

Melosuavines A–H, Cytotoxic Bisindole Alkaloid Derivatives from *Melodinus suaveolens*

Ya-Ping Liu, Yun-Li Zhao, Tao Feng, Gui-Guang Cheng, Bao-Hong Zhang, Yan Li, Xiang-Hai Cai* and Xiao-Dong Luo*

Supporting Information

Figure 1S. Selected HMBC correlations of Melosuavine A (**1**);

Figure 2S. Selected ROESY (\leftrightarrow) correlations of Melosuavine A (**1**);

Figure 3S. Selected HMBC and ^1H – ^1H COSY correlations of Melosuavine D (**4**);

Figure 4S. Selected ROESY (\leftrightarrow) correlations of Melosuavine D (**4**);

Figure 5S. Selected HMBC and ^1H – ^1H COSY correlations of Melosuavine G (**7**);

Figure 6S. Selected ROESY (\leftrightarrow) correlations of Melosuavine G (**7**);

Figure 7S-13S. NMR and MS spectra of Melosuavine A (**1**);

Figure 14S-20S. NMR and MS spectra of Melosuavine B (**2**);

Figure 21S-27S. NMR and MS spectra of Melosuavine C (**3**);

Figure 28S-35S. NMR and MS spectra of Melosuavine D (**4**);

Figure 36S-43S. NMR and MS spectra of Melosuavine E (**5**);

Figure 44S-49S. NMR and MS spectra of Melosuavine F (**6**);

Figure 50S-57S. NMR and MS spectra of Melosuavine G (**7**);

Figure 58S-64S. NMR and MS spectra of Melosuavine H (**8**);

Figure 65S-71S. NMR and MS spectra of Tenuicausine (**9**);

Figure 72S-74S. NMR and MS spectra of Melodinine J (**10**).

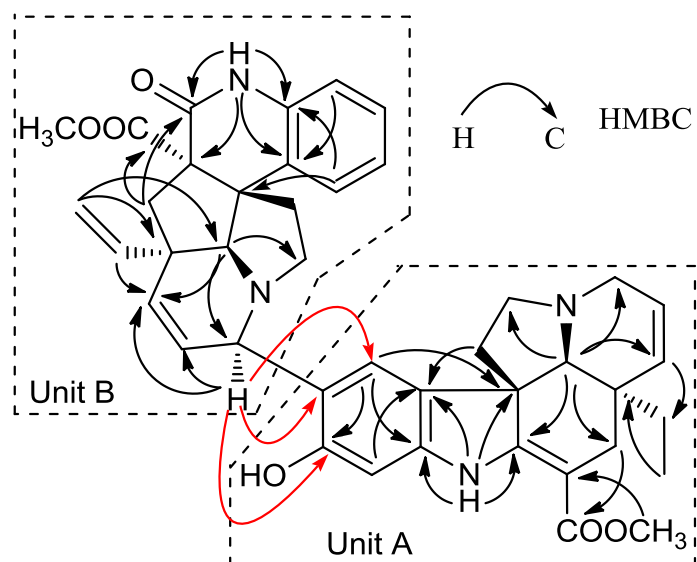


Figure 1S. Selected HMBC correlations of Melosuavine A (**1**).

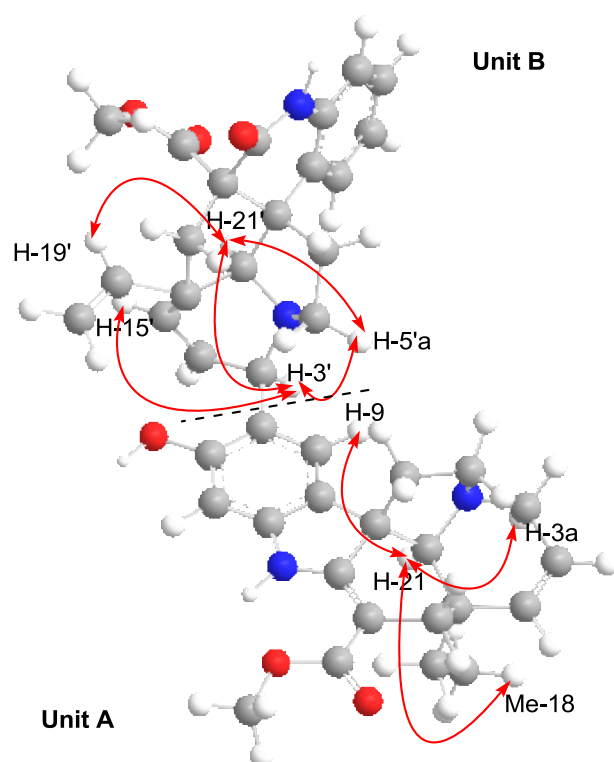


Figure 2S. Selected ROESY (\leftrightarrow) correlations of Melosuavine A (**1**).

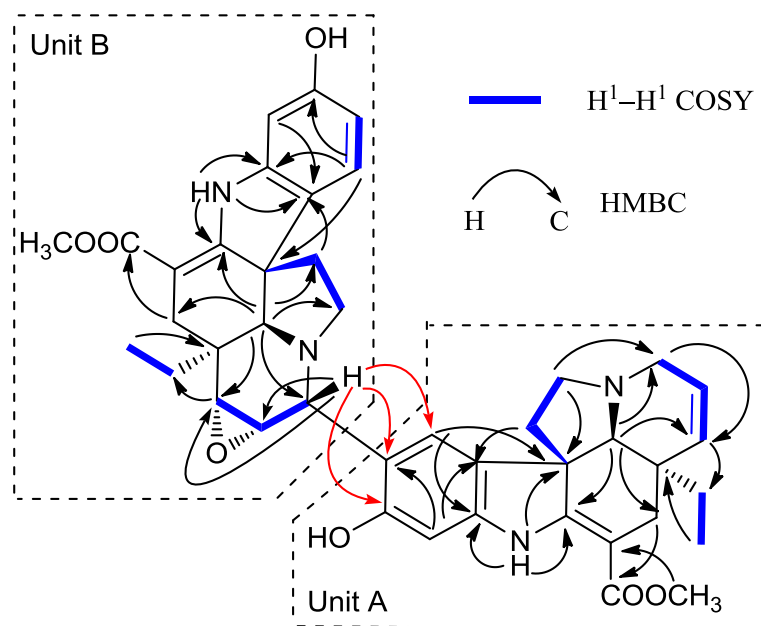


Figure 3S. Selected HMBC and ¹H-¹H COSY correlations of Melosuavine D (4).

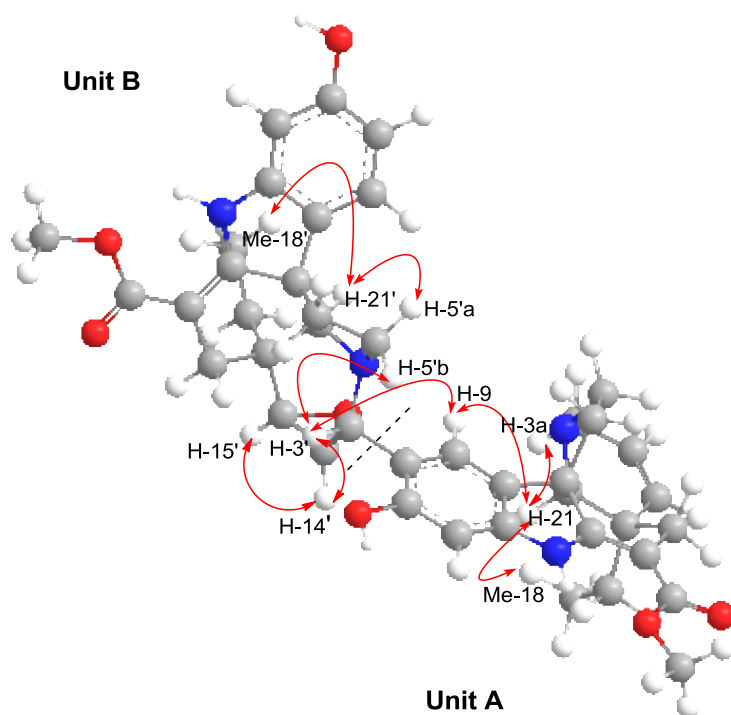


Figure 4S. Selected ROESY (\leftrightarrow) correlations of Melosuavine D (**4**).

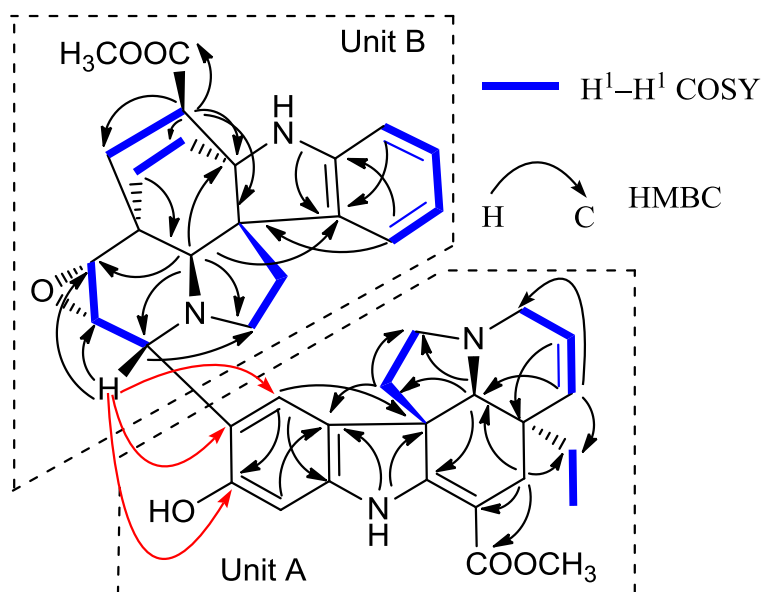


Figure 5S. Selected HMBC and ^1H - ^1H COSY correlations of Melosuavine G (7).

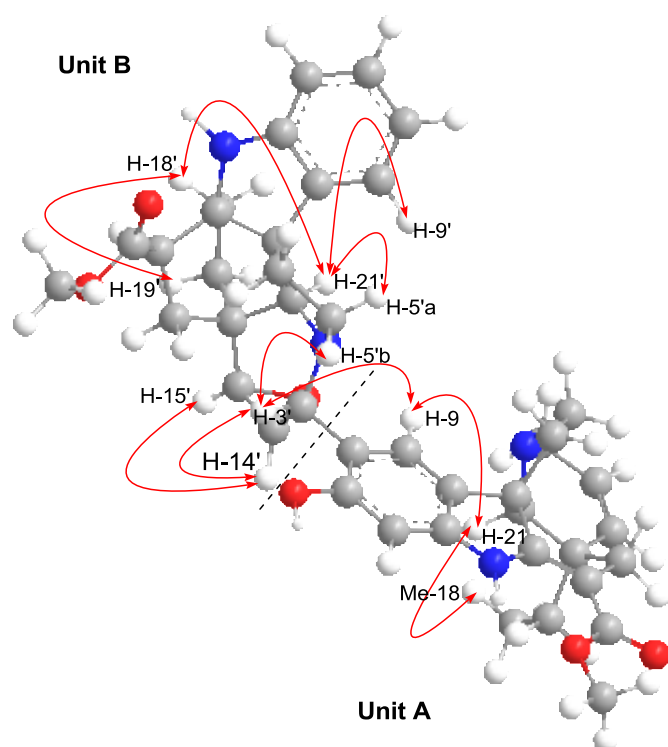


Figure 6S. Selected ROESY (\leftrightarrow) correlations of Melosuavine G (**7**).

Figure 7S. ^1H NMR of Melosuavine A (**1**) in acetone- d_6 .

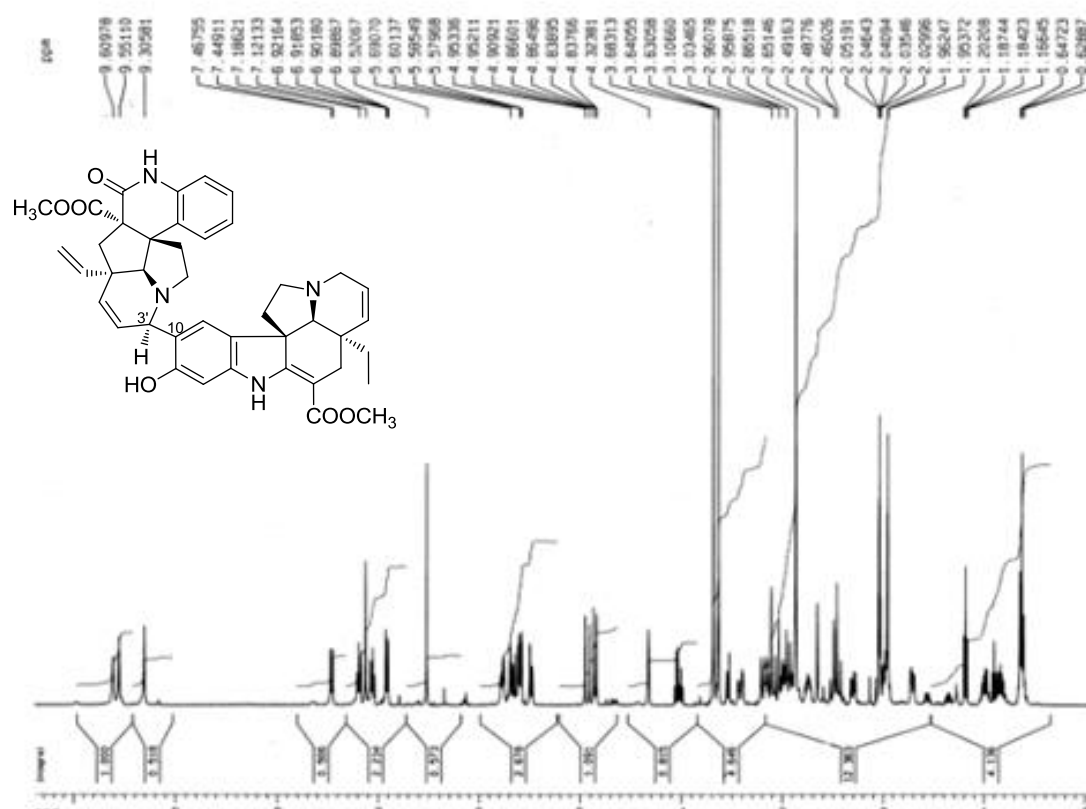


Figure 8S. ^{13}C NMR and DEPT of Melosuavine A (**1**) in acetone- d_6 .

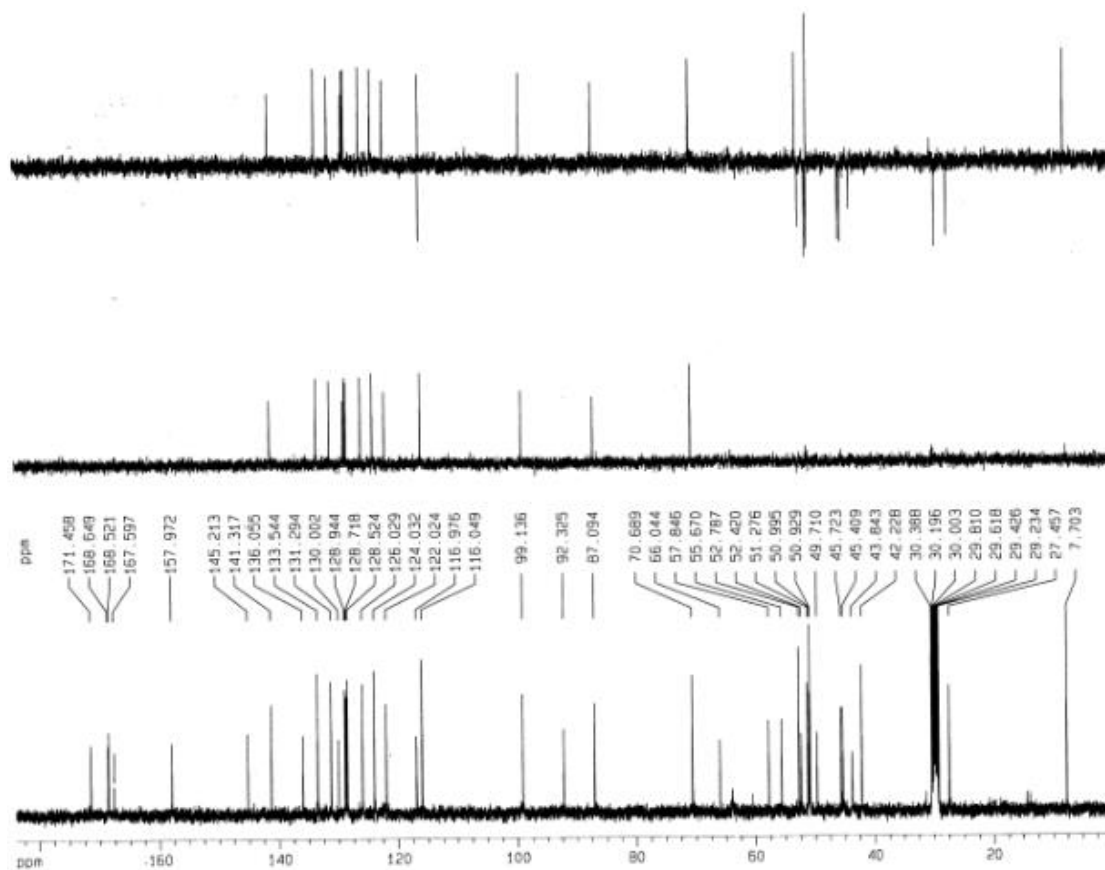


Figure 9S. HSQC of Melosuavine A (**1**) in acetone- d_6 .

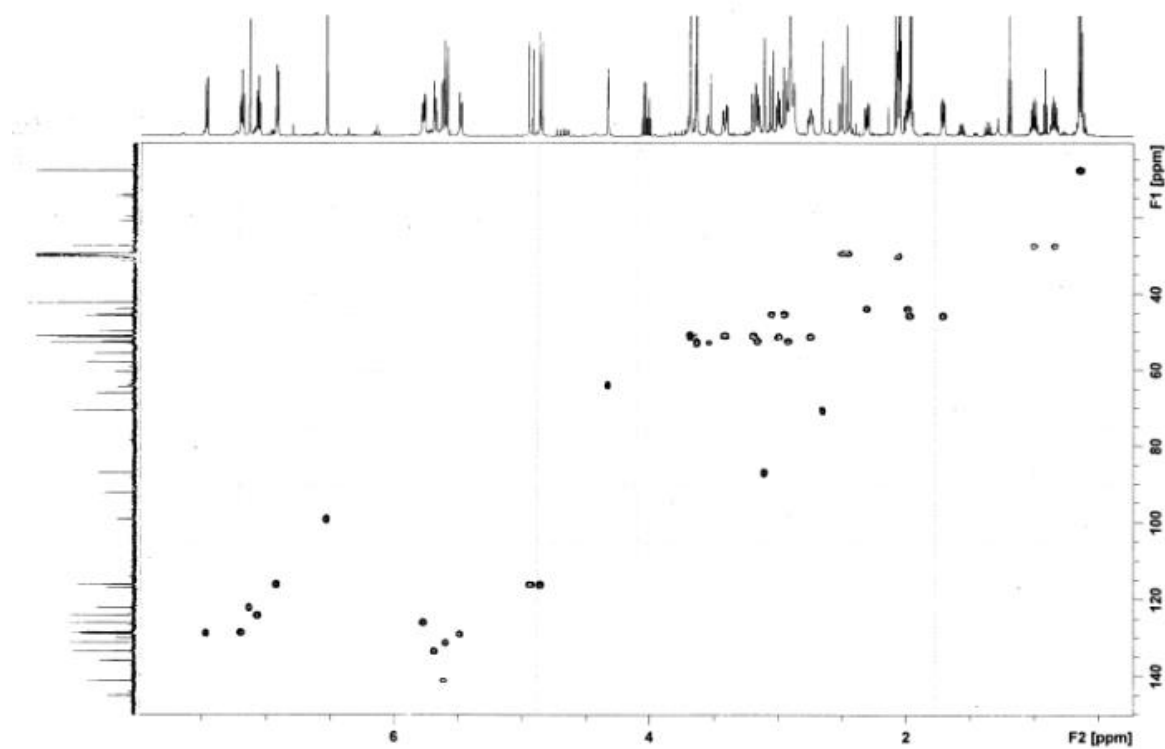


Figure 10S. HMBC of Melosuavine A (**1**) in acetone- d_6 .

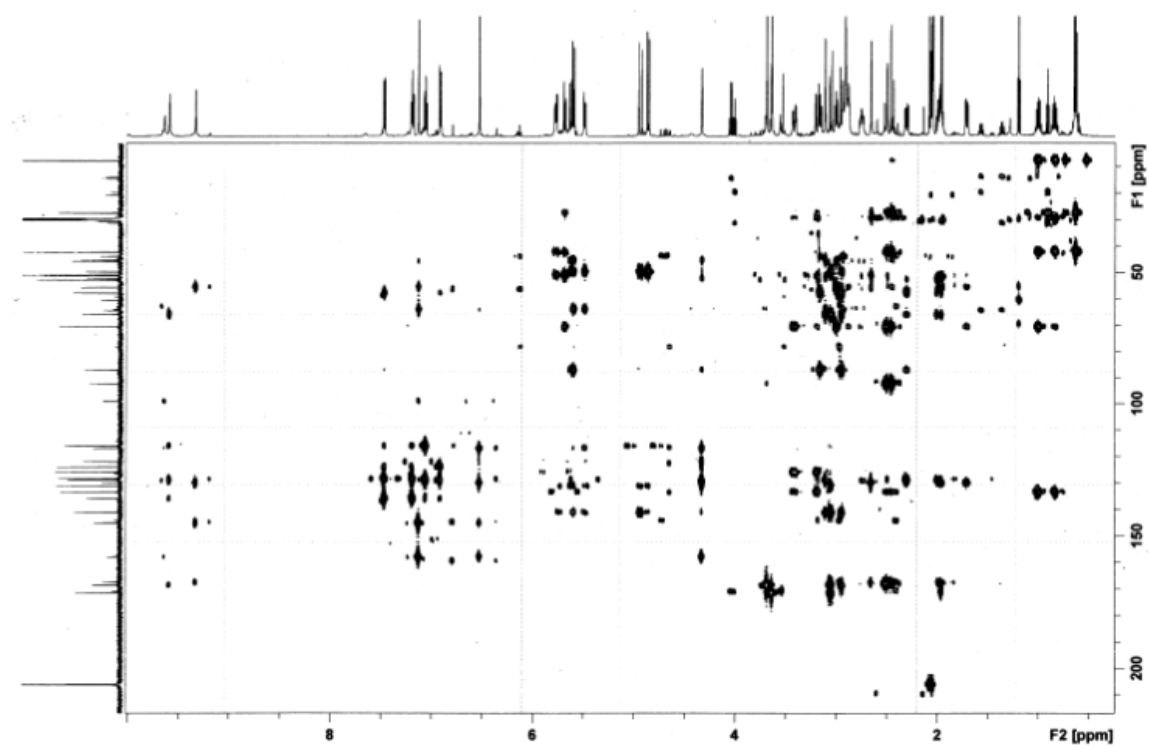


Figure 11S. ROESY of Melosuavine A (**1**) in acetone- d_6 .

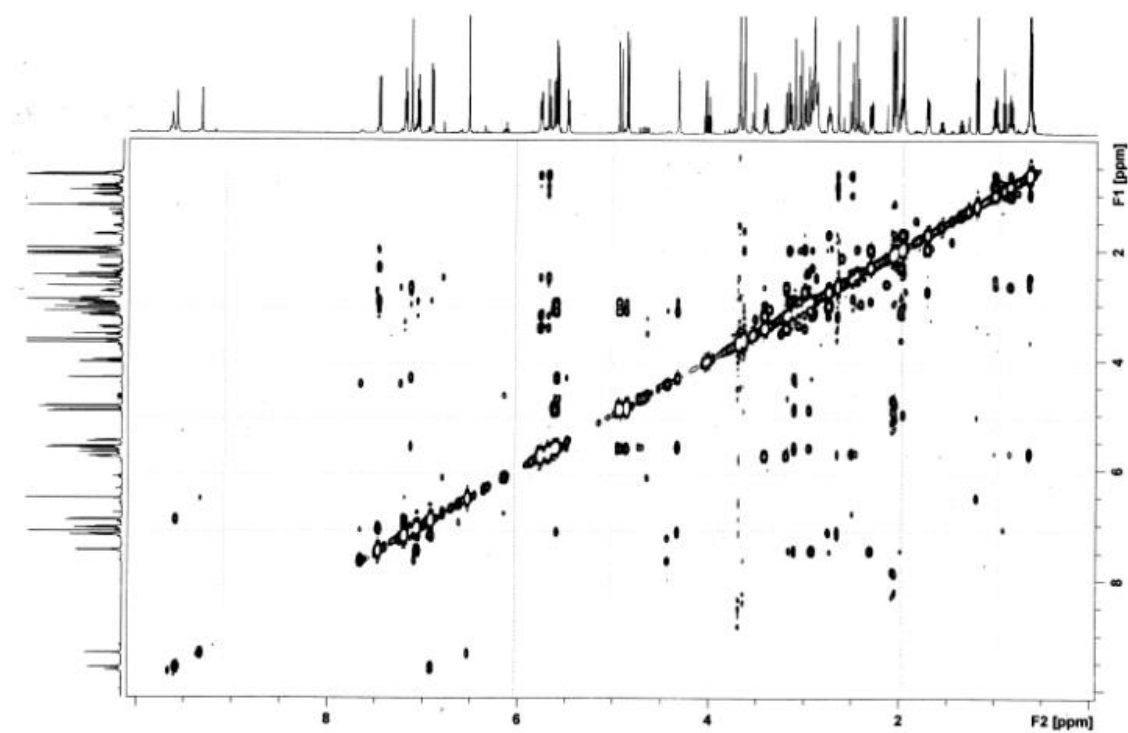


Figure 12S. EIMS of Melosuavine A (**1**).

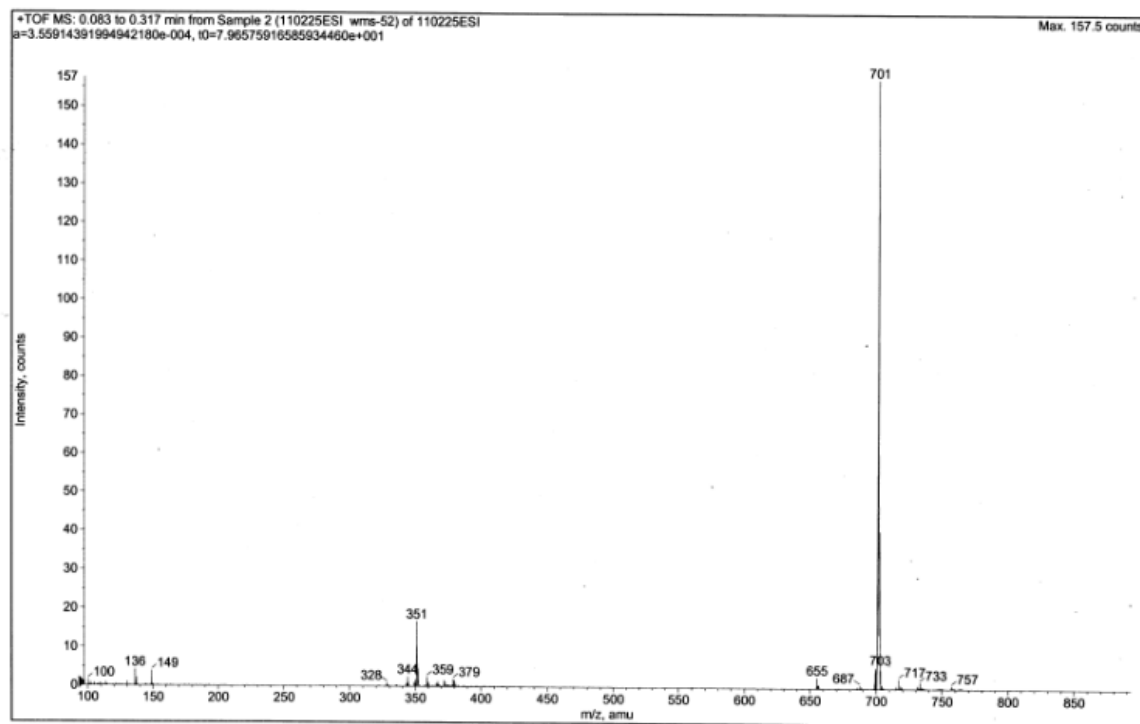


Figure 13S. HREIMS of Melosuavine A (**1**) in acetone-*d*₆.

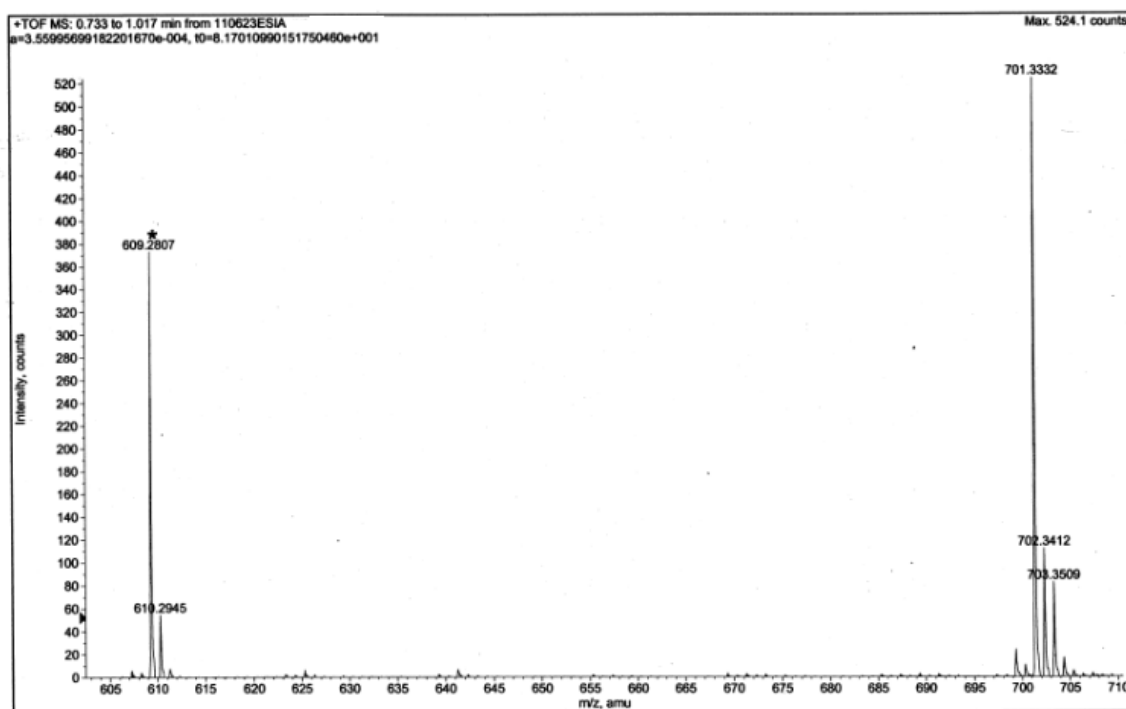


Figure 14S. ^1H NMR of Melosuavine B (**2**) in acetone- d_6 .

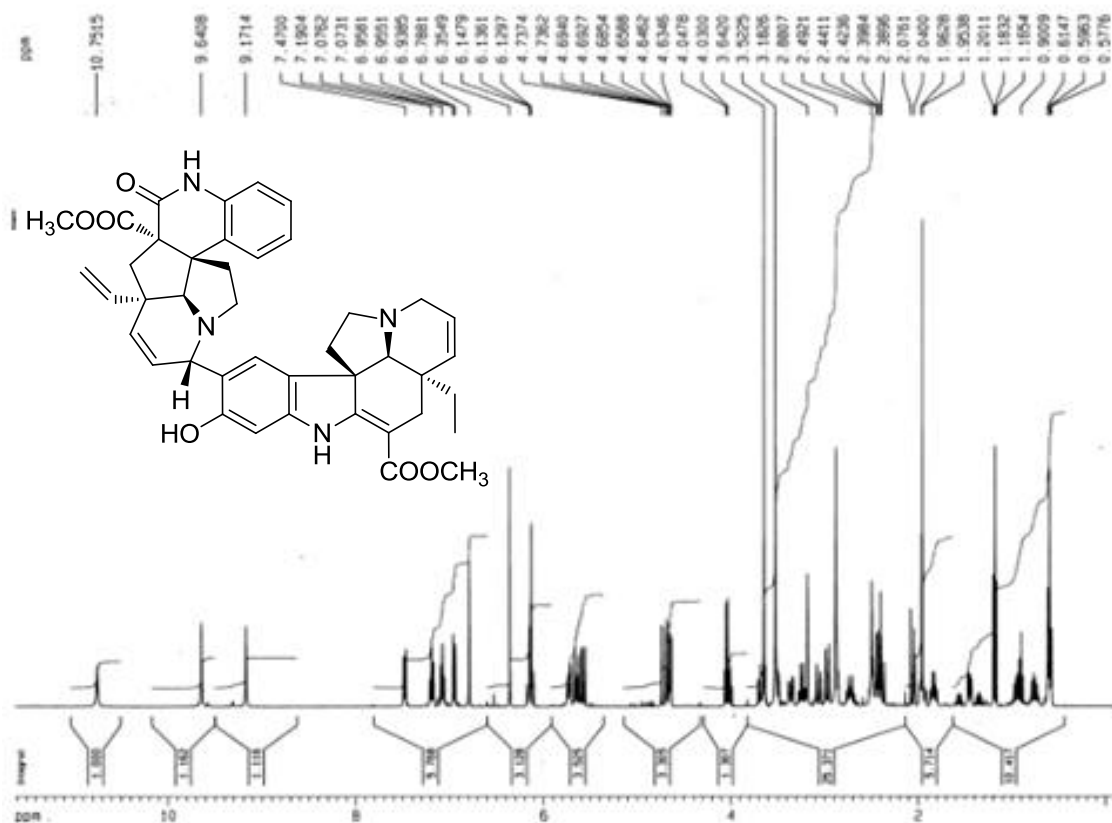


Figure 15S. ^{13}C NMR and DEPT of Melosuavine B (**2**) in acetone- d_6 .

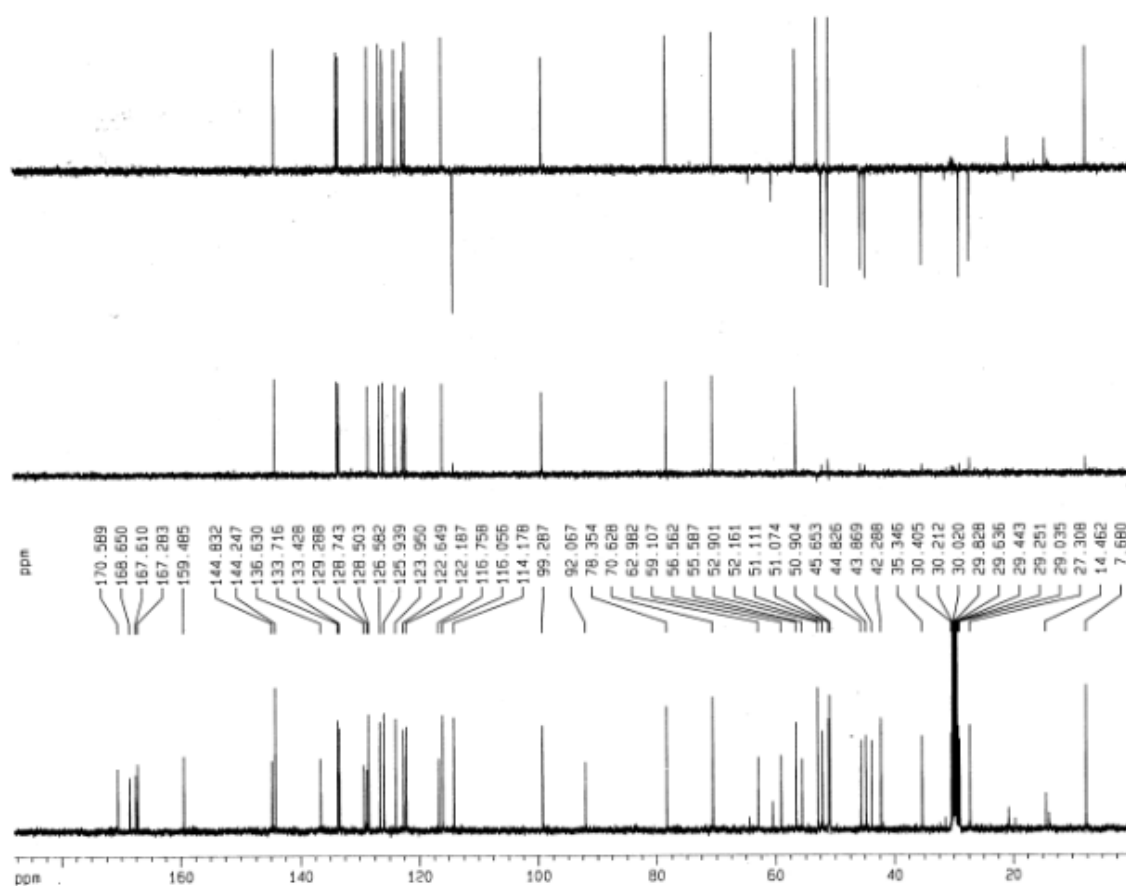


Figure 16S. HSQC of Melosuavine B (**2**) in acetone- d_6 .

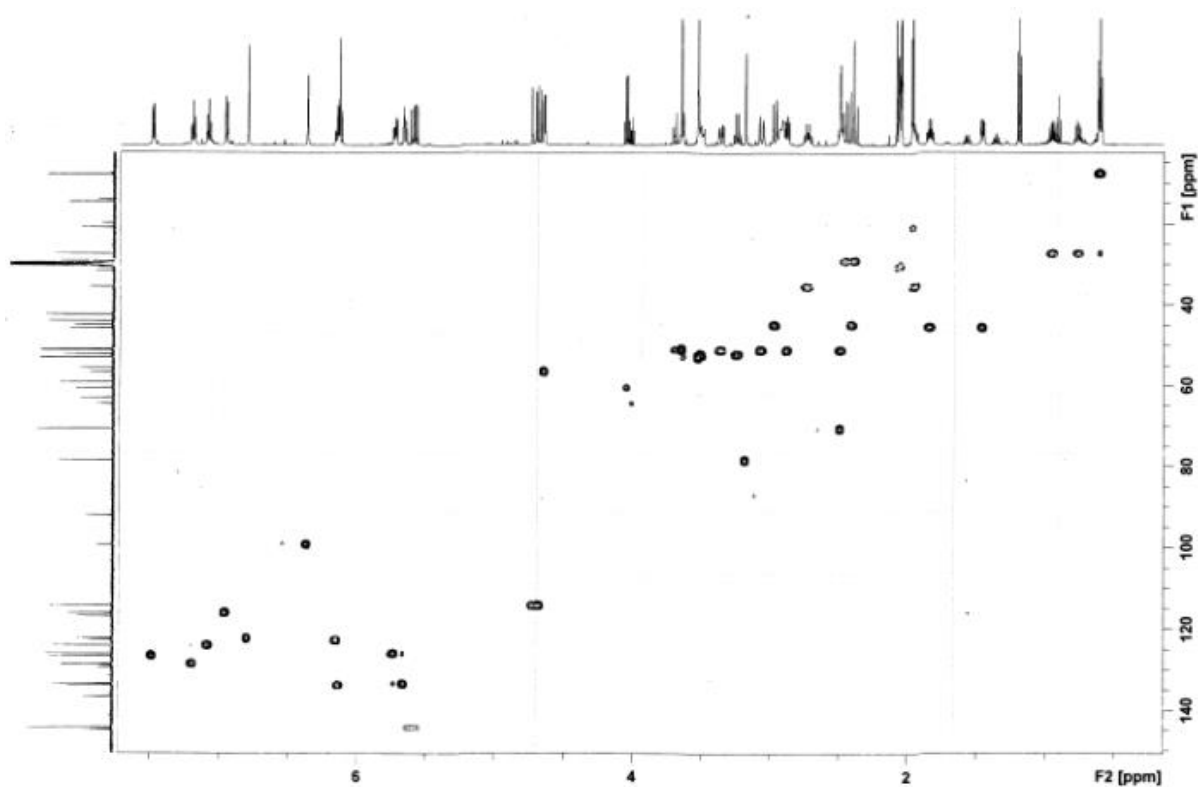


Figure 17S. HMBC of Melosuavine B (**2**) in acetone- d_6 .

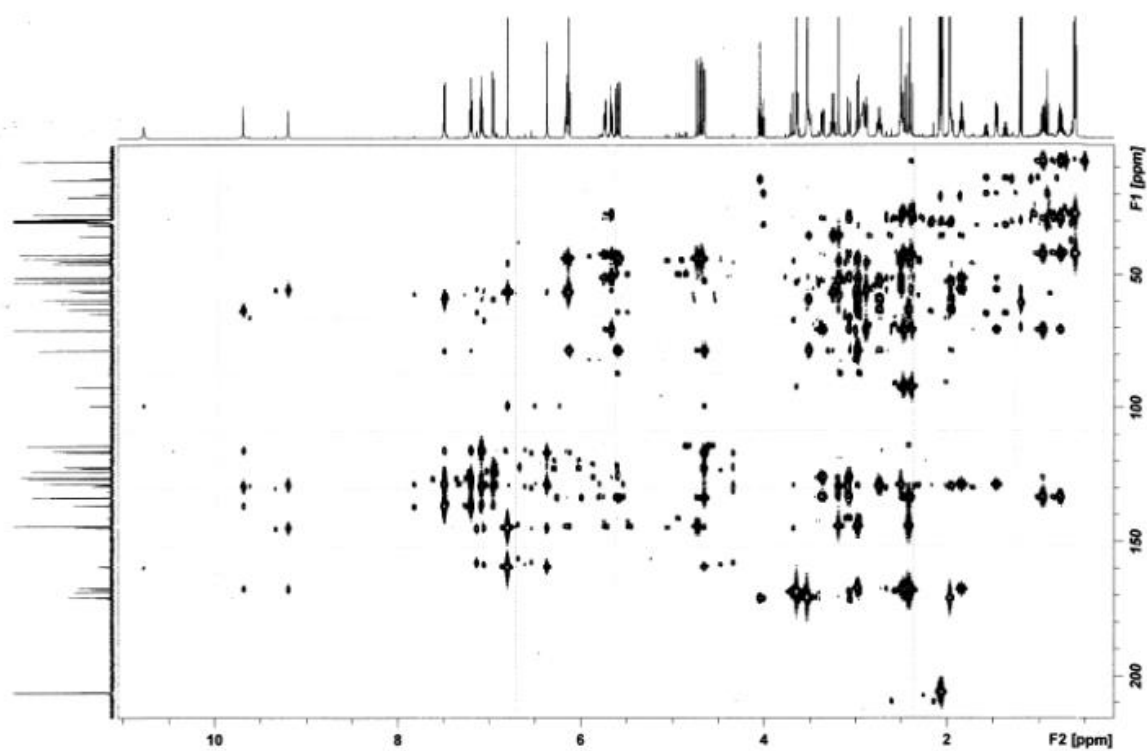


Figure 18S. ROESY of Melosuavine B (**2**) in acetone- d_6 .

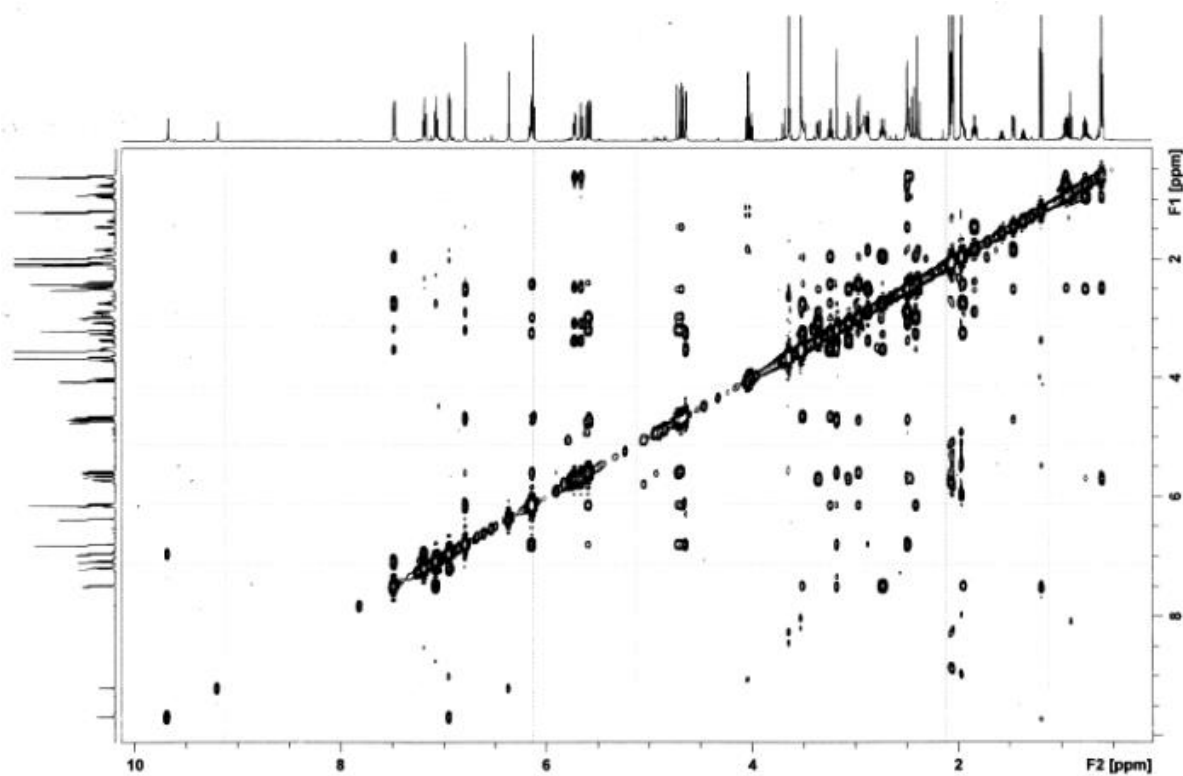


Figure 19S. ESIMS of Melosuavine B (2).

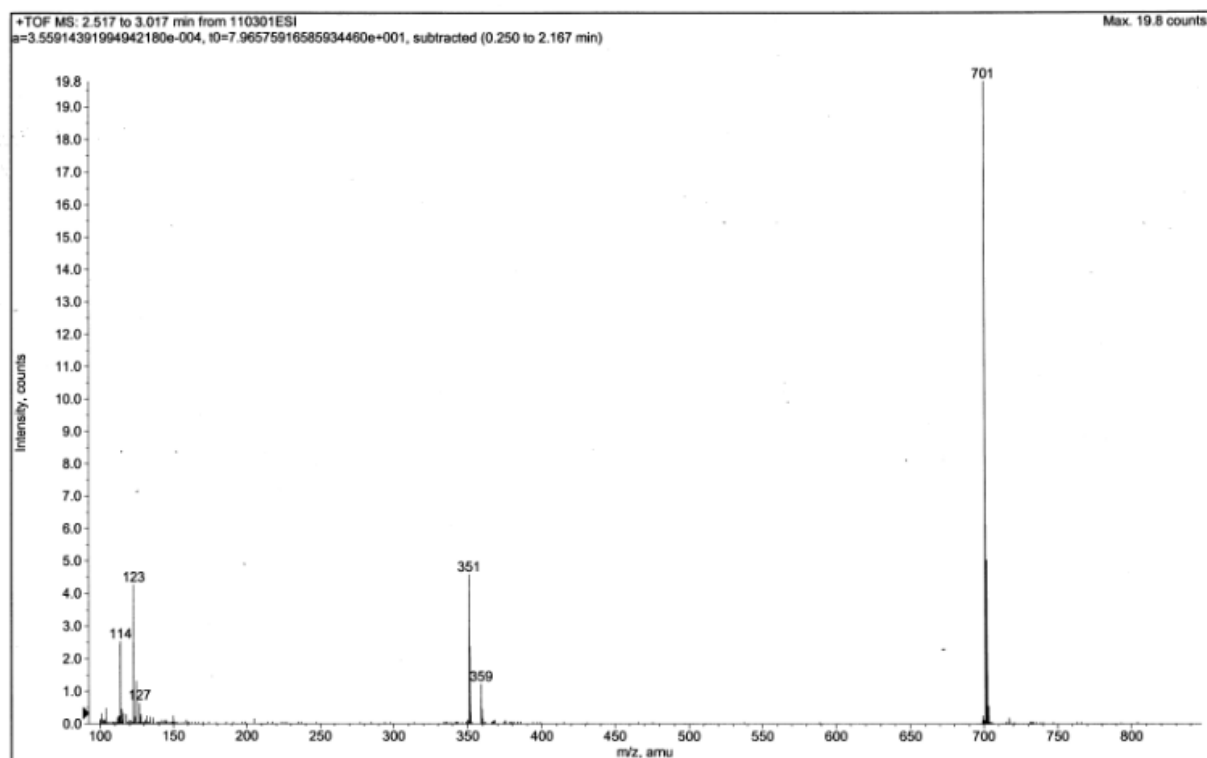


Figure 20S. HRESIMS of Melosuavine B (2).

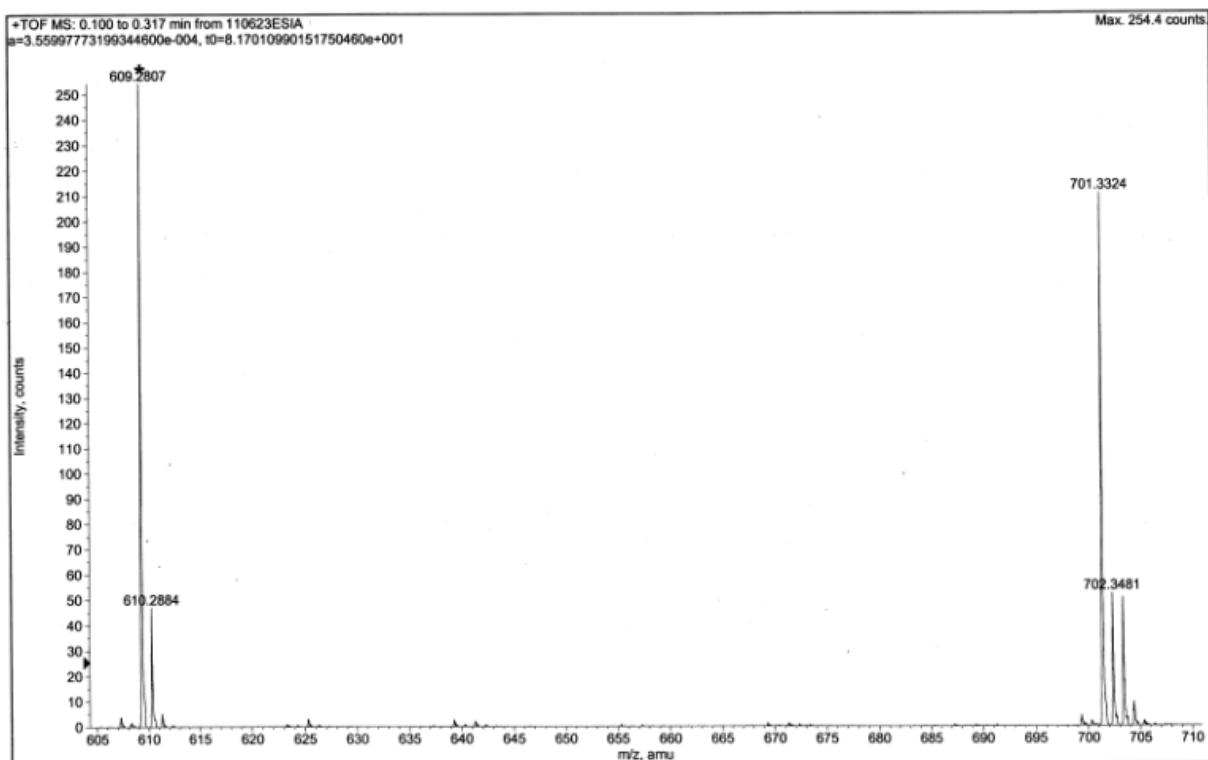


Figure 21S. ^1H NMR of Melosuavine C (**3**) in methanol- d_4 .

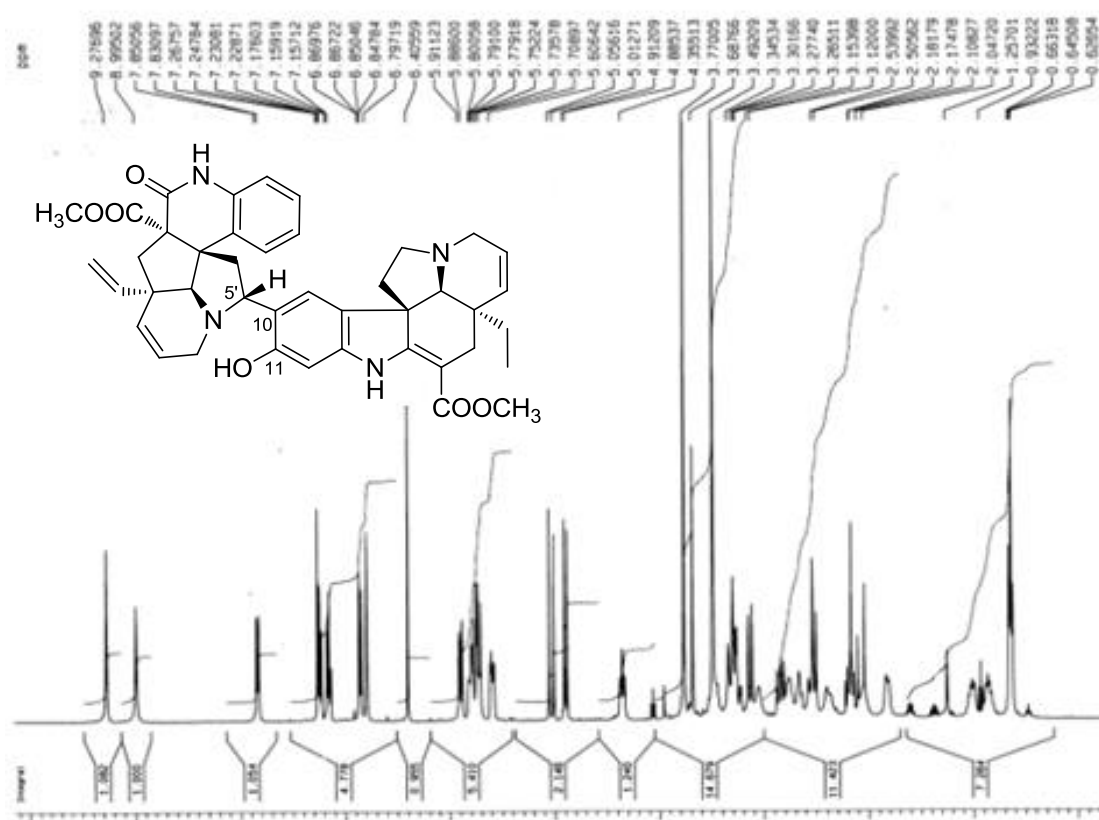


Figure 22S. ^{13}C NMR and DEPT of Melosuavine C (**3**) in methanol- d_4 .

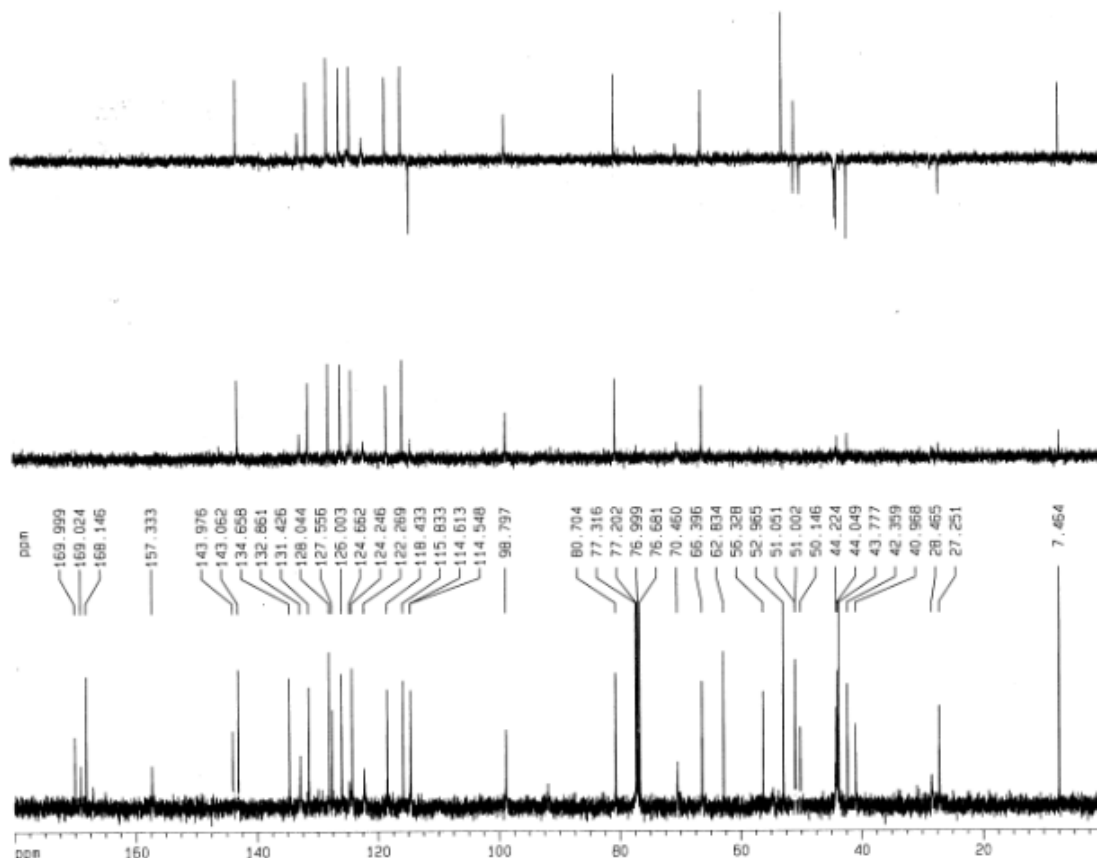


Figure 23S. HSQC of Melosuavine C (**3**) in methanol- d_4 .

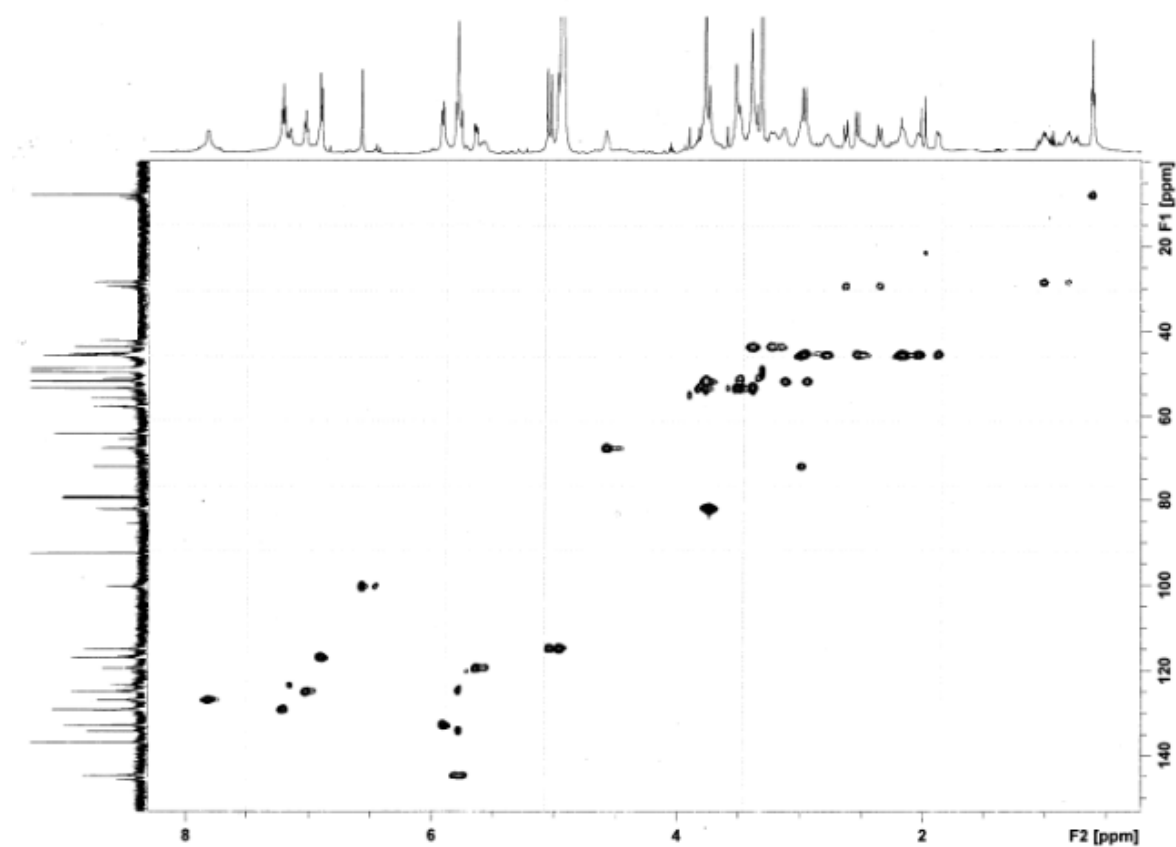


Figure 24S. HMBC of Melosuavine C (**3**) in methanol- d_4 .

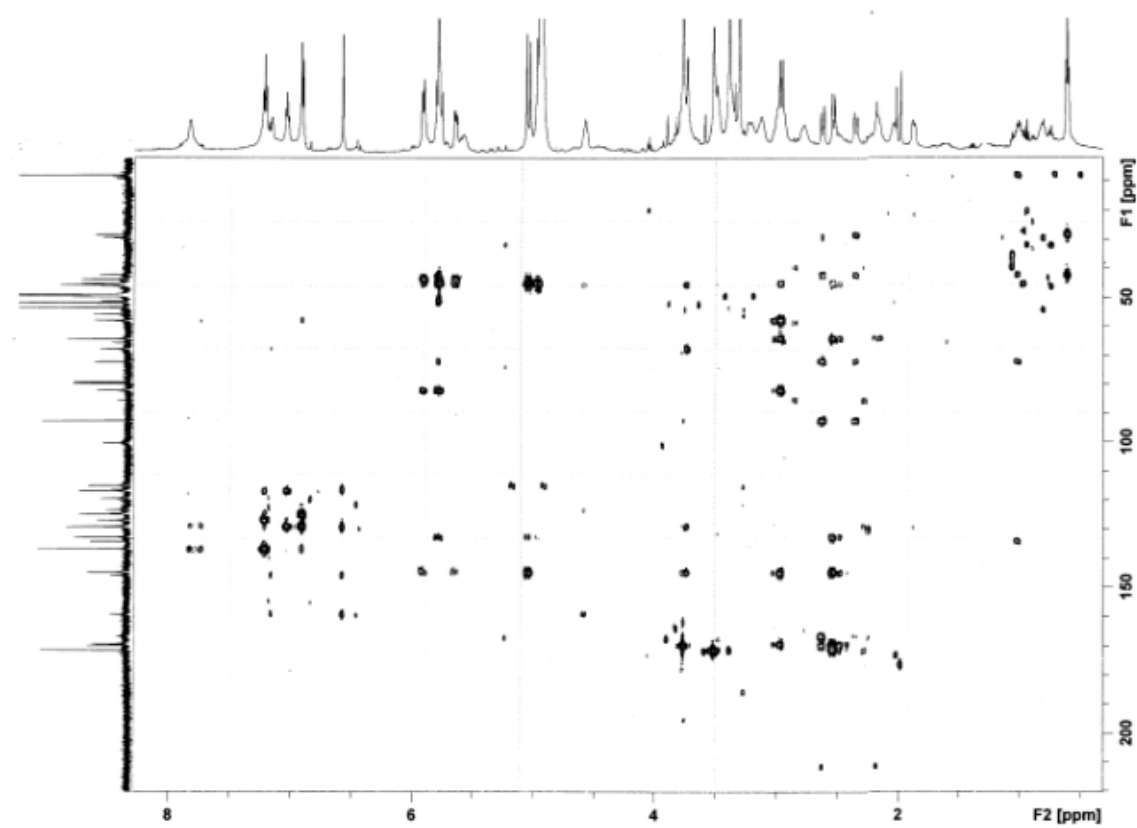


Figure 25S. ROESY of Melosuavine C (**3**) in methanol- d_4 .

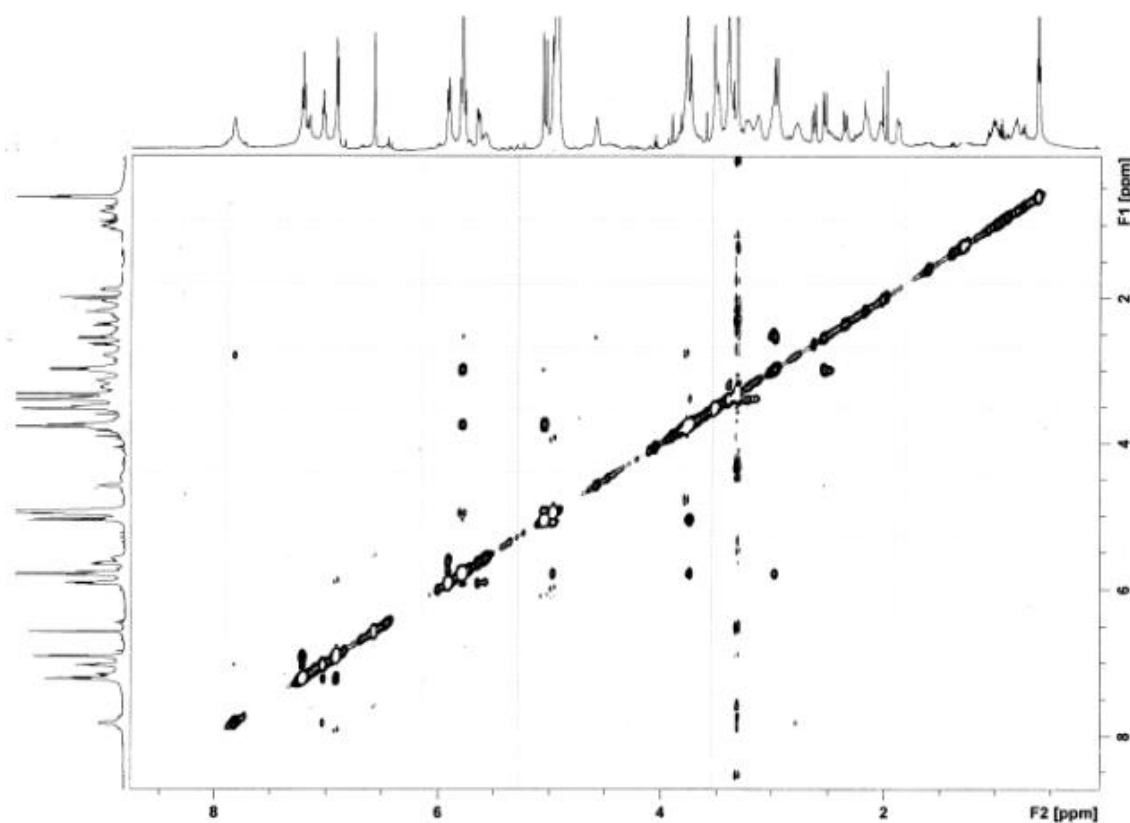


Figure 26S. EIMS of Melosuavine C (**3**).

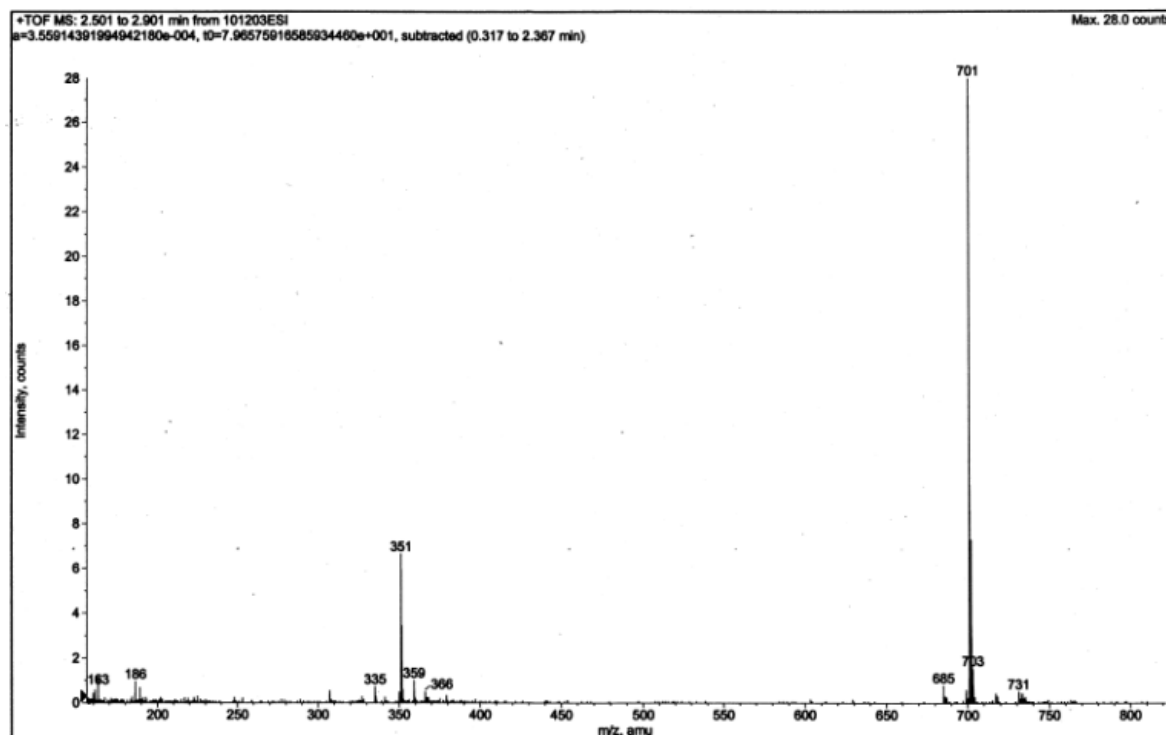


Figure 27S. HREIMS of Melosuavine C (**3**).

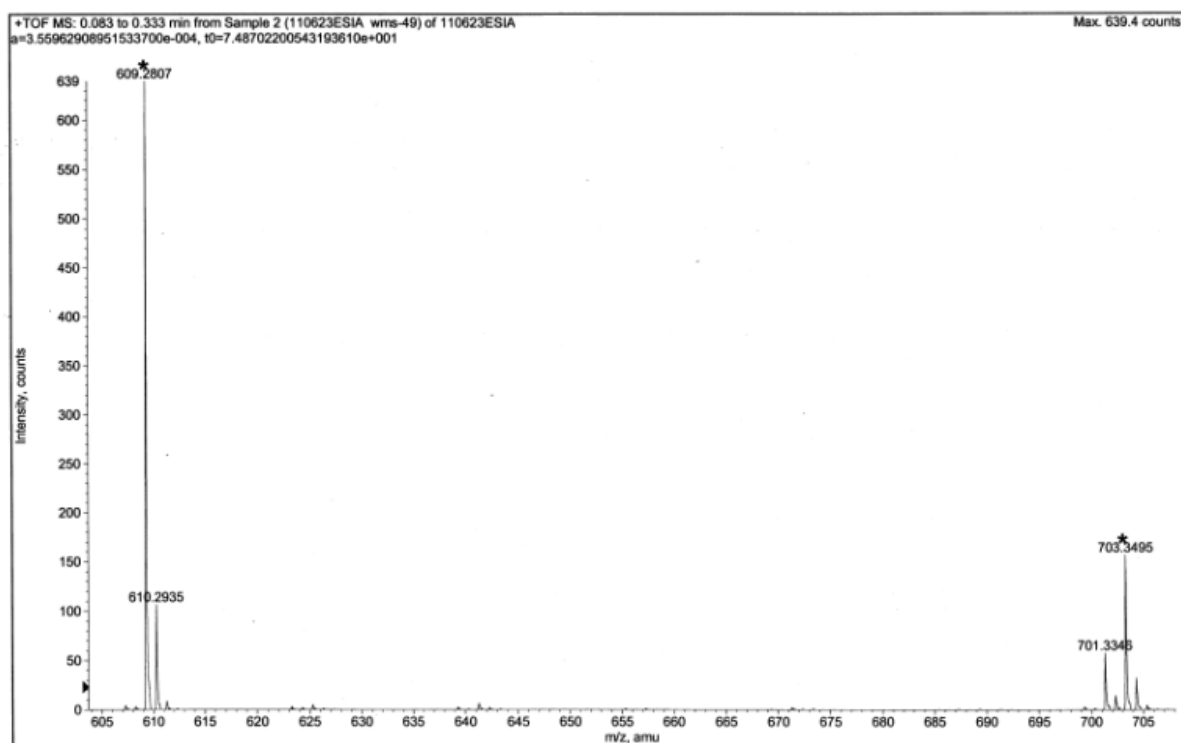


Figure 28S. ^1H NMR of Melosuavine D (**4**) in DMSO.

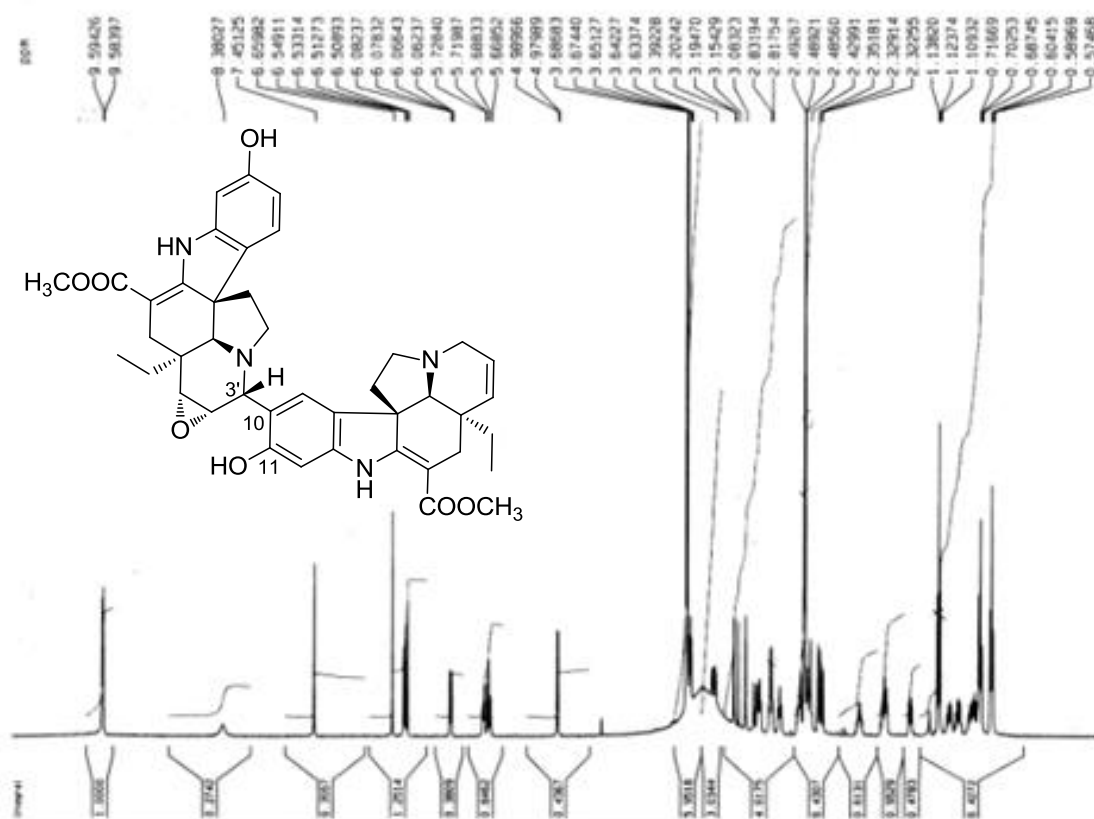


Figure 29S. ^{13}C NMR and DEPT of Melosuavine D (**4**) in DMSO.

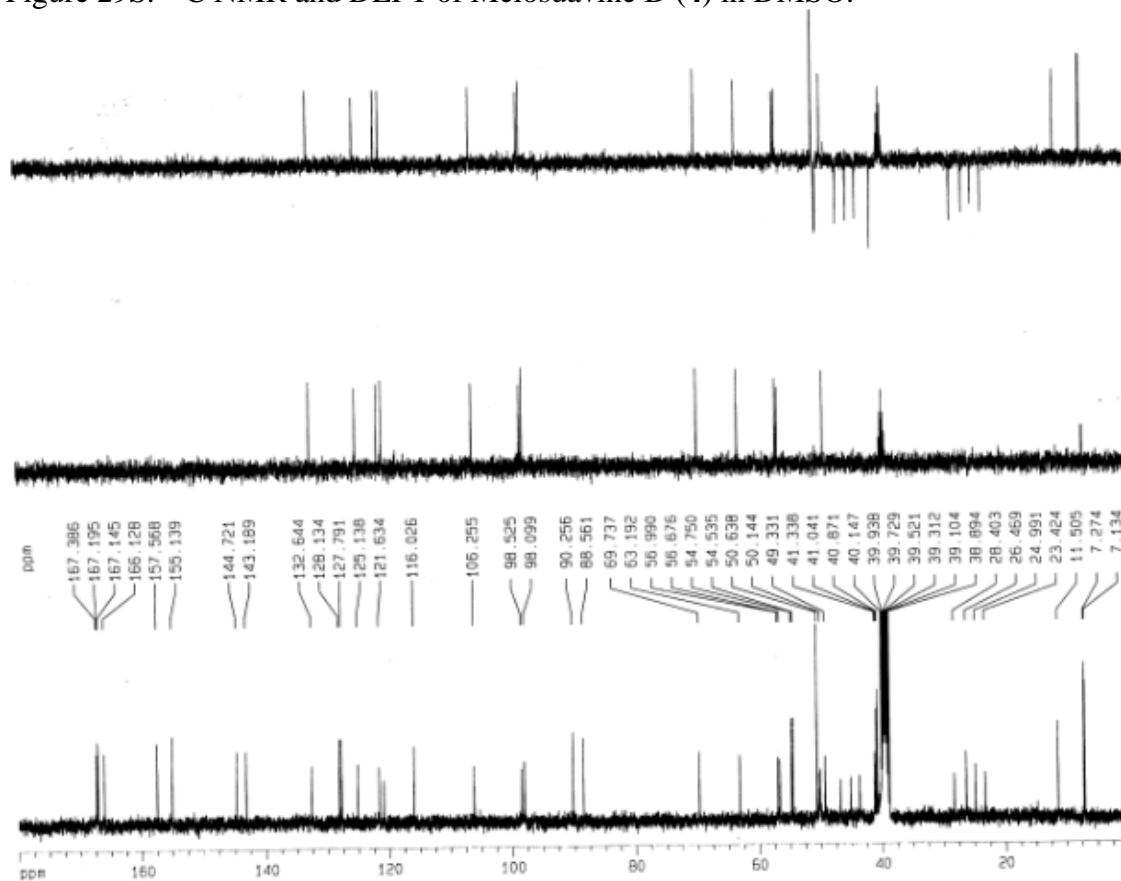


Figure 30S. HSQC of Melosuavine D (**4**) in DMSO.

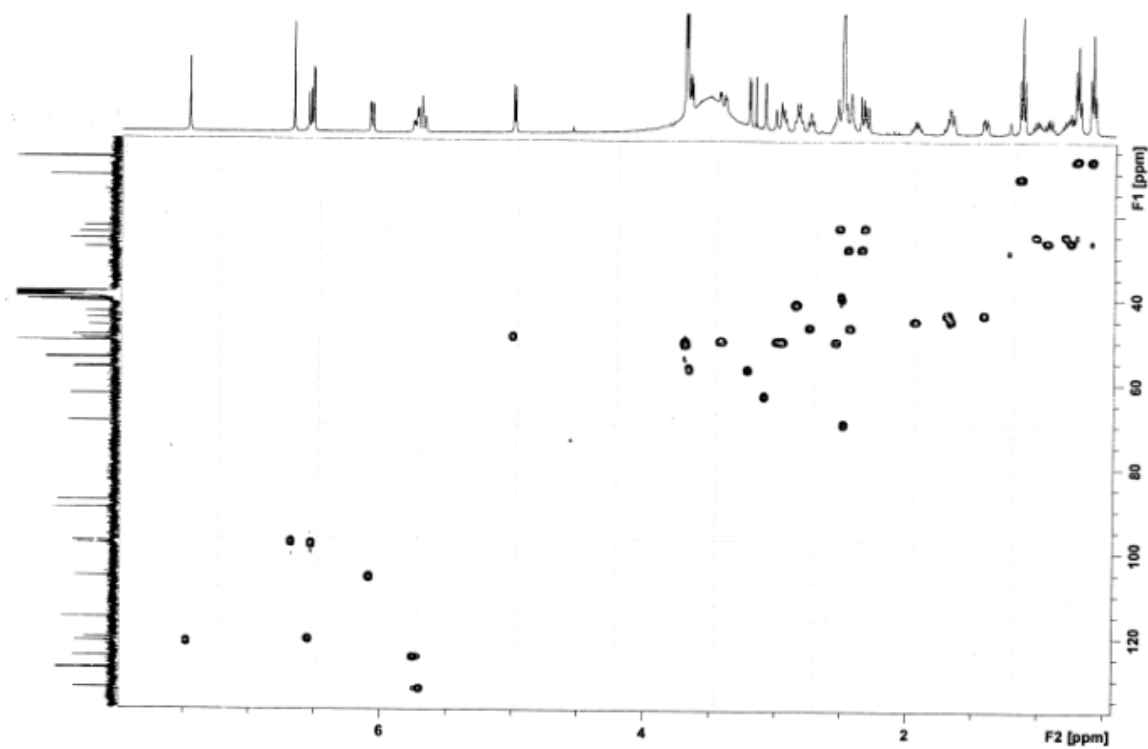


Figure 31S. HMBC of Melosuavine D (**4**) in DMSO.

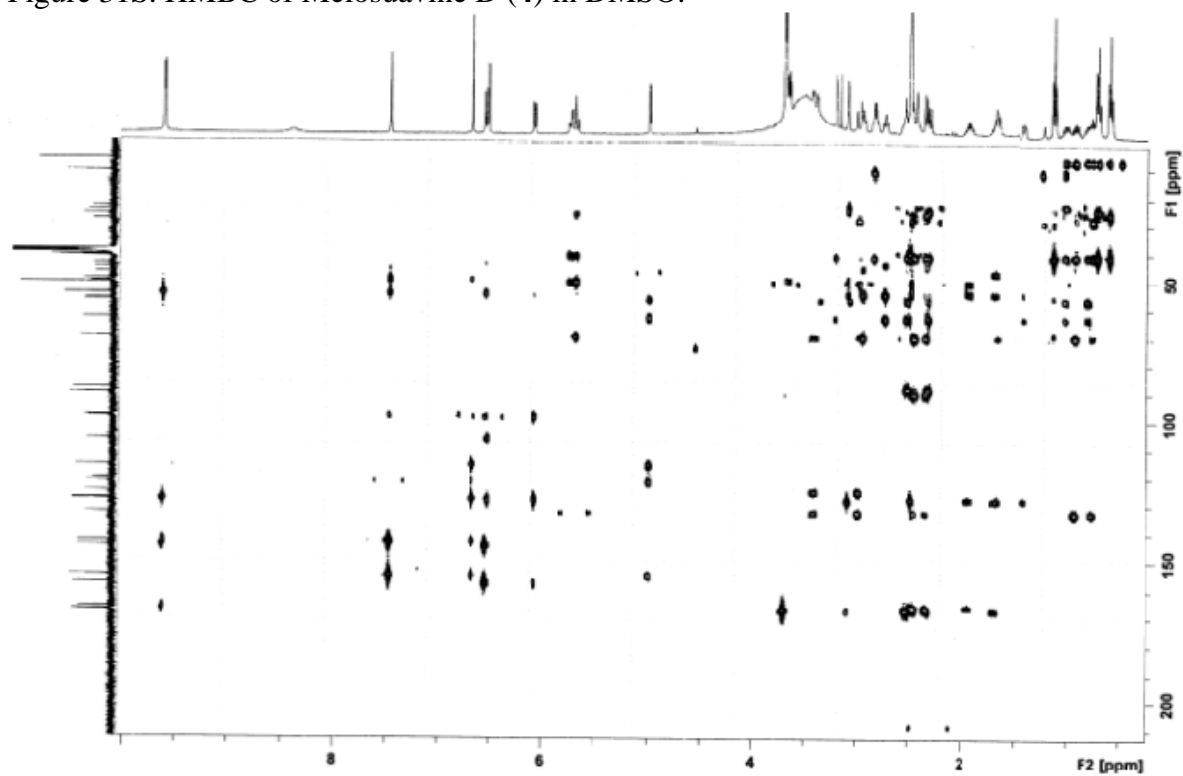


Figure 32S. ^1H - ^1H COSY of Melosuavine D (**4**) in DMSO.

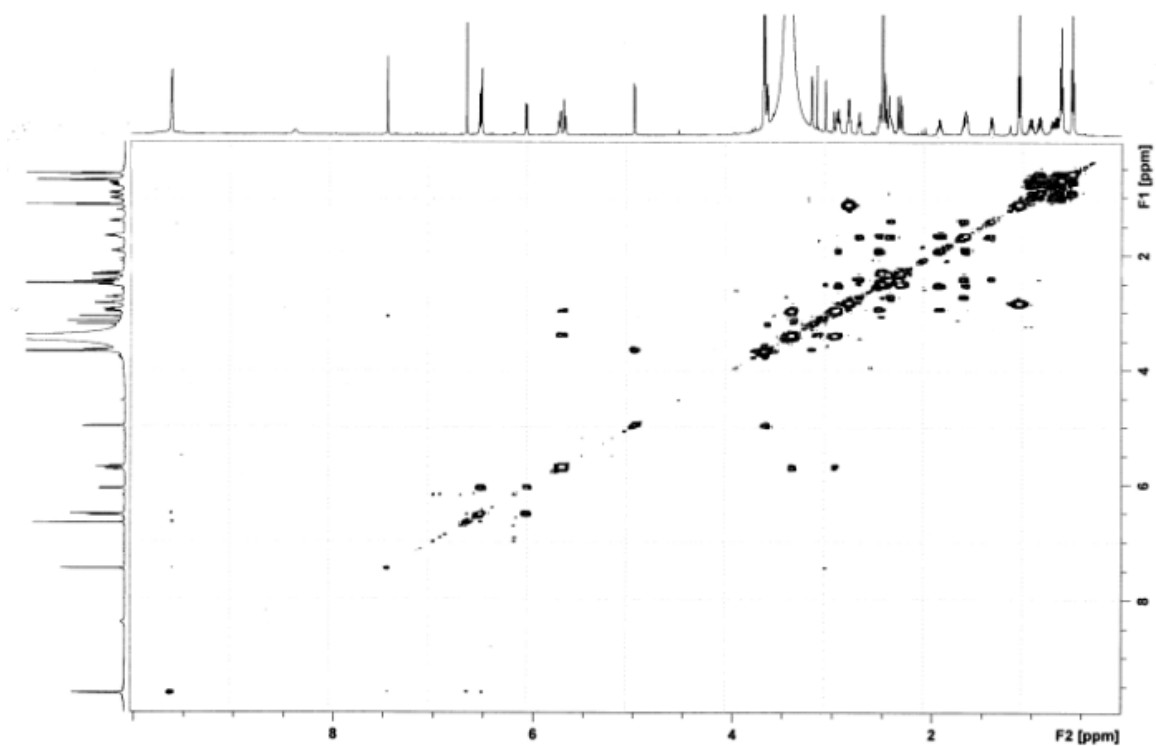


Figure 33S. ROESY of Melosuavine D (**4**) in DMSO.

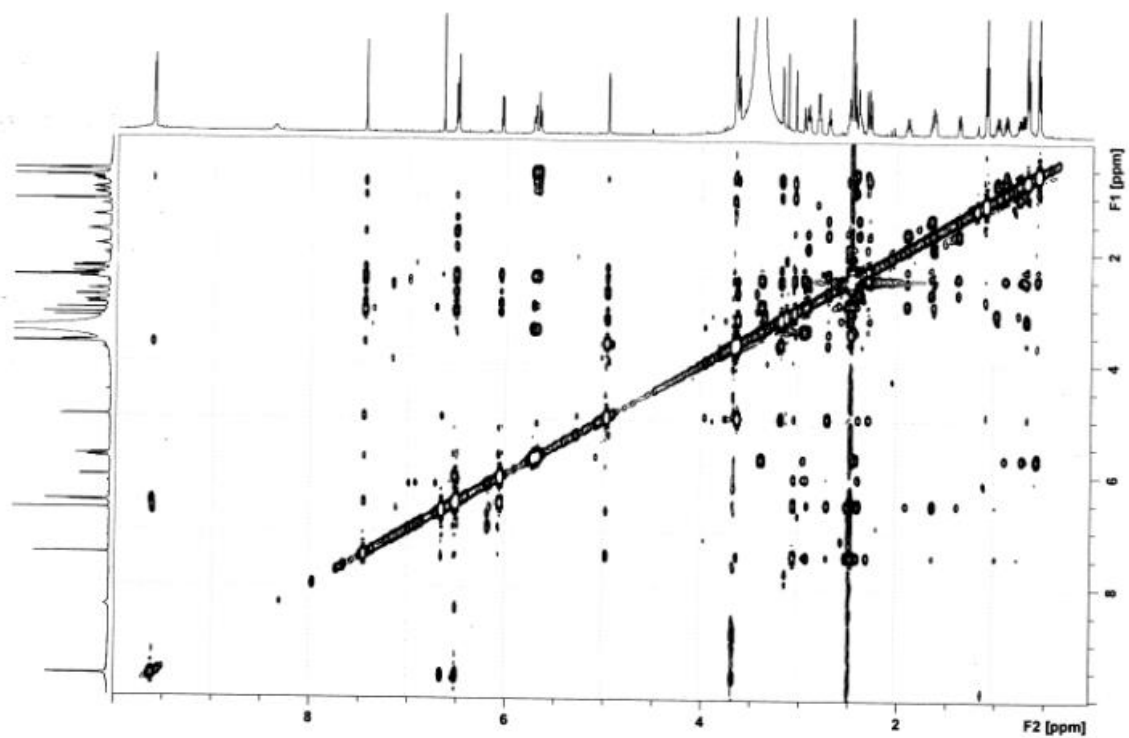


Figure 34S. ESIMS of Melosuavine D (**4**).

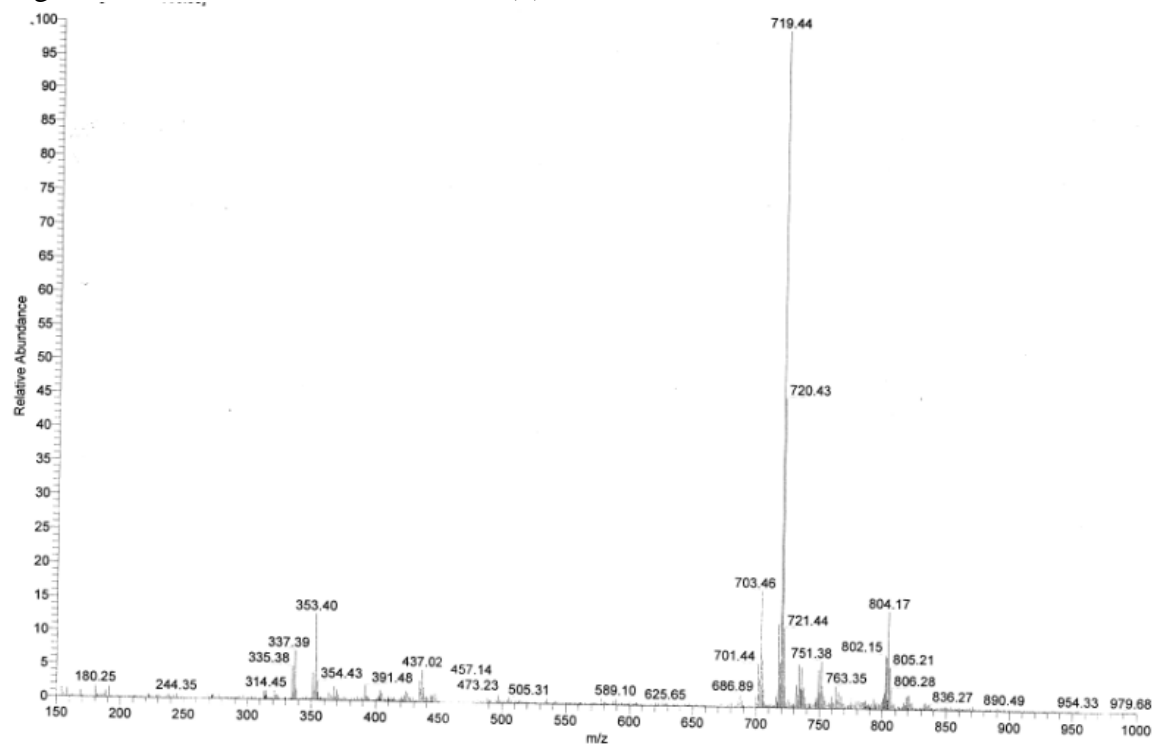


Figure 35S. HRESIMS of Melosuavine D (**4**).

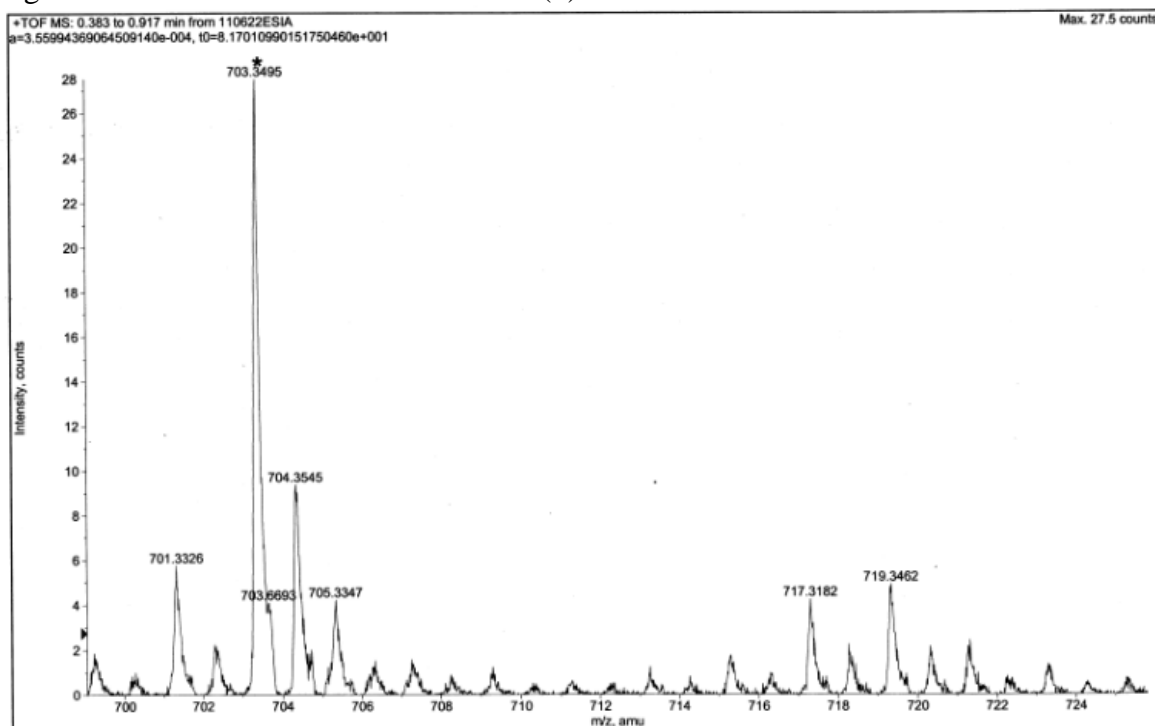


Figure 36S. ^1H NMR of Melosuavine E (**5**) in acetone- d_6 .

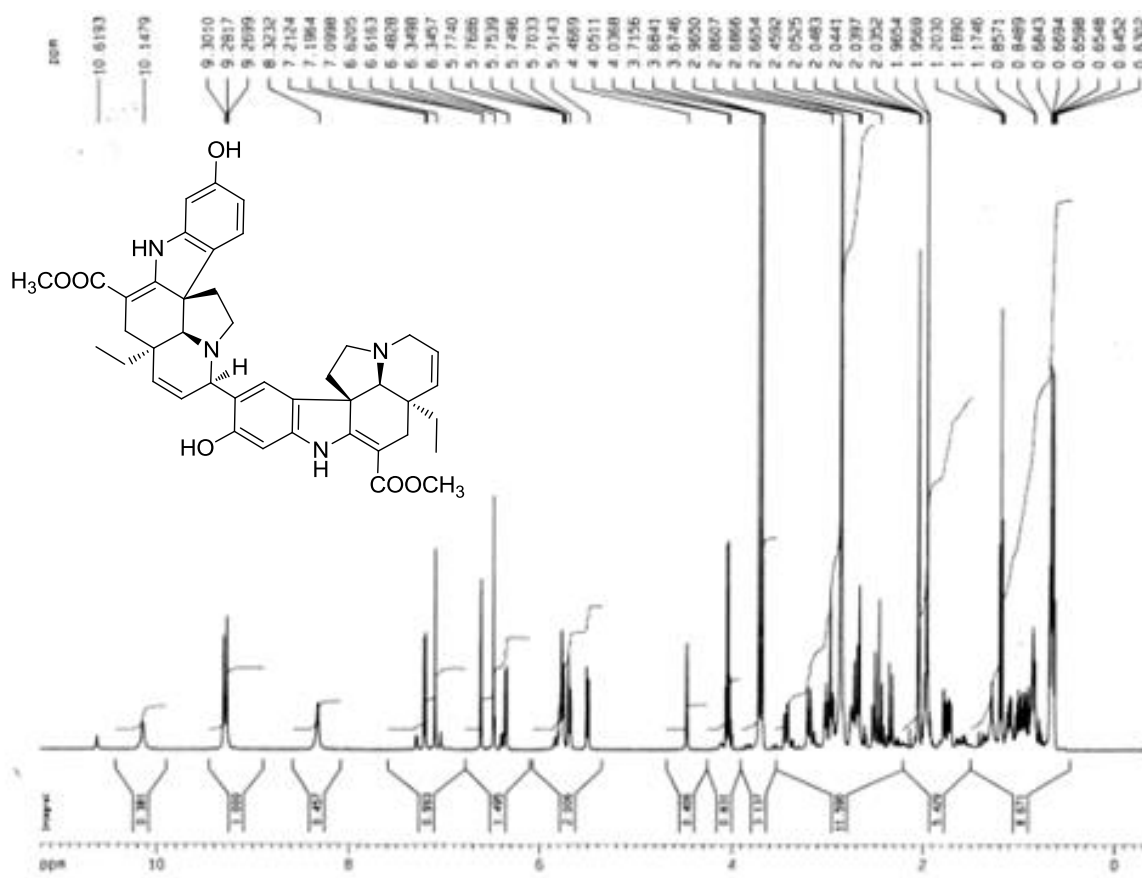


Figure 37S. ^{13}C NMR and DEPT of Melosuavine E (**5**) in acetone- d_6 .

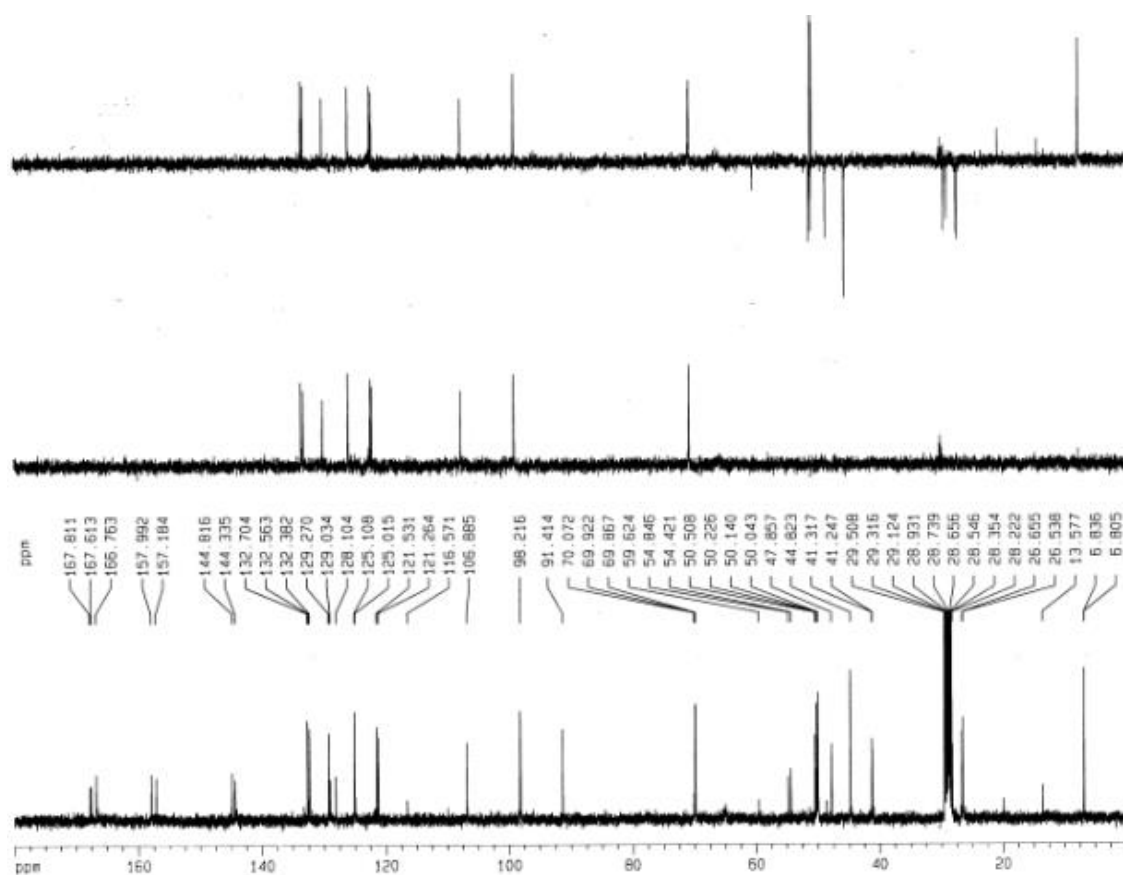


Figure 38S. HSQC of Melosuavine E (**5**) in acetone- d_6 .

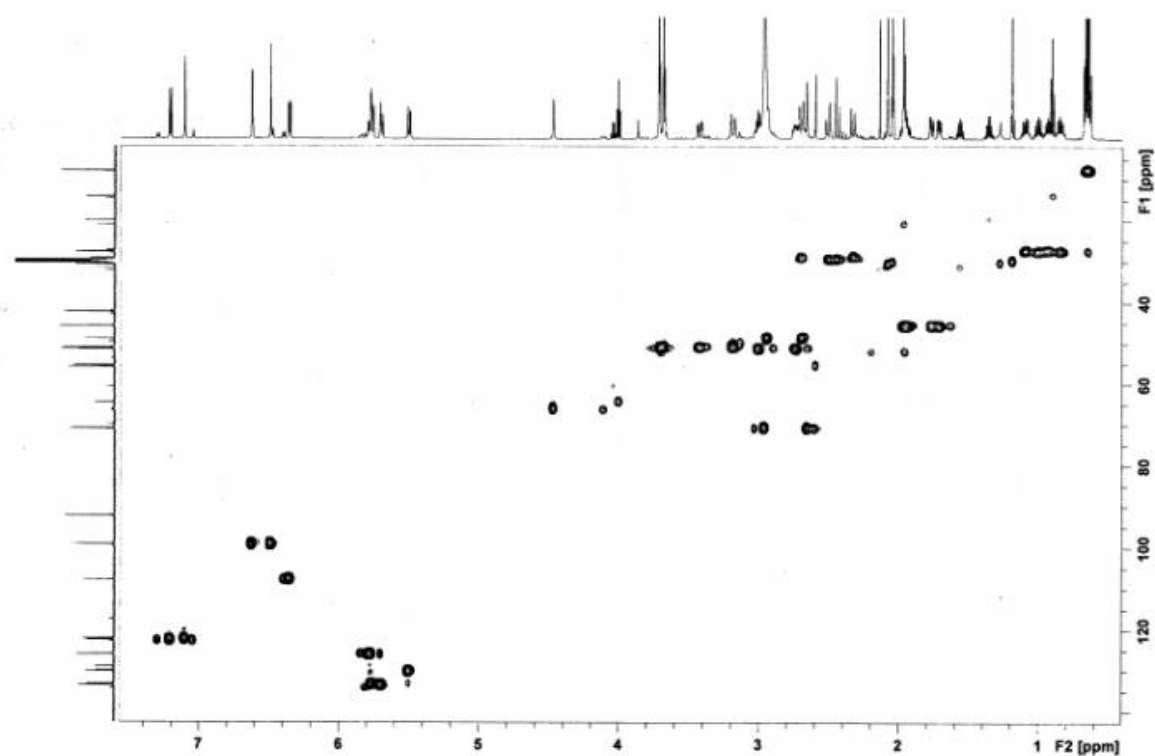


Figure 39S. HMBC of Melosuavine E (**5**) in acetone- d_6 .

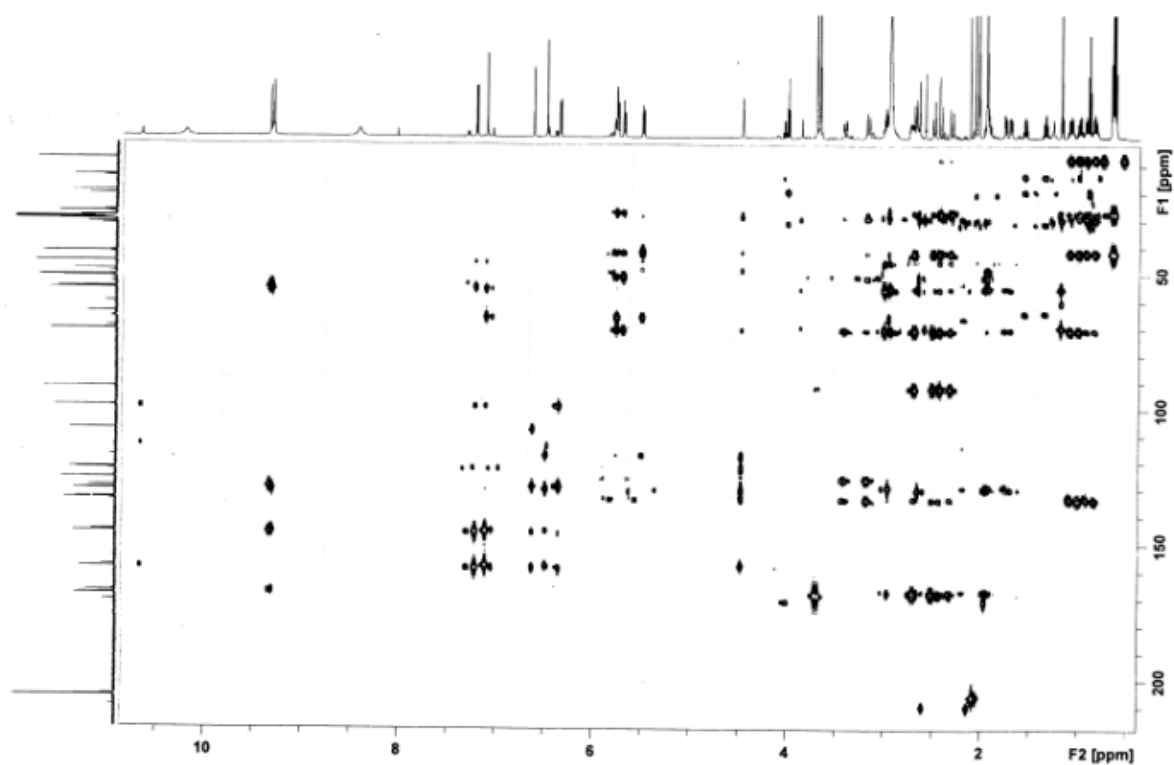


Figure 40S. ^1H - ^1H -ROSY of Melosuavine E (**5**) in acetone- d_6 .

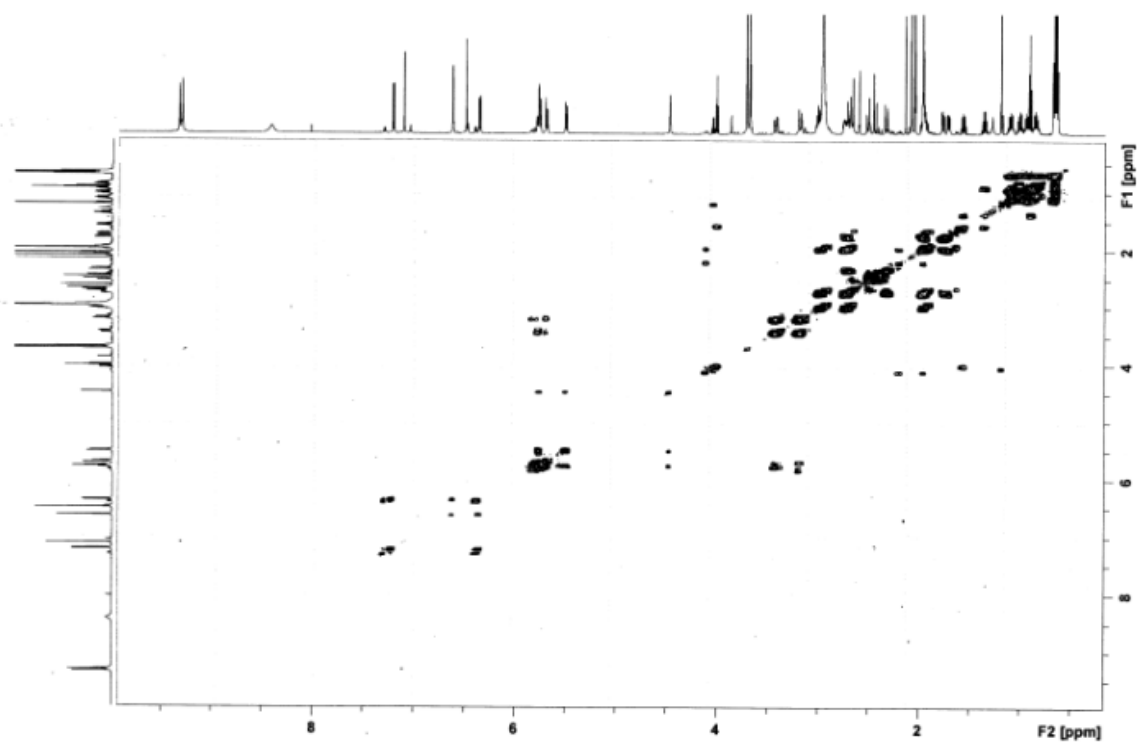


Figure 41S. ROESY of Melosuavine E (**5**) in acetone- d_6 .

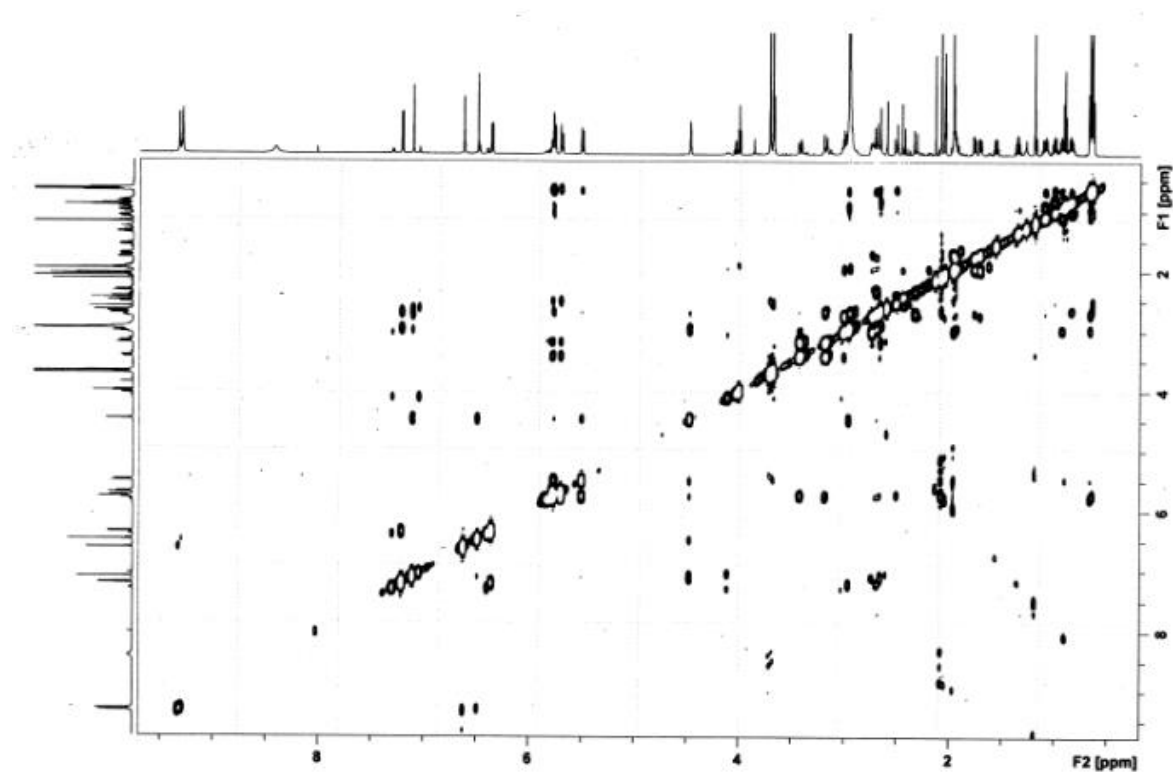


Figure 42S. EIMS of Melosuavine E (**5**).

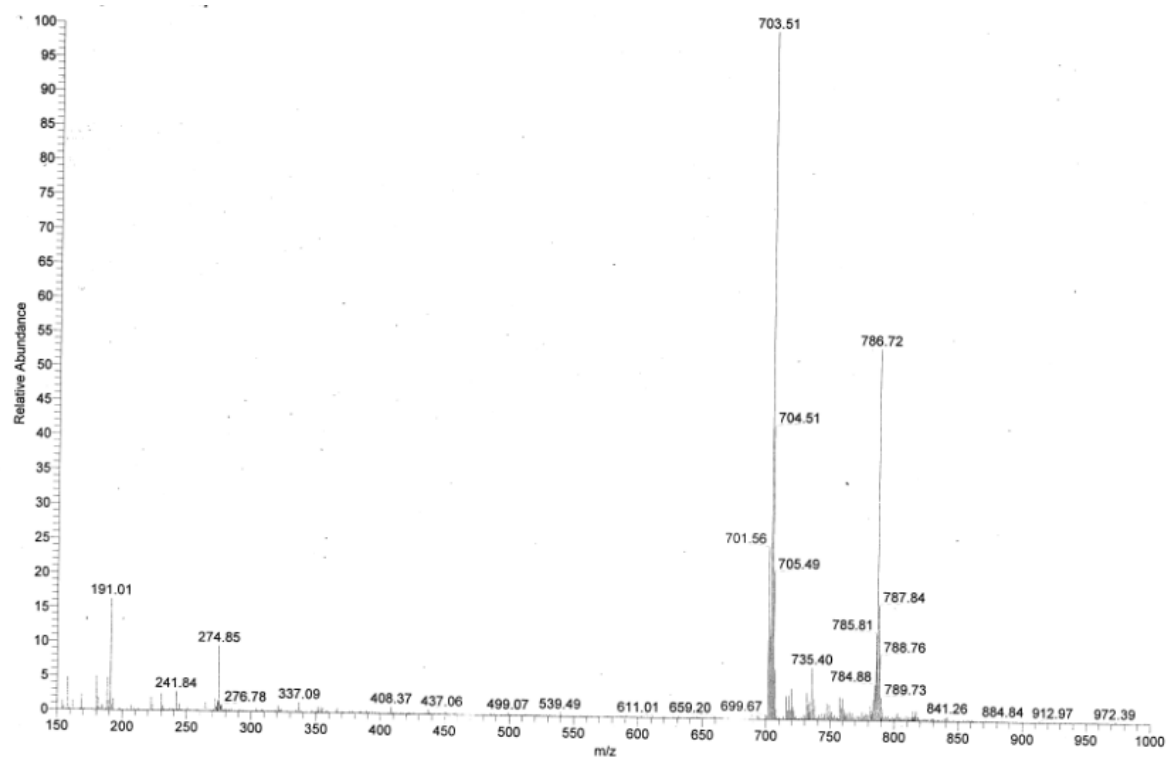


Figure 43S. HREIMS of Melosuavine E (**5**).

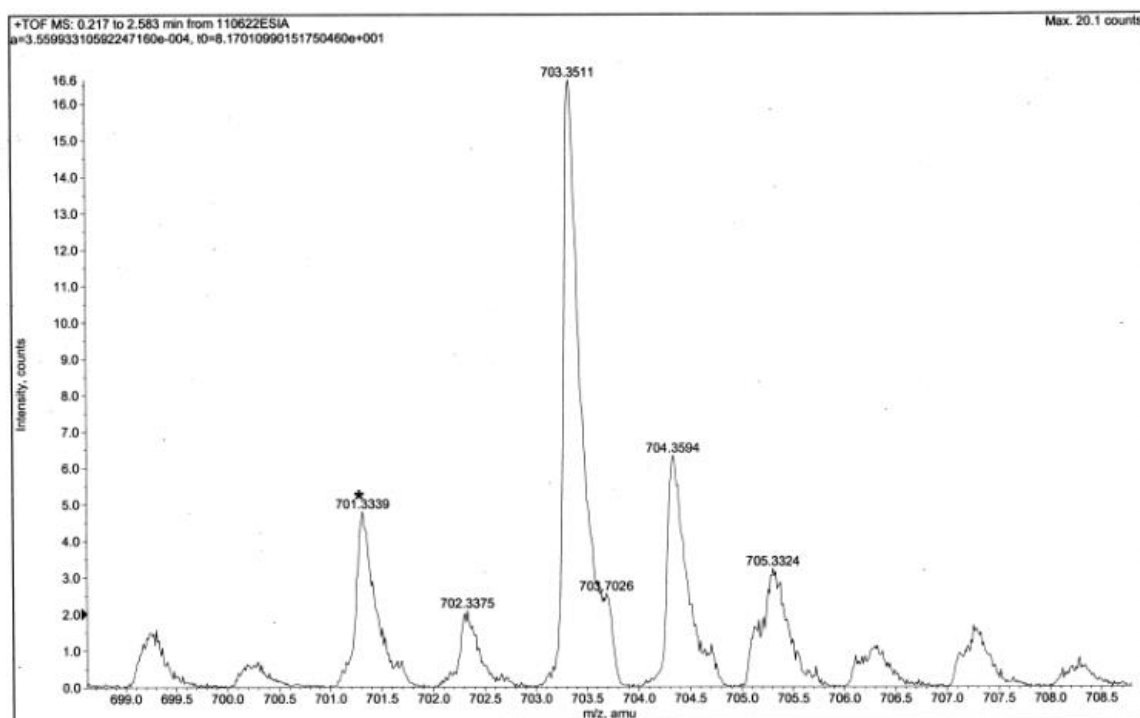


Figure 44S. ^1H NMR of Melosuavine F (**6**) in acetone- d_6 .

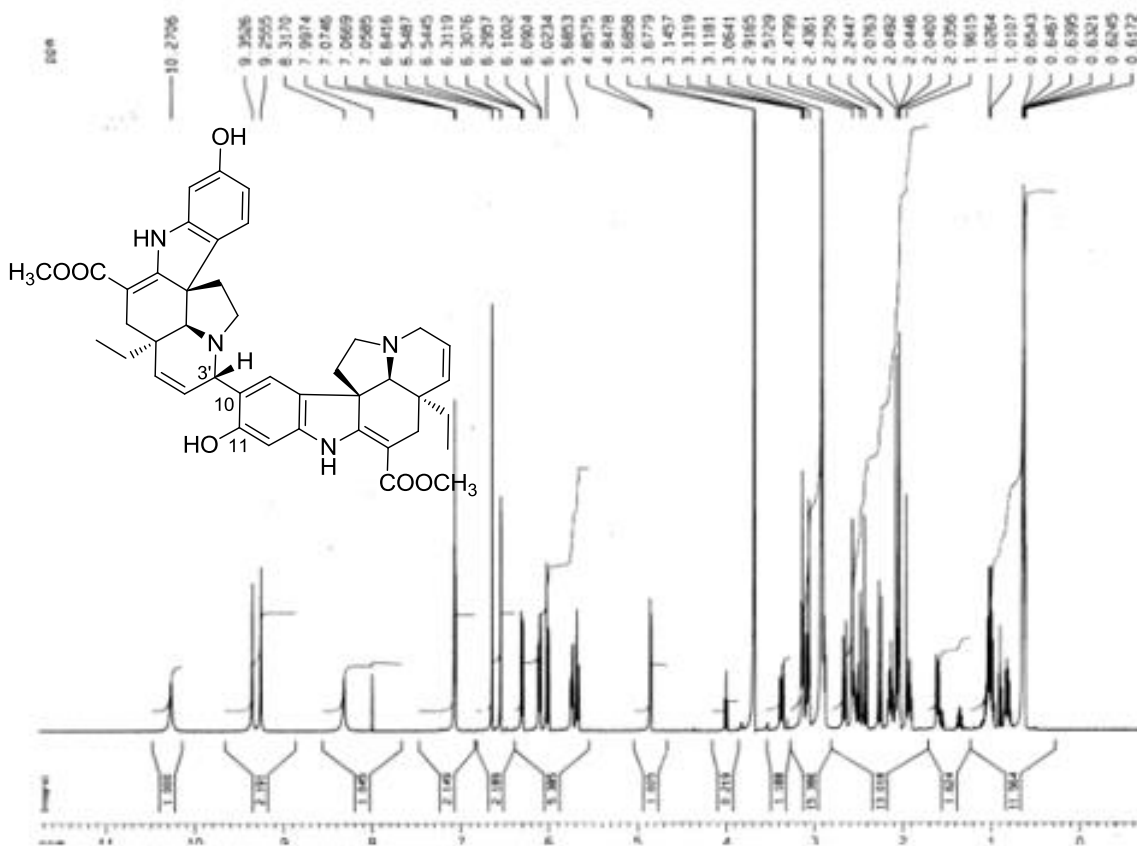


Figure 45S. ^{13}C NMR and DEPT of Melosuavine F (**6**) in acetone- d_6 .

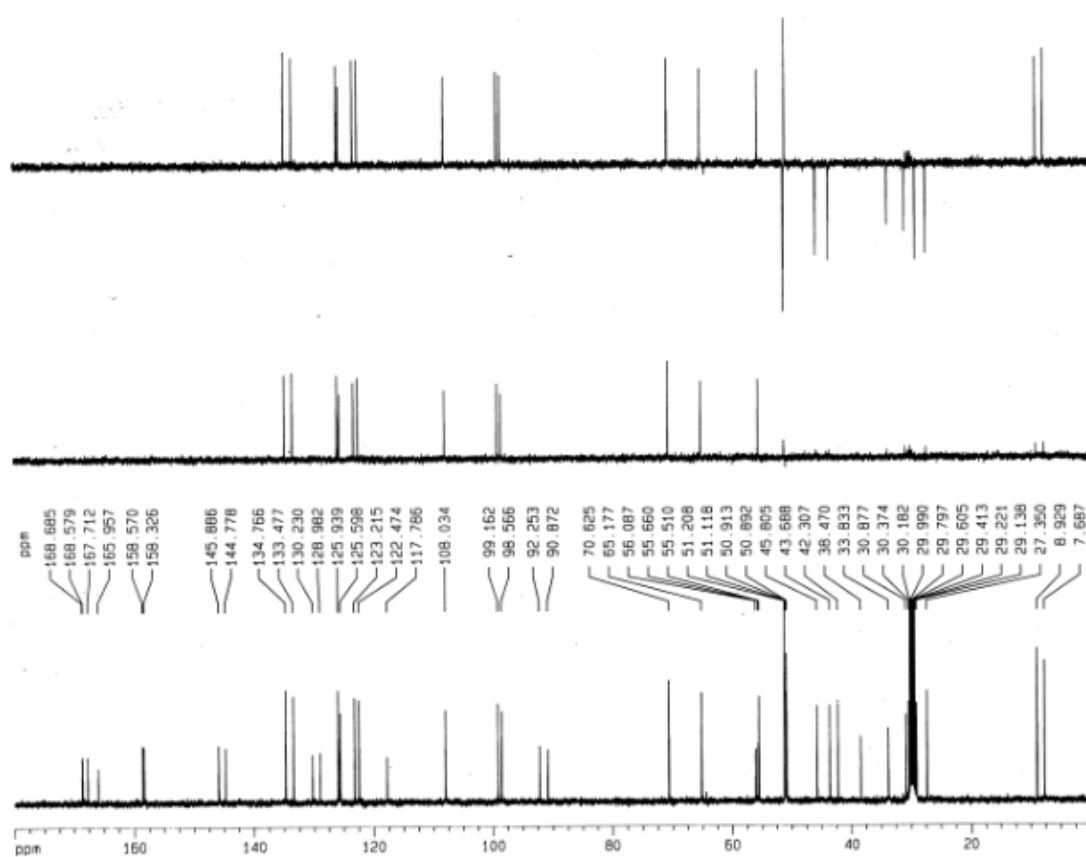


Figure 46S. HSQC of Melosuavine F (**6**) in acetone- d_6 .

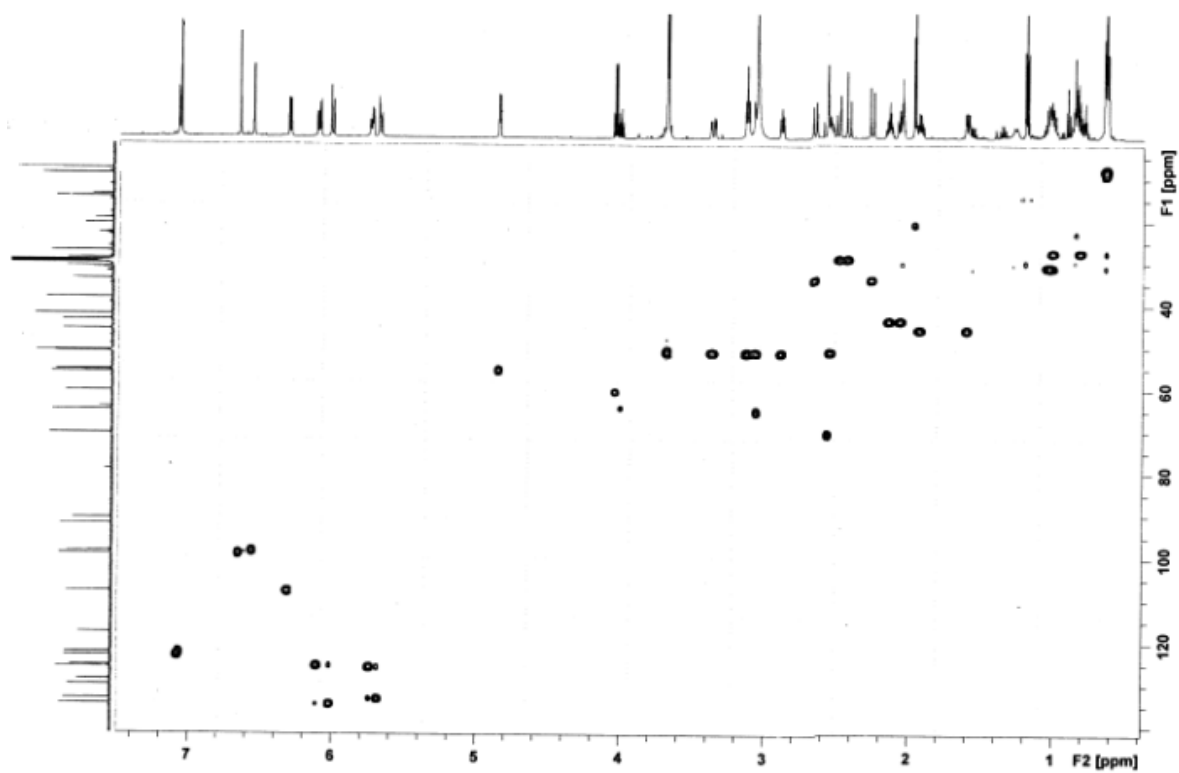


Figure 47S. HMBC of Melosuavine F (**6**) in acetone-*d*₆.

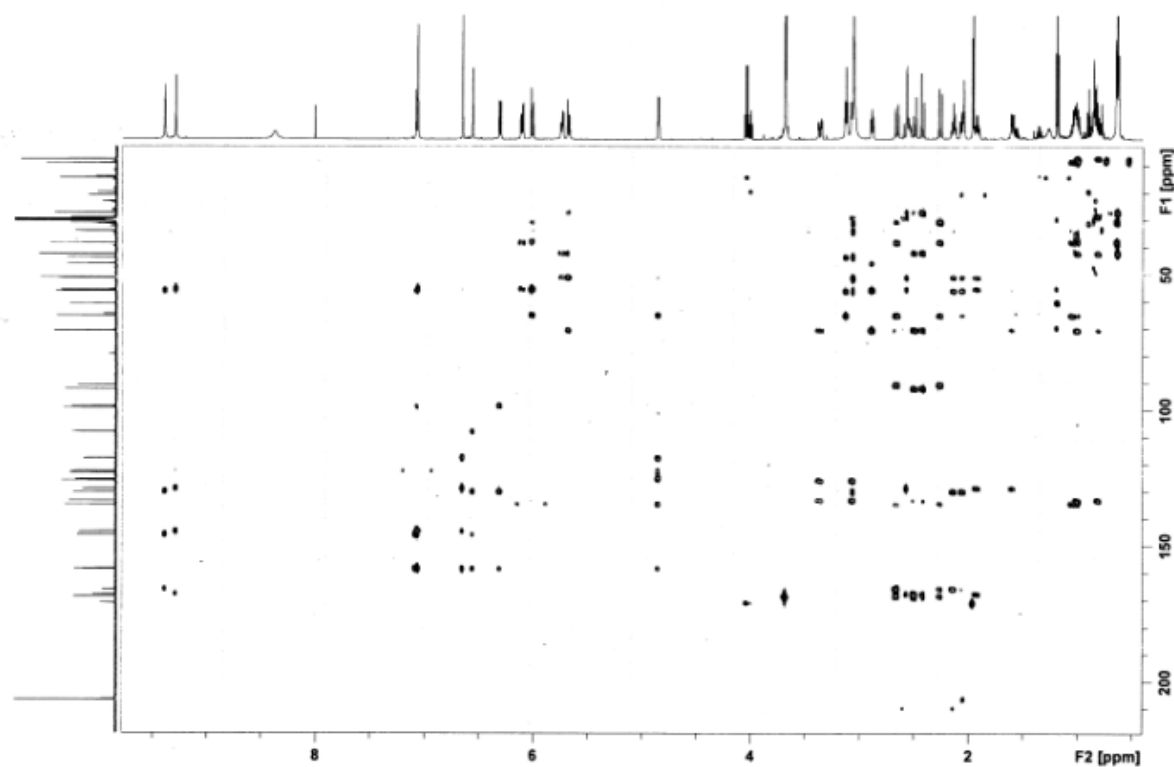


Figure 48S. HREIMS of Melosuavine F (**6**).

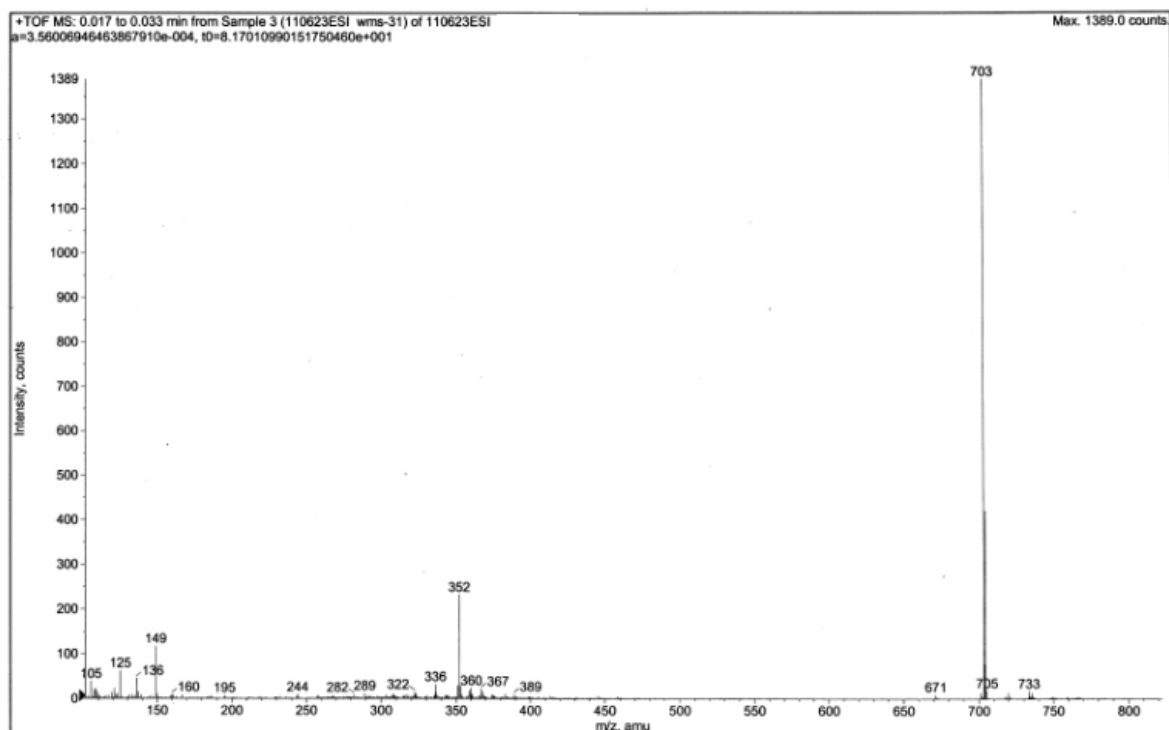


Figure 49S. HREIMS of Melosuavine F (6).

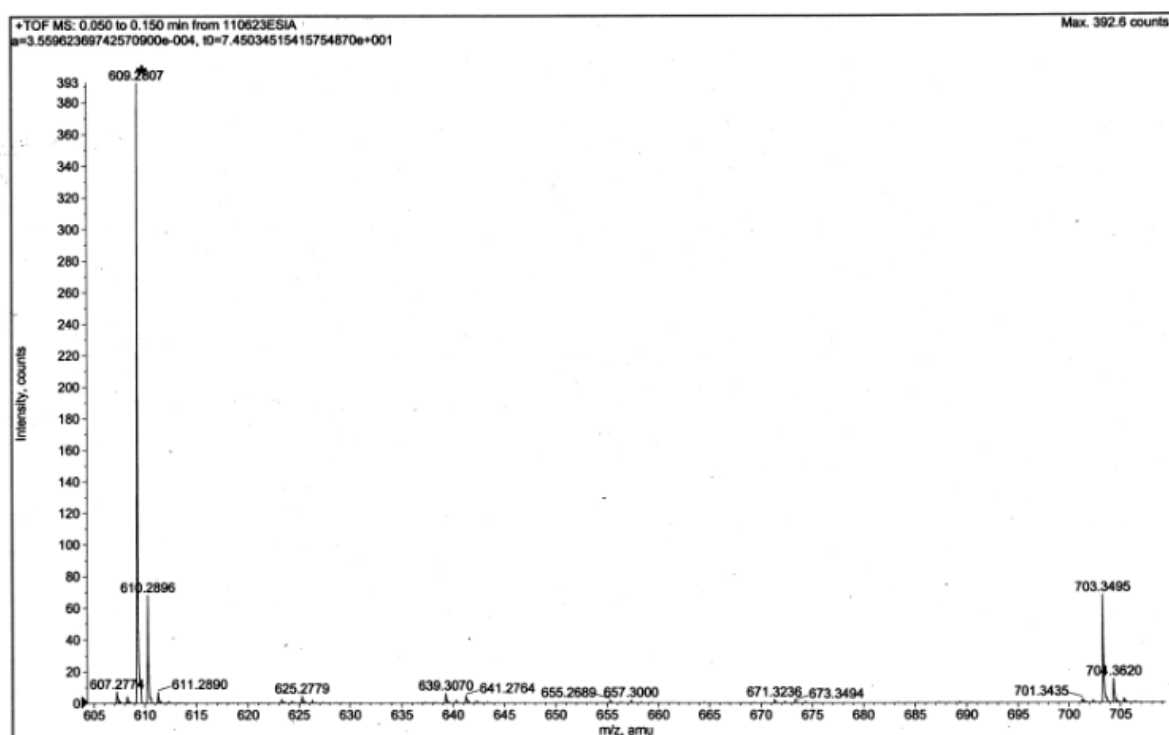


Figure 50S. ^1H NMR of Melosuavine G (7) in acetone- d_6 .

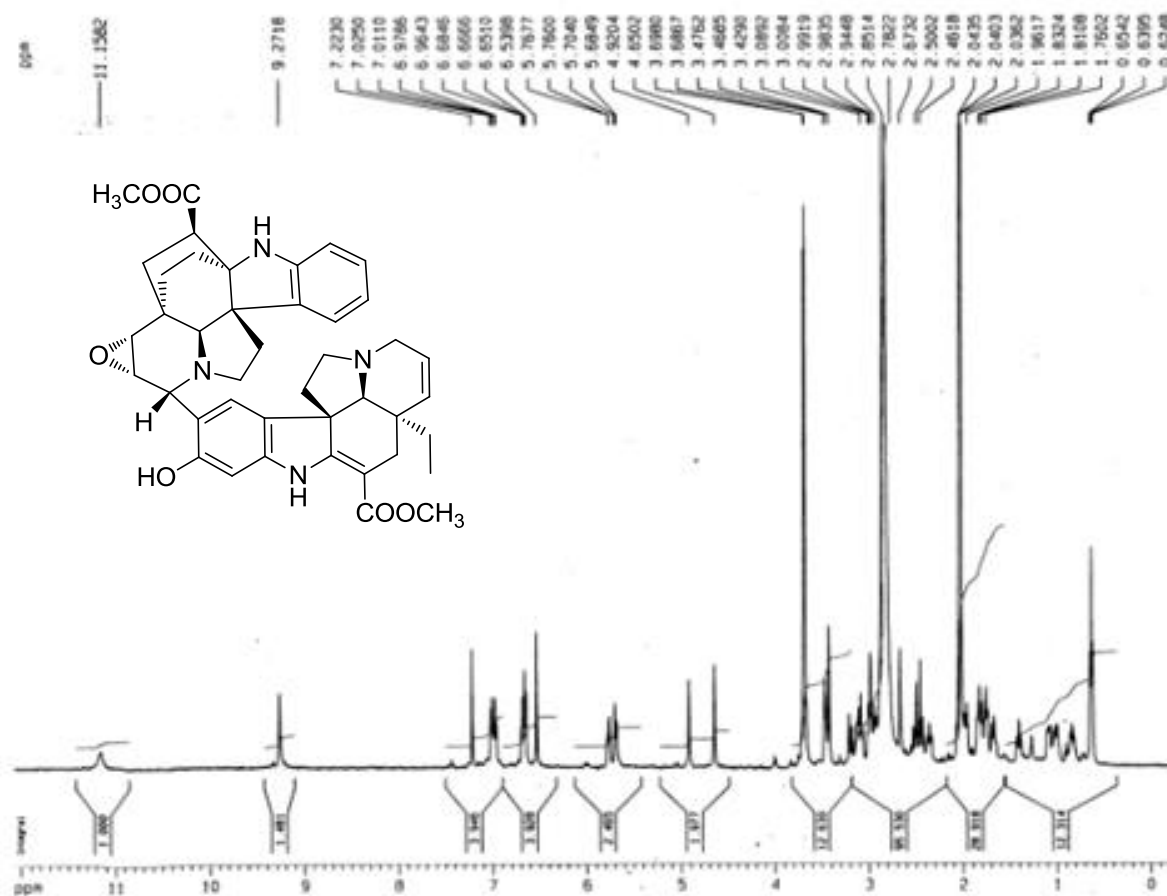


Figure 51S. ^{13}C NMR and DEPT of Melosuavine G (**7**) in acetone- d_6 .

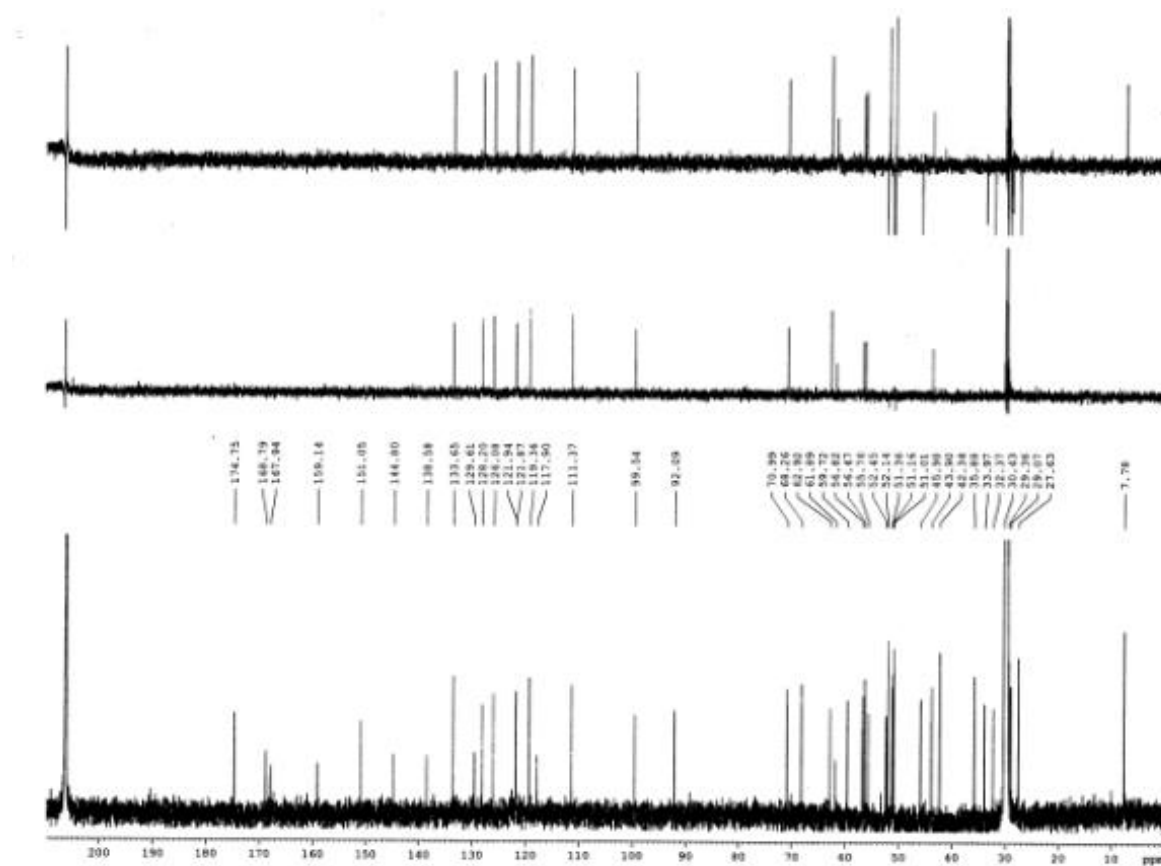


Figure 52S. HSQC of Melosuavine G (**7**) in acetone- d_6 .

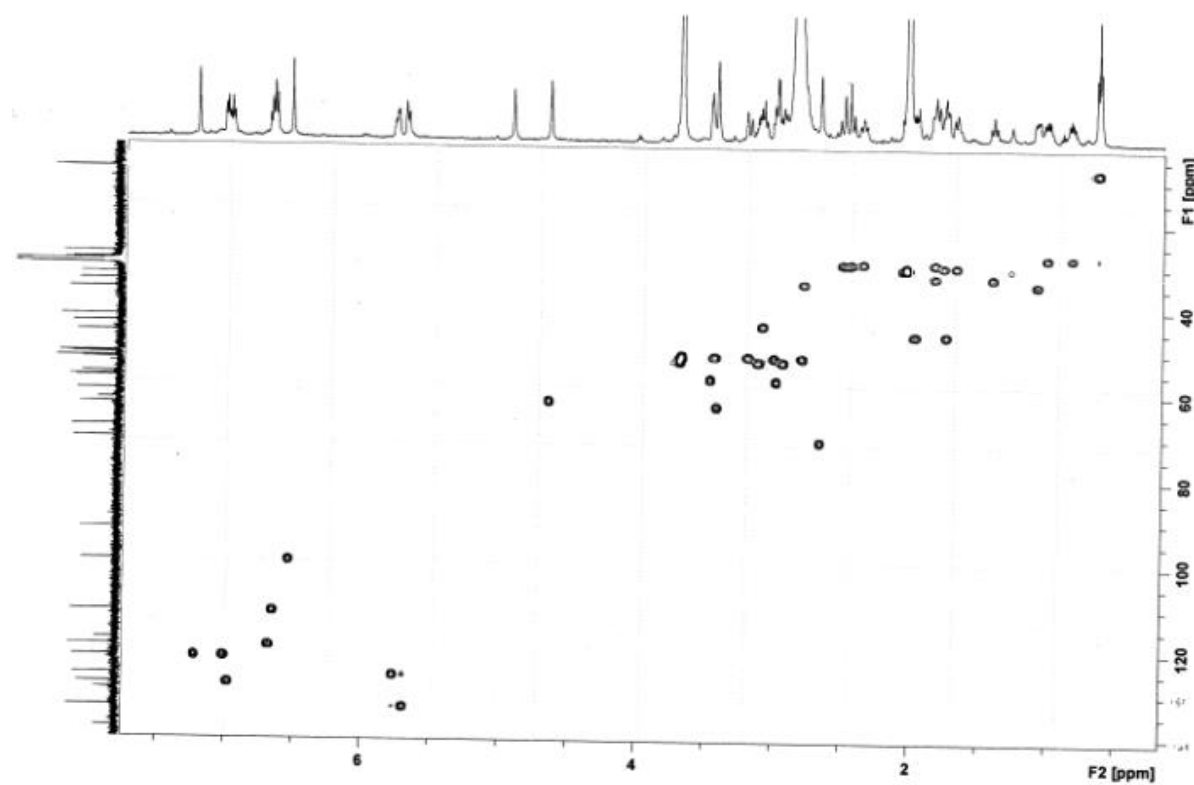


Figure 53S. HMBC of Melosuavine G (7) in acetone- d_6 .

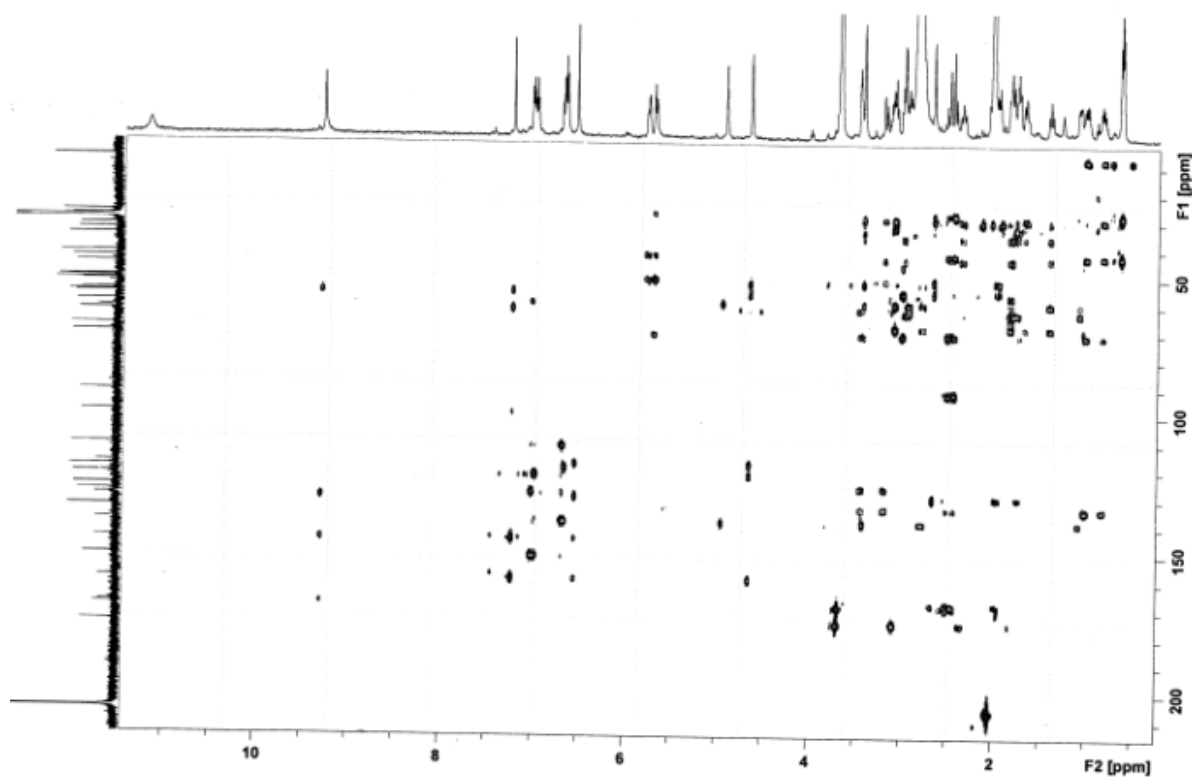


Figure 54S. ^1H - ^1H -COSY of Melosuavine G (7) in acetone- d_6 .

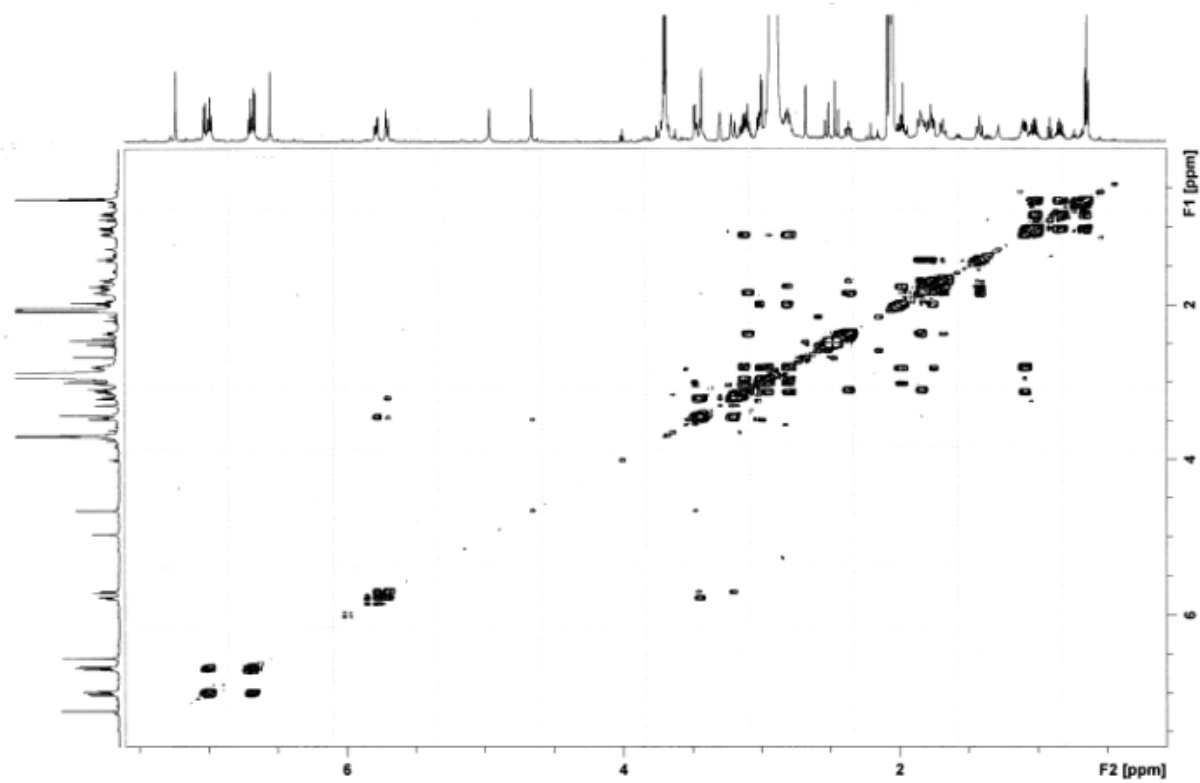


Figure 55S. ROESY of Melosuavine G (**7**) in acetone- d_6 .

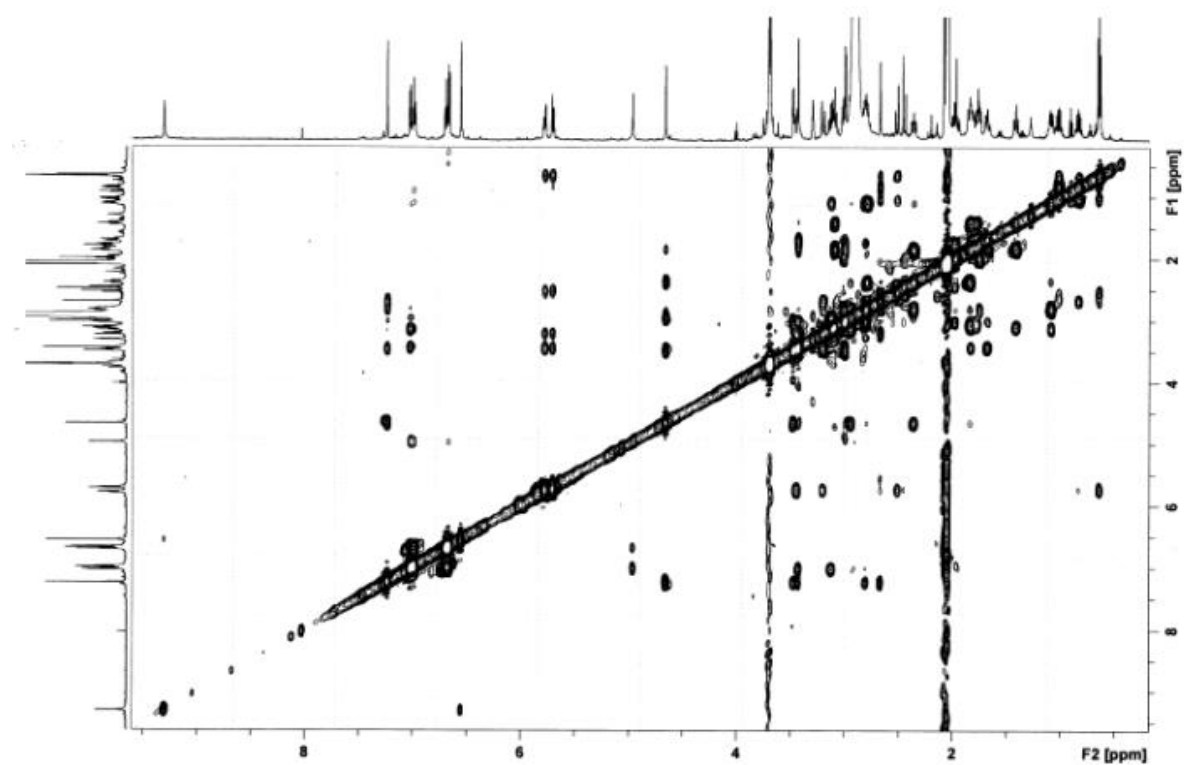


Figure 56S. ESIMS of Melosuavine G (**7**).

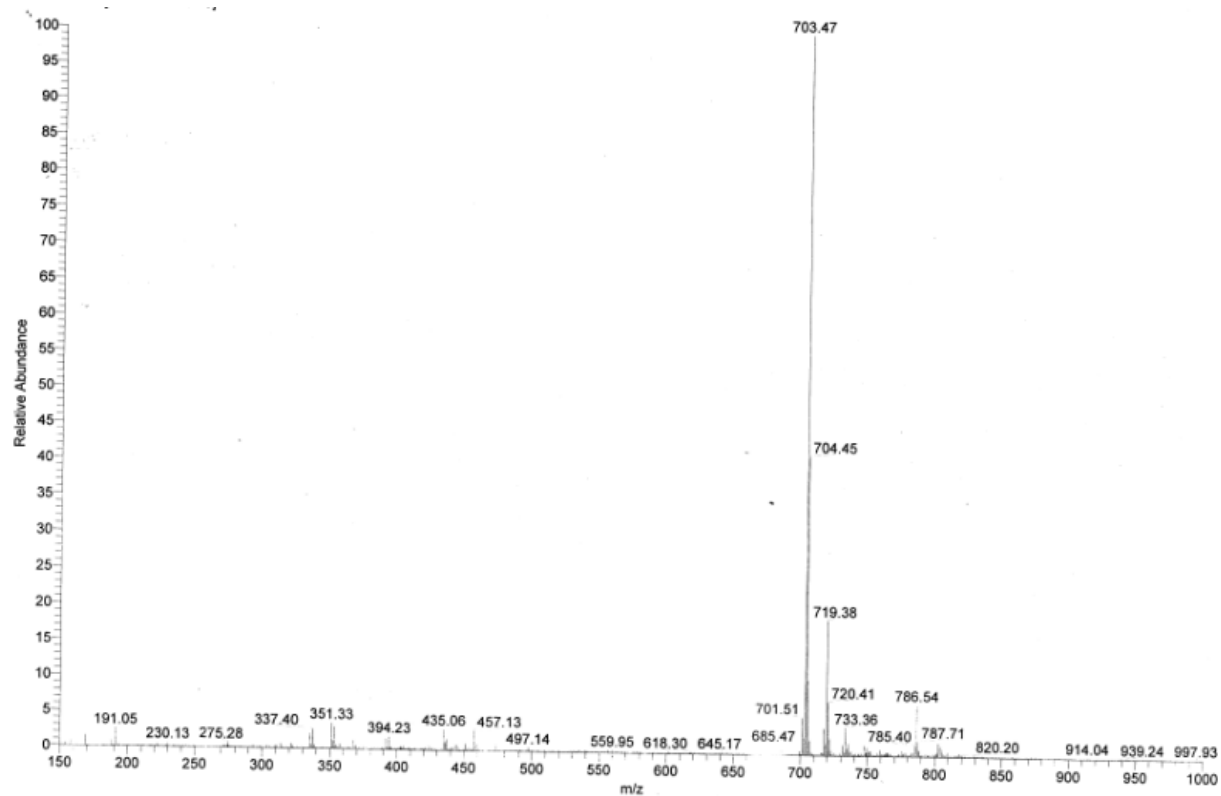


Figure 57S. HRESIMS of Melosuavine G (7).

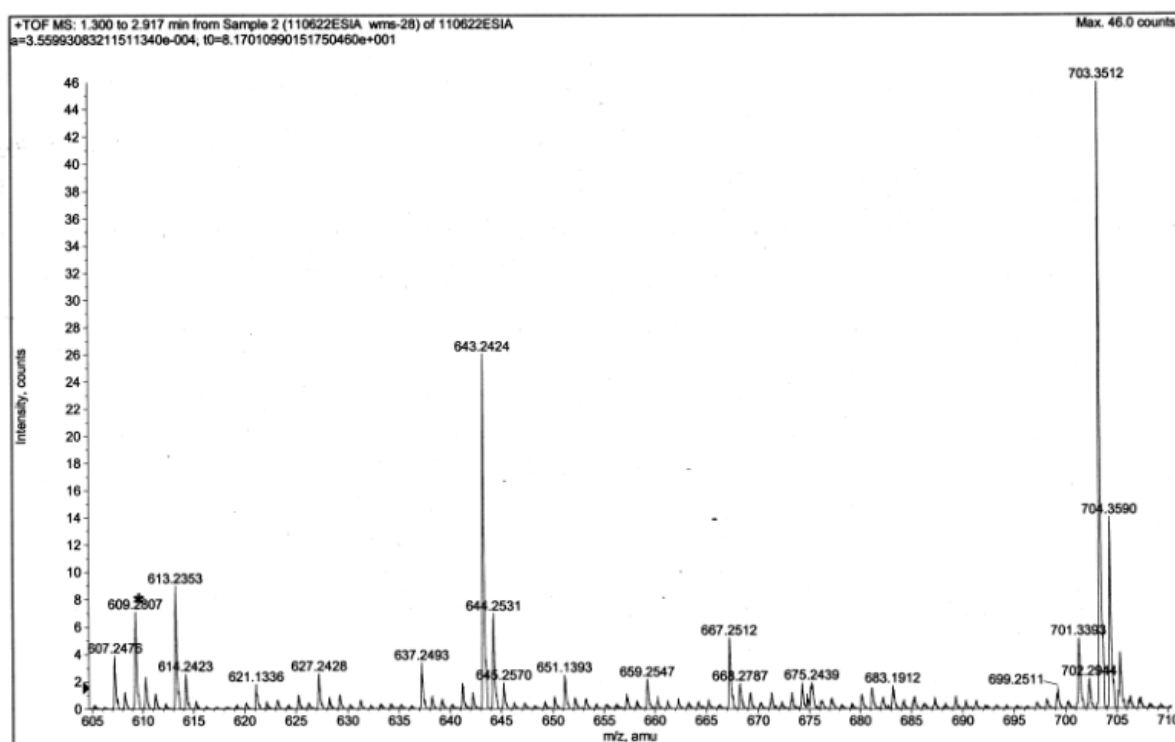


Figure 58S. ^1H NMR of Melosuavine H (**8**) in acetone- d_6 .

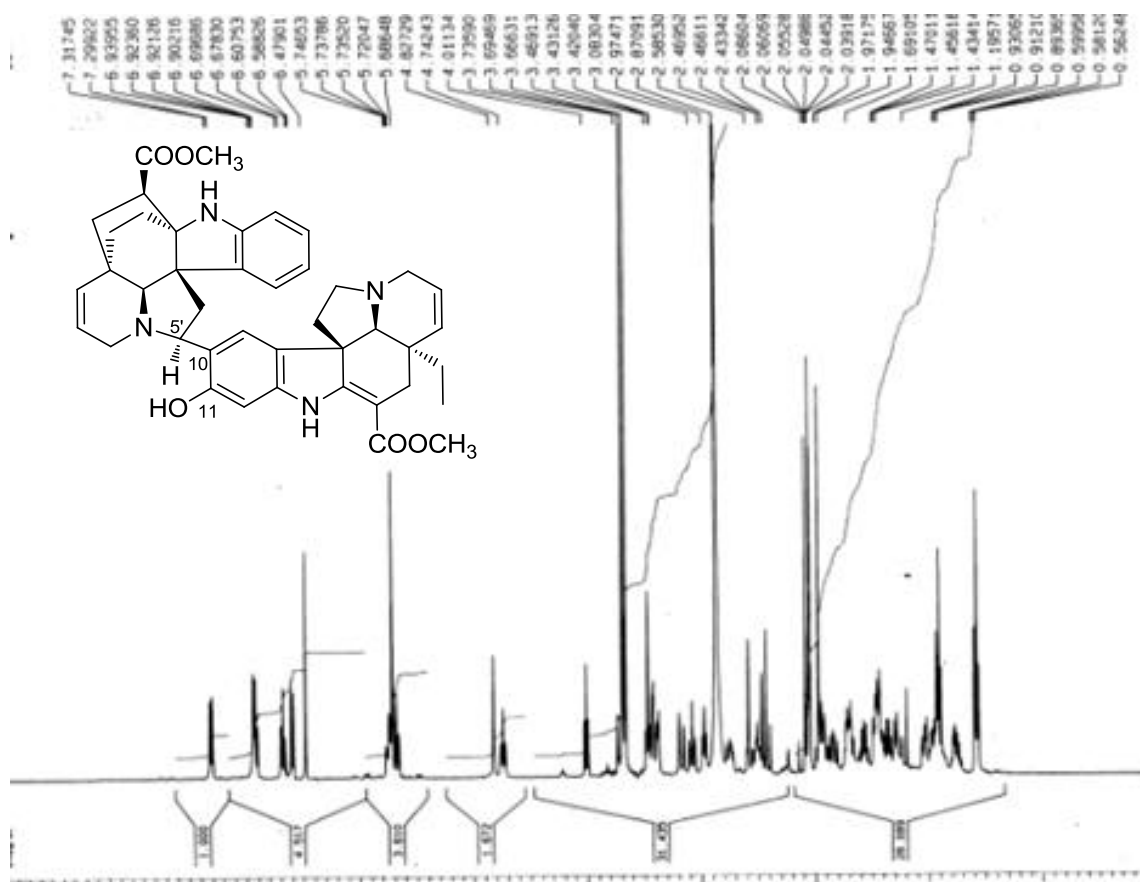


Figure 59S. ^{13}C NMR and DEPT of Melosuavine H (**8**) in acetone- d_6 .

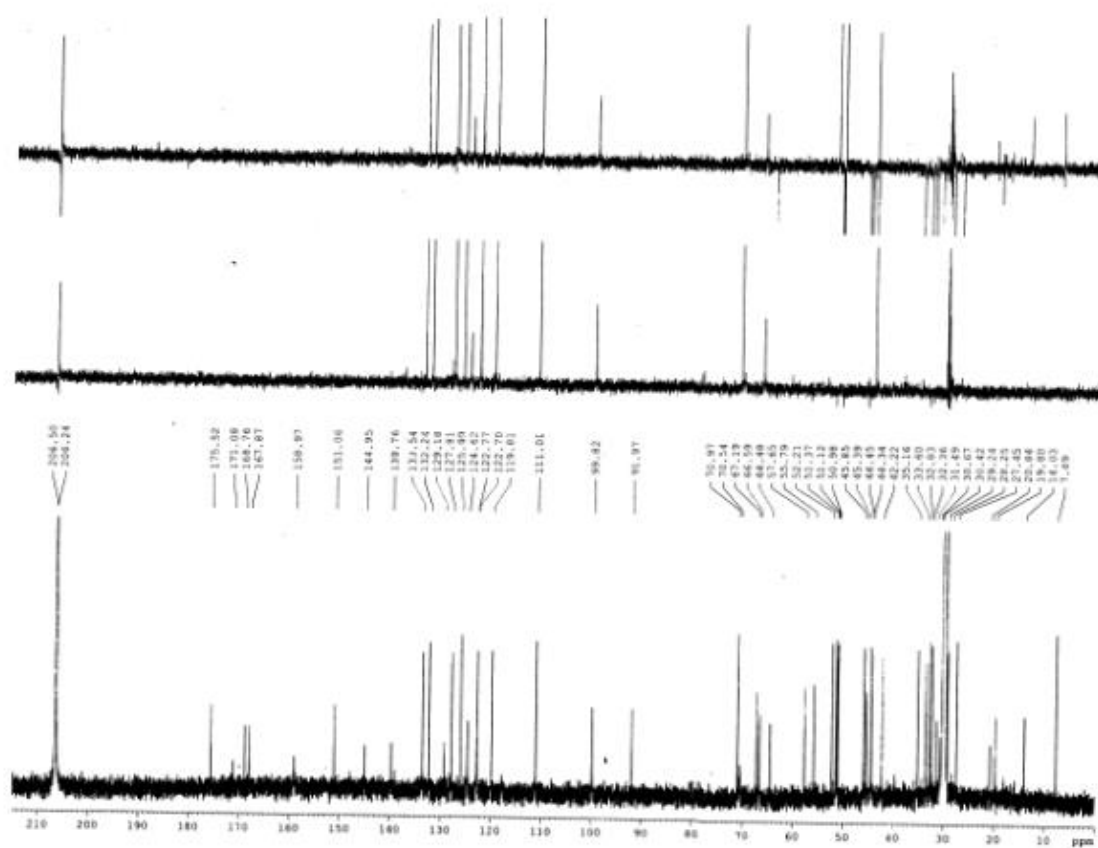


Figure 60S. HSQC of Melosuavine H (**8**) in acetone- d_6 .

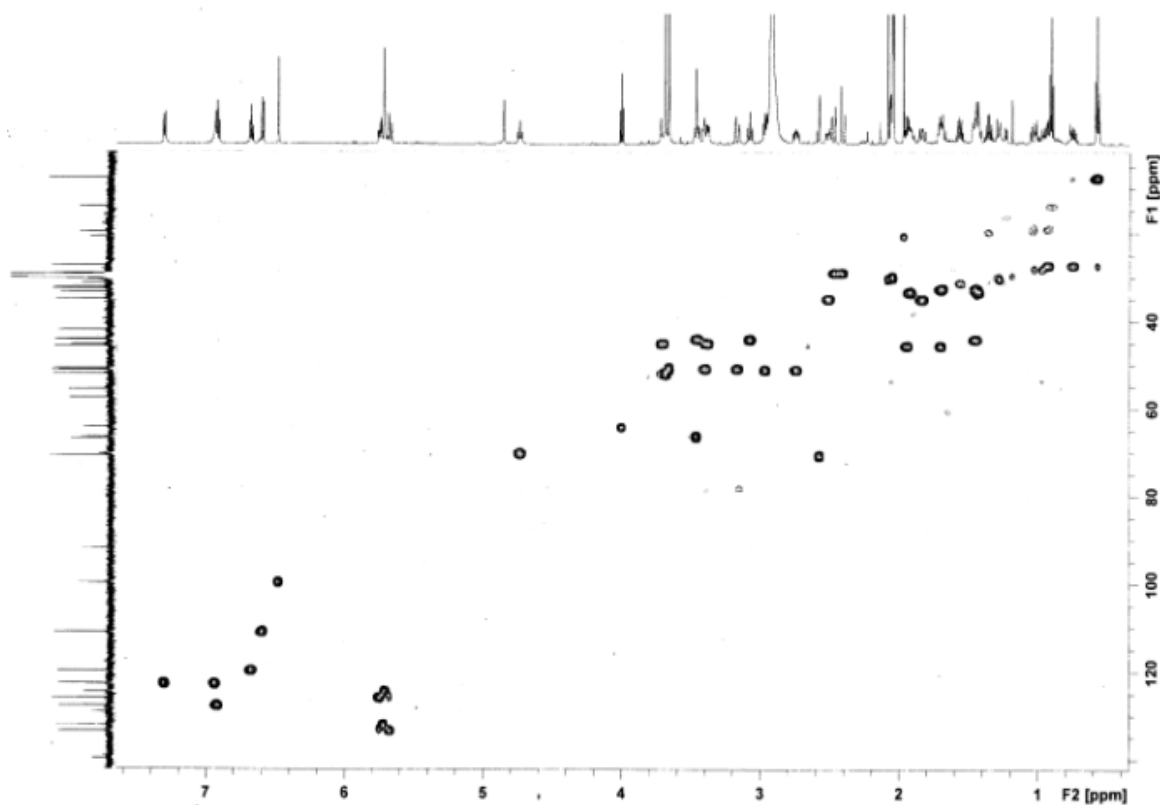


Figure 61S. HMBC of Melosuavine H (**8**) in acetone- d_6 .

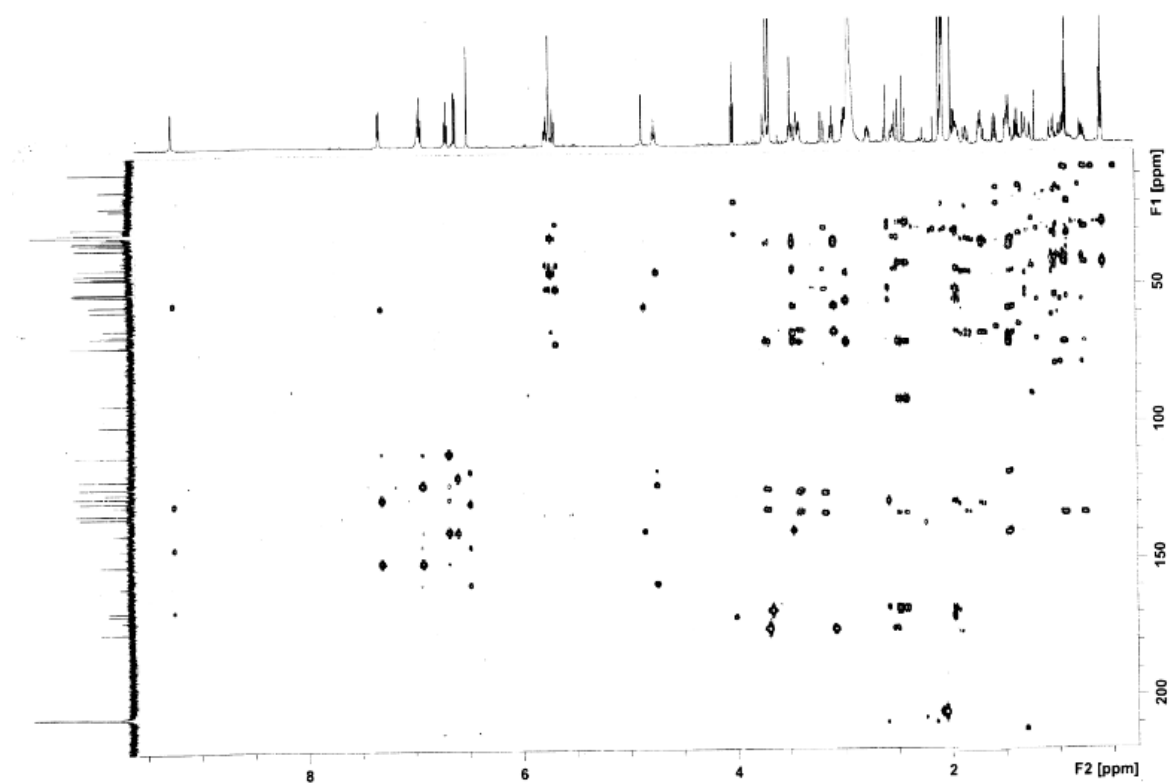


Figure 62S. ROESY of Melosuavine H (**8**) in acetone- d_6 .

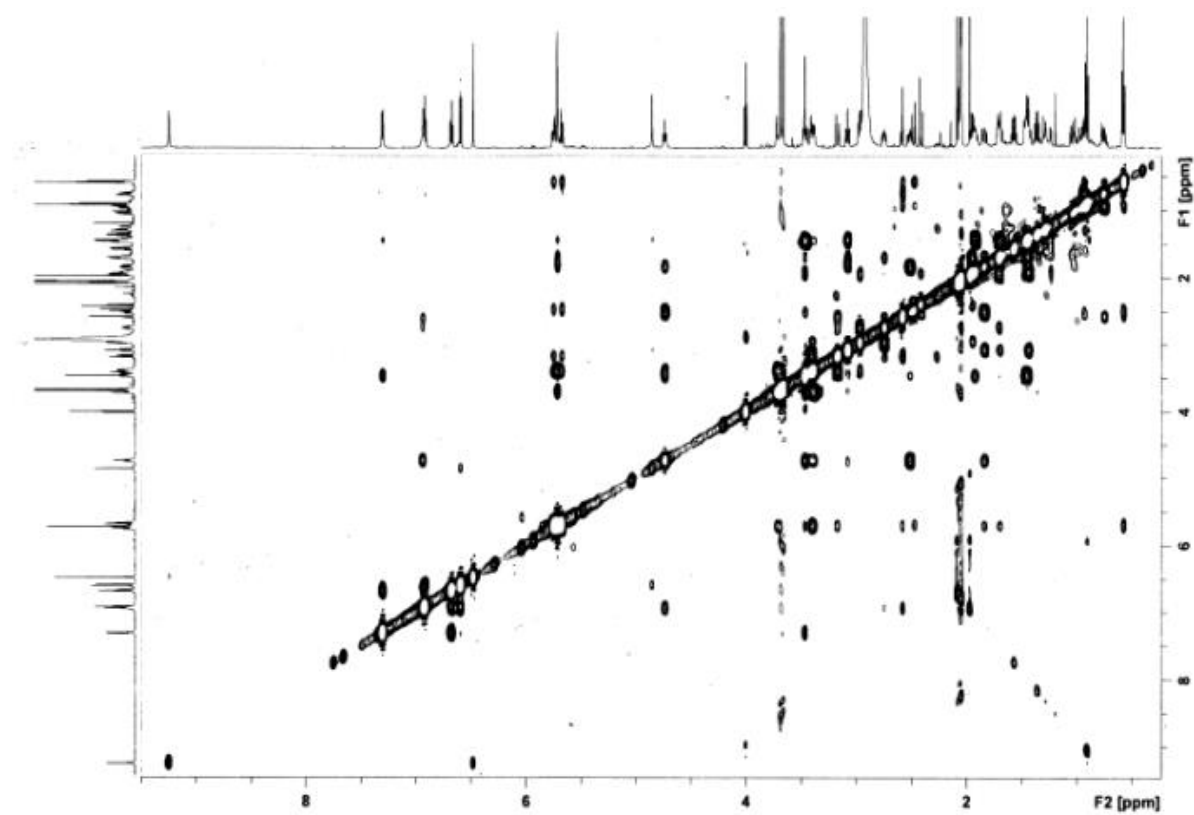


Figure 63S. ESIMS of Melosuavine H (**8**).

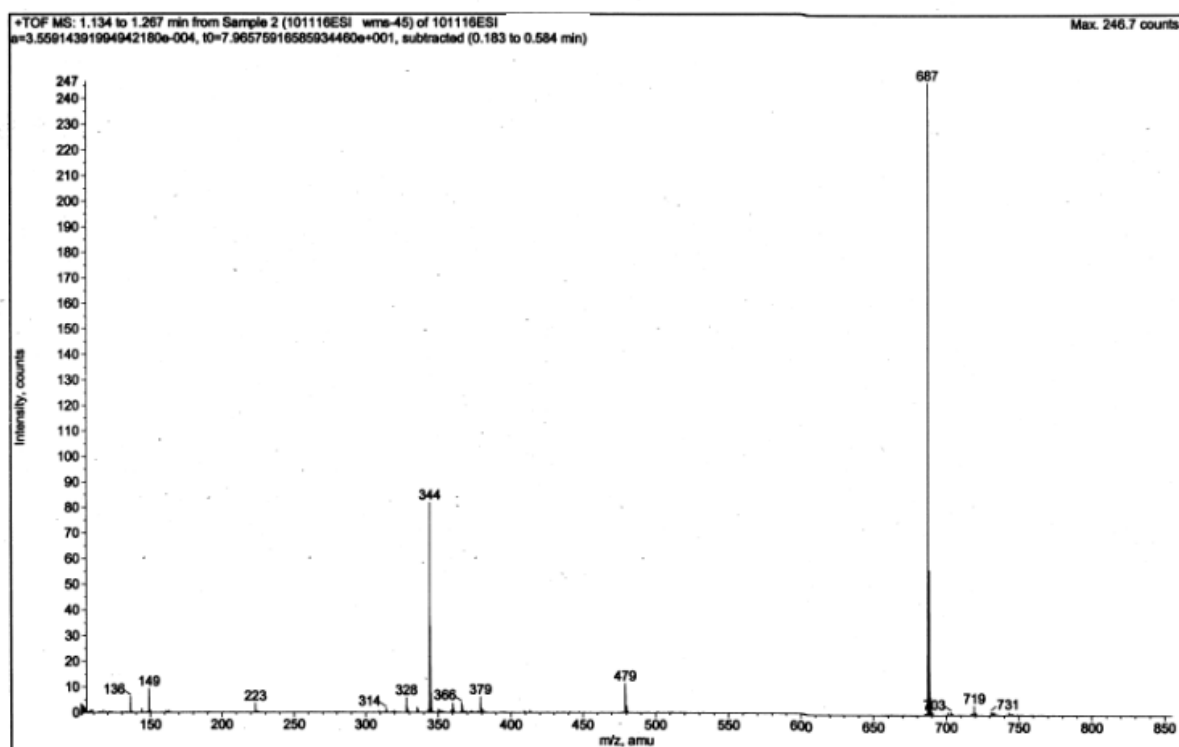


Figure 64S. HRESIMS of Melosuavine H (**8**).

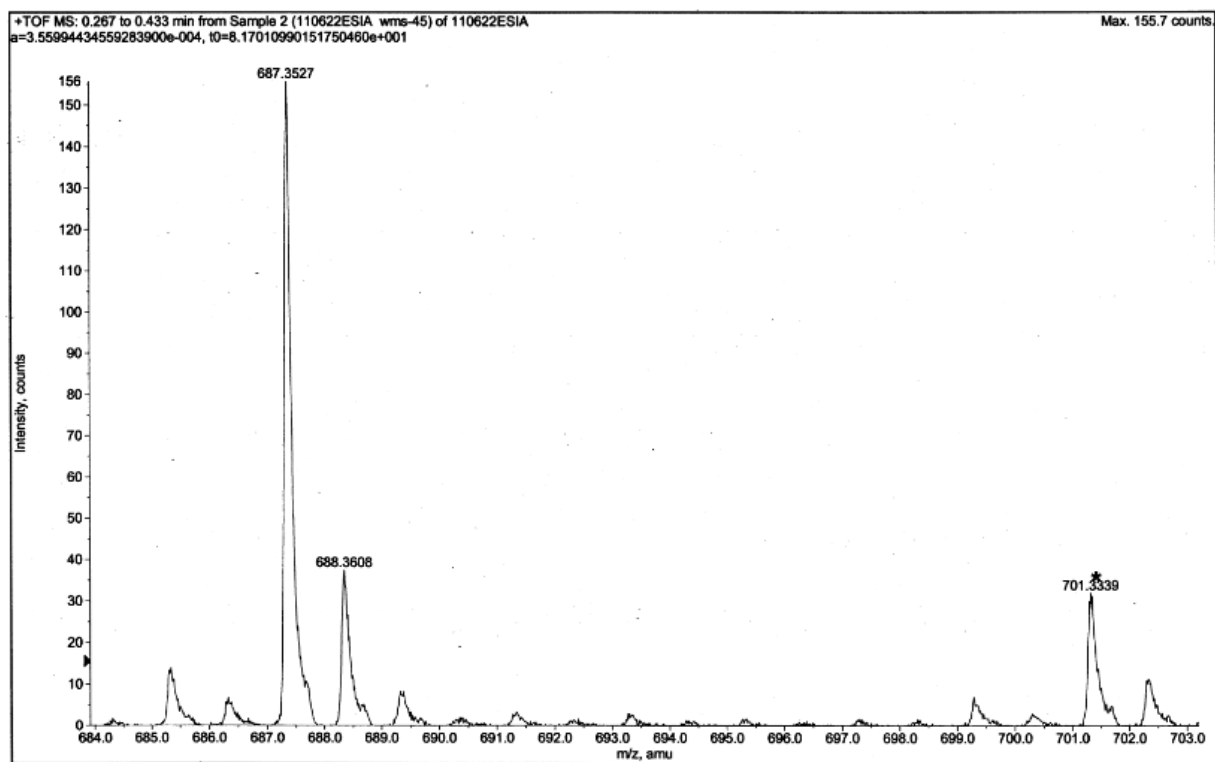


Figure 65S. ^1H NMR of Tenuicausine (**9**) in acetone- d_6 .

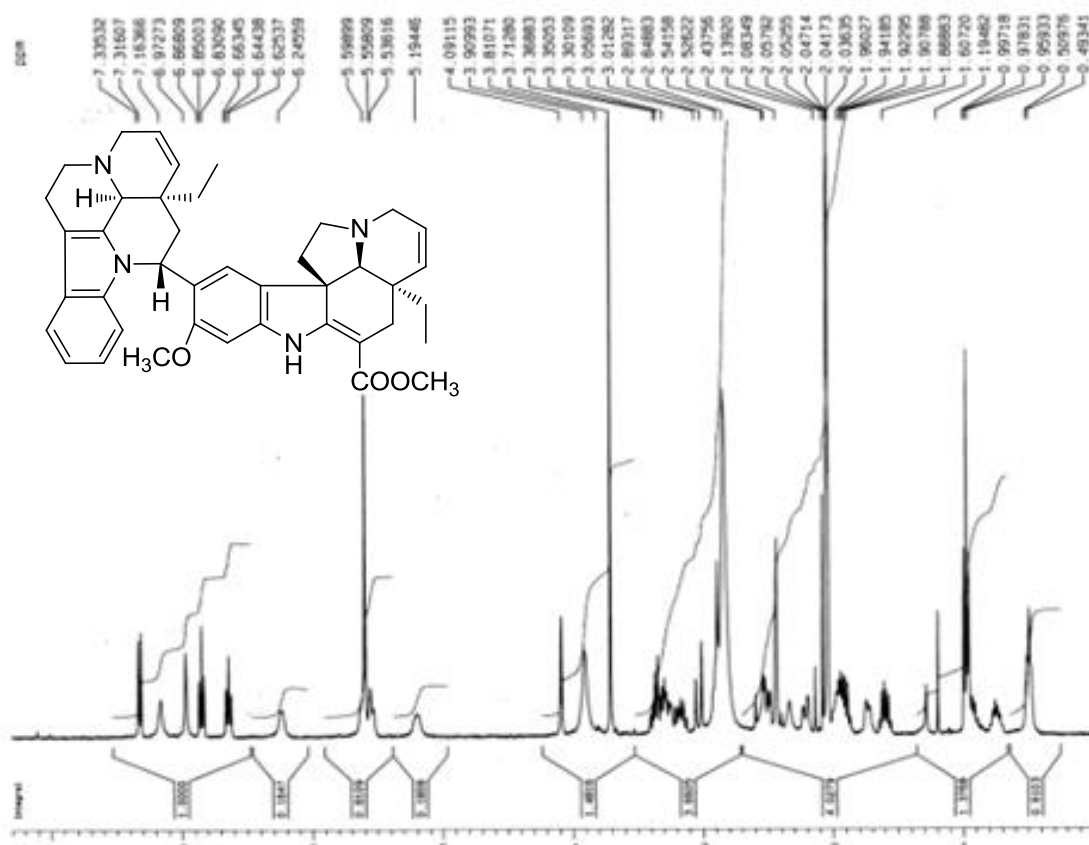


Figure 66S. ^{13}C NMR and DEPT of Tenuicausine (**9**) in acetone- d_6 .

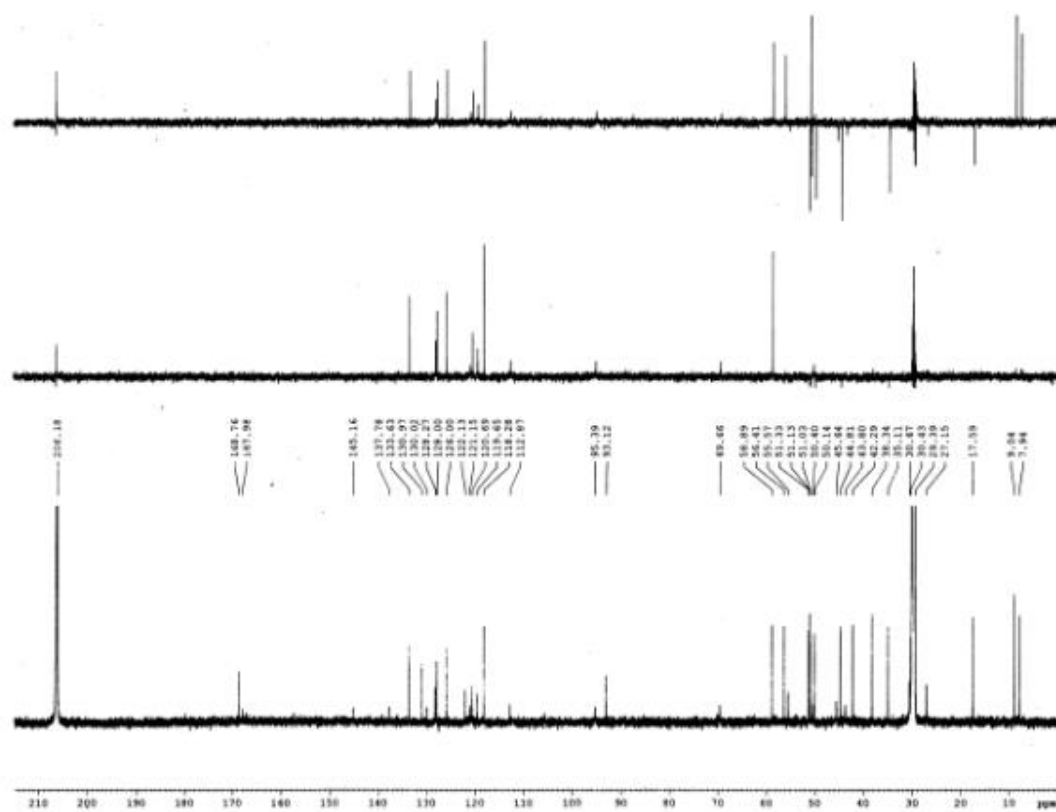


Figure 67S. HSQC of Tenuicausine (9) in acetone- d_6 .

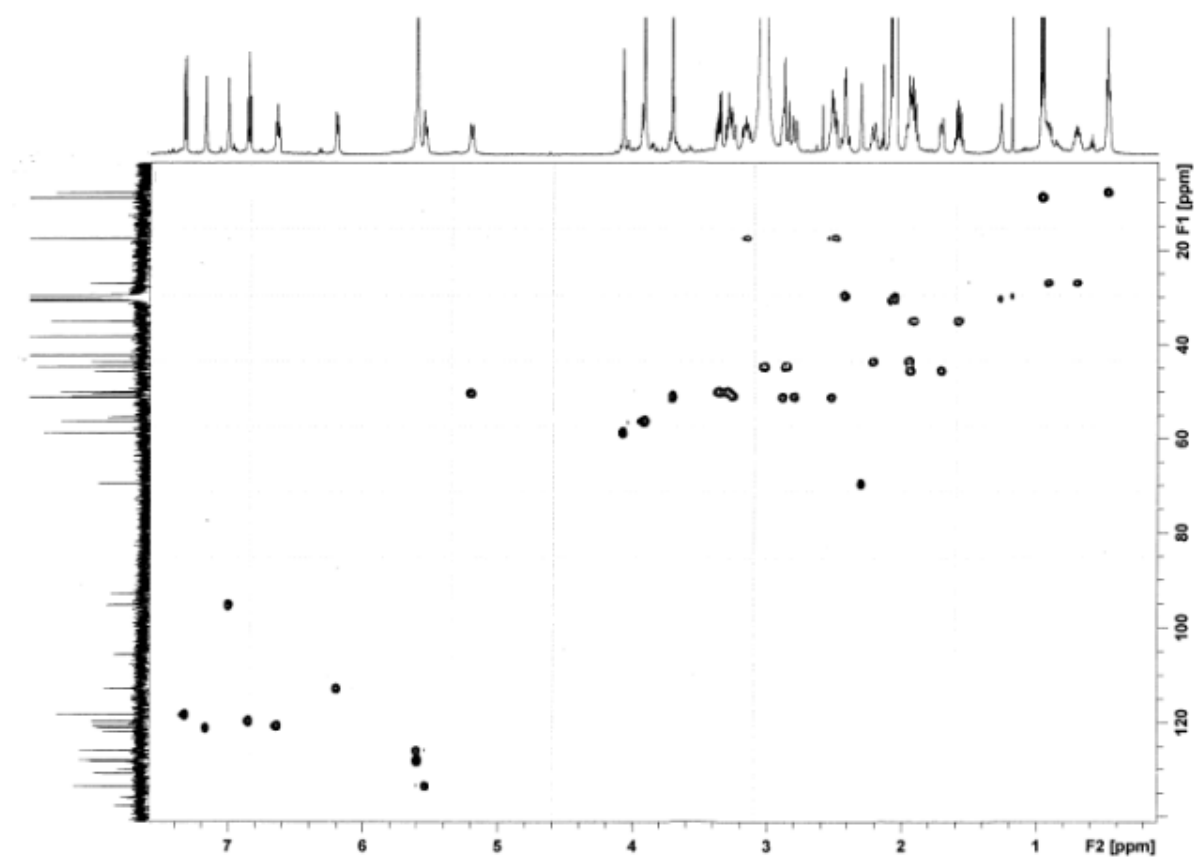


Figure 68S. HMBC of Tenuicausine (9) in acetone- d_6 .

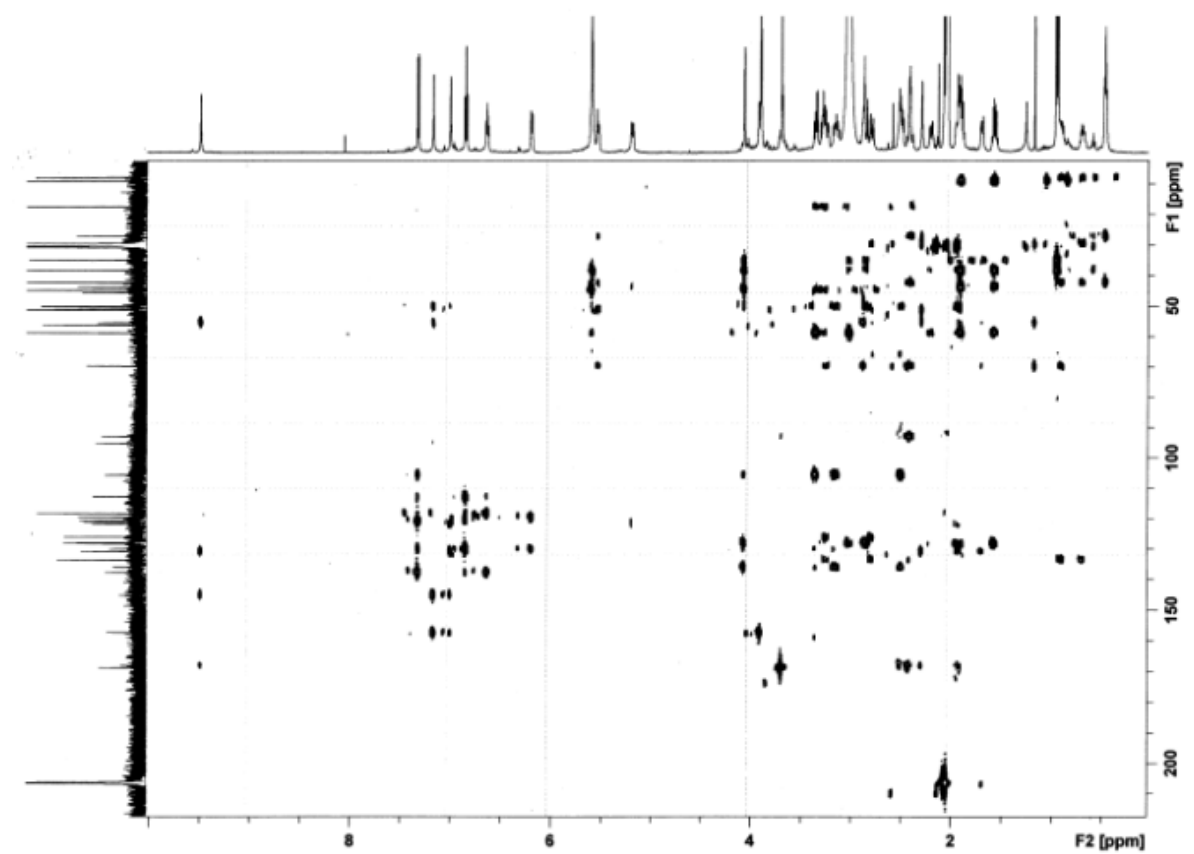


Figure 69S. ROESY of Tenuicausine (9) in acetone-*d*₆.

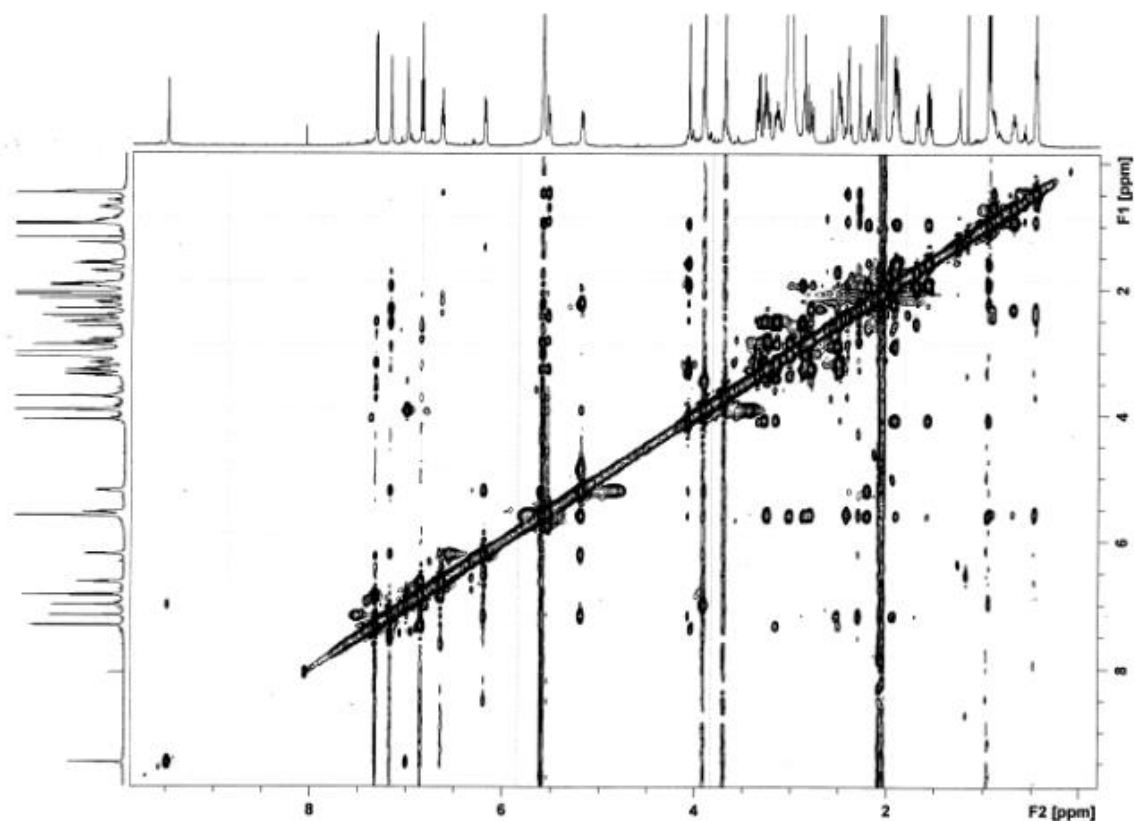


Figure 70S. ESIMS of Tenuicausine (9).

Mass Spectrum List Report					
Analysis Info			Acquisition Date 4/13/2011 2:53:22 PM		
Analysis Name D:\DATA\2011\file110414\wms-62000.d			Operator QIYAN		
Method ms_ptservice.m			Instrument HCT		
Sample Name					
Comment balance method					
<hr/>					
Acquisition Parameter					
Ion Source Type ESI		Ion Polarity Positive		Alternating Ion Polarity off	
Mass Range Mode Std/Enhanced		Scan Begin 50 m/z		Scan End 1400 m/z	
Capillary Exit 139.2 Volt		Skimmer 40.0 Volt		Trap Drive 76.1	
Accumulation Time 100 μ s		Averages 7 Spectra		Auto MS/MS off	

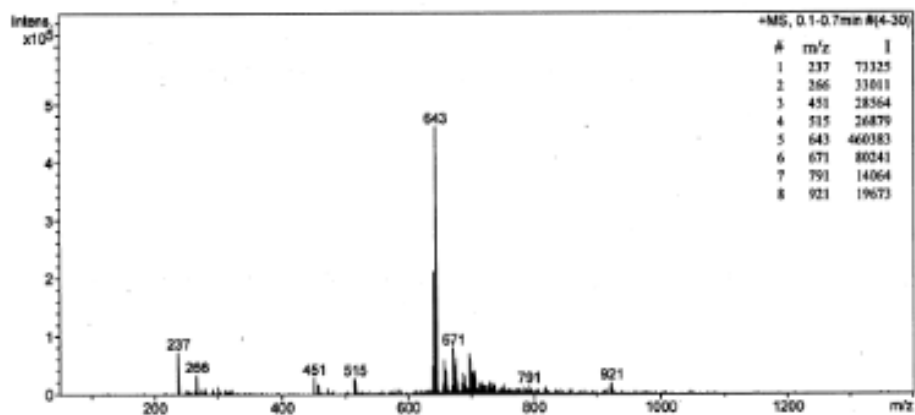


Figure 71S. HRESIMS of Tenuicausine (9).

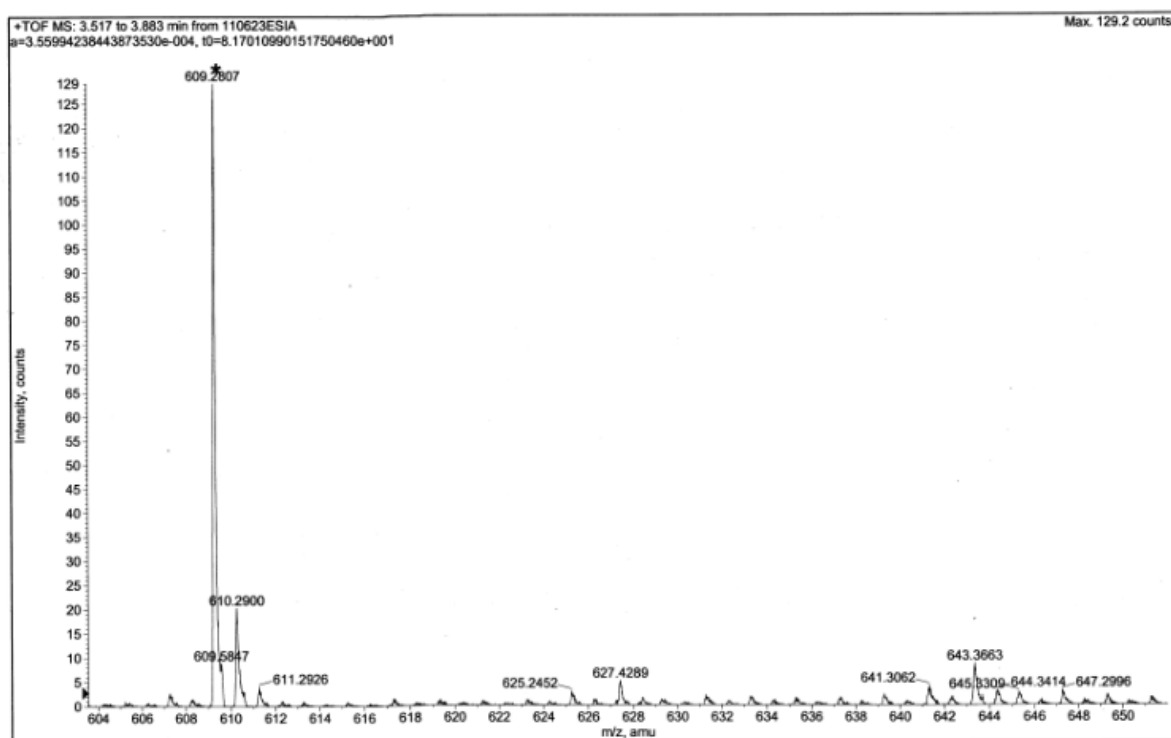
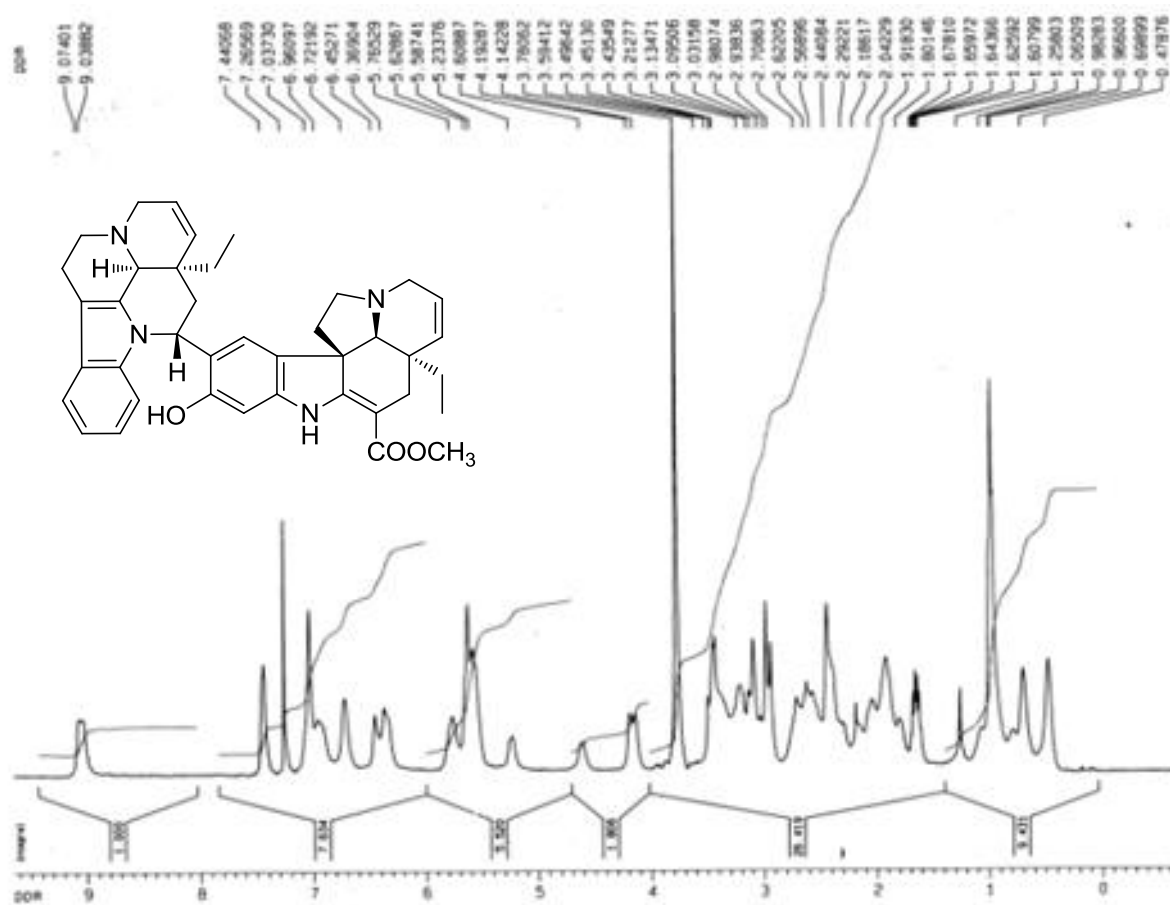


Figure 72S. ^1H NMR of Melodinine J (10) in acetone- d_6 .



157.29
156.46

153.80

142.76

138.40
135.07
134.26
132.96
128.56
127.50
126.91
125.20
124.26
118.87
116.58
117.40
111.75

104.38

96.33

90.76

76.23
76.03
75.83

68.53
57.53
54.74
54.14
50.10
49.83
49.12
48.80
48.50
43.75
42.39
40.80
40.05
39.93
39.45
36.45
36.37
29.51
36.43
36.37
36.37
36.23
36.16
36.09
31.16
28.11
26.11
26.05
26.05

8.43
7.40

Mass Spectrum List Report

Analysis Info		Acquisition Date 4/19/2011 4:02:03 PM	
Analysis Name	D:\DATA\2011file\110419\wms-64b000.d	Operator	QUYAN
Method	ms_ptservice.m	Instrument	HCT
Sample Name			
Comment	balance method		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Enhanced	Scan Begin	100 m/z	Scan End	1400 m/z
Capillary Exit	203.5 Volt	Skimmer	40.0 Volt	Trap Drive	136.8
Accumulation Time	500 μ s	Averages	7 Spectra	Auto MS/MS	off

#	m/z	I
1	369	149449
2	597	108897
3	629	1694791
4	1279	68429