00 Hz
SP4: 0.00 Hz
SP5: 0.00 Hz
SP6: 0.00 Hz
SP7: 15.00 Hz
SP8: 12.00 Hz
SP9: 40.00 Hz
PFG: 1000.00 umm

F1 - Acquisition parameters

NUC1: 1H
TD: 128
SFO1: 500.132610 MHz
FIDRES: 46.876680 Hz
AQ: 12.000 sec
PULPROG: zgpg30

F2 - Processing parameters

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SF: 500.1326000 MHz
WDW: SINC
SSB: 0
LB: 0.00 Hz
GB: 0
RC: 4.00

F1 - Processing parameters

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SF: 500.1326115 MHz
WDW: SINC
SSB: 0
LB: 0.00 Hz
GB: 0

2D NMR data parameters

EX2: 18.00 um
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F2D1: 19.520 um
F1D1: 460.00 Hz
F2D2: 0.441 um
D2H: 200.00 Hz
F1D2: 0.360 um
F1D3: 460.00 Hz
F2D3: 0.520 um
F1D4: 200.00 Hz
F2D4: 0.441 um
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F2D6: 19.520 um
F2D7: 19.520 um

Figure 14. ROESY spectrum of bistenuifolin B (2)

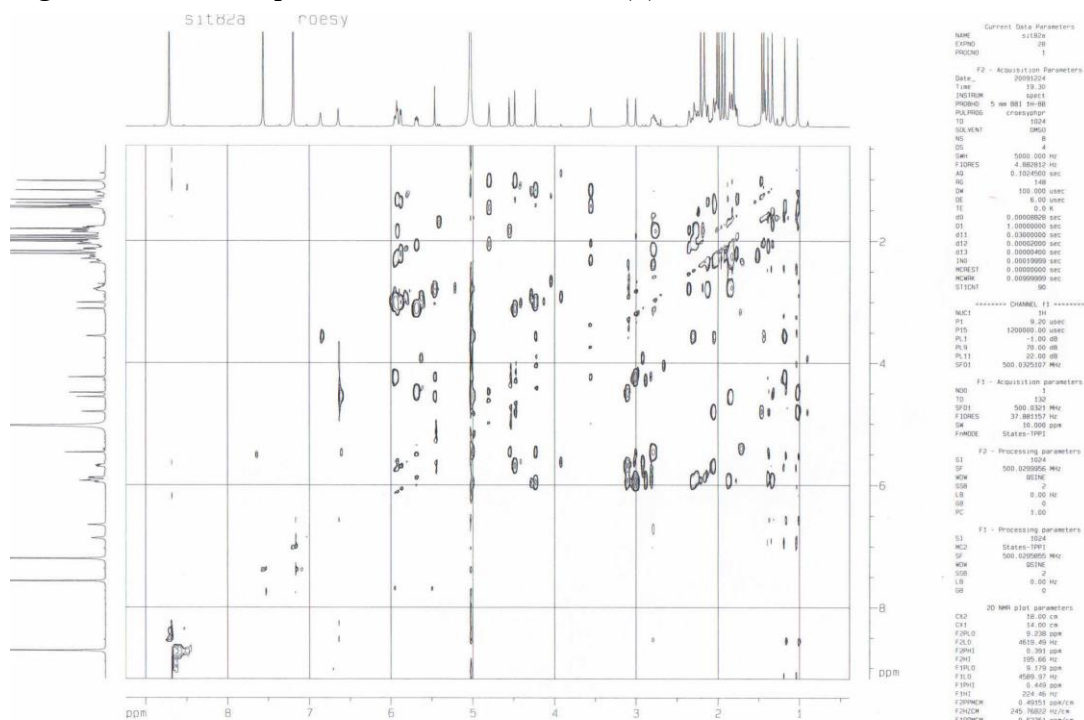
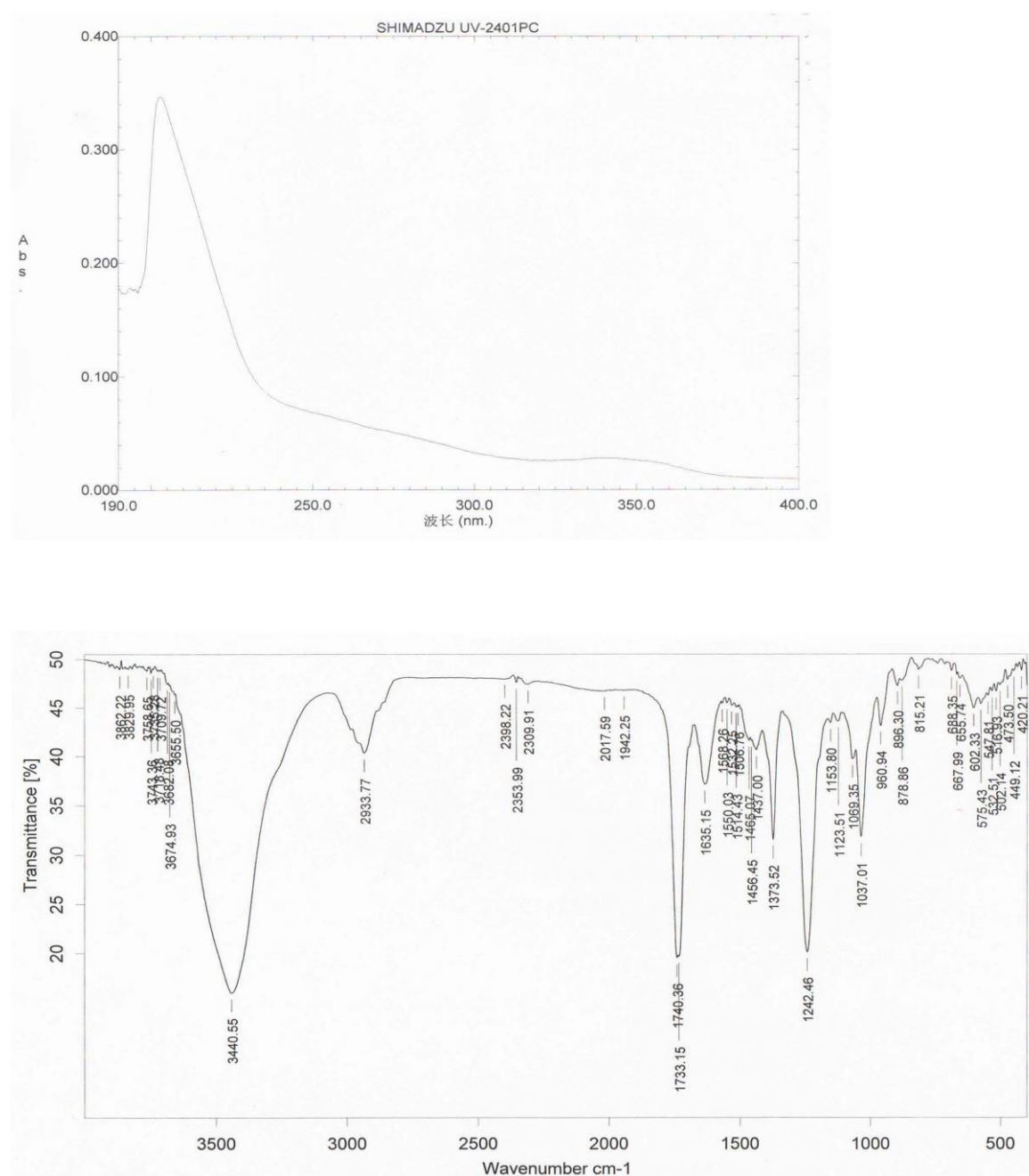


Figure 15. HRESIMS spectrum of bistenuifolin B (2)



	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:

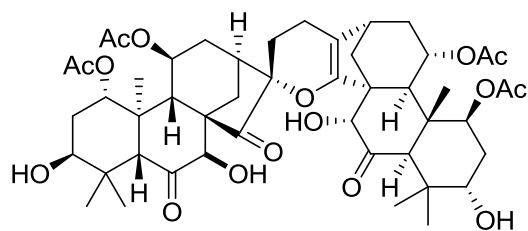


Figure 17. ^1H NMR spectrum of bistenuifolin C (3)

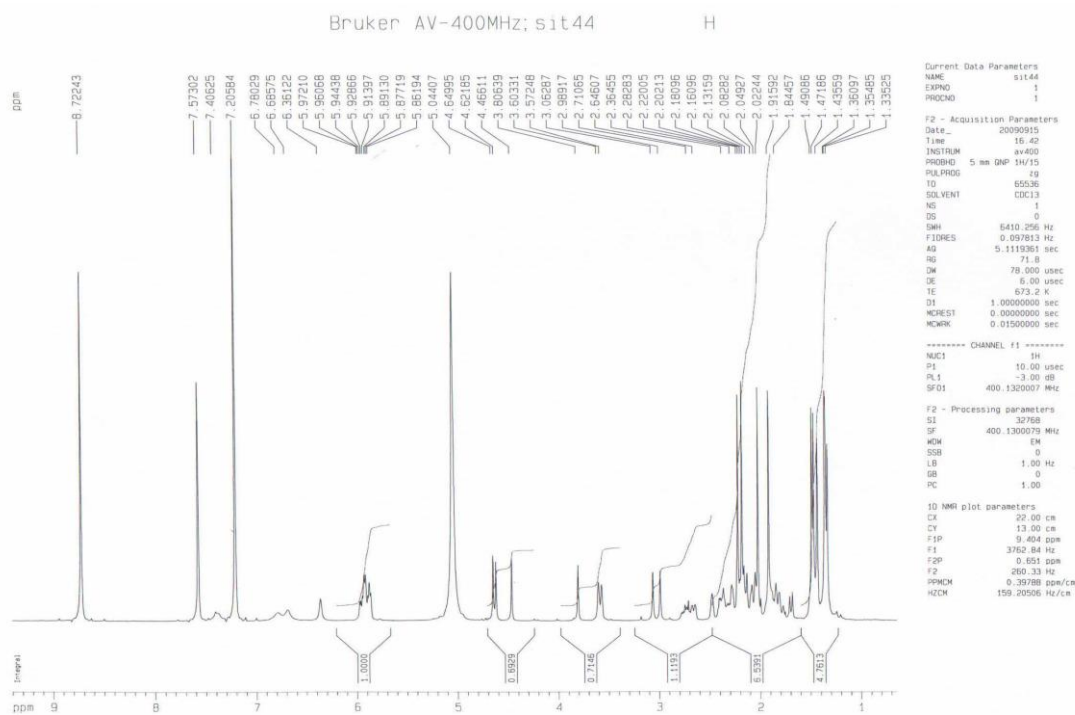


Figure 18. ^{13}C NMR spectrum of bistenuifolin C (3)

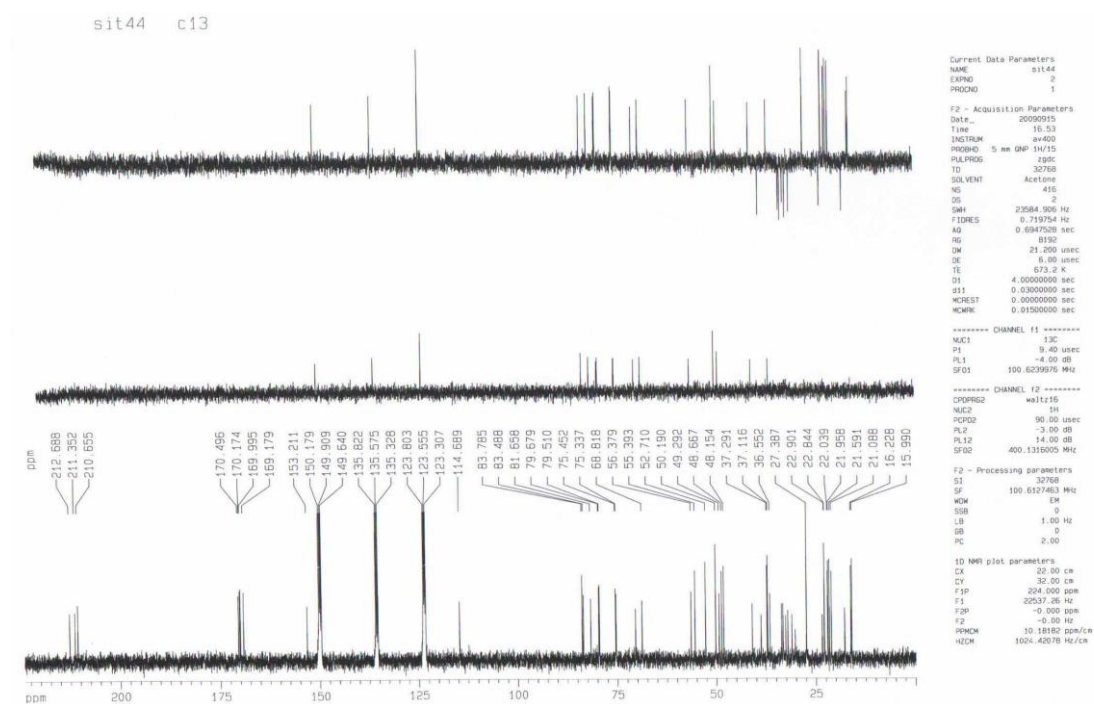


Figure 19. HSQC spectrum of bistenuifolin C (3)

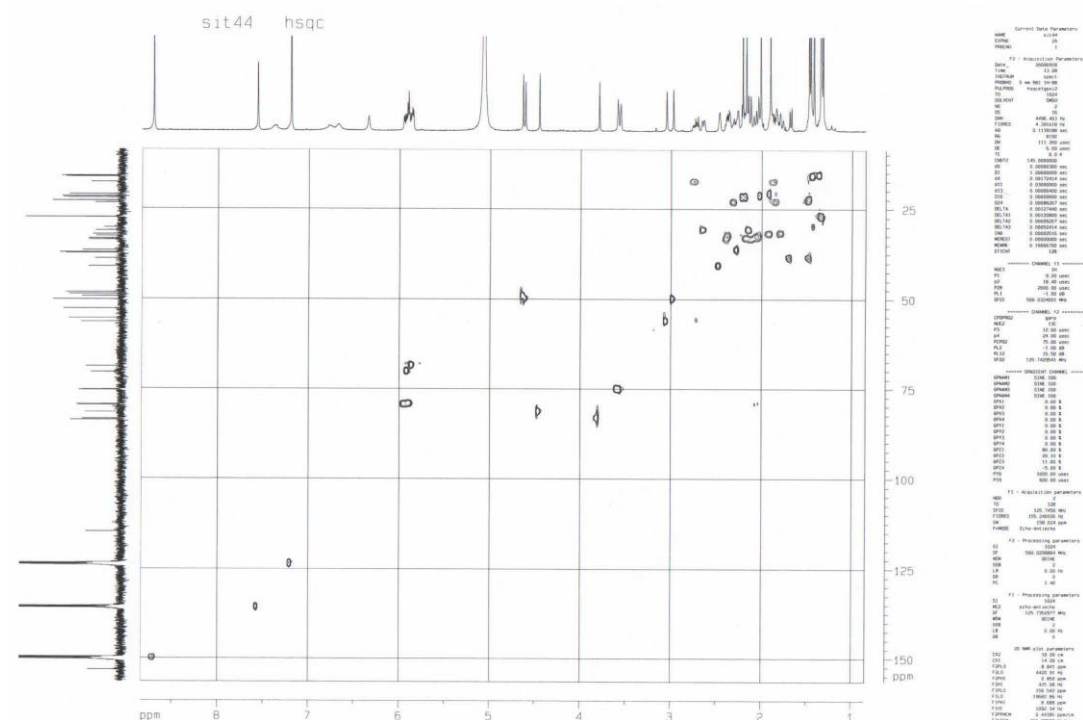


Figure 20. HMBC spectrum of bistenuifolin C (3)

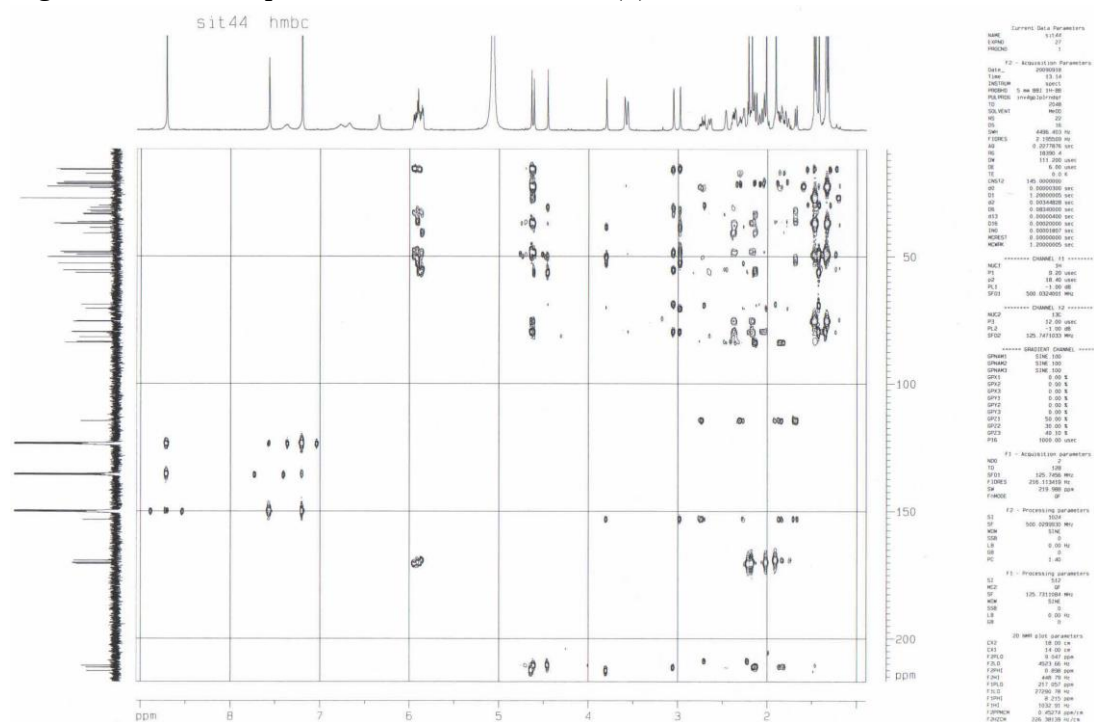


Figure 21. COSY spectrum of bistenuifolin C (3)

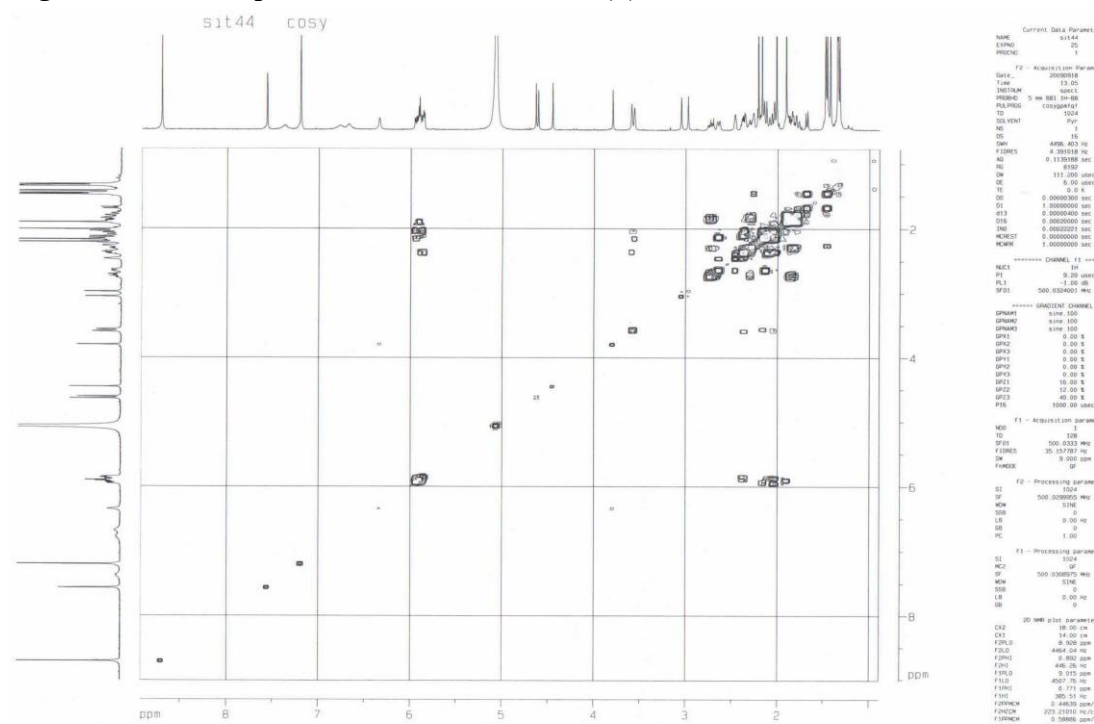


Figure 22. ROESY spectrum of bistenuifolin C (3)

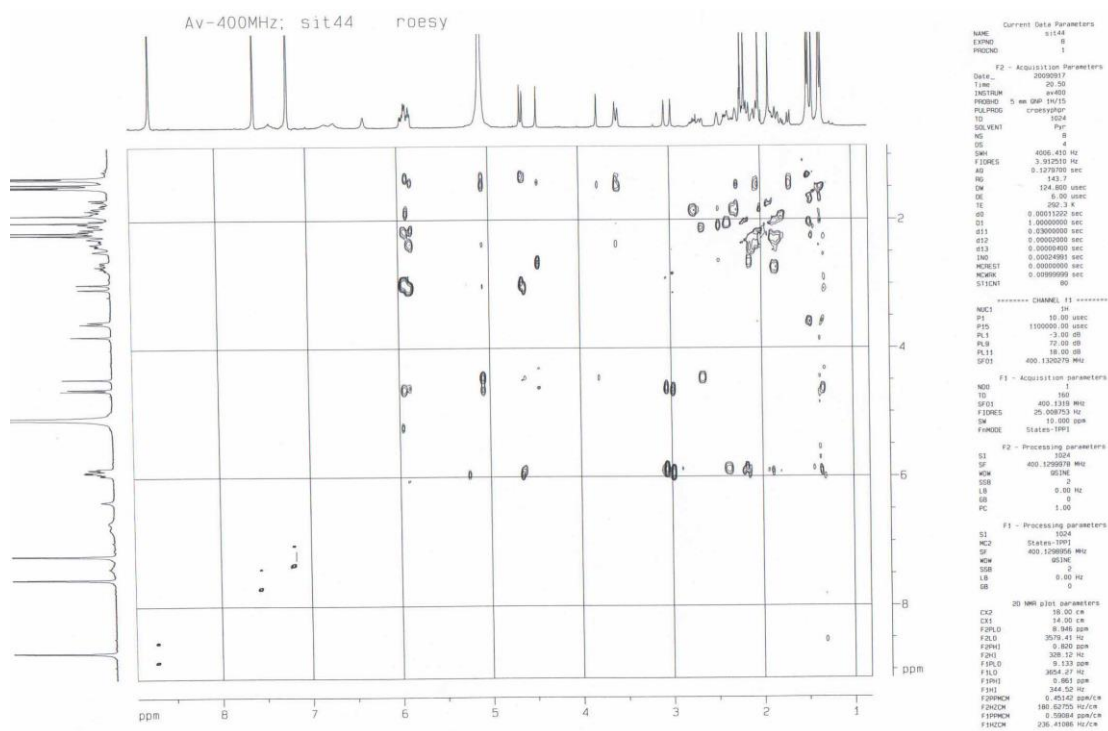
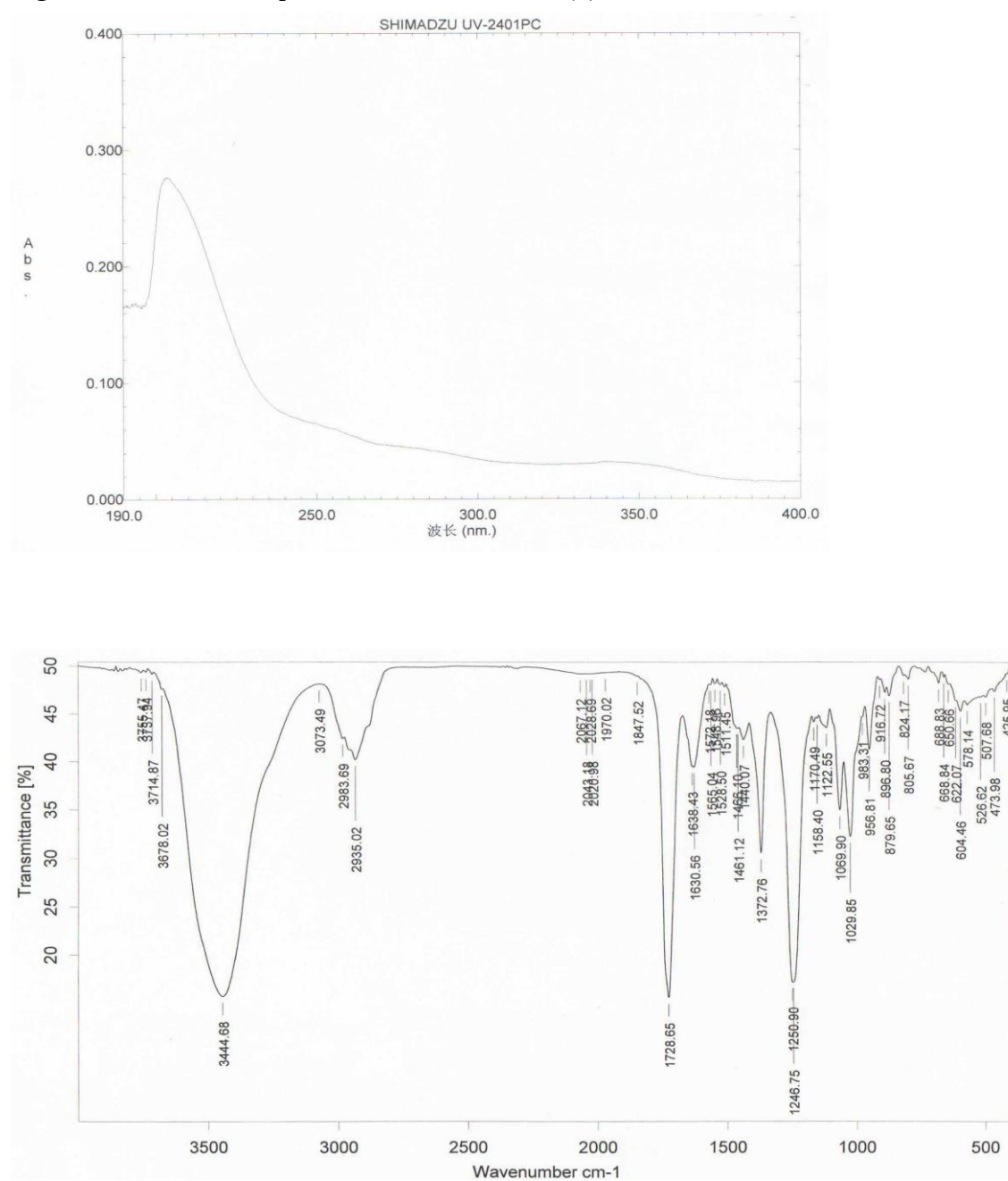


Figure 23. HRESIMS spectrum of bistenuifolin C (3)



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



For compound 4:

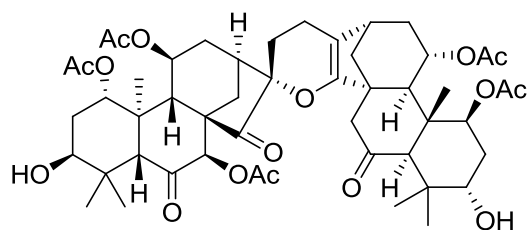


Figure 25. ^1H NMR spectrum of bistenuifolin D (4)

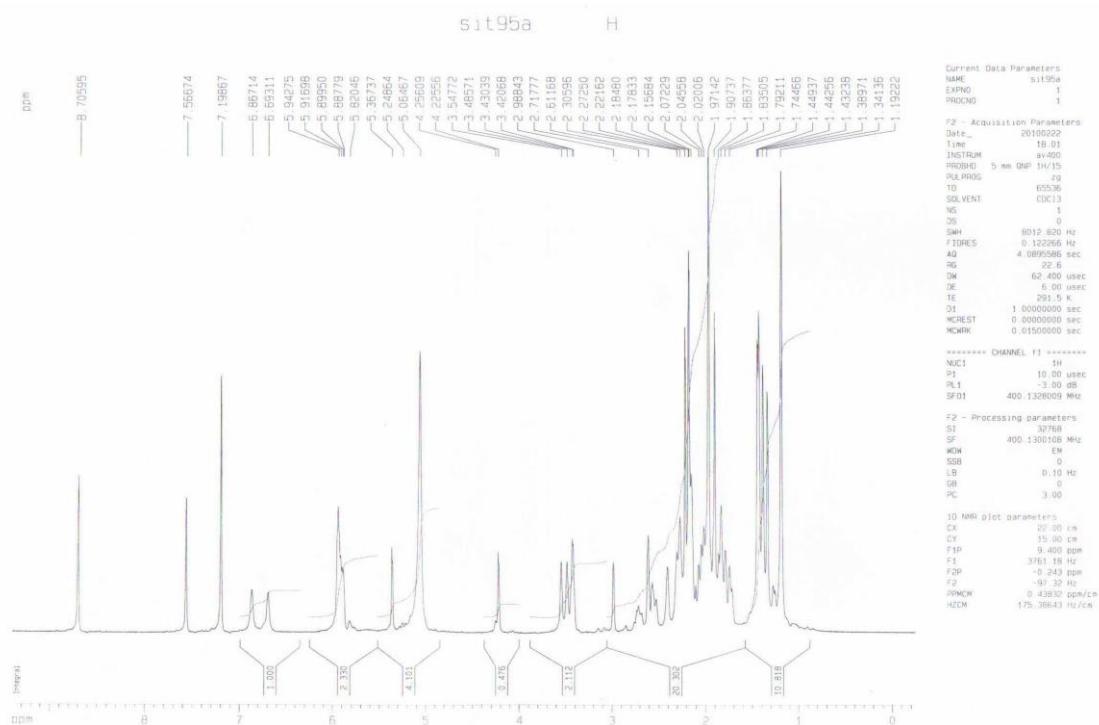


Figure 26. ^{13}C NMR spectrum of bistenuifolin D (4)

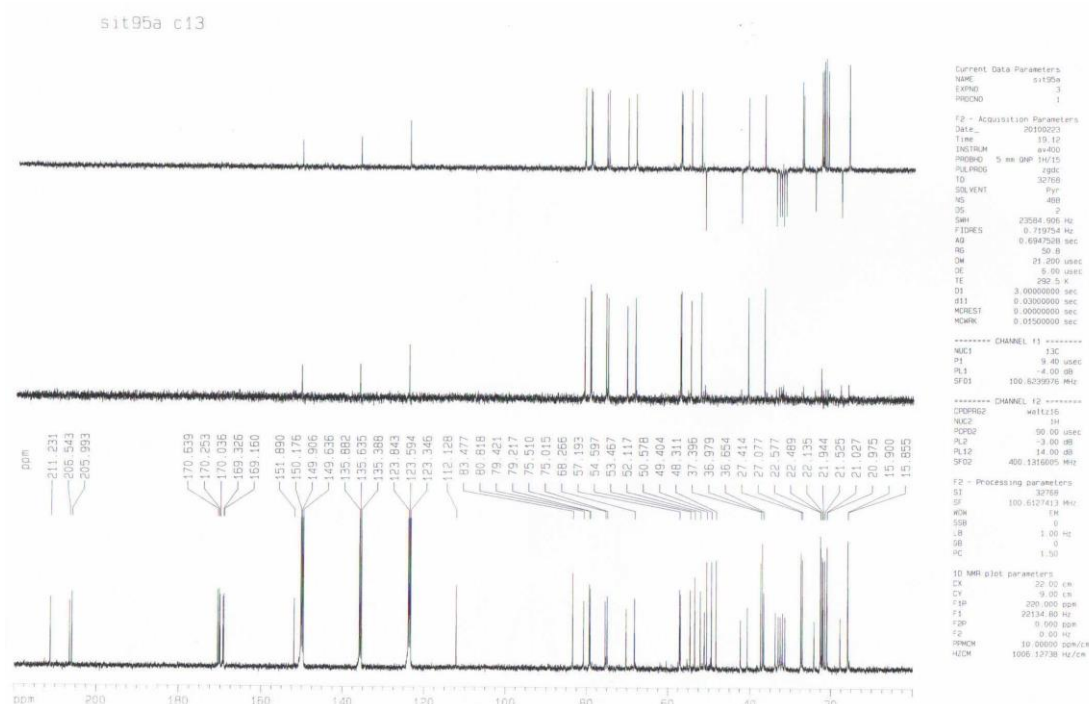


Figure 27. HSQC spectrum of bistenuifolin D (4)

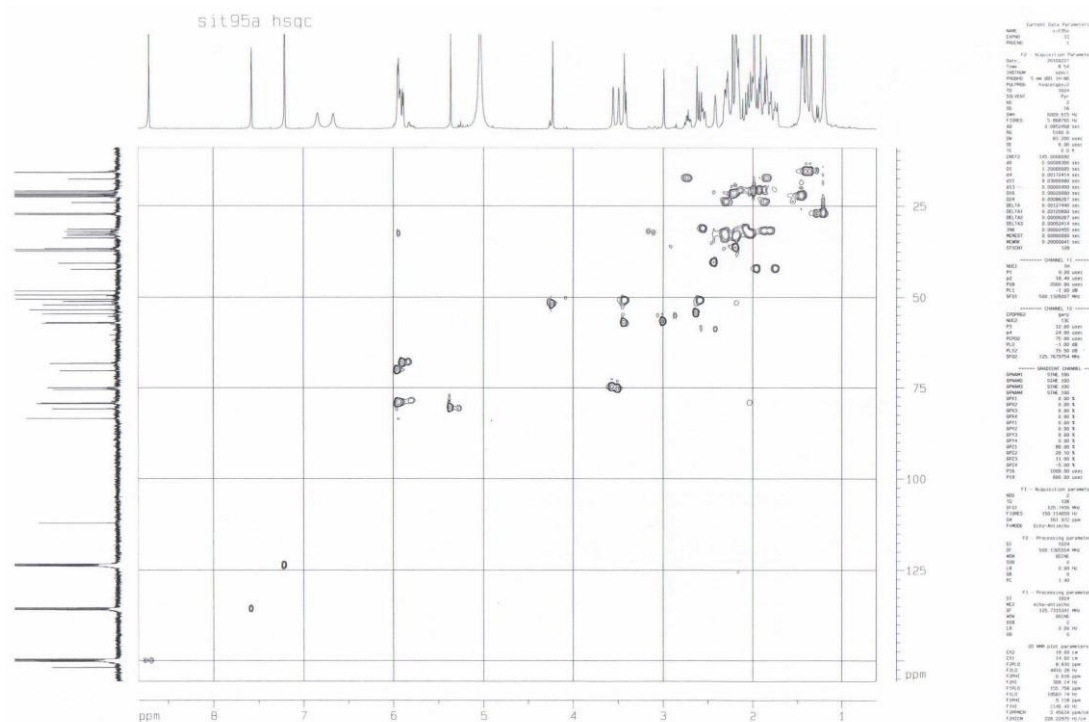


Figure 28. HMBC spectrum of bistenuifolin D (4)

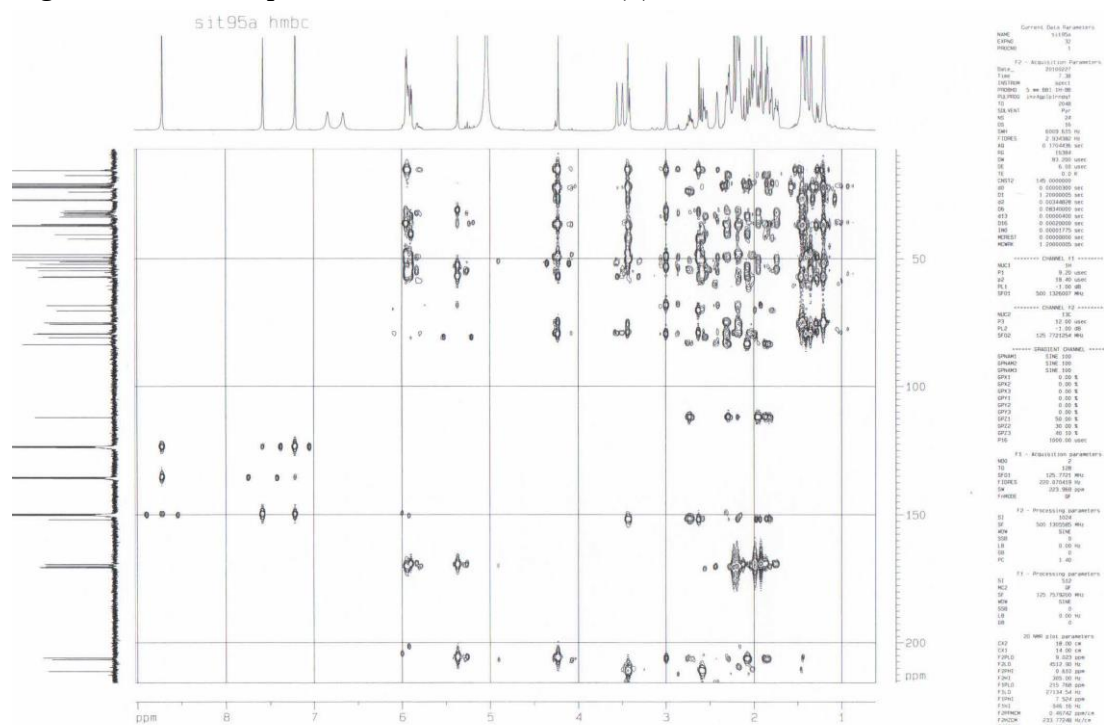


Figure 29. COSY spectrum of bistenuifolin D (4)

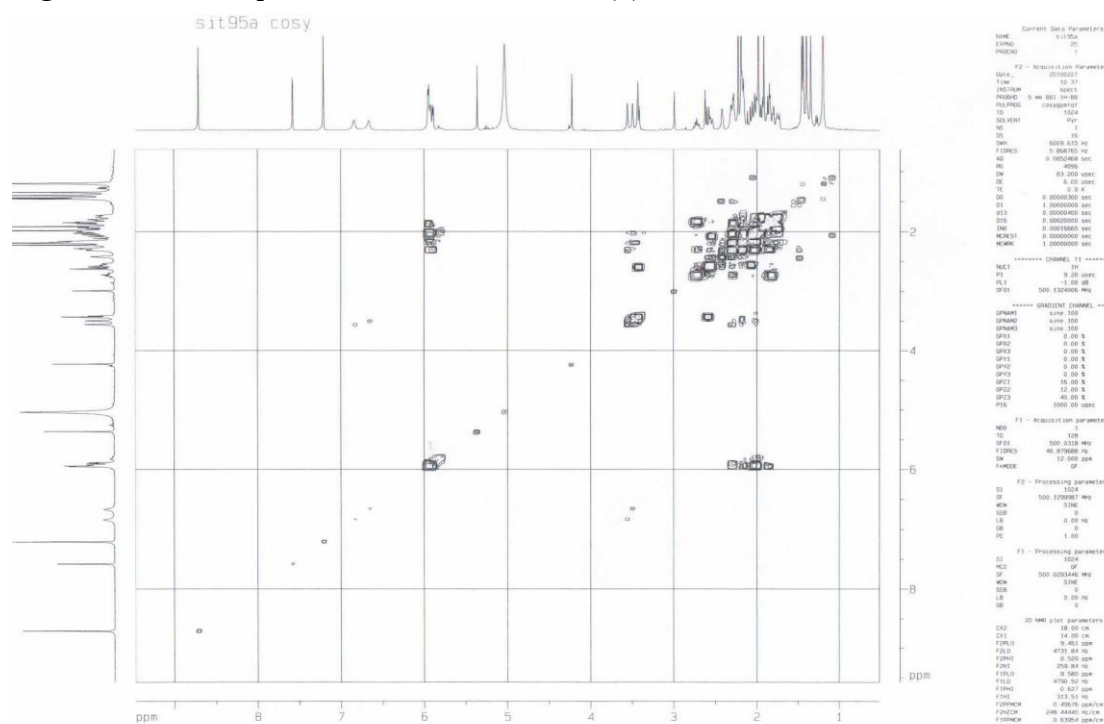


Figure 30. ROESY spectrum of bistenuifolin D (4)

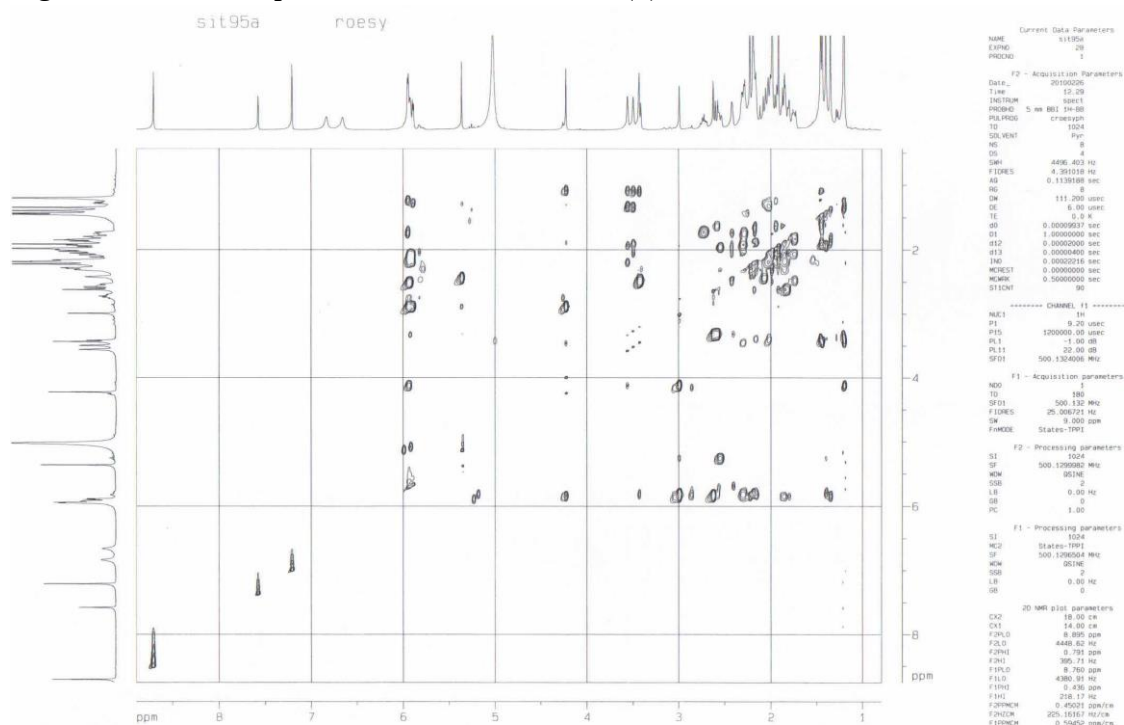
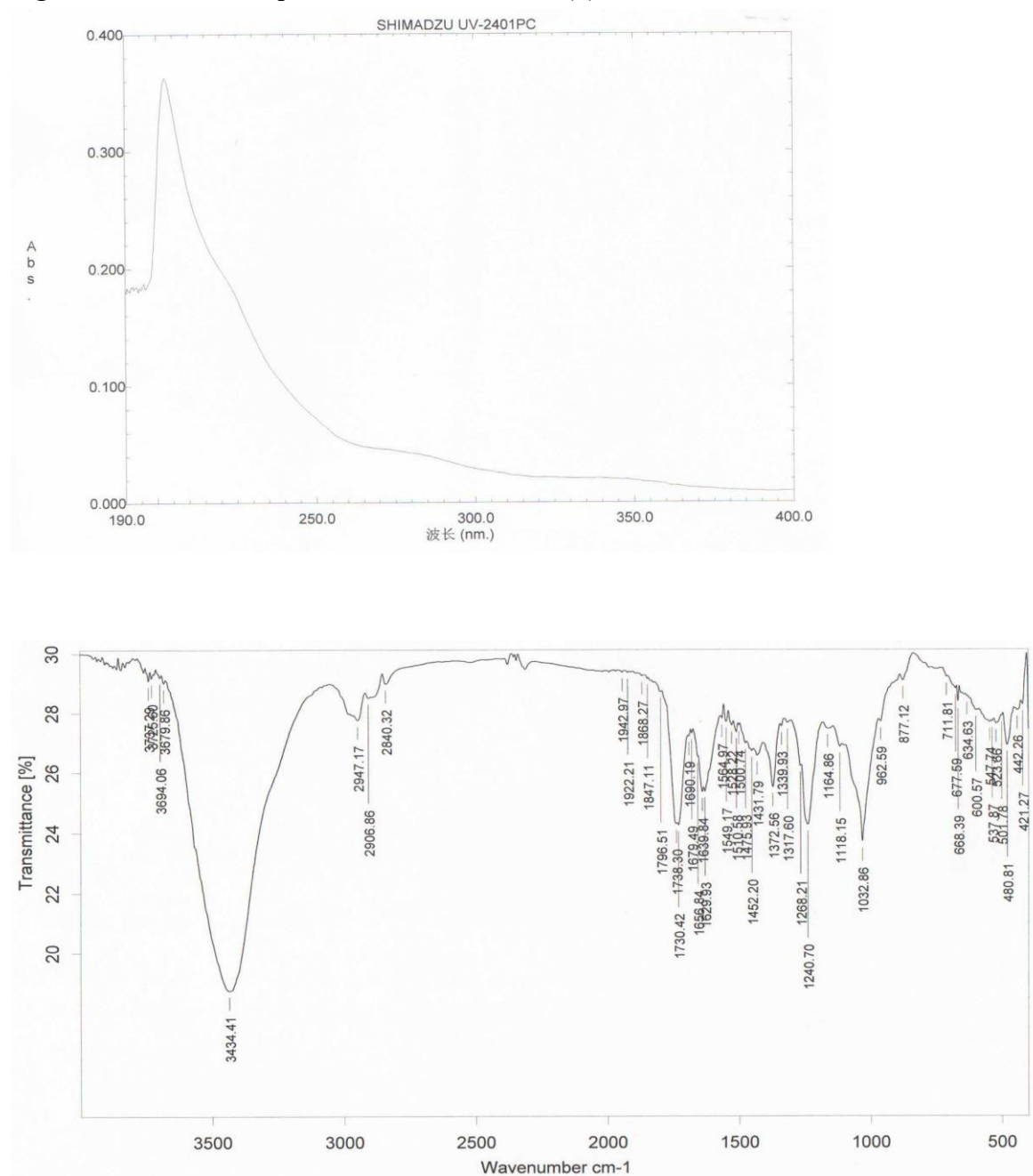


Figure 31. HRESIMS spectrum of bistenuifolin D (4)



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



For compound 5:

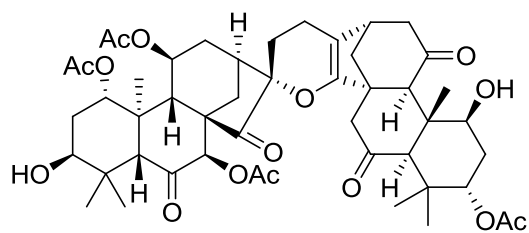


Figure 33. ^1H NMR spectrum of bistenuifolin E (5)

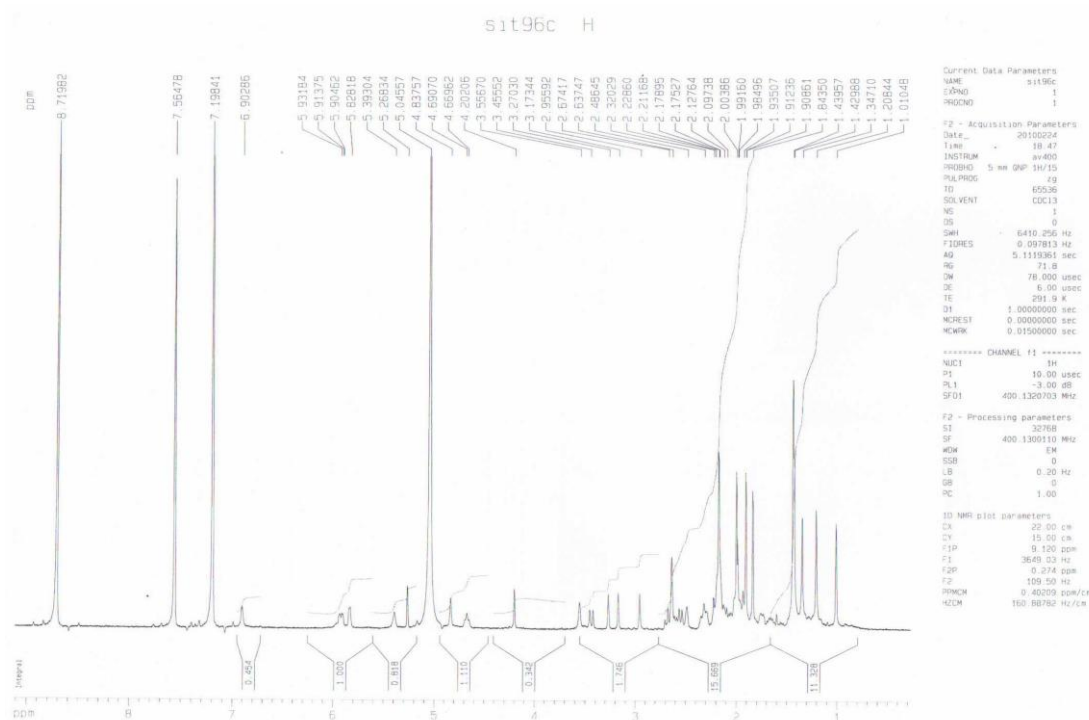


Figure 34. ^{13}C NMR spectrum of bistenuifolin E (5)

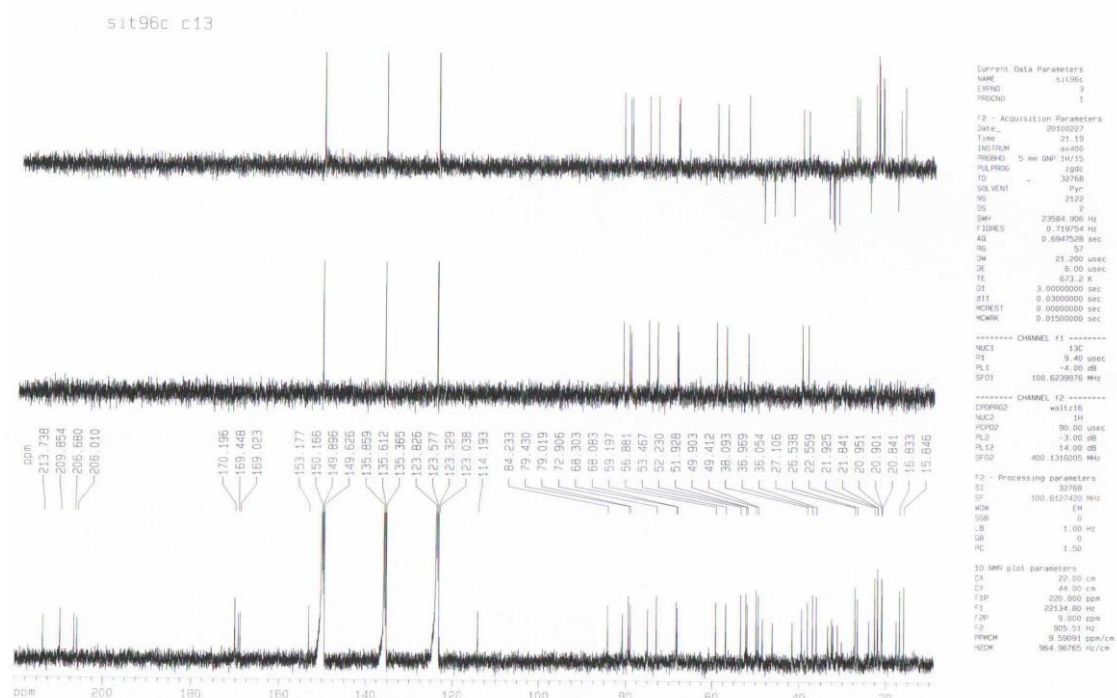
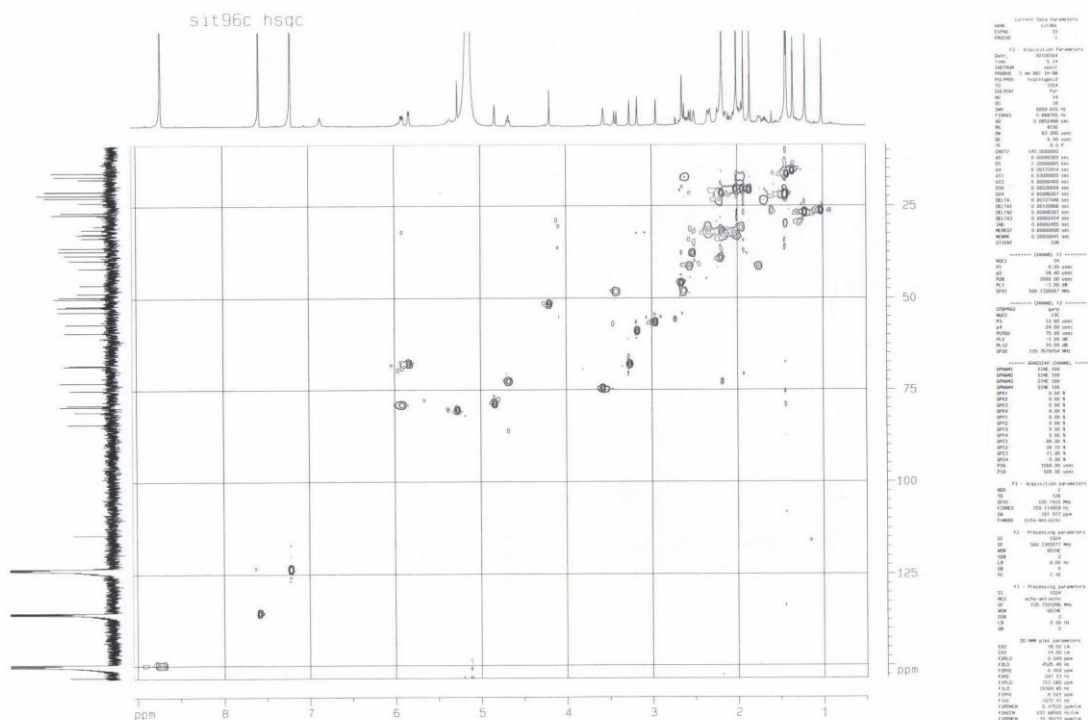


Figure 35. HSQC spectrum of bistenuifolin E (5)



5it96c hmbc

Current Data Parameters

NAME 5it96c
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

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NS 1024
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SW 16000.000 MHz
F2PRES 2.134262 MHz
AQ 0.1774260 sec
RG 327.500 um
WDW EM
SSB 0.000000
LB 0.30 Hz
GB 0
PC 1.000000
MAP 0.000000
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PROCNO 1

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AQ 0.0200000 sec
RG 4096.0
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GPR163 0.00100000
GPR164

Figure 38. ROESY spectrum of bistenuifolin E (5)

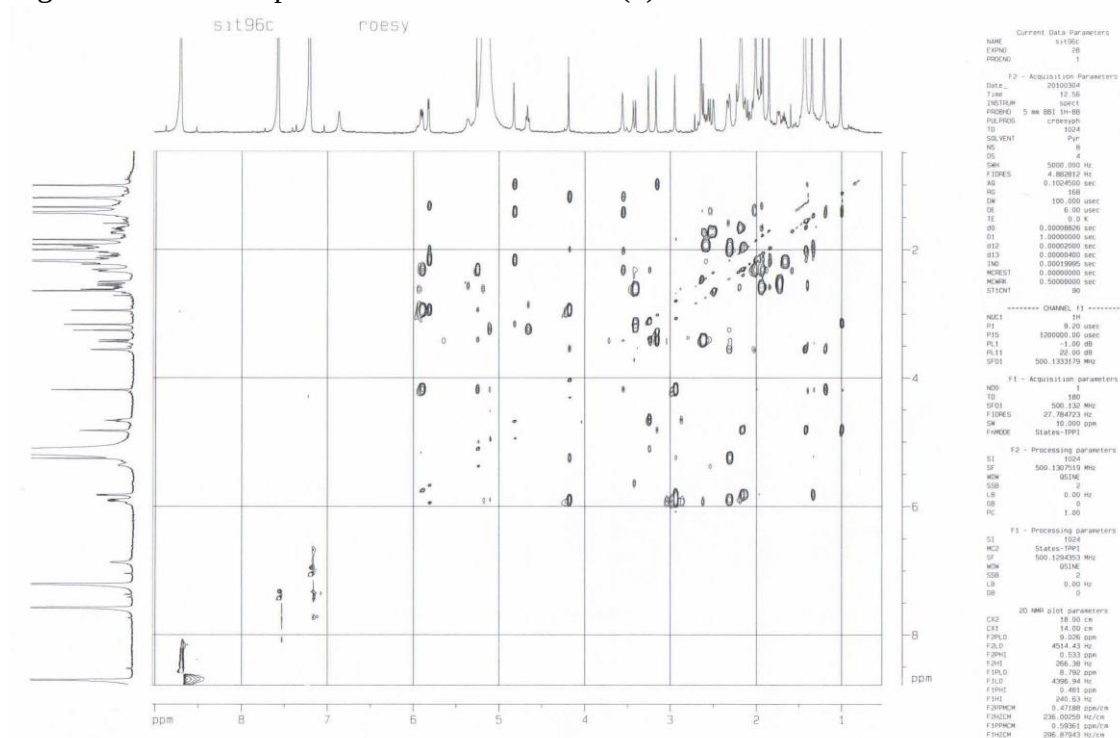
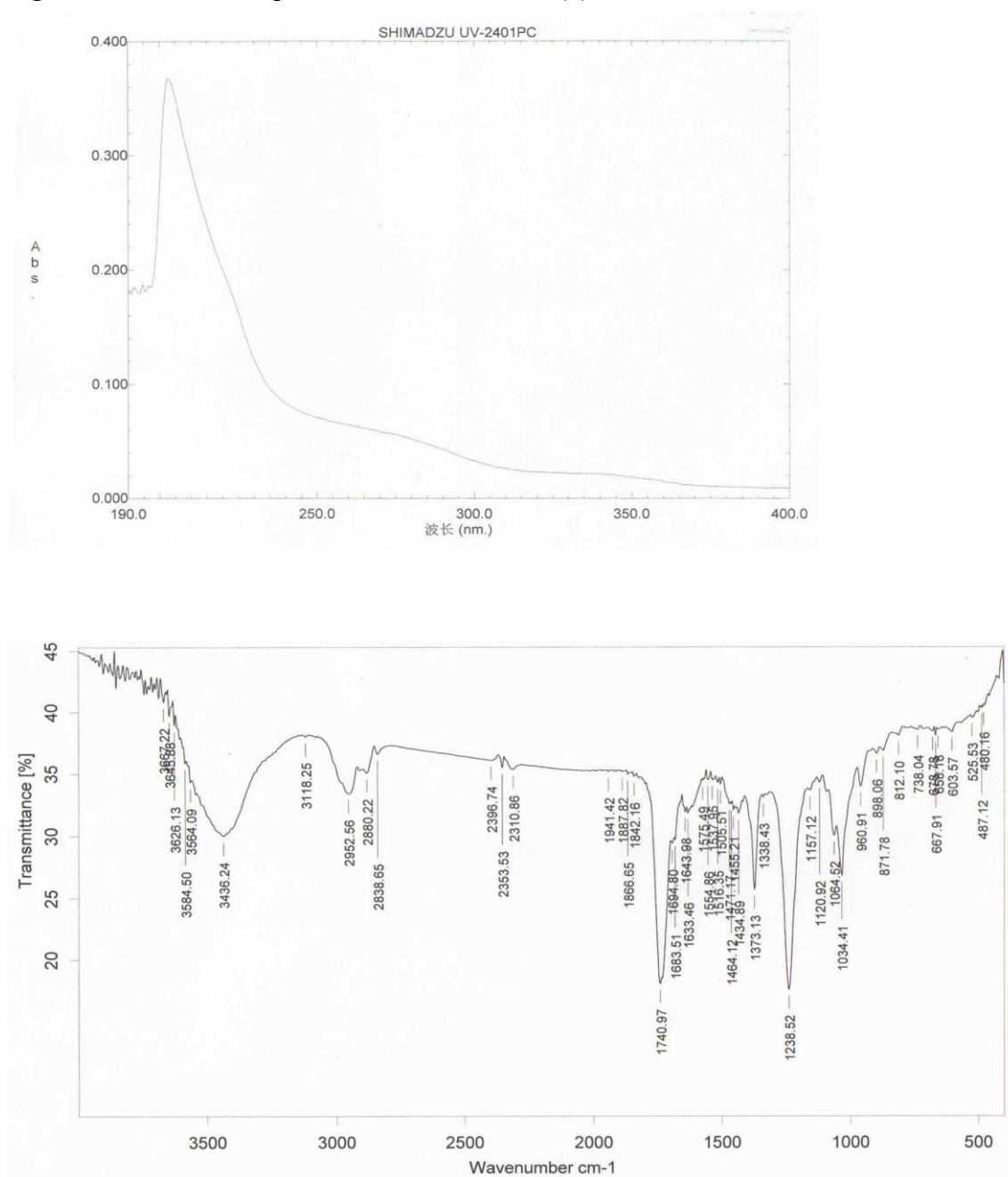


Figure 39. HRESIMS spectrum of bistenuifolin E (5)



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



For compound 6:

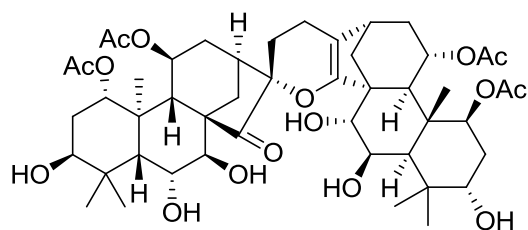


Figure 41. ^1H NMR spectrum of bistenuifolin F (6)

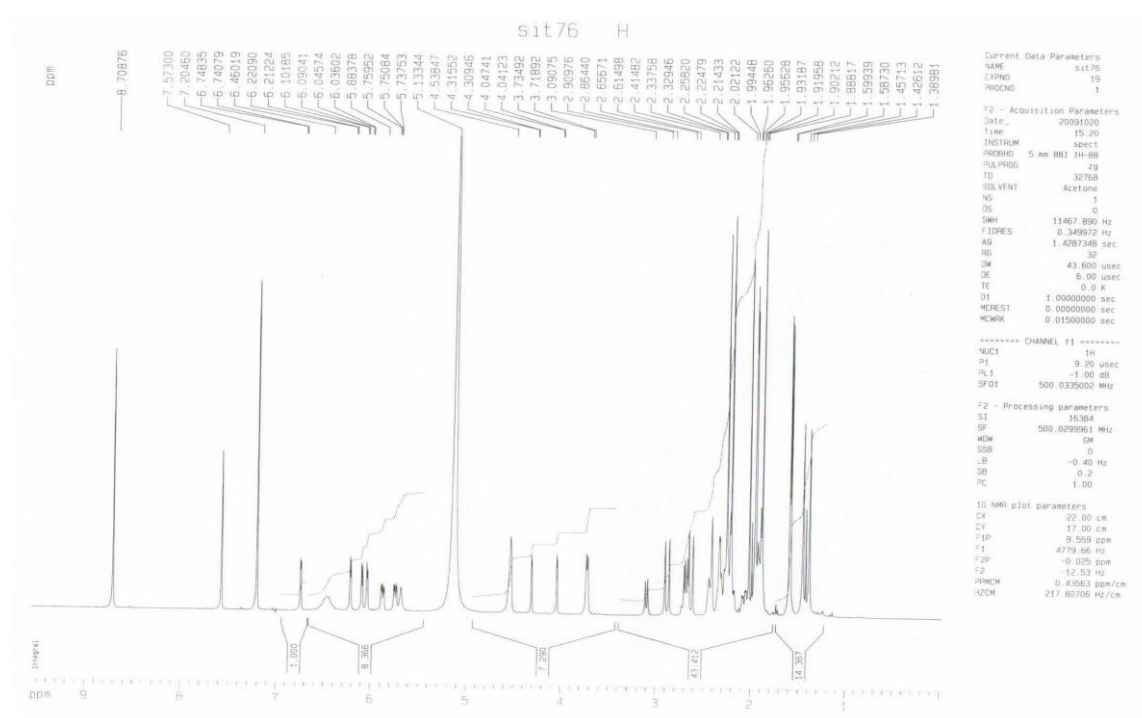


Figure 42. ^{13}C NMR spectrum of bistenuifolin F (6)

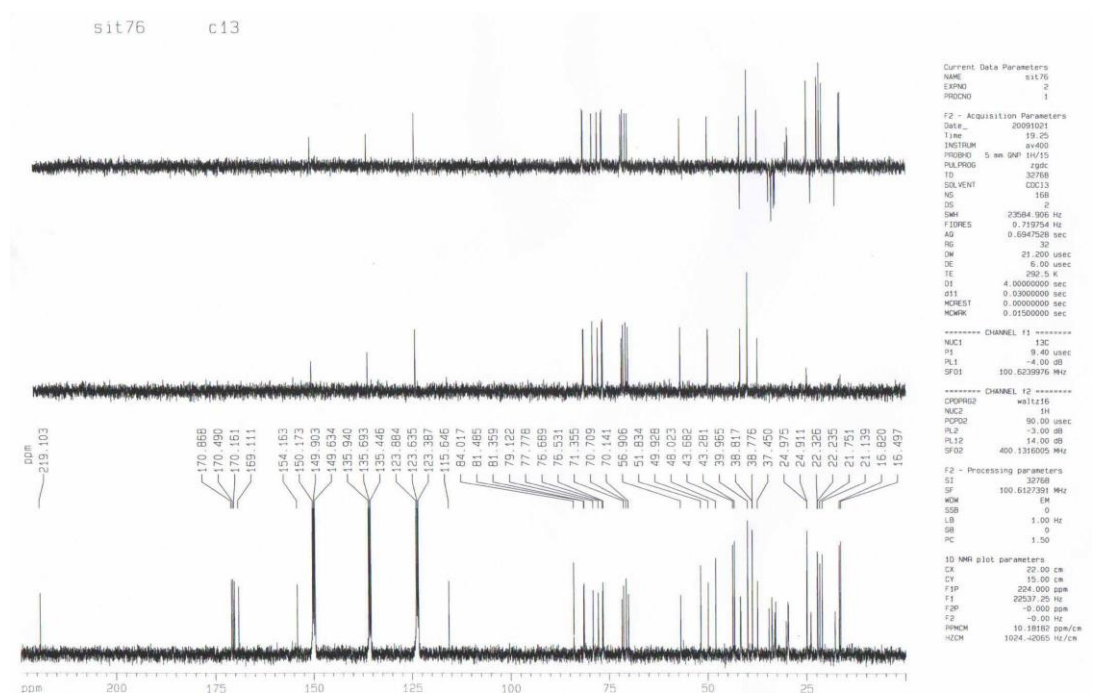


Figure 43. HSQC spectrum of bistenuifolin F (6)

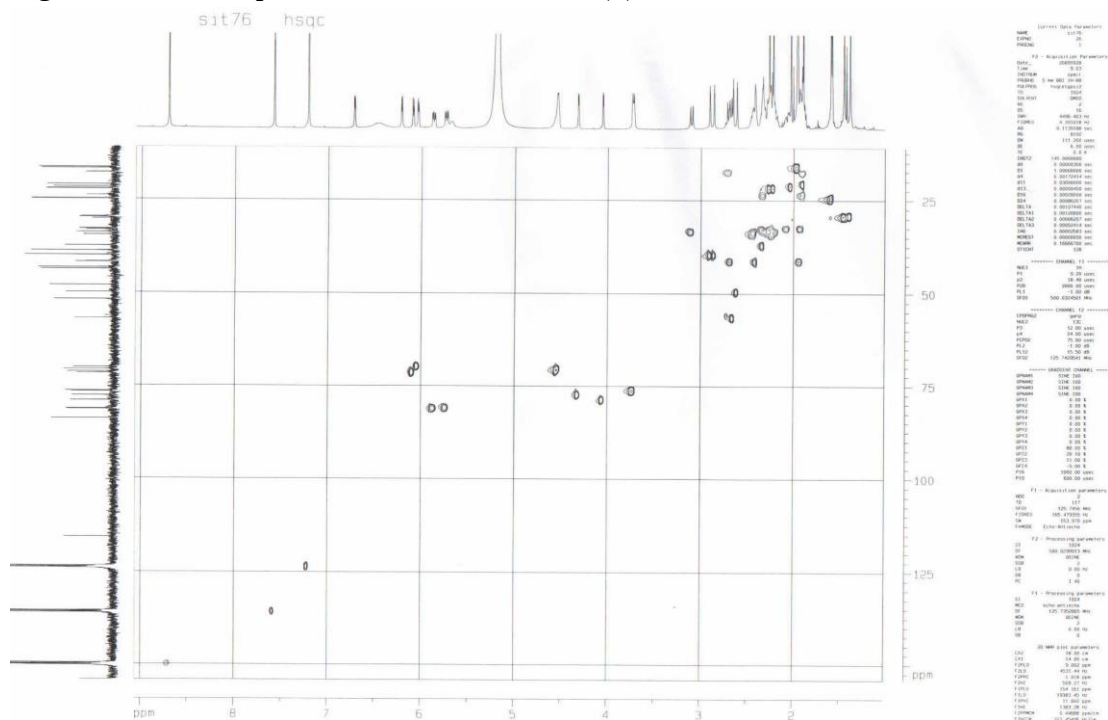


Figure 44. HMBC spectrum of bistenuifolin F (6)

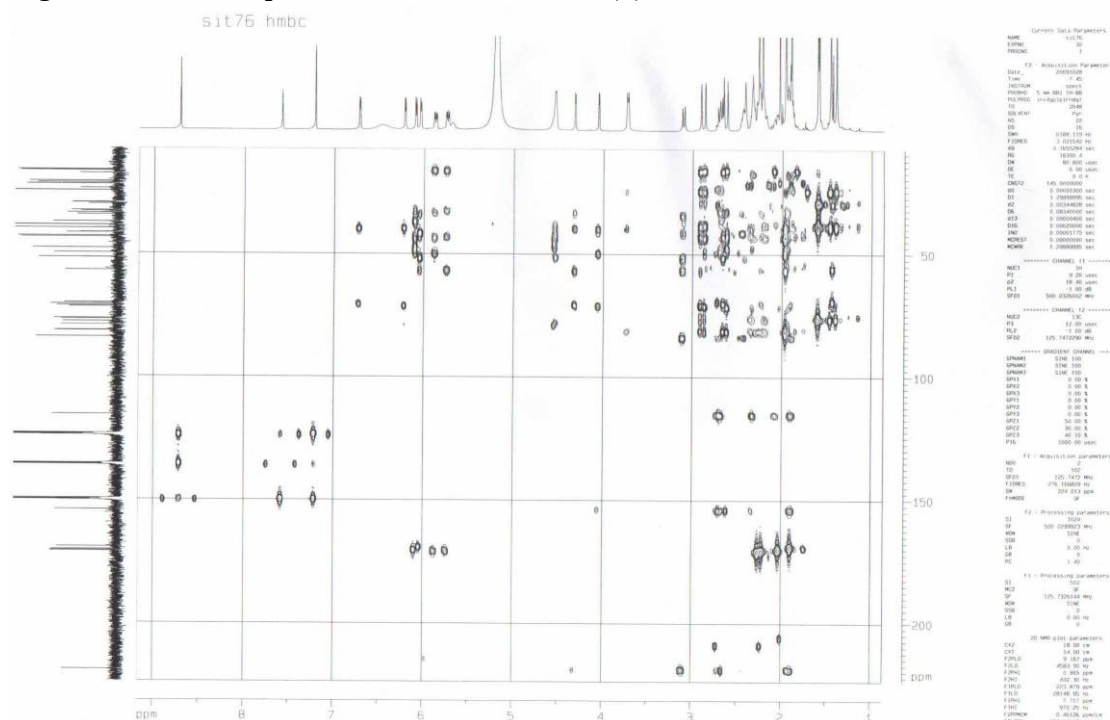


Figure 45. COSY spectrum of bistenuifolin F (6)

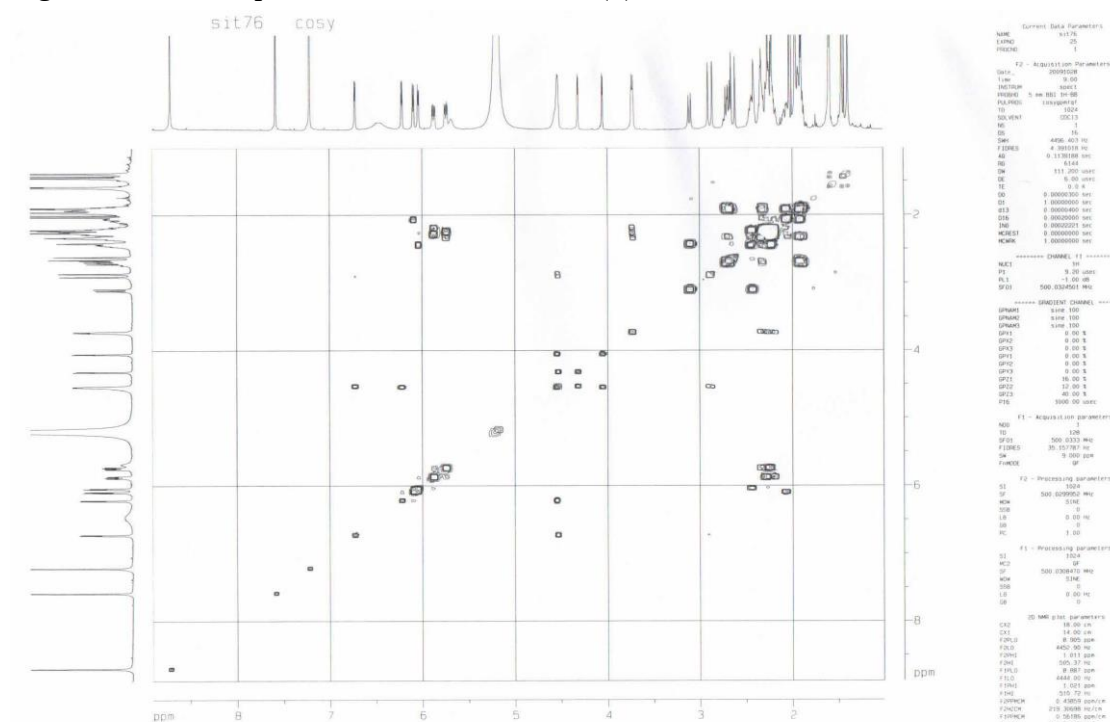


Figure 46. ROESY spectrum of bistenuifolin F (6)

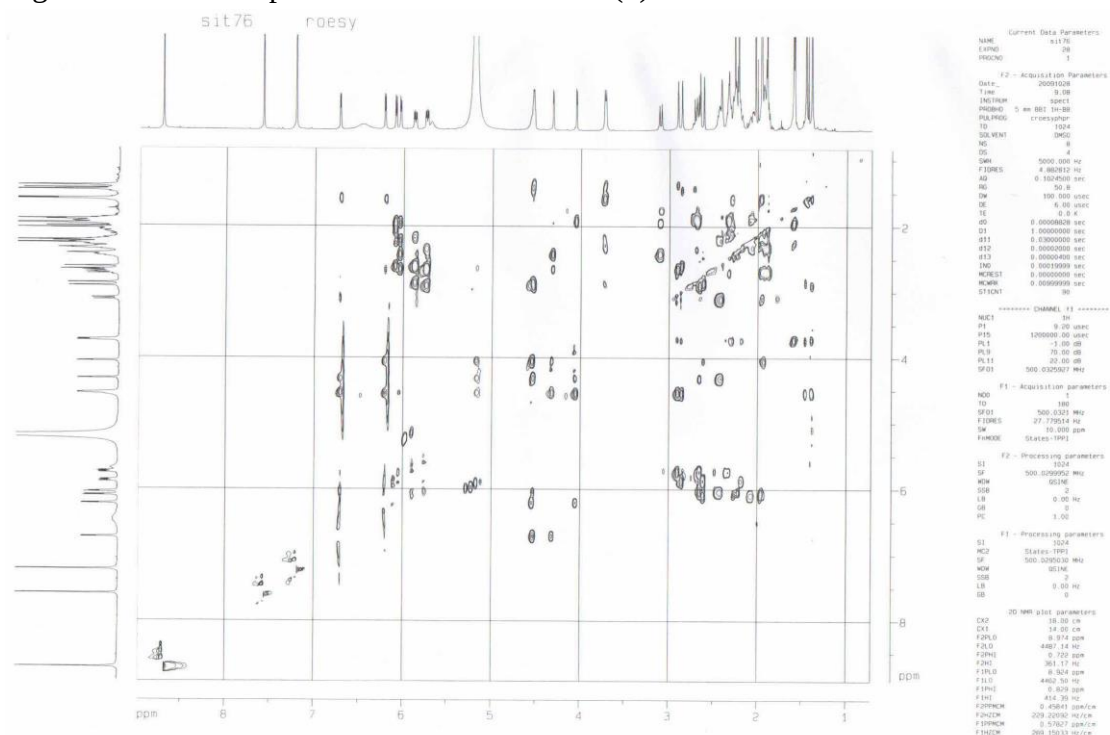
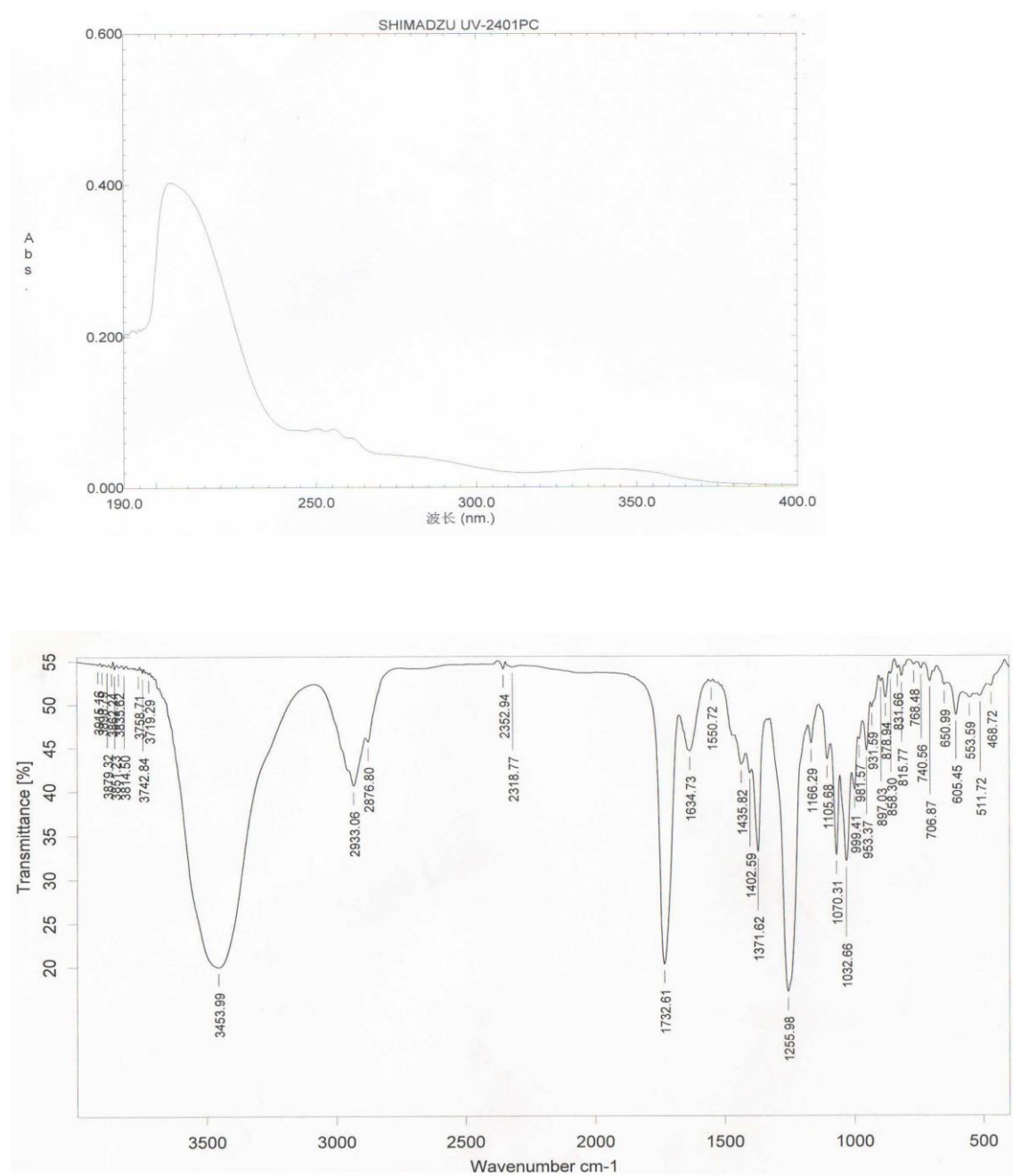


Figure 47. HRESIMS spectrum of bistenuifolin F (6)



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



For compound 7:

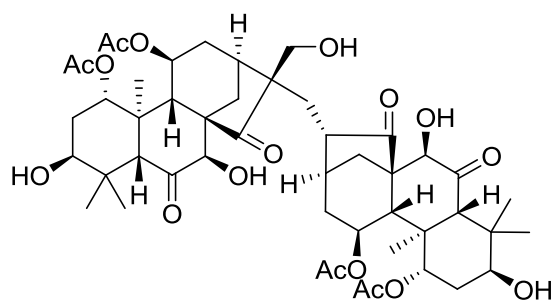


Figure 49. ^1H NMR spectrum of bistenuifolin G (7)

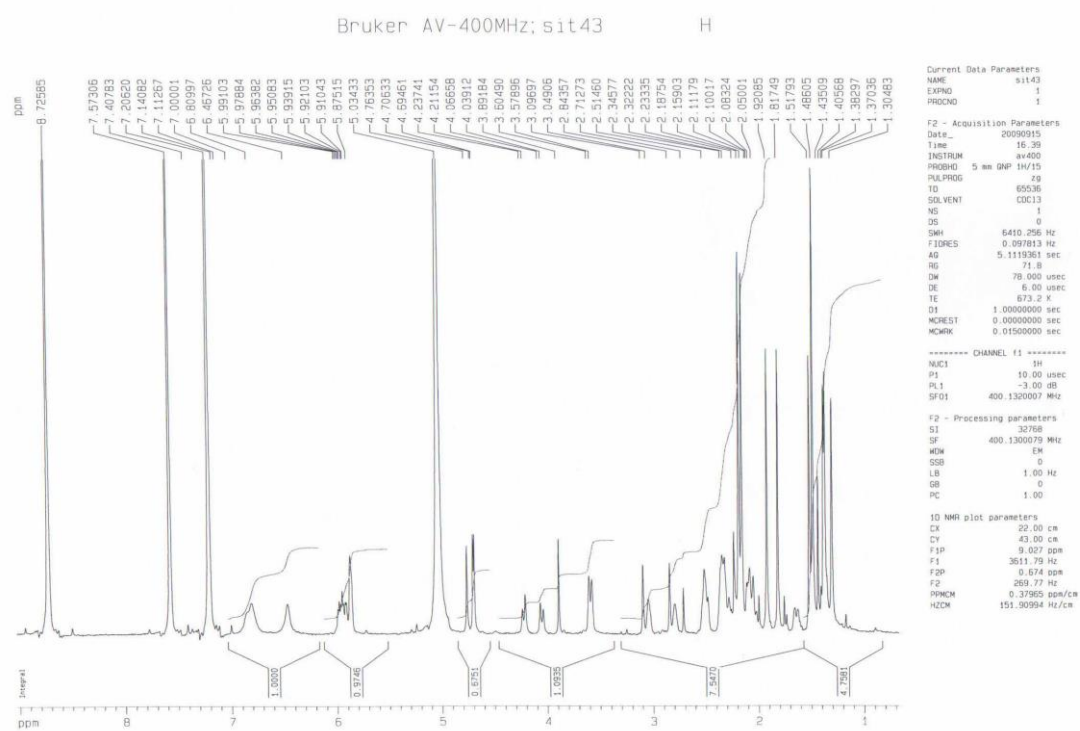


Figure 50. ^{13}C NMR spectrum of bistenuifolin G (7)

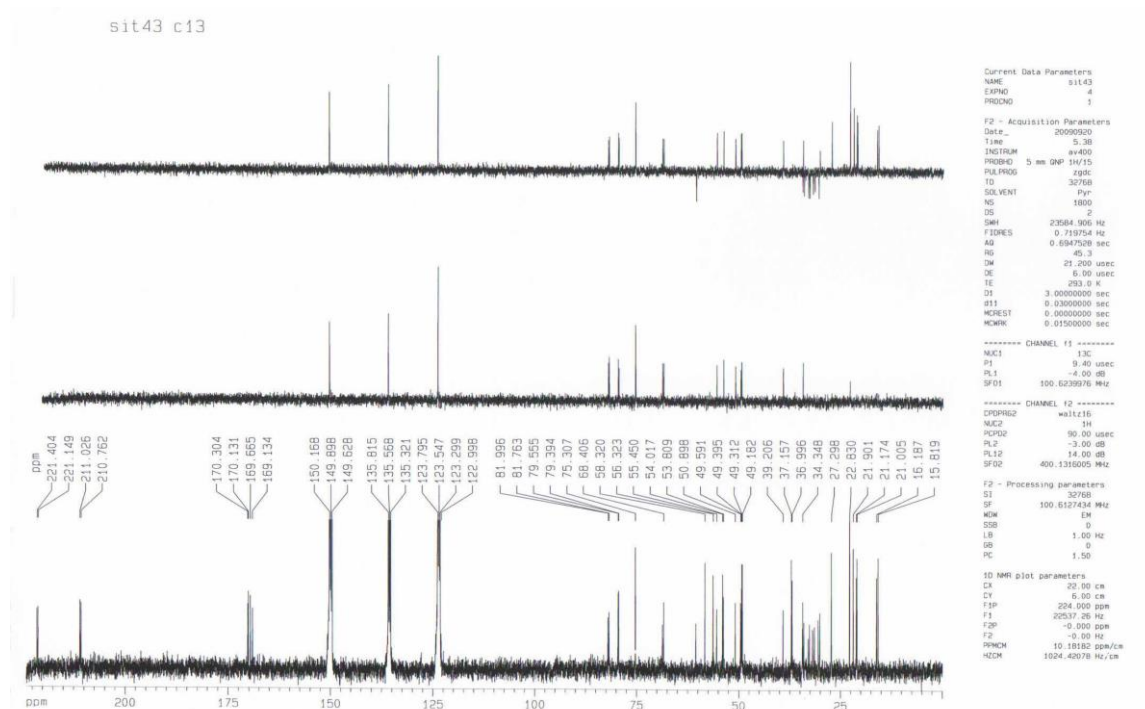
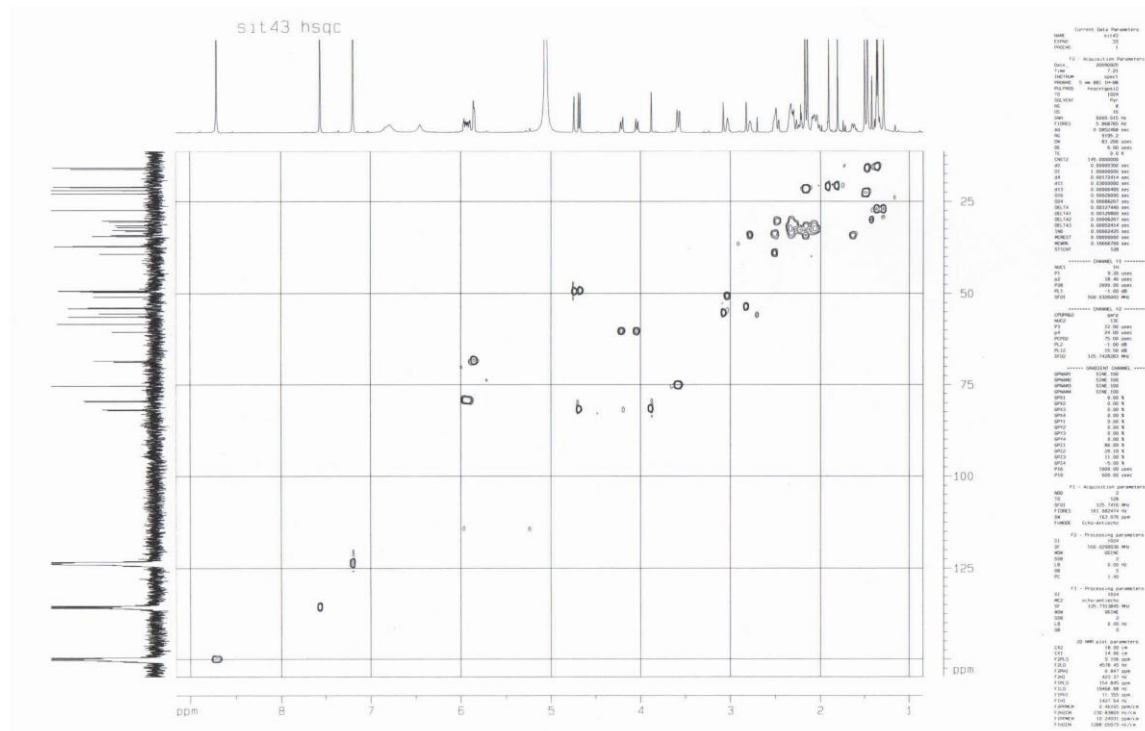


Figure 51. HSQC spectrum of bistenuifolin G (7)



[illegible]

Figure 54. ROESY spectrum of bistenuifolin G (7)

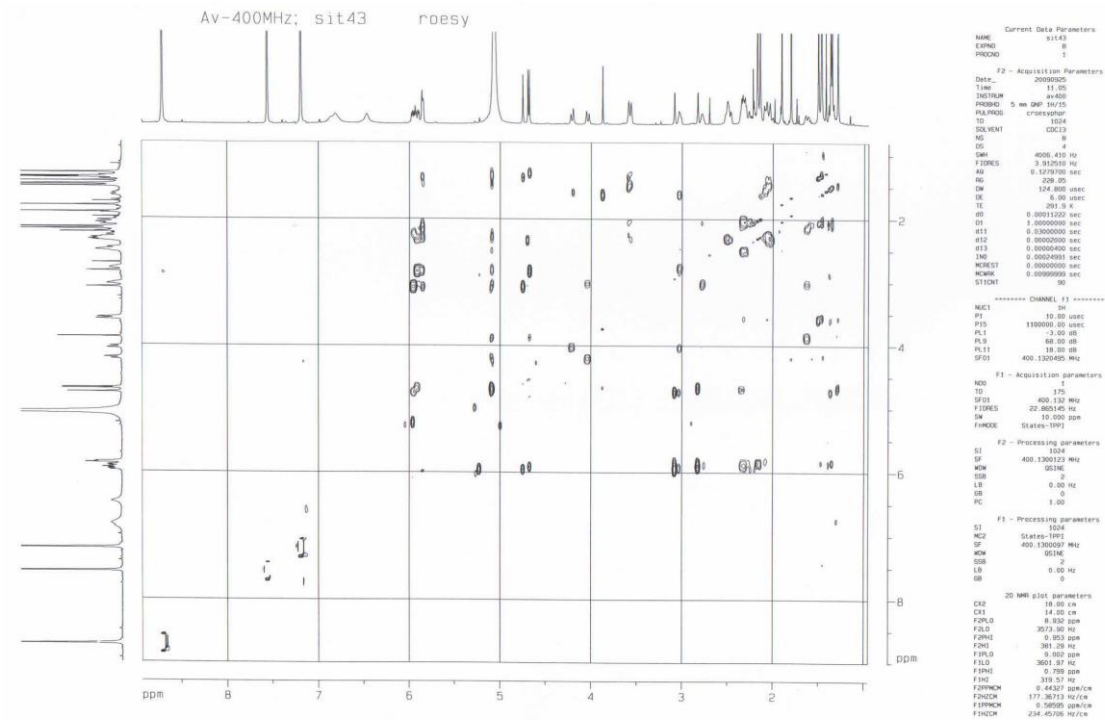


Figure 55. HRESIMS spectrum of bistenuifolin G (7)

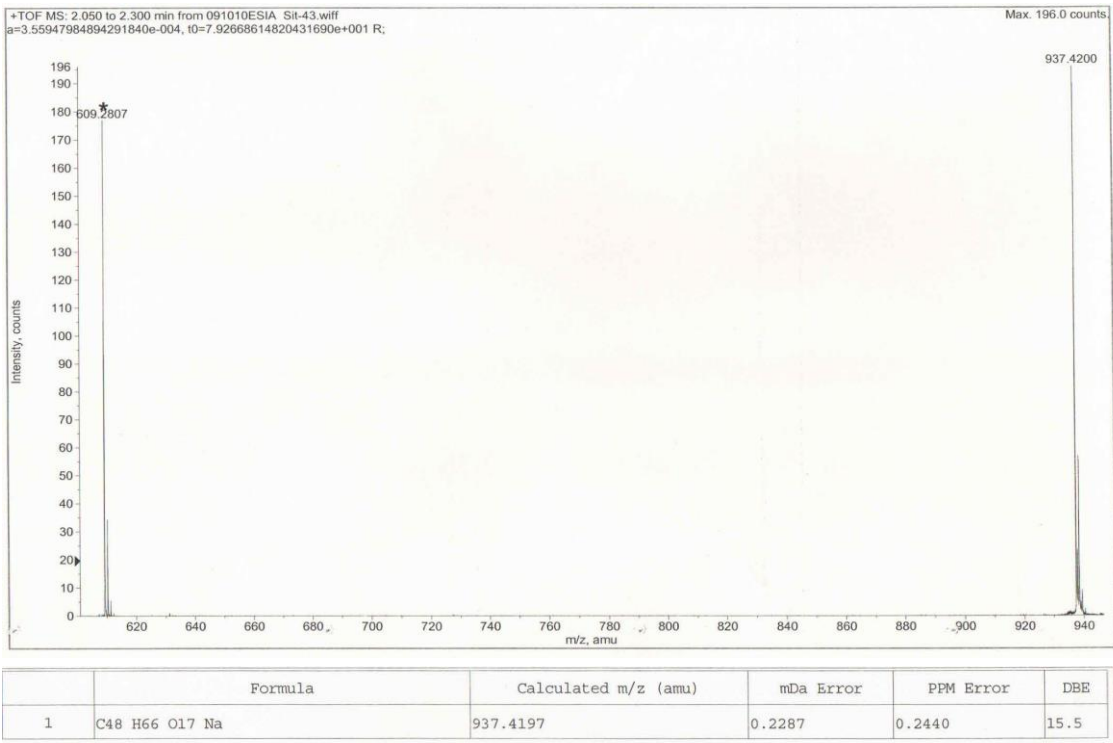
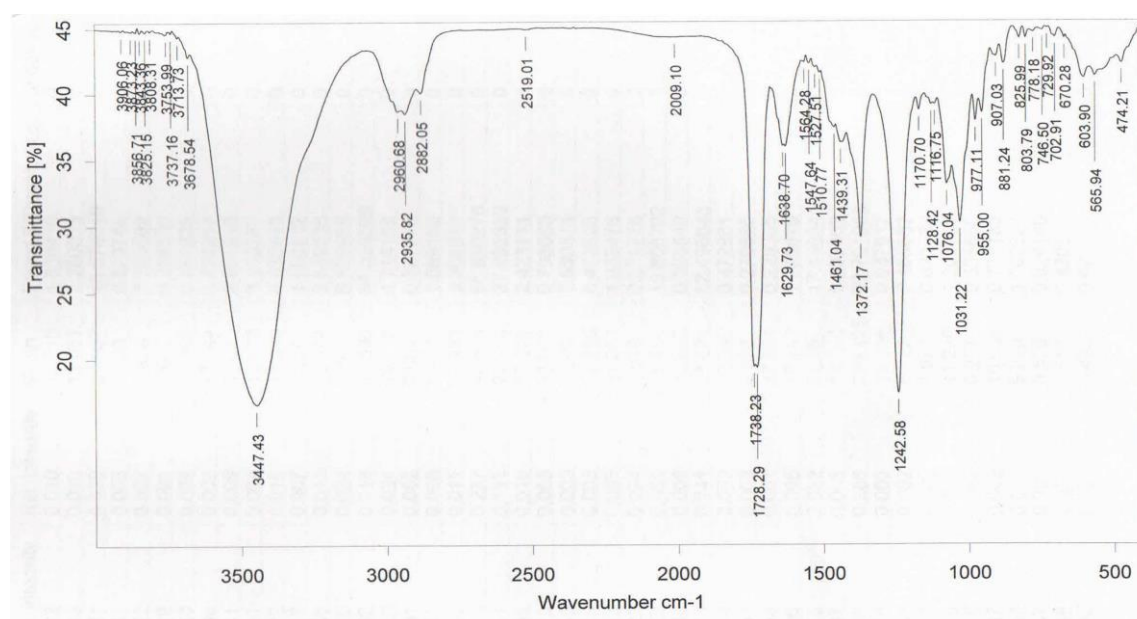
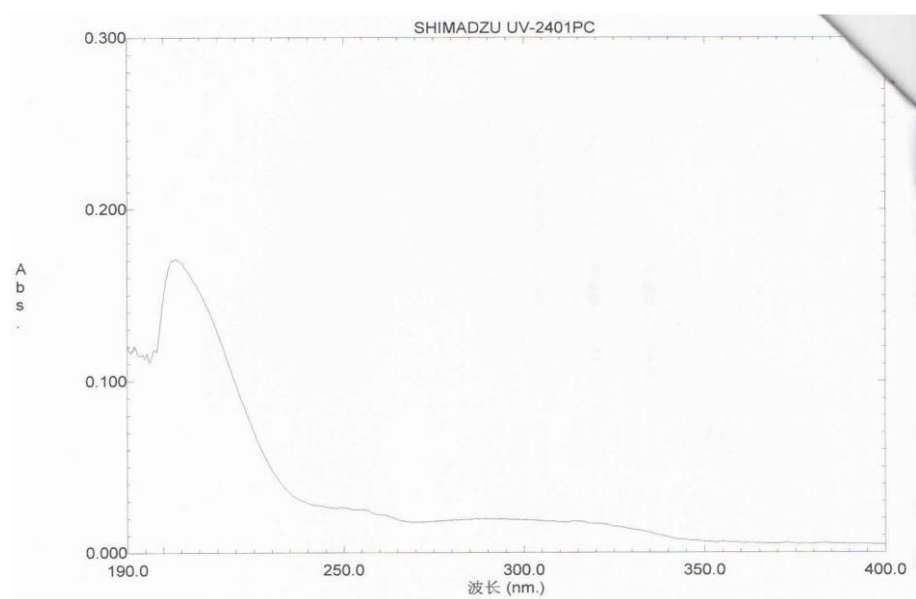


Figure 56. UV and IR spectra of bistenuifolin G (7)



For compound 8:

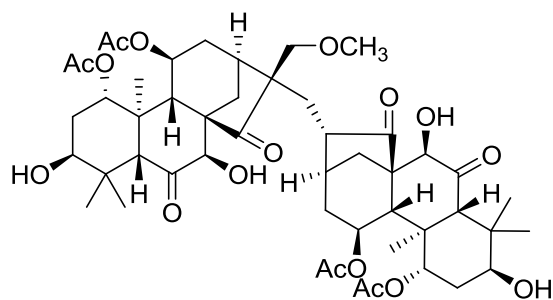


Figure 57. ^1H NMR spectrum of bistenuifolin H (8)

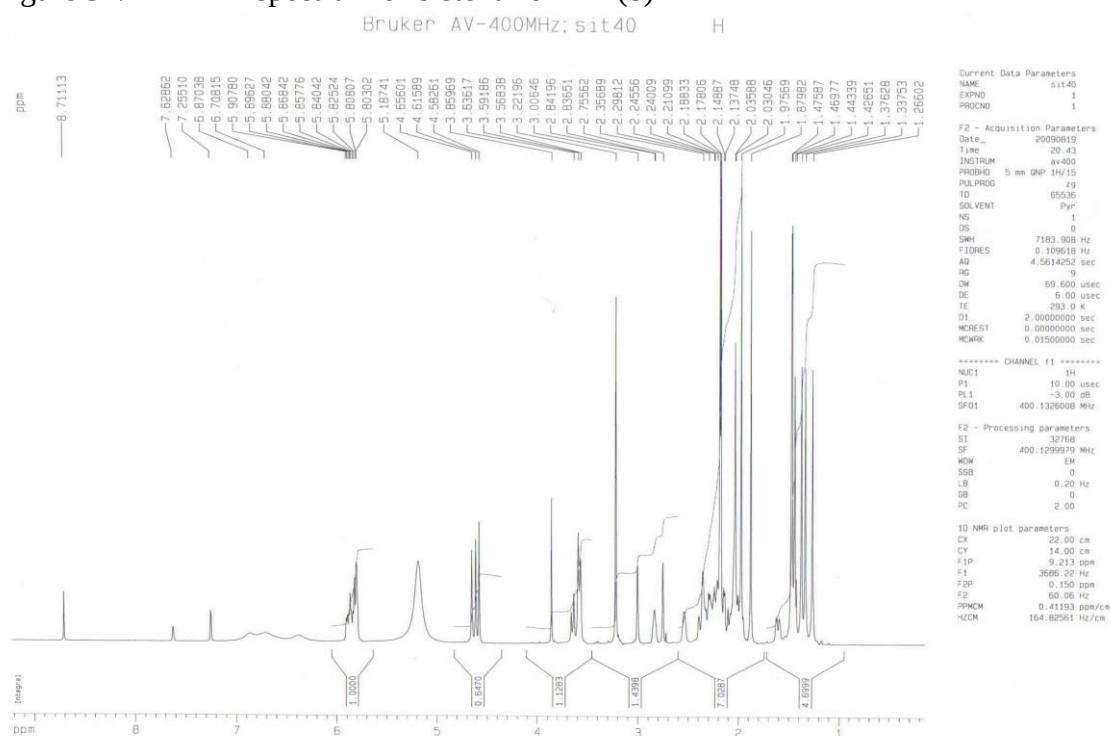


Figure 58. ^{13}C NMR spectrum of bistenuifolin H (**8**)

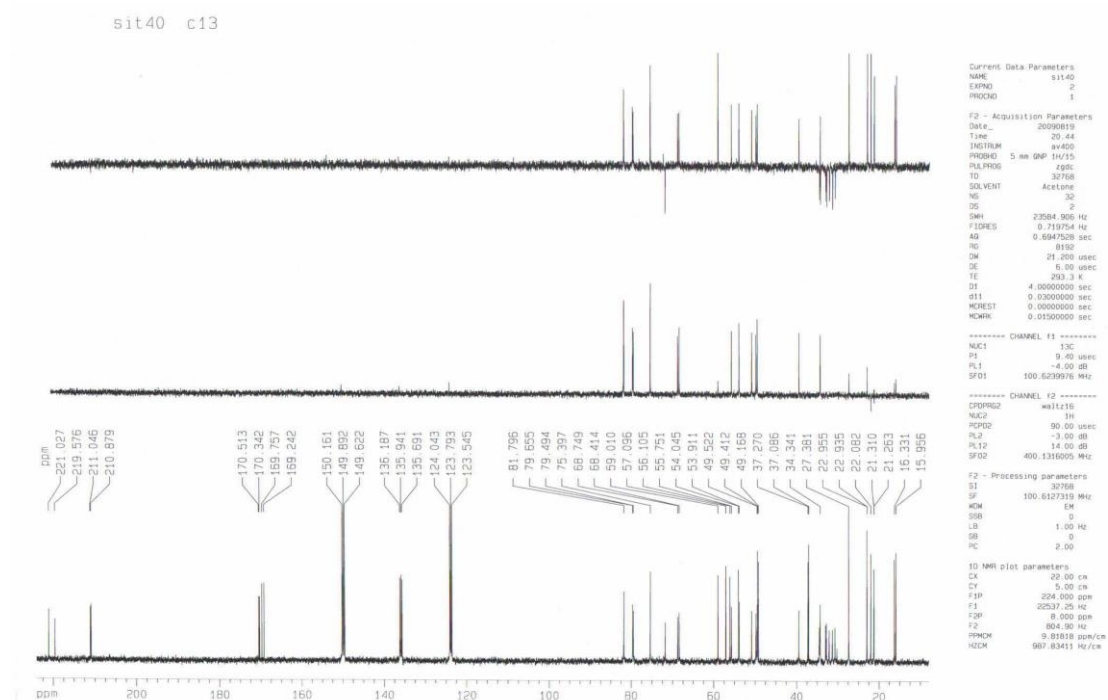
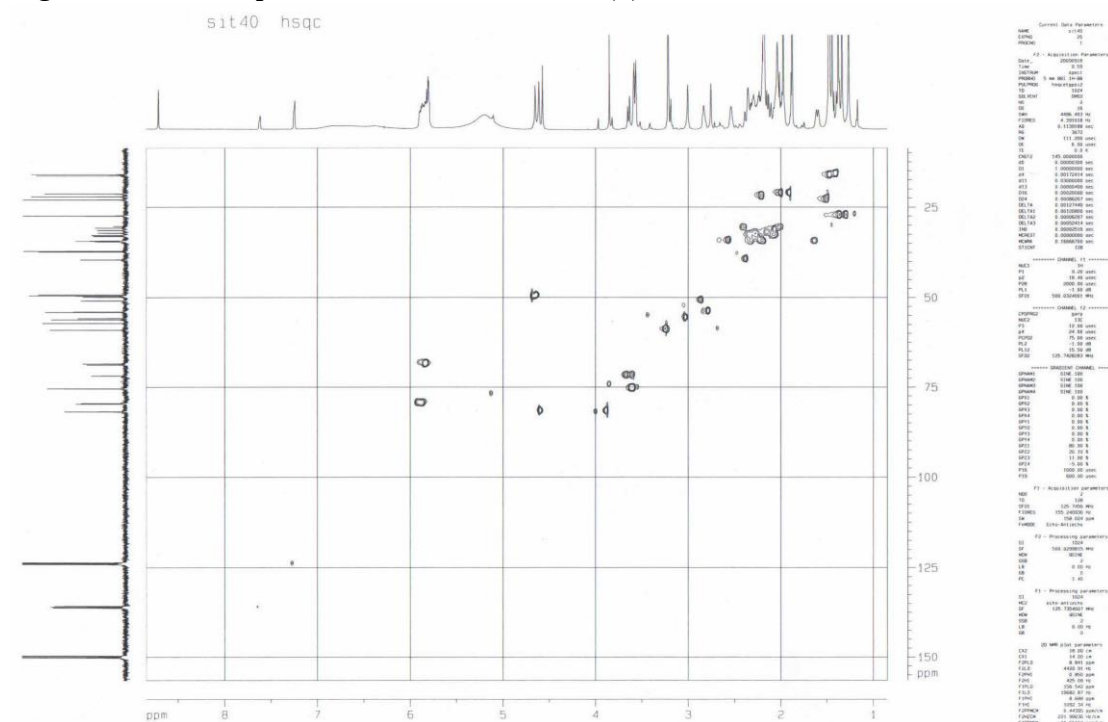


Figure 59. HSQC spectrum of bistenuifolin H (**8**)



sat40 hmbc

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PROCNO	1

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NUC52	1H
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NUC54	1H
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NUC58	1H
NUC59	13C

sit40 cosy

NAME sit40
EXPNO 2
PROCNO 1

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AQ 0.118189 sec
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DE 0.000000 sec
TE 300.2 K
DO 0.0000300 sec
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d13 0.00000000 sec
d19 0.00000000 sec
fno 0.00000001 sec
PCPD1 0.00000000 sec
HEMW 1.00000000 sec

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SFO1 500.1324001 MHz

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GRABMS time 100
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GP9 0.00 %
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FIDRES 35.157787 Hz
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FUNDRC SF

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LB 0.00 Hz
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F1 - Processing parameters
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WDW EPM
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LB 0.00 Hz
GB 0

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CN1 16.00 Hz
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FAPM 0.850 um
FAPL 406.26 Hz
FAPLO 9.015 um
FASLP 406.26 Hz
FAPM 0.771 um
FASLP 406.26 Hz
FAPM 0.44533 um/V
FAPCH 20.21615 mV/A
FAPCH 0.58886 um/V
FAPCH 206.48647 mV/A

Figure 62. ROESY spectrum of bistenuifolin H (8)

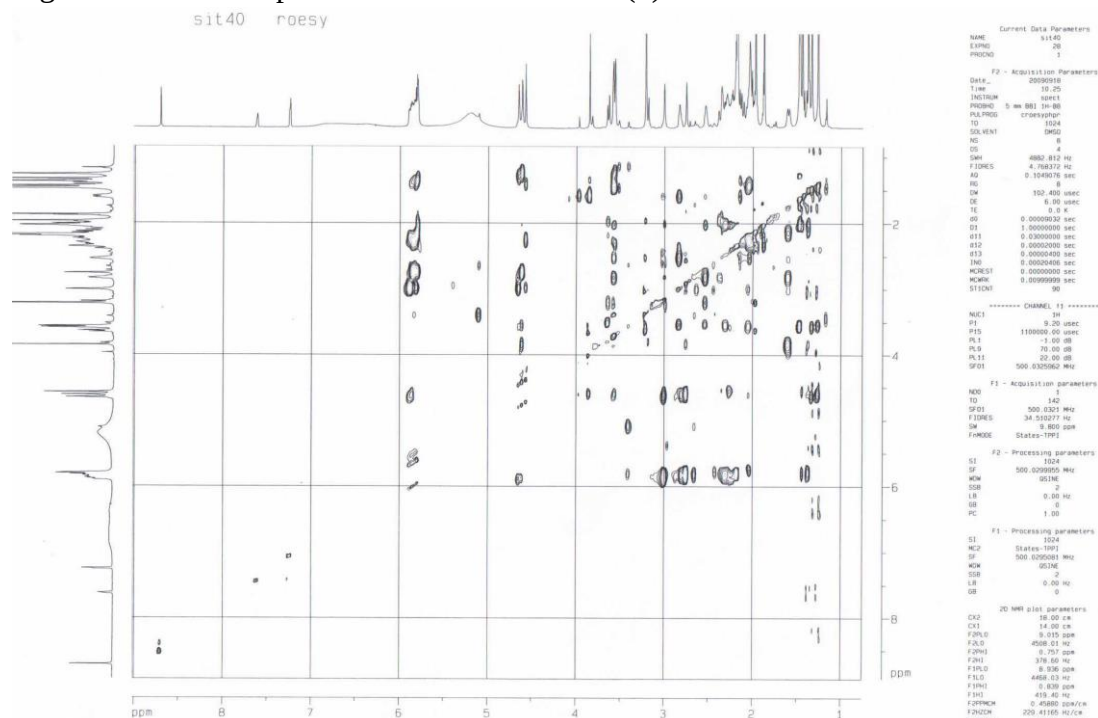
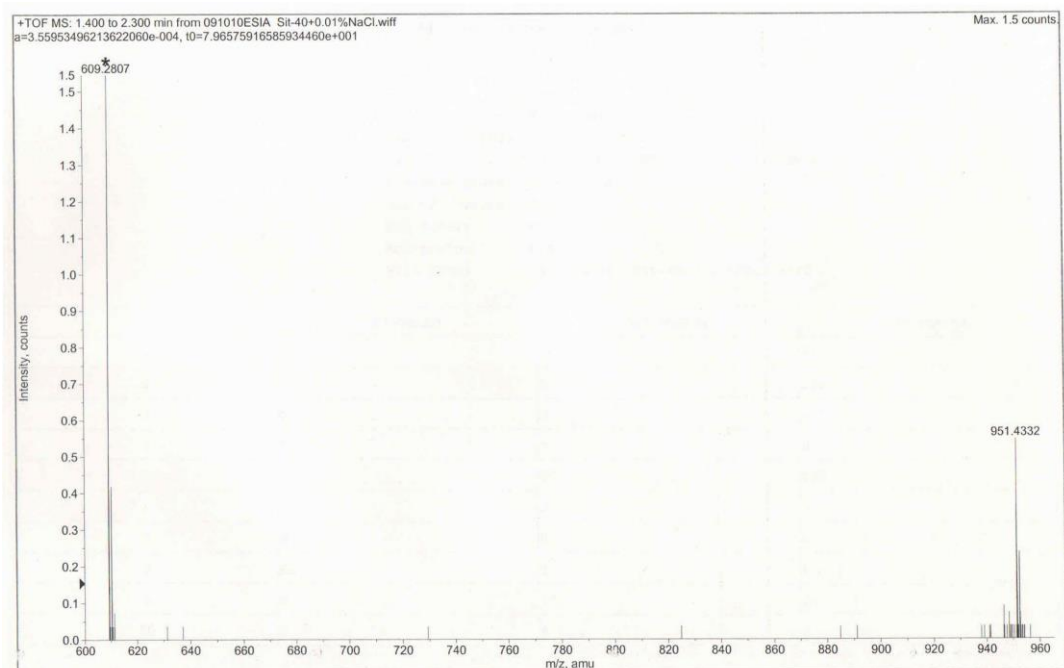
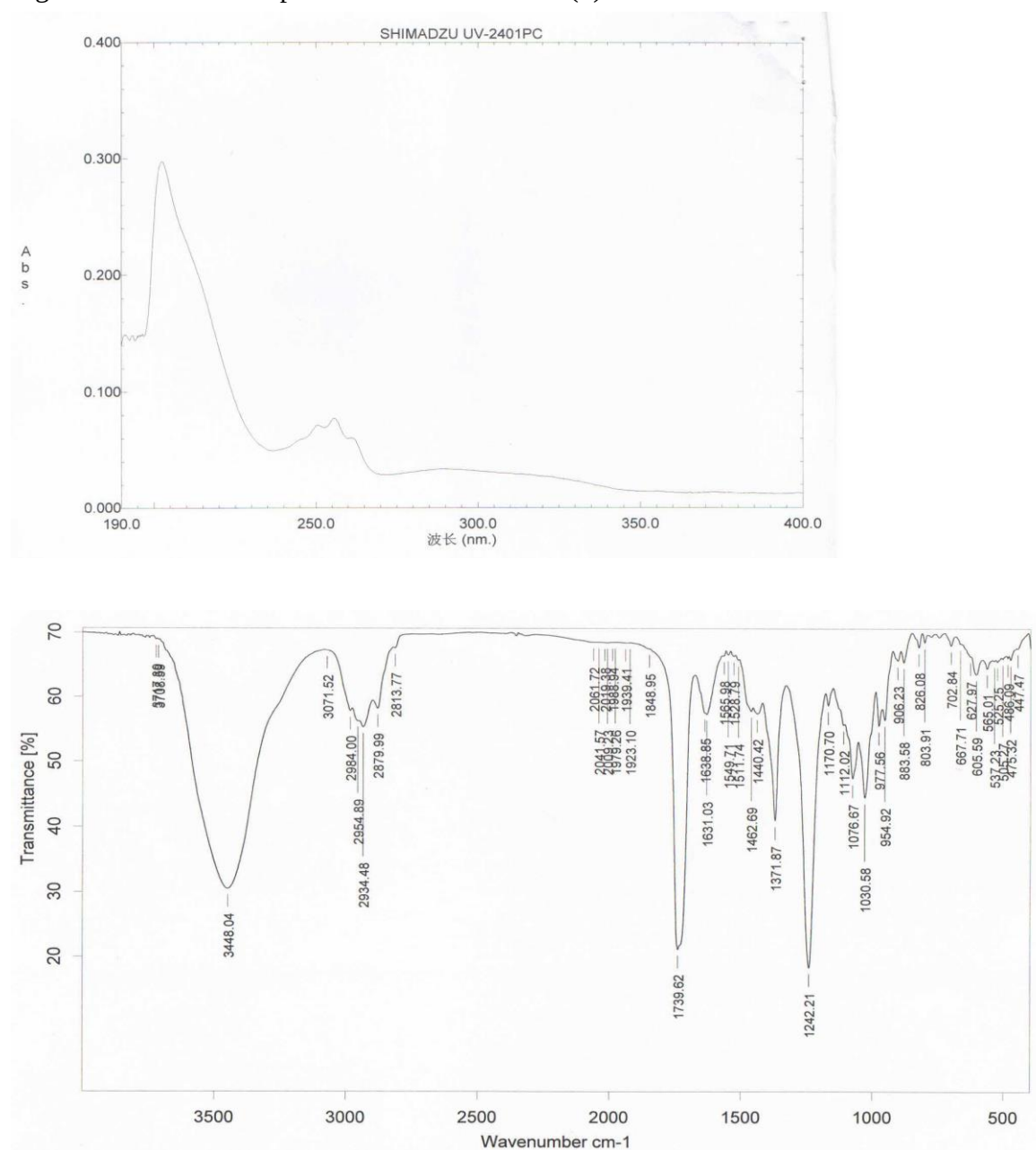


Figure 63. HRESIMS spectrum of bistenuifolin H (8)



	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:

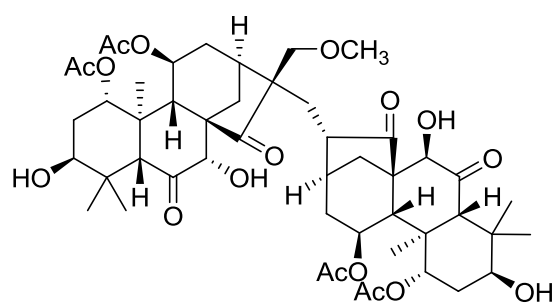


Figure 65. ^1H NMR spectrum of bistenuifolin I (9)

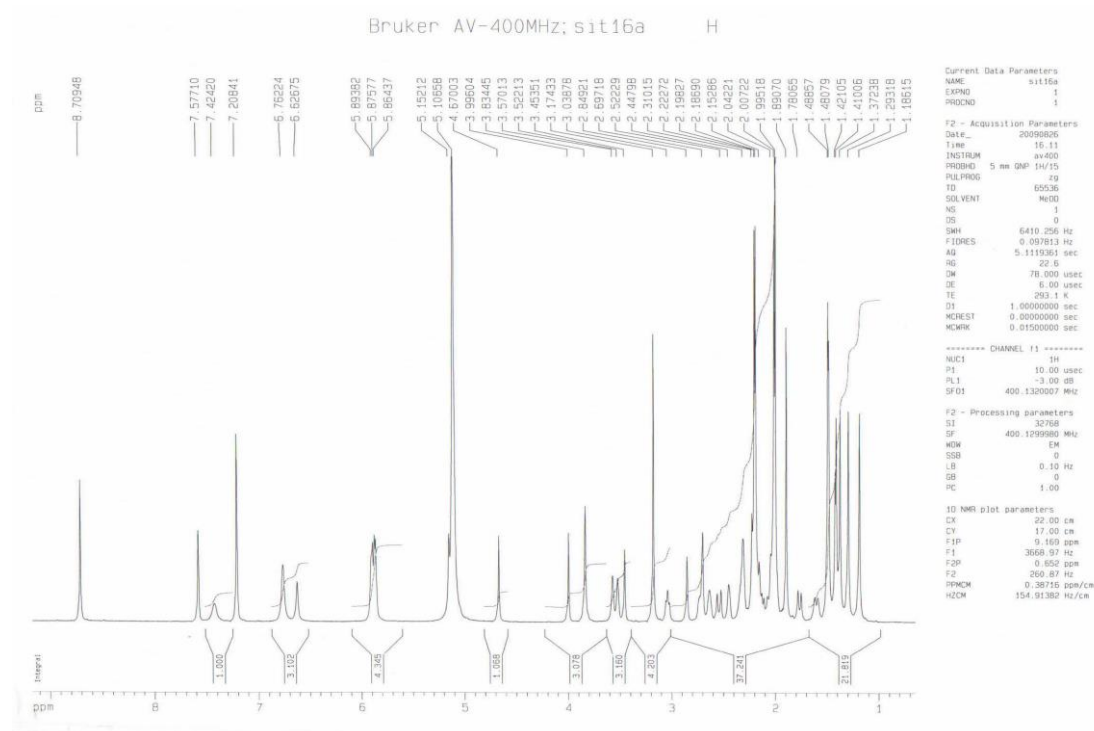


Figure 66. ^{13}C NMR spectrum of bistenuifolin I (9)

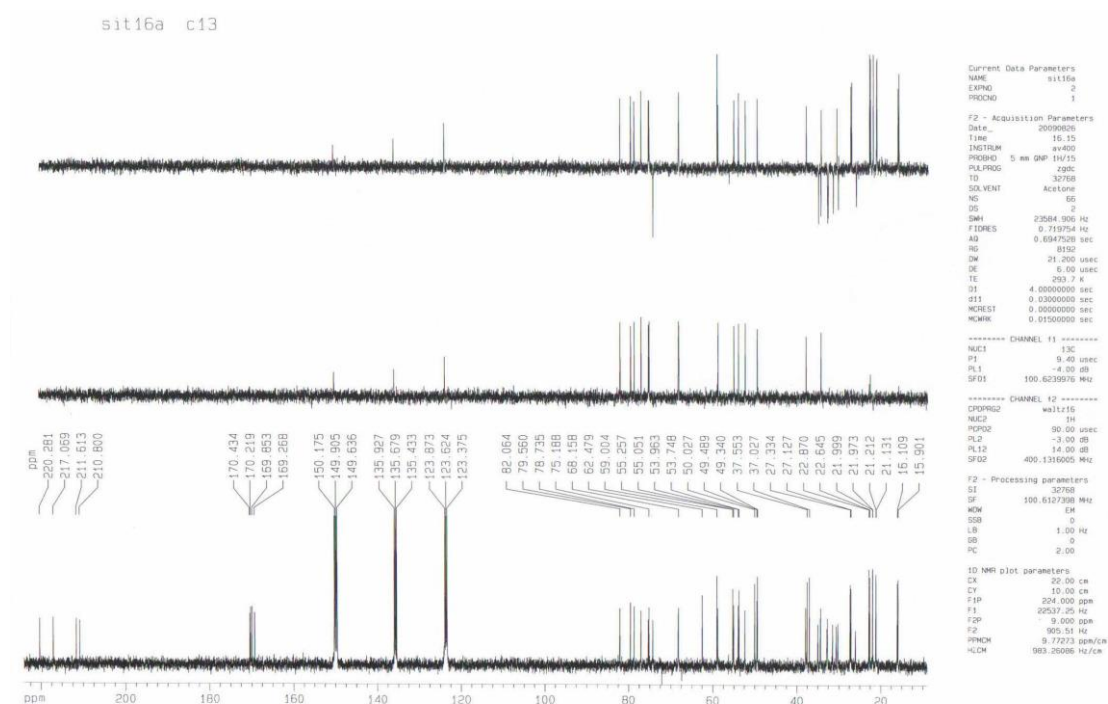
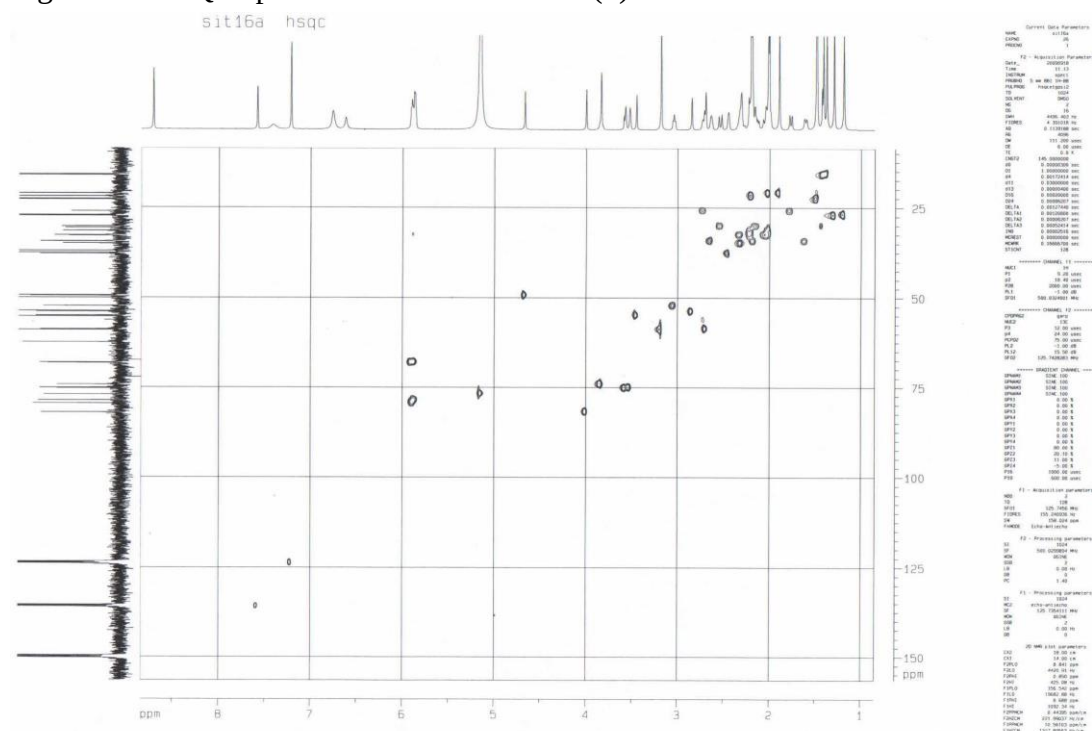


Figure 67. HSQC spectrum of bistenuifolin I (9)



[illegible]

2D COSY NMR spectrum of compound 16a. The x-axis is labeled 'ppm' and ranges from 1 to 9. The y-axis is labeled 'ppm' and ranges from 1 to 9. The plot shows diagonal peaks and off-diagonal cross-peaks indicating scalar coupling between protons. 1D ¹H NMR spectra are projected along the top and left axes. The top spectrum is labeled 'sit16a cosy'.

Current Data Parameters

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EXPNO	25
PROCNO	1

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TD	1328
SOLVENT	pyr
DS	4
TMF	400.453 Hz
FIDRES	4.101010 Hz
AQ	0.191010 sec
RG	111.250 uHz
DE	6.00 uHz
TE	0.2 K
DW	0.0000000 sec
DT	0.0000000 sec
ETD	0.0000000 sec
TEB	0.0000000 sec
IND	0.0000000 sec
MCHEST	0.0000000 sec
MCHEM	1.0000000 sec

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PL3	-1.00 uHz
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******* GRABF1 CHANNEL *******

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QPMW35	0.00 Hz
QPMW36	0.00 Hz
QPMW37	0.00 Hz
QPMW38	0.00 Hz
QPMW39	0.00 Hz
QPMW40	0.00 Hz
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QPMW44	0.00 Hz
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QPMW47	0.00 Hz
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QPMW86	0.00 Hz
QPMW87	0.00 Hz
QPMW88	0.00 Hz
QPMW89	0.00 Hz
QPMW90	0.00 Hz
QPMW91	0.00 Hz
QPMW92	0.00 Hz
QPMW93	0.00 Hz
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QPMW95	0.00 Hz
QPMW96	0.00 Hz
QPMW97	0.00 Hz
QPMW98	0.00 Hz
QPMW99	0.00 Hz
QPMW100	0.00 Hz

F1 - Acquisition parameters

NUC1	13C
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PL3	500.000000 MHz
QF1	500.000000 MHz
QF3	20.127777 MHz
SW	0.000000 MHz
FWHM	0.000000 MHz

F2 - Processing parameters

SI	1328
SF	500.000000 MHz
WDW	EM
SSB	0.00 MHz
LB	0.00 MHz
GB	0.00 MHz
PC	1.00

F1 - Processing parameters

SI	1328
SF	500.000000 MHz
WDW	EM
SSB	0.00 MHz
LB	0.00 MHz
GB	0.00 MHz
PC	1.00

2D NMR plot parameters

EX1	10.00 uHz
EX2	10.00 uHz
EX3	

Figure 70. ROESY spectrum of bistenuifolin I (9)

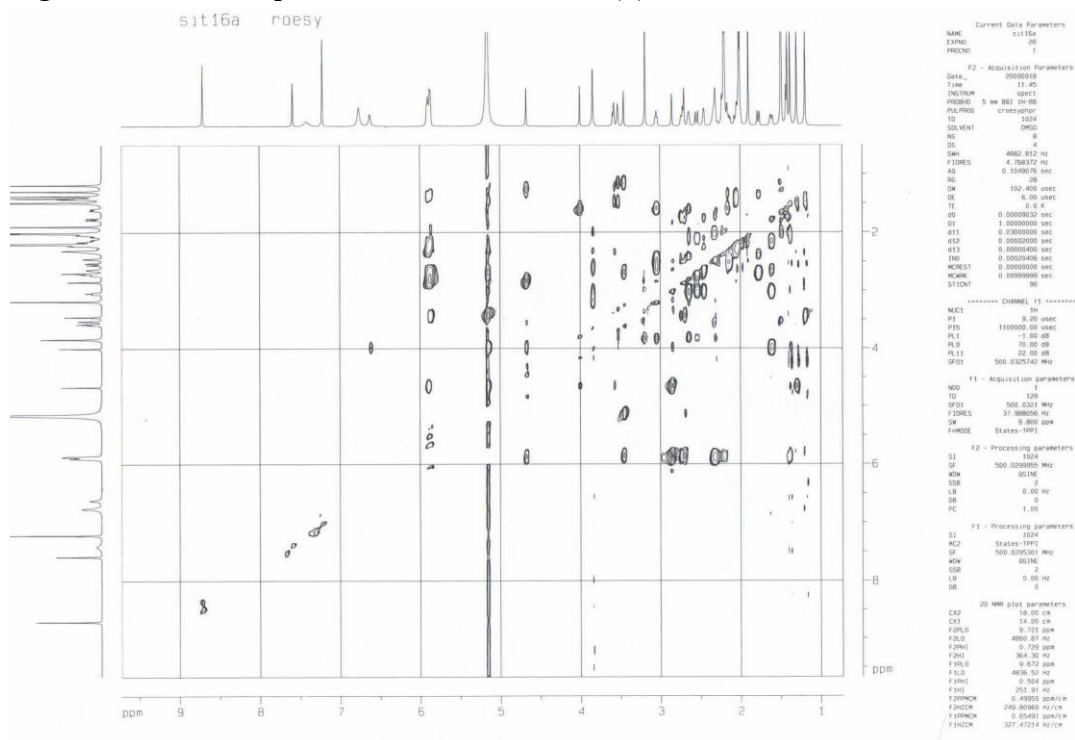


Figure 71. HRESIMS spectrum of bistenuifolin I (9)

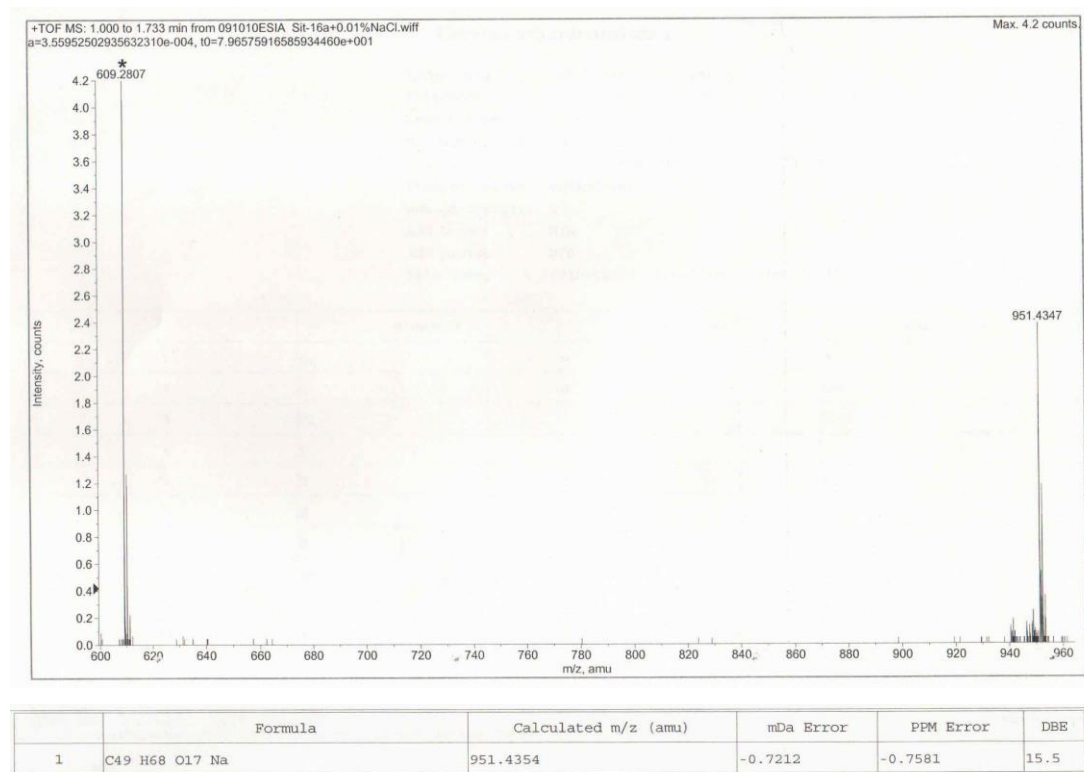
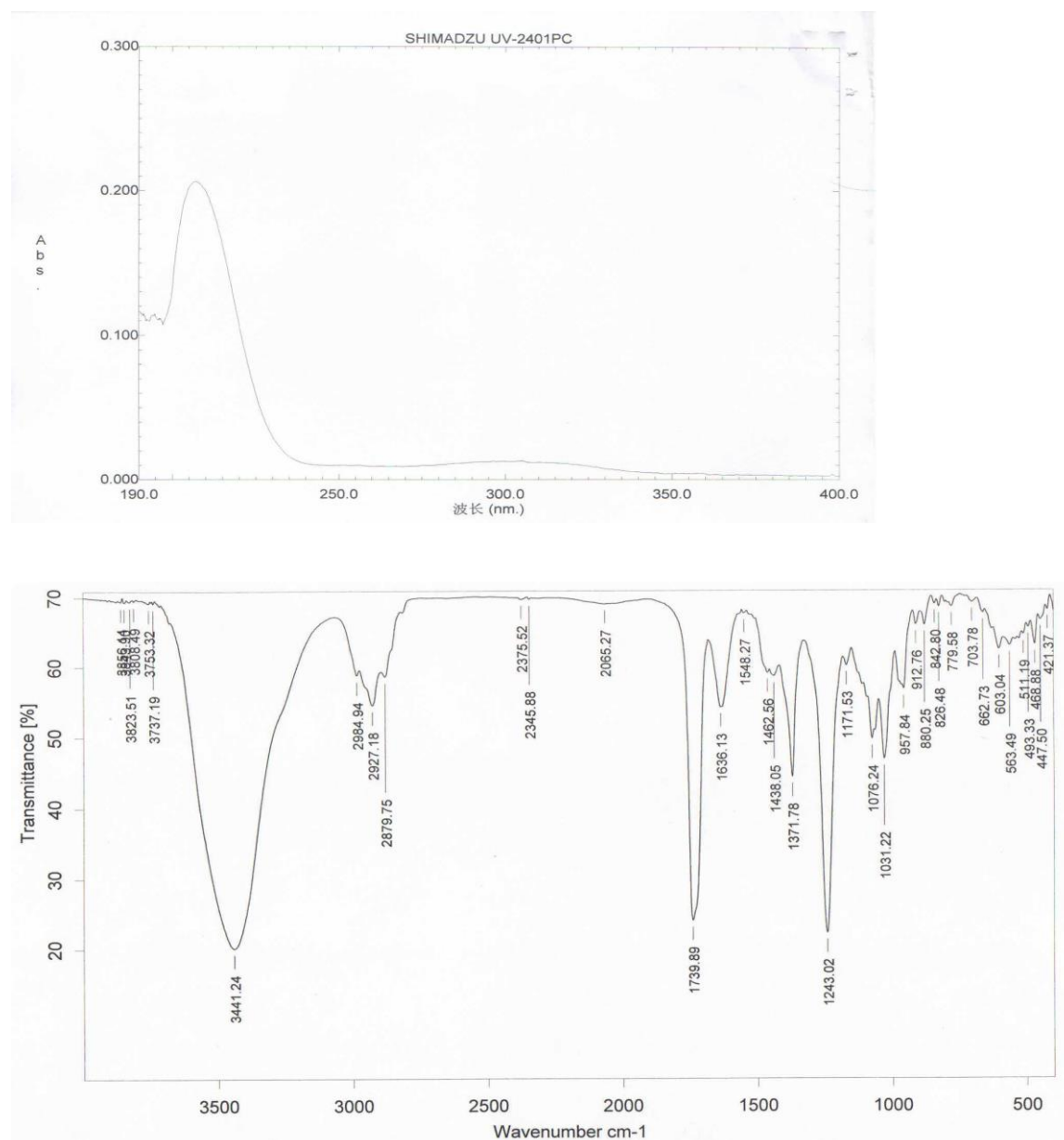


Figure 72. UV and IR spectra of bistenuifolin I (9)



For compound 10:

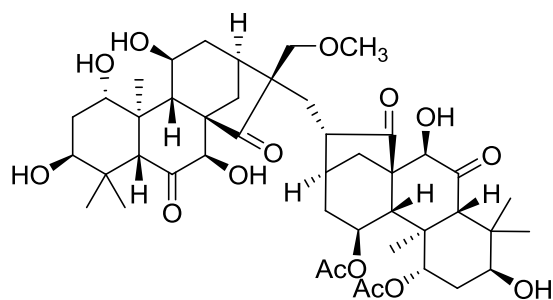


Figure 73. ^1H NMR spectrum of bistenuifolin J (**10**)

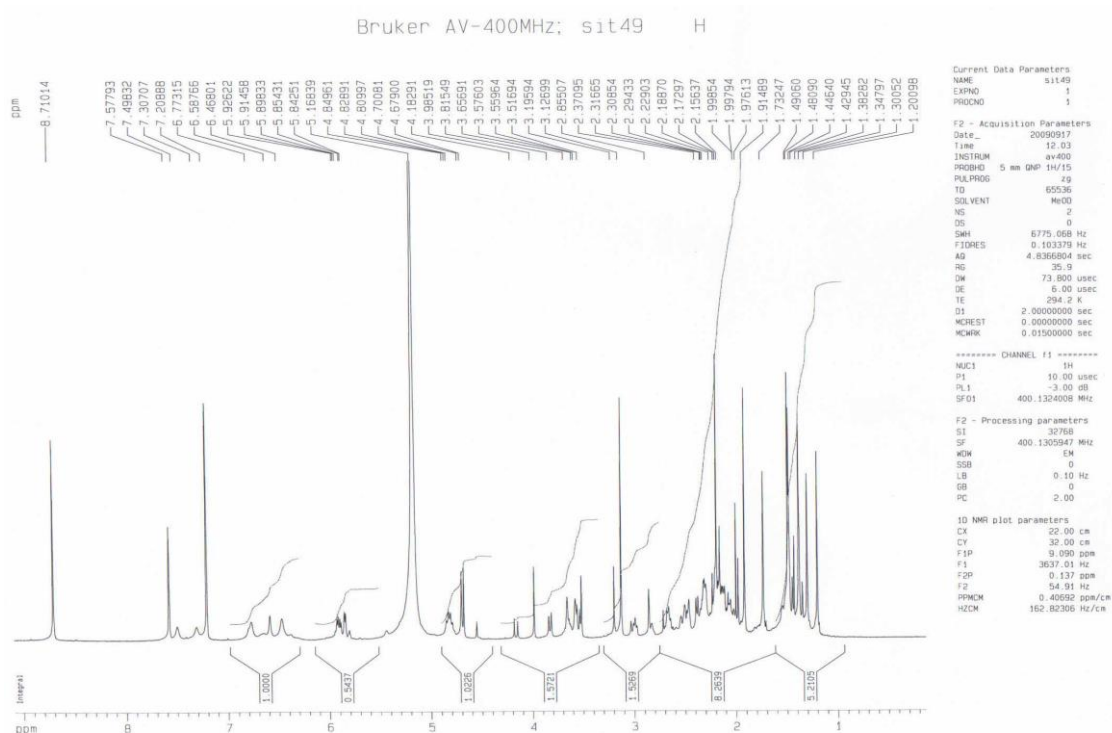


Figure 74. ^{13}C NMR spectrum of bistenuifolin J (10)

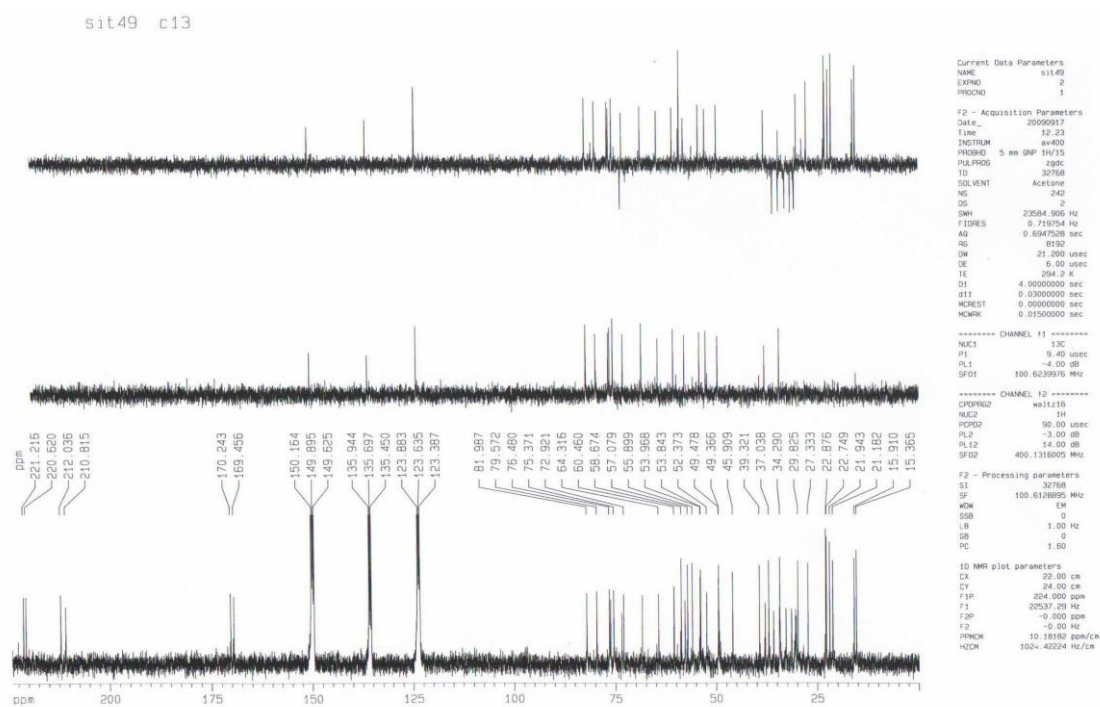
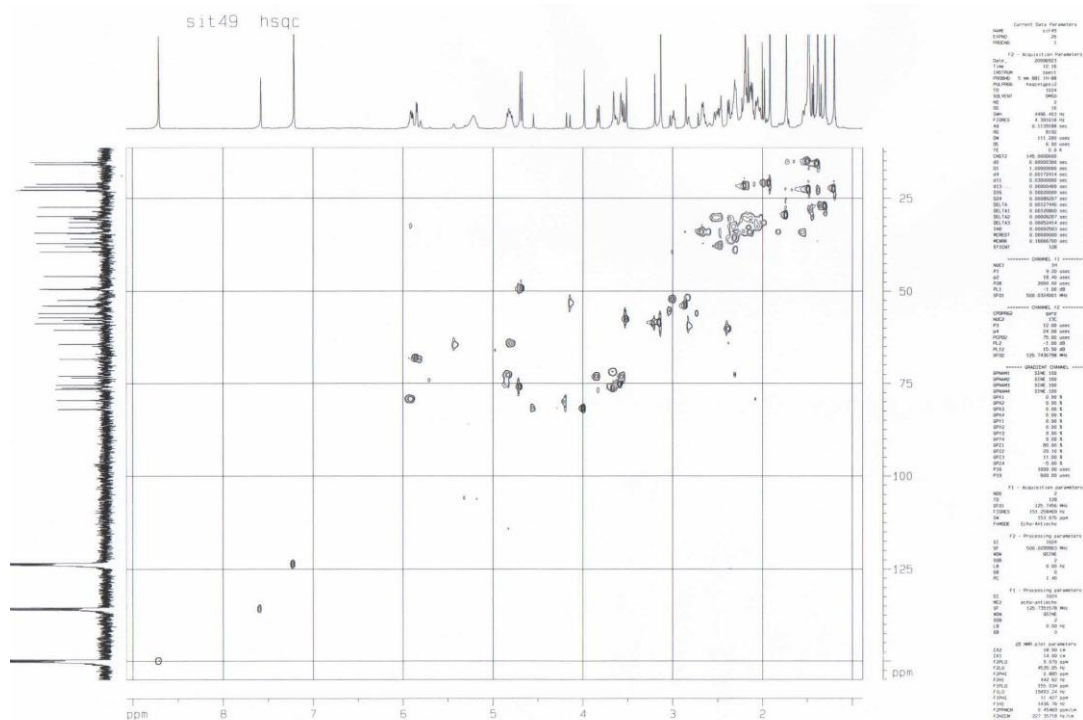


Figure 75. HSQC spectrum of bistenuifolin J (10)



5pt4 data hmbc

Current Data Parameters

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EXPNO     2
PROCNO    1
F2 - Acquisition Parameters
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Time      12.32
INSTRUM   spect
PROBHD    5 mm BBO 1H-13
PULPROG   zgpg30
TD         65536
SOLVENT   H2O
NS         2048
DS         4
SS         10
AQ         0.000180000
RG          32
FIDRES    0.000180000
AQRES     0.000180000
RGRES     0.000180000
F2 - Processing parameters
SI         32768
SF          500.136
WDW         EM
SSB         0
LB          3.00
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PC          1.00
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PC92        0.000000000
PC93        0.000000000
PC94        0.000000000
PC95        0.000000000
PC96        0.000000000
PC97        0.000000000
PC98        0.000000000
PC99        0.000000000
PC100       0.000000000

```

14a

1H NMR (400 MHz, CDCl₃)

Chemical structure of 14a: CC1=CC=C(C=C1)C(=O)N2C(=O)C(=O)N2C3=CC=CC=C3

1D Spectrum (Top):

- 8.0 ppm (s, 1H)
- 7.5 ppm (s, 1H)
- 7.4 ppm (s, 1H)
- 7.3 ppm (s, 1H)
- 7.2 ppm (s, 1H)
- 7.1 ppm (s, 1H)
- 7.0 ppm (s, 1H)
- 6.9 ppm (s, 1H)
- 6.8 ppm (s, 1H)
- 6.7 ppm (s, 1H)
- 6.6 ppm (s, 1H)
- 6.5 ppm (s, 1H)
- 6.4 ppm (s, 1H)
- 6.3 ppm (s, 1H)
- 6.2 ppm (s, 1H)
- 6.1 ppm (s, 1H)
- 6.0 ppm (s, 1H)
- 5.9 ppm (s, 1H)
- 5.8 ppm (s, 1H)
- 5.7 ppm (s, 1H)
- 5.6 ppm (s, 1H)
- 5.5 ppm (s, 1H)
- 5.4 ppm (s, 1H)
- 5.3 ppm (s, 1H)
- 5.2 ppm (s, 1H)
- 5.1 ppm (s, 1H)
- 5.0 ppm (s, 1H)
- 4.9 ppm (s, 1H)
- 4.8 ppm (s, 1H)
- 4.7 ppm (s, 1H)
- 4.6 ppm (s, 1H)
- 4.5 ppm (s, 1H)
- 4.4 ppm (s, 1H)
- 4.3 ppm (s, 1H)
- 4.2 ppm (s, 1H)
- 4.1 ppm (s, 1H)
- 4.0 ppm (s, 1H)
- 3.9 ppm (s, 1H)
- 3.8 ppm (s, 1H)
- 3.7 ppm (s, 1H)
- 3.6 ppm (s, 1H)
- 3.5 ppm (s, 1H)
- 3.4 ppm (s, 1H)
- 3.3 ppm (s, 1H)
- 3.2 ppm (s, 1H)
- 3.1 ppm (s, 1H)
- 3.0 ppm (s, 1H)
- 2.9 ppm (s, 1H)
- 2.8 ppm (s, 1H)
- 2.7 ppm (s, 1H)
- 2.6 ppm (s, 1H)
- 2.5 ppm (s, 1H)
- 2.4 ppm (s, 1H)
- 2.3 ppm (s, 1H)
- 2.2 ppm (s, 1H)
- 2.1 ppm (s, 1H)
- 2.0 ppm (s, 1H)
- 1.9 ppm (s, 1H)
- 1.8 ppm (s, 1H)
- 1.7 ppm (s, 1H)
- 1.6 ppm (s, 1H)
- 1.5 ppm (s, 1H)
- 1.4 ppm (s, 1H)
- 1.3 ppm (s, 1H)
- 1.2 ppm (s, 1H)
- 1.1 ppm (s, 1H)
- 1.0 ppm (s, 1H)
- 0.9 ppm (s, 1H)
- 0.8 ppm (s, 1H)
- 0.7 ppm (s, 1H)
- 0.6 ppm (s, 1H)
- 0.5 ppm (s, 1H)
- 0.4 ppm (s, 1H)
- 0.3 ppm (s, 1H)
- 0.2 ppm (s, 1H)
- 0.1 ppm (s, 1H)

2D Correlation Plot (Bottom):

- Diagonal peaks: 1D spectrum.
- Off-diagonal cross-peaks: Correlations between protons.
- Strong correlations in the aromatic region (6-8 ppm).
- Correlations in the aliphatic region (1-4 ppm).

Figure 78. ROESY spectrum of bistenuifolin J (10)

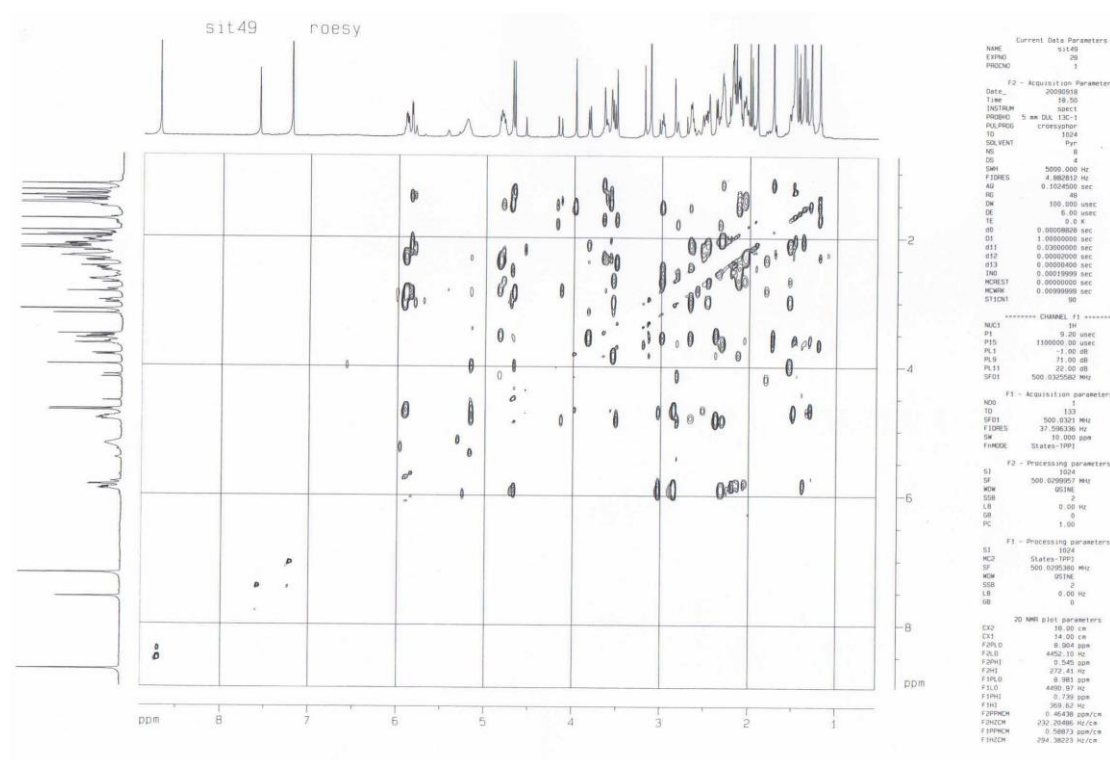
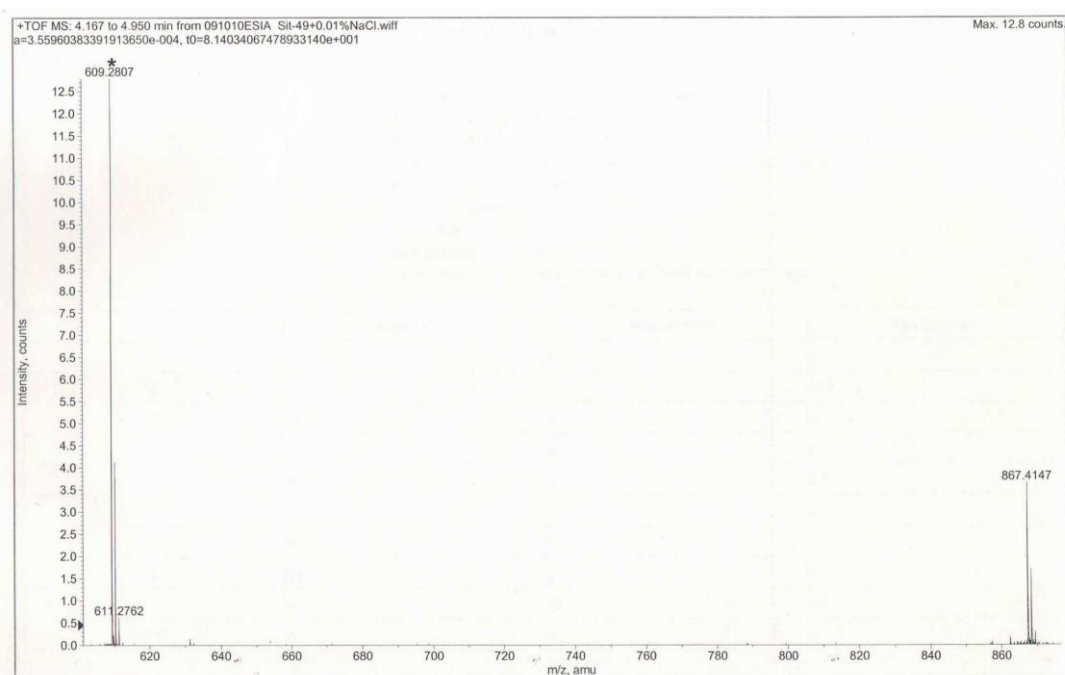
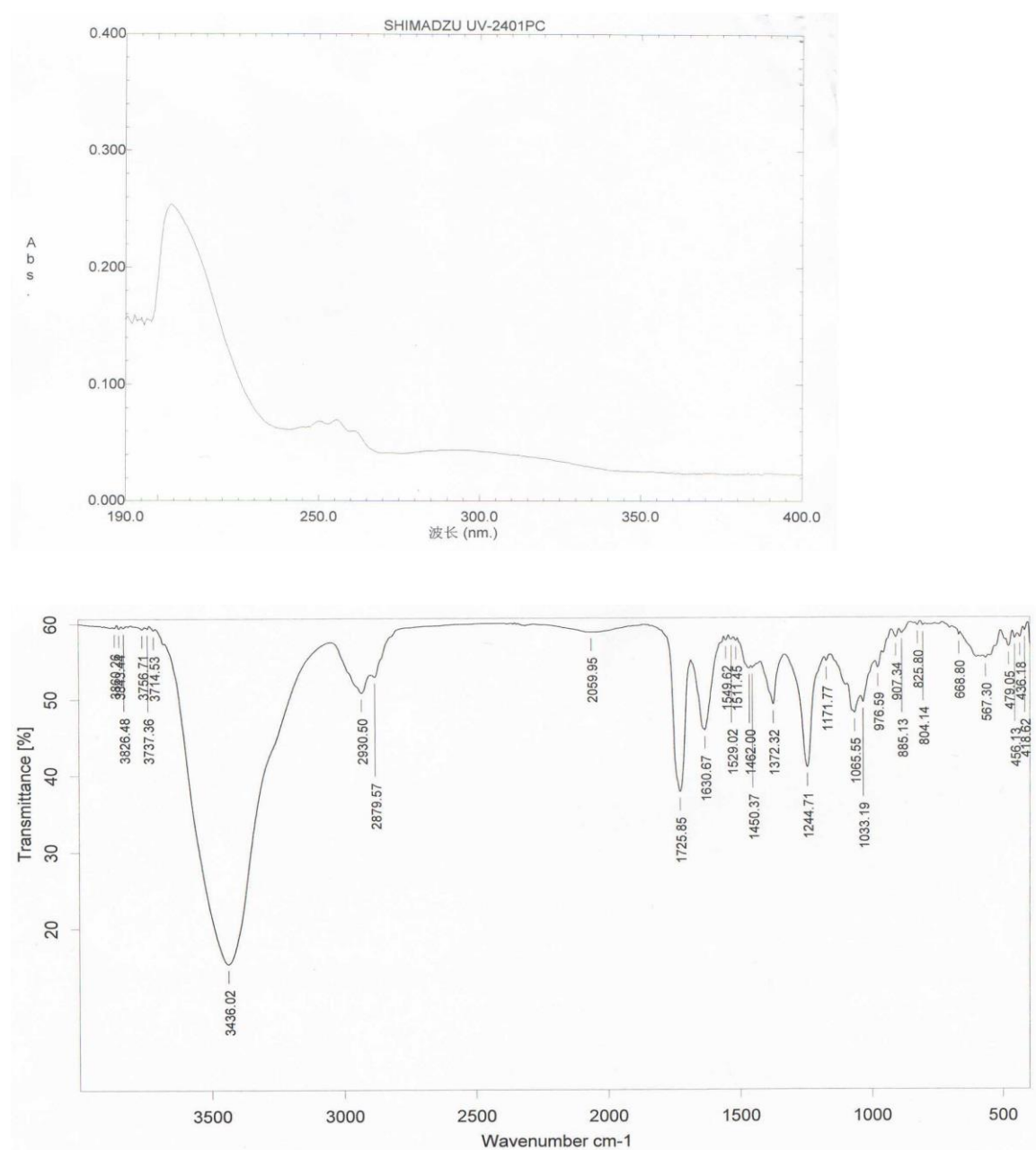


Figure 79. HRESIMS spectrum of bistenuifolin J (10)



	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C ₄₅ H ₆₄ O ₁₅ Na	867.4142	0.4081	0.4705	13.5

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



For compound 11:

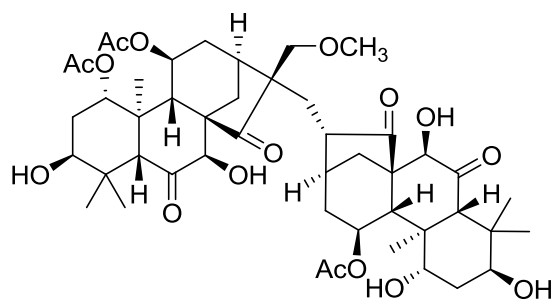


Figure 81. ^1H NMR spectrum of bistenuifolin K (**11**)

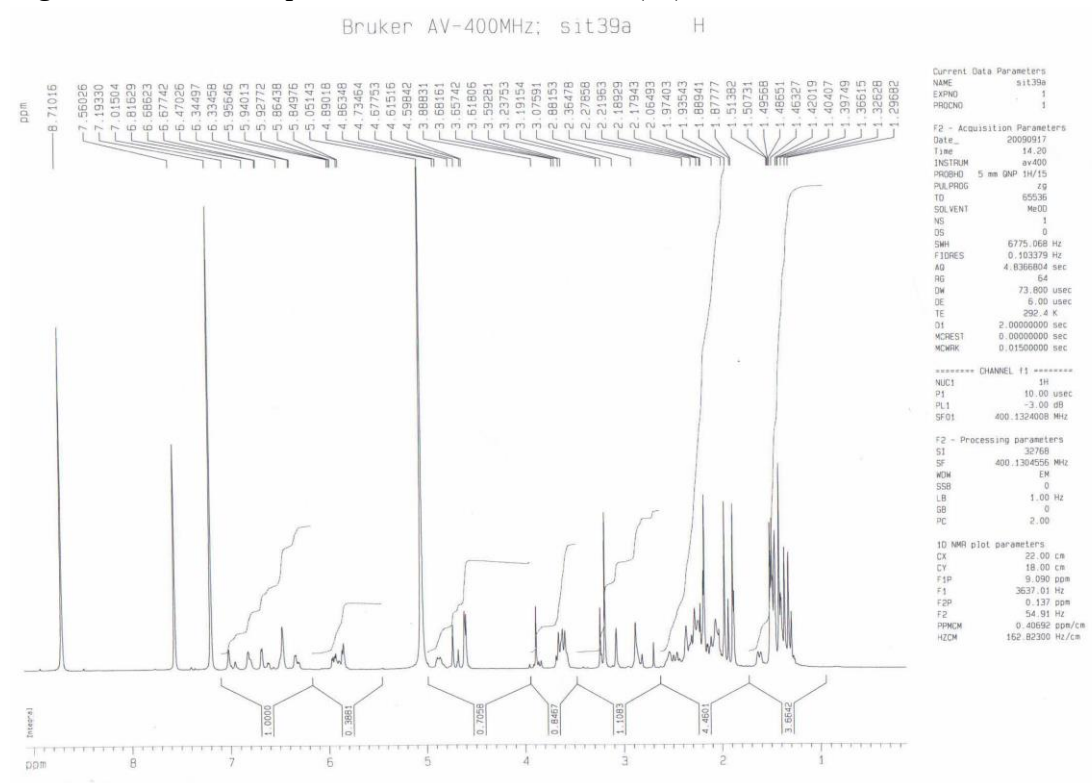


Figure 82. ^{13}C NMR spectrum of bistenuifolin K (**11**)

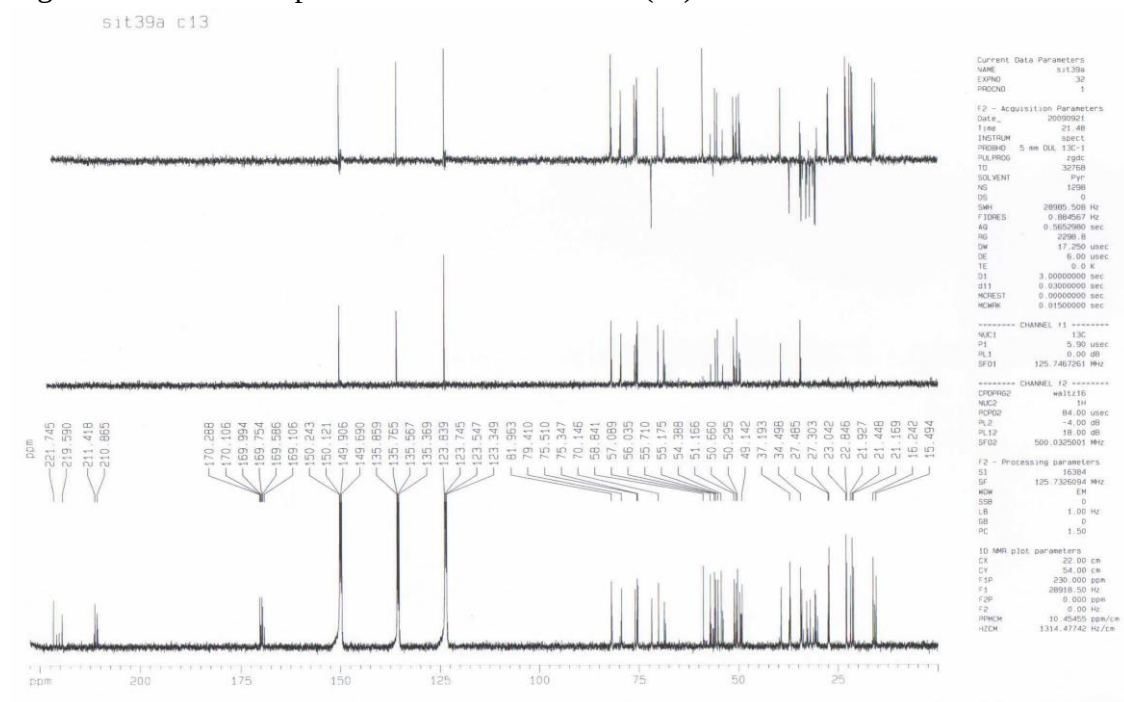


Figure 83. HSQC spectrum of bistenuifolin K (**11**)

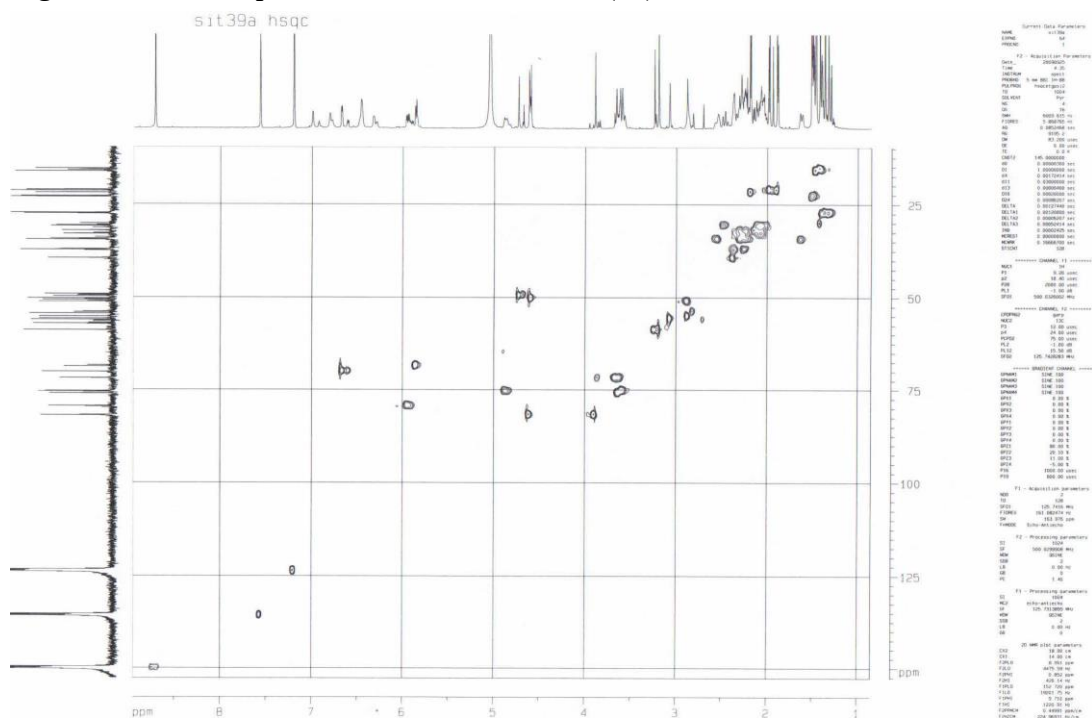


Figure 84. HMBC spectrum of bistenuifolin K (11)

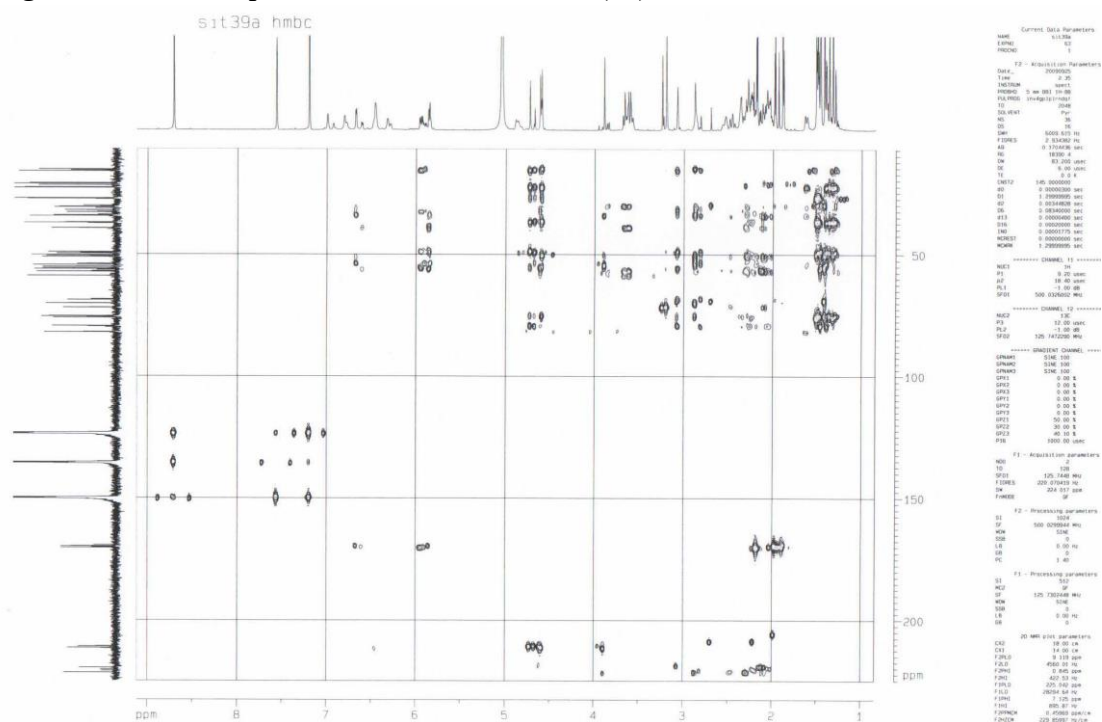


Figure 85. COSY spectrum of bistenuifolin K (11)

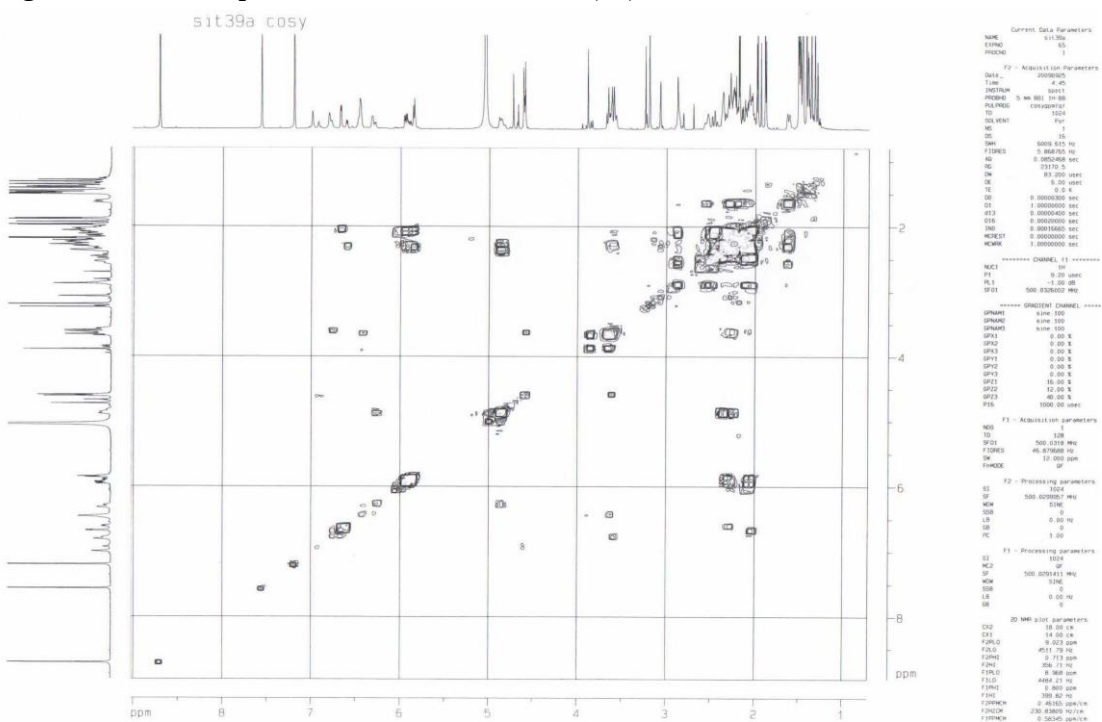


Figure 86. ROESY spectrum of bistenuifolin K (11)

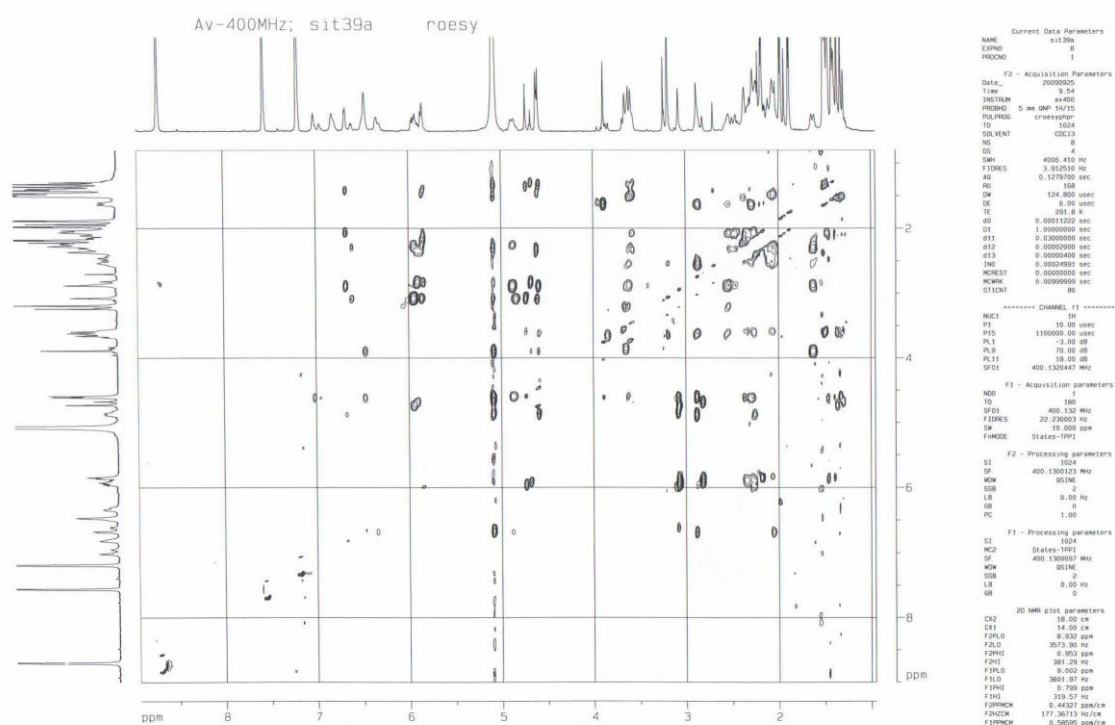
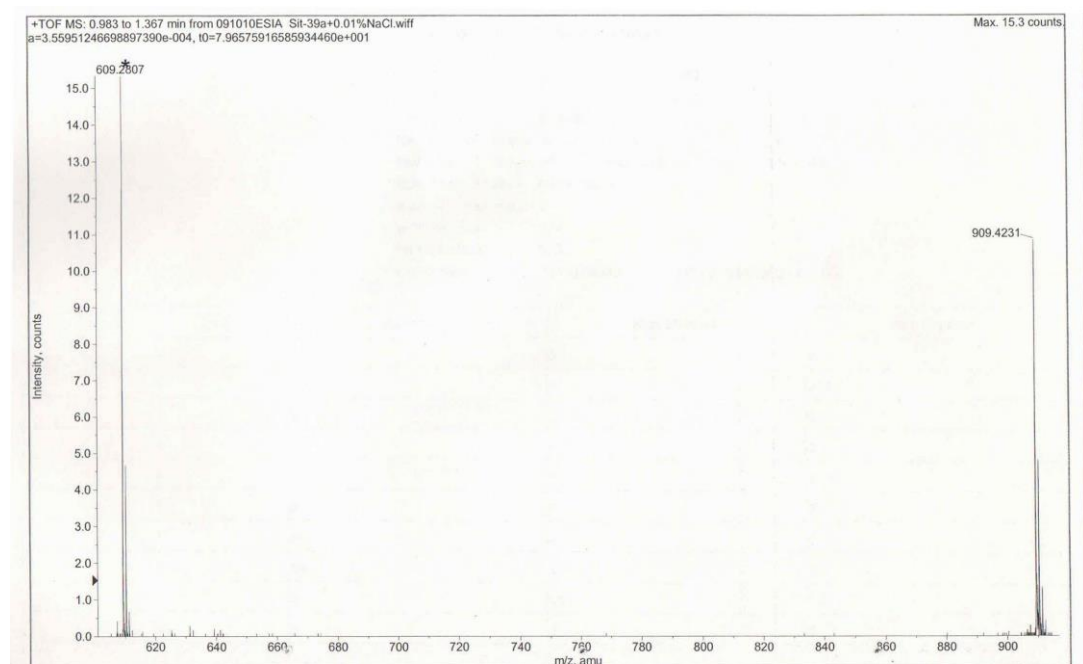
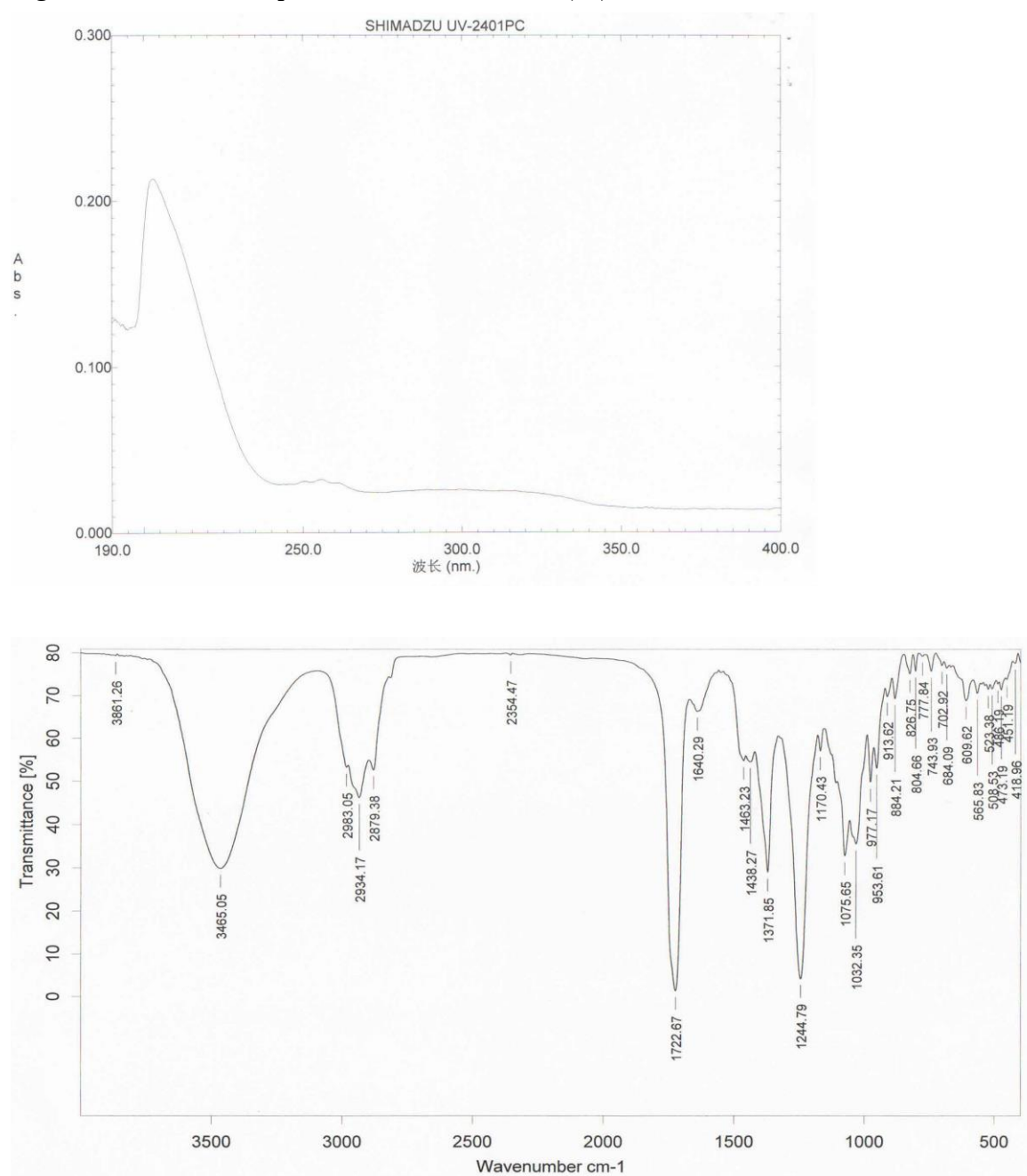


Figure 87. HRESIMS spectrum of bistenuifolin K (11)



	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:

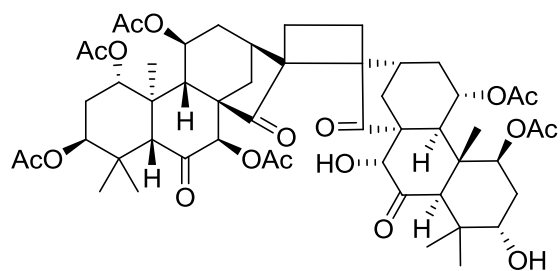


Figure 89. ^1H NMR spectrum of bistenuifolin L (12)

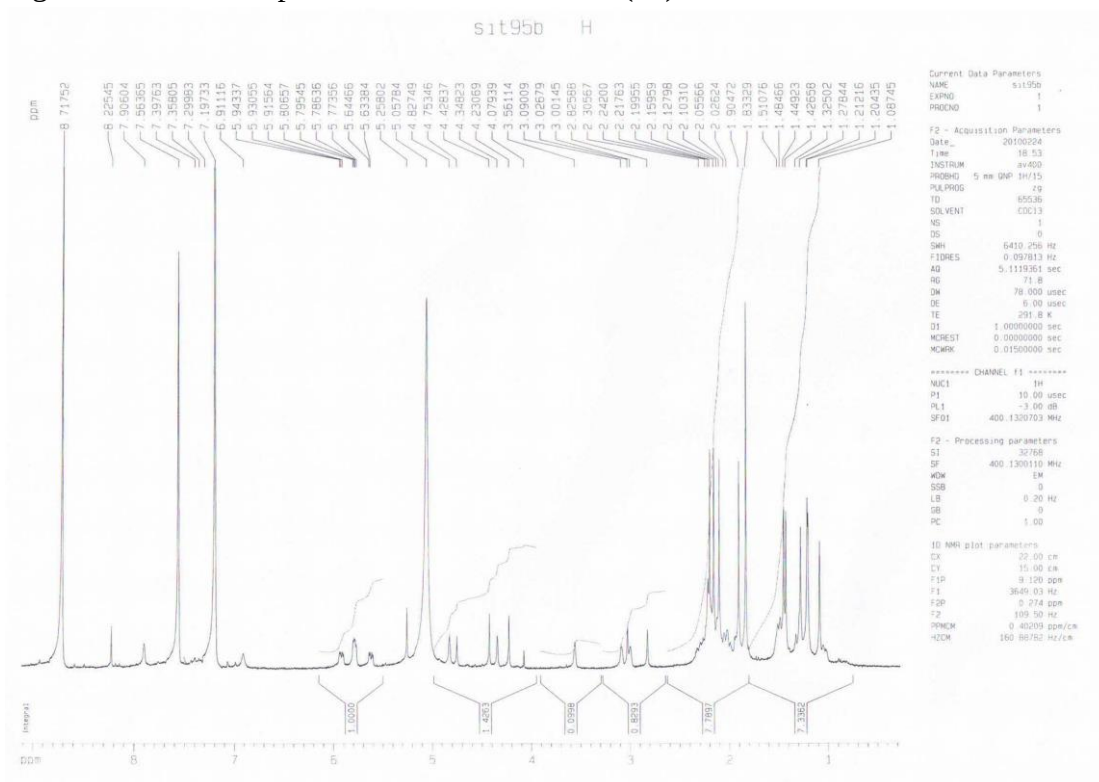


Figure 90. ^{13}C NMR spectrum of bistenuifolin L (12)

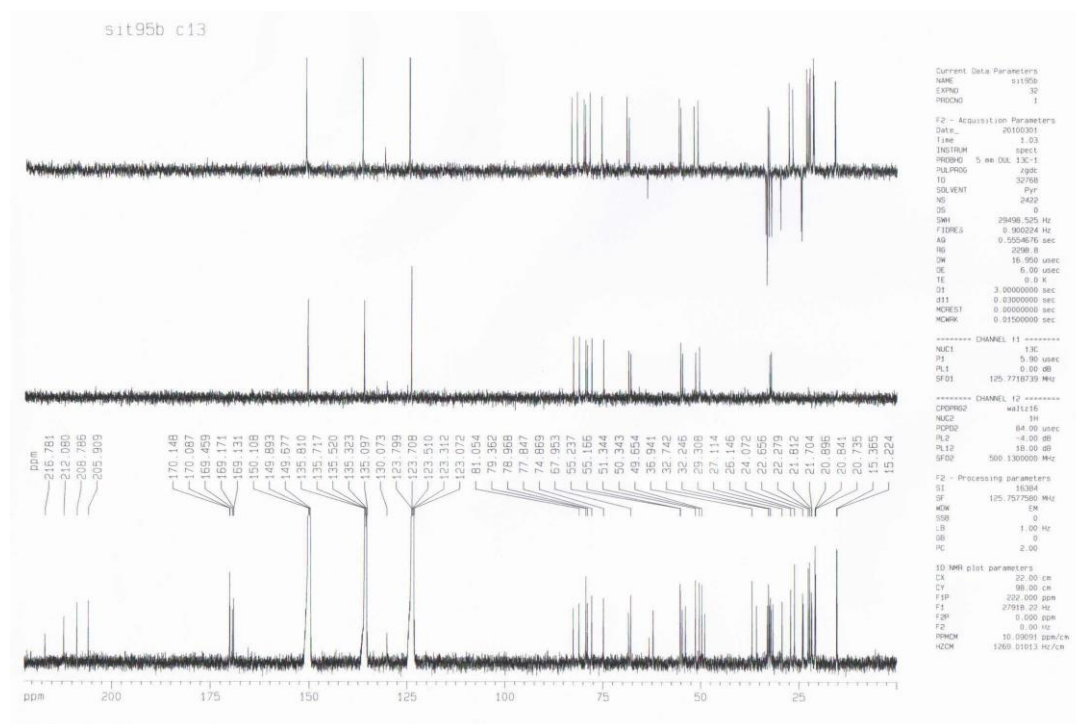
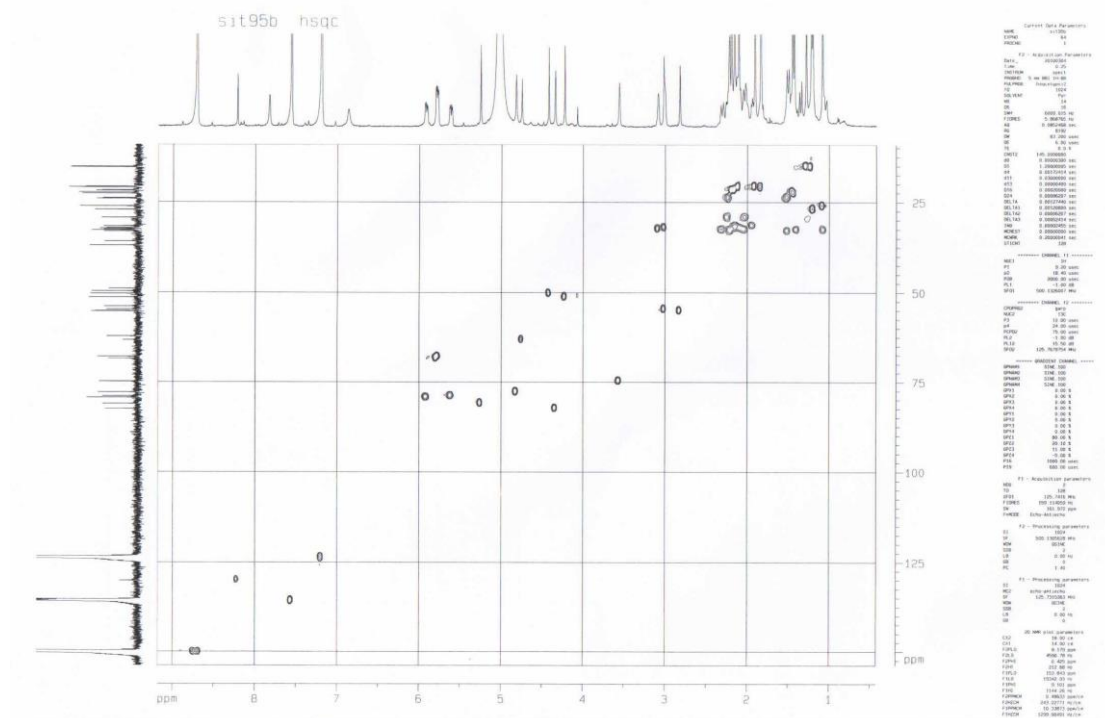


Figure 91. HSQC spectrum of bistenuifolin L (12)



[illegible][illegible]

Figure 94. ROESY spectrum of bistenuifolin L (12)

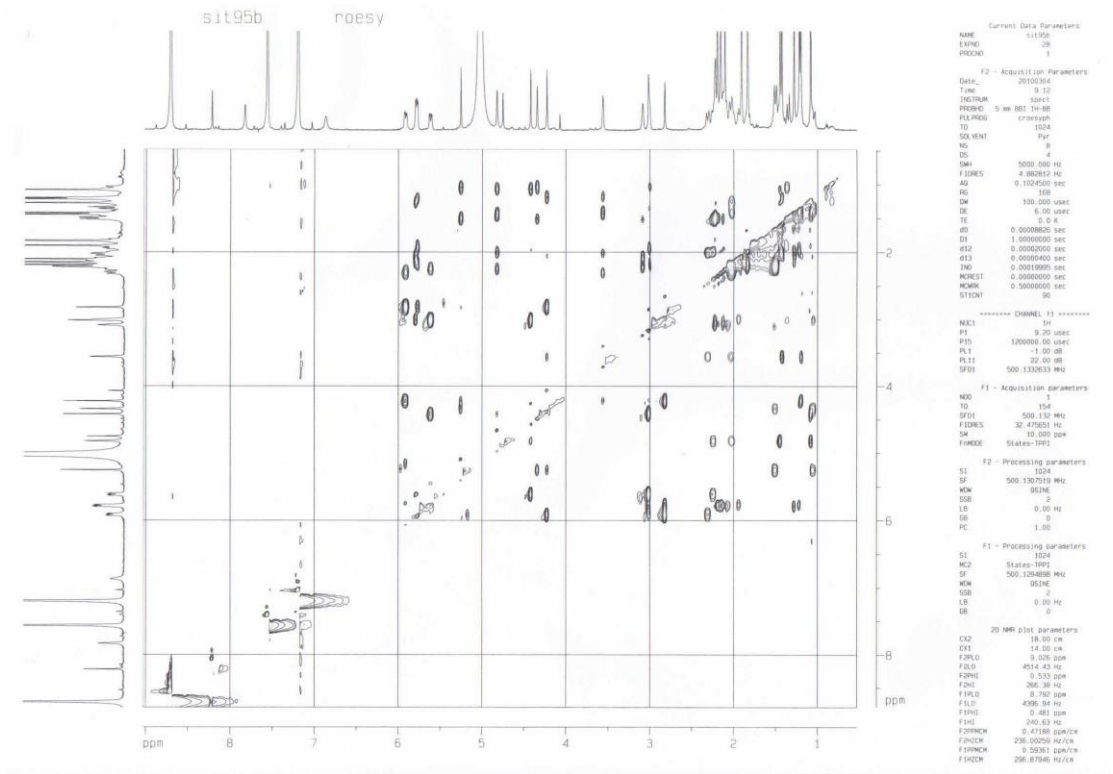


Figure 95. HRESIMS spectrum of bistenuifolin L (12)

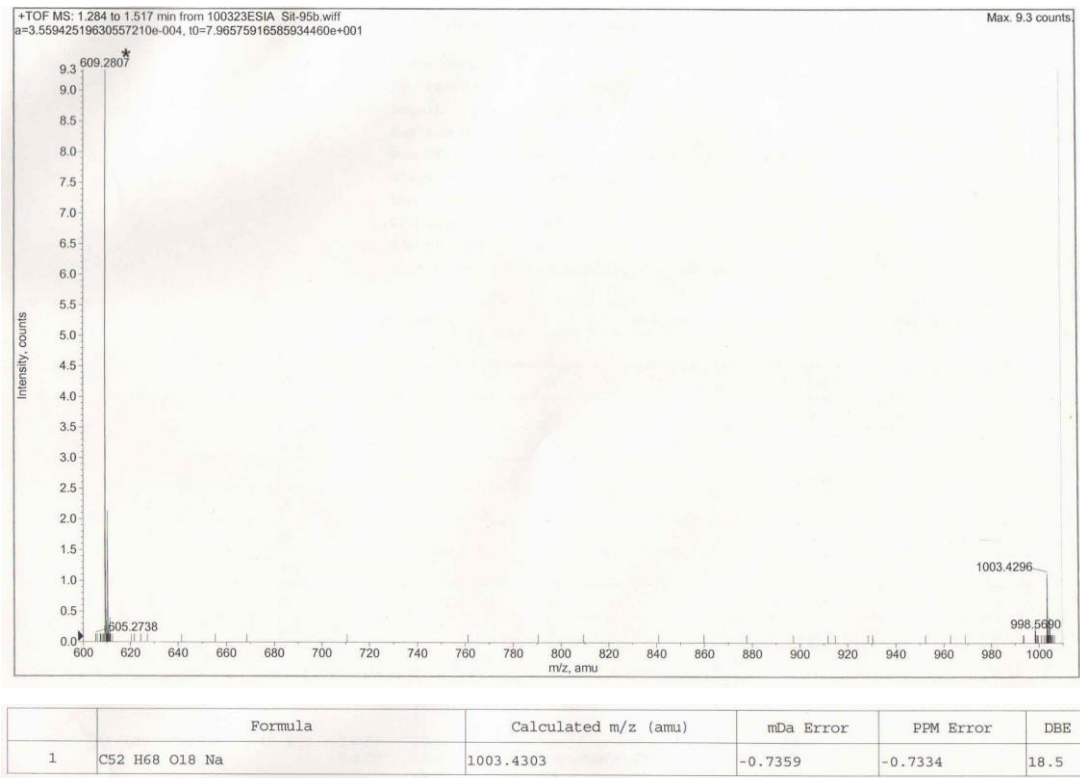
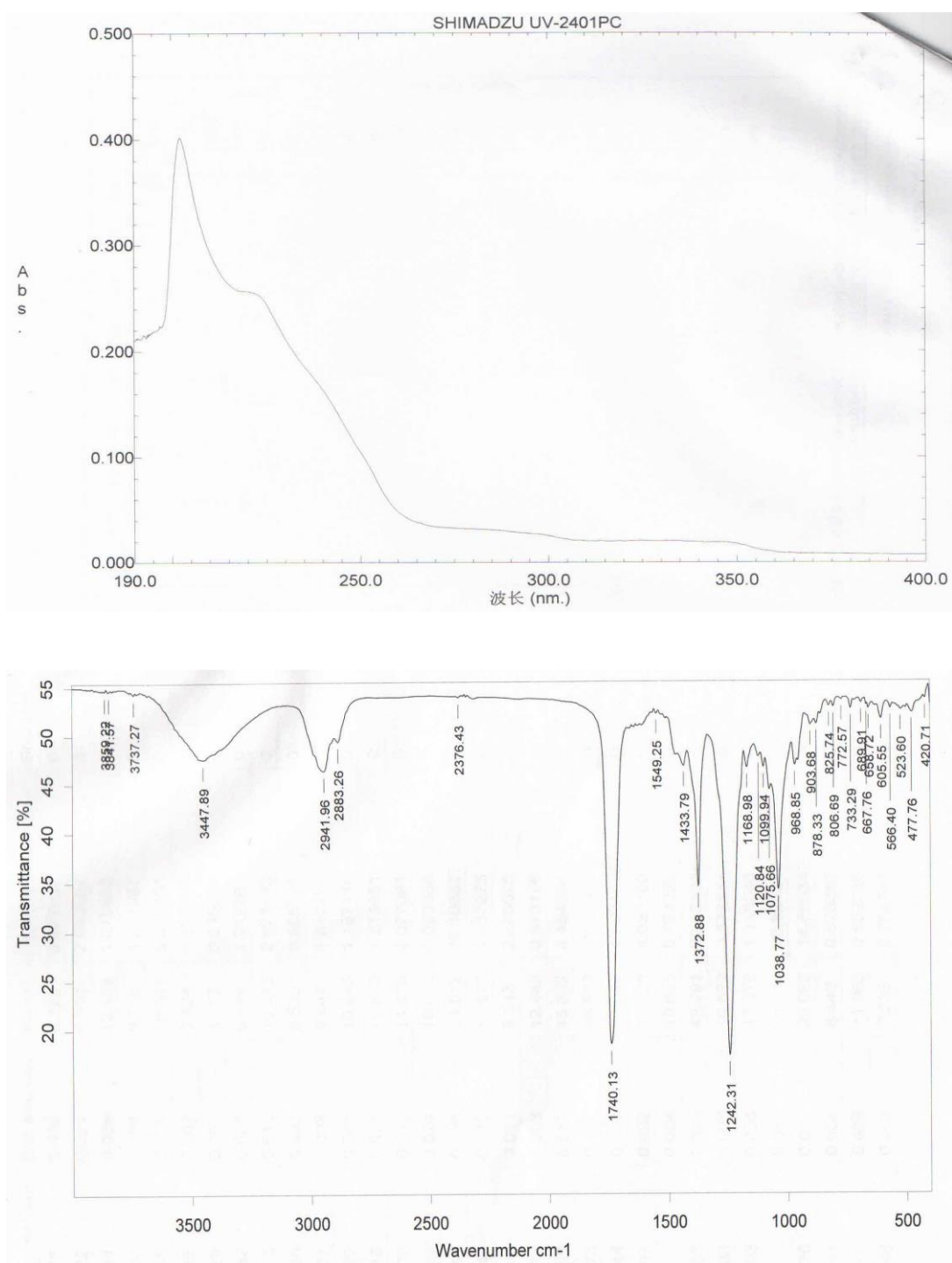


Figure 96. UV and IR spectra of bistenuifolin L (**12**)



For compound 13:

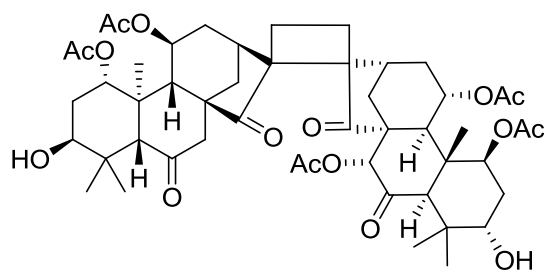


Figure 97. ^1H NMR spectrum of bistenuifolin M (13)

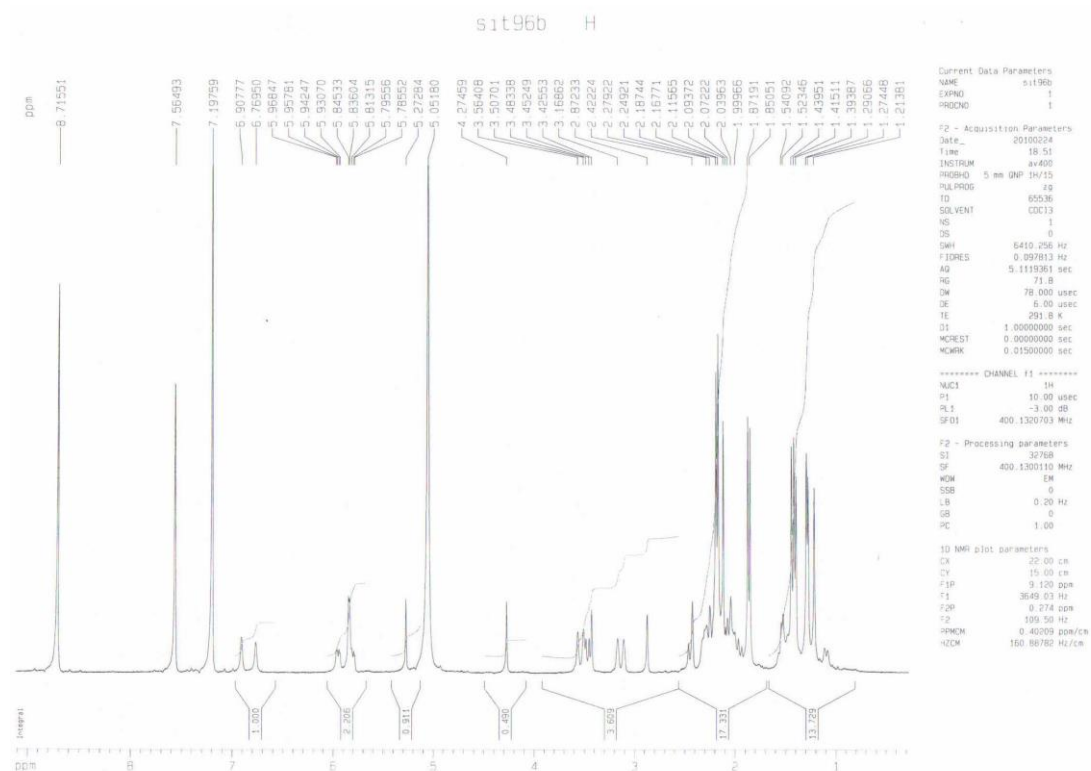


Figure 98. ^{13}C NMR spectrum of bistenuifolin M (13)

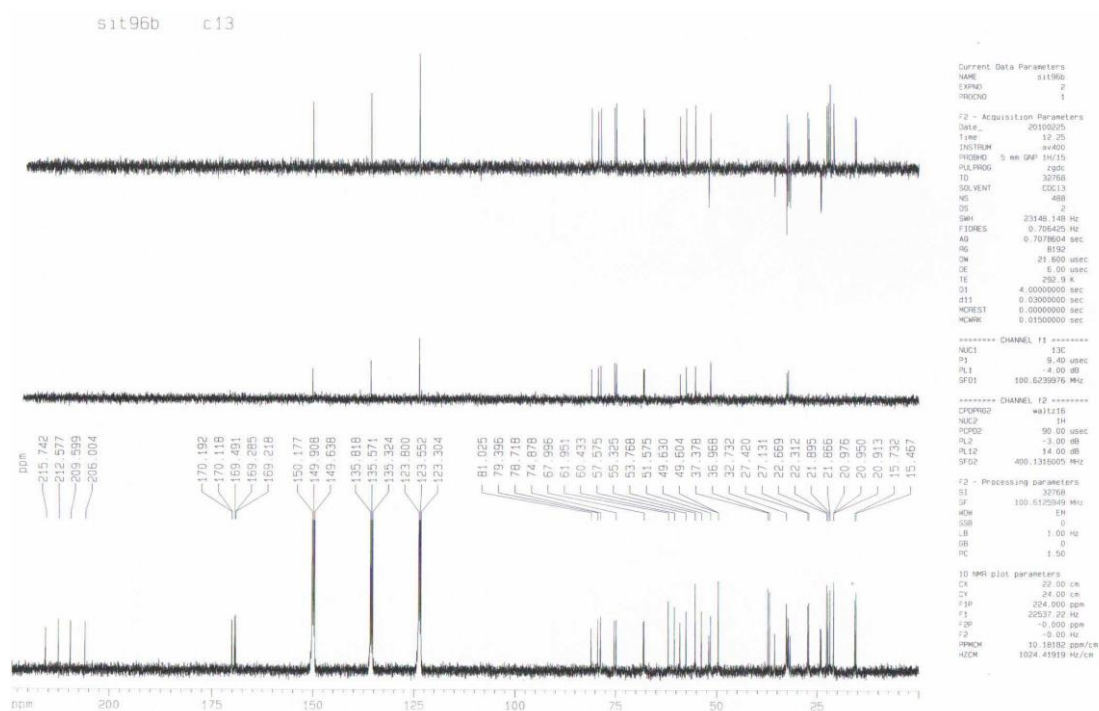
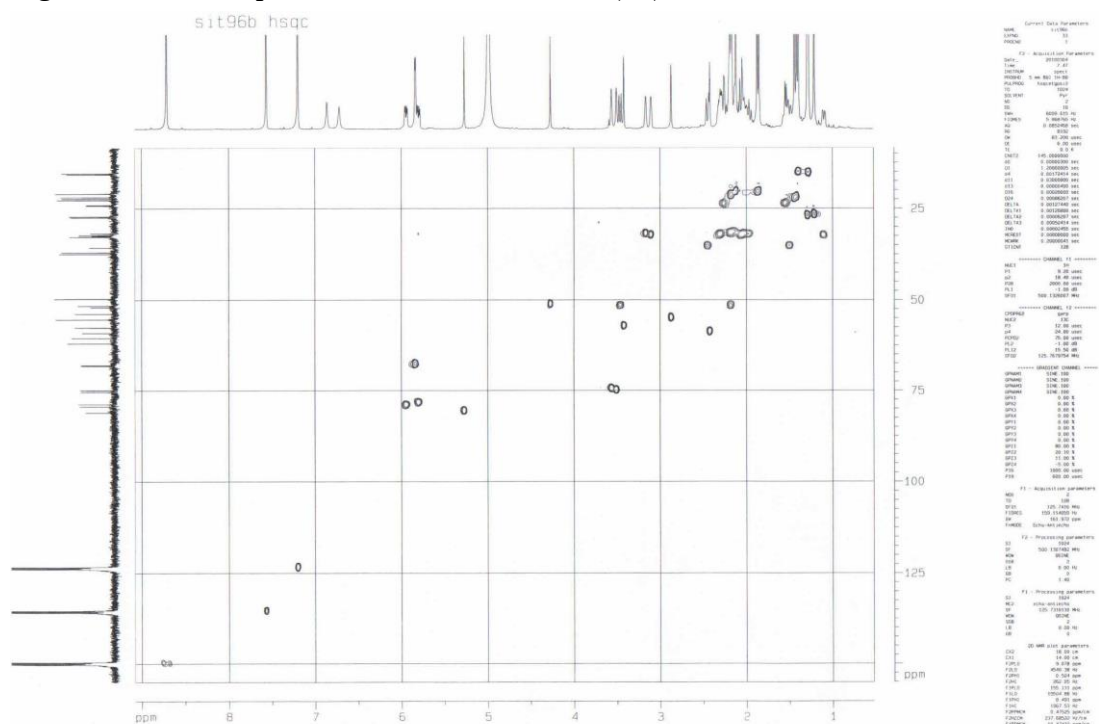


Figure 99. HSQC spectrum of bistenuifolin M (13)



51t96b hmbc

Export Data Parameters
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 Project 1

F2 - Acquisition Parameters
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 Time 8:15
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 F2 200MHZ
 SOLVENT Py
 NS 32
 DS 4
 SWH 6000.000 MHz
 FIDRES 2.532400 MHz
 AQ 0.150436 sec
 RG 2048
 DA 83.200 uS
 DE 5.00 uS
 TE 300.2 K

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 P1 9.00 uS
 PL1 -1.00 dB
 SFO1 500.130000 MHz

===== CHANNEL f1 =====
 NU2 126
 P2 12.00 uS
 PL2 -1.00 dB
 SFO2 100.628100 MHz

===== ORIGIN =====
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 GNAME2 126
 GNAME3 126
 GPR1 0.00 %
 GPR2 0.00 %
 GPR3 0.00 %
 GPR4 0.00 %
 GPR5 0.00 %
 GPR6 0.00 %
 GPR7 0.00 %
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 GPR9 0.00 %
 GPR10 0.00 %
 GPR11 0.00 %
 GPR12 0.00 %
 GPR13 0.00 %
 GPR14 0.00 %
 GPR15 0.00 %

F2 - Acquisition Parameters
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 DS 4
 SWH 125.7448 MHz
 FIDRES 2.000000 MHz
 DA 204.017 sec
 TE 300.2 K

F2 - Processing parameters
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 SF 500.130000 MHz
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 LB 0.391
 GB 0
 PC 0.00 %
 OR 0
 GC 0.40

F3 - Processing parameters
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 SF 100.628100 MHz
 W 512
 LB 0.391
 GB 0
 PC 0.00 %
 OR 0
 GC 0.40

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 F3 8.00 (4)
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 F96 160.731 (4)
 F97 160.731 (4)
 F98 160.731 (4)
 F99 160.731 (4)
 F100 160.731 (4)

[illegible]

Figure 102. ROESY spectrum of bistenuifolin M (13)

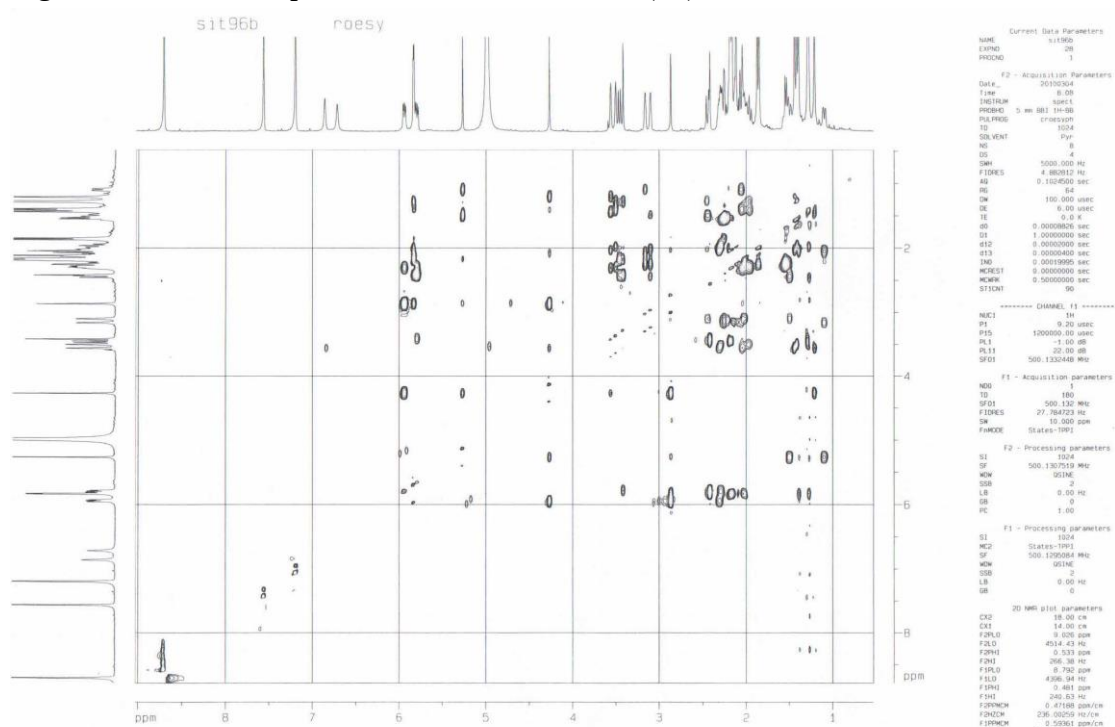
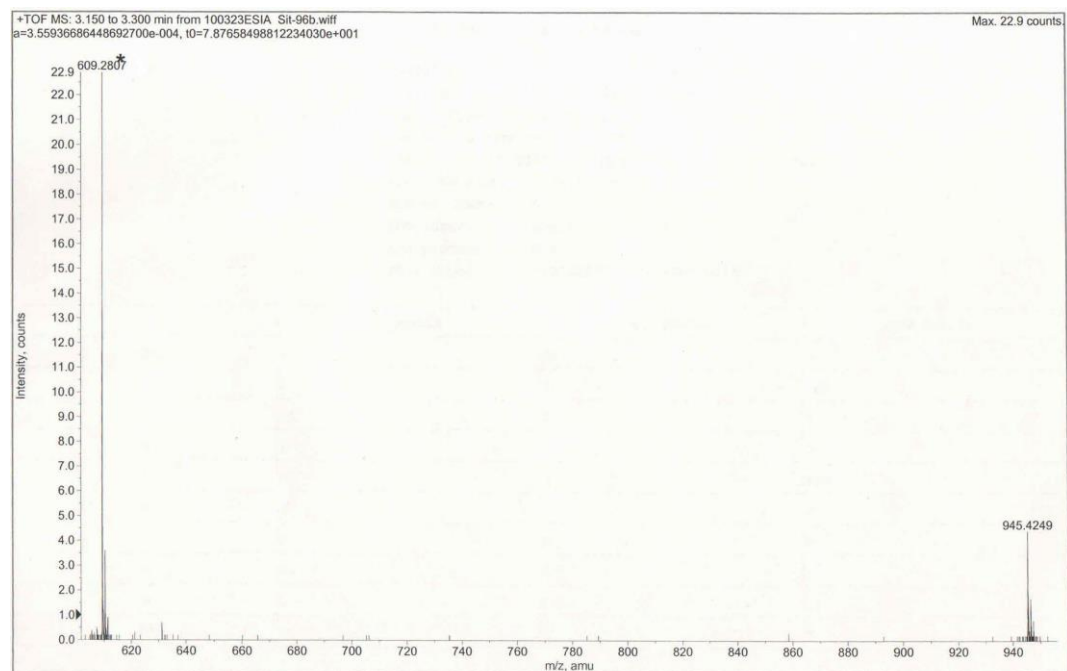
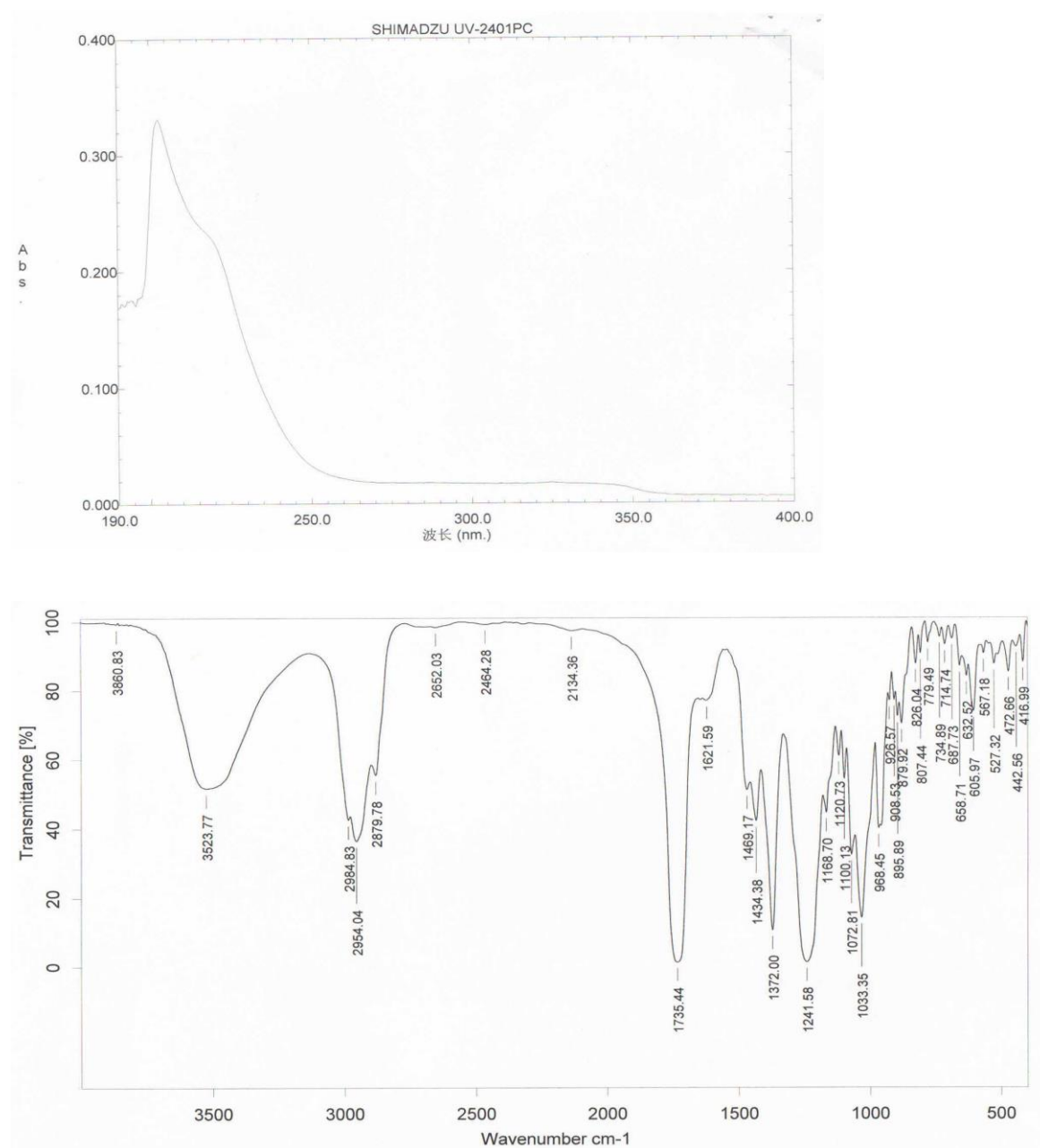


Figure 103. HRESIMS spectrum of bistenuifolin M (13)

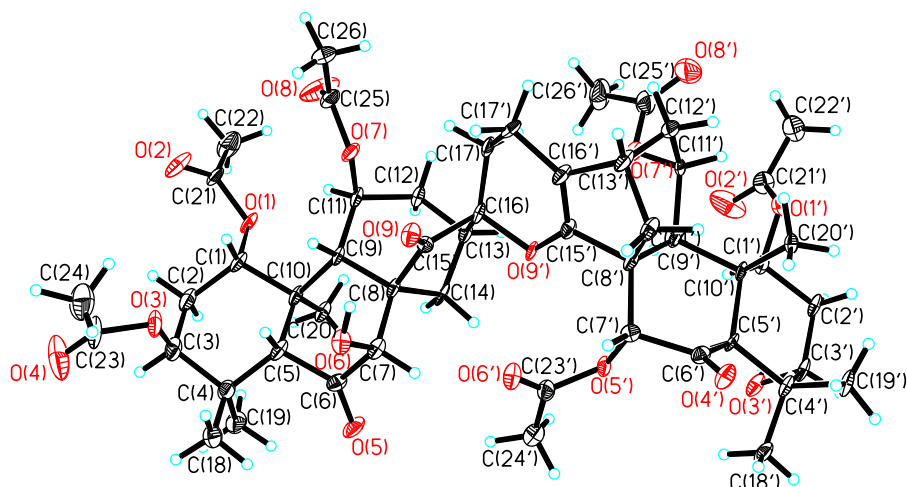


	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C50 H66 O16 Na	945.4248	0.0434	0.0459	17.5

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 ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} 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)

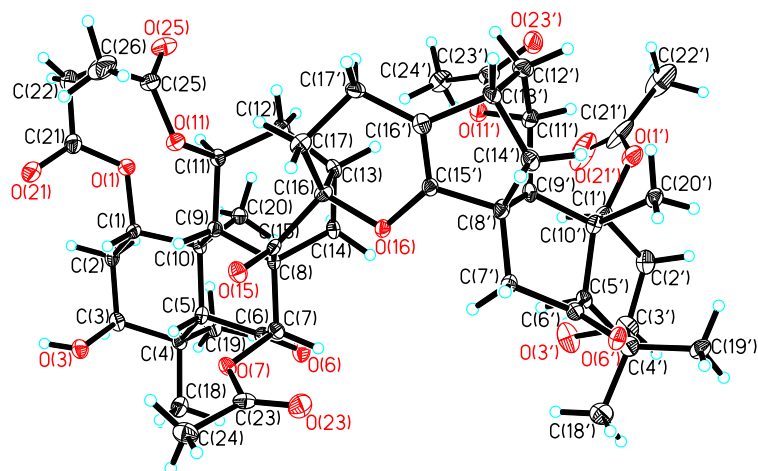
O(18')-C(18')-H(18C)	108.8
C(4')-C(18')-H(18C)	108.8
O(18')-C(18')-H(18D)	108.8
C(4')-C(18')-H(18D)	108.8
H(18C)-C(18')-H(18D)	107.7
C(19')-C(4')-C(18')	105.41(18)
C(19')-C(4')-C(5')	114.4(2)
C(18')-C(4')-C(5')	109.97(19)
C(19')-C(4')-C(3')	109.39(19)
C(18')-C(4')-C(3')	109.1(2)
C(5')-C(4')-C(3')	108.44(17)
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 ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 4. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
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)

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

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: