Supplementary Materials

Antimicrobial Terpenoids from South China Sea Soft Coral *Lemnalia* sp.

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Content

1. Antibacterial and Antiviral Activity of the Isolated Compounds 1-13

Table S1. Antibacterial and antiviral activity of the isolated compounds **1-13**.

No.	MIC (against *Staphylococcus aureus*, μg/mL)	MIC (against *Bacillus subtilis*, μg/mL)	Inhibition rate at 30 μM (against H1N1)	Inhibition rate at 50 μM (against HSV-1)
1	> 128	> 128	84.50%	0.60%
2	> 128	> 128	100.00%	5.10%
3	> 128	> 128	77.60%	32.10%
4	> 128	> 128	88.50%	0.00%
5	8	8	2.20%	0.00%
6	4	16	5.40%	0.00%
7	4	16	21.70%	0.00%
8	16	8	15.60%	0.00%
9	> 128	> 128	2.20%	13.70%
10	16	8	0.00%	0.00%
11	> 128	16	49.40%	50%
12	> 128	16	2.70%	0.00%
13	> 128	8	1.40%	0.00%
Penicillin G	1	1	——	——
Acyclovir	——	——	97.00%	93.70%

2. Regression analysis of experimental vs calculated ^{13}C NMR chemical shifts of compound 1 and 2

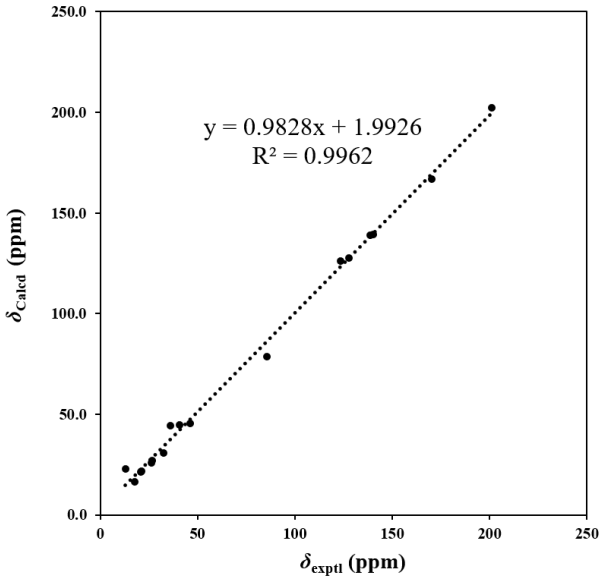


Figure S1. Regression analysis of experimental vs calculated ^{13}C NMR chemical shifts of (4S,5S,8R)-**1** at the GIAO/mPW1PW91/6-31G (d, p) level using DP4+ method. The linear fitting is shown as dashed line

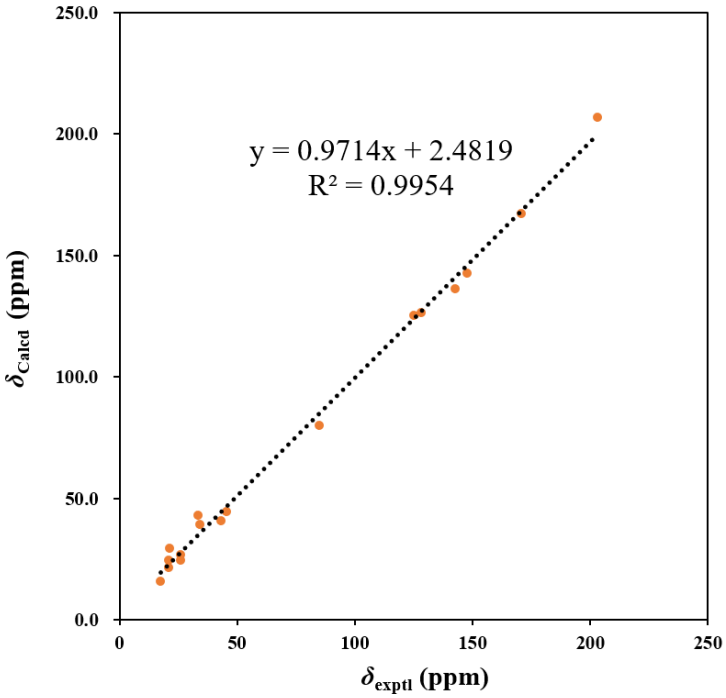


Figure S2. Regression analysis of experimental vs calculated ^{13}C NMR chemical shifts of (4S,5S,8S)-**2** at the GIAO/mPW1PW91/6-31G (d, p) level using DP4+ method. The linear fitting is shown as dashed line

3. Calculated ECD spectrum of (2*S*,4*S*,5*S*,6*R*,7*S*)-4 and experimental ECD spectrum of 4

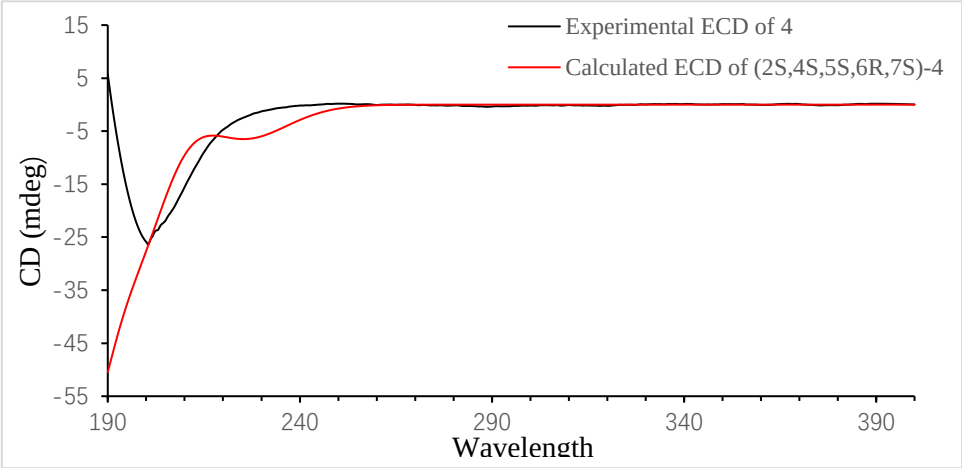


Figure S3. Calculated ECD spectrum of (2*S*,4*S*,5*S*,6*R*,7*S*)-**4** and experimental ECD spectrum of **4**

4. Calculated ECD spectrum of (1*R*,5*S*,6*R*,7*R*,10*R*,11*S*)-10 and experimental ECD spectrum of 10

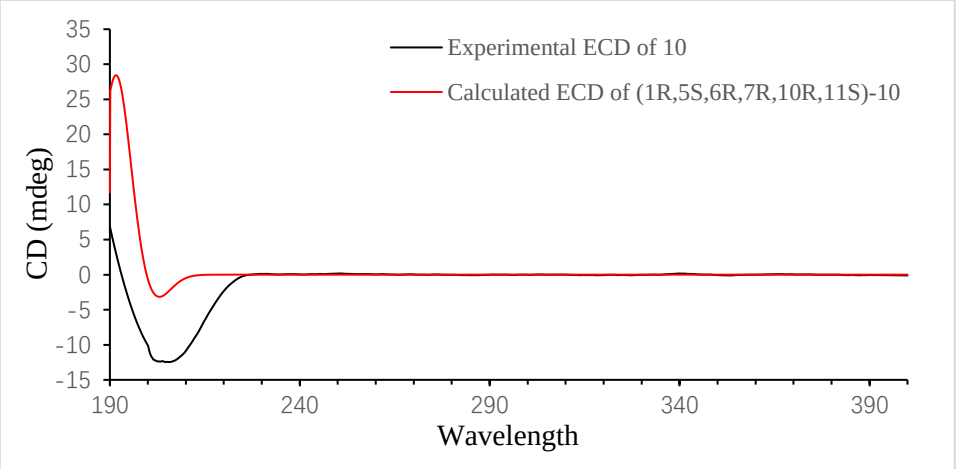


Figure S4. Calculated ECD spectrum of (1*R*,5*S*,6*R*,7*R*,10*R*,11*S*)-**10** and experimental ECD spectrum of **10**

5. Spectroscopic data for lineolemnene E (1)

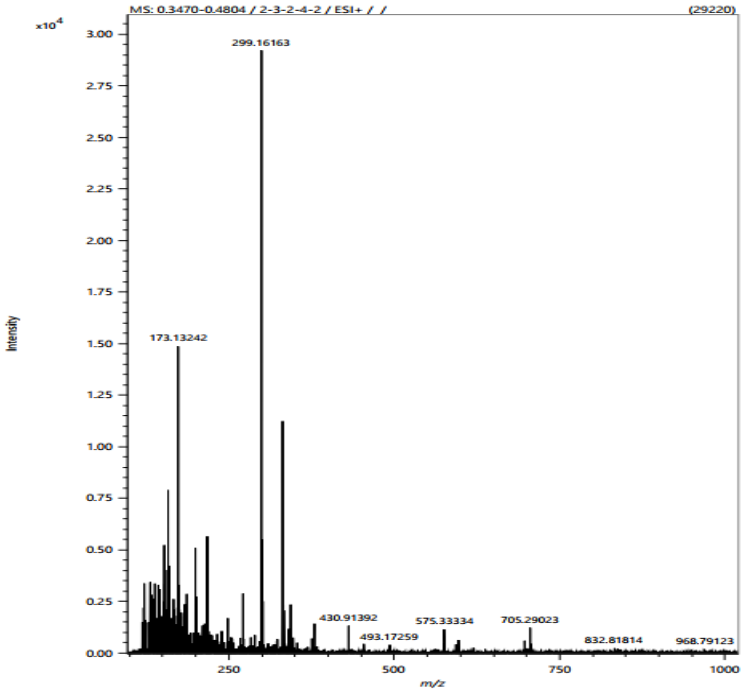


Figure S5. HRESIMS spectrum of lineolemnene E (**1**)

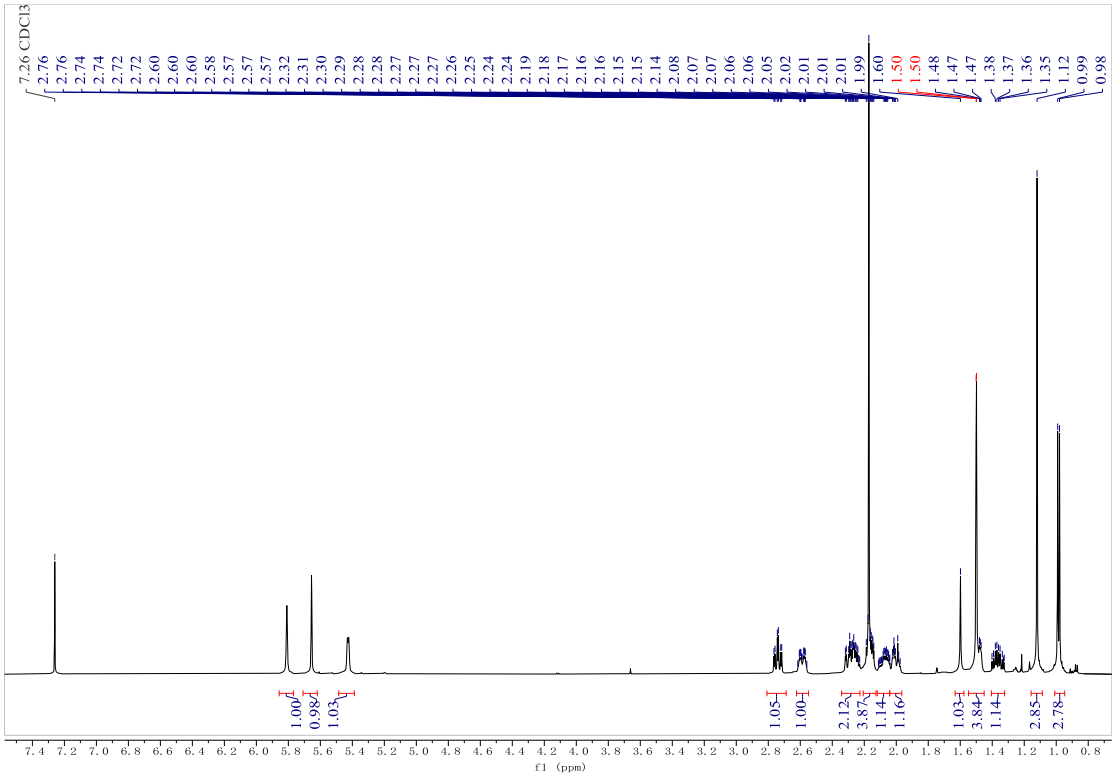


Figure S6. ^{1}H-NMR spectrum of lineolemnene E (**1**) in $CDCl_3$

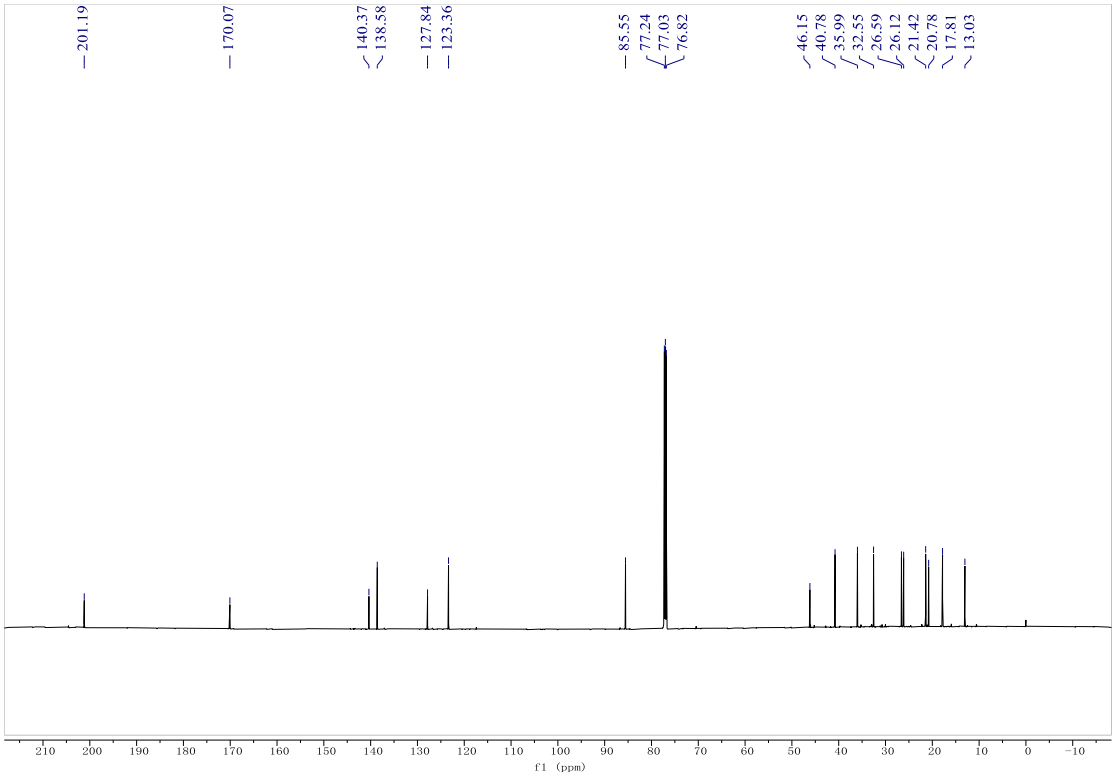


Figure S7. ^{13}C-NMR spectrum of lineolemnene E (**1**) in $CDCl_3$

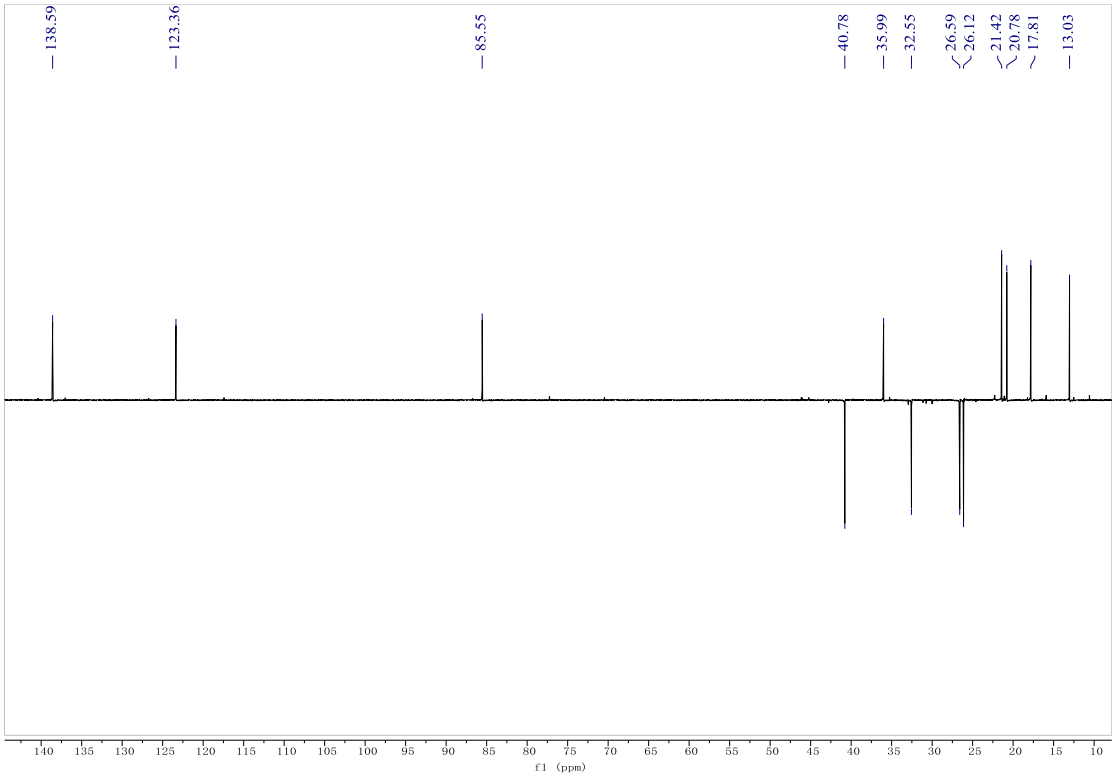


Figure S8. Dept 135° spectrum of lineolemnene E (**1**) in $CDCl_3$

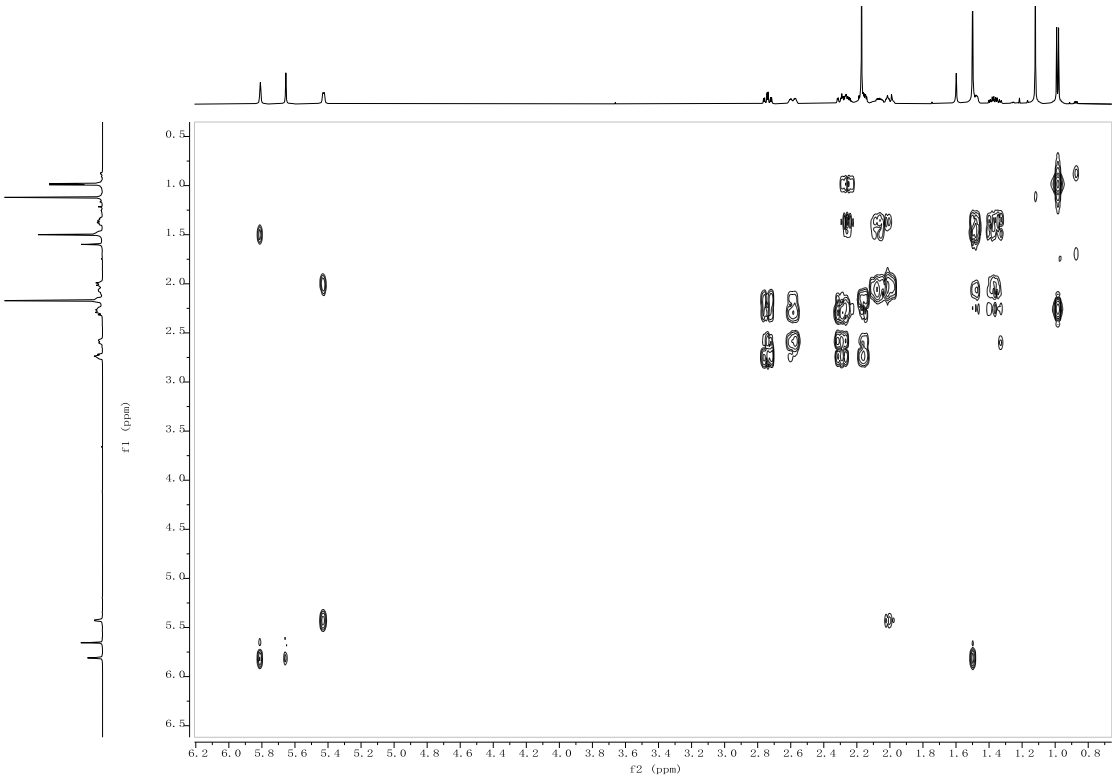


Figure S9. ^{1}H-^{1}H COSY spectrum of lineolemnene E (**1**) in $CDCl_3$

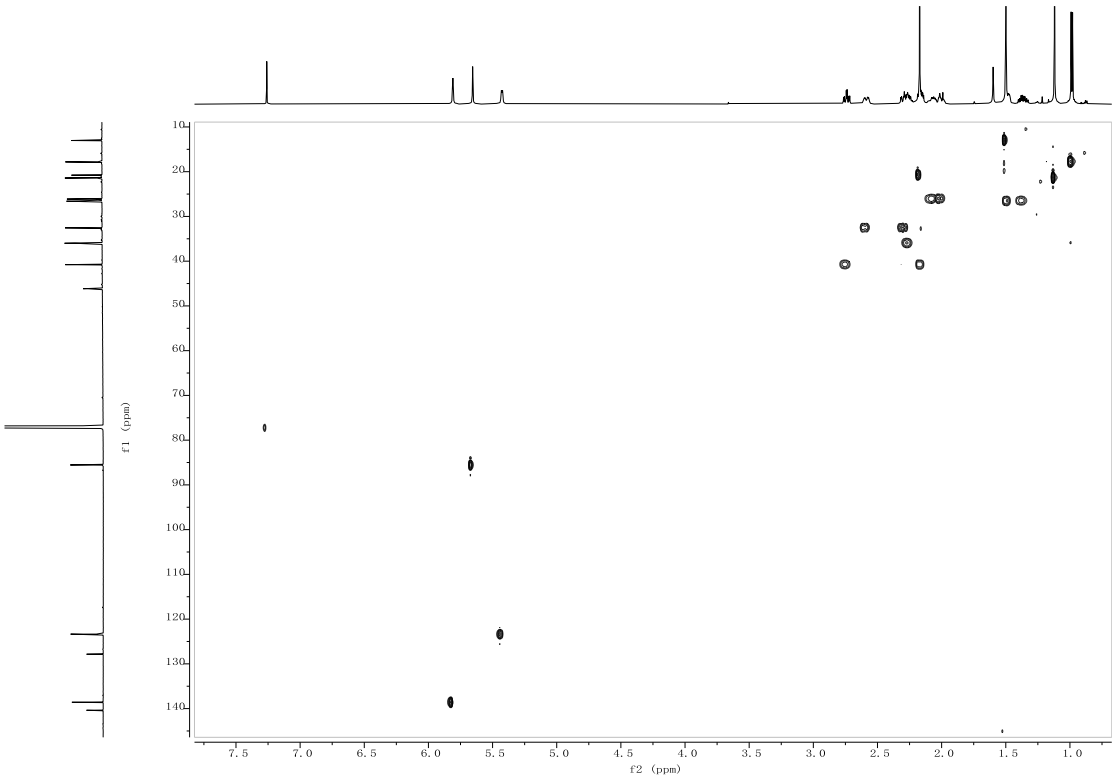


Figure S10. HSQC spectrum of lineolemnene E (**1**) in $CDCl_3$

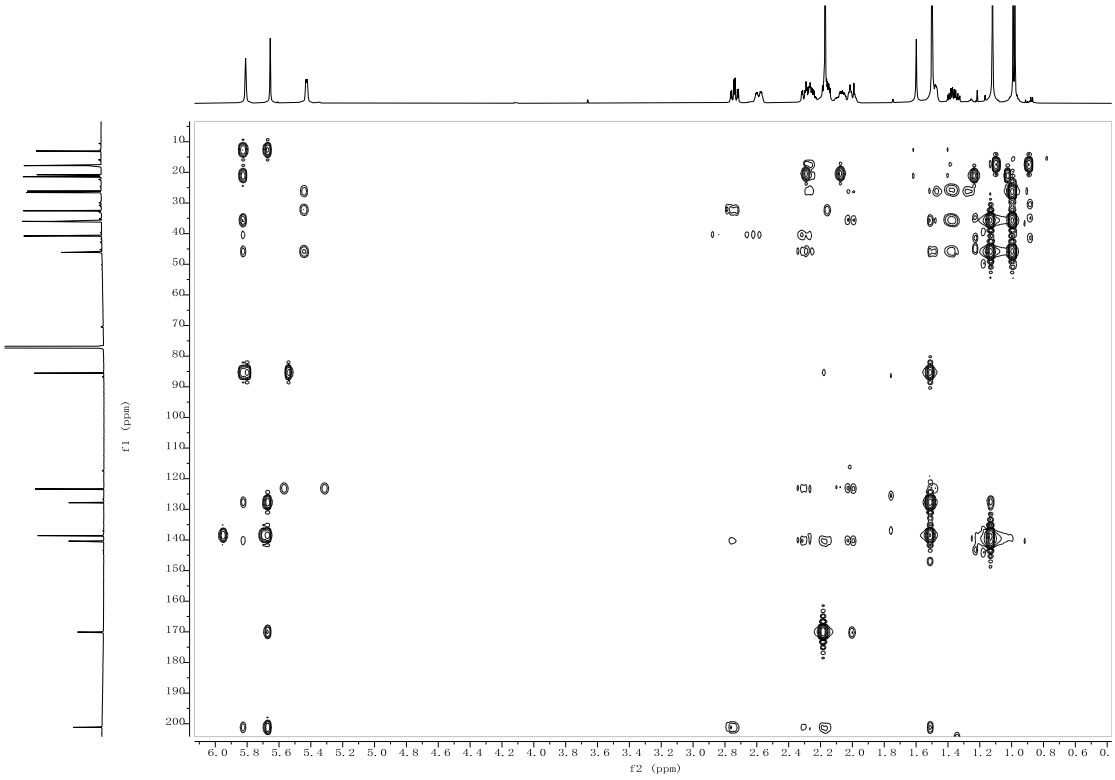


Figure S11. HMBC spectrum of lineolemnene E (**1**) in $CDCl_3$

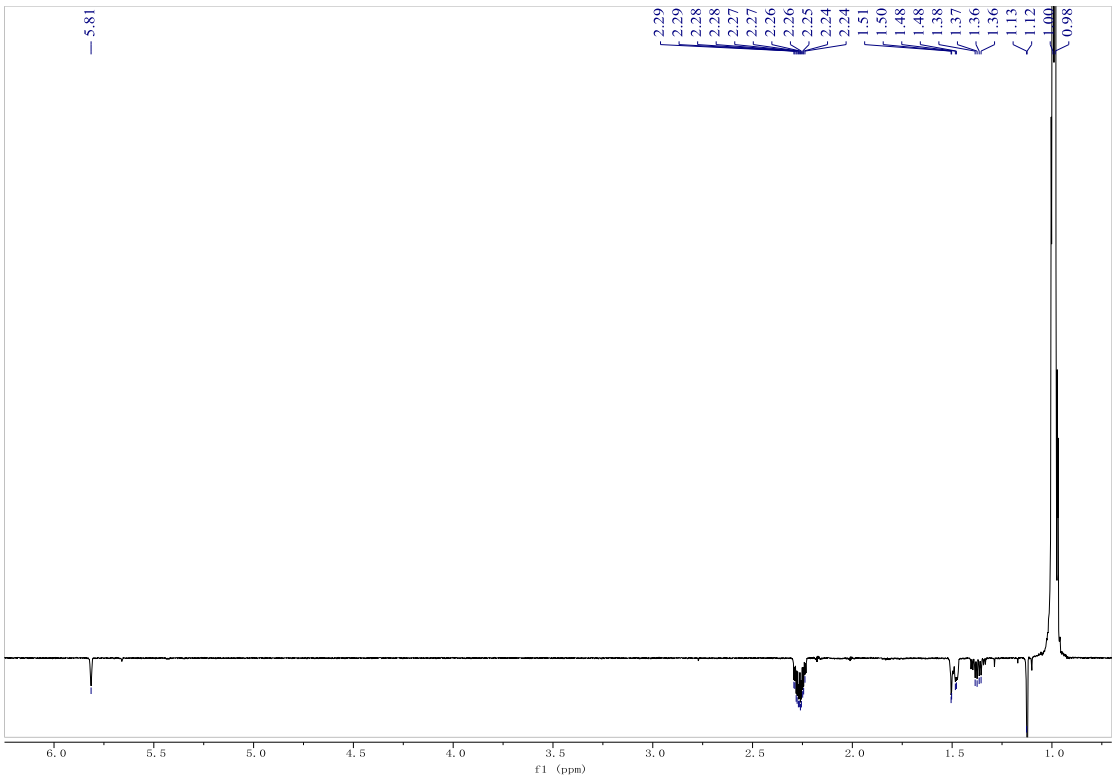


Figure S12. NOESY spectrum of lineolemnene E (**1**) in $CDCl_3$

6. Spectroscopic data for lineolemnene F (2)

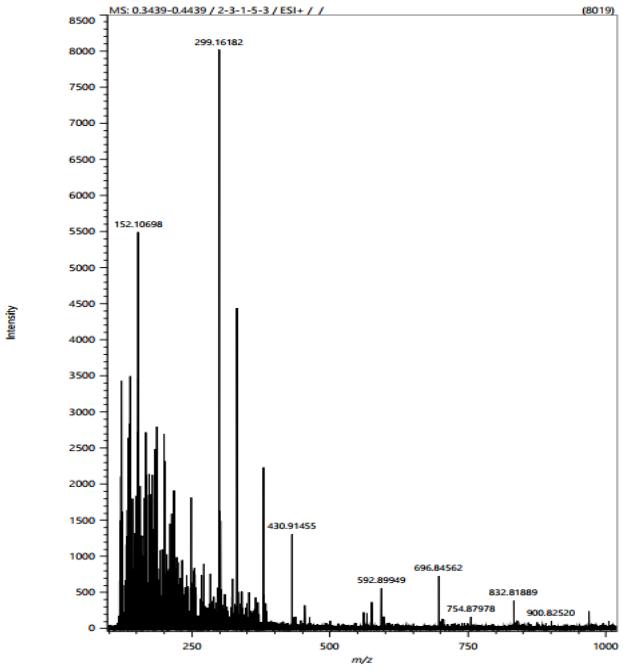


Figure S13. HRESIMS spectrum of lineolemnene F (**2**)

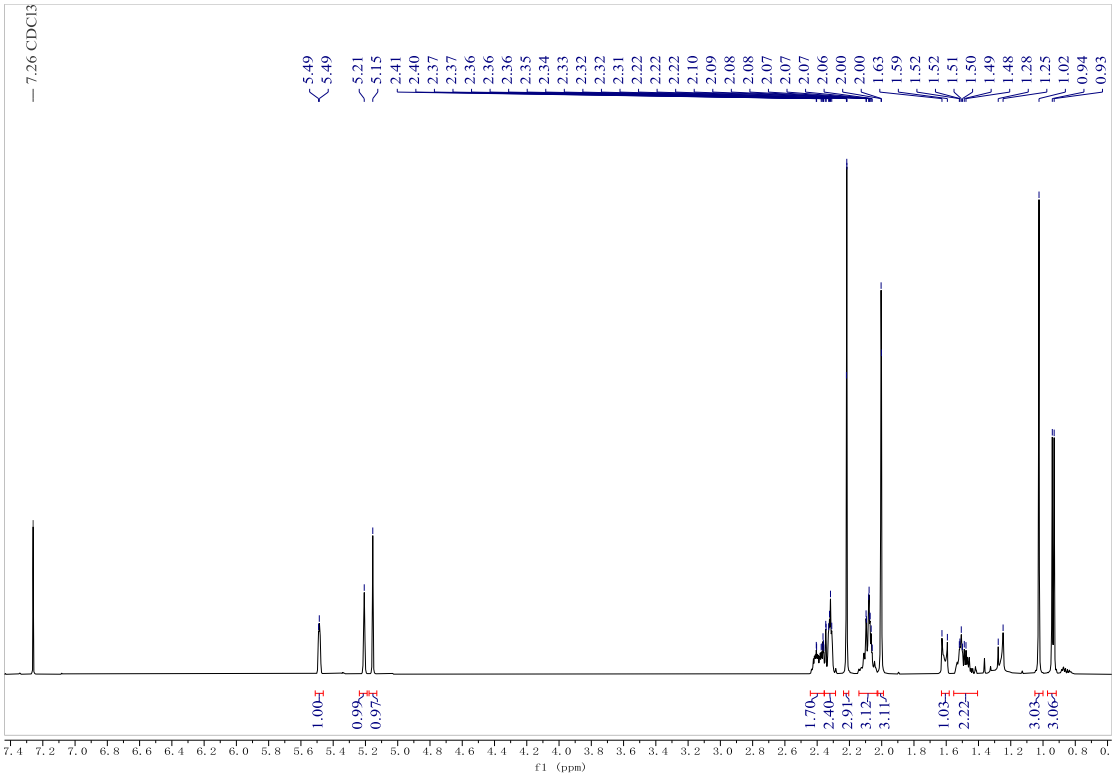


Figure S14. ^{1}H-NMR spectrum of lineolemnene F (**2**) in $CDCl_3$

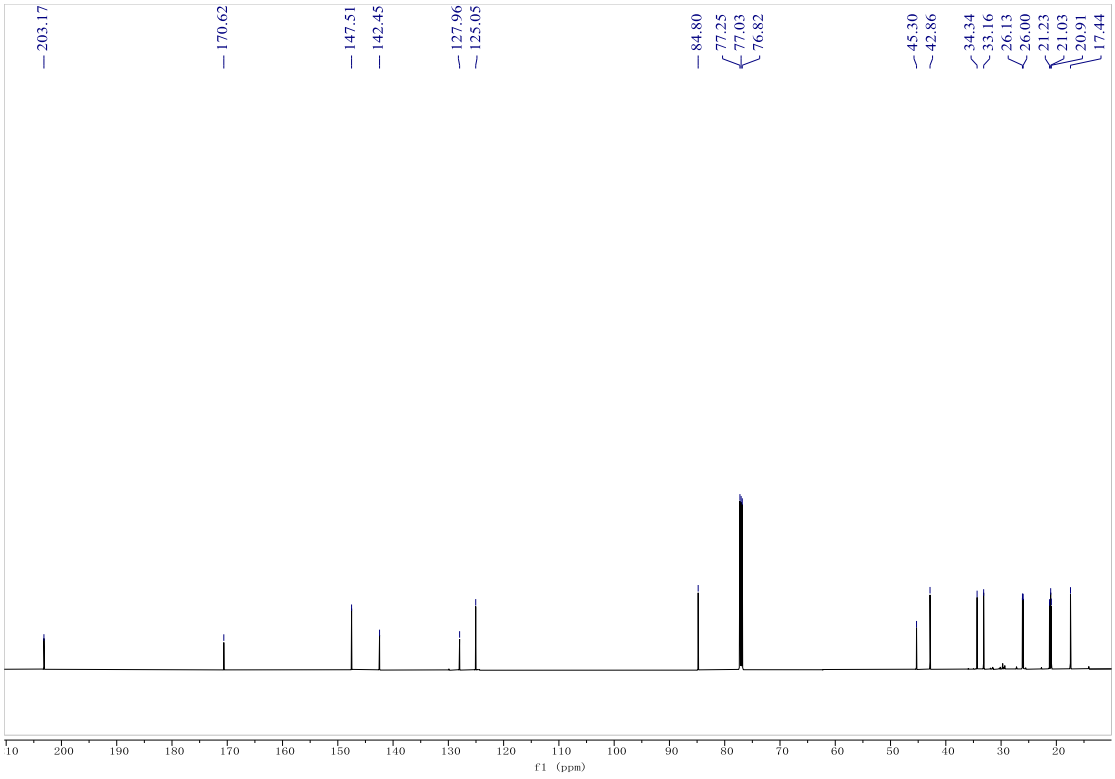


Figure S15. ^{13}C-NMR spectrum of lineolemnene F (**2**) in $CDCl_3$

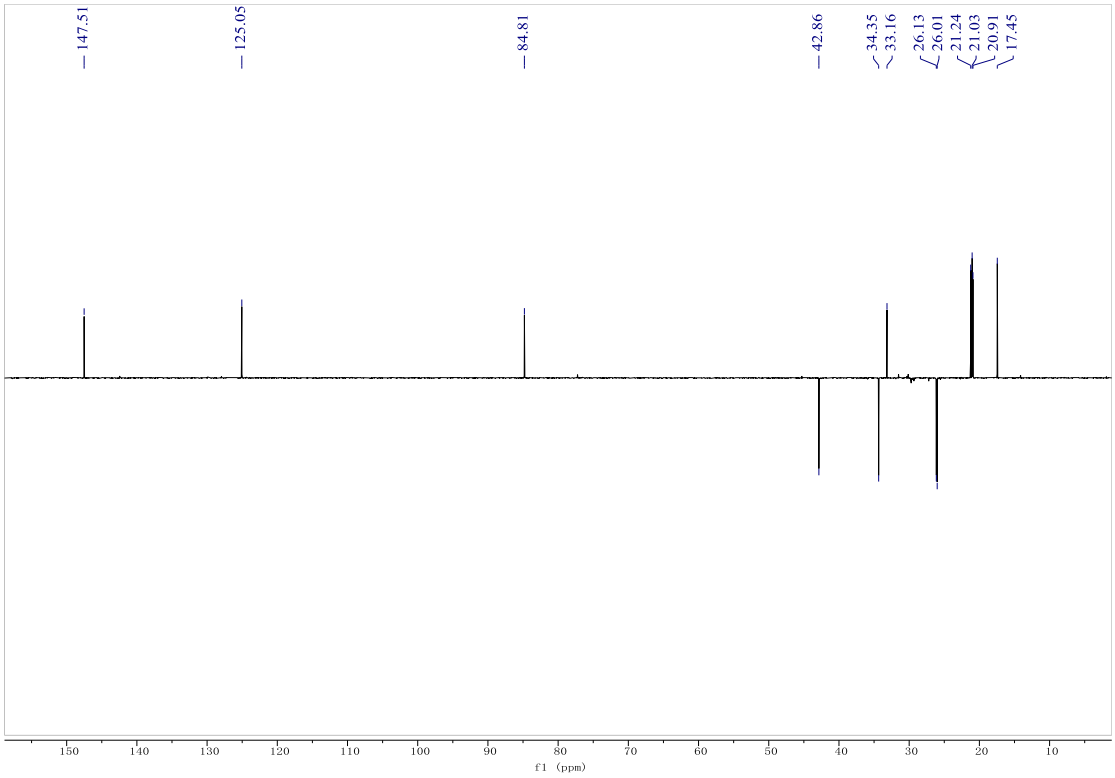


Figure S16. Dept 135° spectrum of lineolemnene F (**2**) in $CDCl_3$

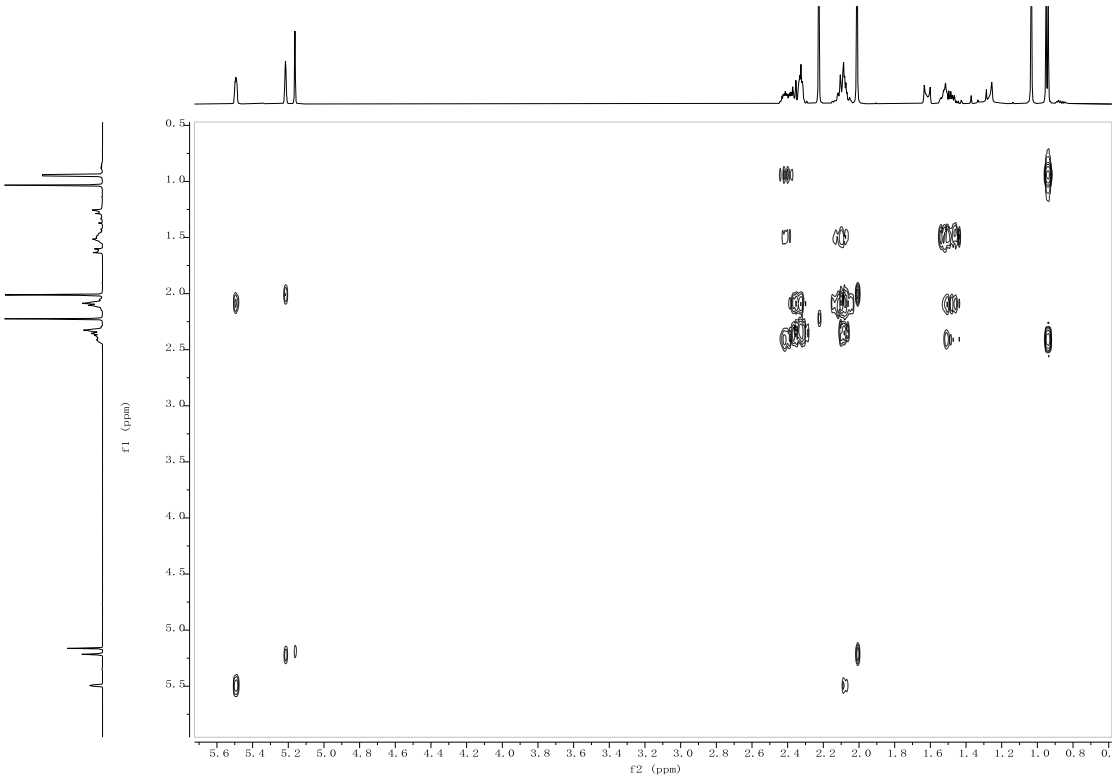


Figure S17. ^{1}H-^{1}H COSY spectrum of lineolemnene F (**2**) in $CDCl_3$

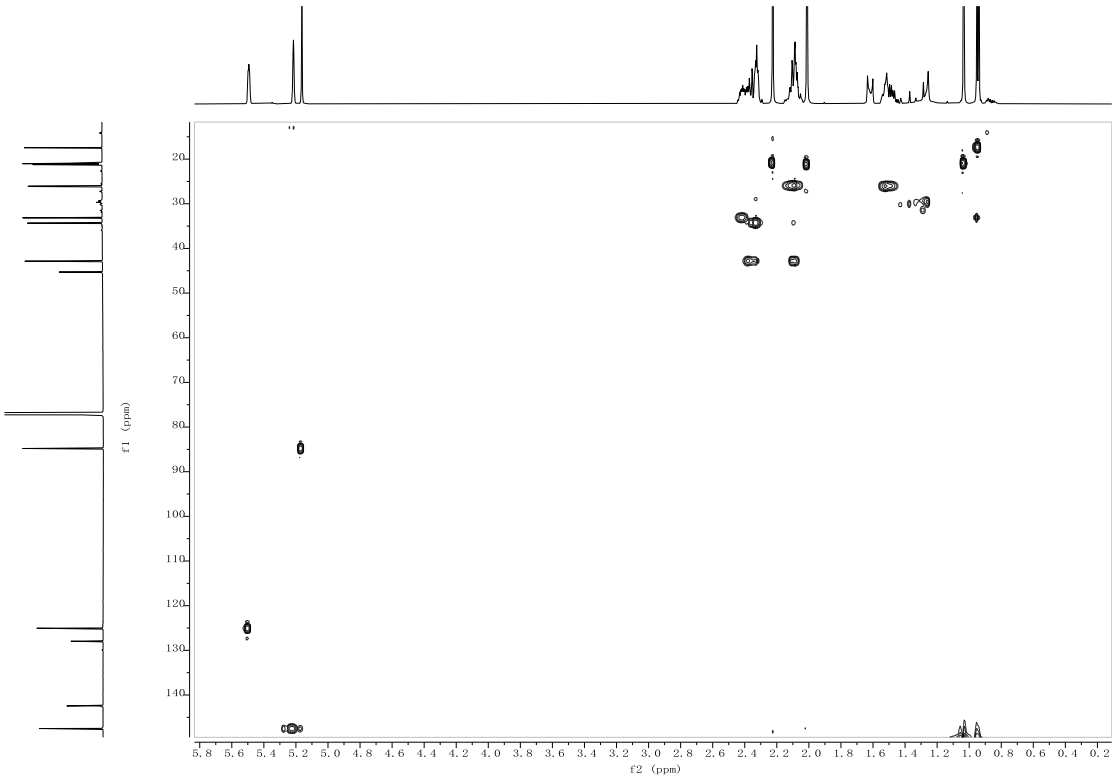


Figure S18. HSQC spectrum of lineolemnene F(**2**) in $CDCl_3$

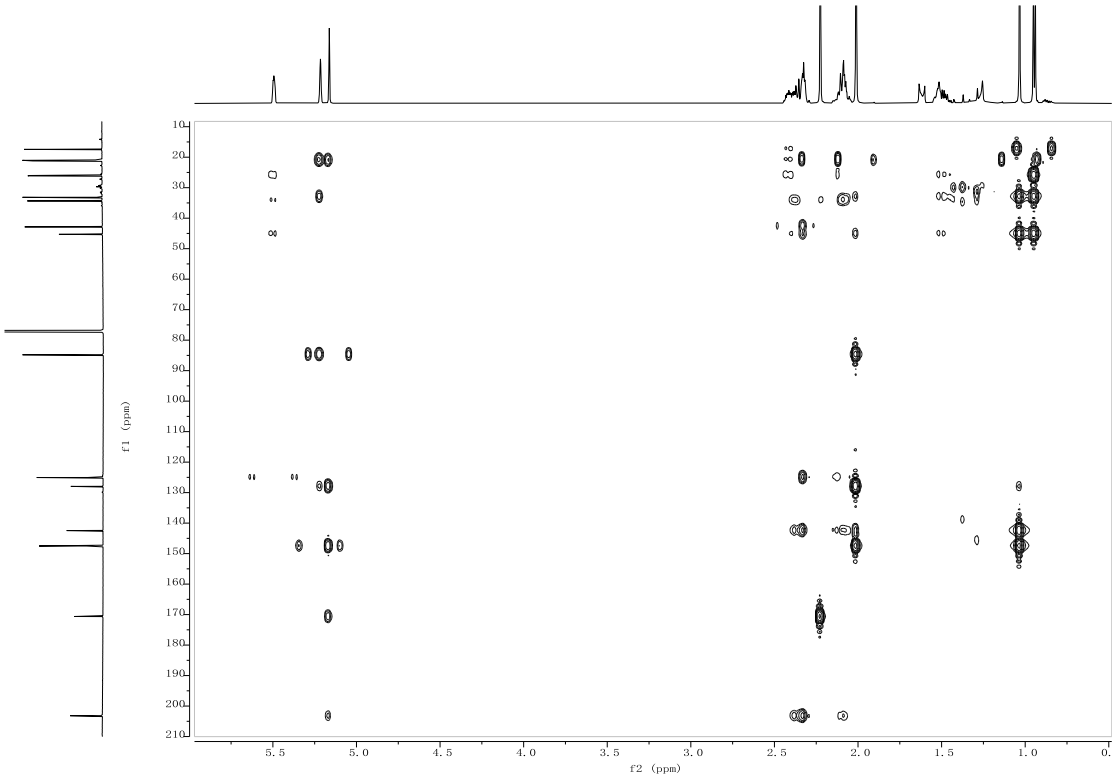


Figure S19. HMBC spectrum of lineolemnene F (**2**) in $CDCl_3$

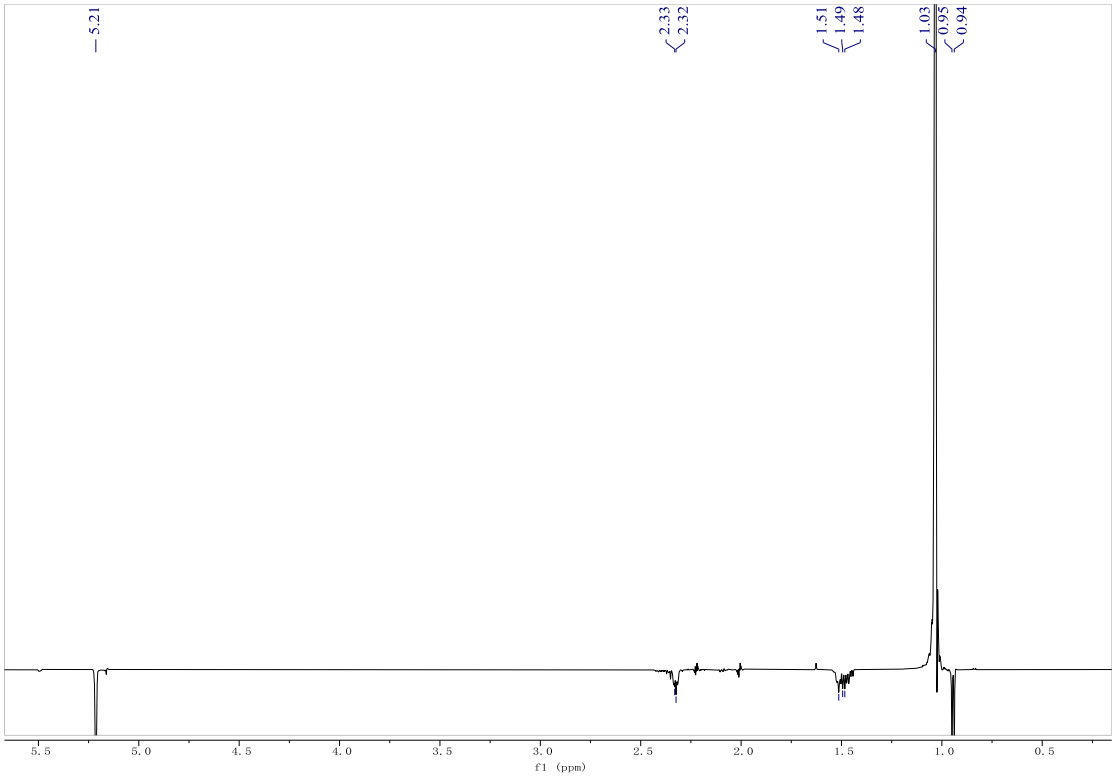


Figure S20. NOESY spectrum of lineolemnene F (**2**) in $CDCl_3$

7. Spectroscopic data for lineolemnene G (3)

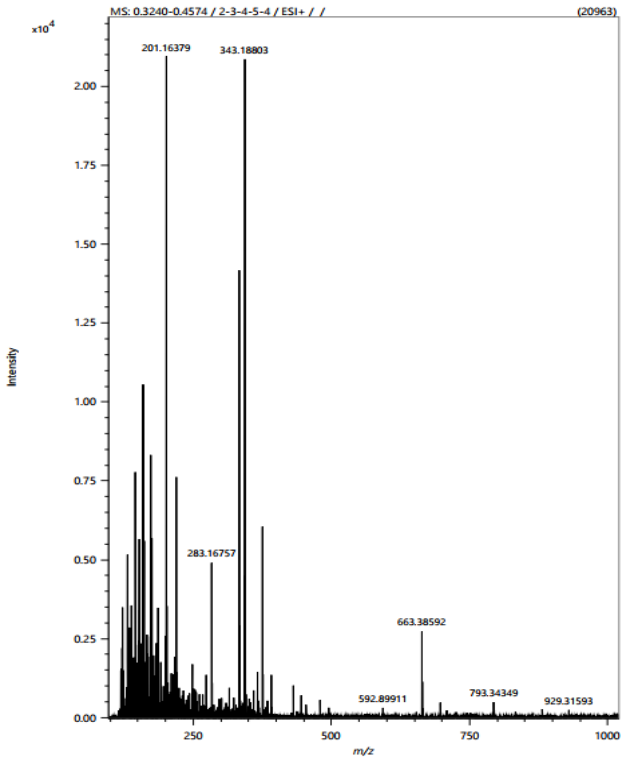


Figure S21. HRESIMS spectrum of lineolemnene G (**3**)

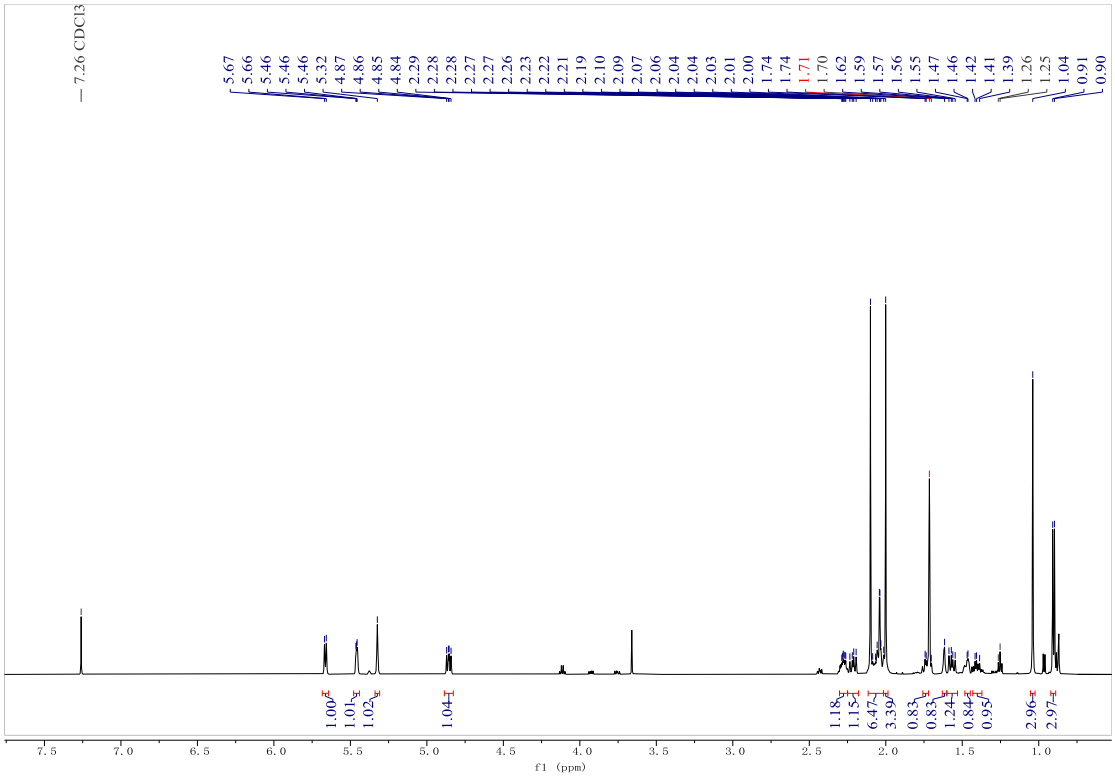


Figure S22. ^{1}H-NMR spectrum of lineolemnene G (**3**) in $CDCl_3$

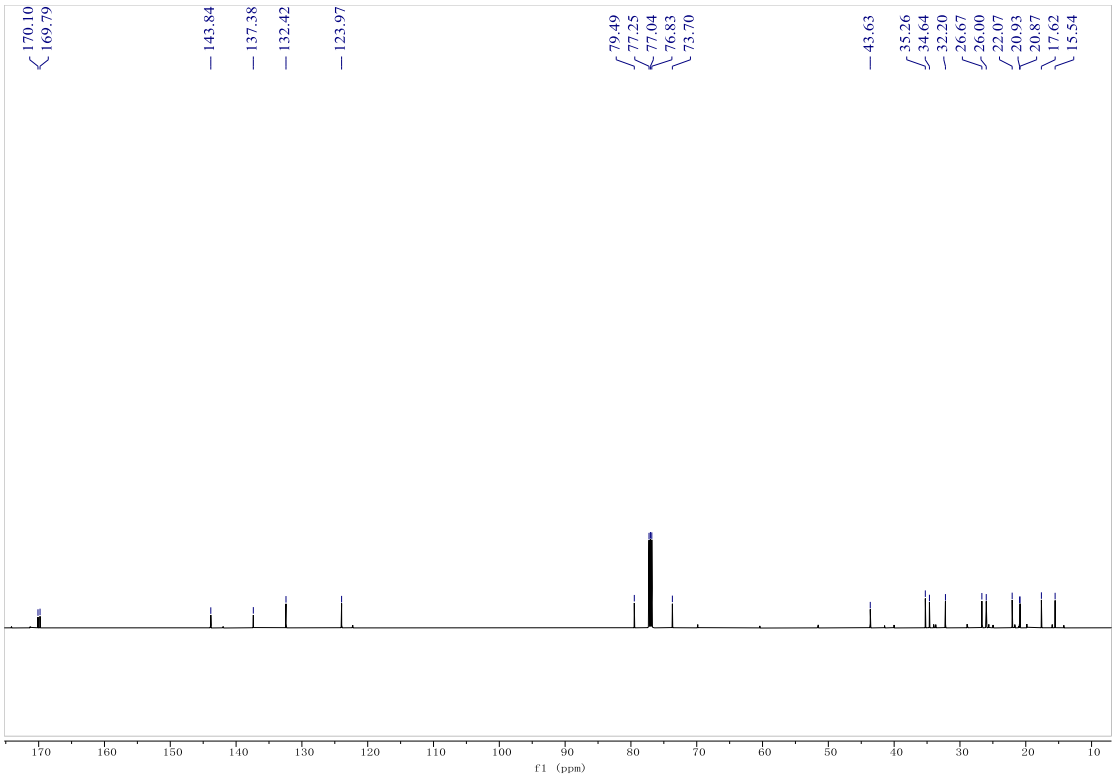


Figure S23. ^{13}C-NMR spectrum of lineolemnene G (**3**) in $CDCl_3$

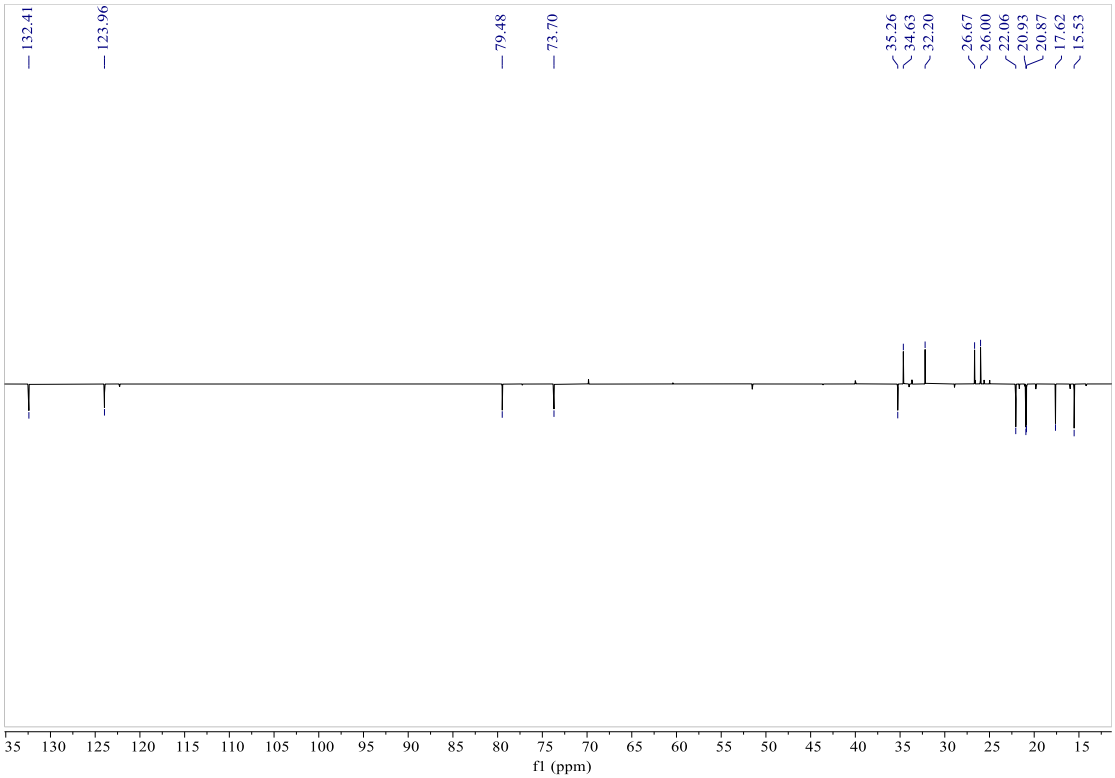


Figure S24. Dept 135° spectrum of lineolemnene G (**3**) in $CDCl_3$

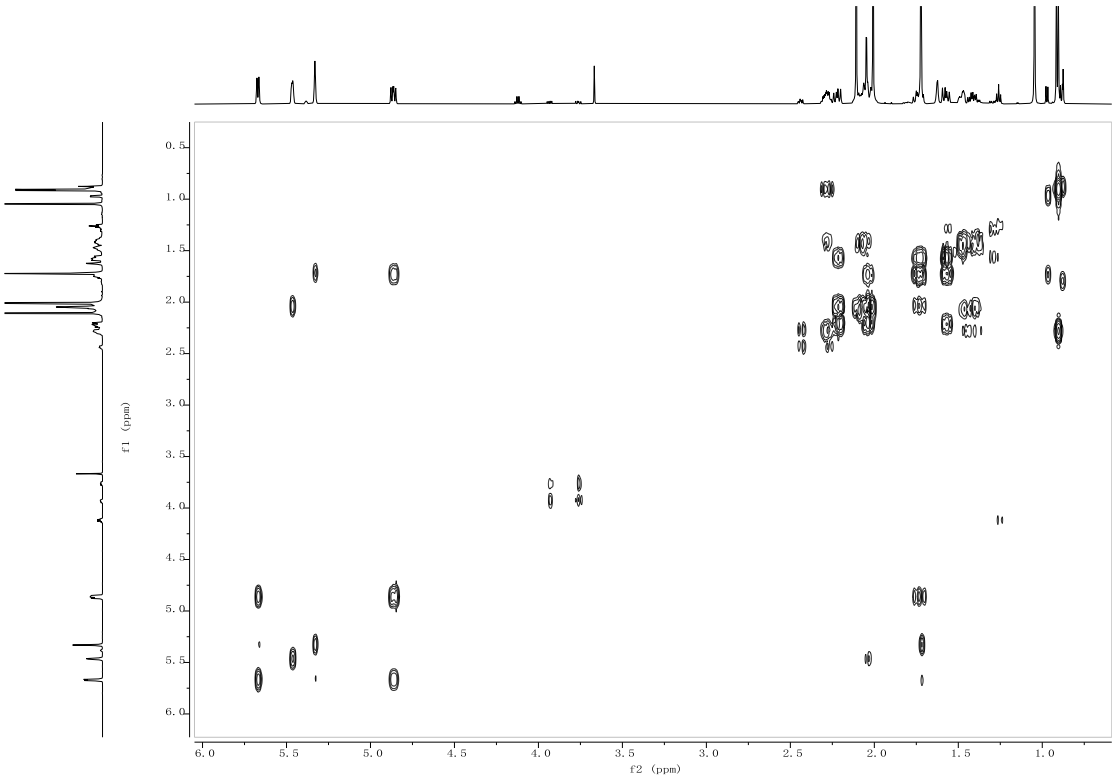


Figure S25. ^{1}H-^{1}H COSY spectrum of lineolemnene G (**3**) in $CDCl_3$

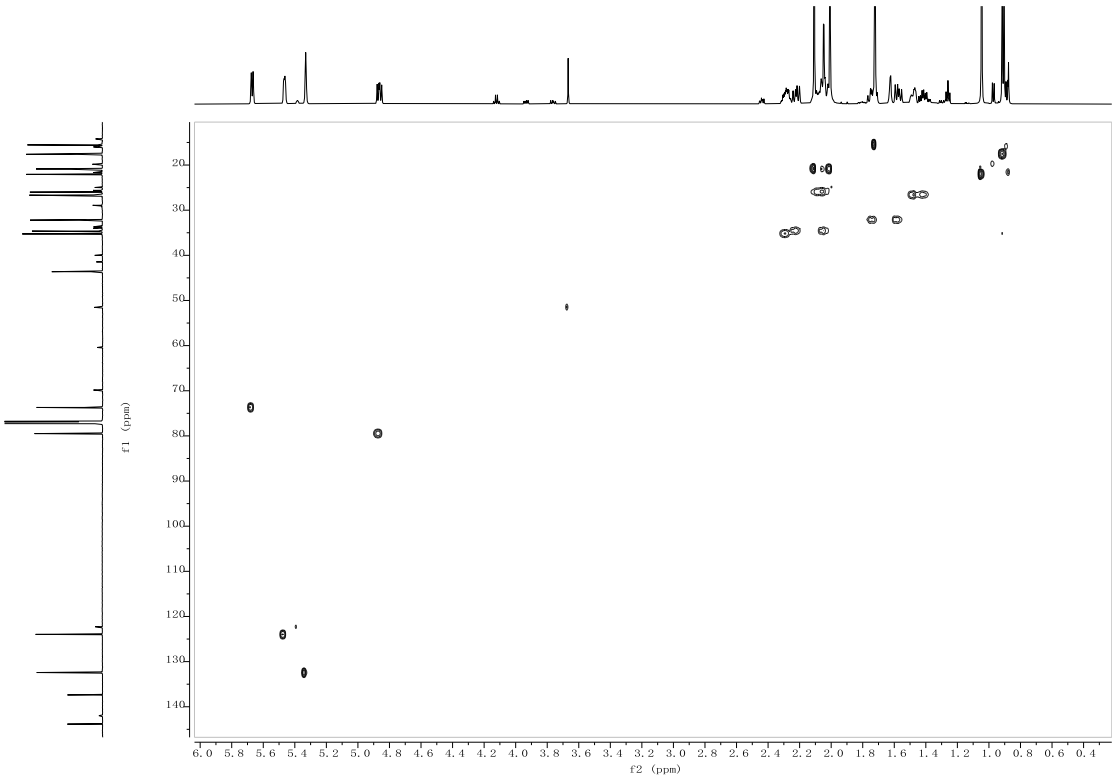


Figure S26. HSQC spectrum of lineolemnene G(**3**) in $CDCl_3$

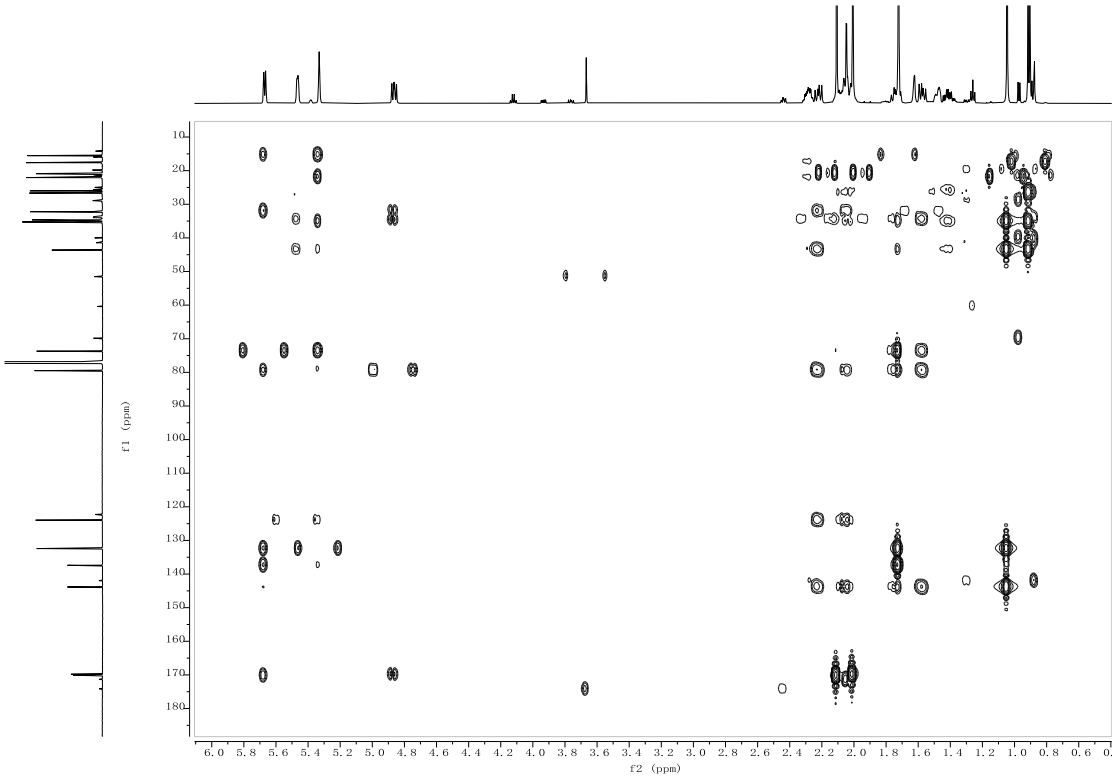
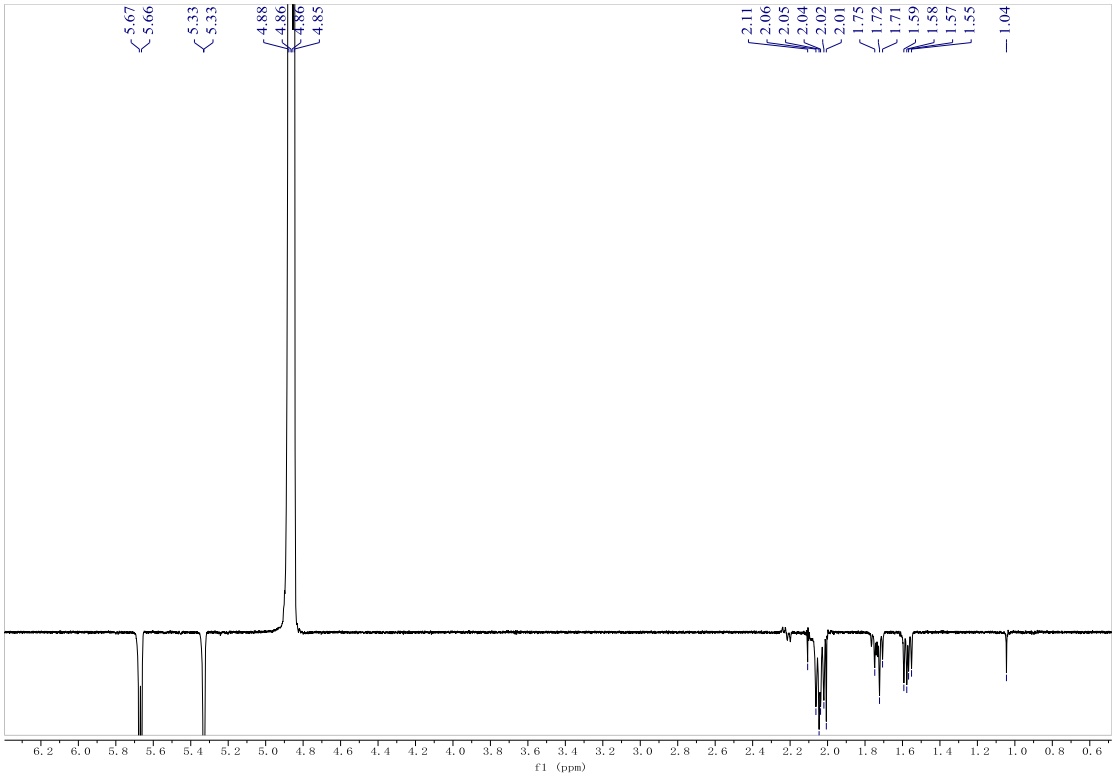


Figure S27. HMBC spectrum of lineolemnene G (**3**) in $CDCl_3$


5.67
5.66
5.33
5.33
4.88
4.86
4.86
4.85
2.11
2.06
2.05
2.04
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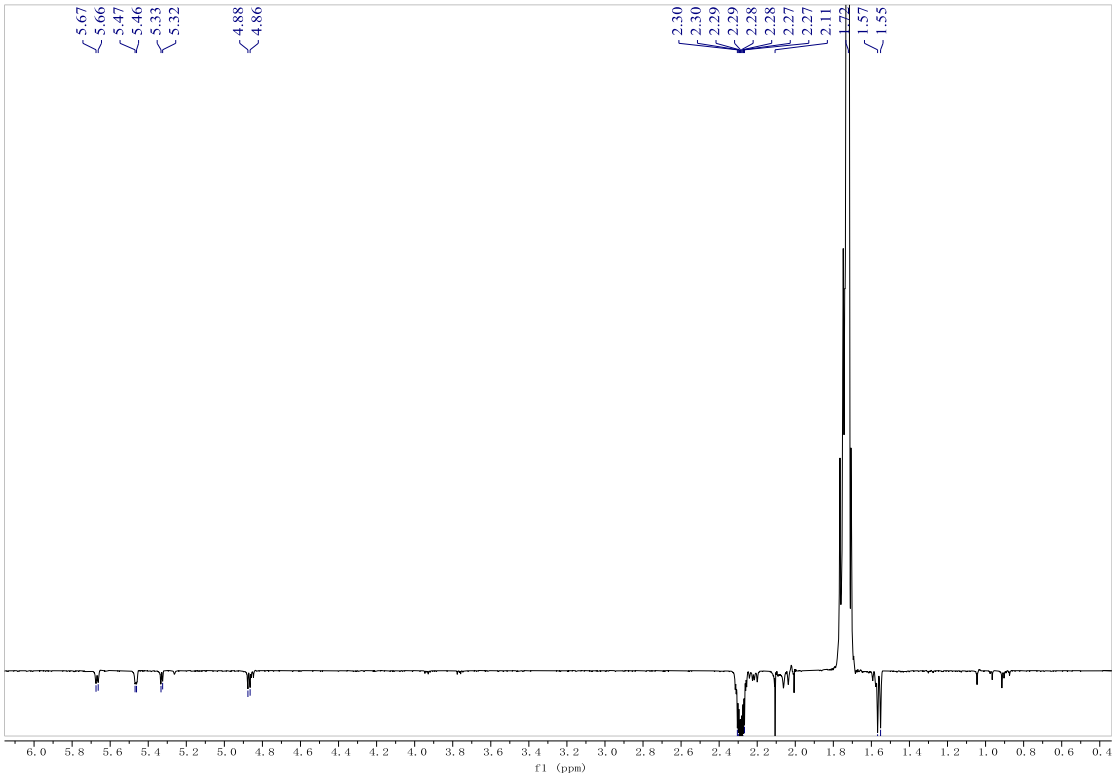
1.59
1.58
1.57
1.55
1.04
f1 (ppm)


5.67
5.66
5.47
5.46
5.33
5.32
4.88
4.86
2.30
2.30
2.29
2.29
2.28
2.28
2.27
2.27
2.11
1.72
1.57
1.55
f1 (ppm)

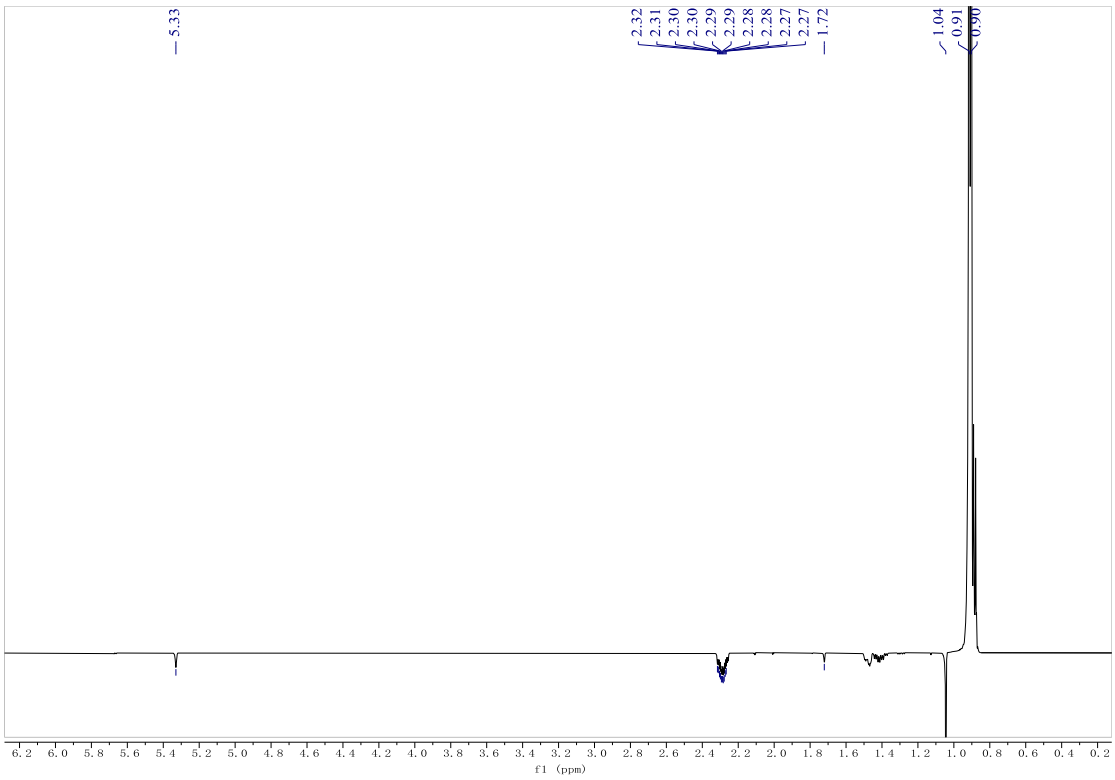


Figure S28. NOESY spectrum of lineolemnene G (**3**) in $CDCl_3$

8. Spectroscopic data for 2-acetoxy-aristolane (4)

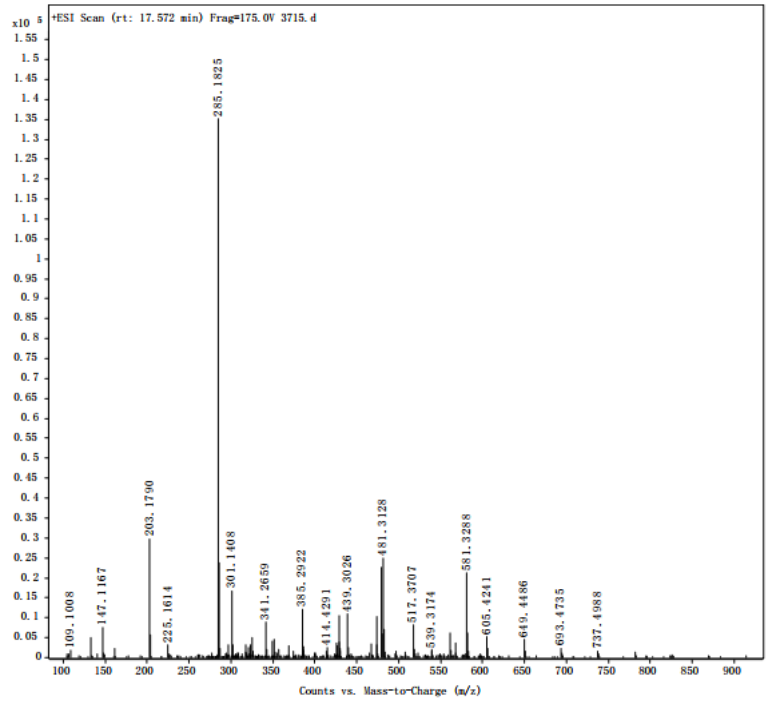


Figure S29. HRESIMS spectrum of 2-acetoxy-aristolane (**4**)

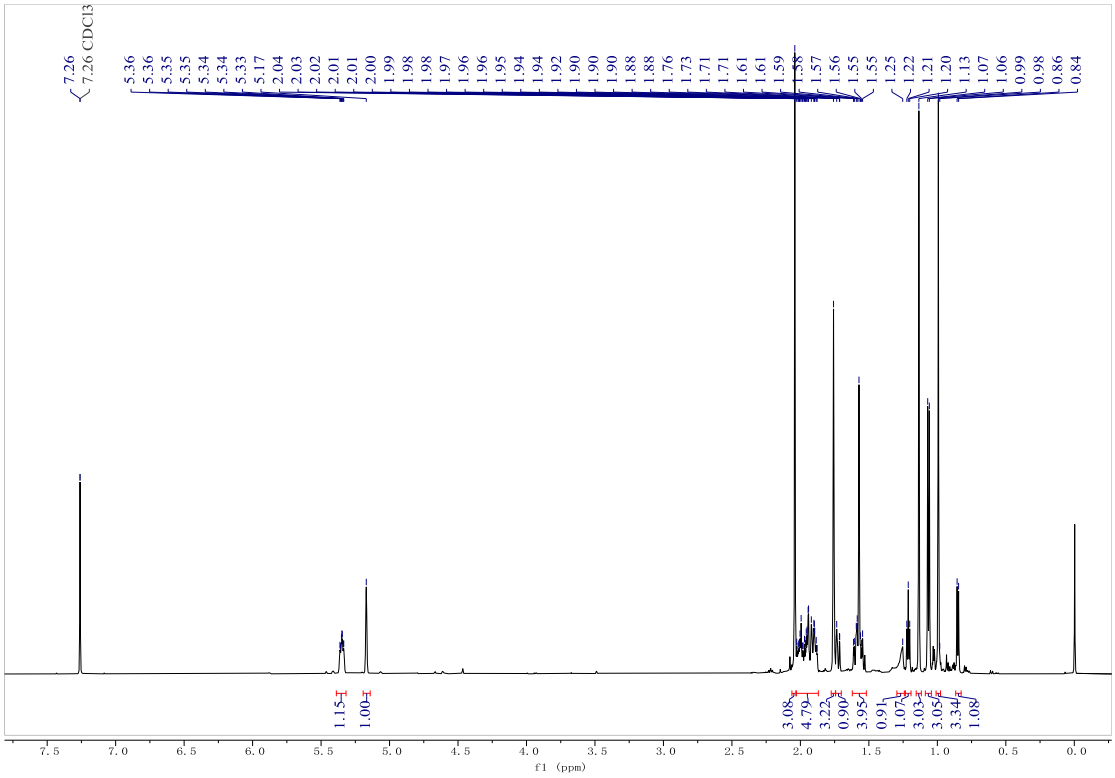


Figure S30. ^{1}H-NMR spectrum of 2-acetoxy-aristolane (**4**) in $CDCl_3$

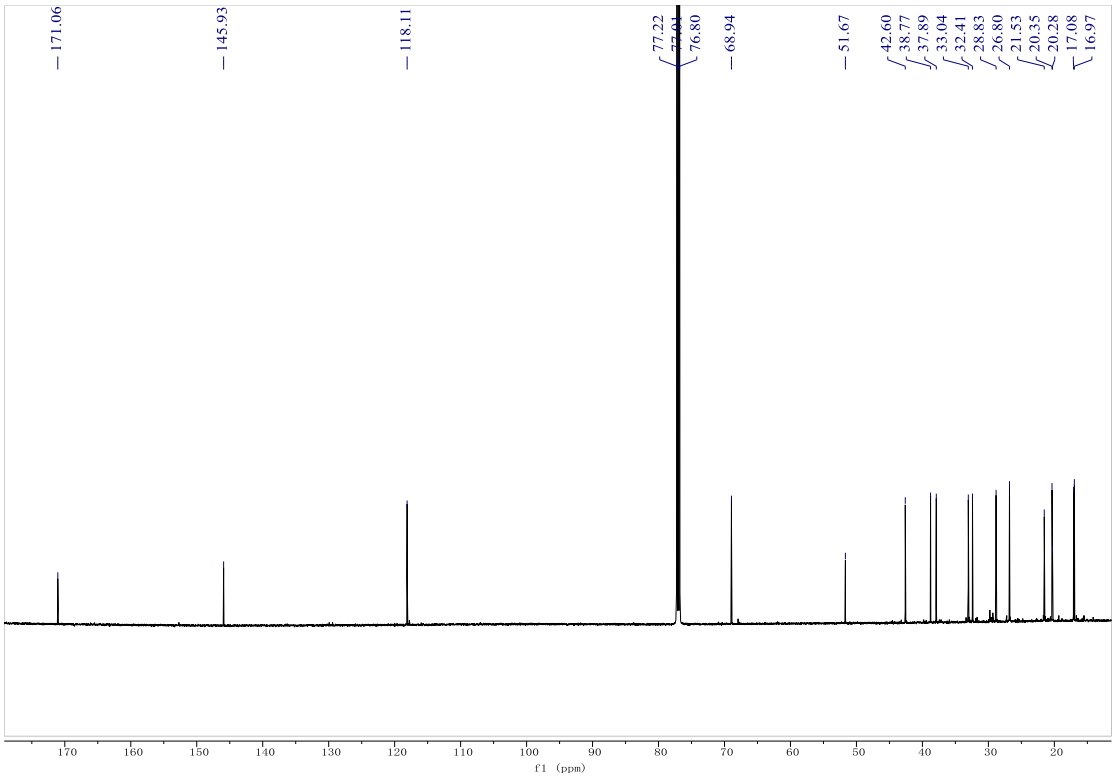


Figure S31. ^{13}C-NMR spectrum of 2-acetoxy-aristolane (**4**) in $CDCl_3$

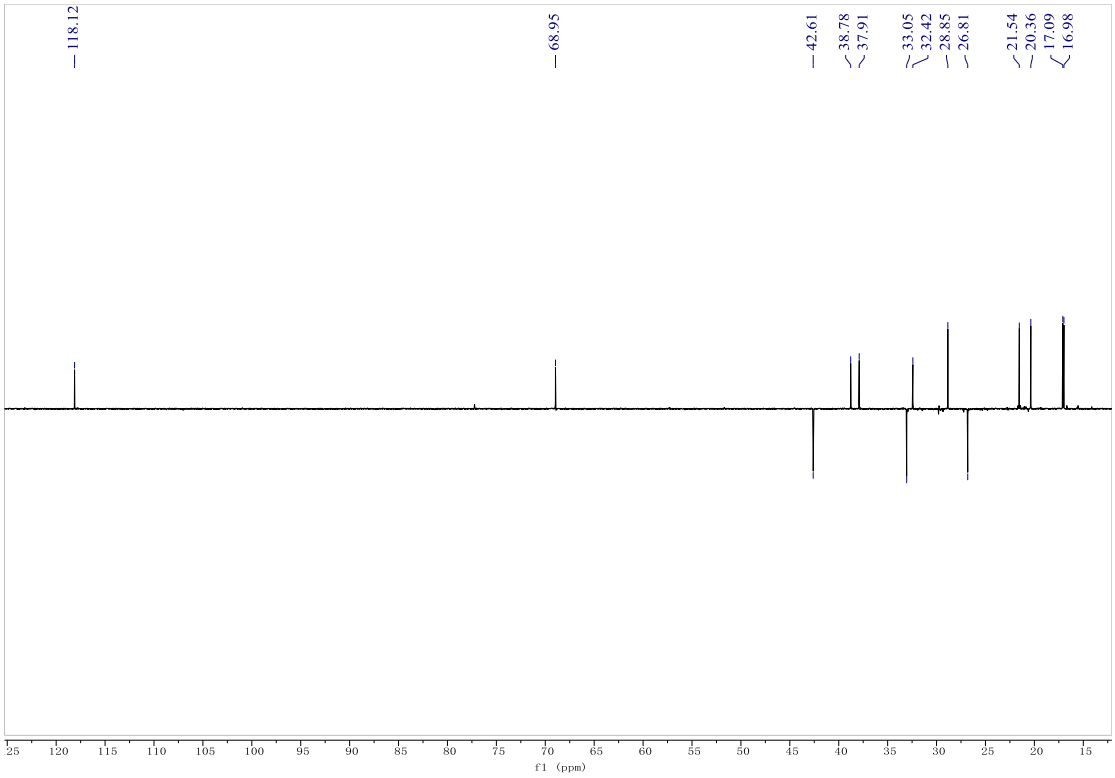


Figure S32. Dept 135° spectrum of 2-acetoxy-aristolane (**4**) in $CDCl_3$

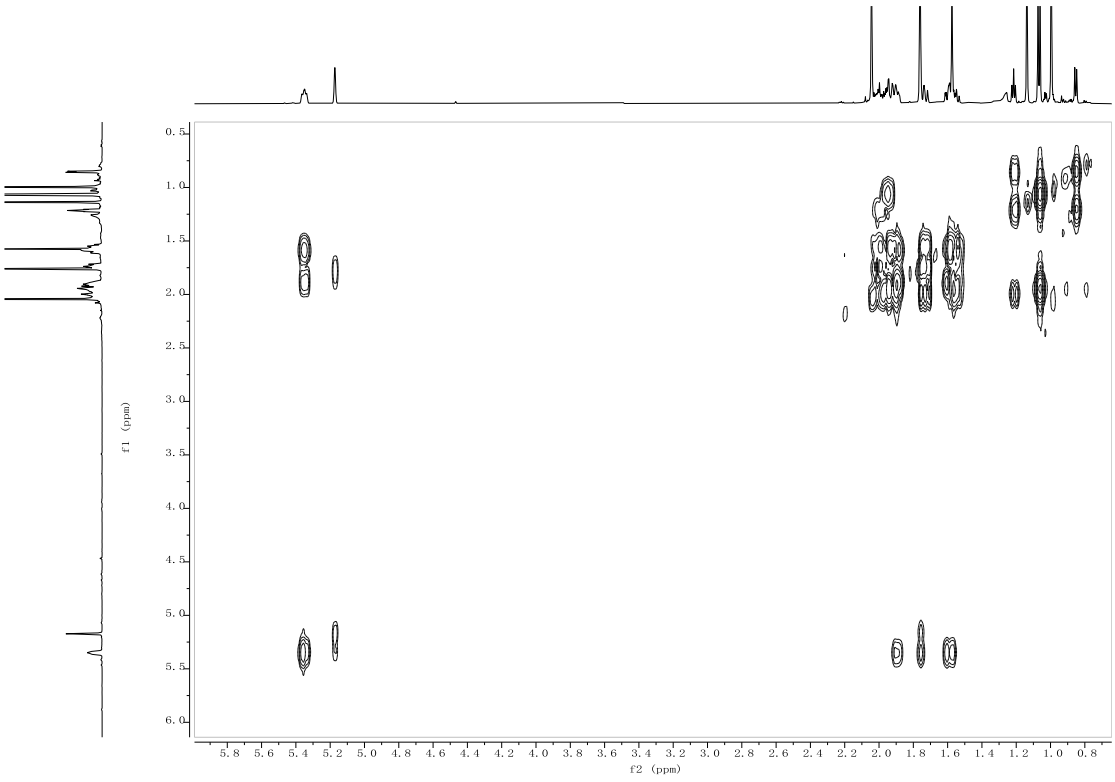


Figure S33. ^{1}H-^{1}H COSY spectrum of 2-acetoxy-aristolane (**4**) in $CDCl_3$

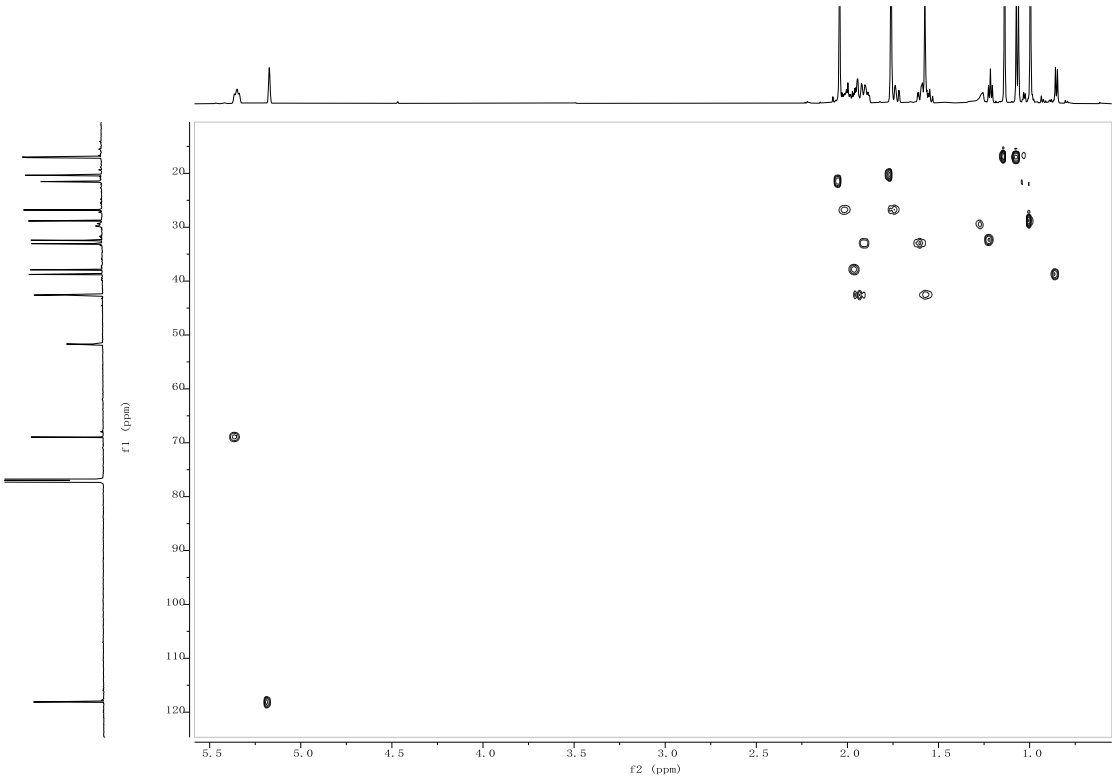


Figure S34. HSQC spectrum of 2-acetoxy-aristolane (**4**) in $CDCl_3$

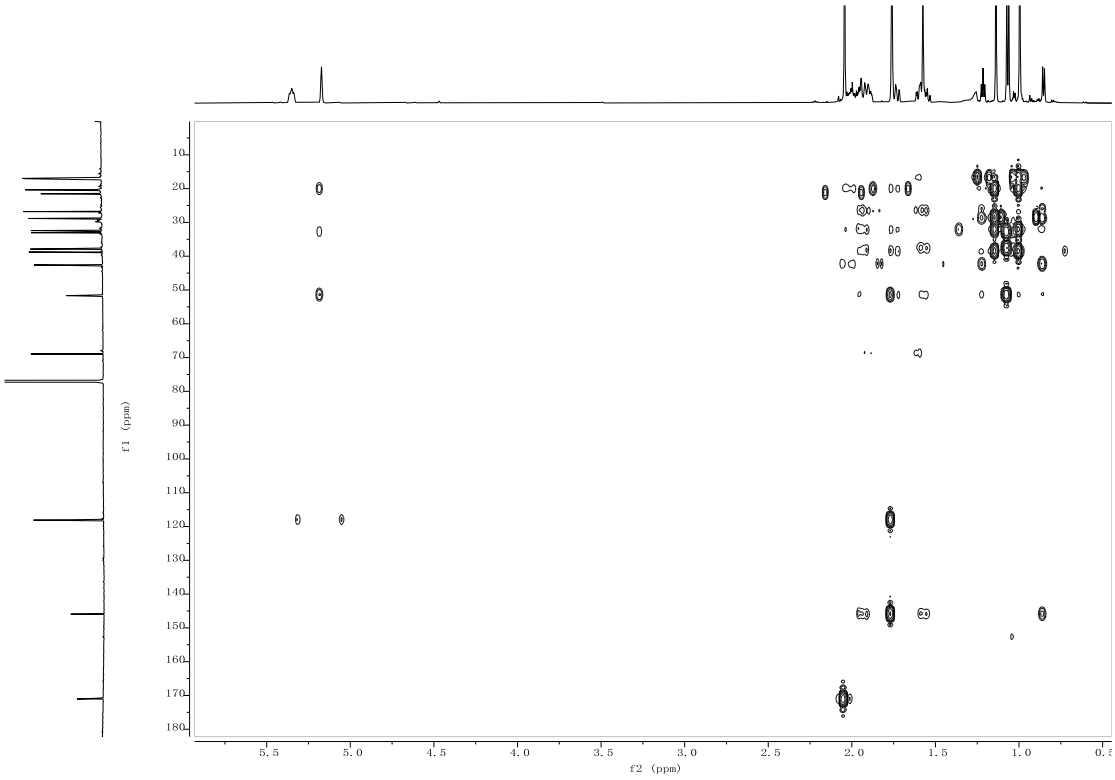


Figure S35. HMBC spectrum of 2-acetoxy-aristolane (**4**) in $CDCl_3$

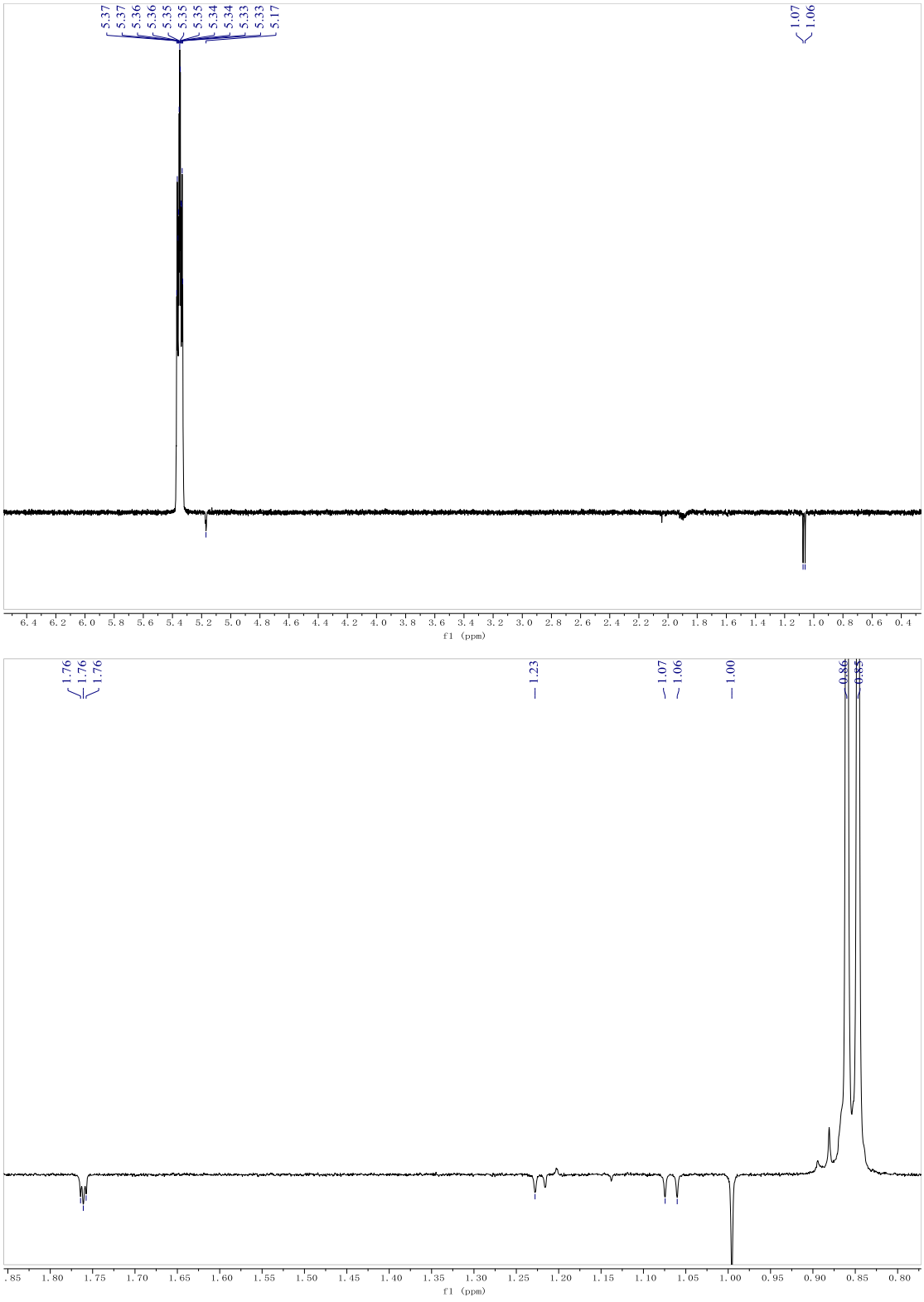


Figure S36. NOESY spectrum of 2-acetoxy-aristolane (**4**) in $CDCl_3$

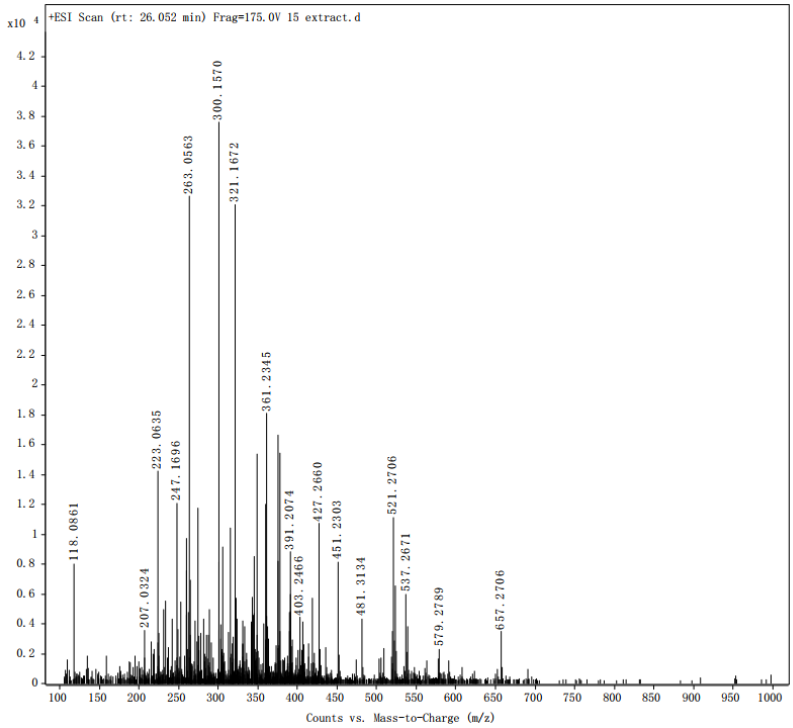


Figure S37. [M + H]+ of **4** extracted from the TIC of *Lemnalia* sp. methanol extract

9. Spectroscopic data for biofloranate A (5)

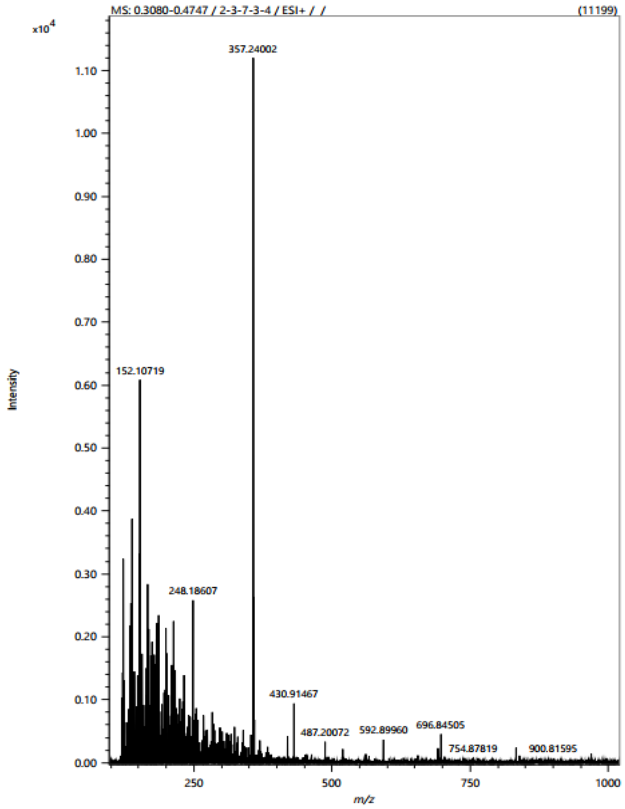


Figure S38. HRESIMS spectrum of biofloranate A (**5**)

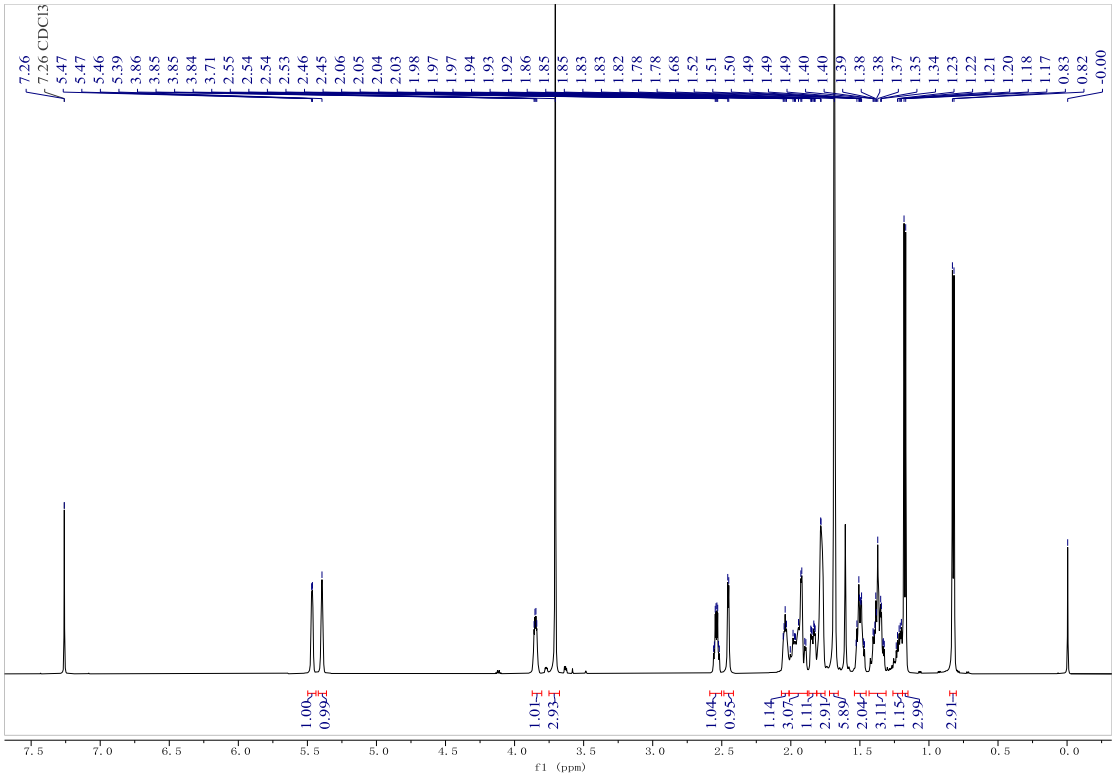


Figure S39. ^{1}H-NMR spectrum of biofloranate A (**5**) in $CDCl_3$

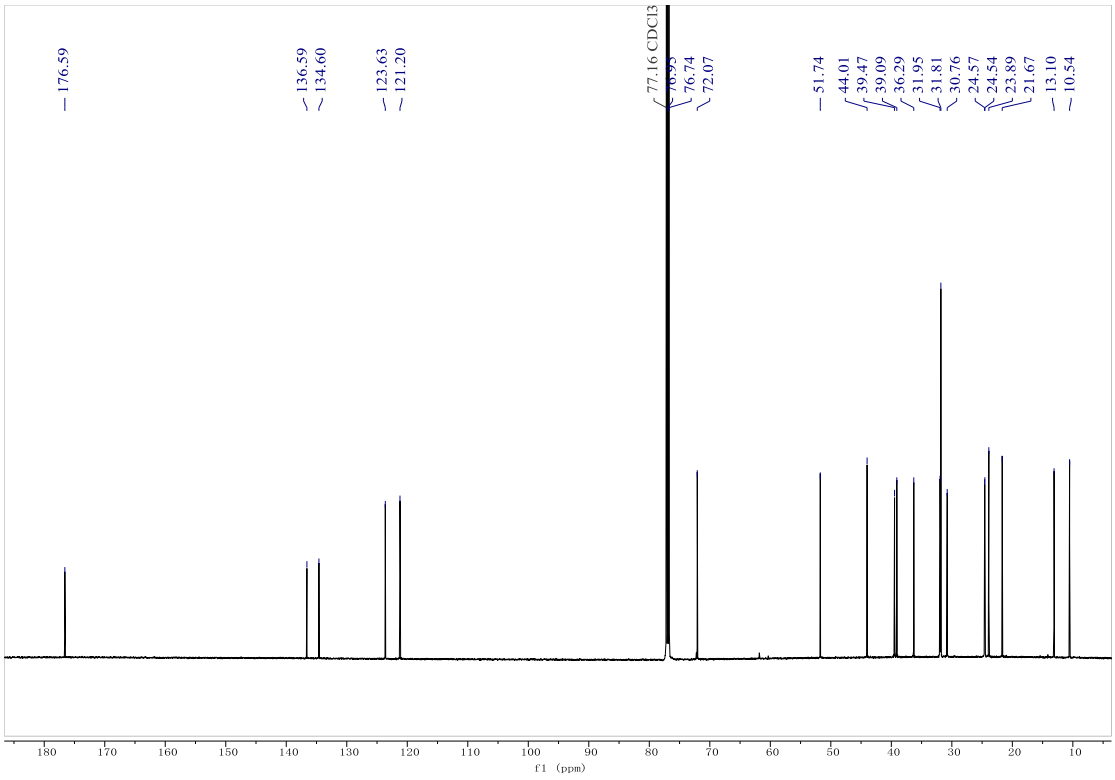


Figure S40. ^{13}C-NMR spectrum of biofloranate A (**5**) in $CDCl_3$

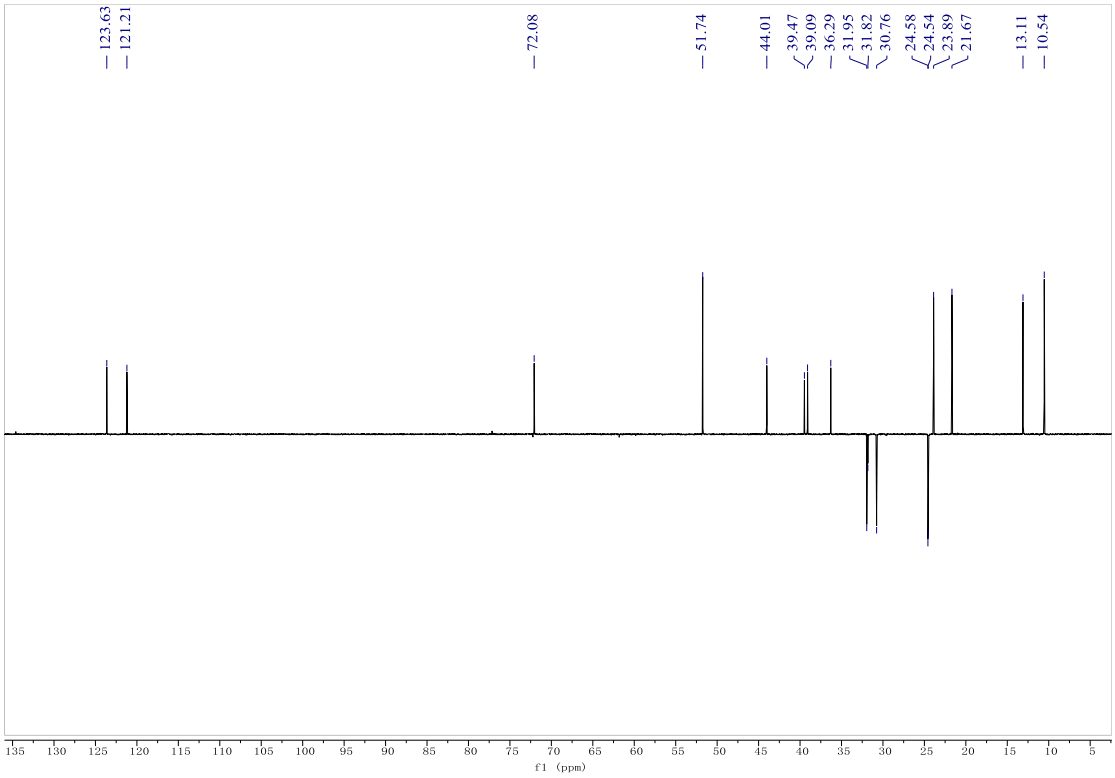


Figure S41. Dept 135° spectrum of biofloranate A (**5**) in $CDCl_3$

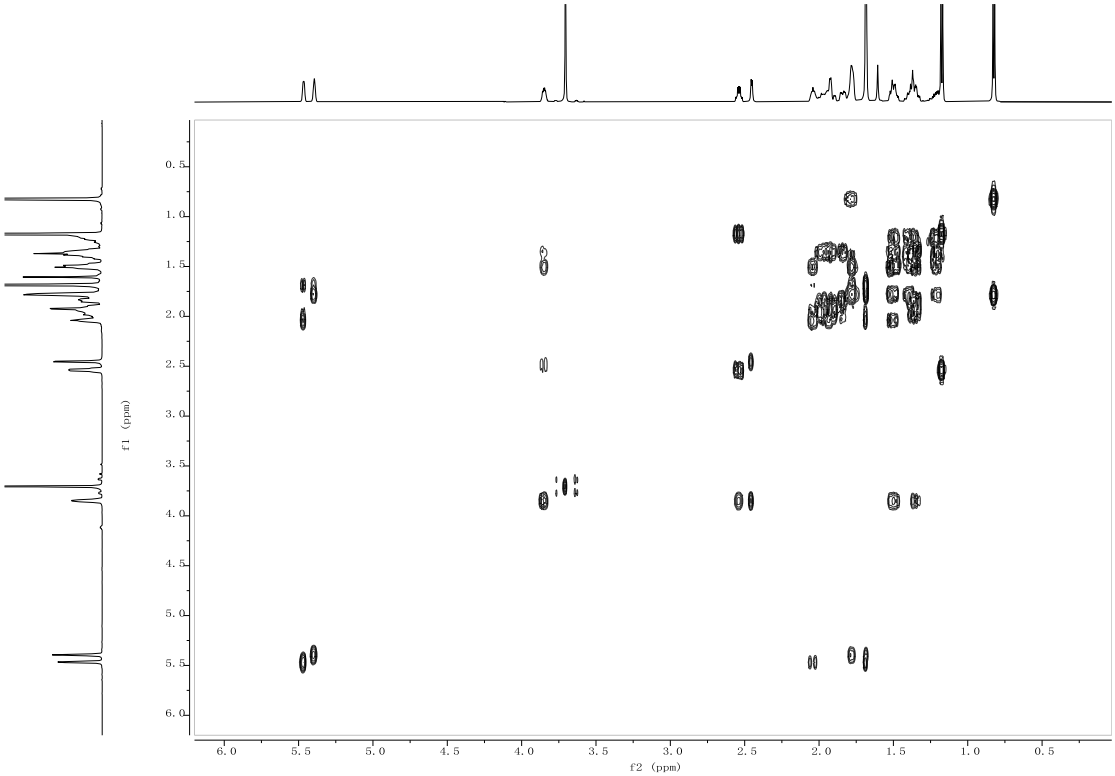


Figure S42. ^{1}H-^{1}H COSY spectrum of biofloranate A (**5**) in $CDCl_3$

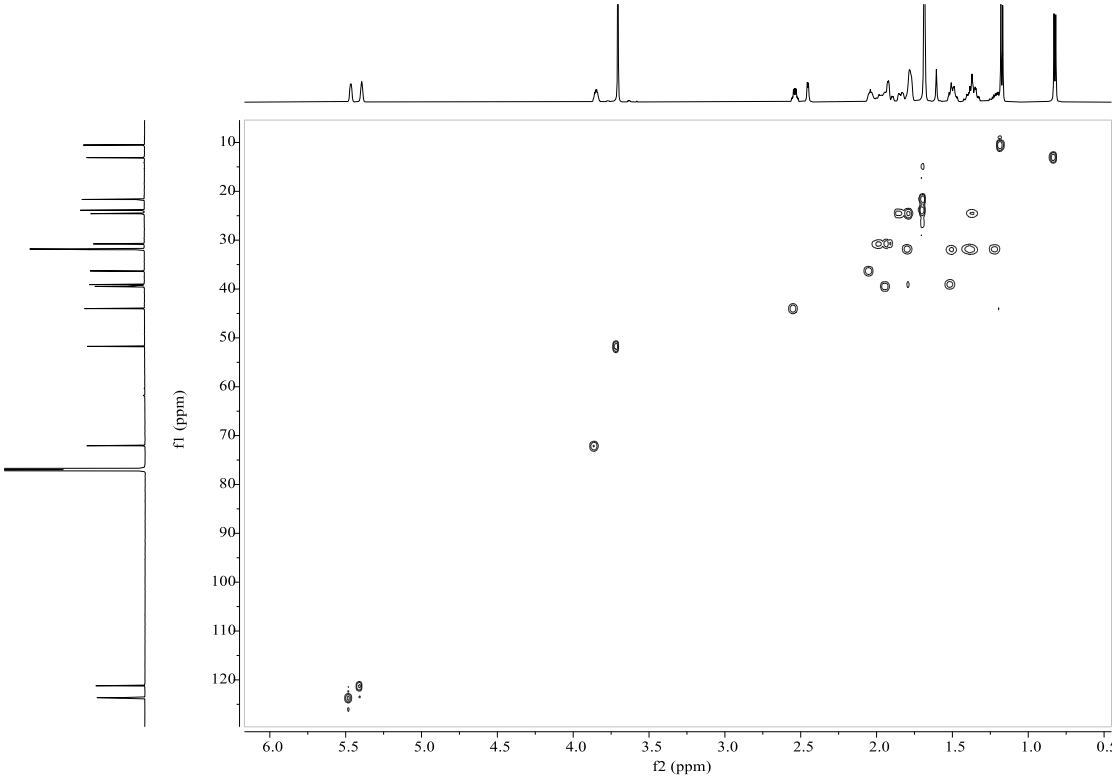


Figure S43. HSQC spectrum of biofloranate A (**5**) in $CDCl_3$

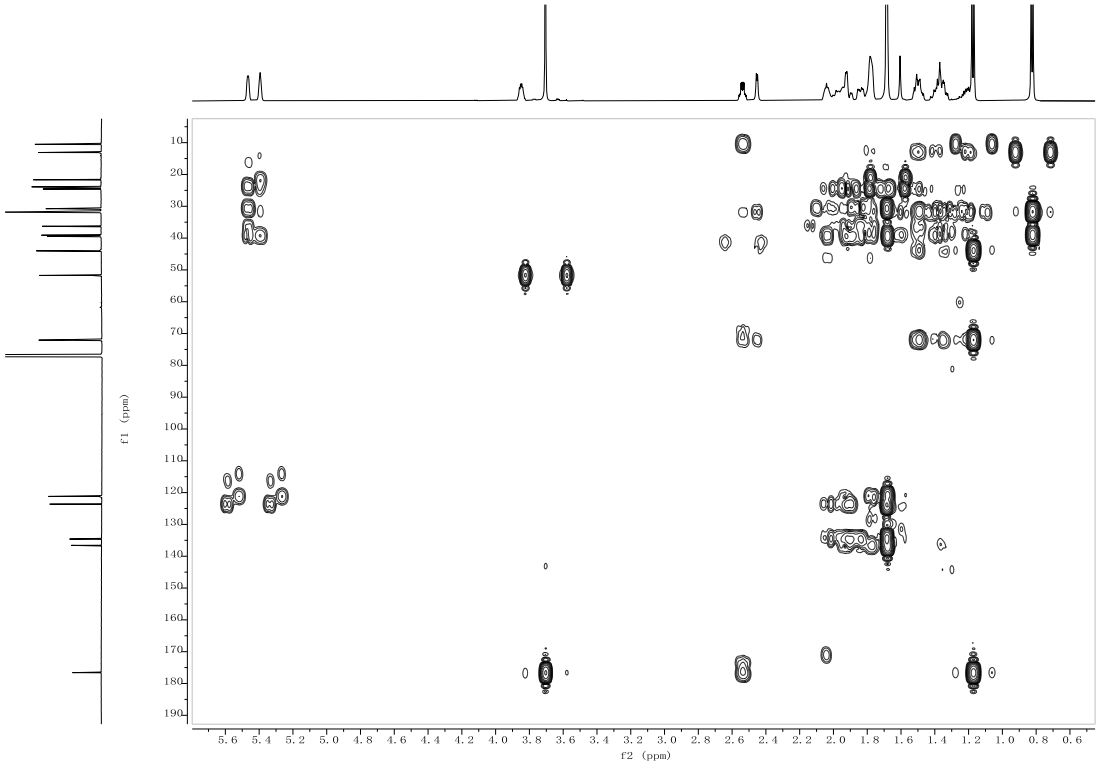


Figure S44. HMBC spectrum of biofloranate A (**5**) in $CDCl_3$

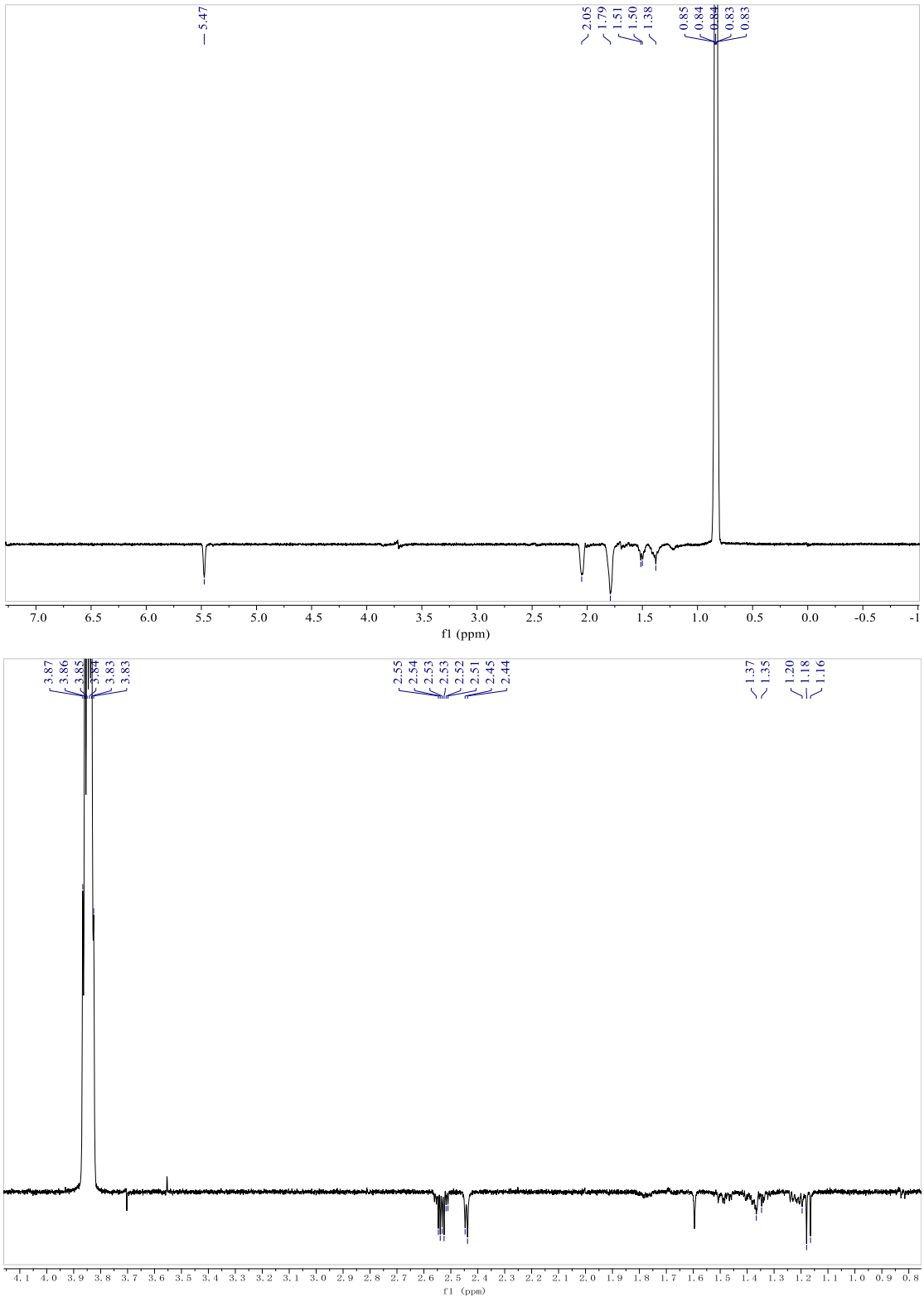


Figure S45. NOESY spectrum of biofloranate A (**5**) in $CDCl_3$

10. Spectroscopic data for biofloranate B (6)

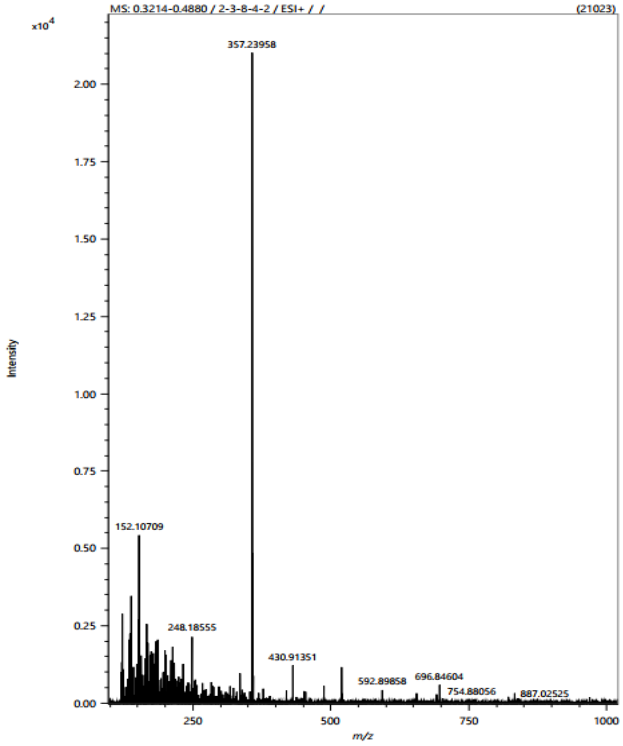


Figure S46. HRESIMS spectrum of biofloranate B (**6**)

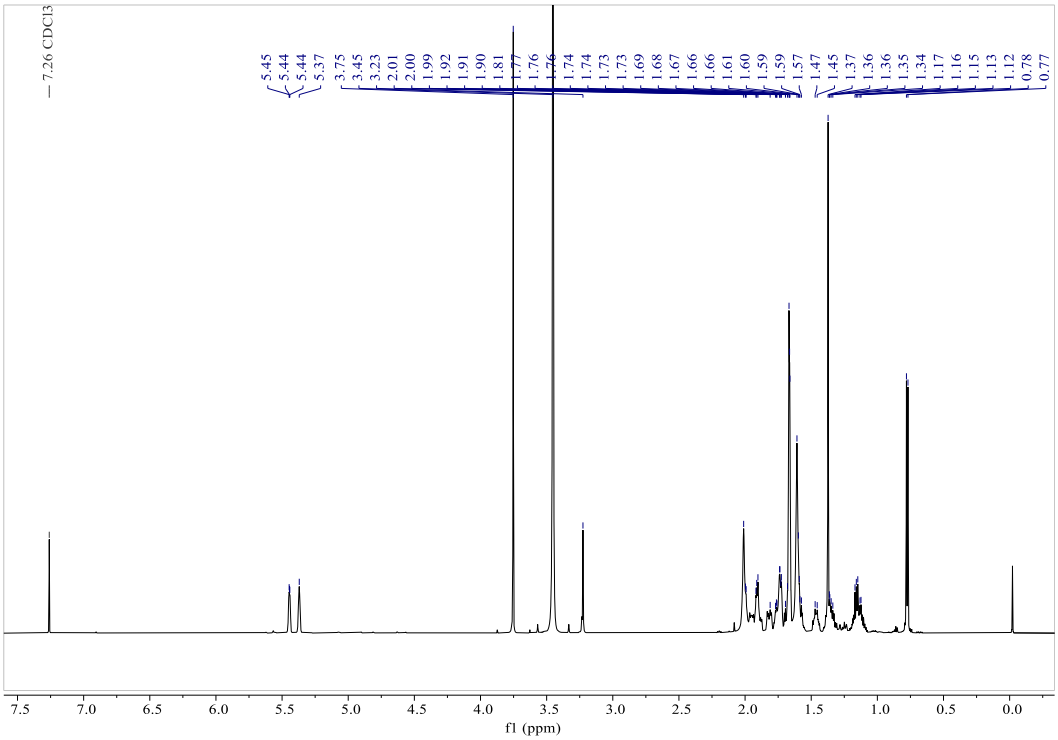


Figure S47. ^{1}H-NMR spectrum of biofloranate B (**6**) in $CDCl_3$

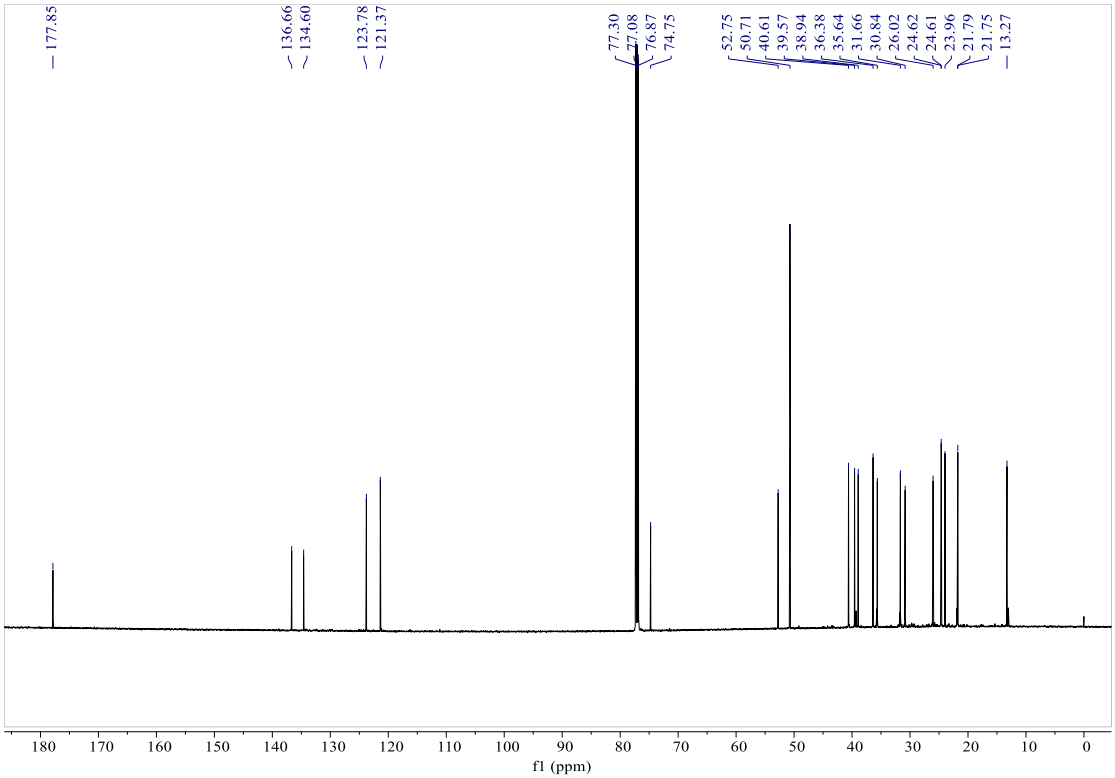


Figure S48. ^{13}C-NMR spectrum of biofloranate B (**6**) in $CDCl_3$

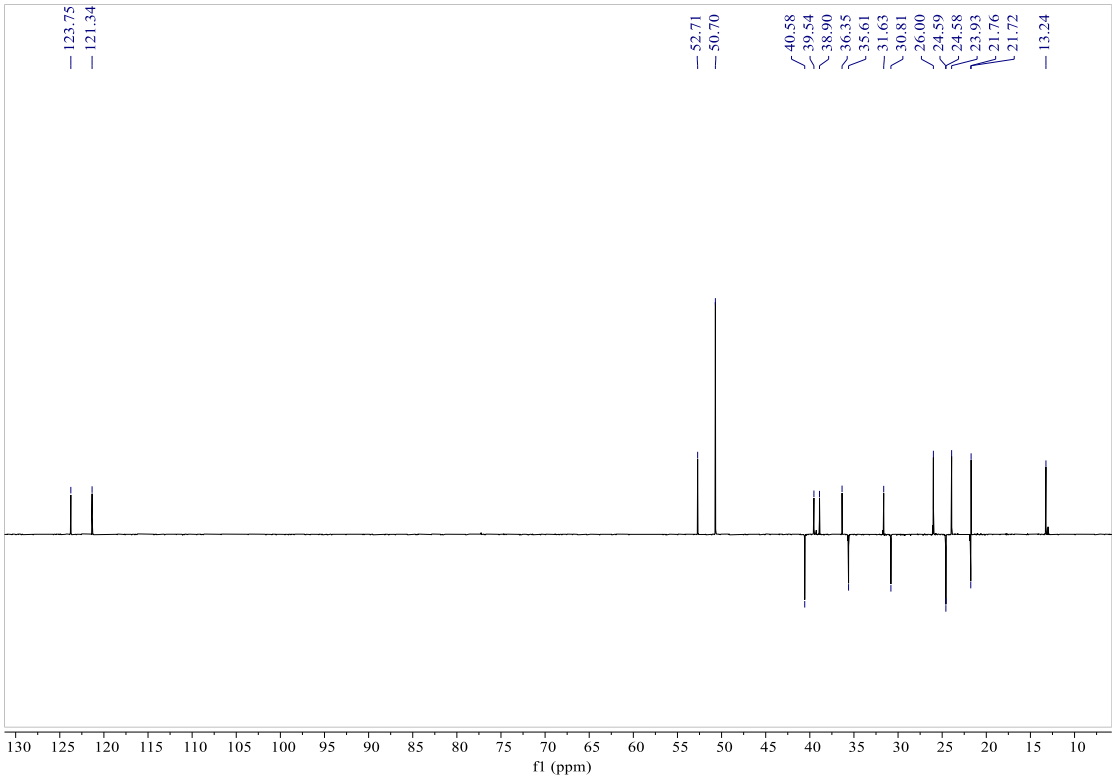


Figure S49. Dept 135° spectrum of biofloranate B (**6**) in $CDCl_3$

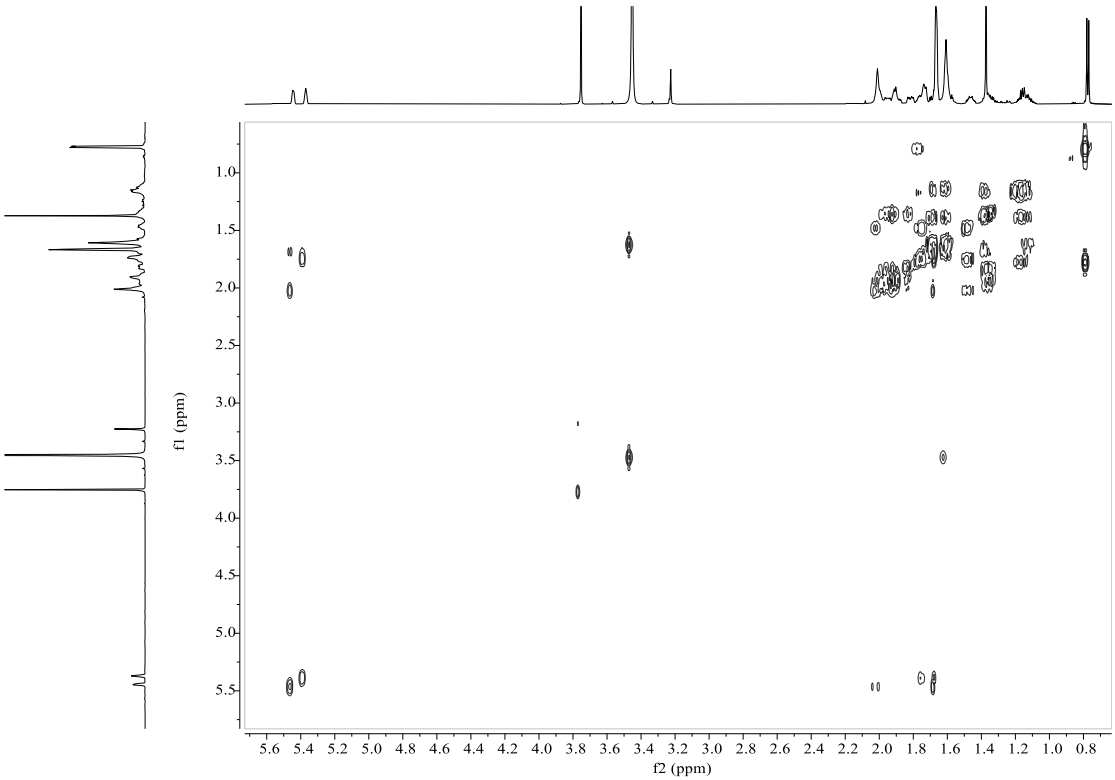


Figure S50. ^{1}H-^{1}H COSY spectrum of biofloranate B (**6**) in $CDCl_3$

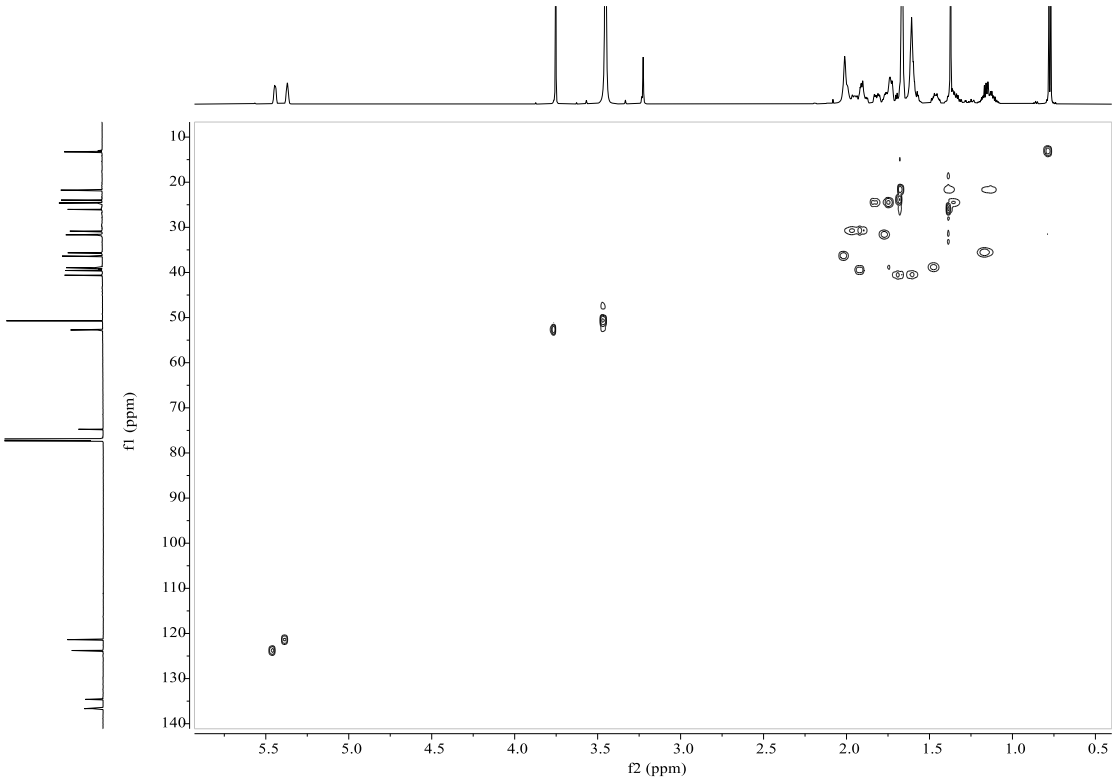


Figure S51. HSQC spectrum of biofloranate B (**6**) in $CDCl_3$

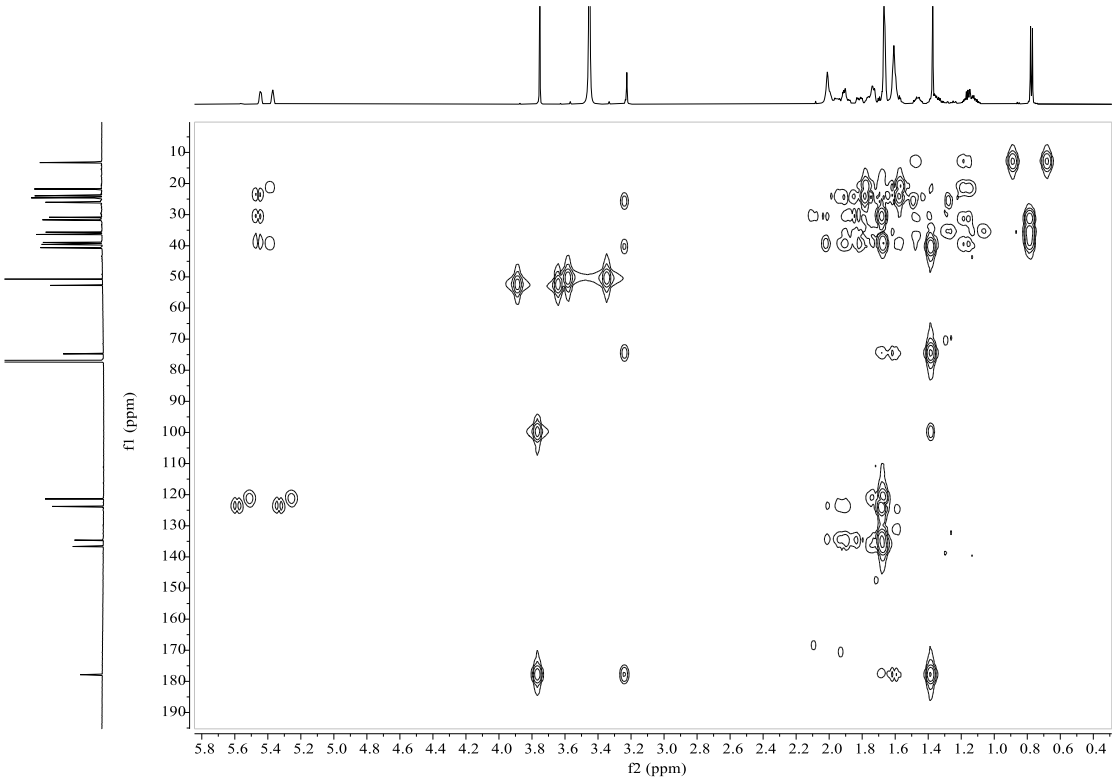


Figure S52. HMBC spectrum of biofloranate B (**6**) in $CDCl_3$

11. Spectroscopic data for biofloranate C (7)

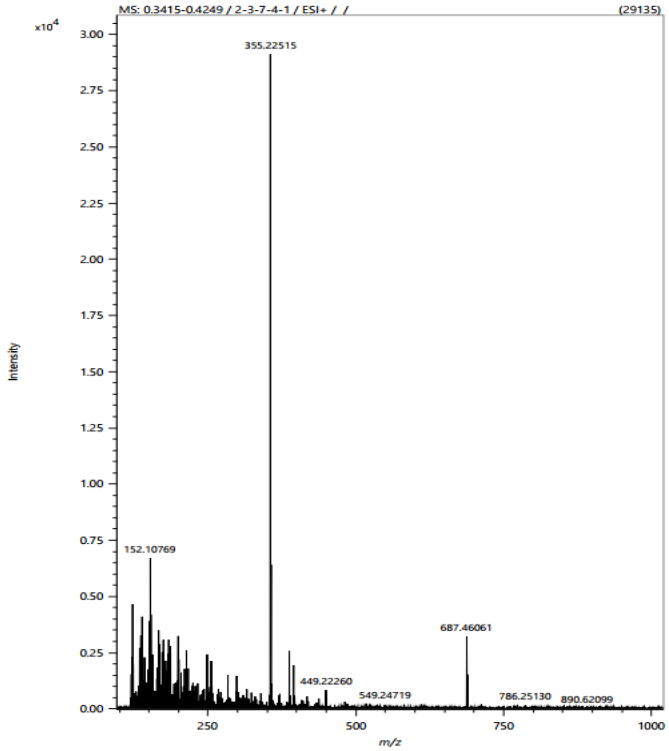


Figure S53. HRESIMS spectrum of biofloranate C (**7**)

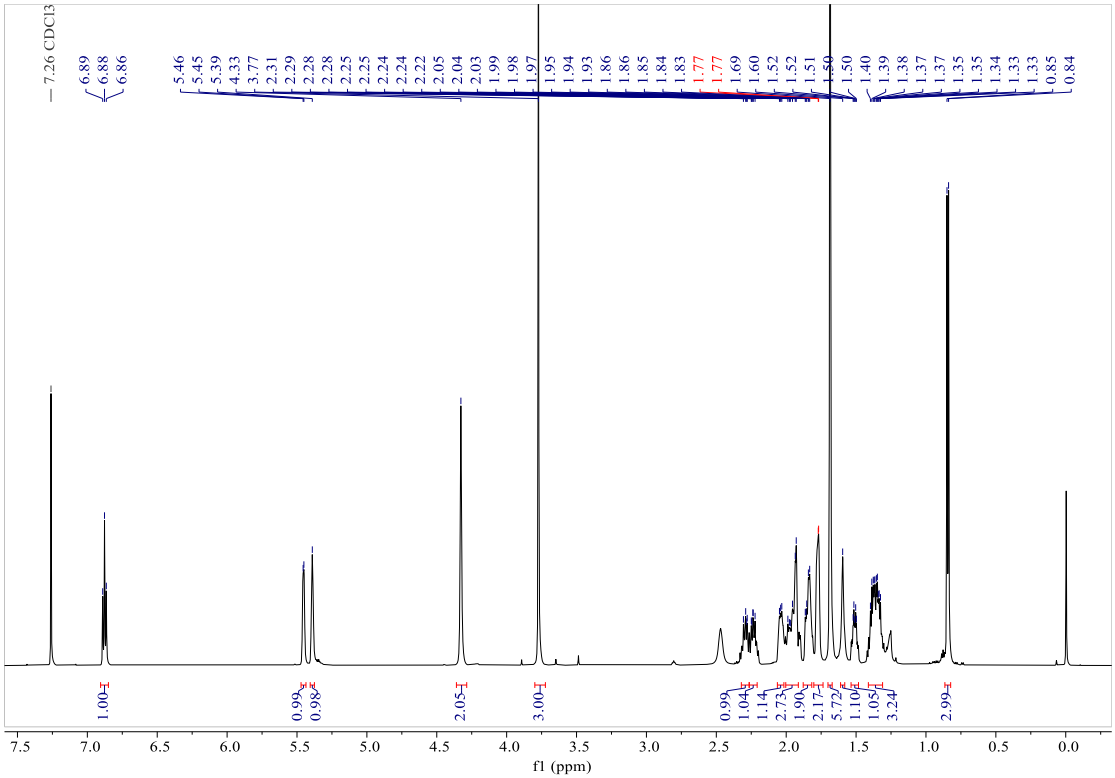


Figure S54. ^{1}H-NMR spectrum of biofloranate C (**7**) in $CDCl_3$

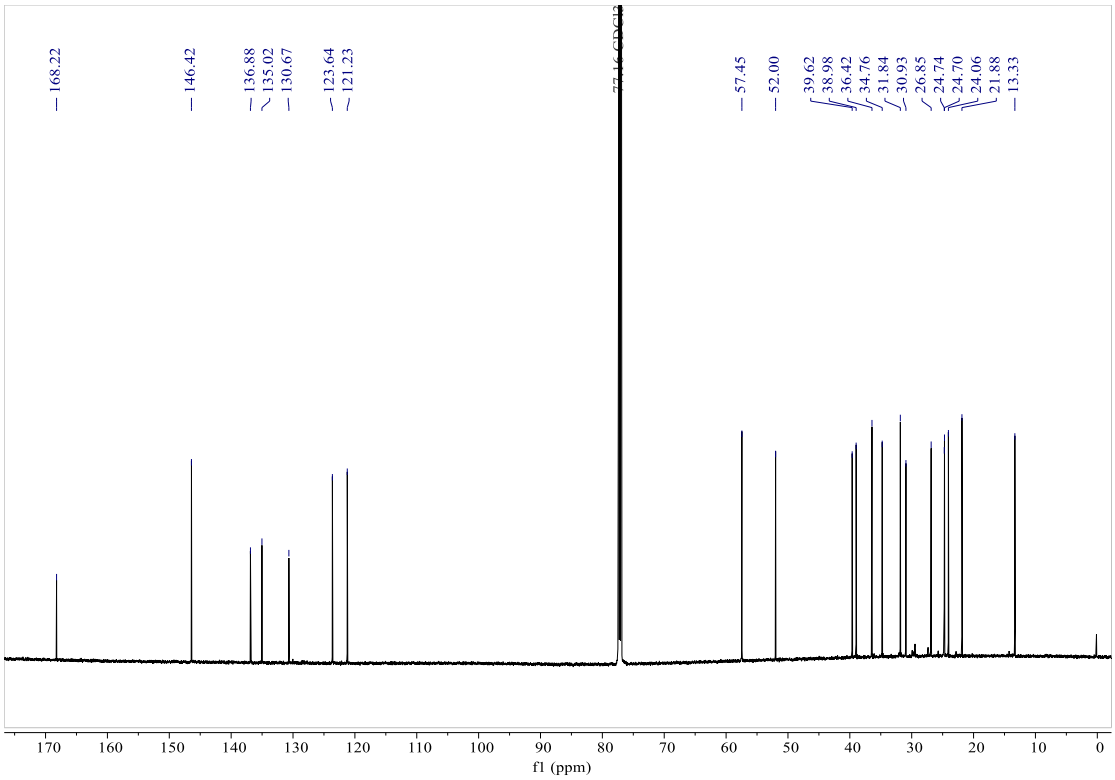


Figure S55. ^{13}C-NMR spectrum of biofloranate C (**7**) in $CDCl_3$

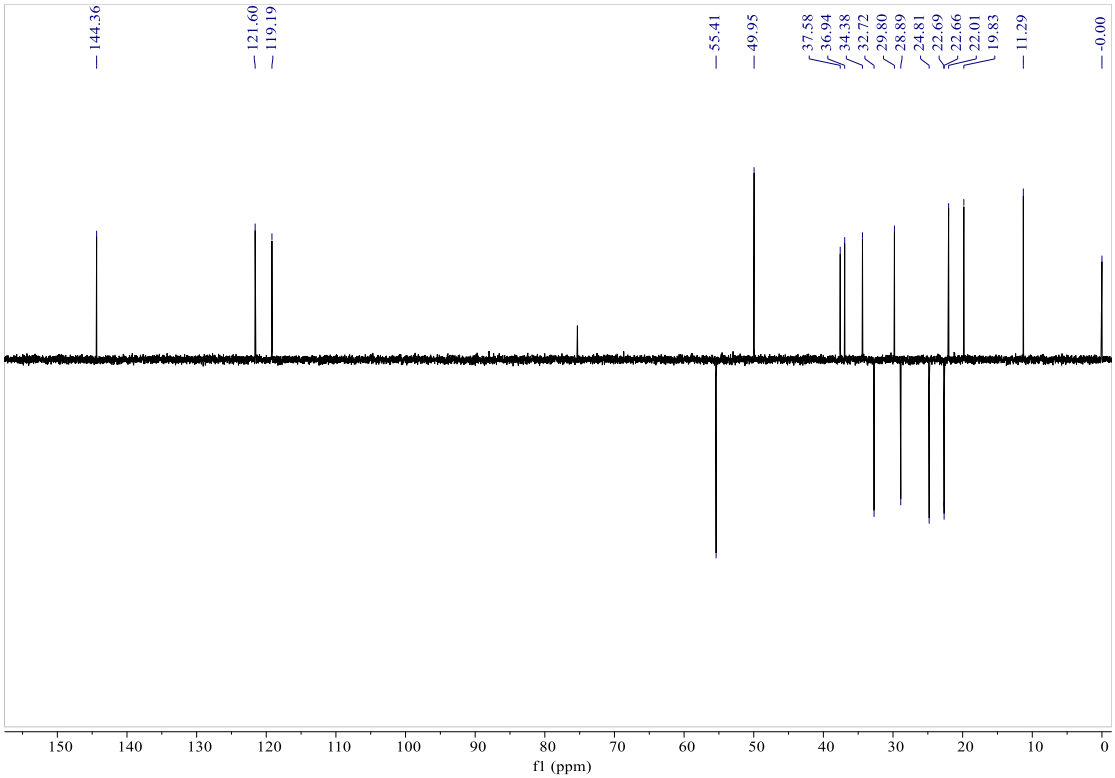


Figure S56. Dept 135° spectrum of biofloranate C (**7**) in $CDCl_3$

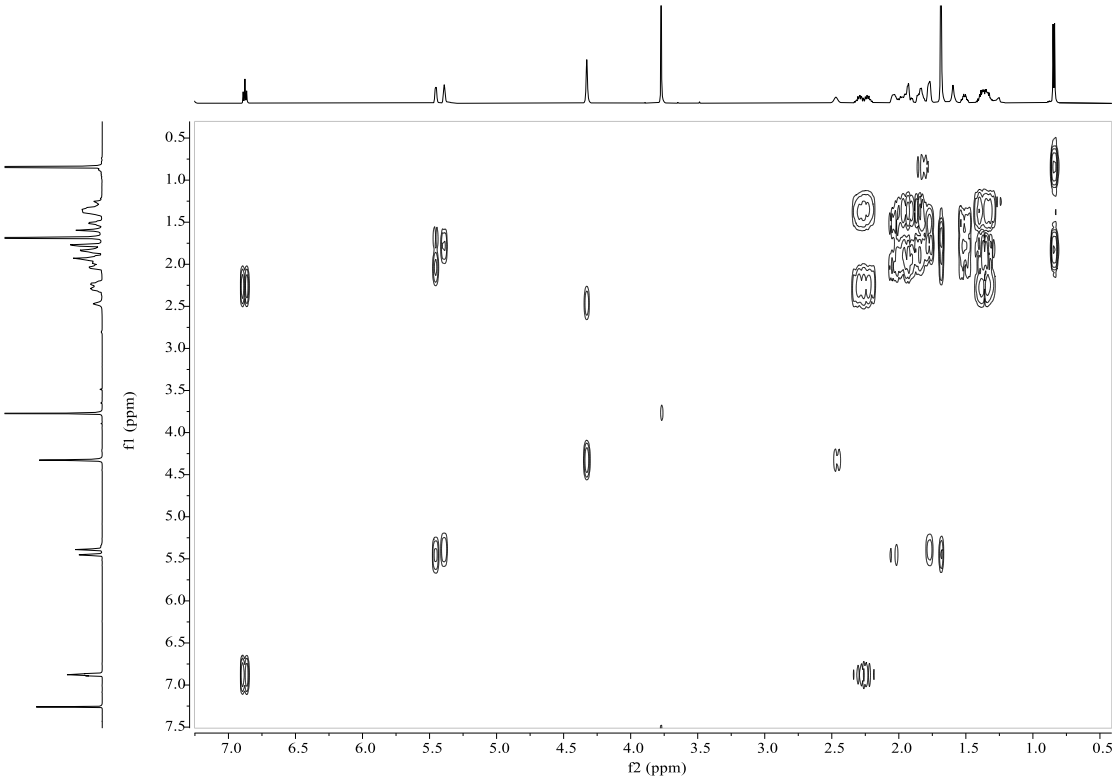


Figure S57. ^{1}H-^{1}H COSY spectrum of biofloranate C (**7**) in $CDCl_3$

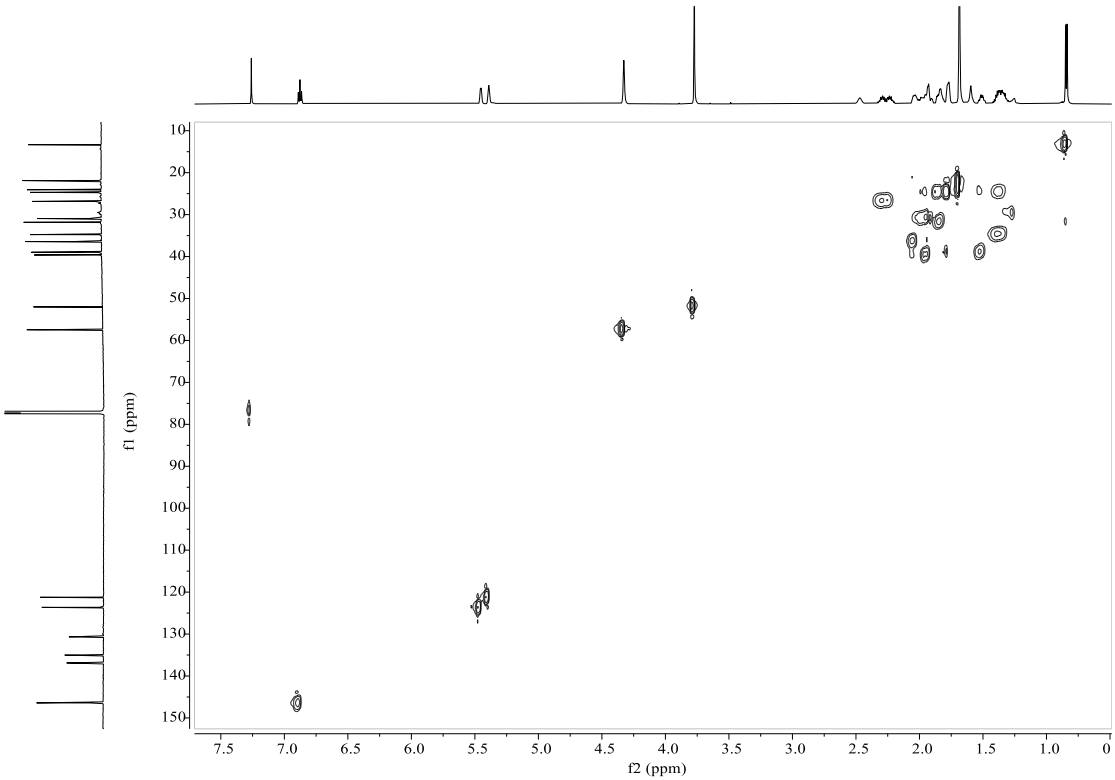


Figure S58. HSQC spectrum of biofloranate C (**7**) in $CDCl_3$

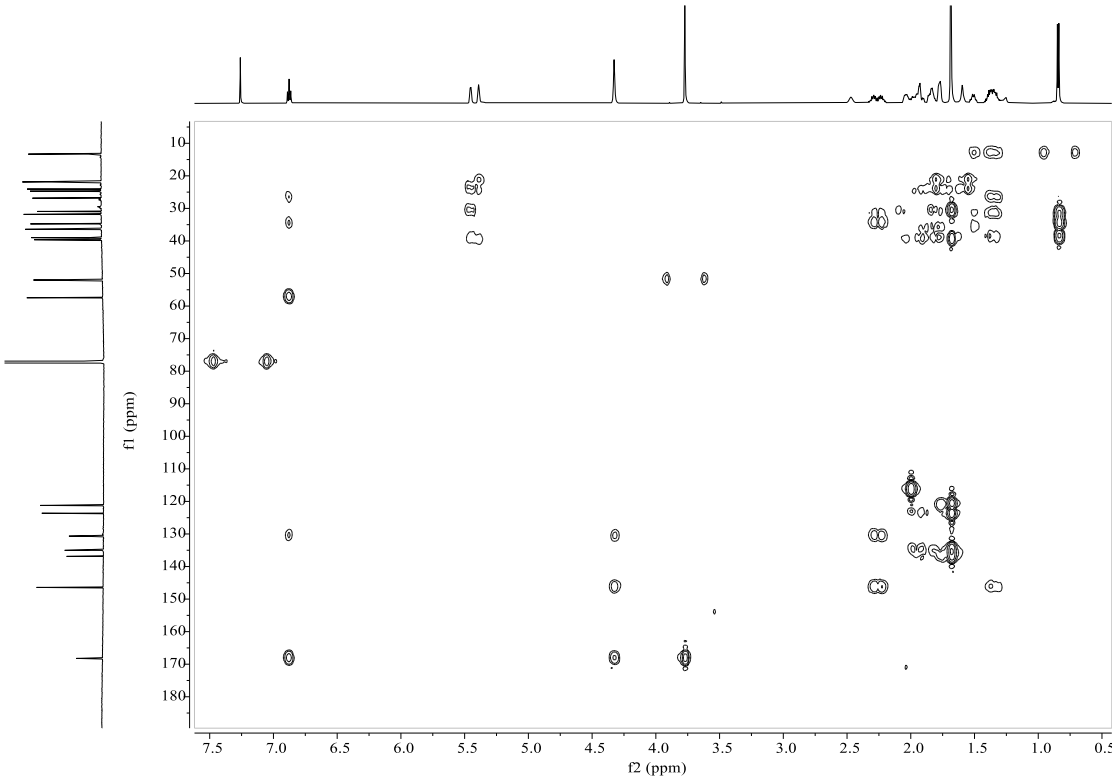


Figure S59. HMBC spectrum of biofloranate C (**7**) in $CDCl_3$

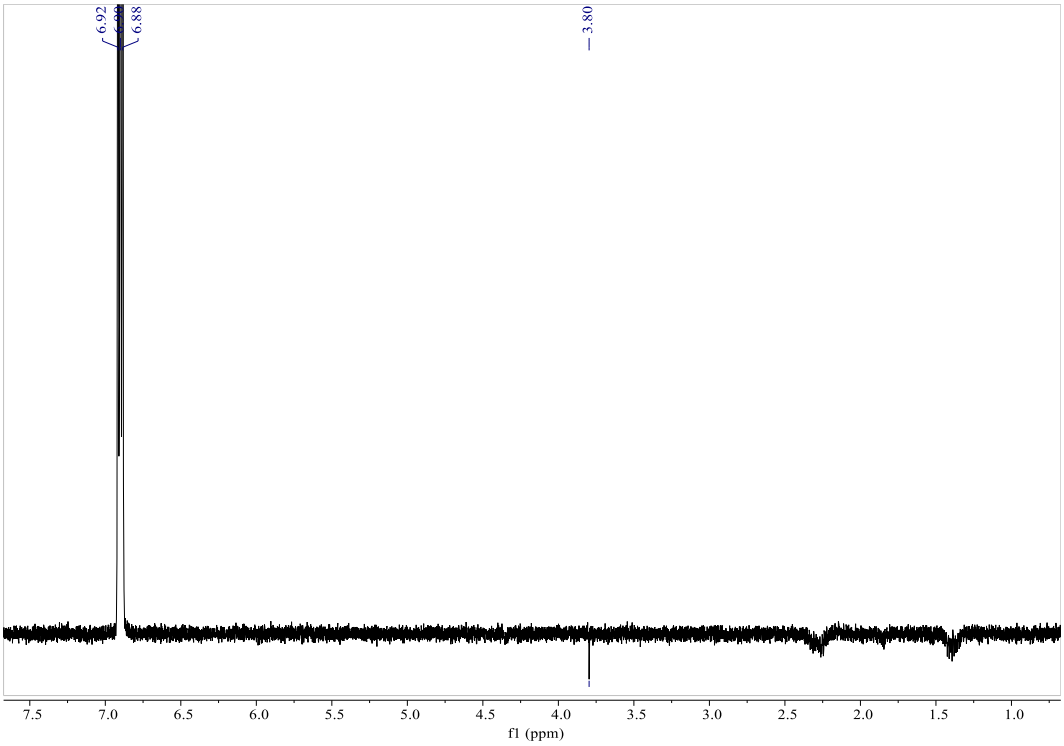


Figure S60. NOESY spectrum of biofloranate C (**7**) in $CDCl_3$

12. Spectroscopic data for biofloranate D (8)

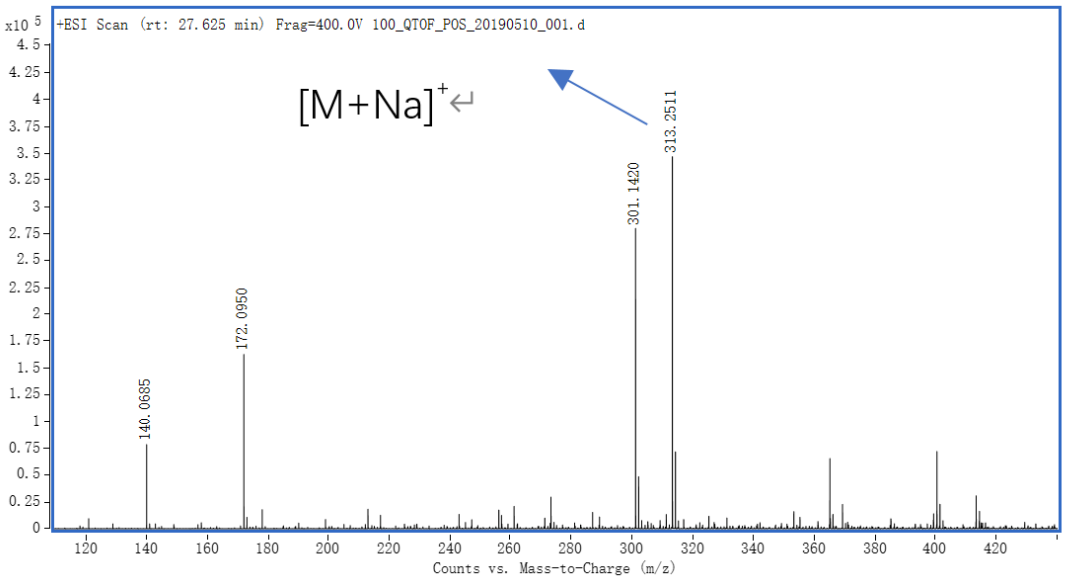


Figure S61. HRESIMS spectrum of biofloranate D (**8**)

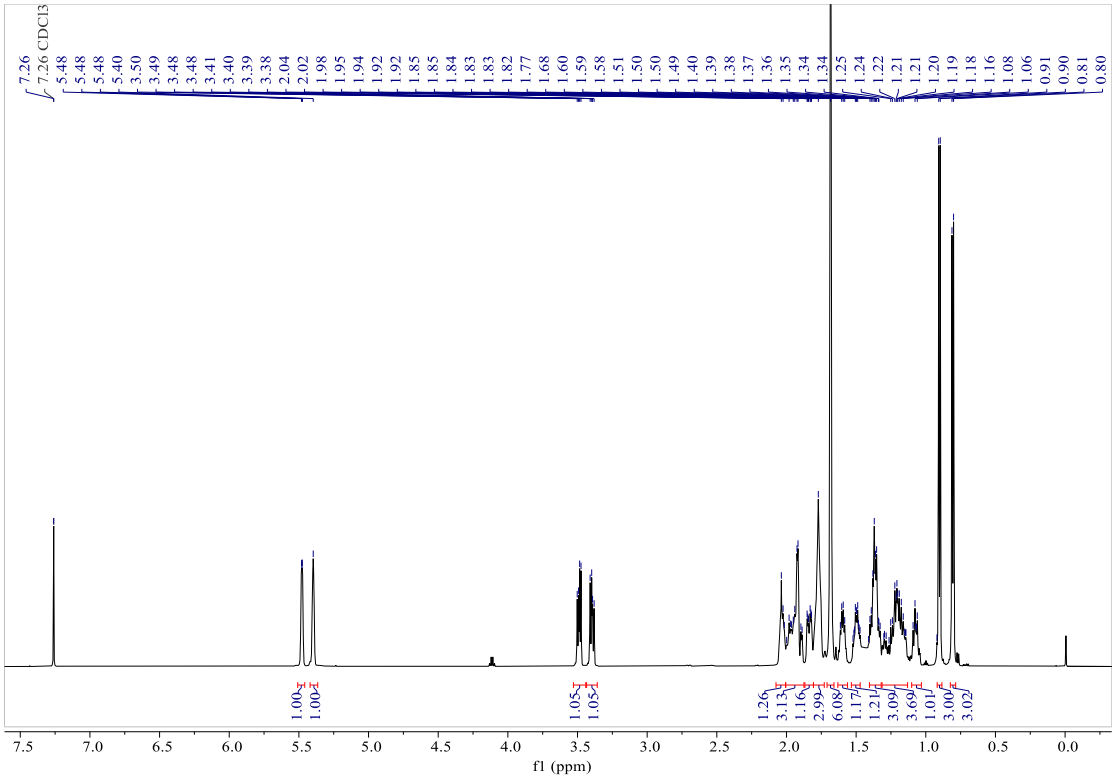


Figure S62. ^{1}H-NMR spectrum of biofloranate D (**8**) in $CDCl_3$

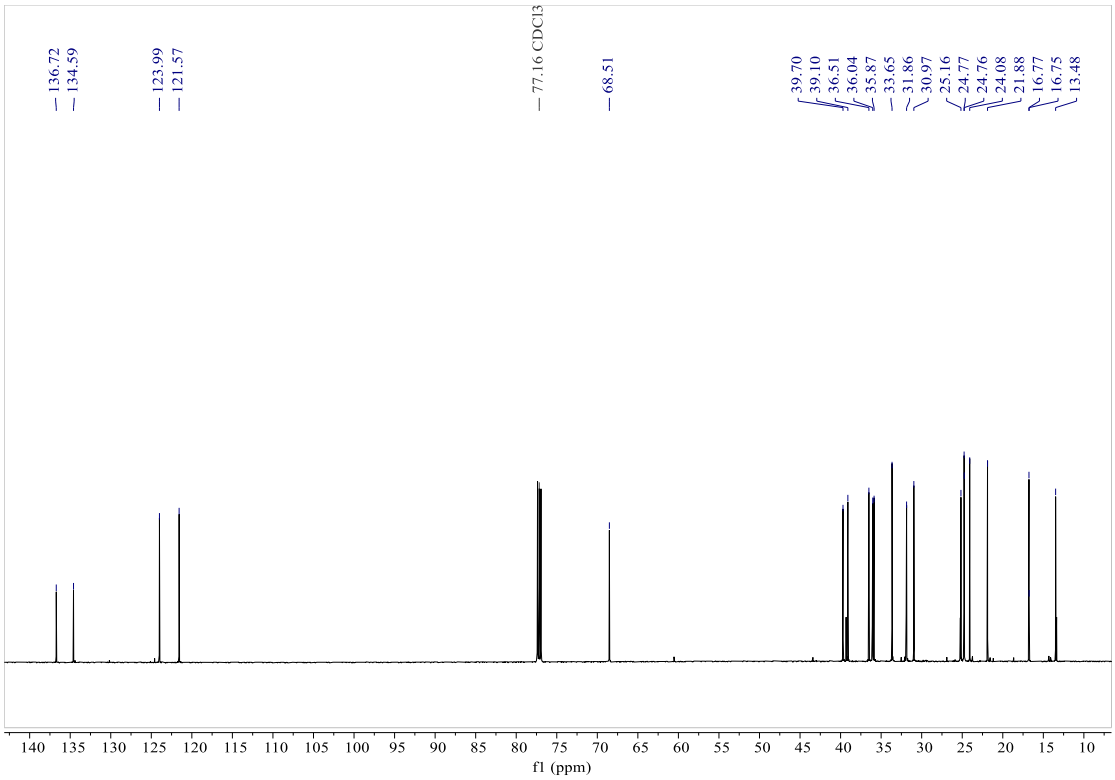


Figure S63. ^{13}C-NMR spectrum of biofloranate D (**8**) in $CDCl_3$

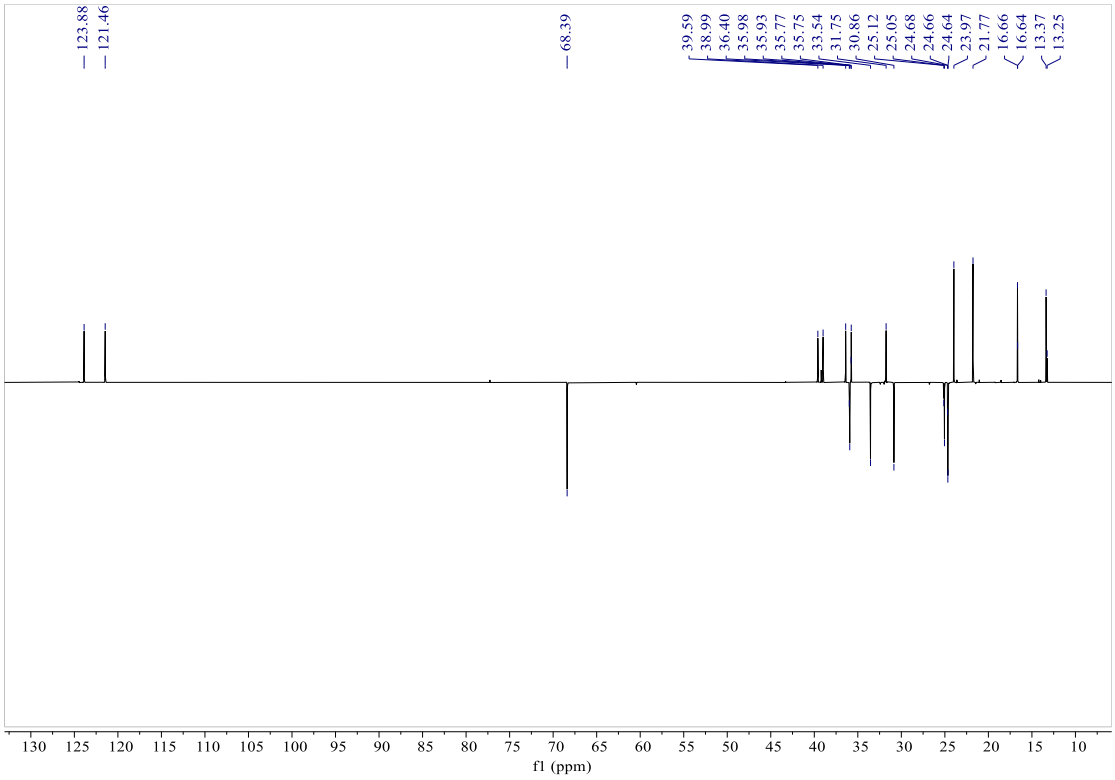


Figure S64. Dept 135° spectrum of biofloranate D (**8**) in $CDCl_3$

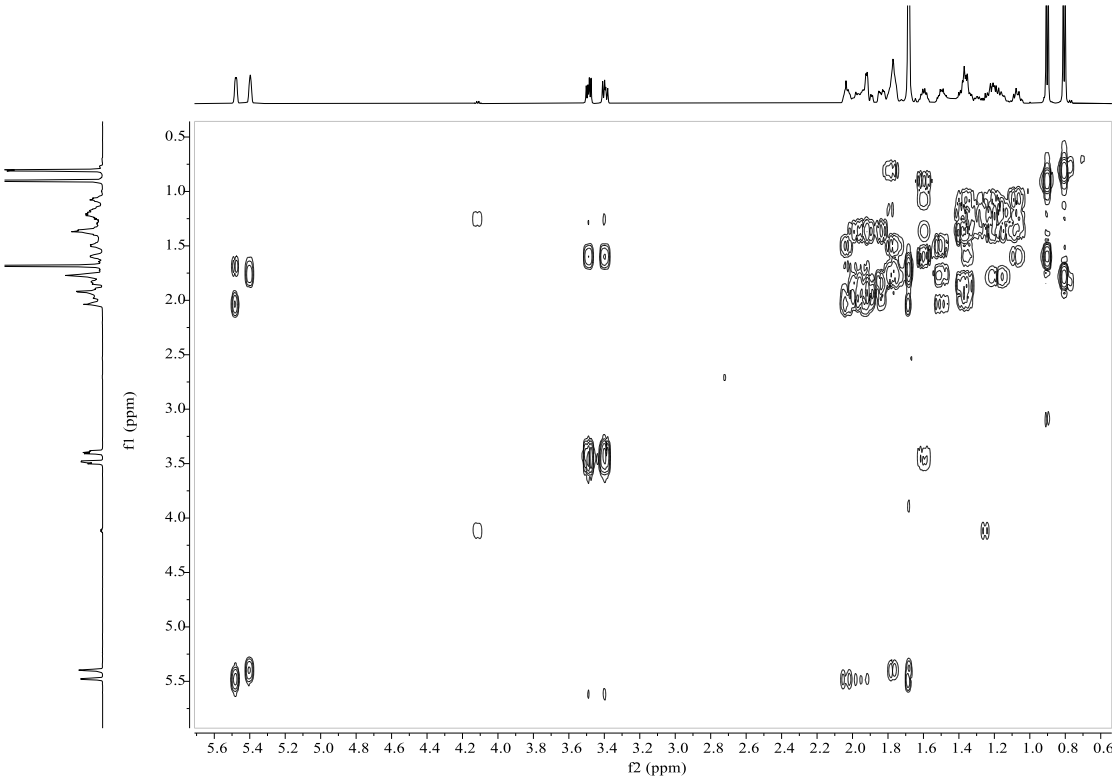


Figure S65. ^{1}H-^{1}H COSY spectrum of biofloranate D (**8**) in $CDCl_3$

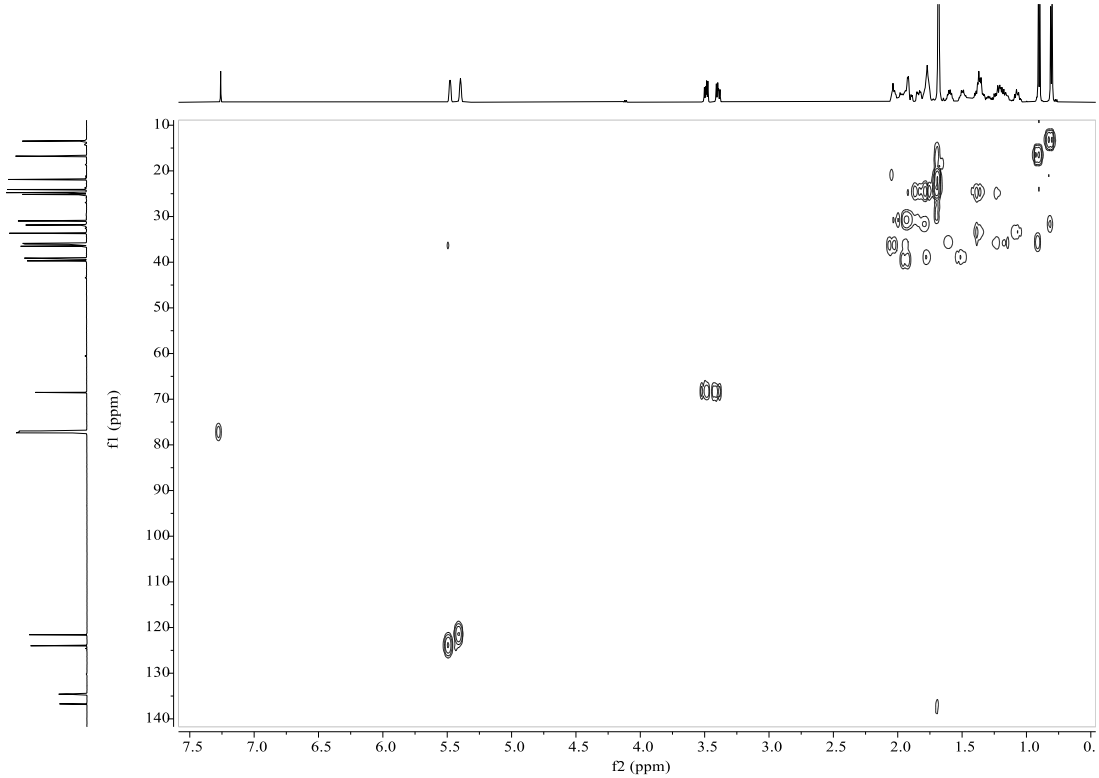


Figure S66. HSQC spectrum of biofloranate D (**8**) in $CDCl_3$

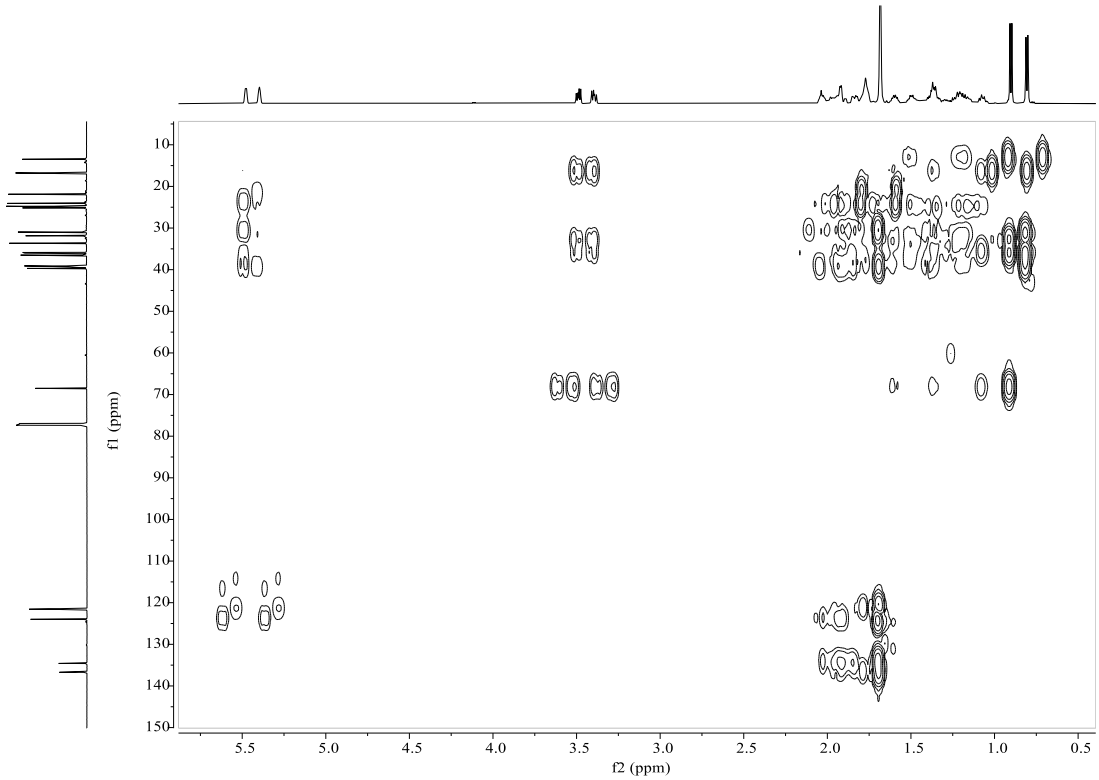


Figure S67. HMBC spectrum of biofloranate D (**8**) in $CDCl_3$

13. Spectroscopic data for euplexaurene D (9)

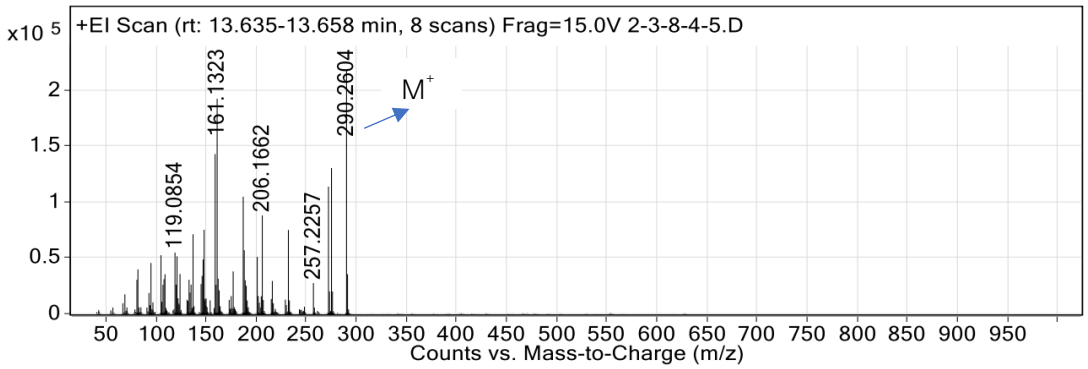


Figure S68. HRESIMS spectrum of euplexaurene D (**9**)

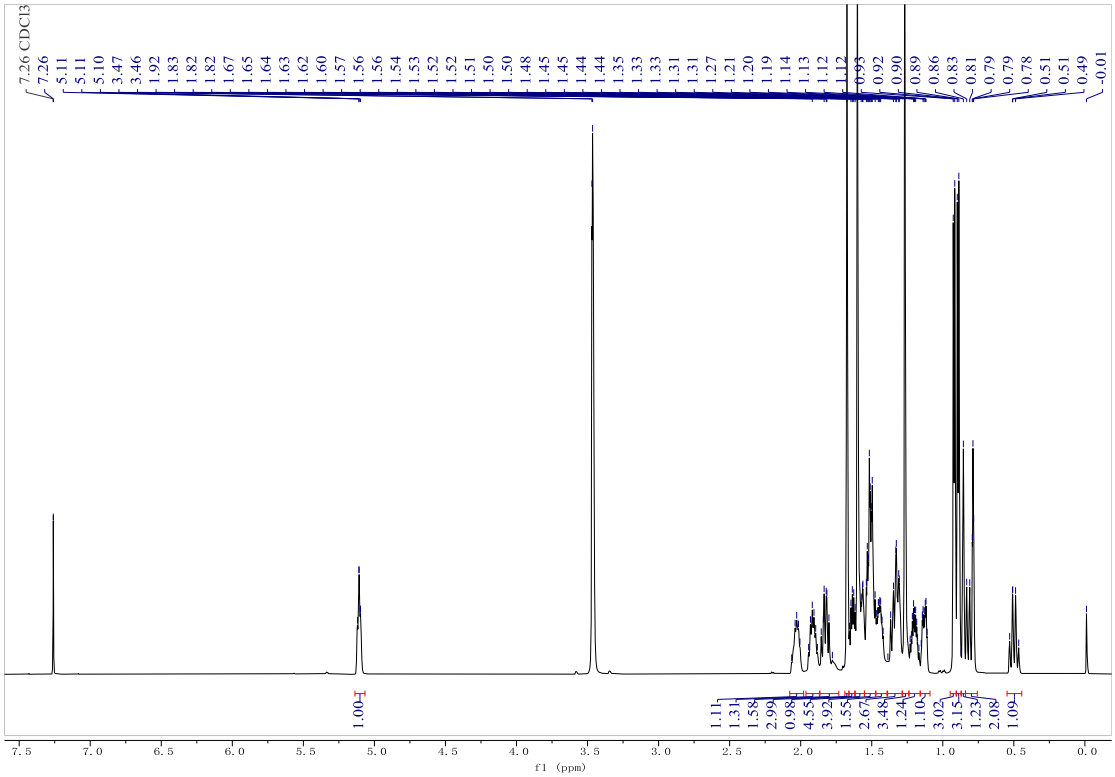


Figure S69. ^{1}H-NMR spectrum of euplexaurene D (**9**) in $CDCl_3$

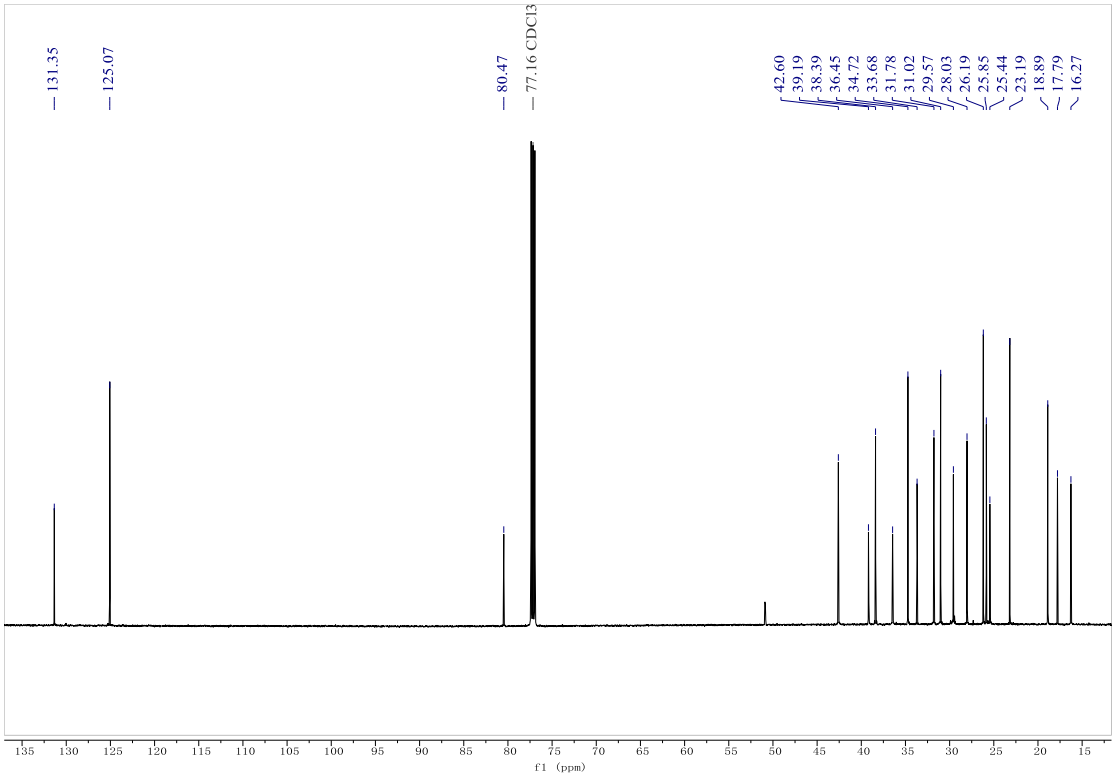


Figure S70. ^{13}C-NMR spectrum of euplexaurene D (**9**) in $CDCl_3$

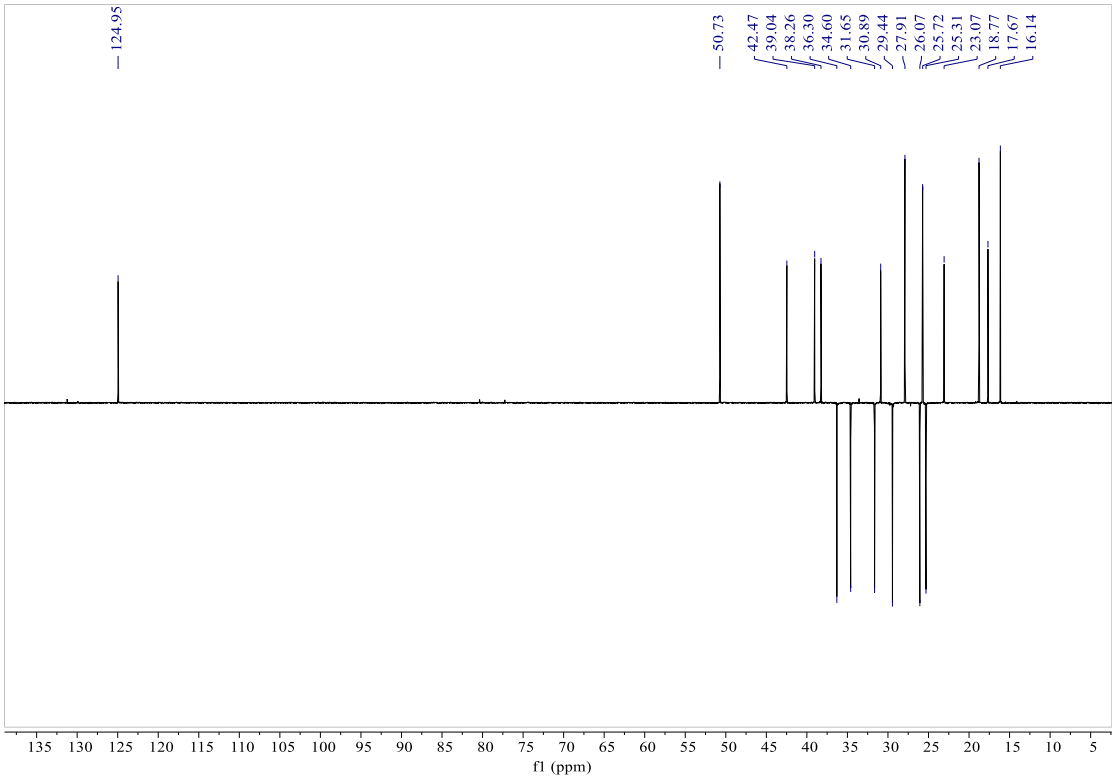


Figure S71. Dept 135° spectrum of euplexaurene D (**9**) in $CDCl_3$

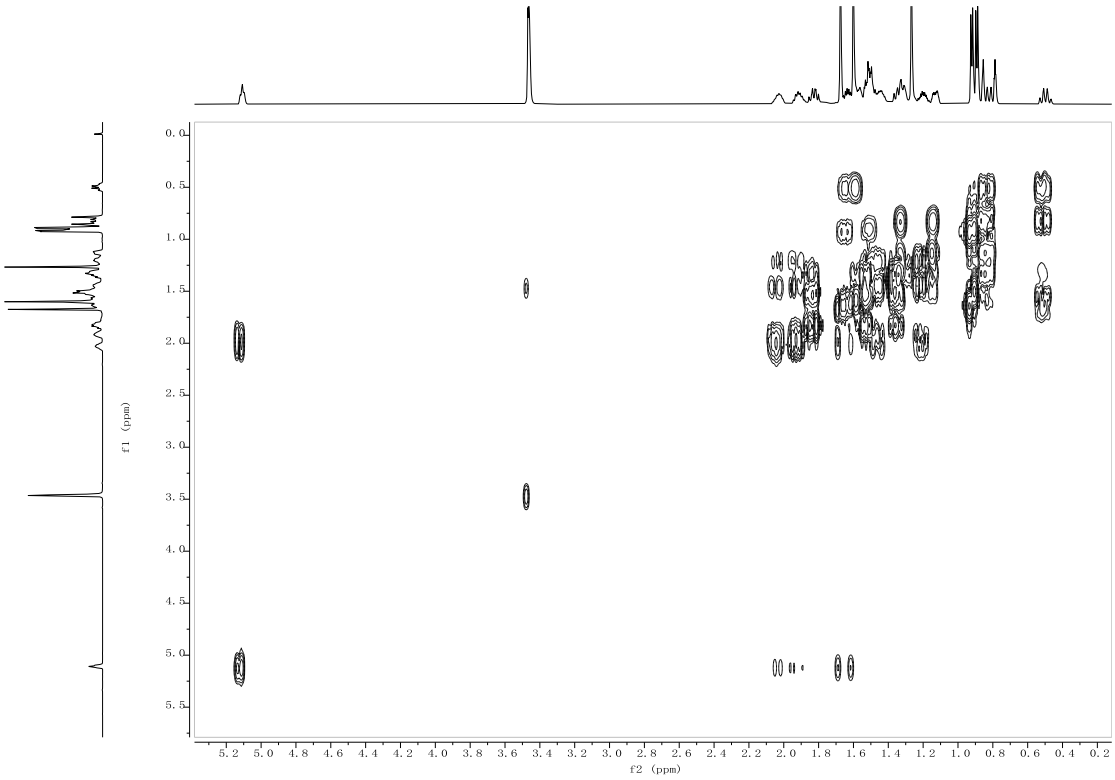


Figure S72. ^{1}H-^{1}H COSY spectrum of euplexaurene D (**9**) in $CDCl_3$

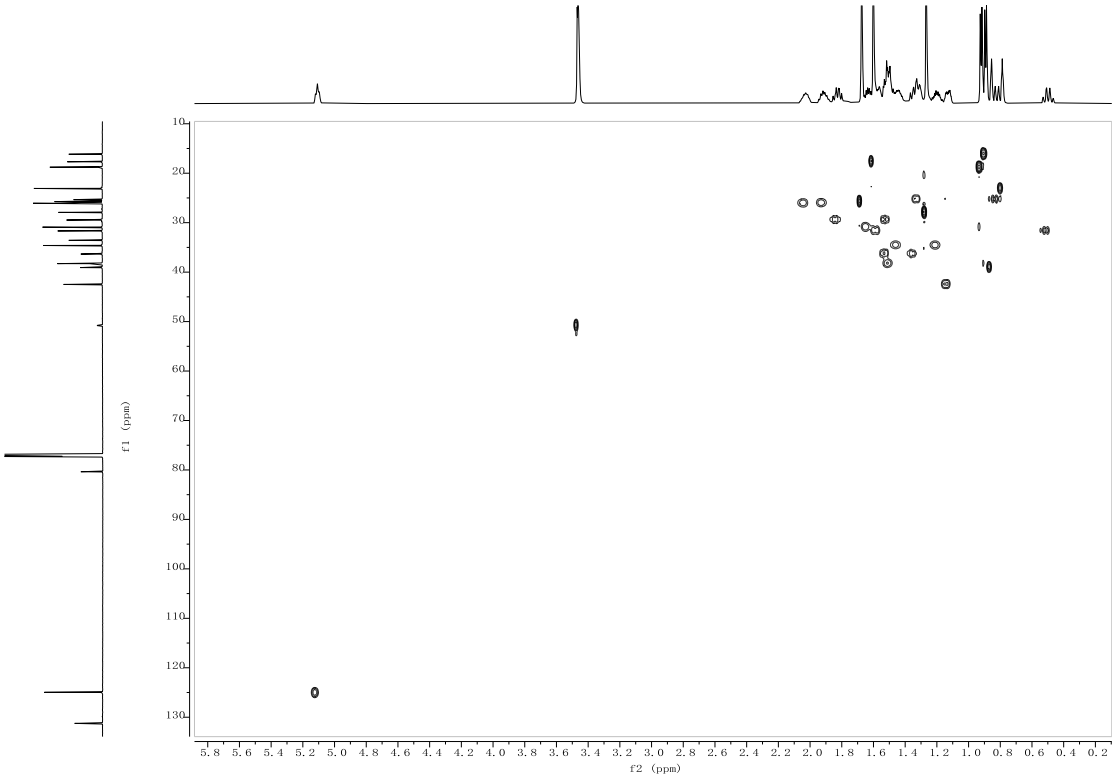


Figure S73. HSQC spectrum of euplexaurene D (**9**) in $CDCl_3$

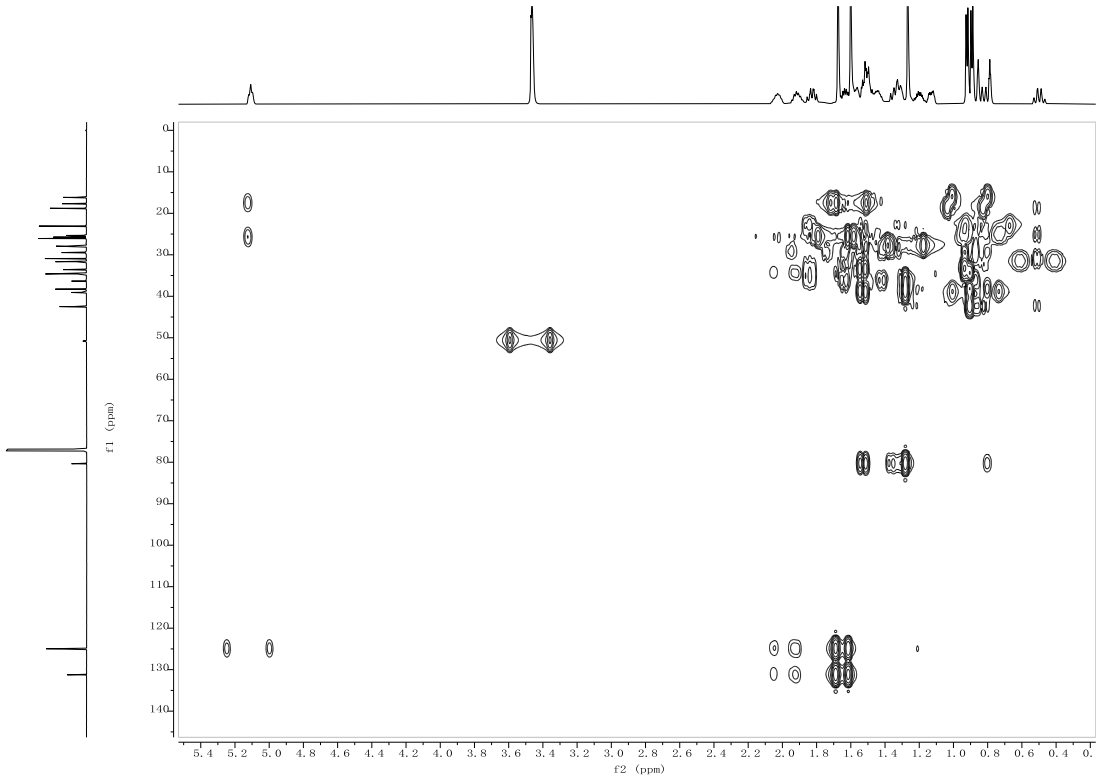
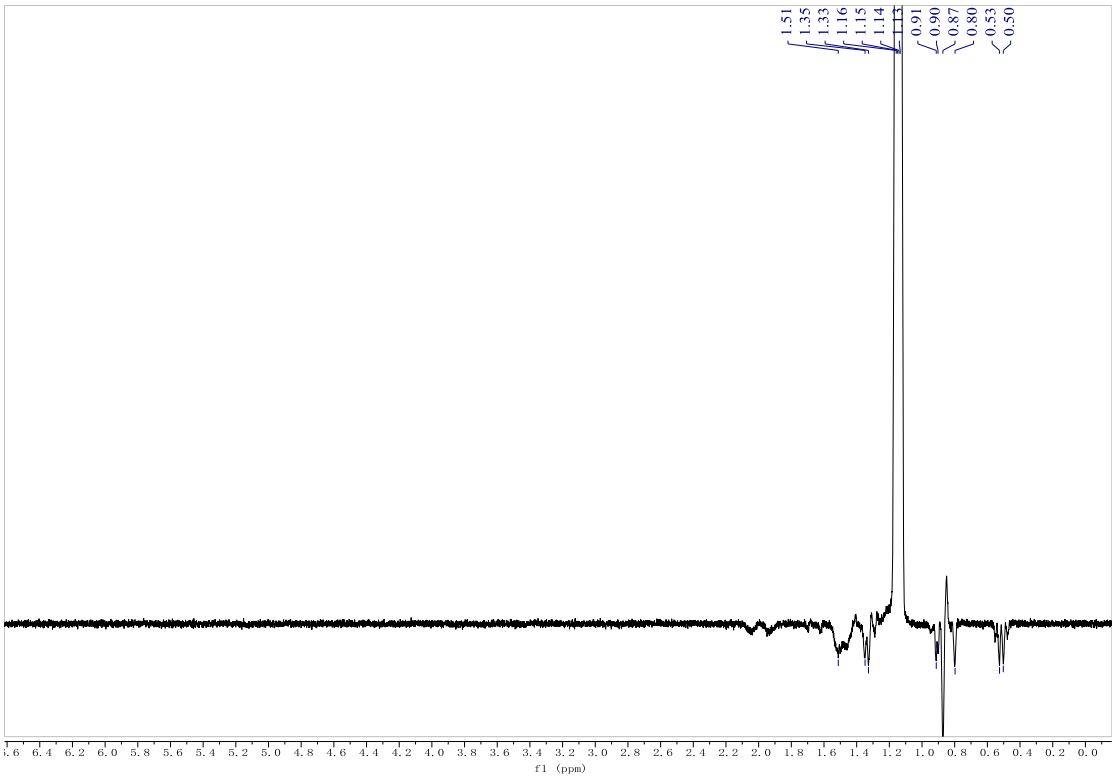


Figure S74. HMBC spectrum of euplexaurene D (**9**) in $CDCl_3$



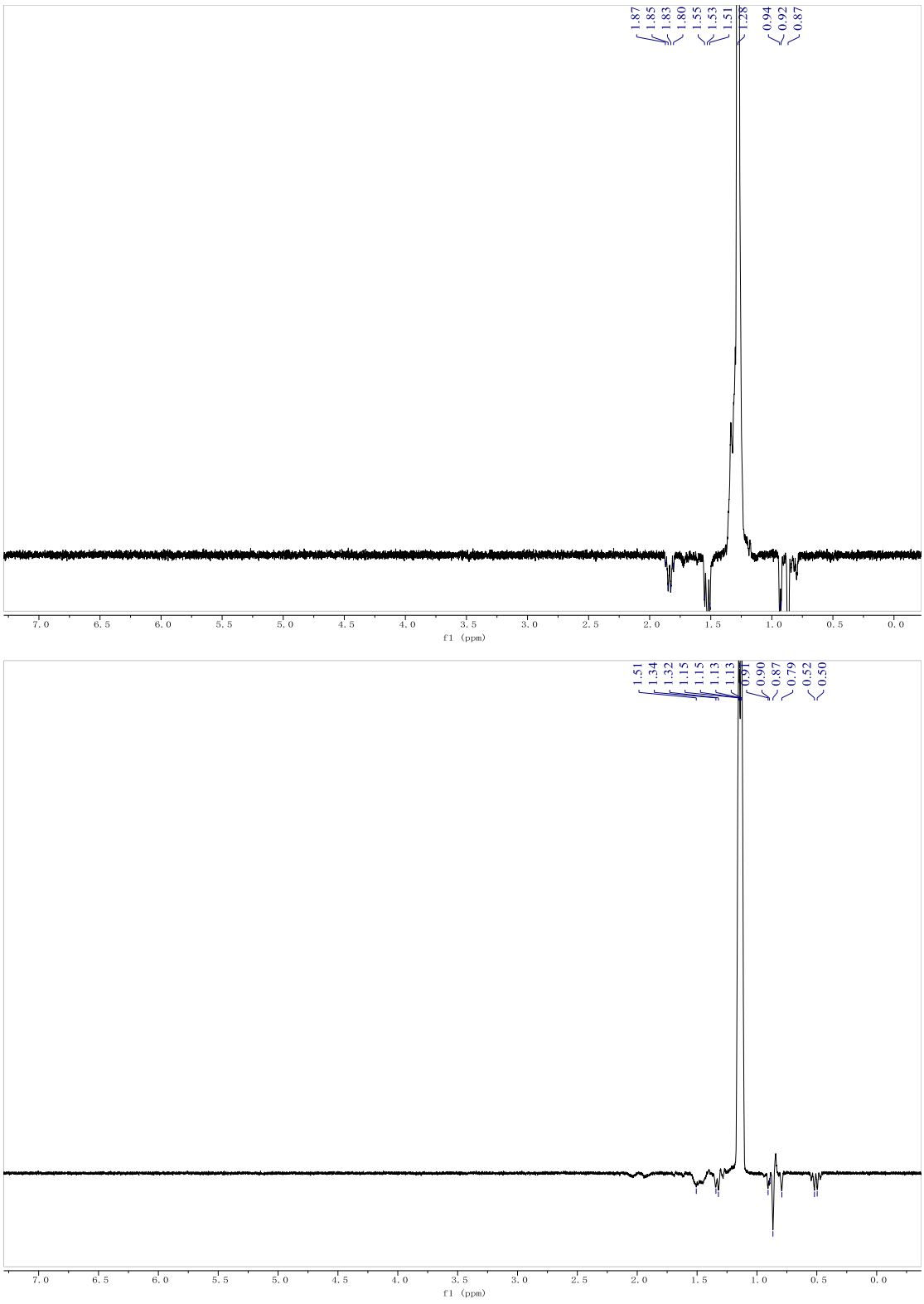
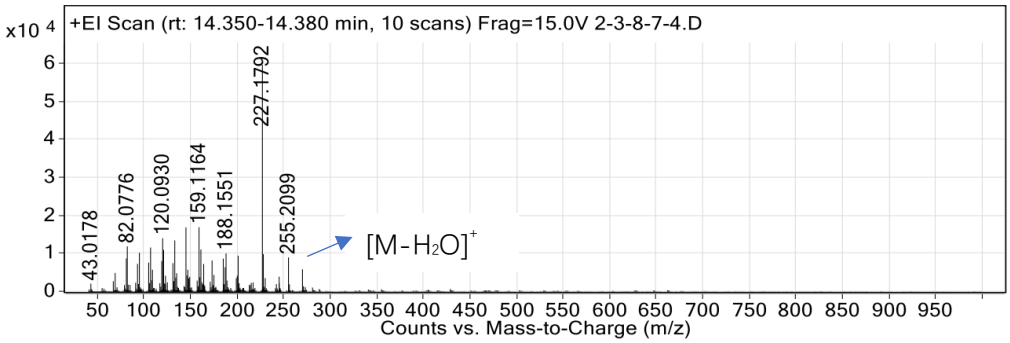


Figure S75. NOESY spectrum of euplexaurene D (**9**) in $CDCl_3$

14. Spectroscopic data for cneorubin K (10)



214.1701		1583.18
215.1783		2193.89
217.194		2309.28
219.1739		861.74
227.1792	1	59650.05
228.1823	1	9764.34
229.1869	1	1146.87
230.202	1	3462.92
231.2056	1	835.83
241.1946		797.61
242.2019		1874.33
245.189	1	3847.64
245.2253		2077.21
246.1928	1	802.48
255.2099	1	8896.82
256.2133	1	1813.48
270.2334	1	5782.26
271.2372	1	1305.07
273.2204		1087.19
281.0514		970.24

Figure S76. HRESIMS spectrum of cneorubin K (**10**)

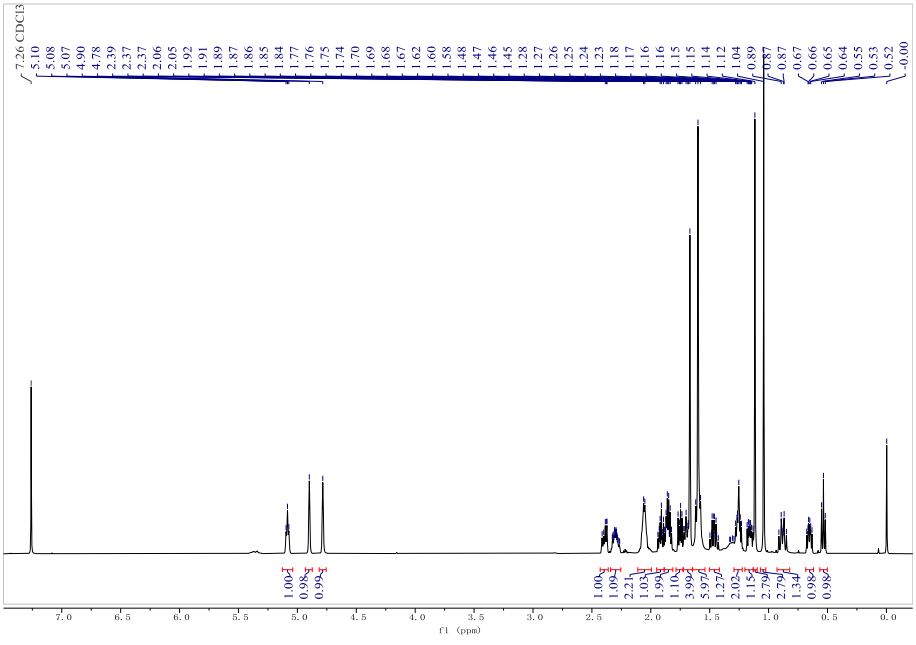


Figure S77. ^{1}H-NMR spectrum of cneorubin K (**10**) in $CDCl_3$

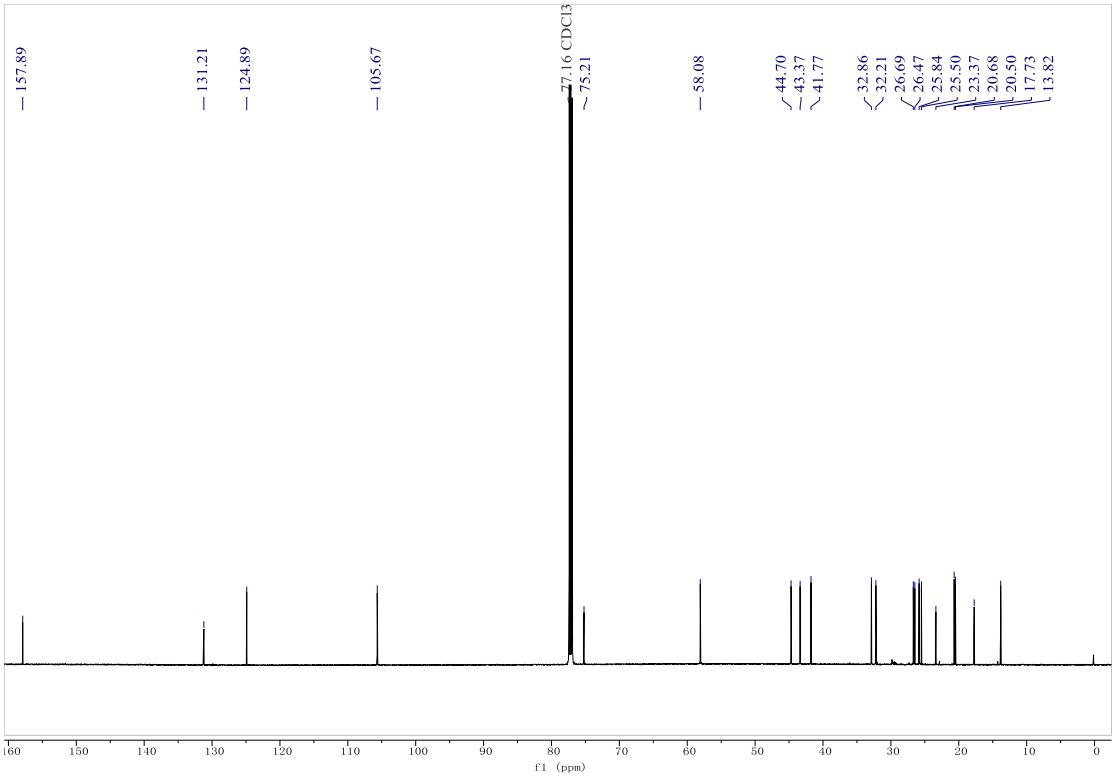


Figure S78. ^{13}C-NMR spectrum of cneorubin K (**10**) in $CDCl_3$

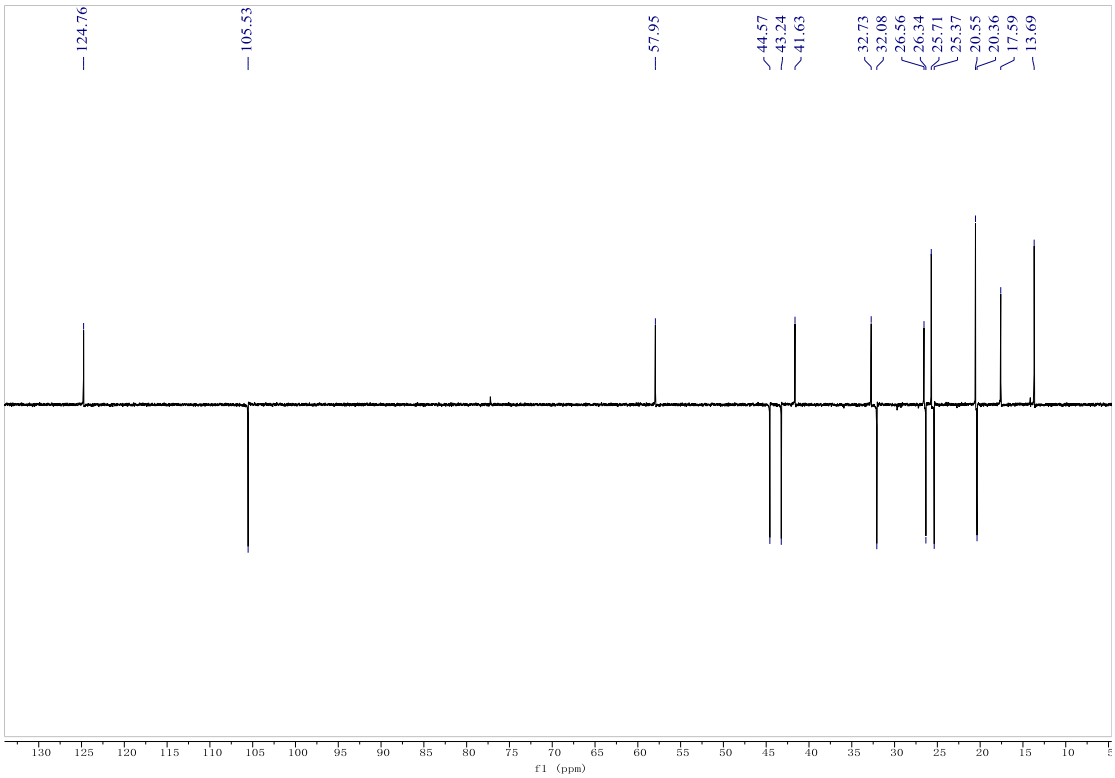


Figure S79. Dept 135° spectrum of cneorubin K (**10**) in $CDCl_3$

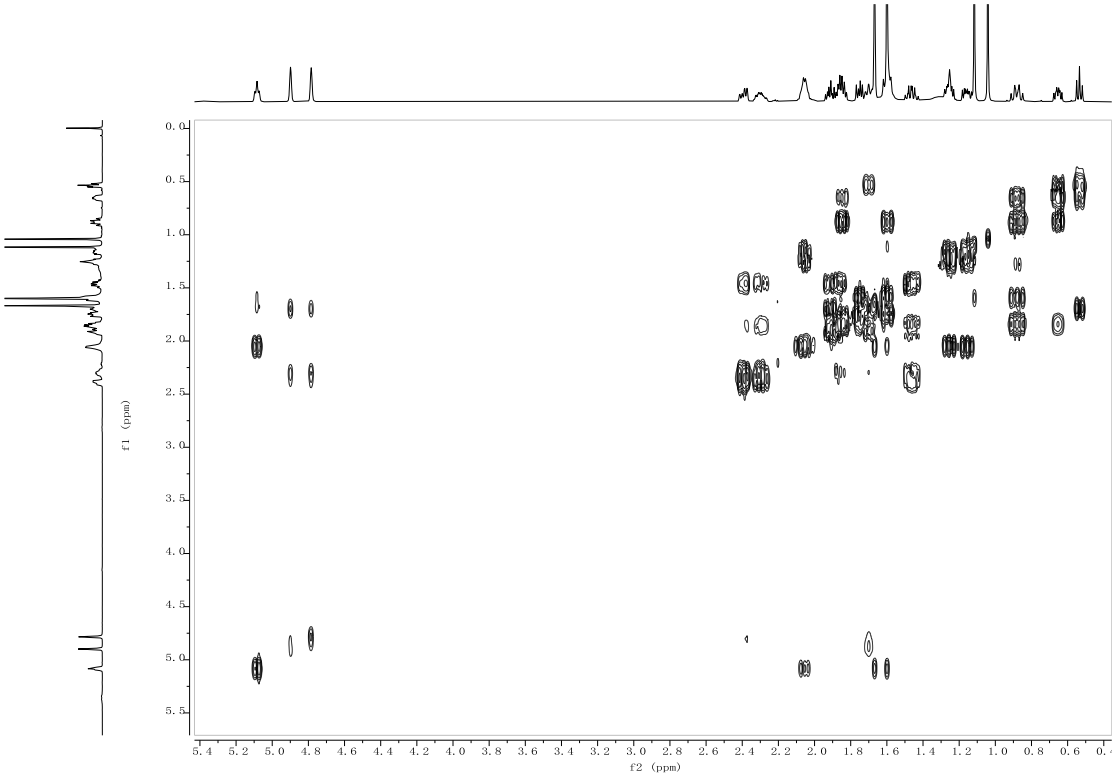


Figure S80. ^{1}H-^{1}H COSY spectrum of cneorubin K (**10**) in $CDCl_3$

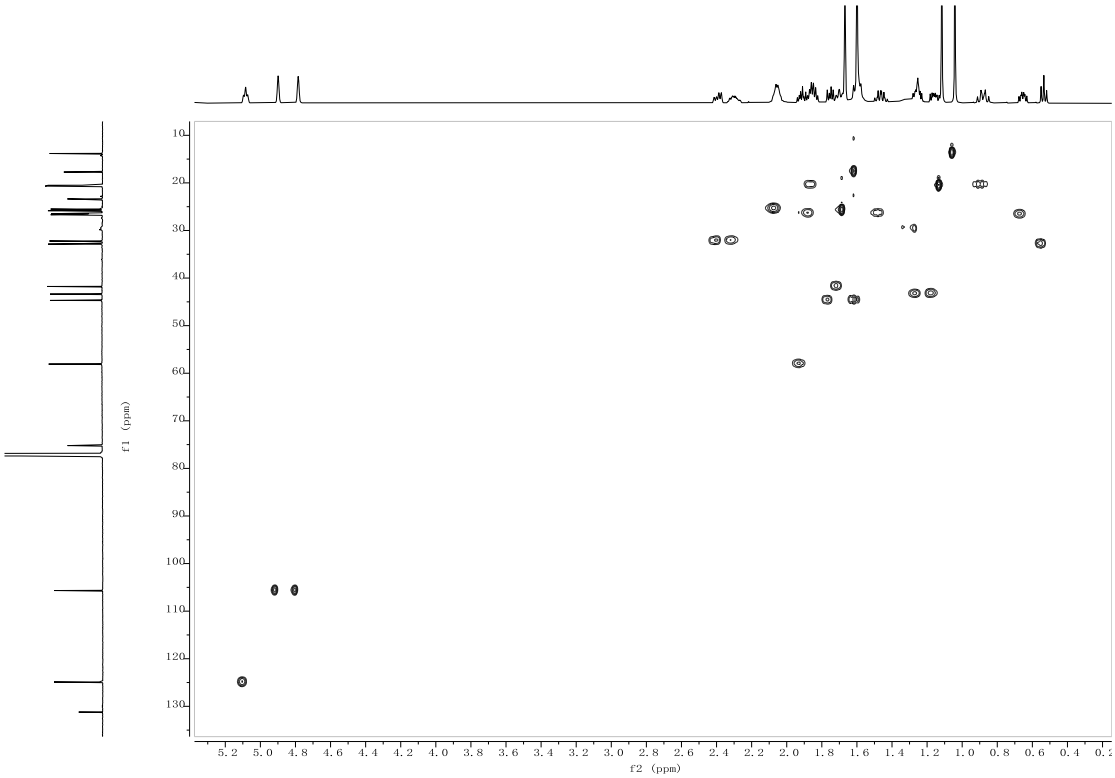


Figure S81. HSQC spectrum of cneorubin K (**10**) in $CDCl_3$

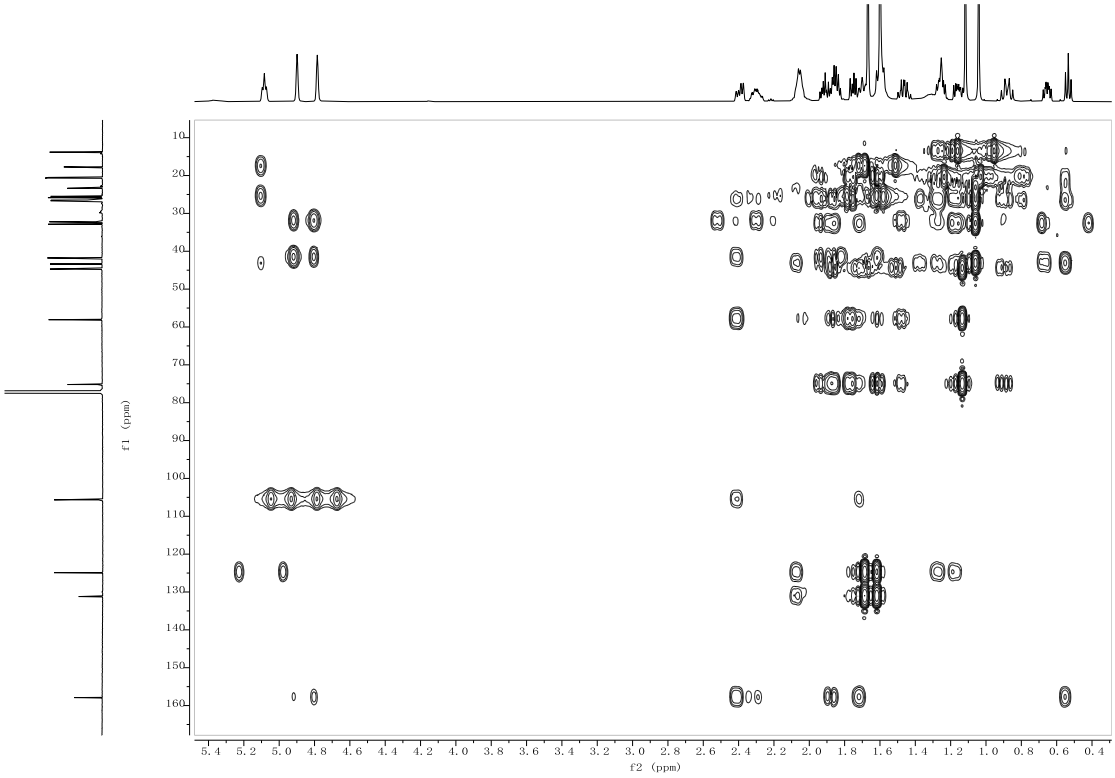
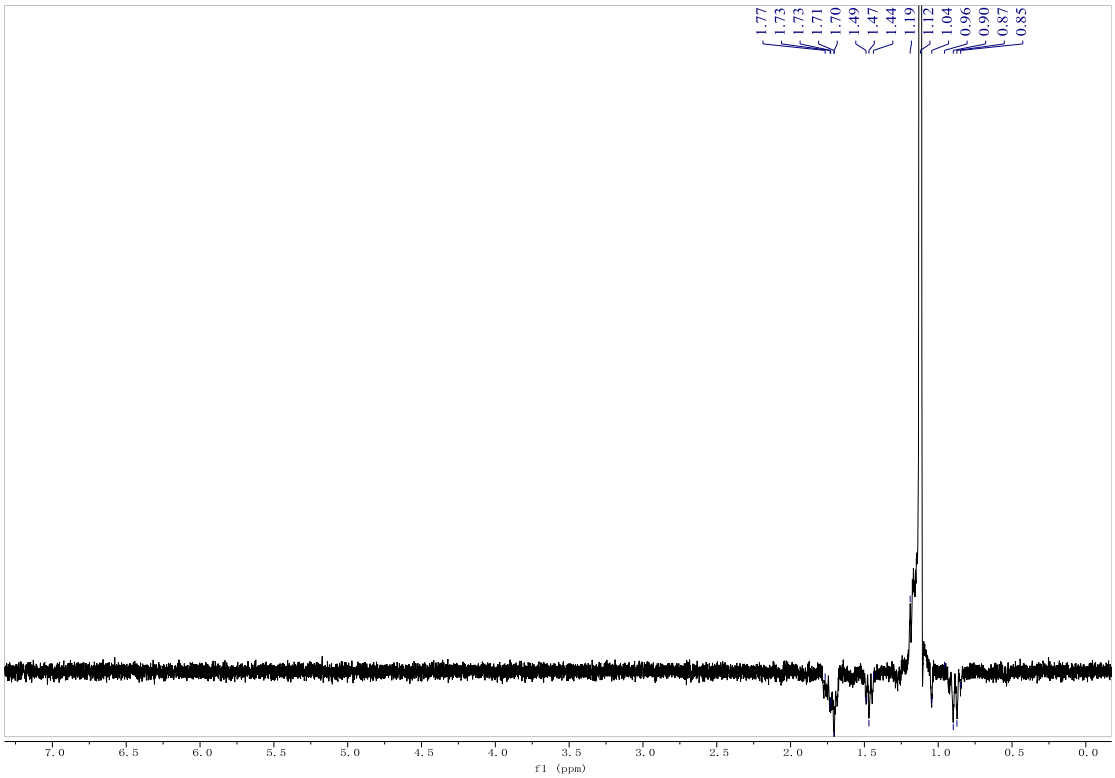
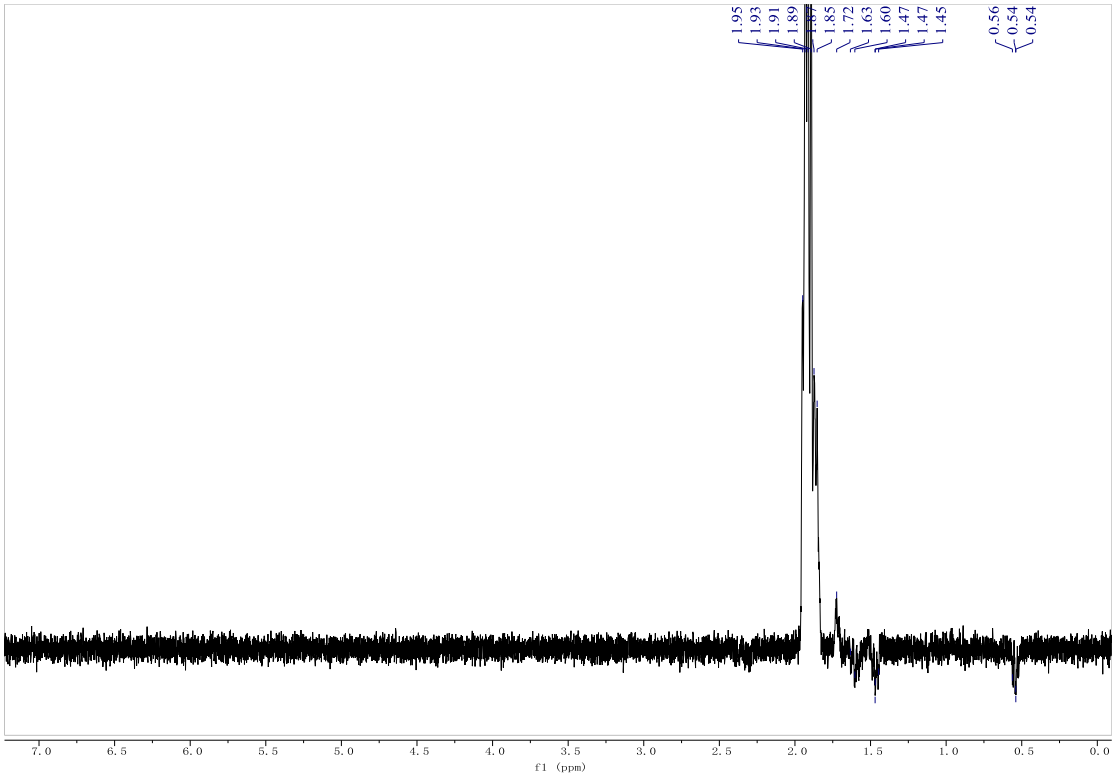
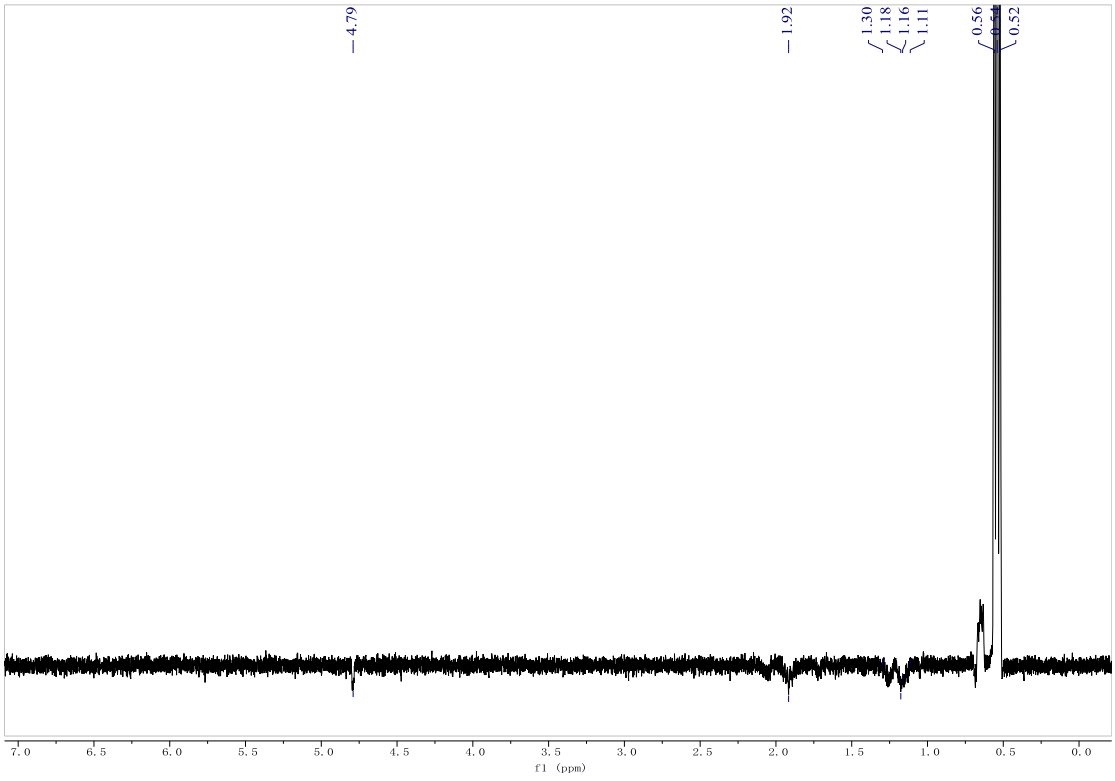


Figure S82. HMBC spectrum of cneorubin K (**10**) in $CDCl_3$




1.95
1.93
1.91
1.89
1.85
1.72
1.63
1.60
1.47
1.47
1.45
0.56
0.54
0.54
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


4.79
1.92
1.30
1.18
1.16
1.11
0.56
0.54
0.52
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

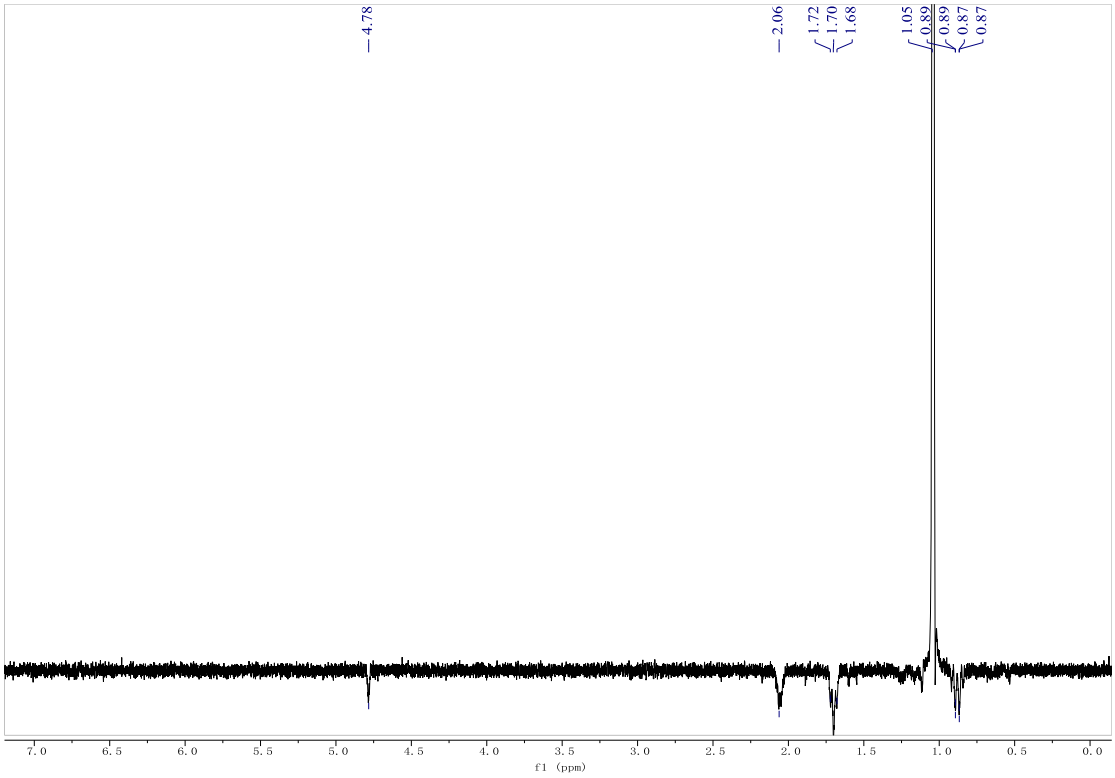


Figure S83. NOESY spectrum of cneorubin K (**10**) in $CDCl_3$

15. ^{1}H-NMR for (*S*)-MTPA and (*R*)-MTPA esters of compound 5 in pyridine-d_5

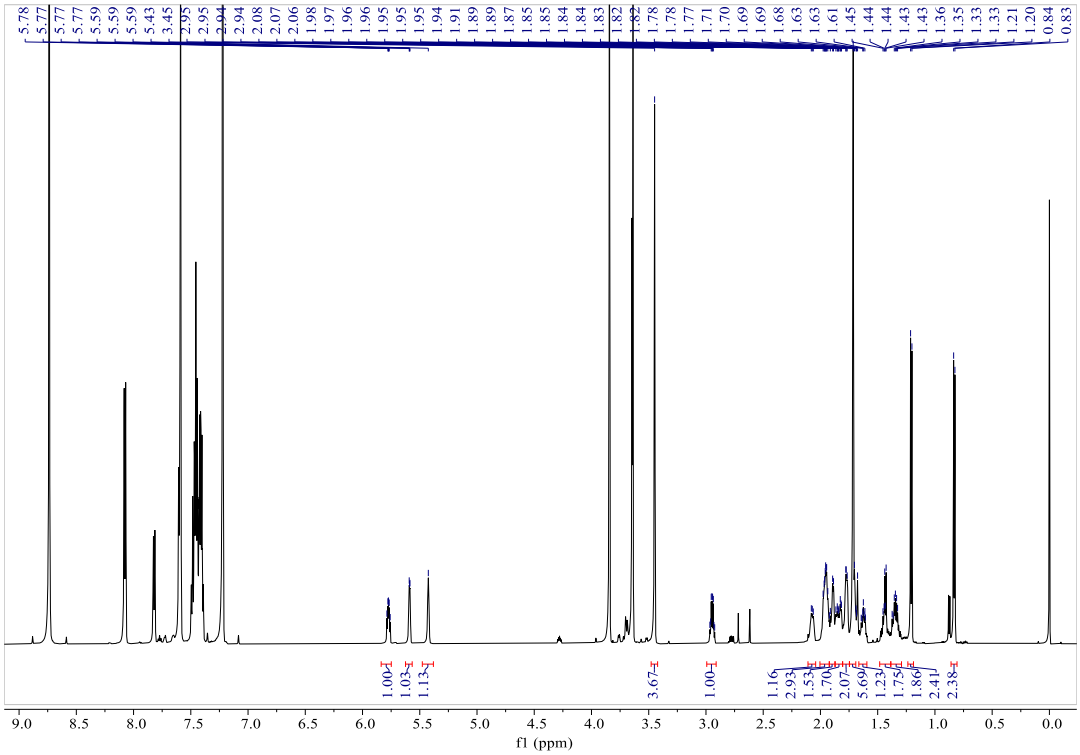


Figure S84. ^{1}H-NMR for (*S*)-MTPA ester of compound **5** in pyridine-d_5

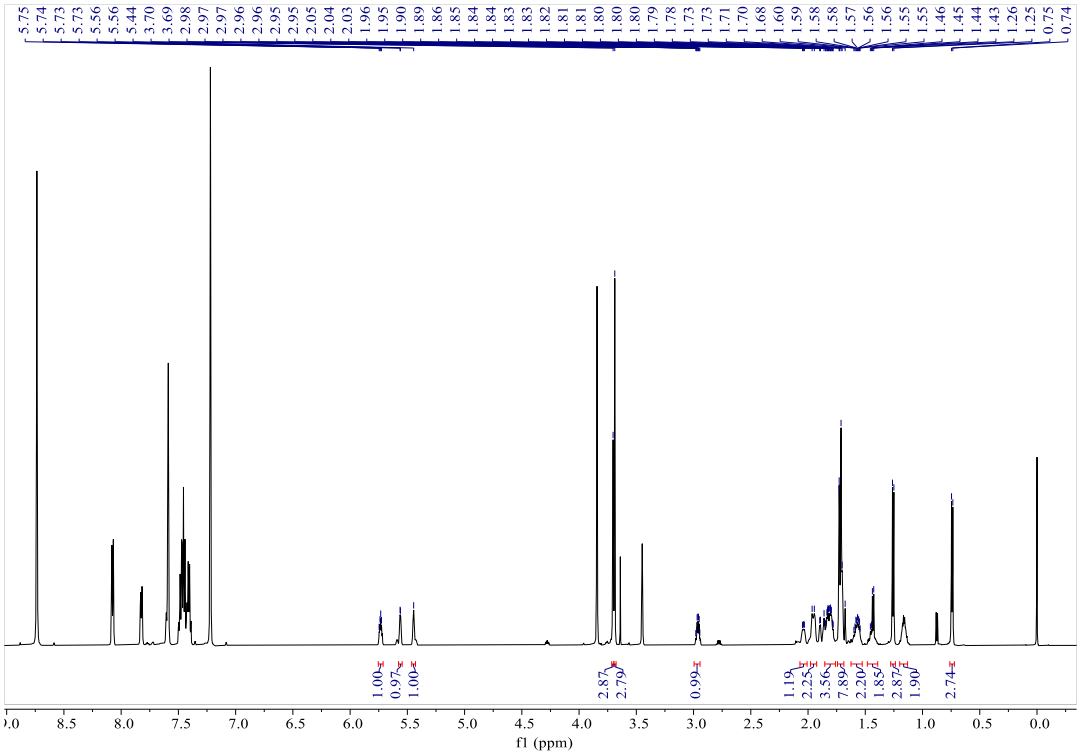


Figure S85. ^{1}H-NMR for (*R*)-MTPA ester of compound **5** in pyridine-d_5

16. Spectroscopic data for known compound cneorubin X (11)

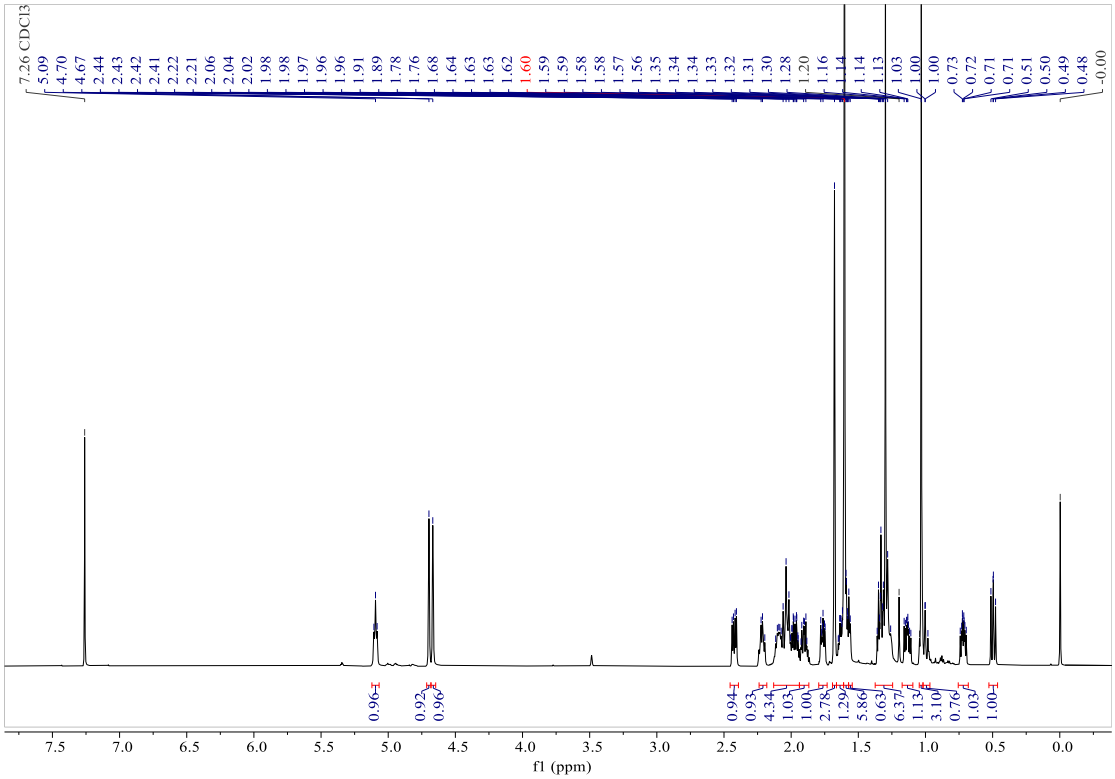


Figure S86. ^{1}H-NMR spectrum of cneorubin X (**11**) in $CDCl_3$

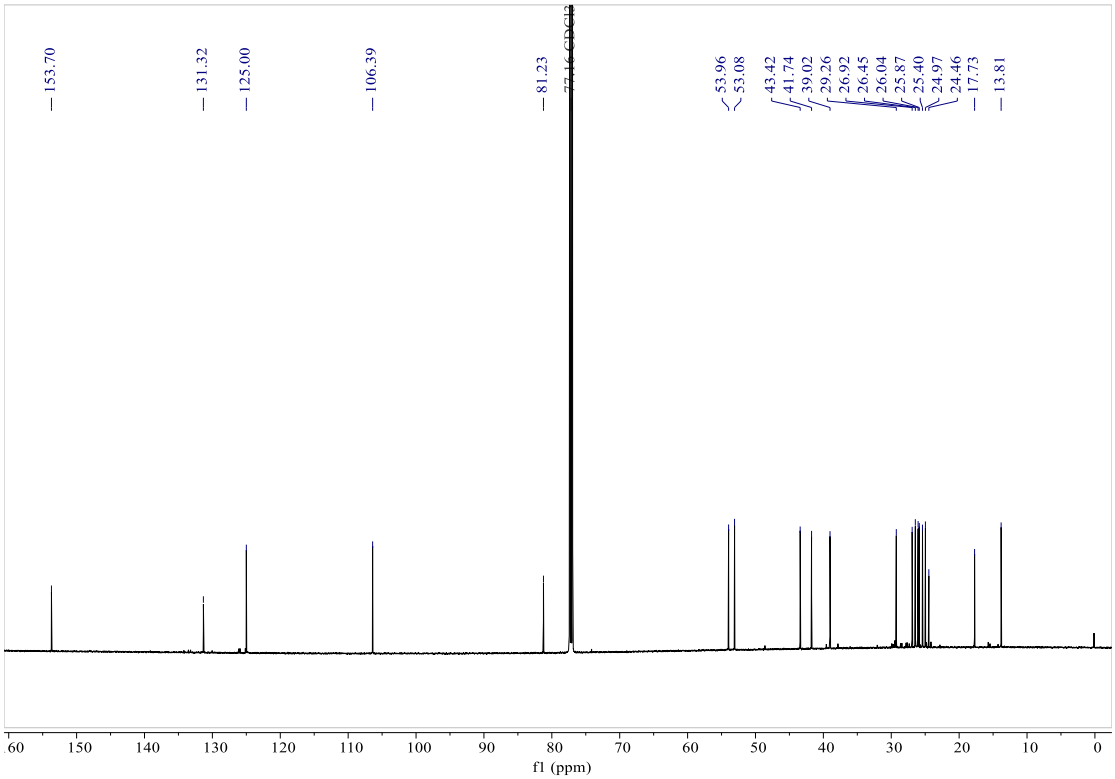


Figure S87. ^{13}C-NMR spectrum of cneorubin X (**11**) in $CDCl_3$

17. Spectroscopic data for known compound obscuronatin (12)

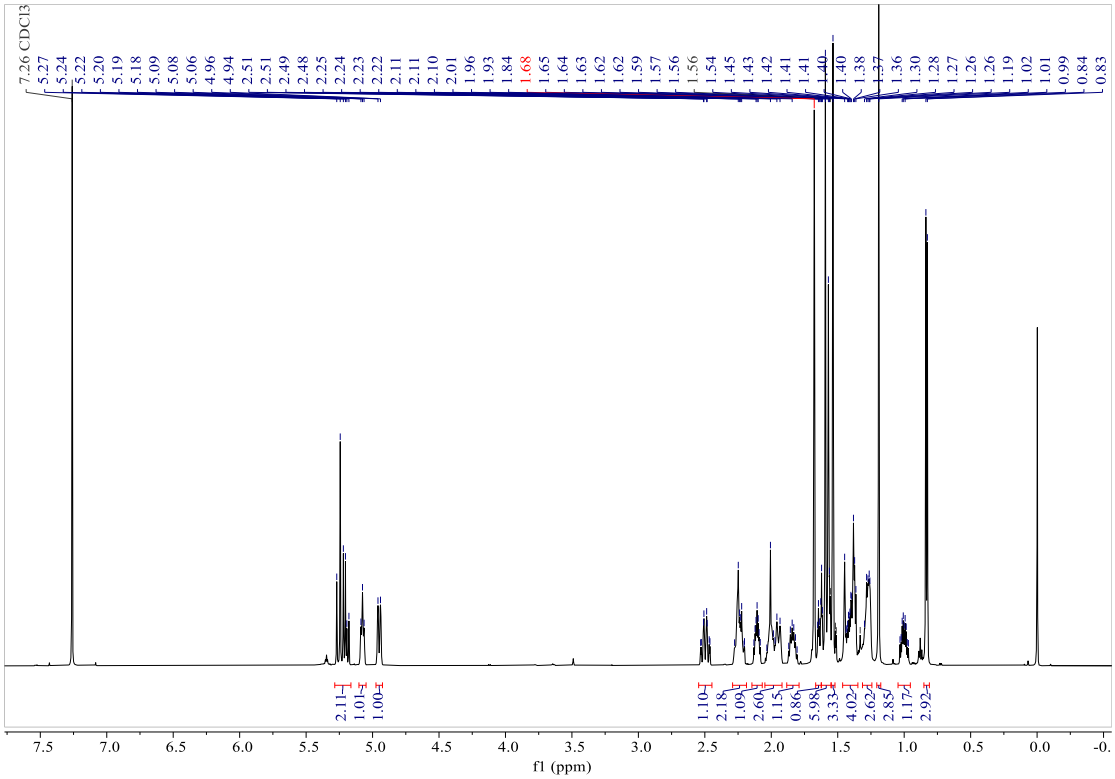


Figure S88. ^{1}H-NMR spectrum of obscuronatin (**12**) in $CDCl_3$

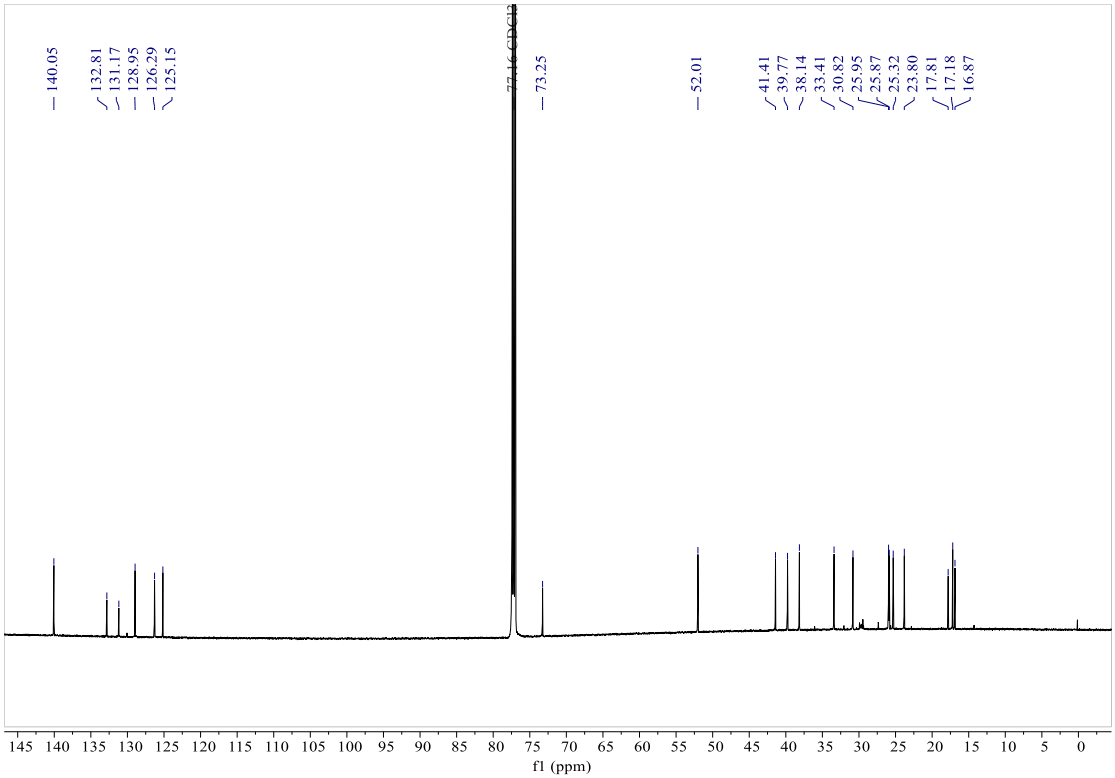


Figure S89. ^{13}C-NMR spectrum of obscuronatin (**12**) in $CDCl_3$

18. Spectroscopic data for known compound dictyotin B (13)

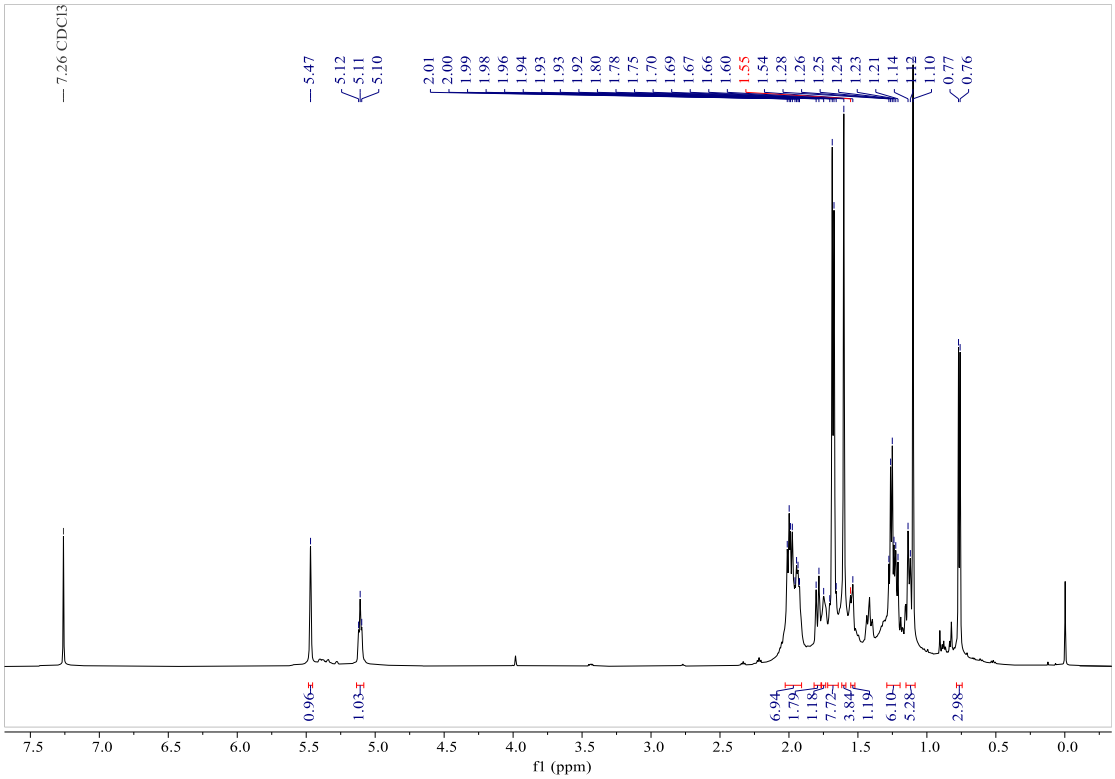


Figure S90. ^{1}H-NMR spectrum of dictyotin B (**13**) in $CDCl_3$

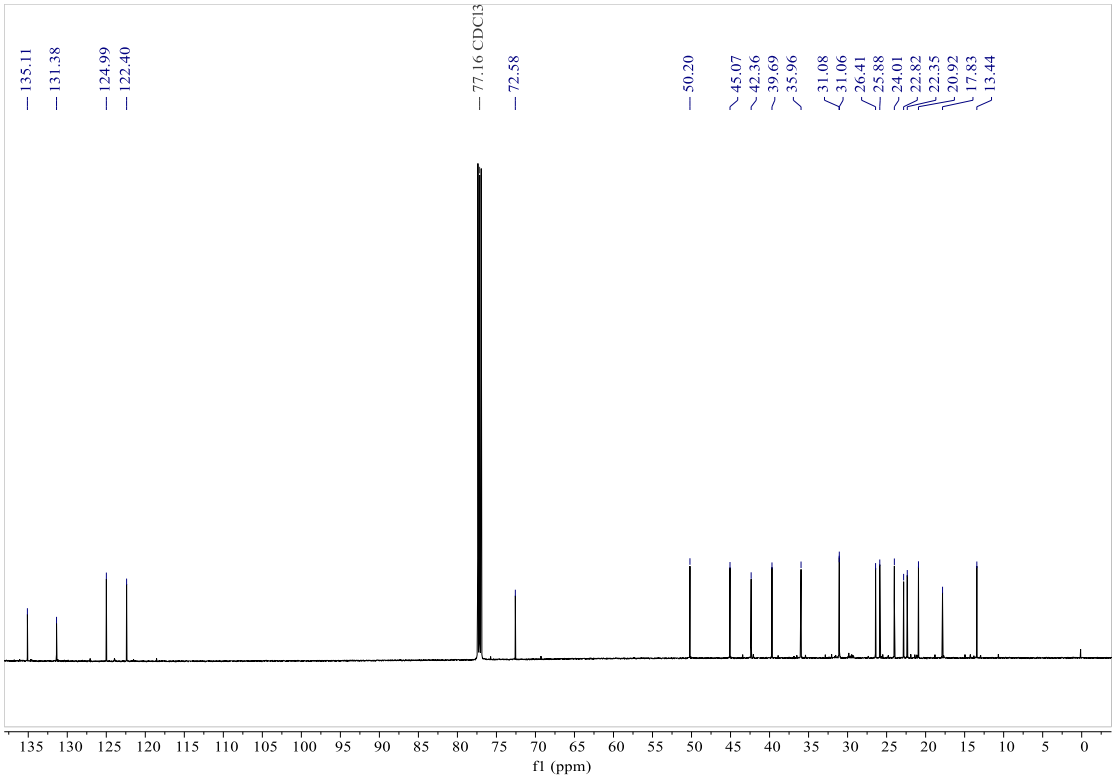


Figure S91. ^{13}C-NMR spectrum of dictyotin B (**13**) in $CDCl_3$