

Supporting Information

Secondary Metabolites with Chemical Diversity from the Marine-derived

Fungus *Pseudallescheria boydii* F19-1 and Their Cytotoxic Activity

Wen-Jian Lan,^{ad} Kun-Teng Wang,^{ab} Meng-Yang Xu,^b Jing-Jing Zhang,^e Chi-Keung Lam,^c

Guo-Hua Zhong,^e Jun Xu,^b De-Po Yang,^{ad} Hou-Jin Li^{*c} and Lai-You Wang^{*b}

^aSchool of Pharmaceutical Sciences, Sun Yat-sen University, Guangzhou 510006, China

^bSchool of Pharmacy, Guangdong Pharmaceutical University; Guangdong Metabolic Diseases Research Center of Integrated Chinese and Western Medicine, Guangzhou 510006, China

^cSchool of Chemistry and Chemical Engineering, Sun Yat-sen University, Guangzhou 510275, China

^dGuangdong Technology Research Center for Advanced Chinese Medicine, Guangzhou 510006, China

^eLab of Insect Toxicology, South China Agricultural University, Guangzhou 510642, China

To whom correspondence should be addressed: wanglaiyou@gdpu.edu.cn

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Figure S1. HR-ESI-MS spectrum of pseuboydone A (**1**)

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LTQ Orbitrap Elite

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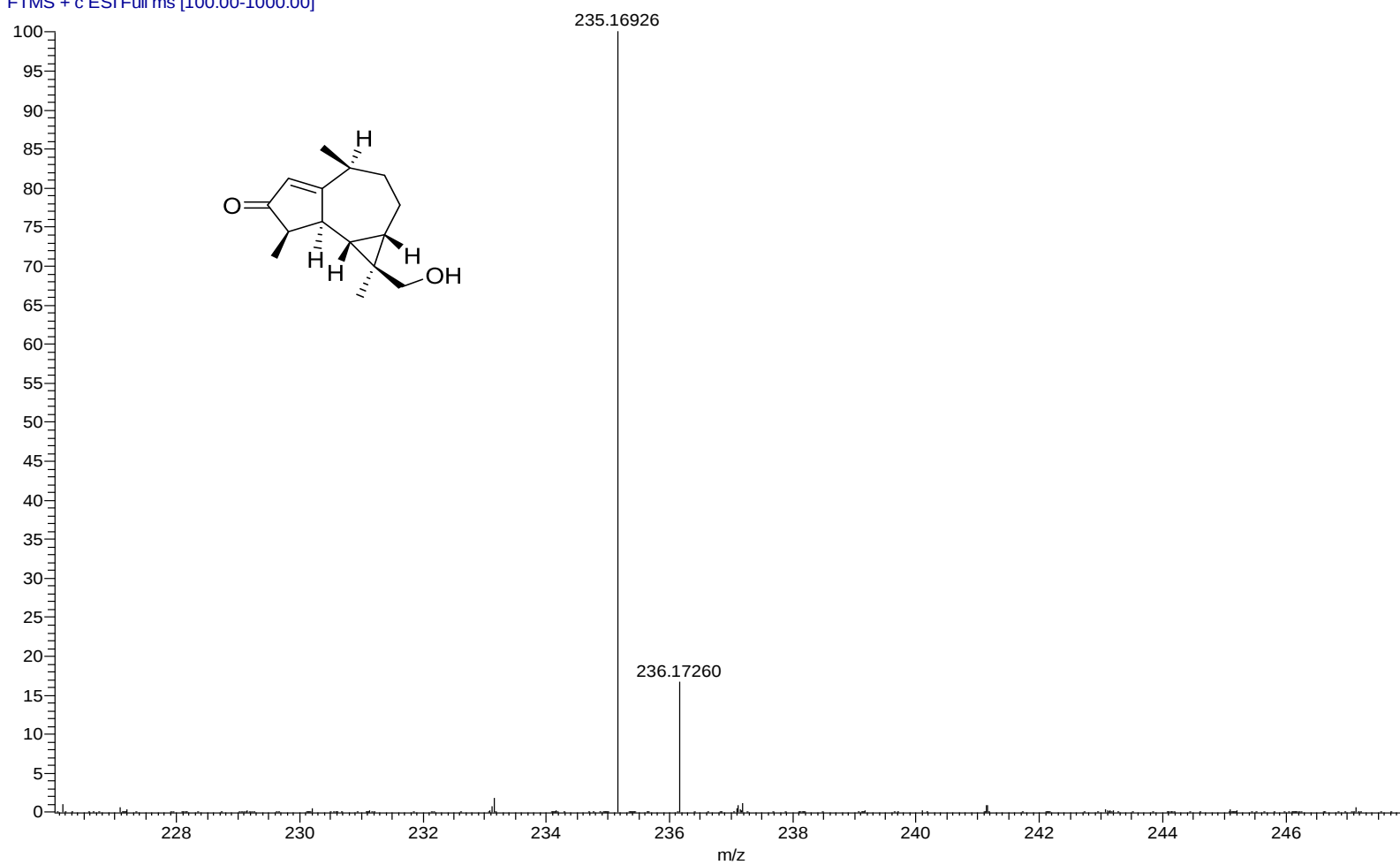


Figure S2. ^1H -NMR spectrum of pseuboydone A (**1**) in CDCl_3 (400MHz)

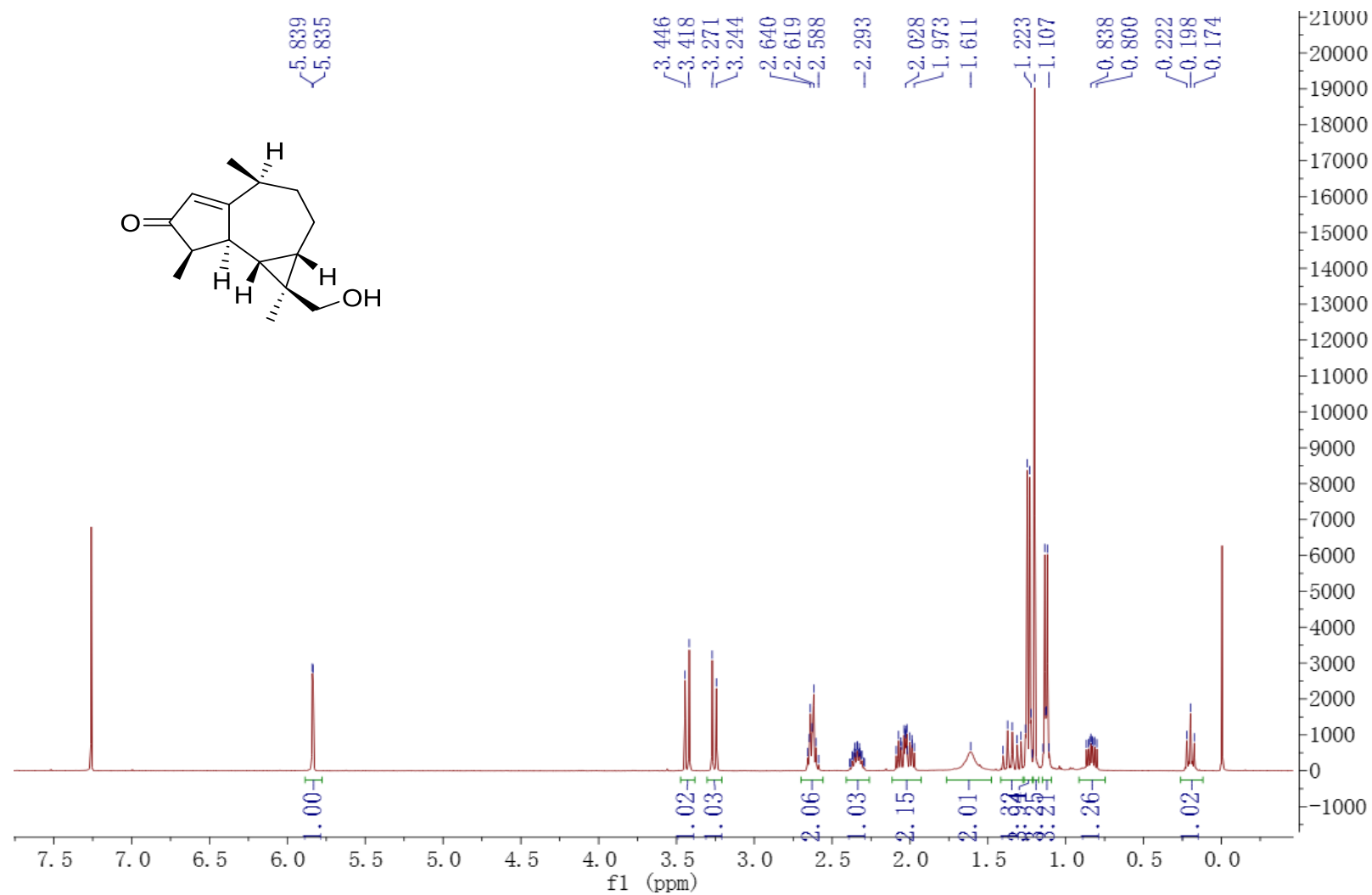


Figure S3. ^{13}C NMR and DEPT spectra of pseuboydone A (**1**) in CDCl_3 (100MHz)

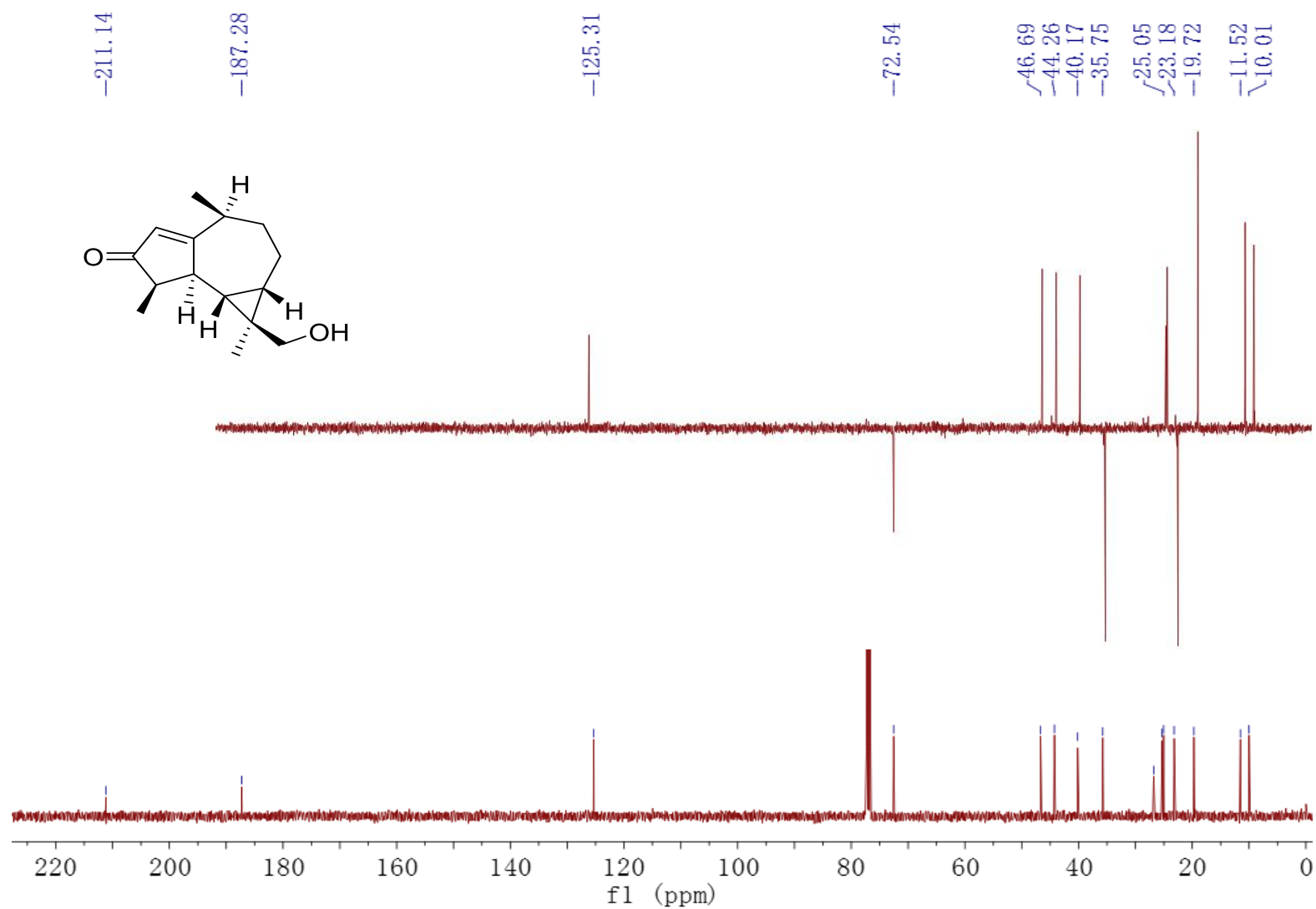


Figure S4. HMQC spectrum of pseuboydone A (**1**) in CDCl₃

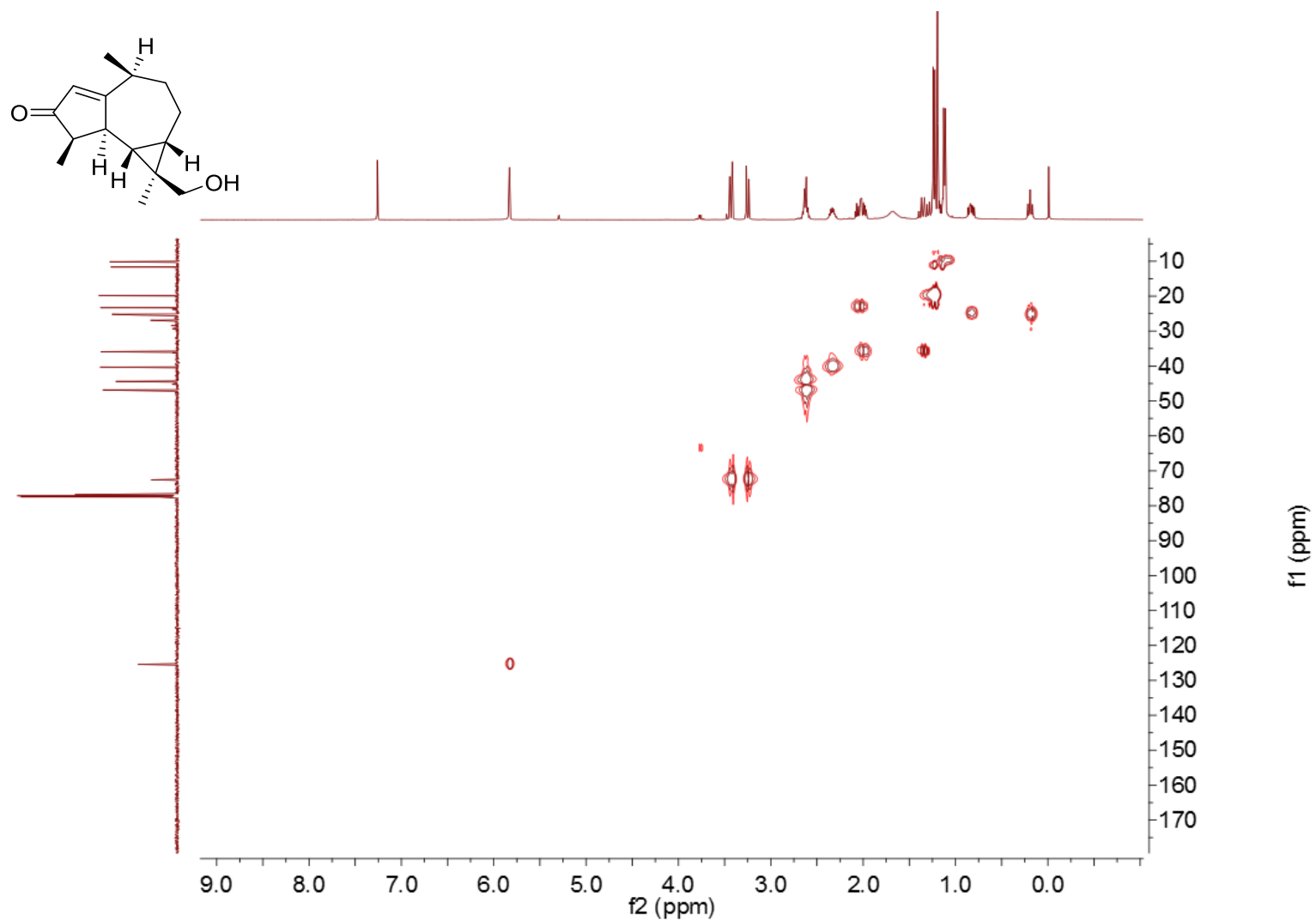


Figure S5. ^1H - ^1H COSY spectrum of pseuboydone A (**1**) in CDCl_3

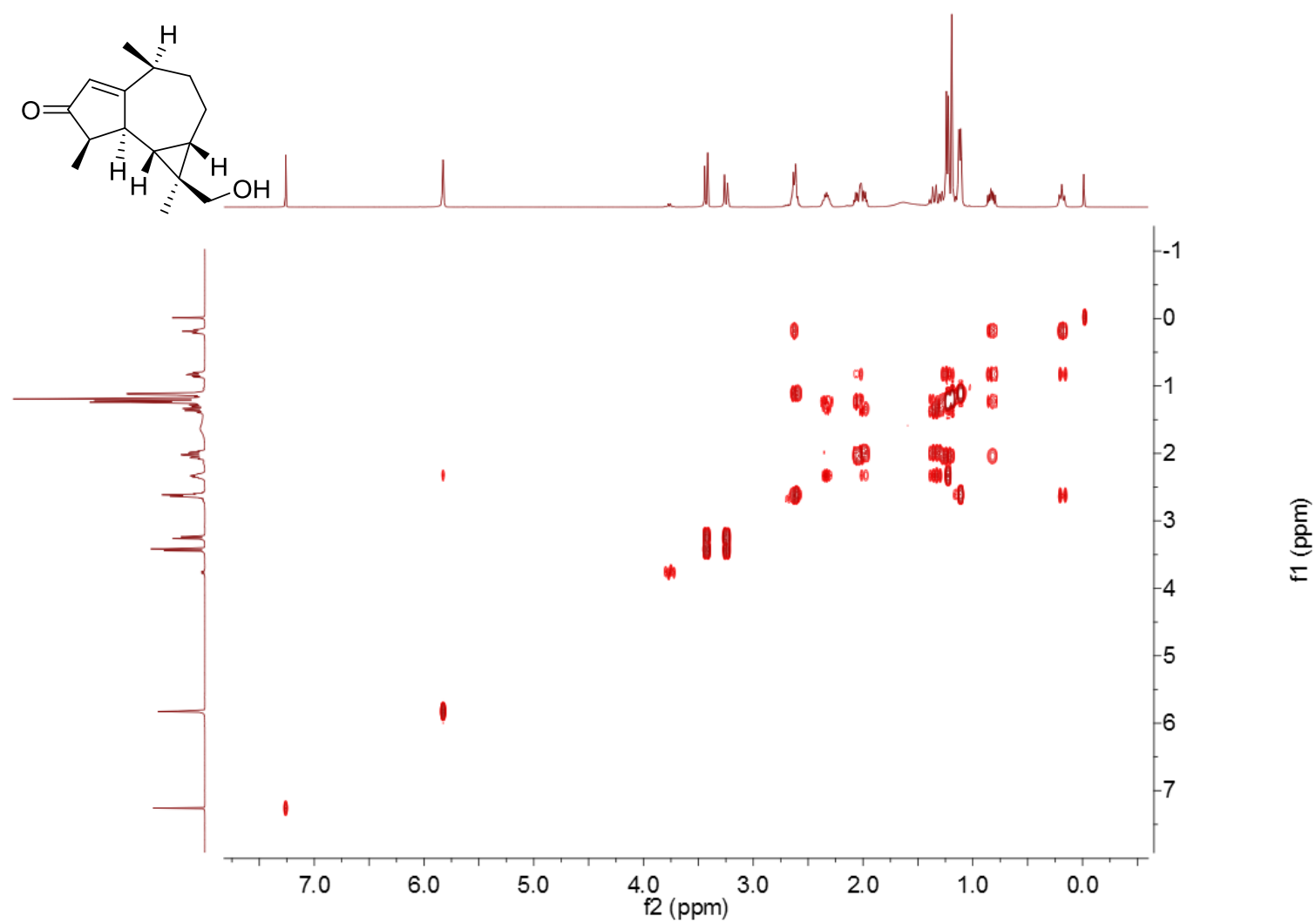


Figure S6. HMBC spectrum of pseuboydone A (**1**) in CDCl₃

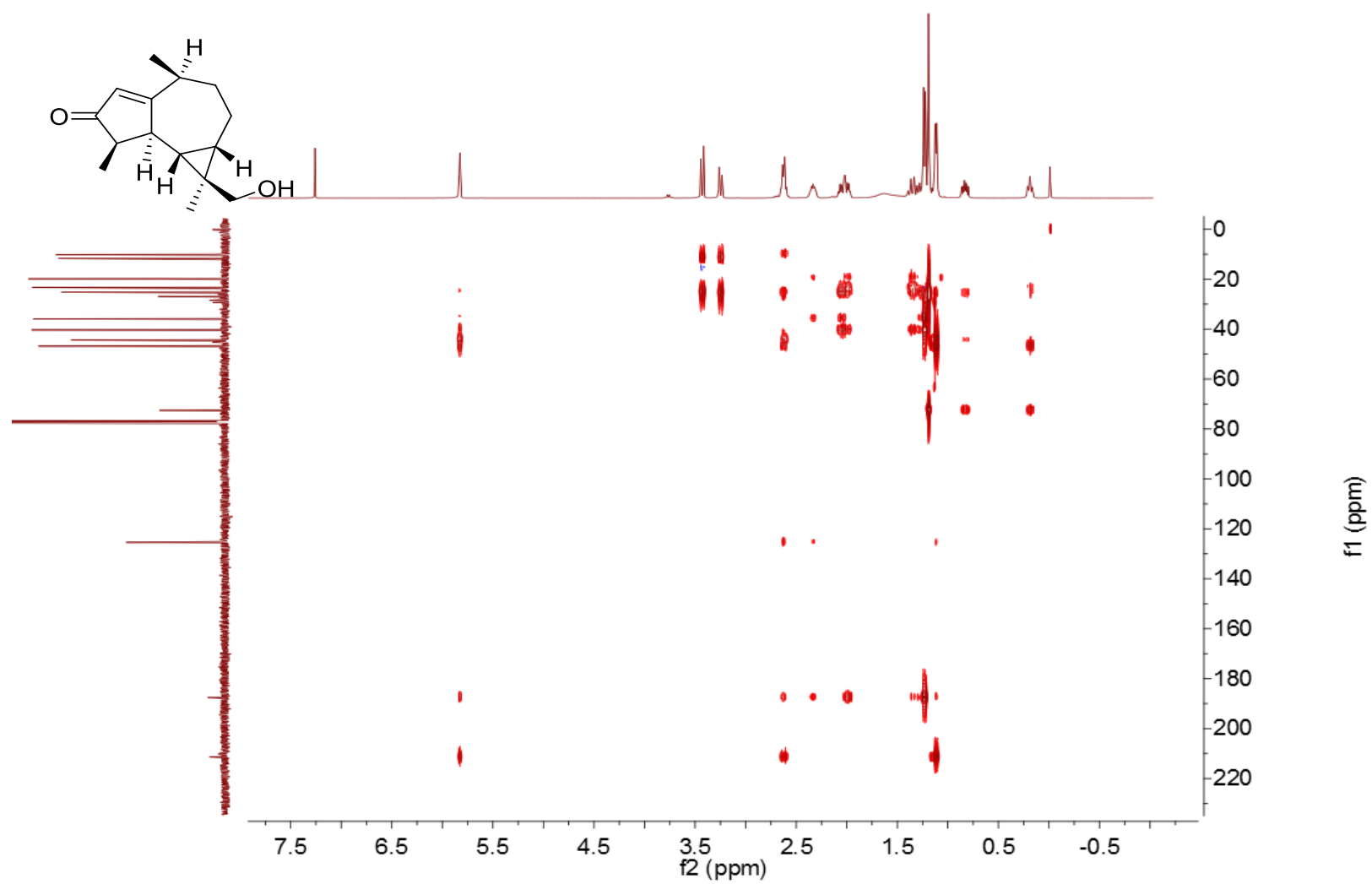


Figure S7. NOESY spectrum of pseudoboydone A (**1**) in CDCl₃

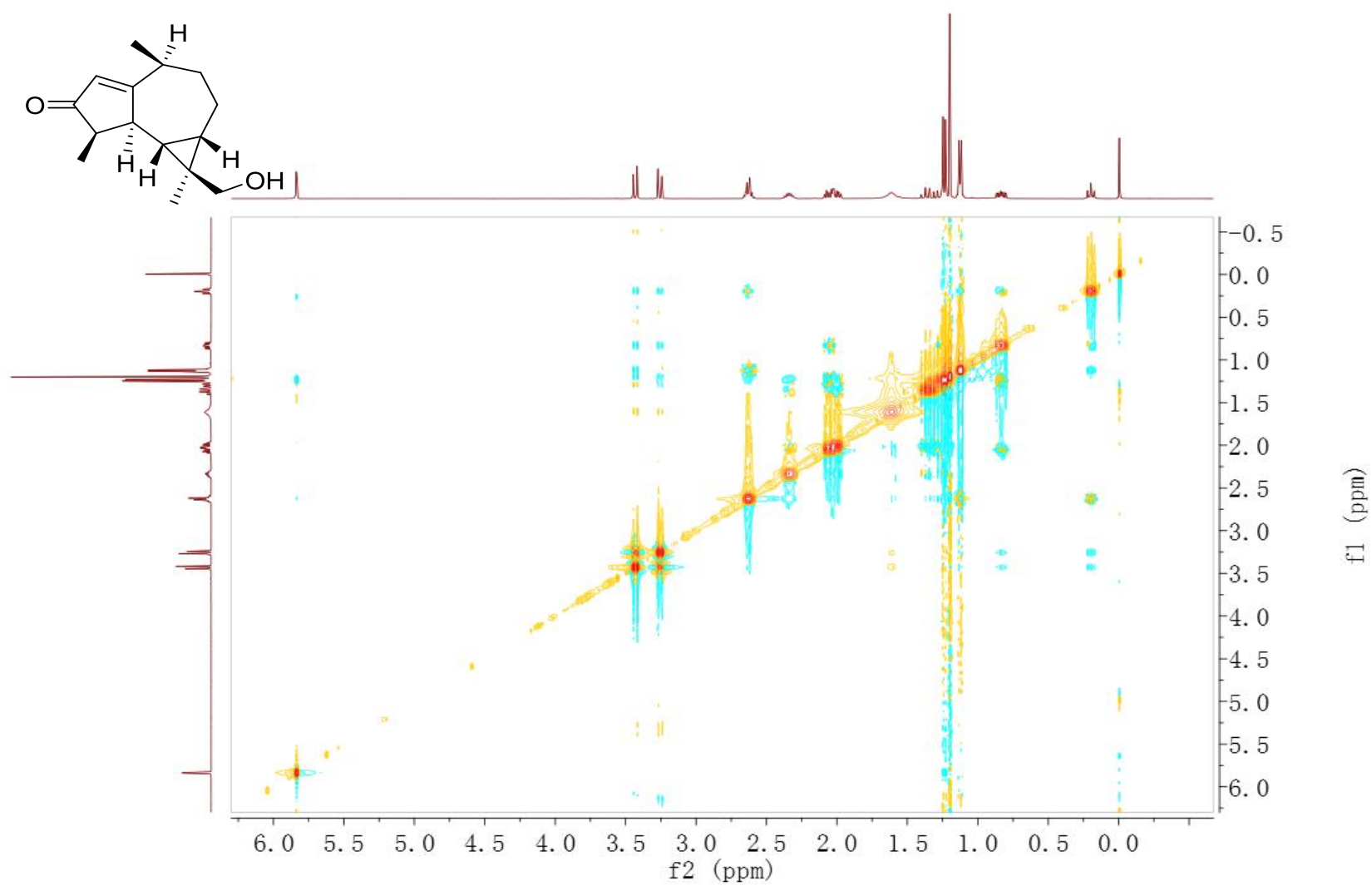


Figure S8. HR-ESI-MS spectrum of pseuboydone B (**2**)

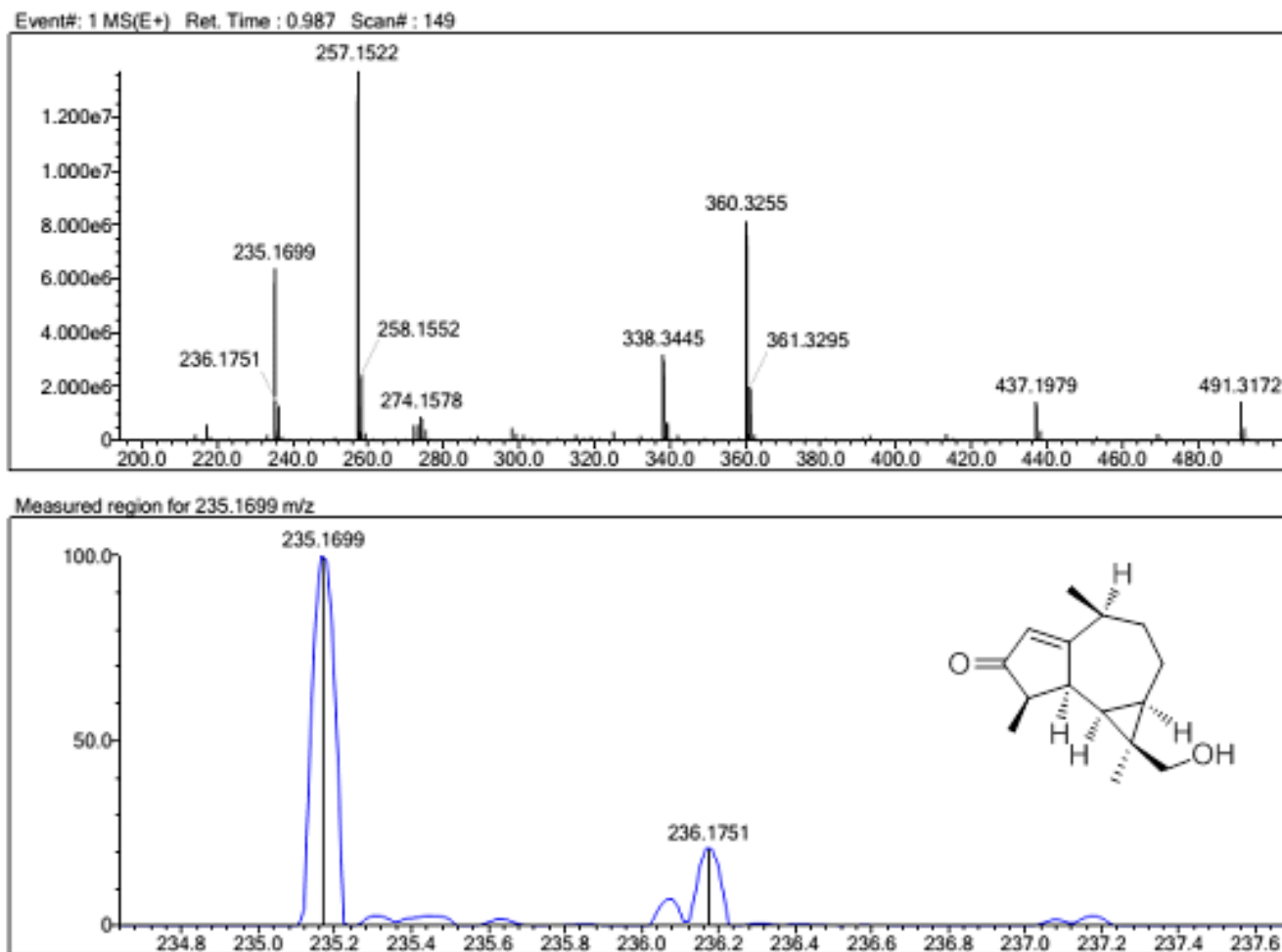


Figure S9. ^1H -NMR spectrum of pseuboydone B (**2**) in CDCl_3 (400MHz)

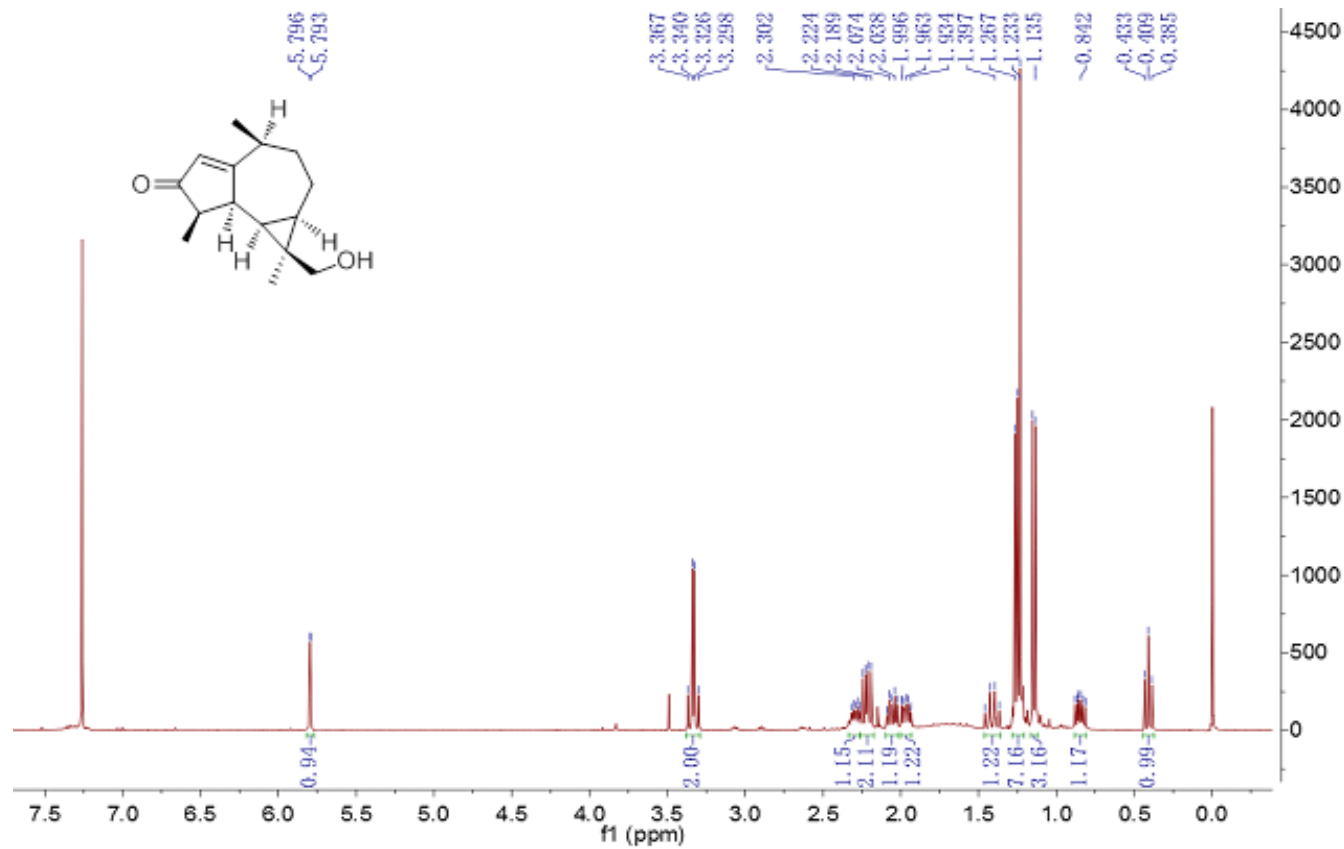


Figure S10. ^{13}C -NMR and DEPT spectra of pseudoboydone B (**2**) in CDCl_3 (100MHz)

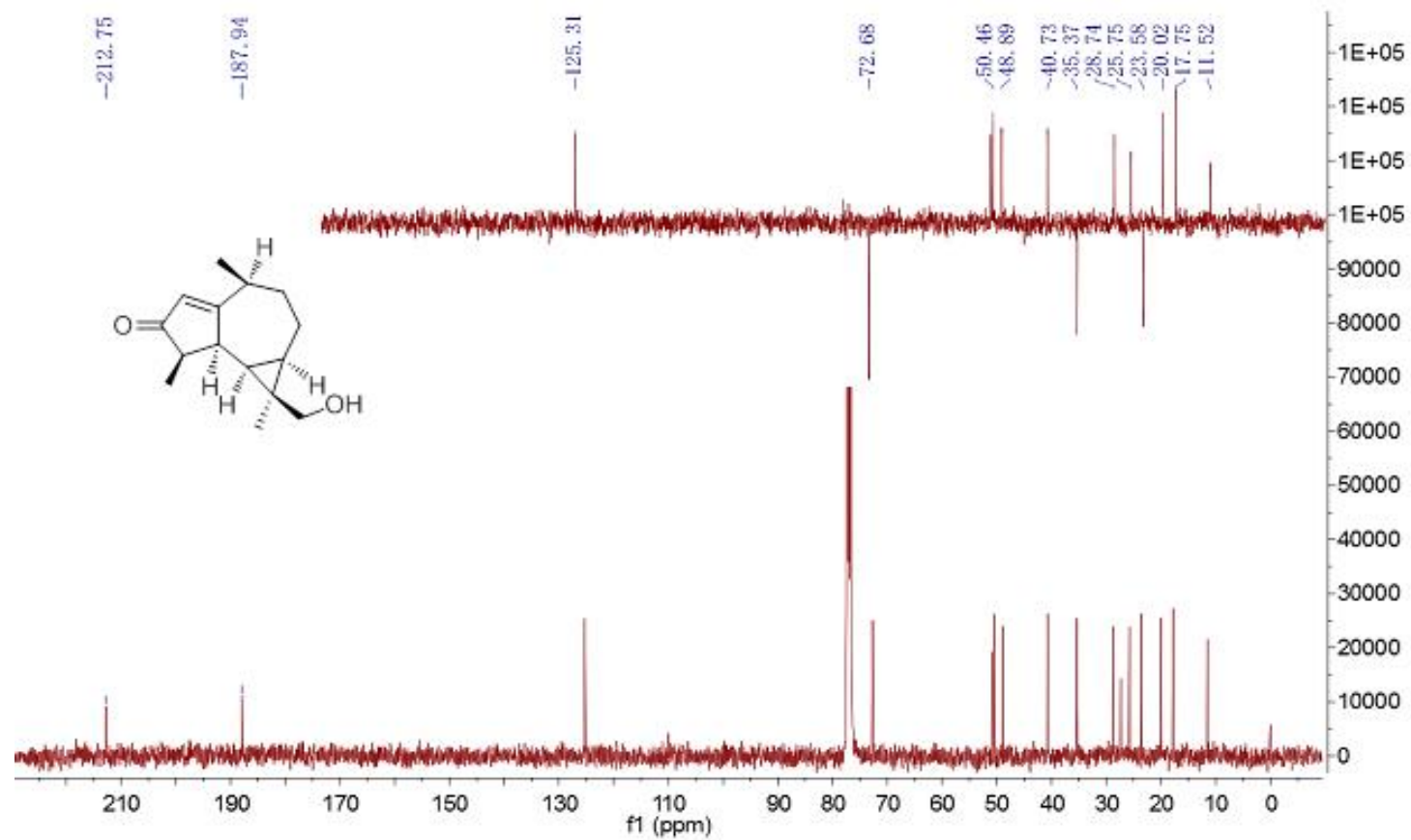


Figure S11. HMQC spectrum of pseuboydone B (**2**) in CDCl₃

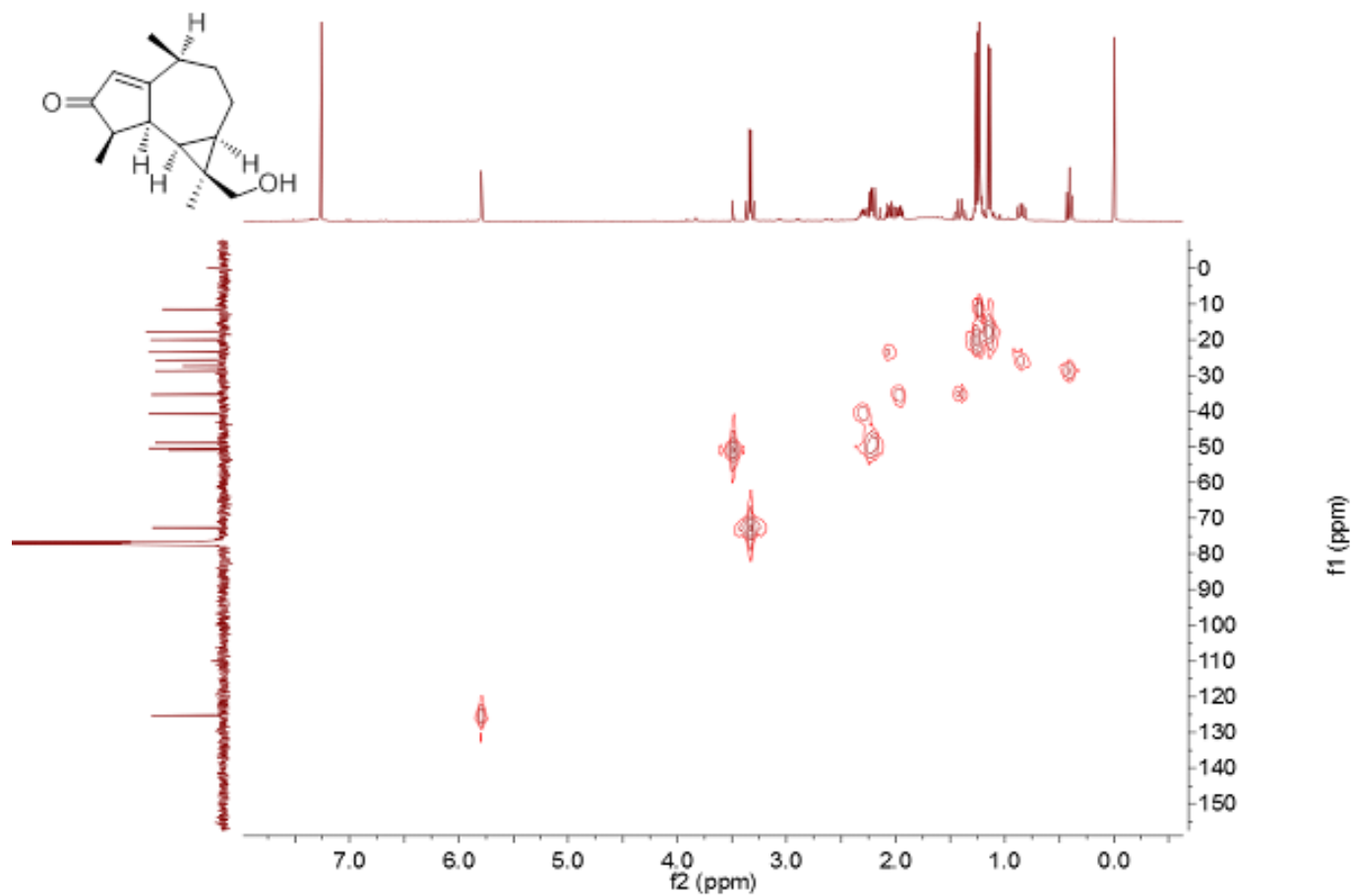


Figure S12. ^1H - ^1H COSY spectrum of pseuboydone B (**2**) in CDCl_3

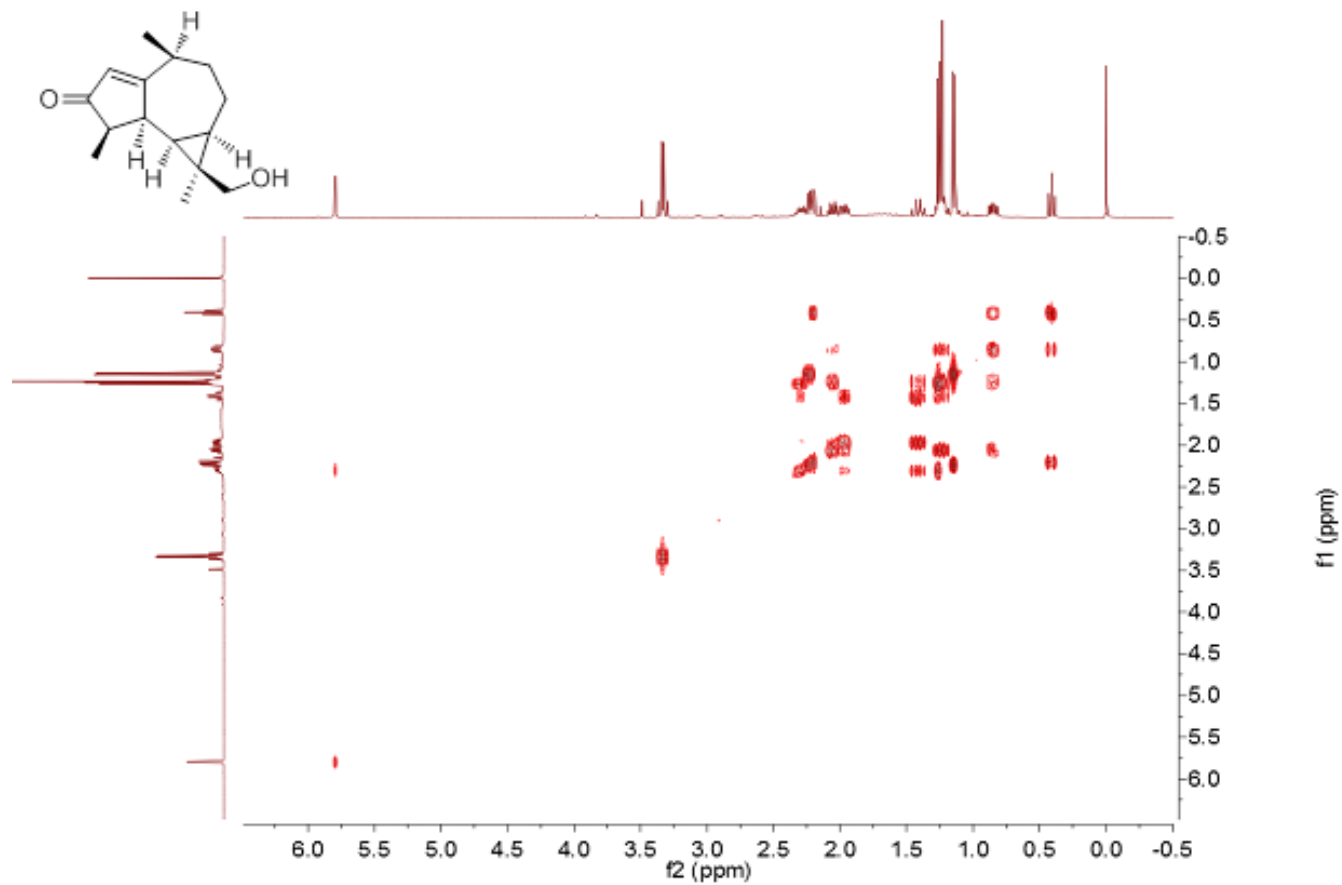


Figure S13. HMBC spectrum of pseuboydone B (**2**) in CDCl₃

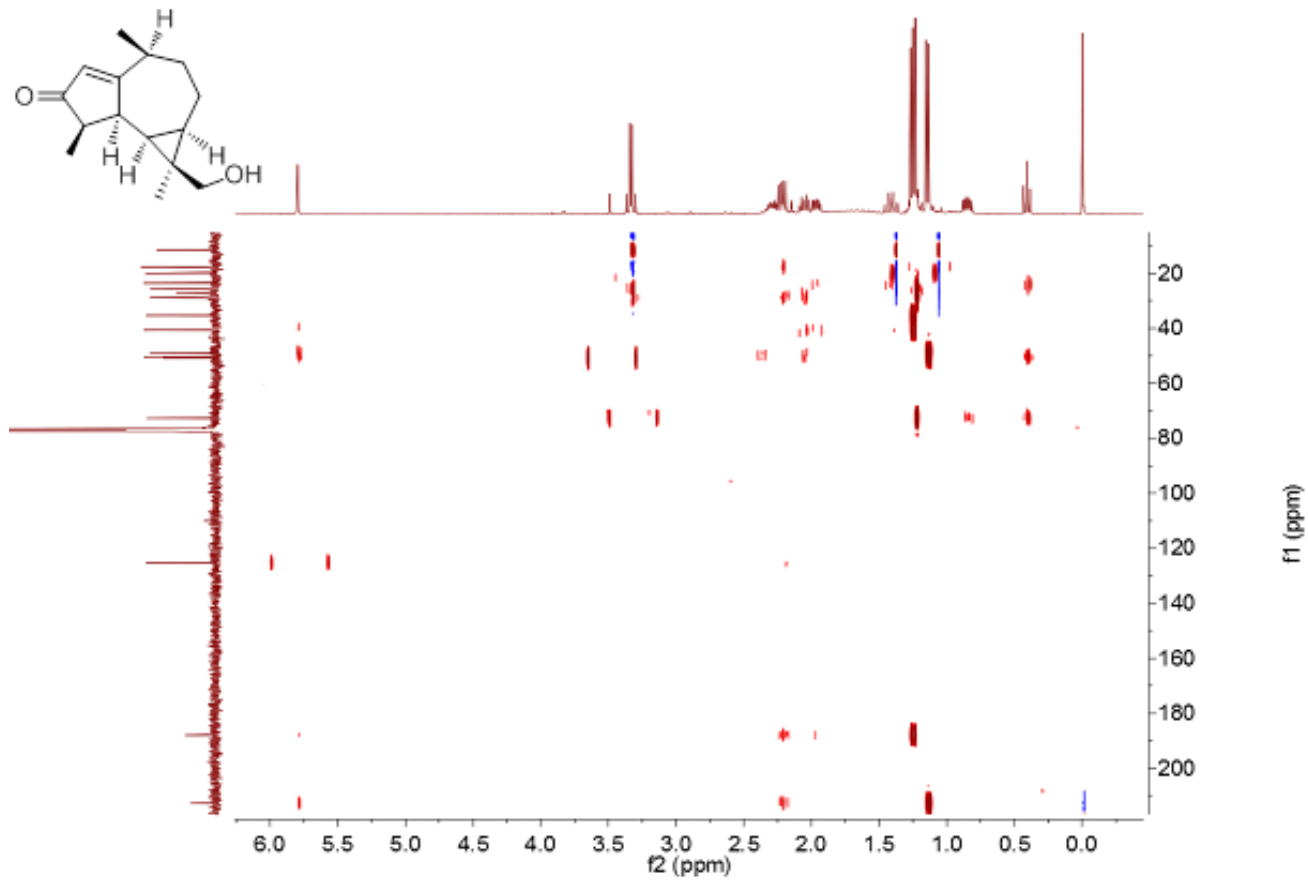


Figure S14. NOESY spectrum of pseuboydone B (**2**) in CDCl₃

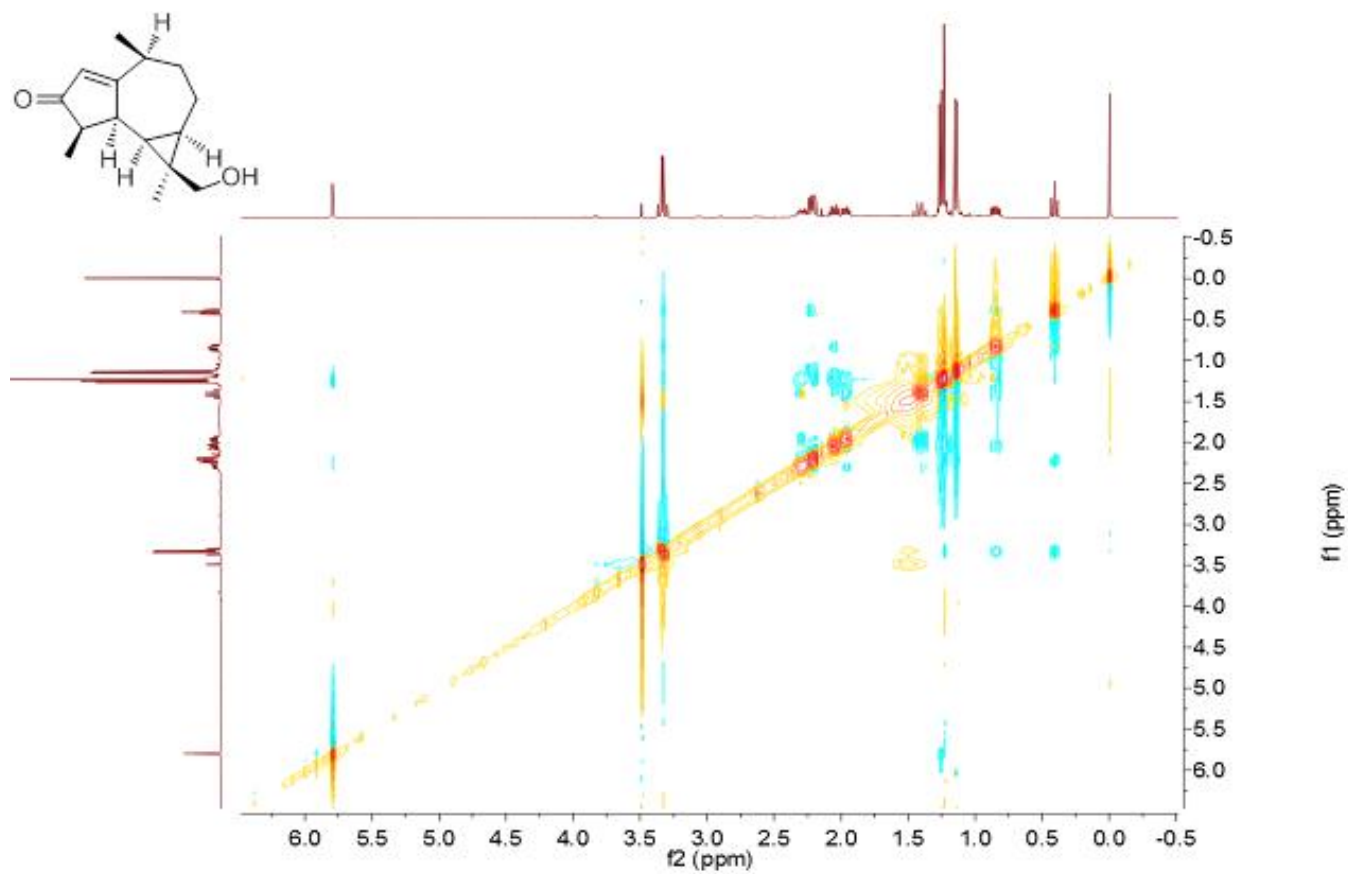


Figure S15. HR-ESI-MS spectrum of pseuboydone C (3)

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19-9s

LTQ Orbitrap Elite

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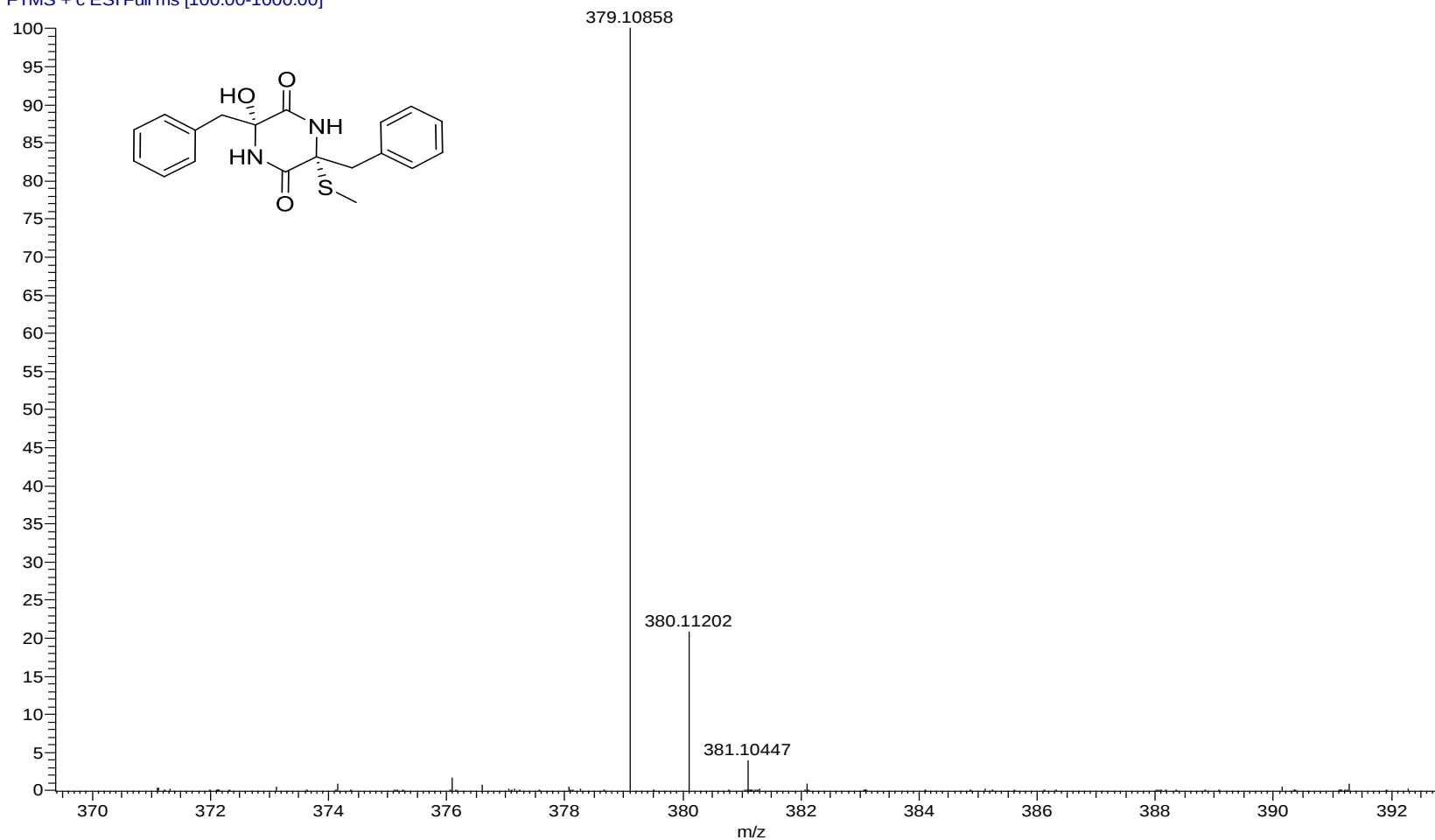


Figure S16. ^1H -NMR spectrum of pseuboydone C (**3**) in $\text{DMSO-}d_6$ (400MHz)

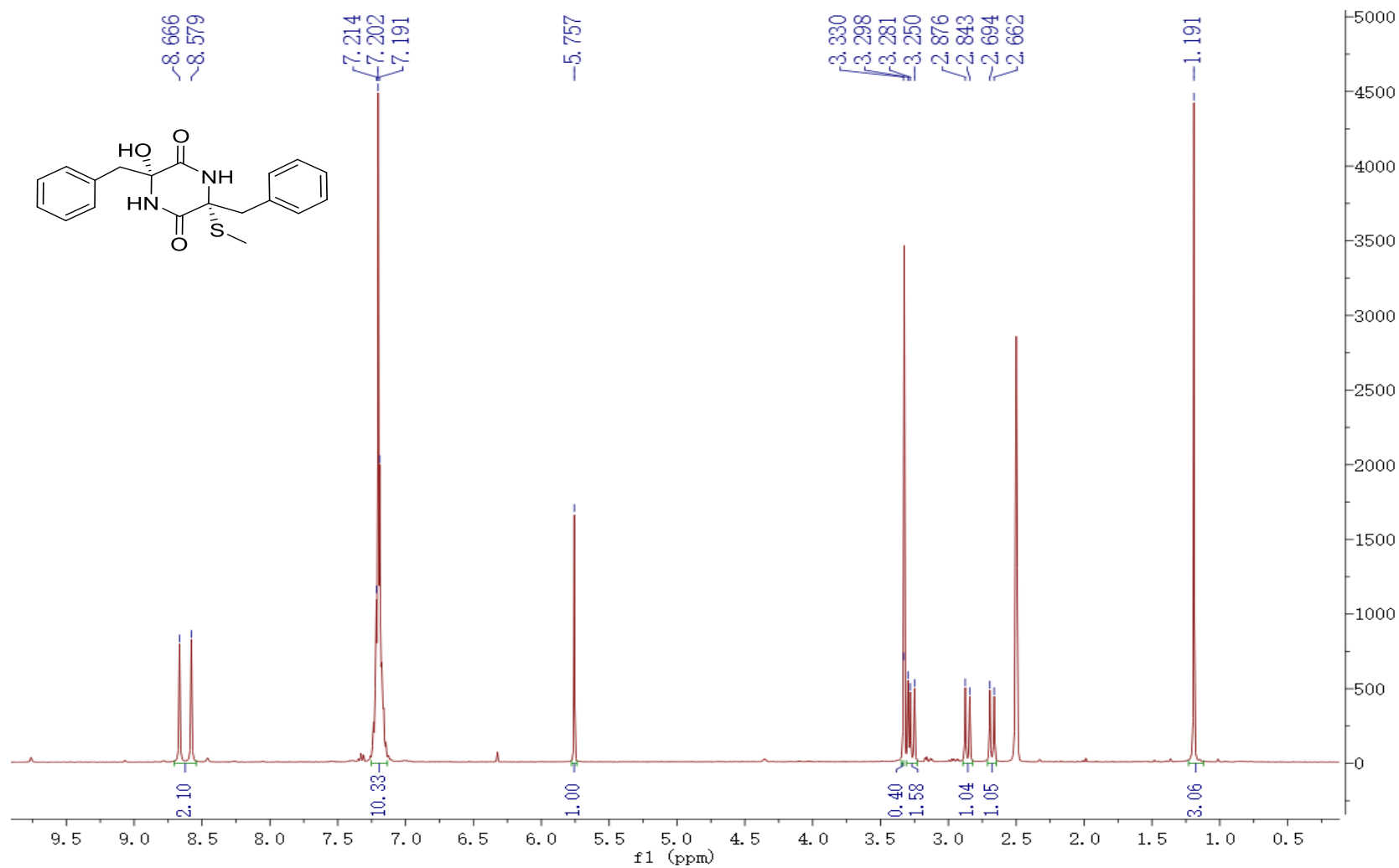


Figure S17. ^{13}C -NMR and DEPT spectra of pseudoydone C (**3**) in $\text{DMSO}-d_6$ (100MHz)

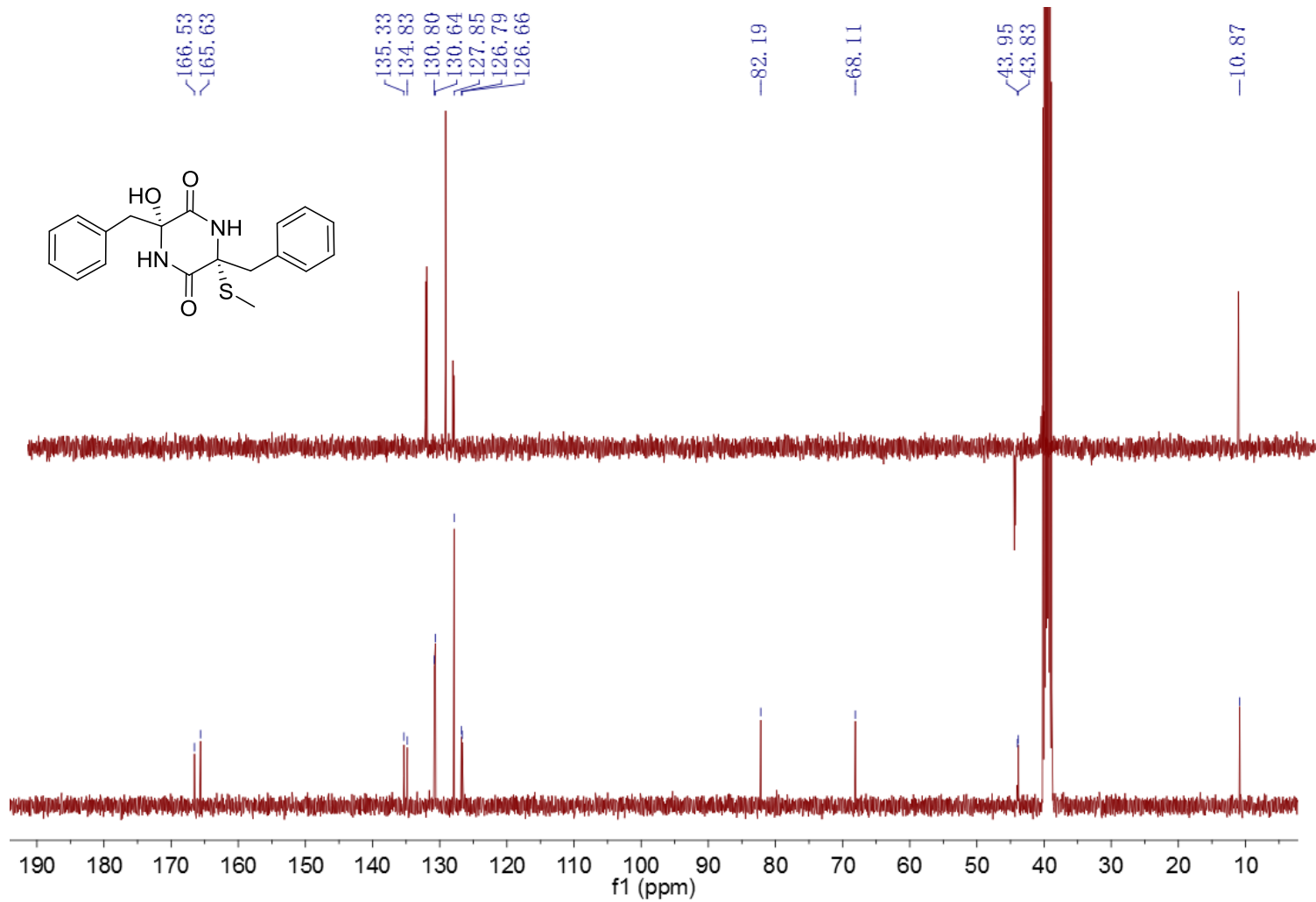


Figure S18. HMQC spectrum of pseuboydone C (**3**) in DMSO- d_6

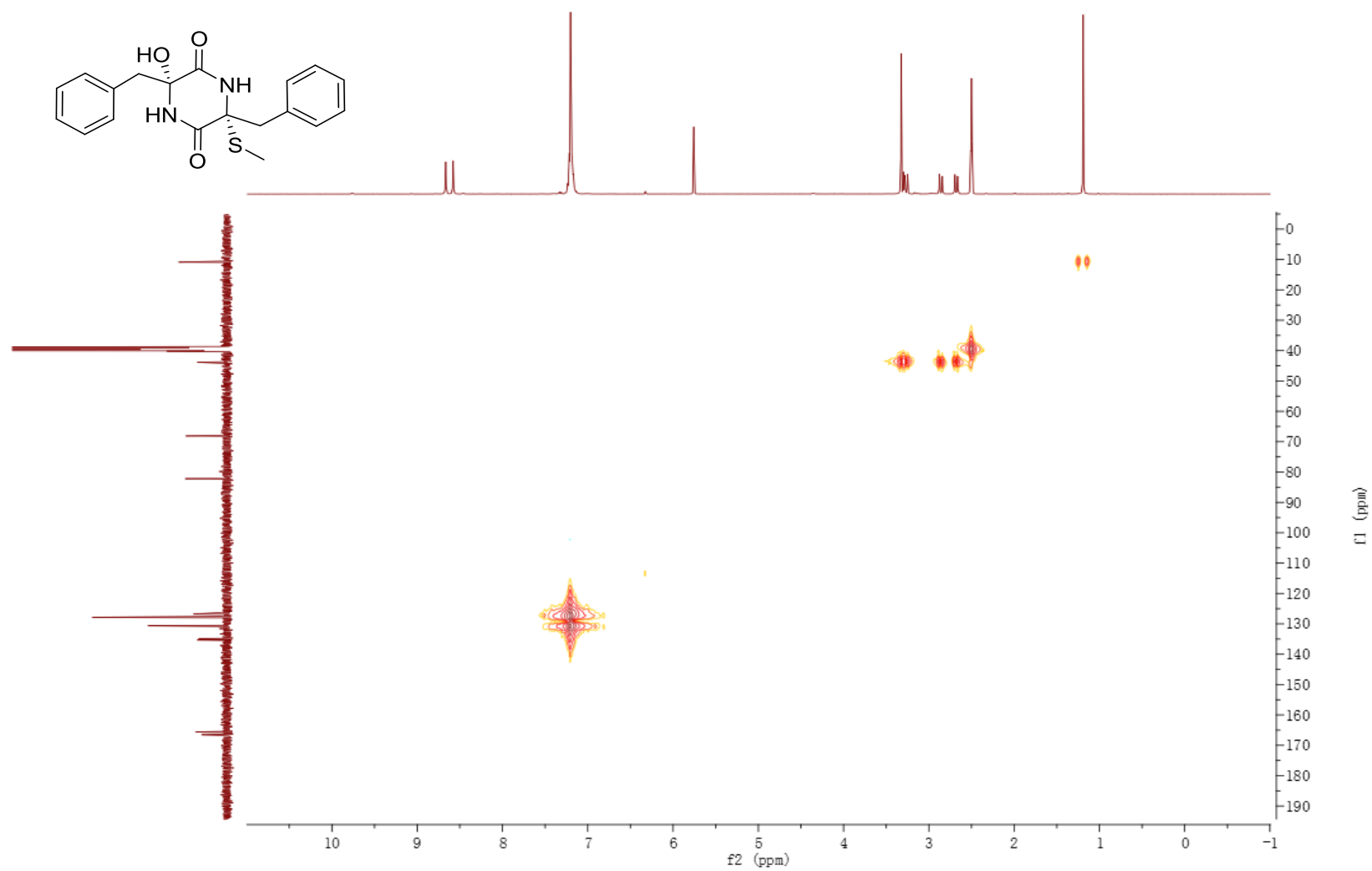


Figure S19. ^1H - ^1H COSY spectrum of pseuboydone C (**3**) in $\text{DMSO-}d_6$

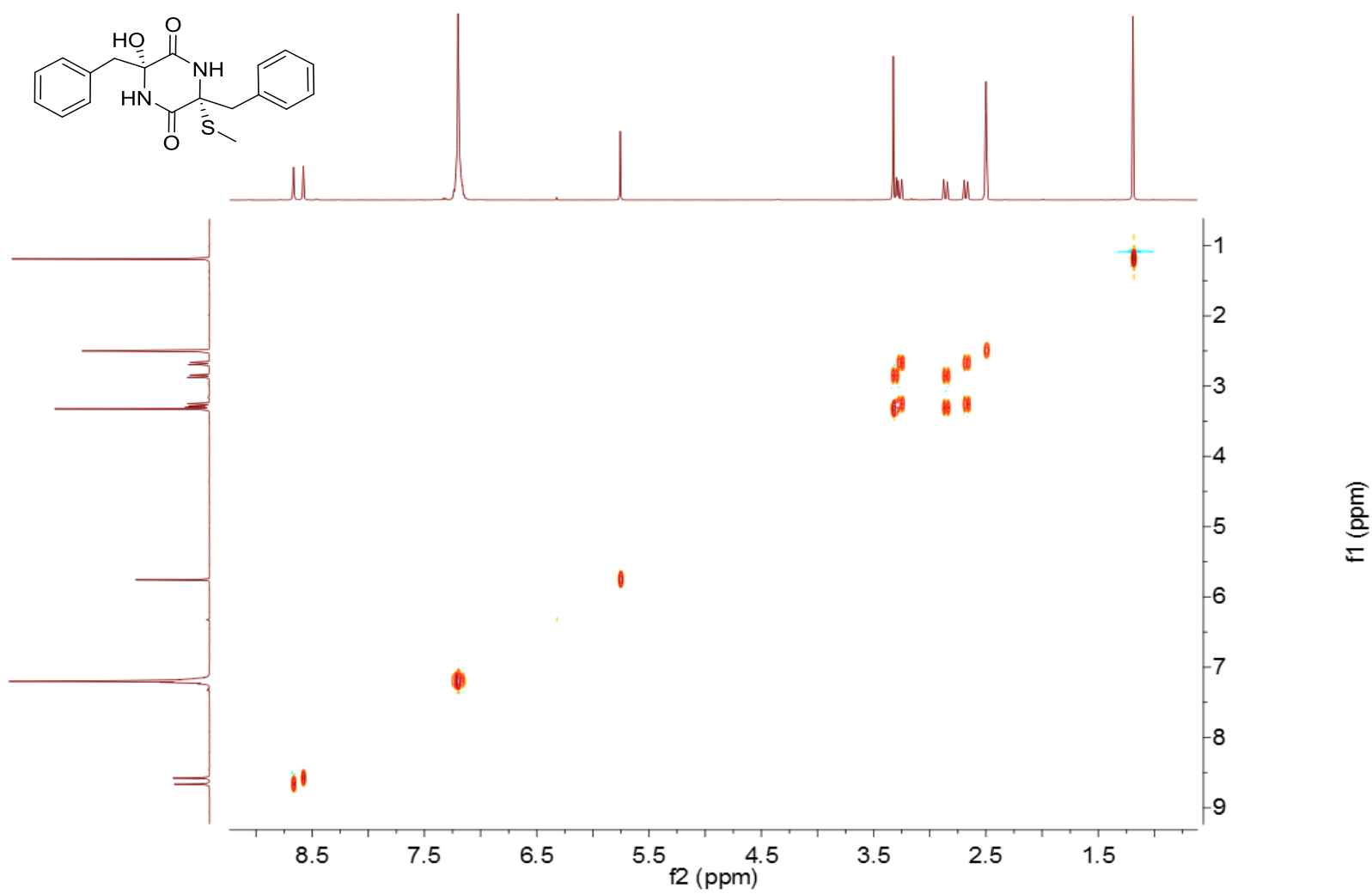


Figure S20. HMBC spectrum of pseuboydone C (**3**) in DMSO- d_6

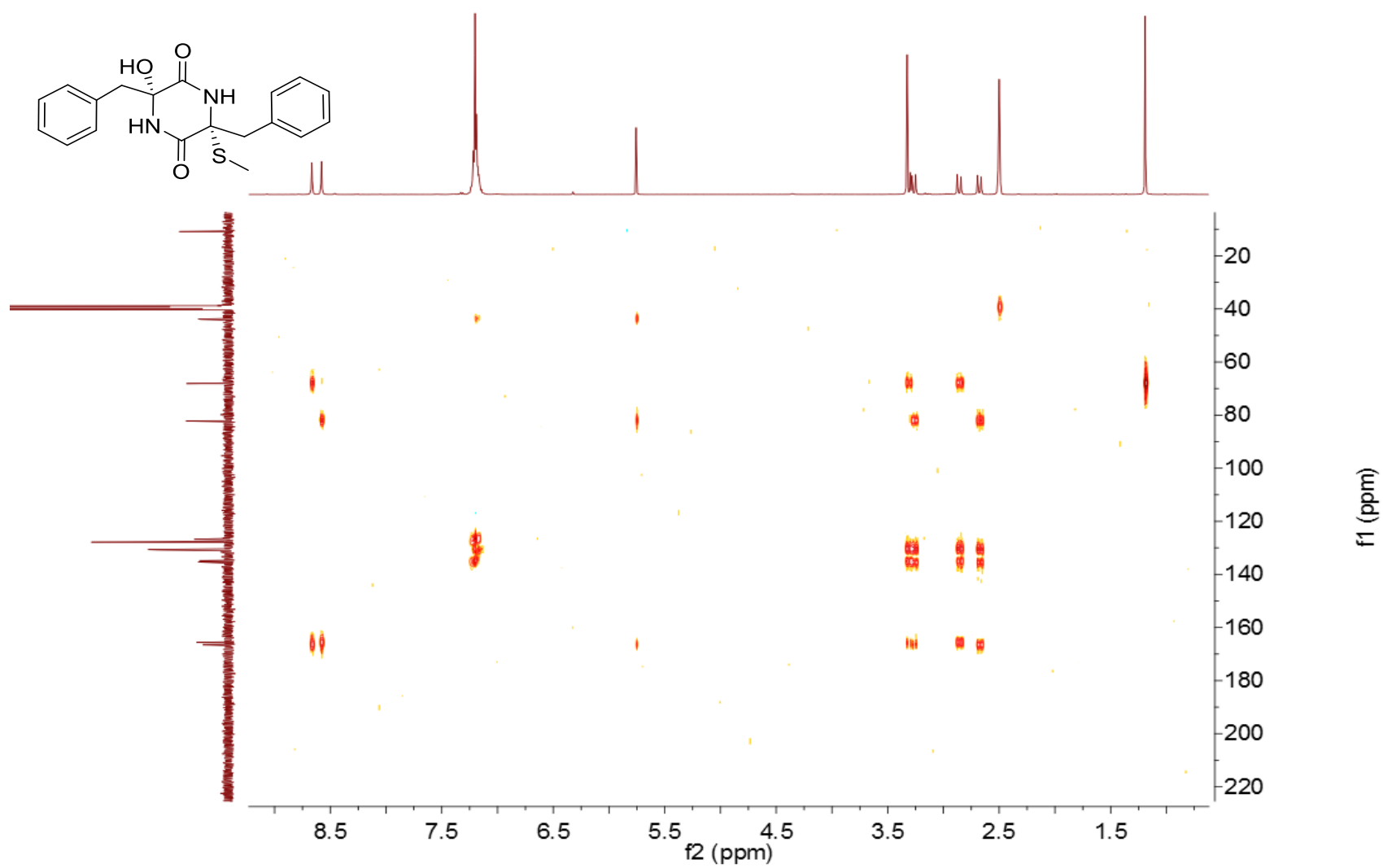


Figure S21. NOESY spectrum of pseuboydone C (**3**) in DMSO- d_6

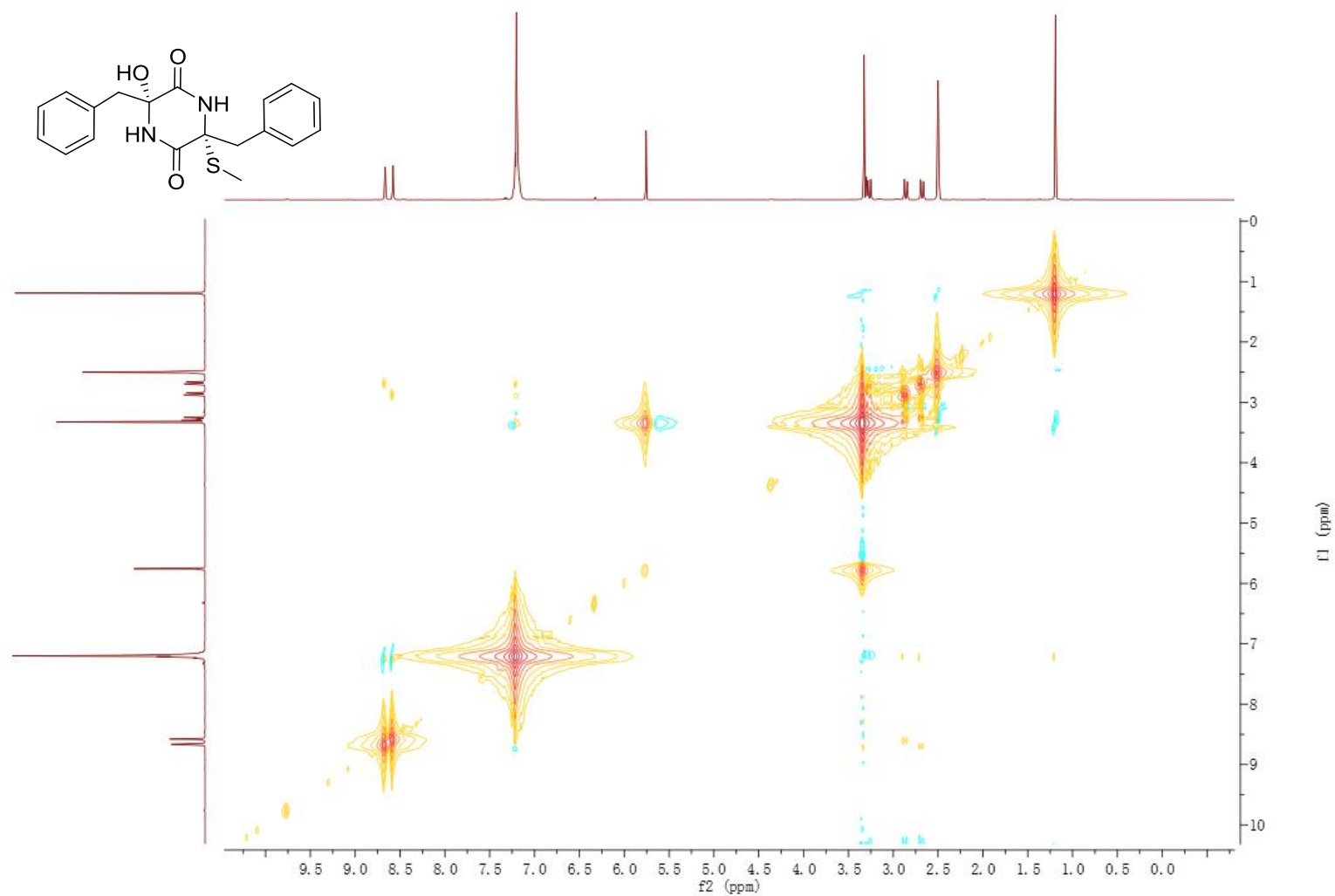
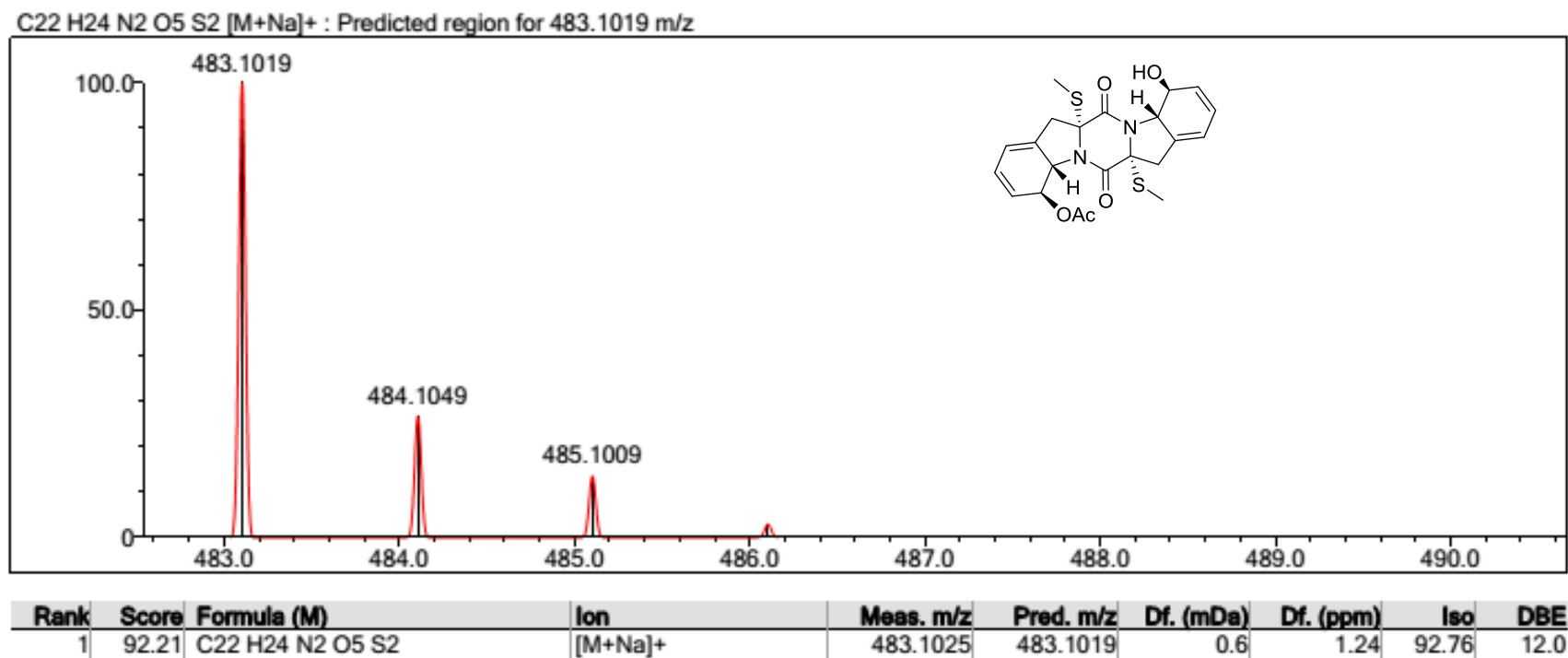


Figure S22. HR-ESI-MS spectrum of pseuboydone D (**4**)



Chemical structure of compound 10 is shown in the top left. The ^1H NMR spectrum (CDCl₃) is displayed below, with chemical shifts (ppm) on the x-axis (0.0 to 9.5) and intensity on the y-axis (0 to 11000). The spectrum shows several peaks, with integration values provided below the baseline.

Chemical shifts (ppm) labeled above the peaks:

- 6.160, 6.133, 6.001, 5.998, 5.978, 5.967, 5.963, 5.952, 5.917, 5.912, 5.885, 5.881, 5.866, 5.861, 5.857, 5.852, 5.747, 5.727, 5.608, 5.594, 5.588, 5.585, 5.157, 5.129, 4.893, 4.857, 4.831, 3.098, 3.066, 3.002, 2.970, 2.899, 2.886, 2.868, 2.853, 2.283, 2.166, 2.095

Integration values (labeled below the baseline):

- 1.00, 2.69, 1.22, 1.20, 0.90, 0.15, 1.12, 1.07, 2.21, 1.20, 1.29, 2.25, 2.72, 2.97, 3.51

Figure S24. ^{13}C -NMR and DEPT spectra of pseuboydone D (**4**) in CDCl_3 (125MHz)

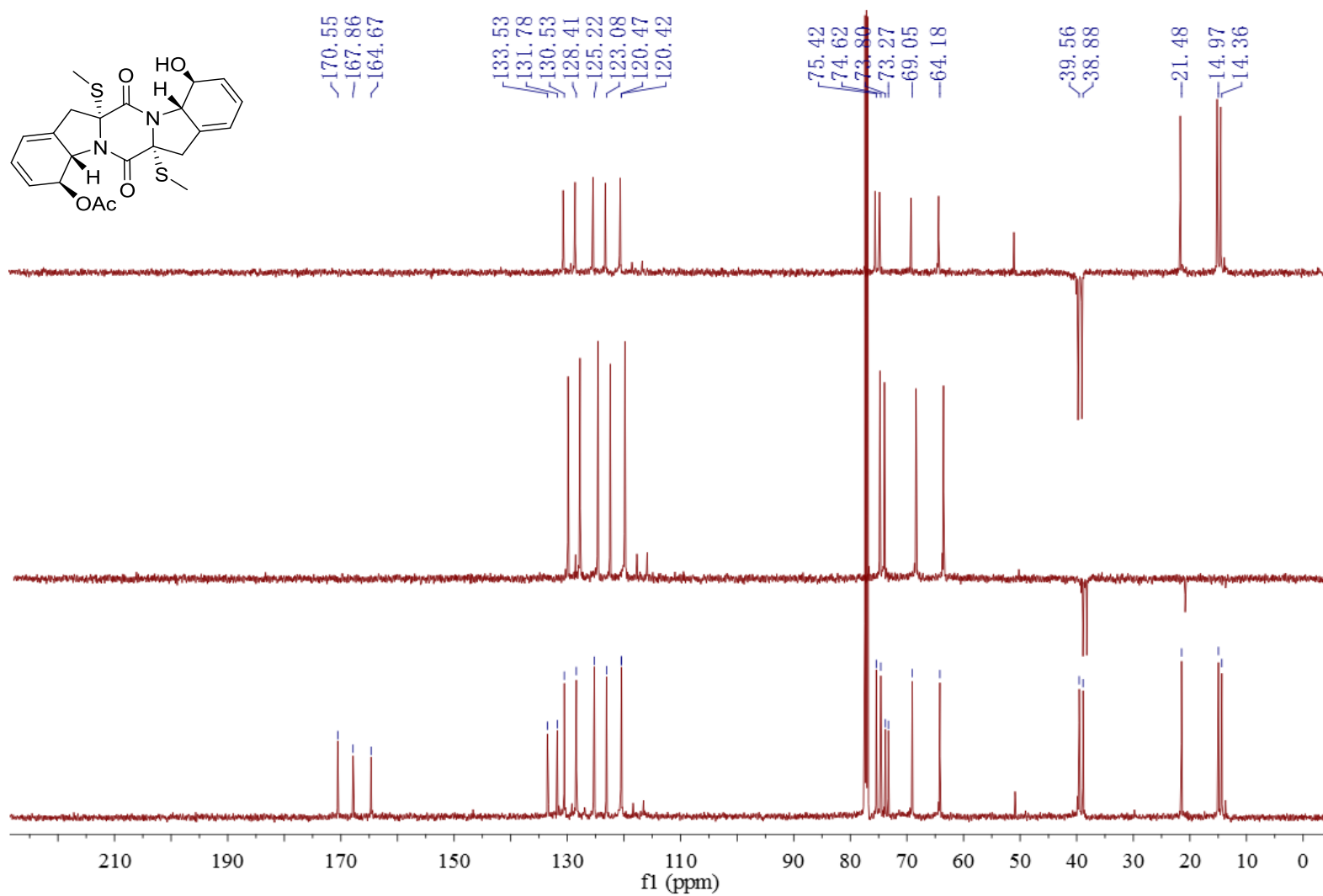


Figure S25. HMQC spectrum of pseuboydone D (**4**) in CDCl₃

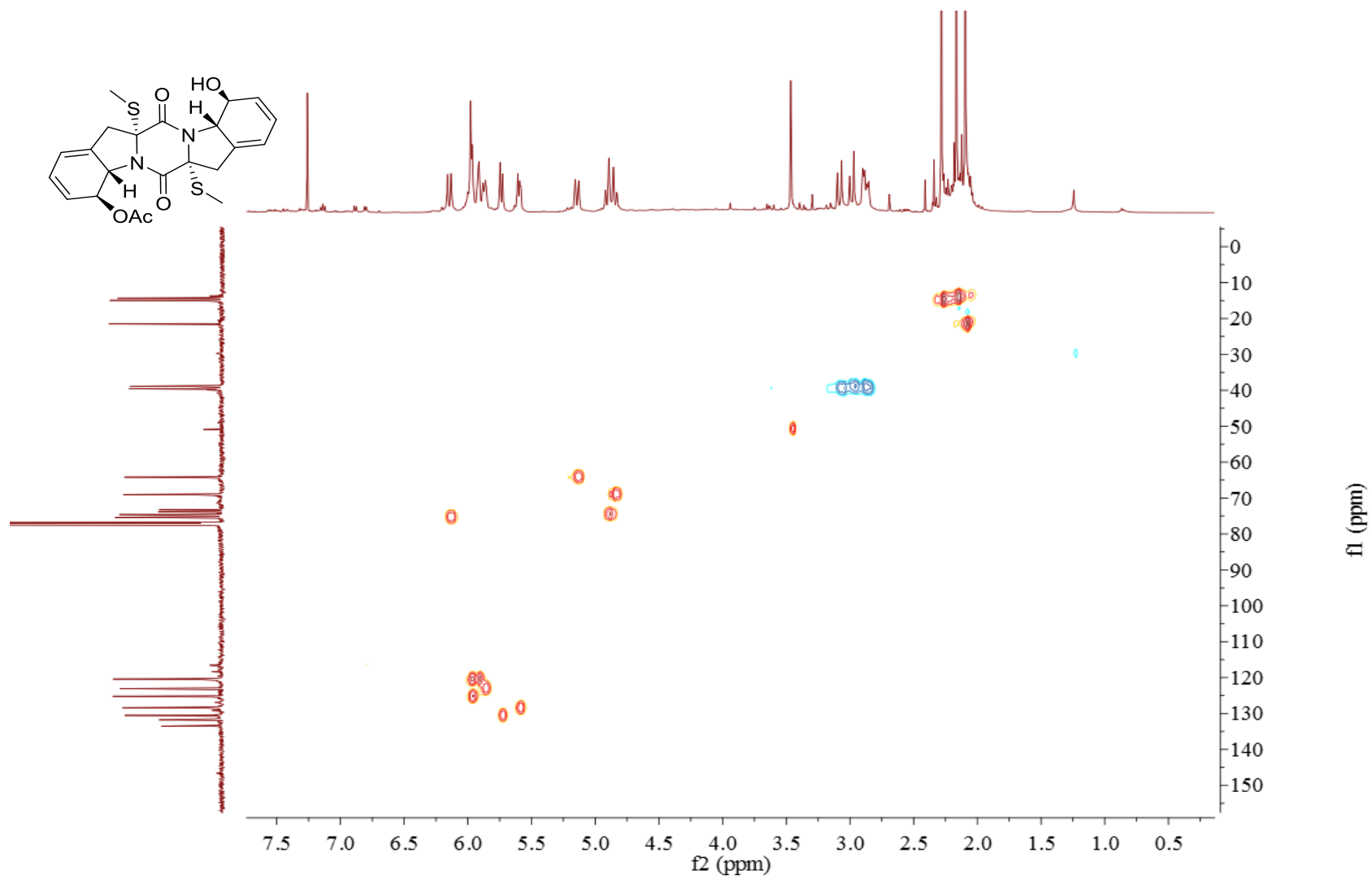


Figure S26. ^1H - ^1H COSY spectrum of pseuboydone D (**4**) in CDCl_3

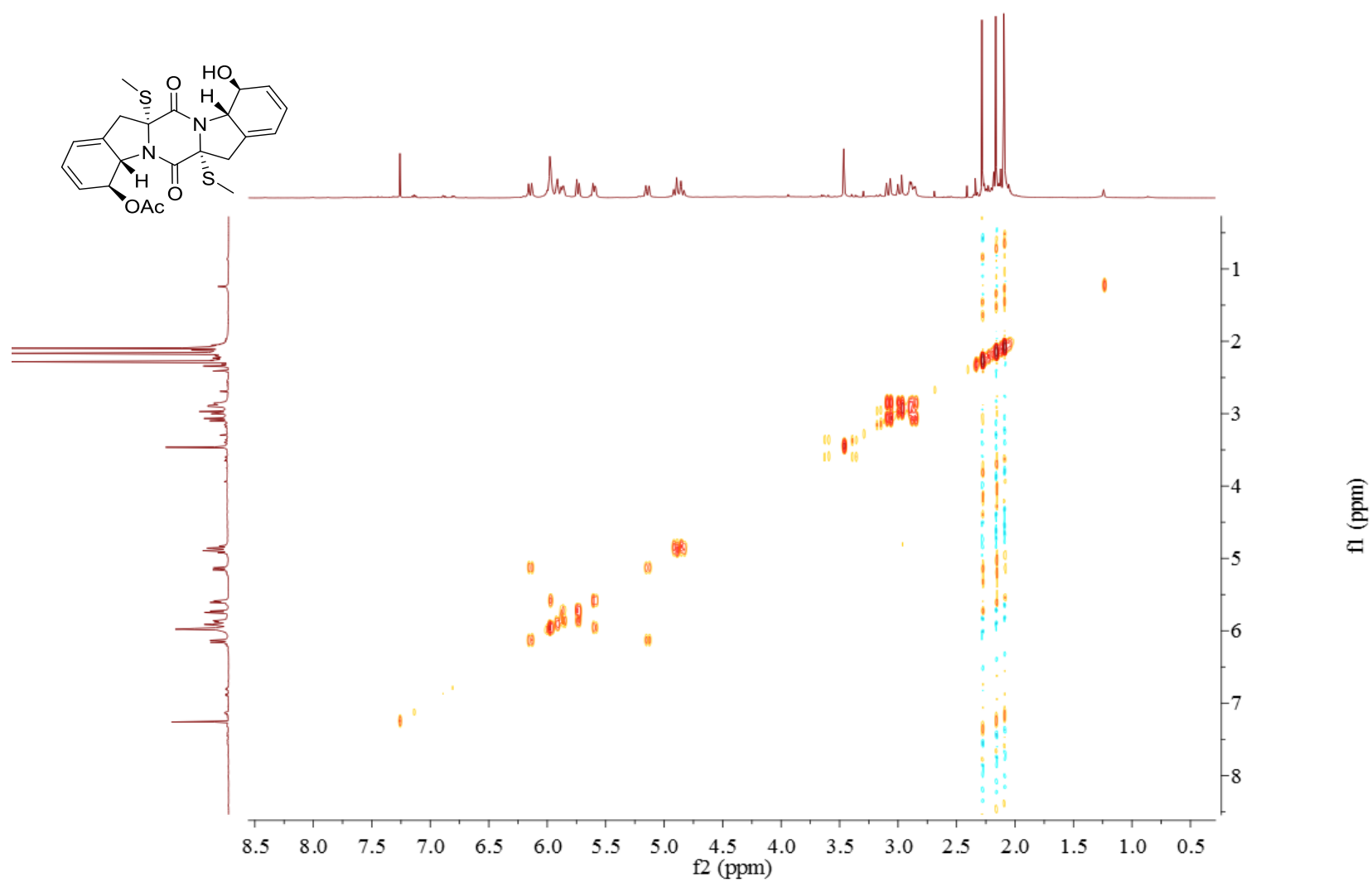


Figure S27. HMBC spectrum of pseuboydone D (**4**) in CDCl₃

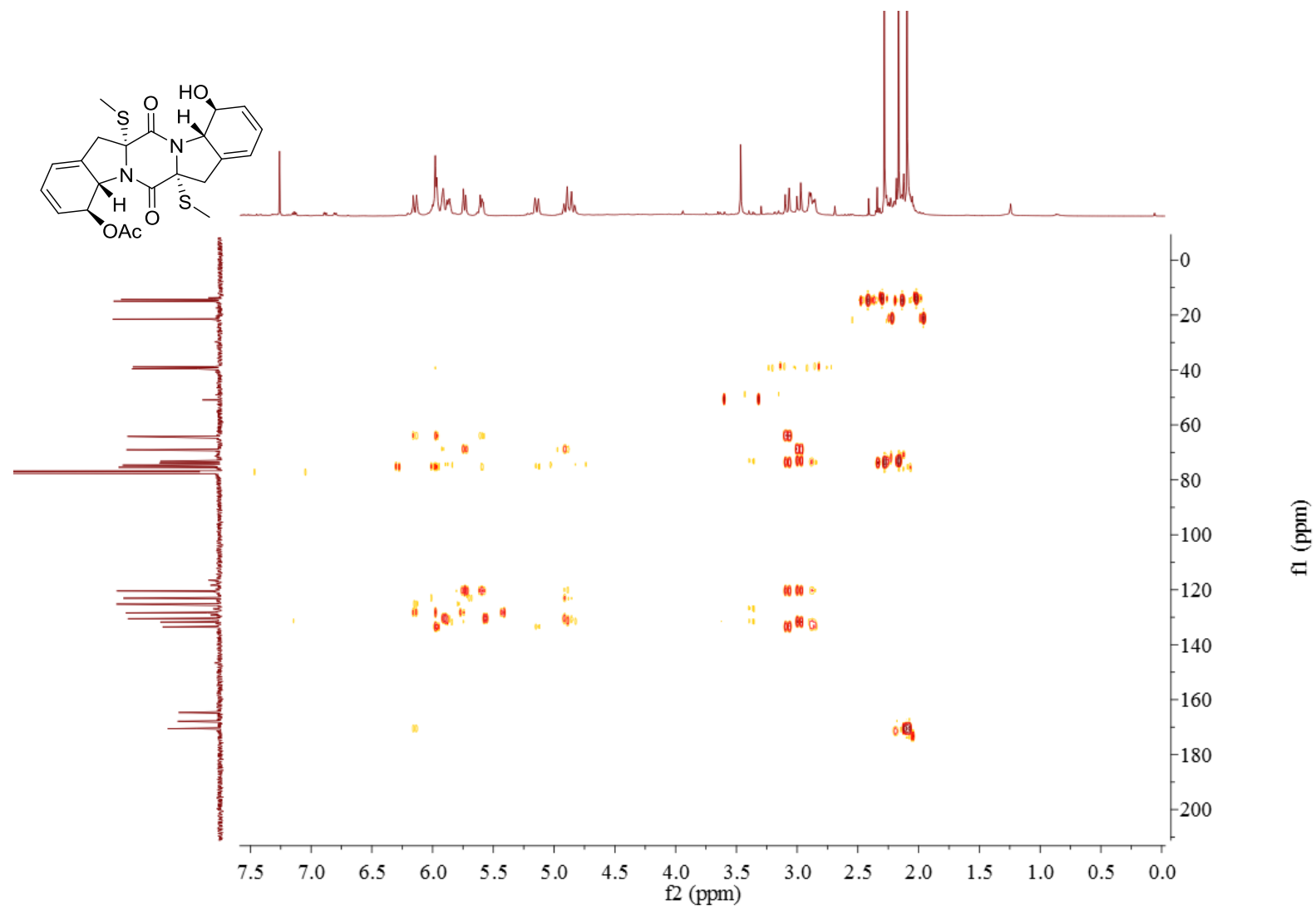


Figure S28. LR-ESI-MS spectrum of haematocin (**5**) in CDCl₃

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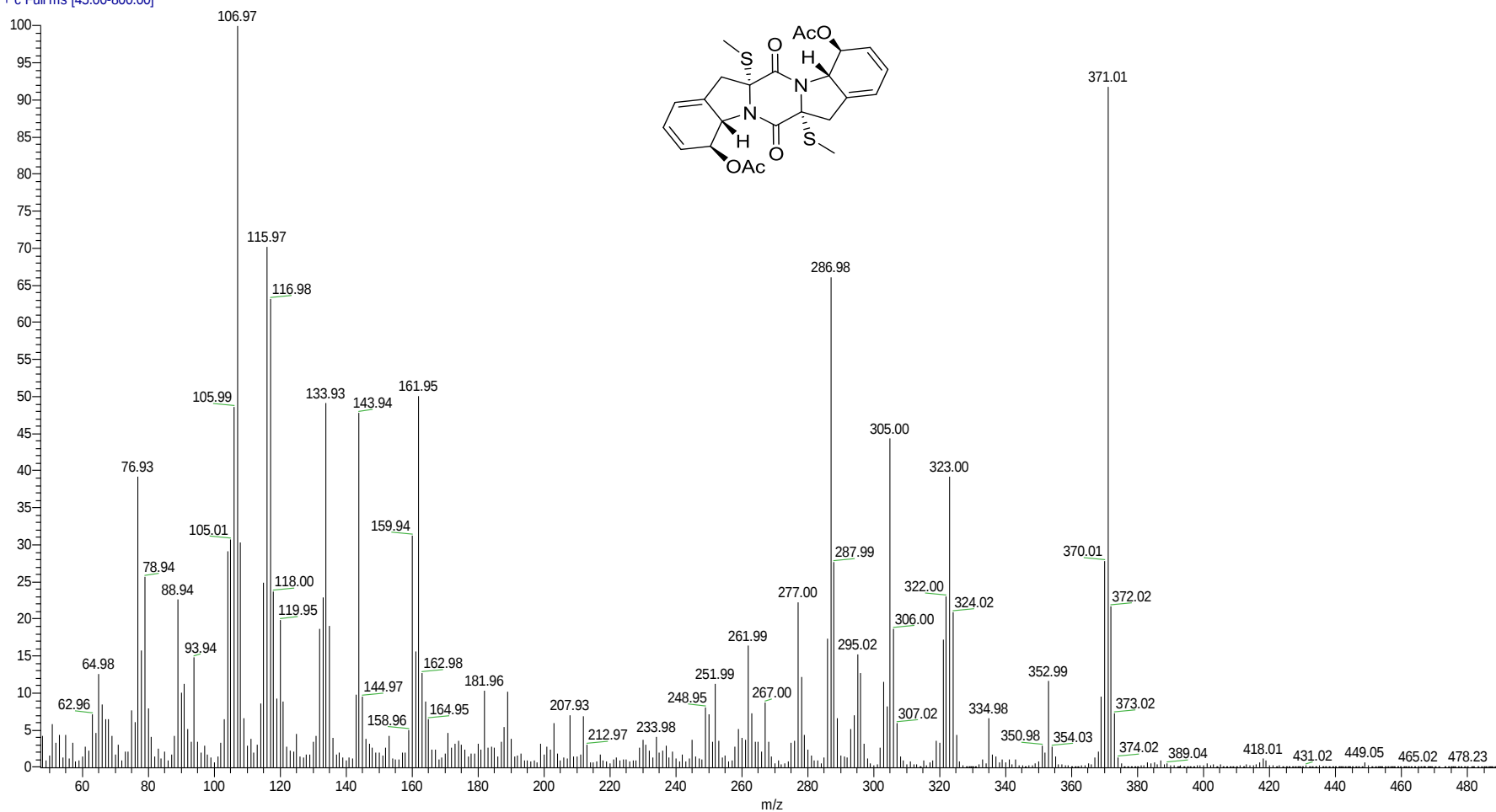


Figure S29. ^1H -NMR spectrum of haematocin (**5**) in CDCl_3

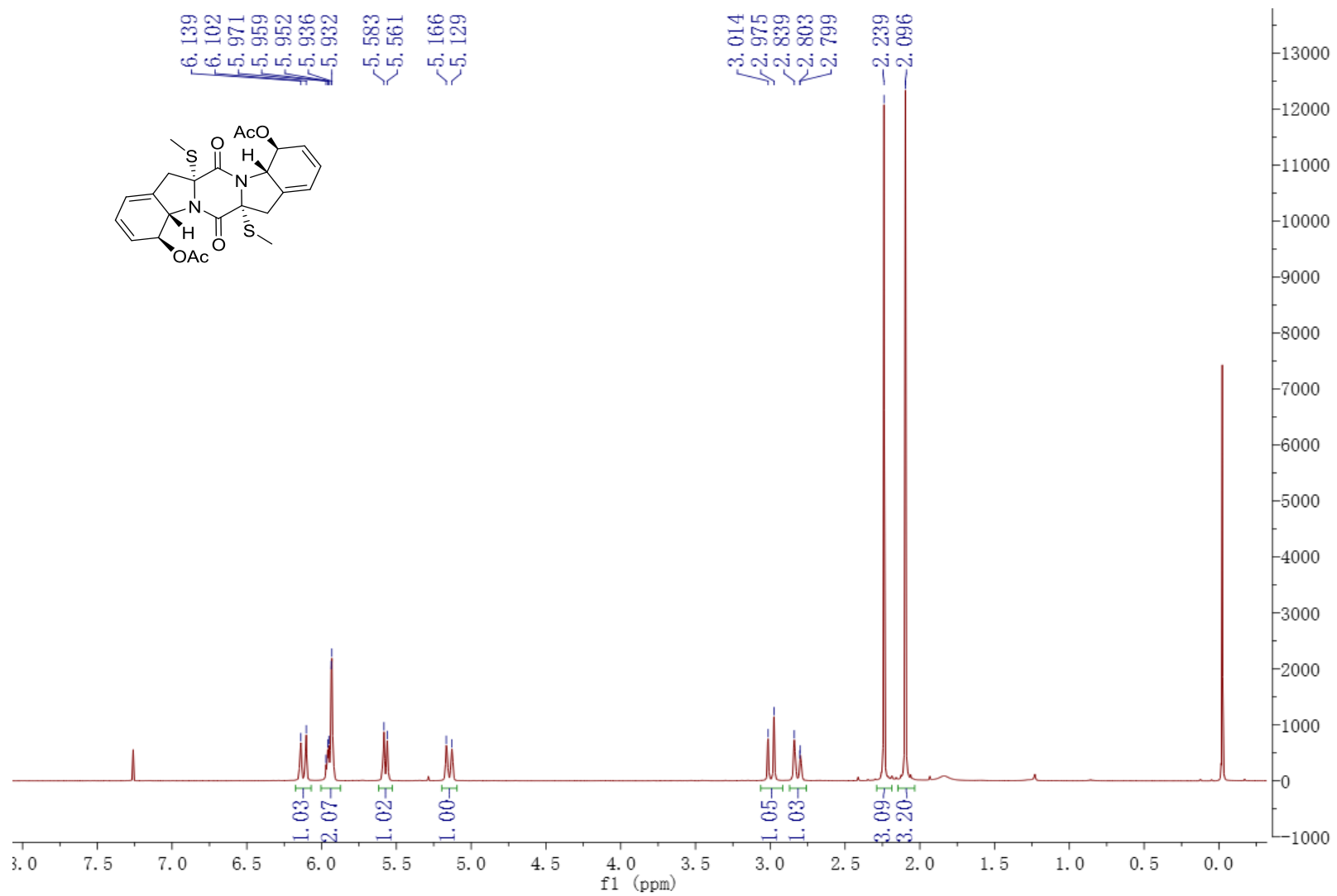


Figure S30. ^{13}C -NMR and DEPT spectra of haematocin (**5**)

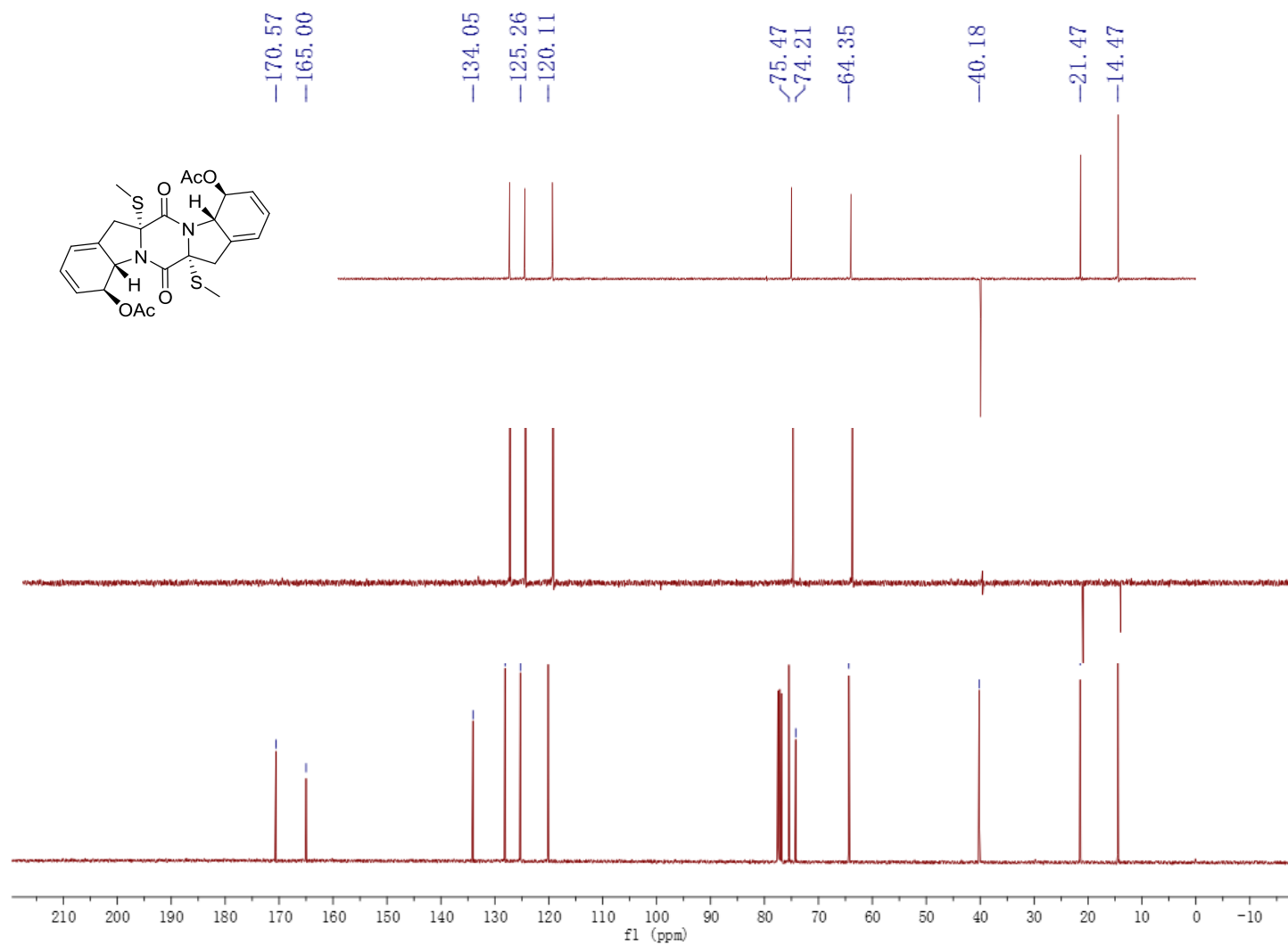


Figure S31. HMQC spectrum of haematocin (**5**) in CDCl₃

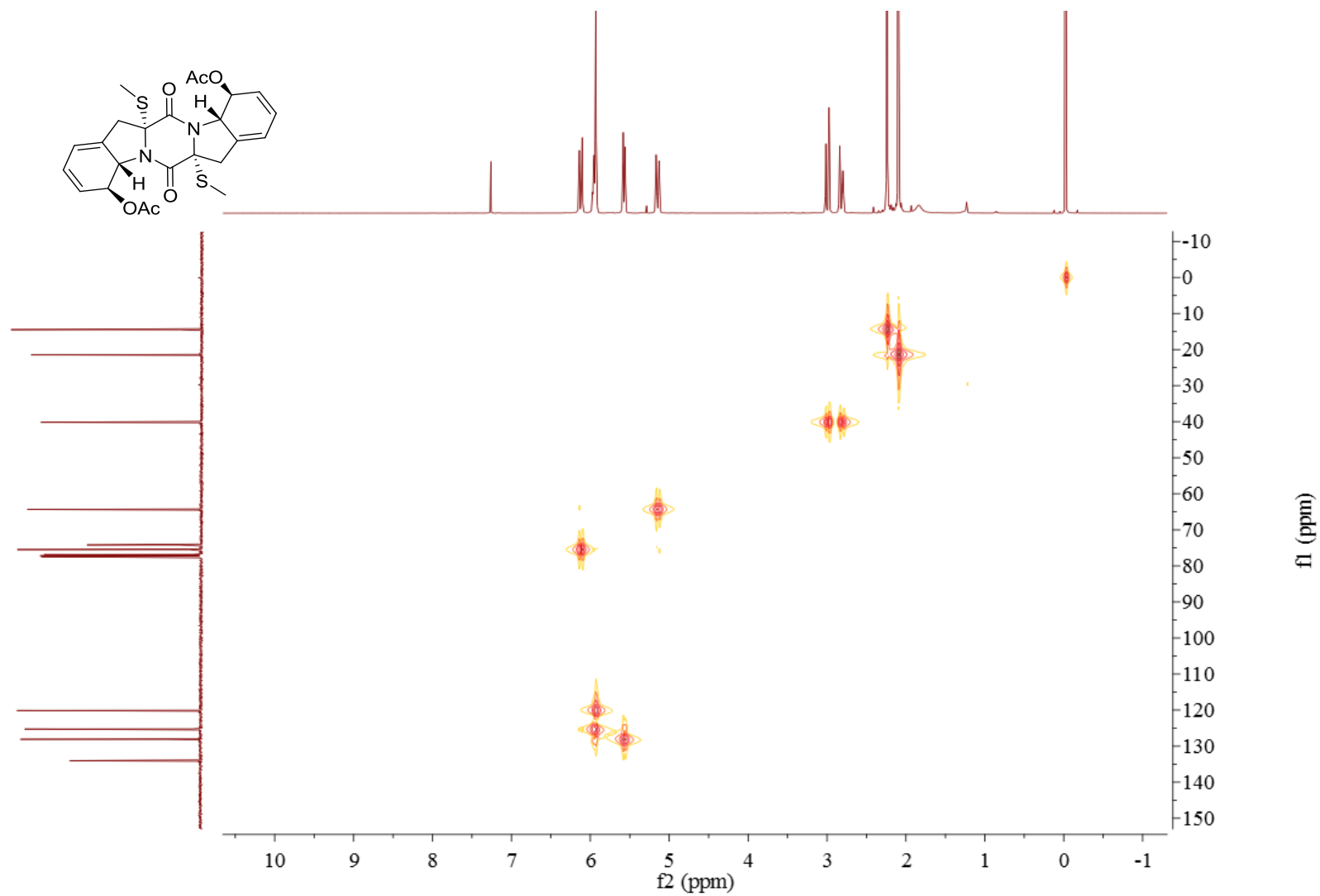


Figure S32. ^1H - ^1H COSY spectrum of haematocin (**5**) in CDCl_3

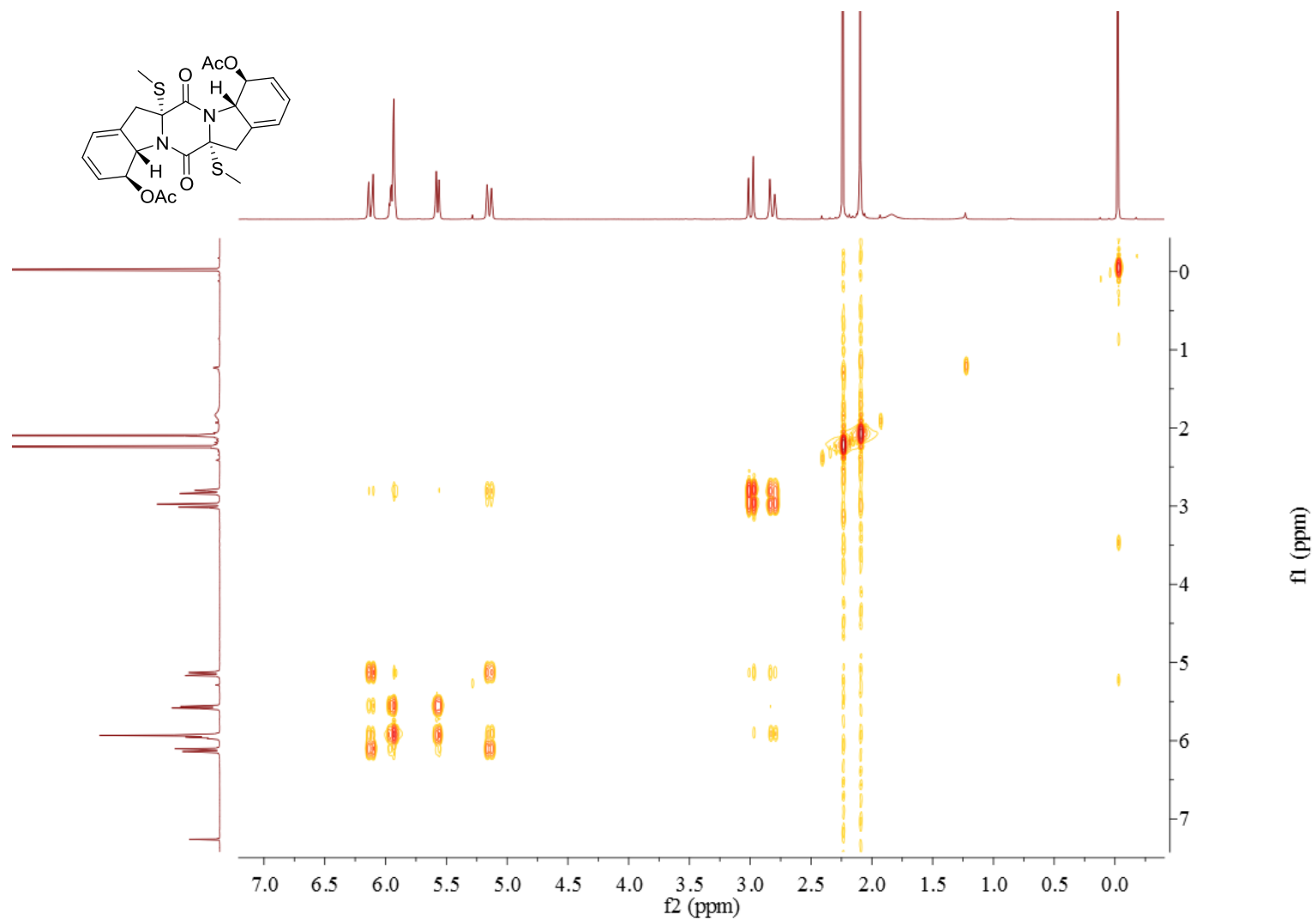


Figure S33. HMBC spectrum of haematocin (**5**) in CDCl₃

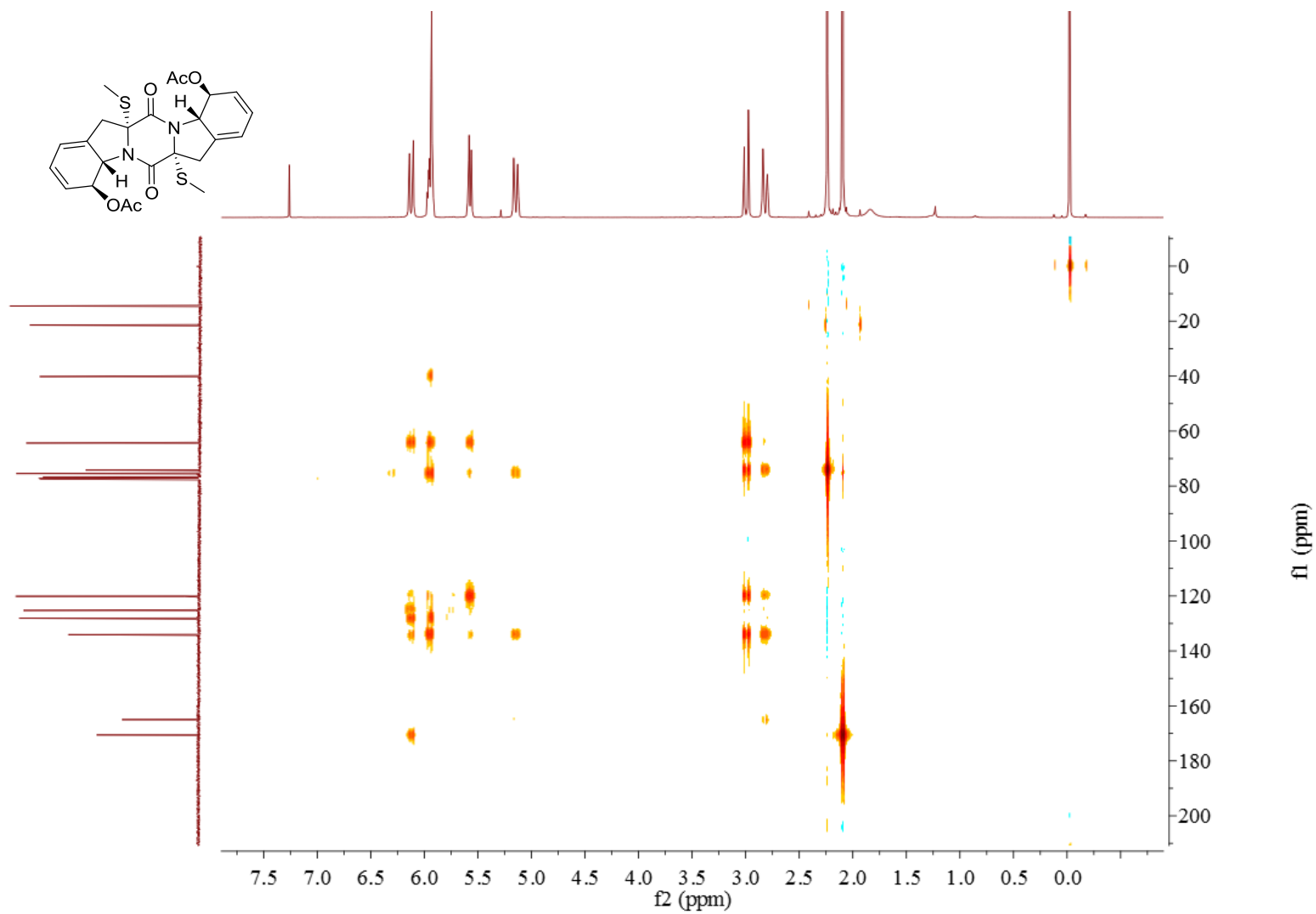


Figure S34. NOESY spectrum of haematocin (5) in CDCl₃

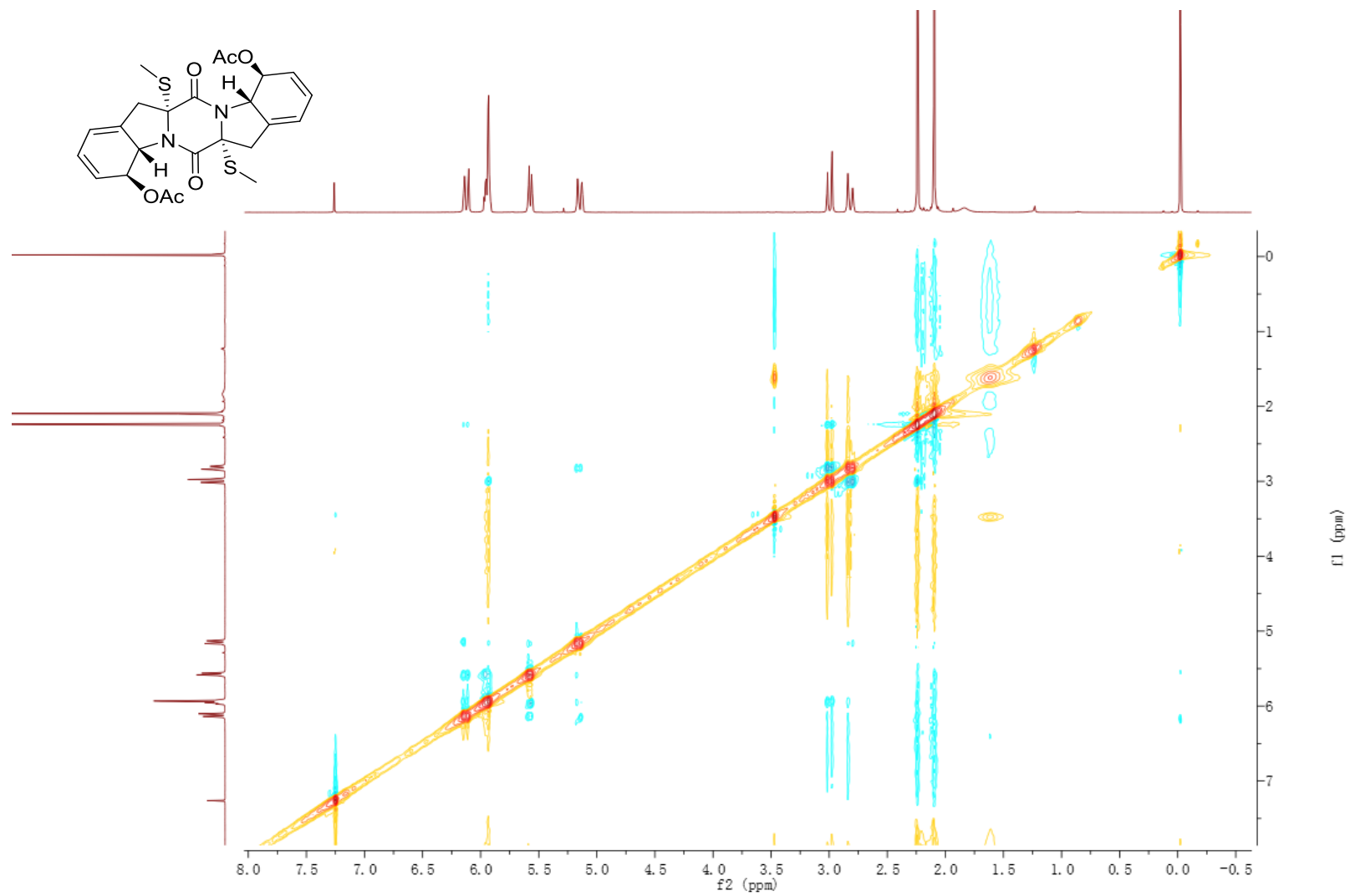


Figure S35. LR-ESI-MS spectrum of boydine A (**6**)

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQ\DATA-LR\13\042603

4/

F24-1_CC22-27_Pre3

042603 #91 RT: 2.34 AV: 1 NL: 4.57E6

T: + c Full ms [45.00-800.00]

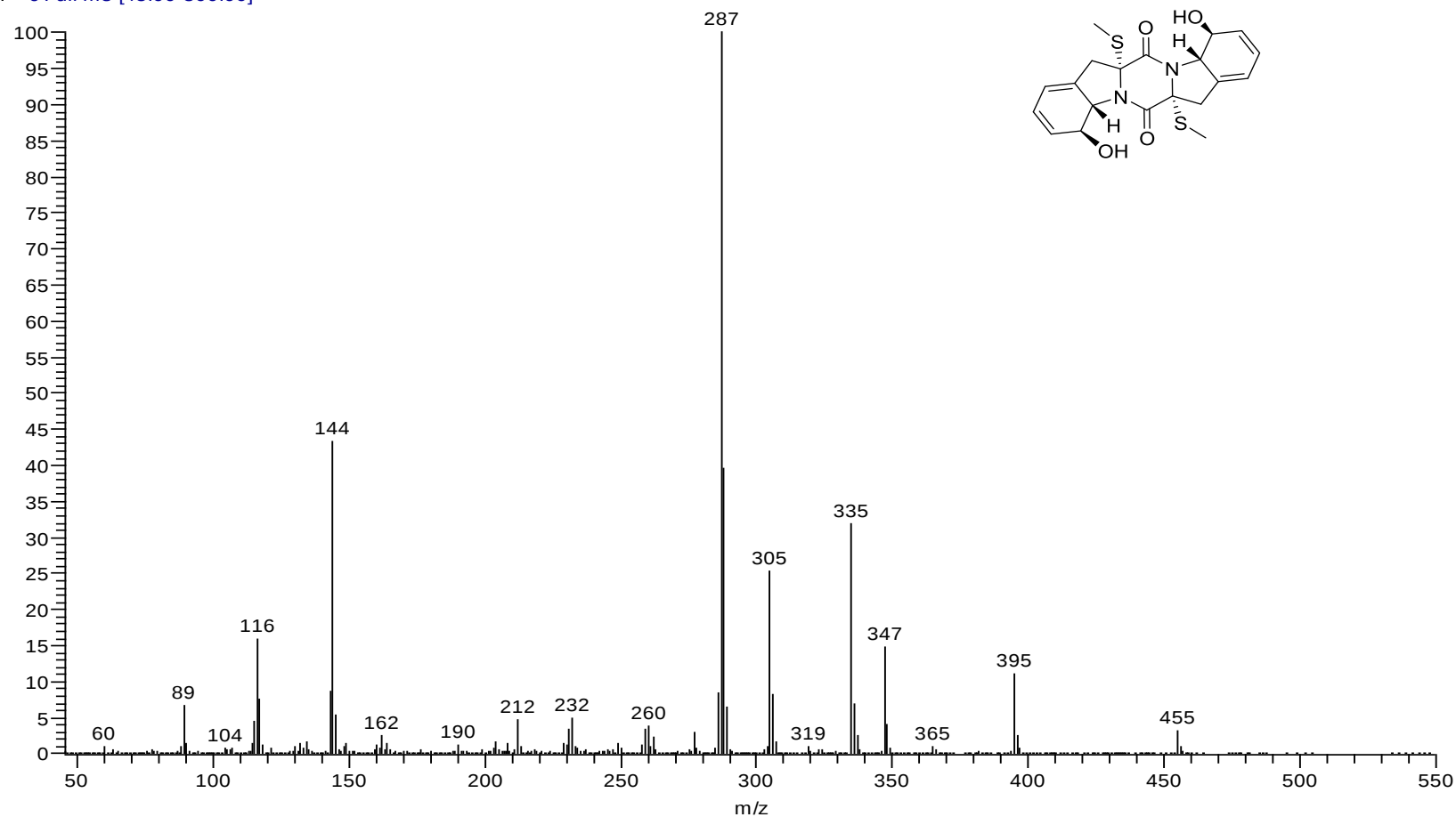


Figure S36. ^1H -NMR spectrum of boydine A (**6**) in CDCl_3 (400MHz)

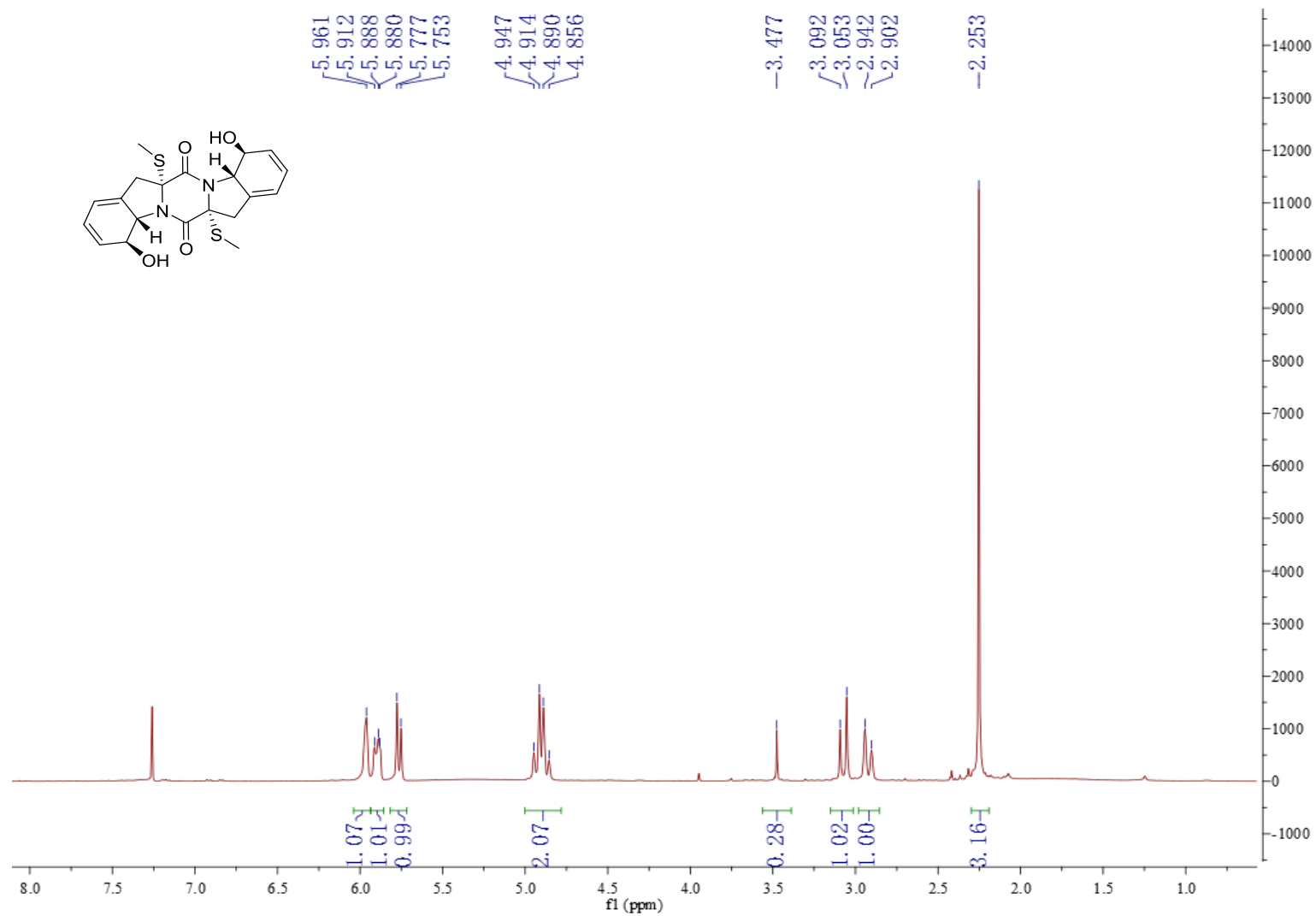


Figure S37. ^{13}C -NMR and DEPT spectra of boydine A (**6**) in CDCl_3 (100MHz)

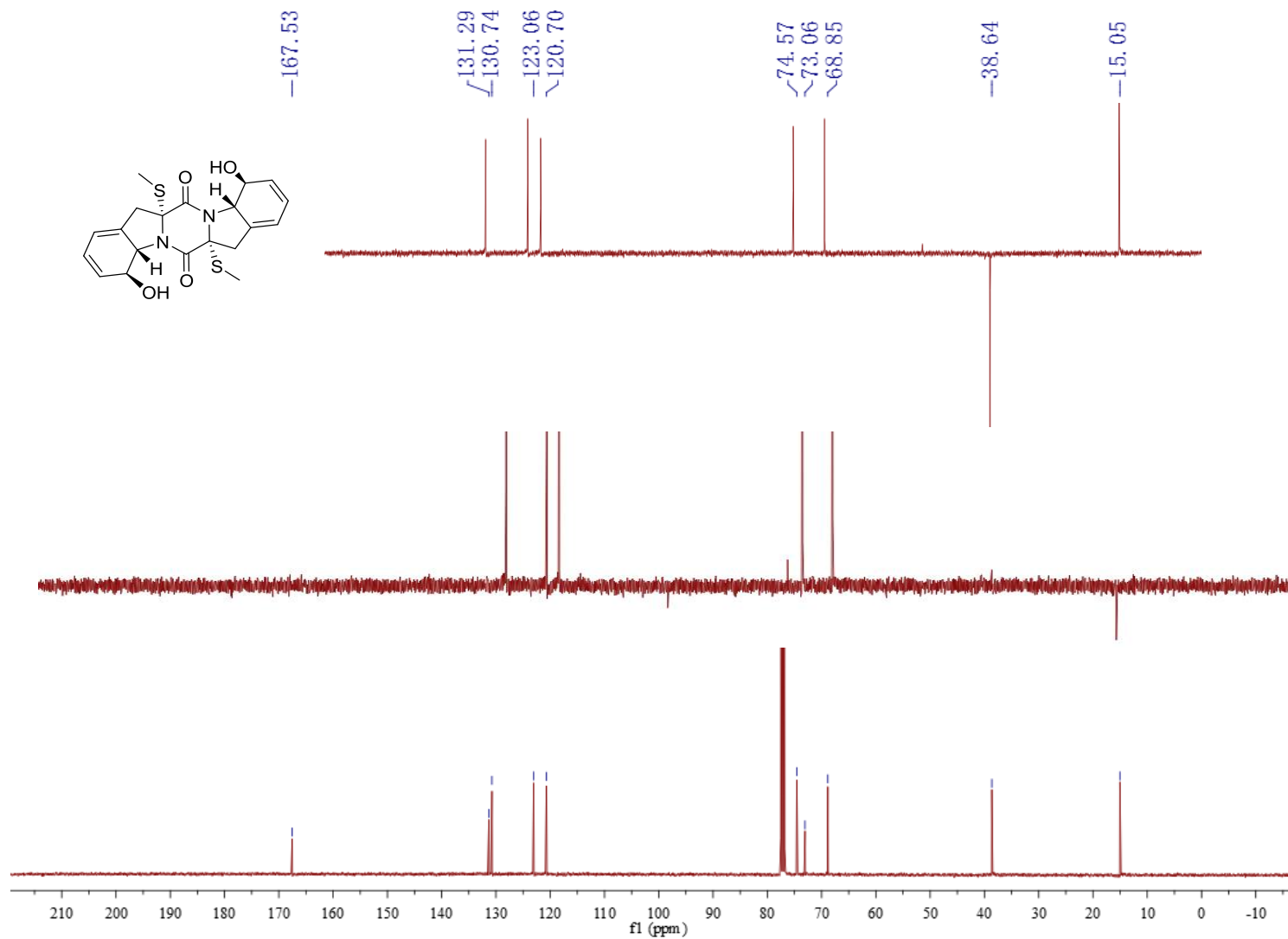


Figure S38. HMQC spectrum of boydine A (**6**) in CDCl₃

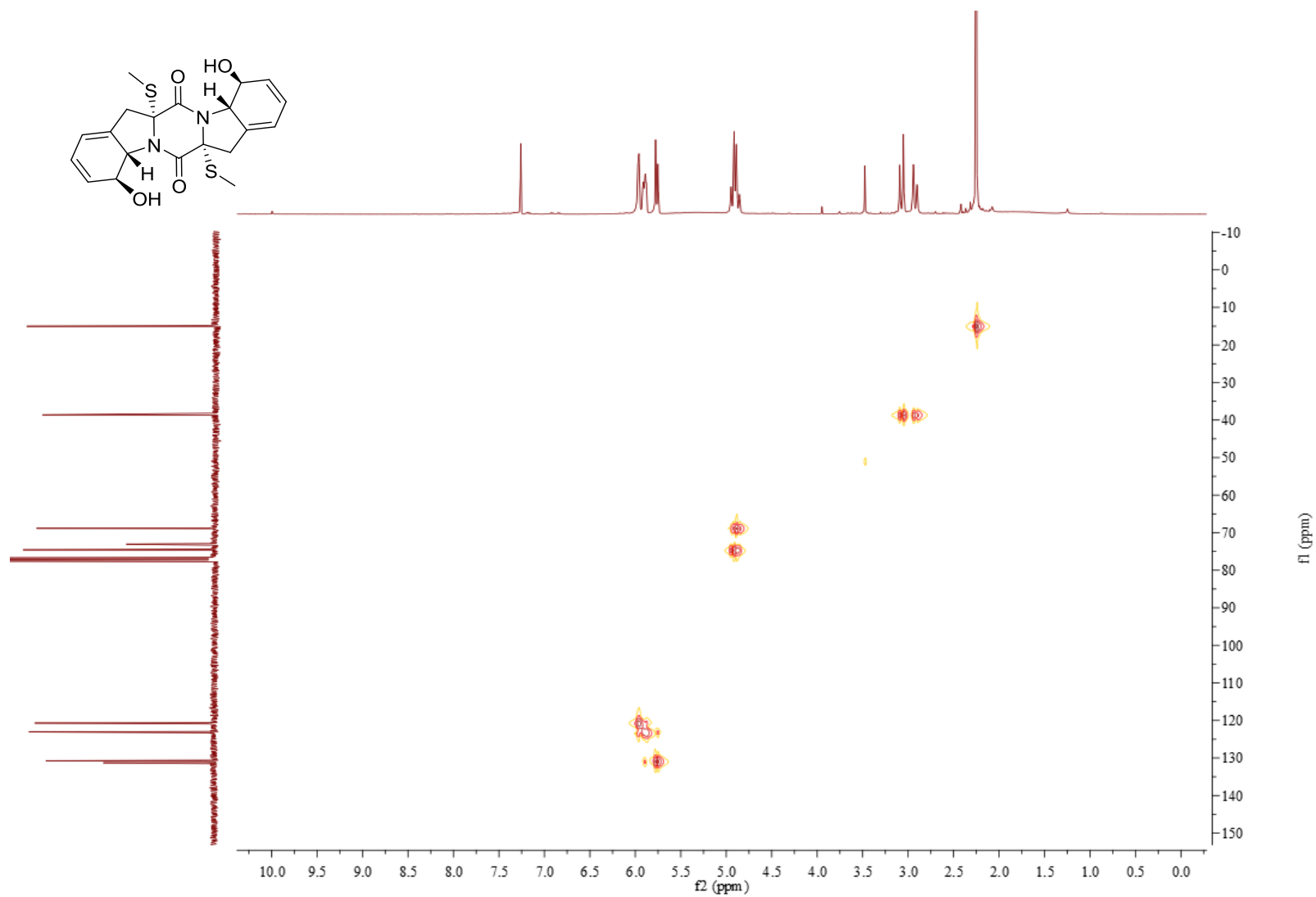


Figure S39. ^1H - ^1H COSY spectrum of boydine A (**6**) in CDCl_3

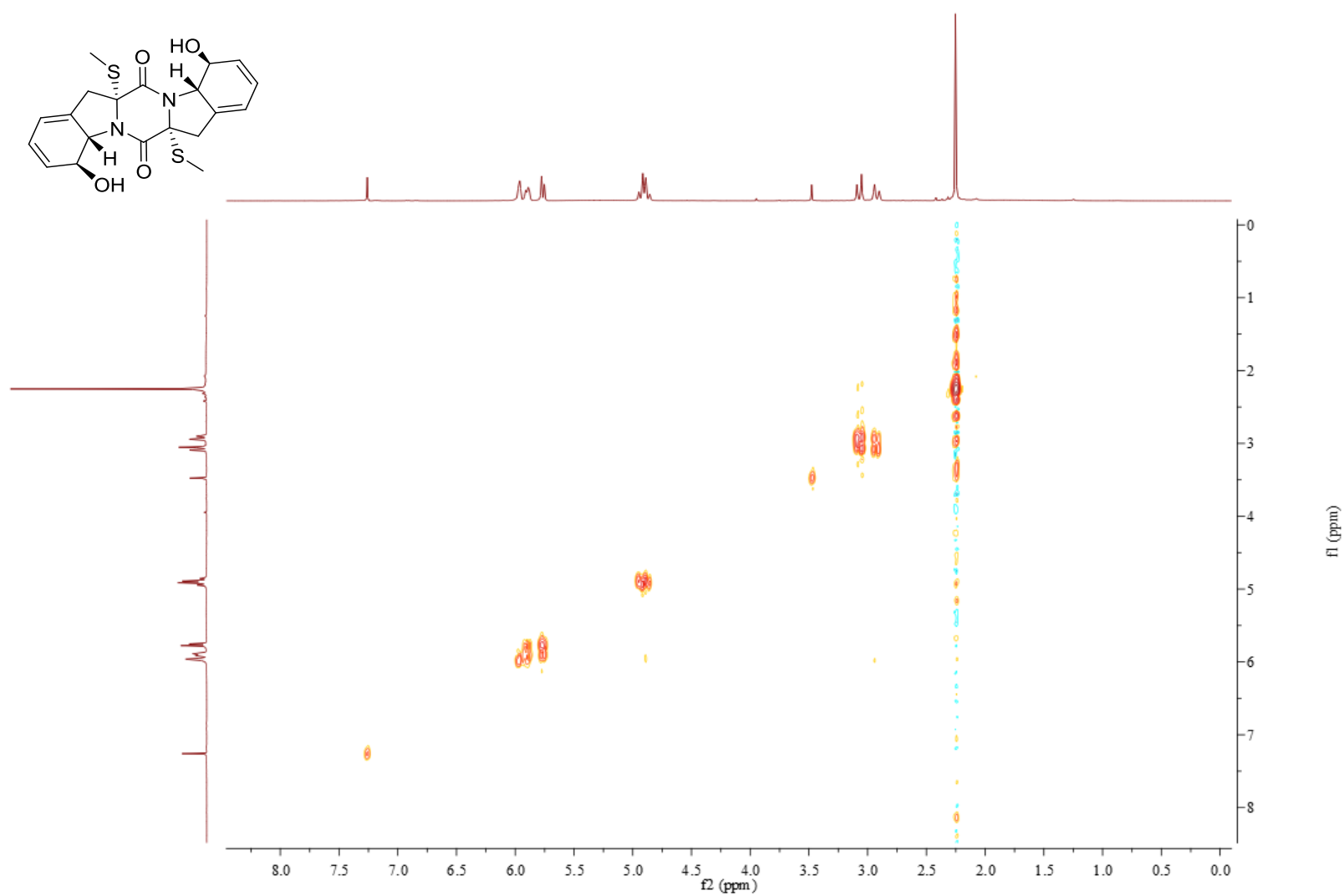


Figure S40. HMBC spectrum of boydine A (**6**) in CDCl₃

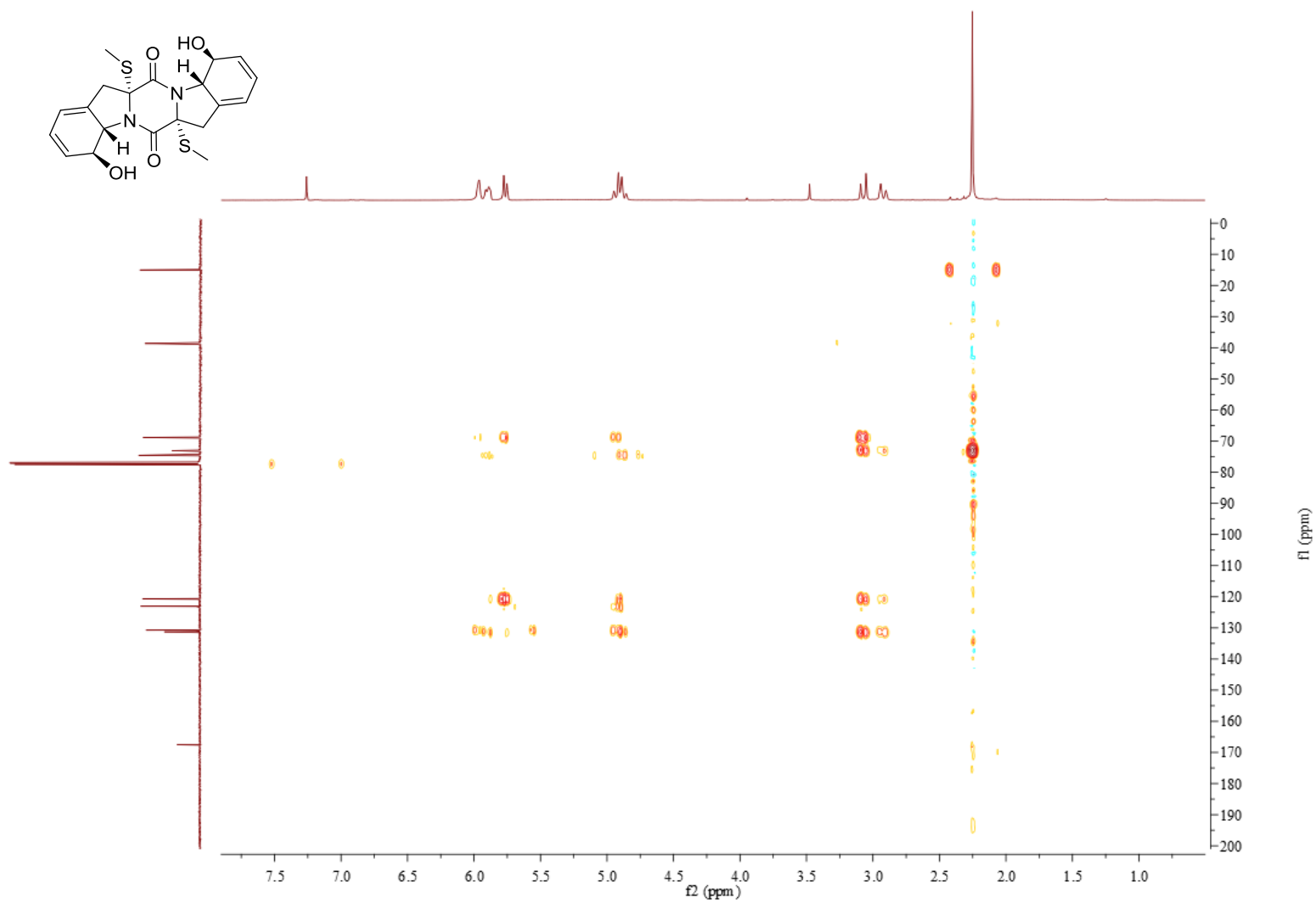


Figure S41. NOESY spectrum of boydine A (**6**) in CDCl₃

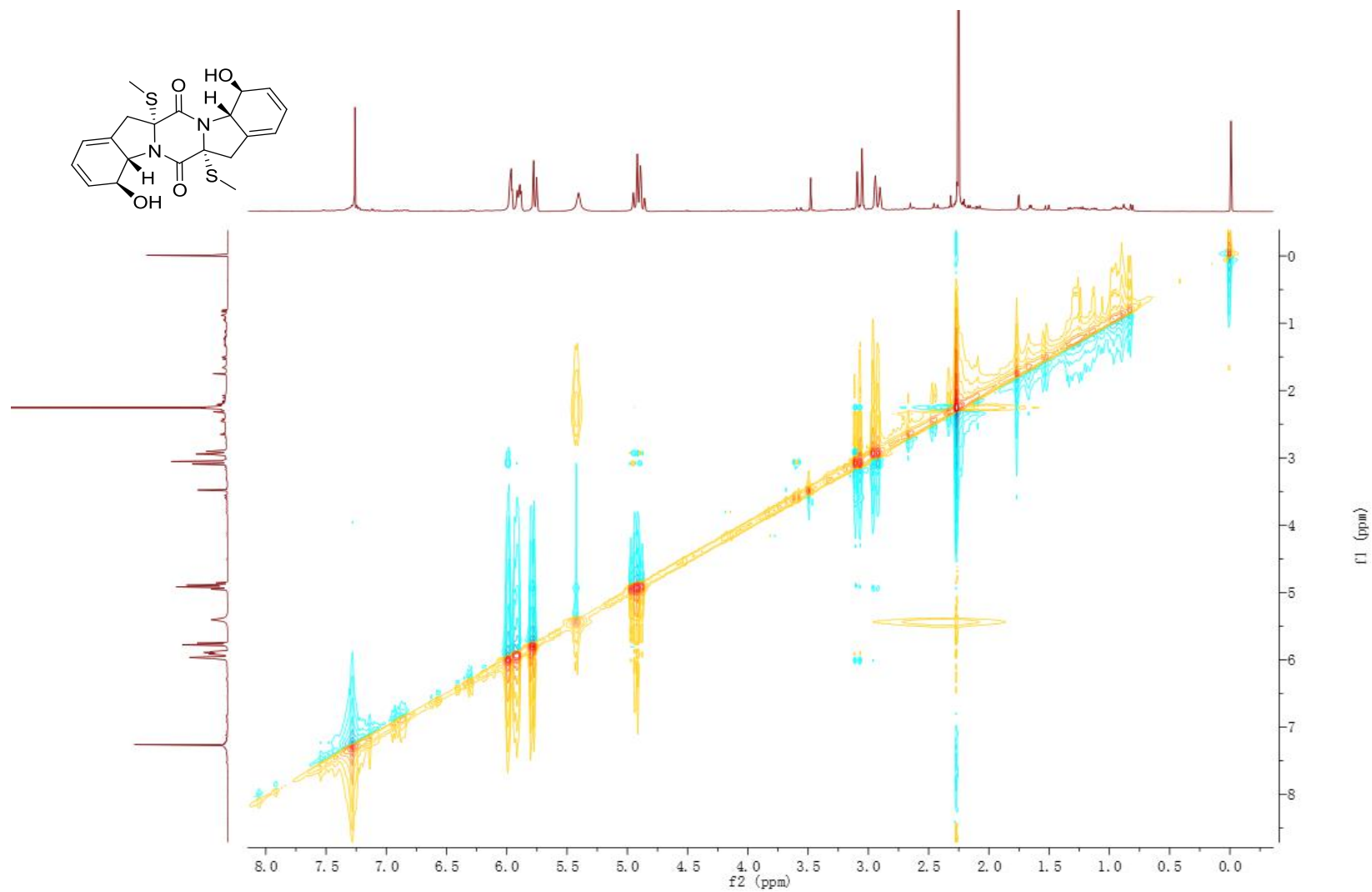


Figure S42. LR-ESI-MS spectrum of boydine B (7)

F19_7_P5 #3-6 RT: 0.15-0.23 AV: 2 SB: 2 0.02-0.11, 0.49 NL: 1.19E7
T: + c ESI Full m s [100.00-2000.00]

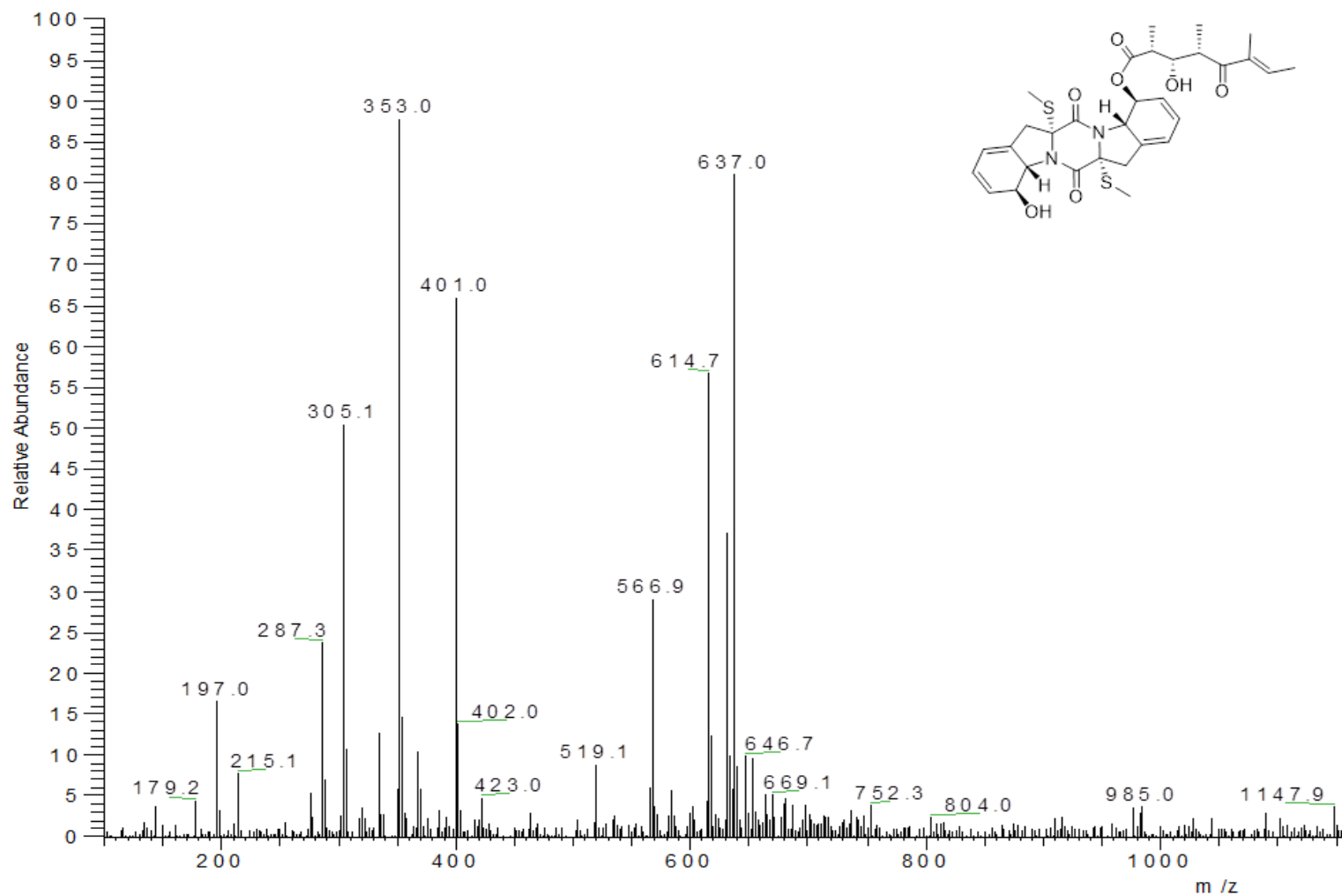


Figure S43. ^1H -NMR spectrum of boydine B (**7**) in CDCl_3 (400MHz)

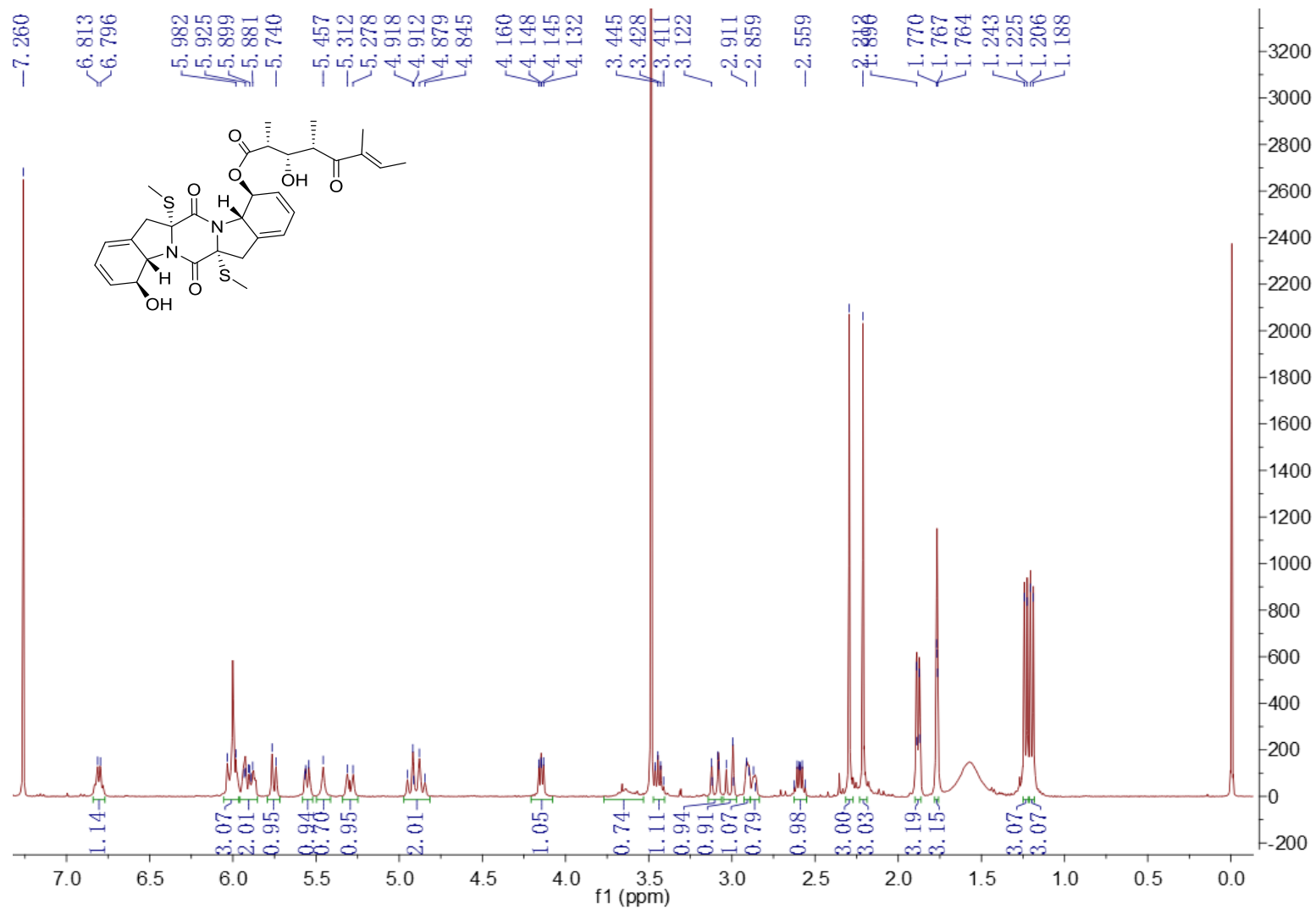


Figure S44. ^{13}C -NMR spectrum of boydine B (7) in CDCl_3 (100MHz)

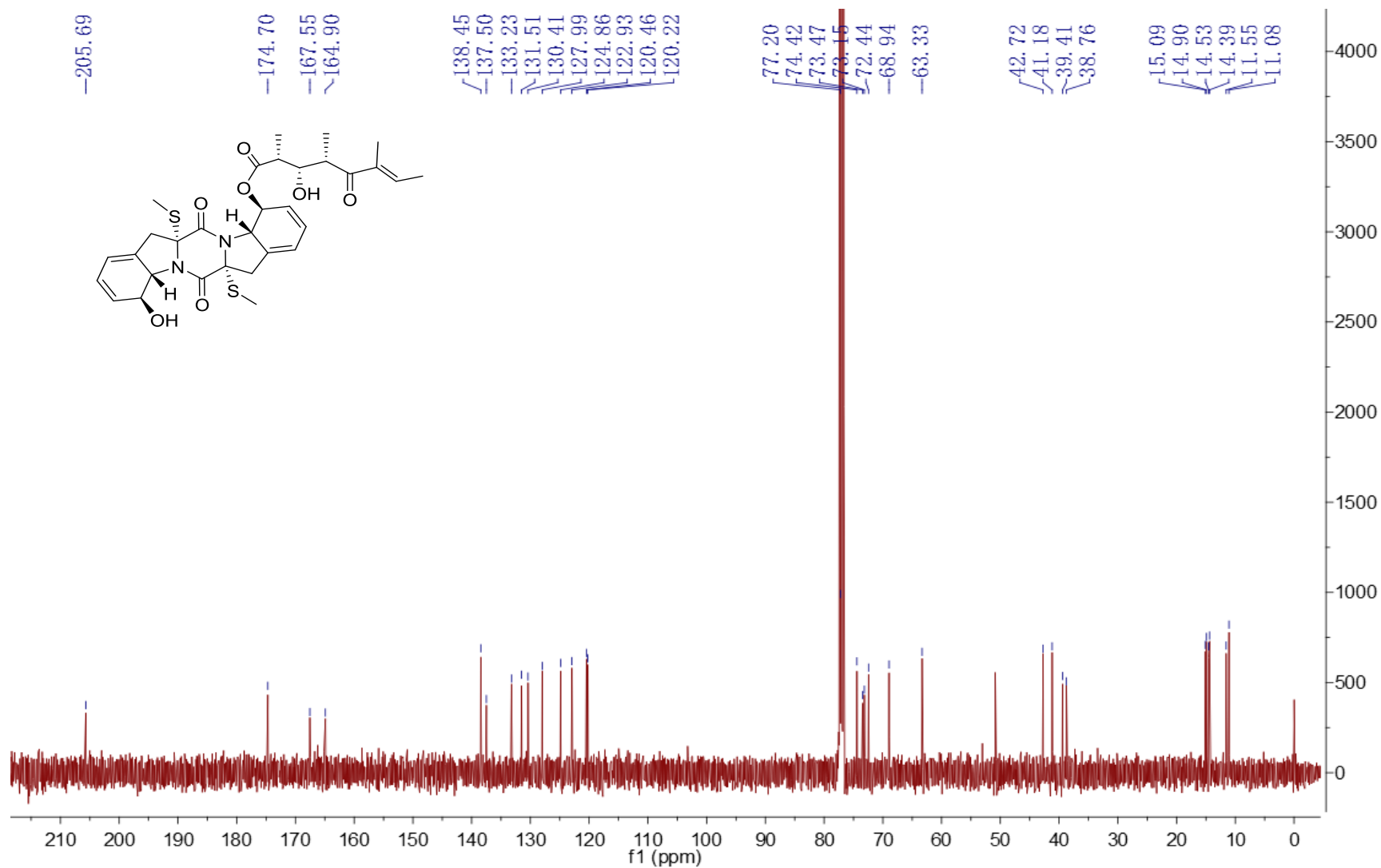


Figure S45. ^1H -NMR spectrum of phomazine B (**8**) in CDCl_3 (400MHz)

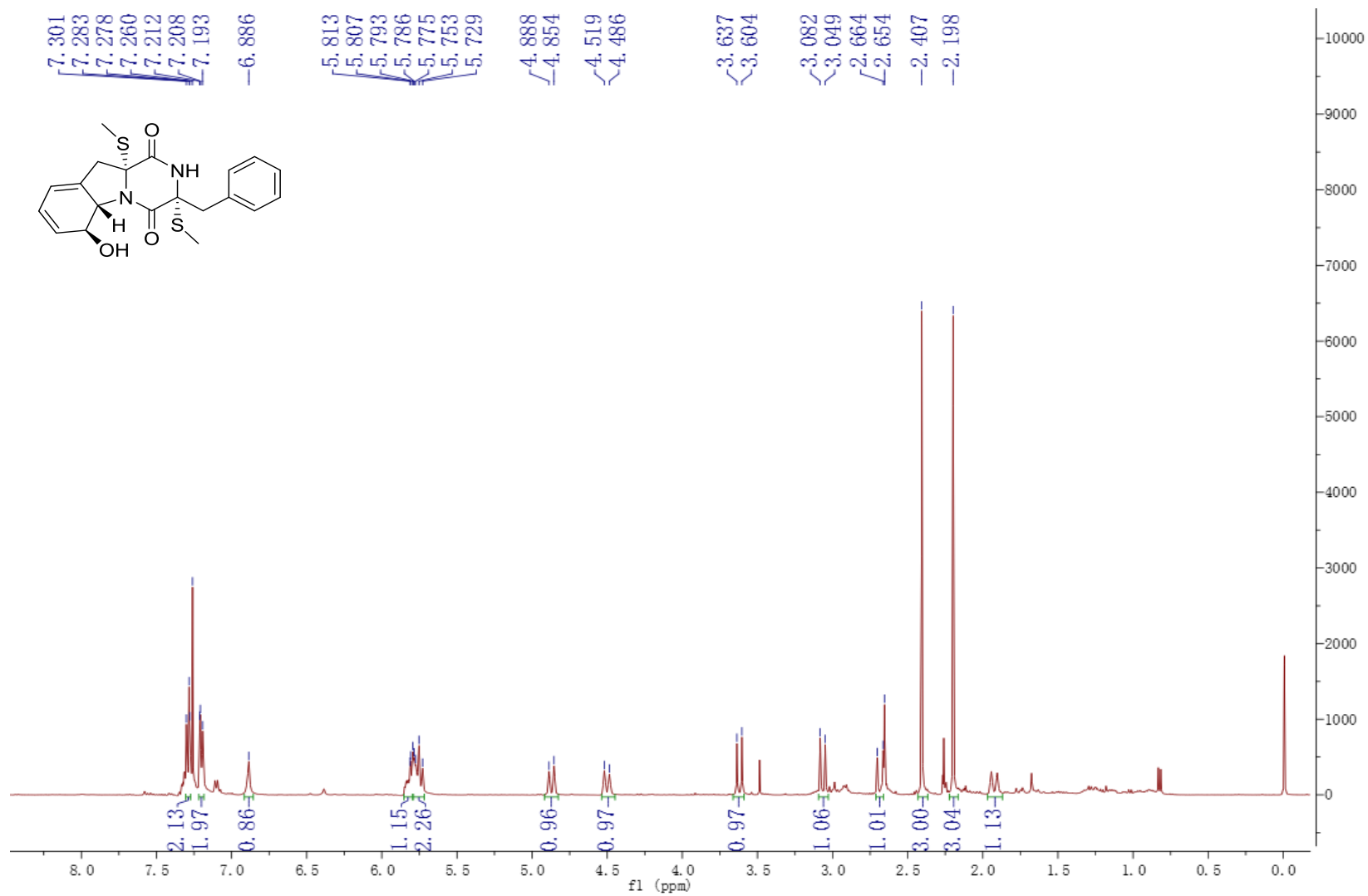


Figure S46. ^{13}C -NMR and DEPT spectra of phomazine B (**8**) in CDCl_3 (100MHz)

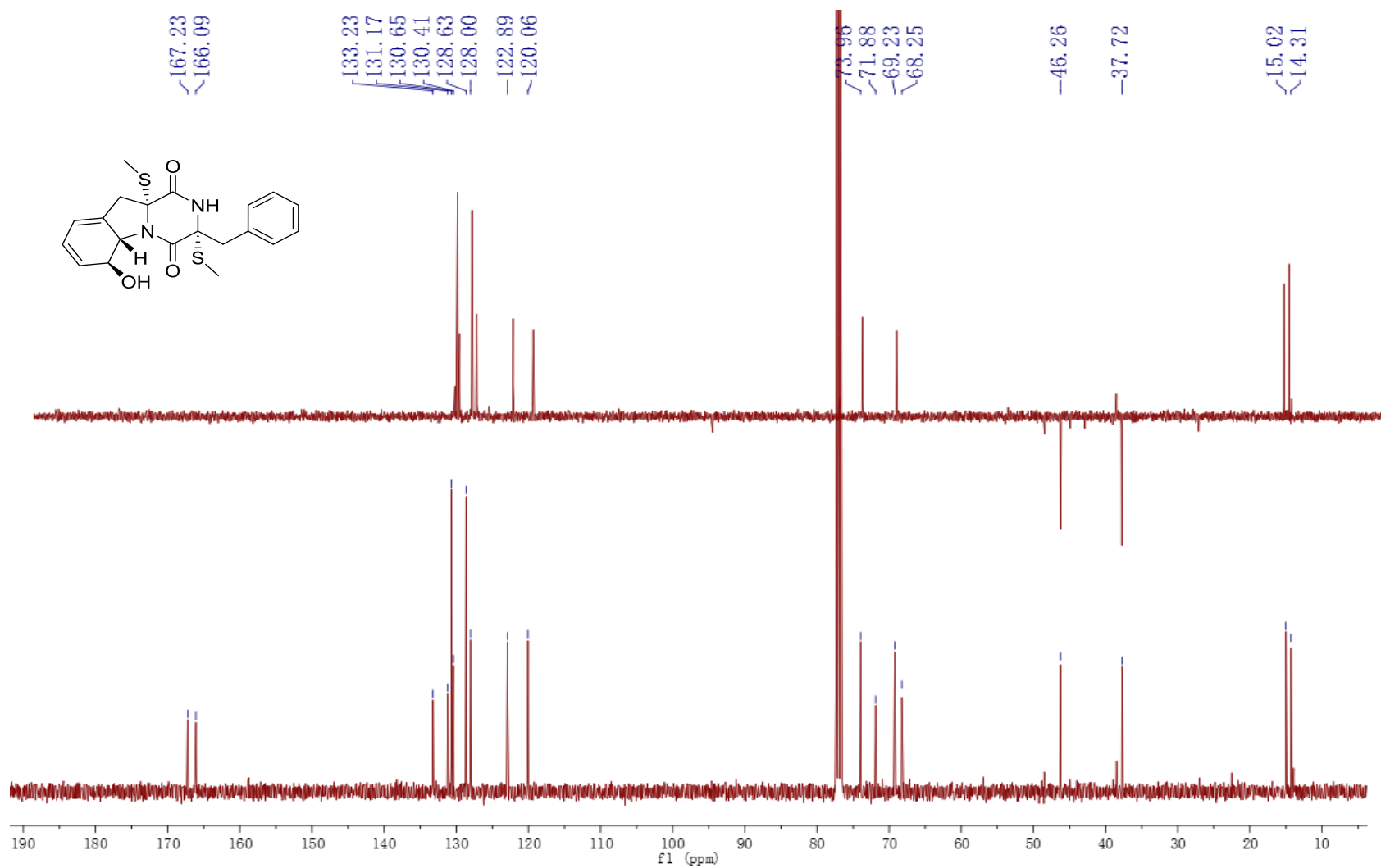


Figure S47. HMQC spectrum of phomazine B (**8**) in CDCl₃

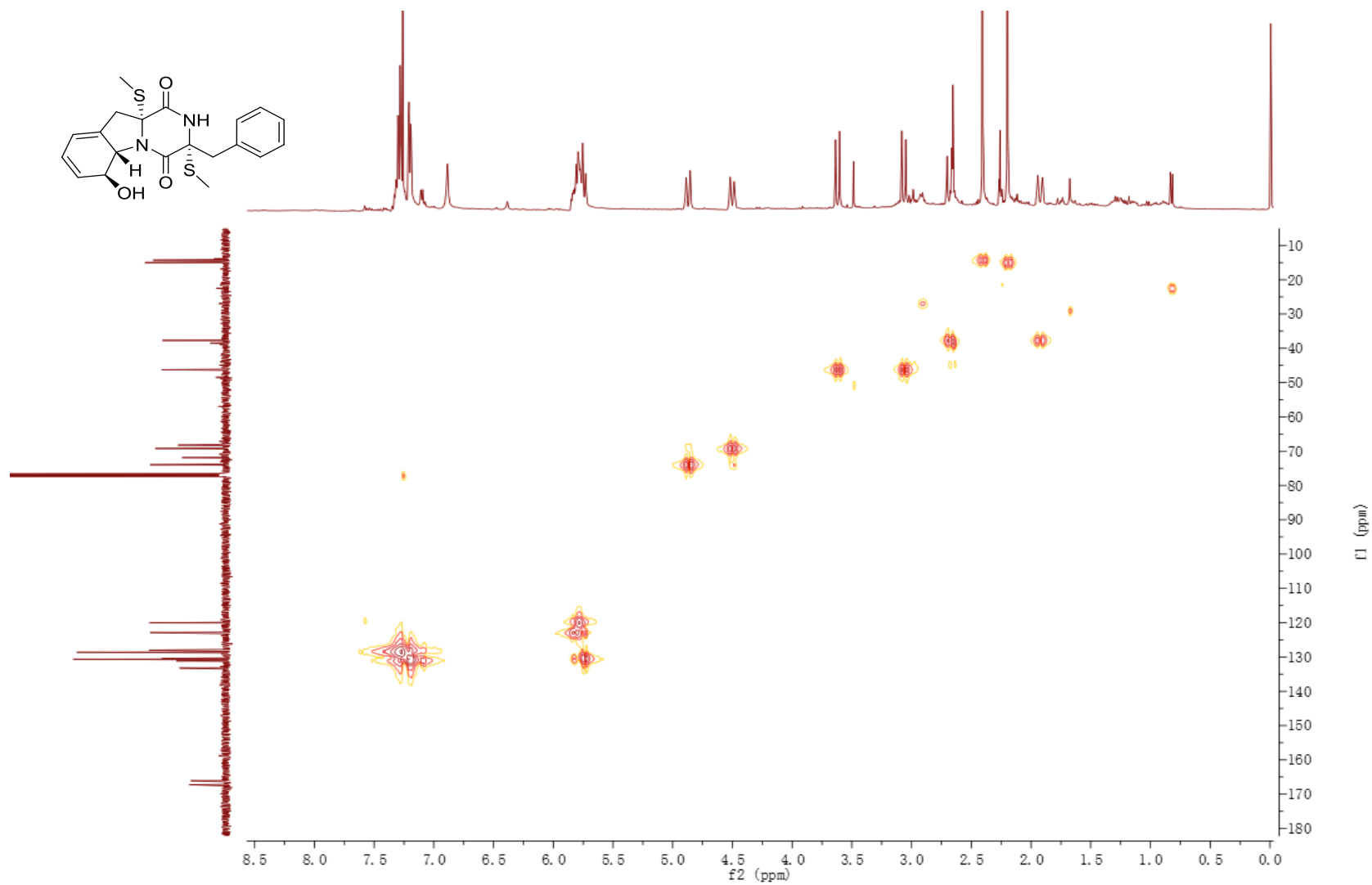


Figure S48. HMBC spectrum of phomazine B (**8**) in CDCl₃

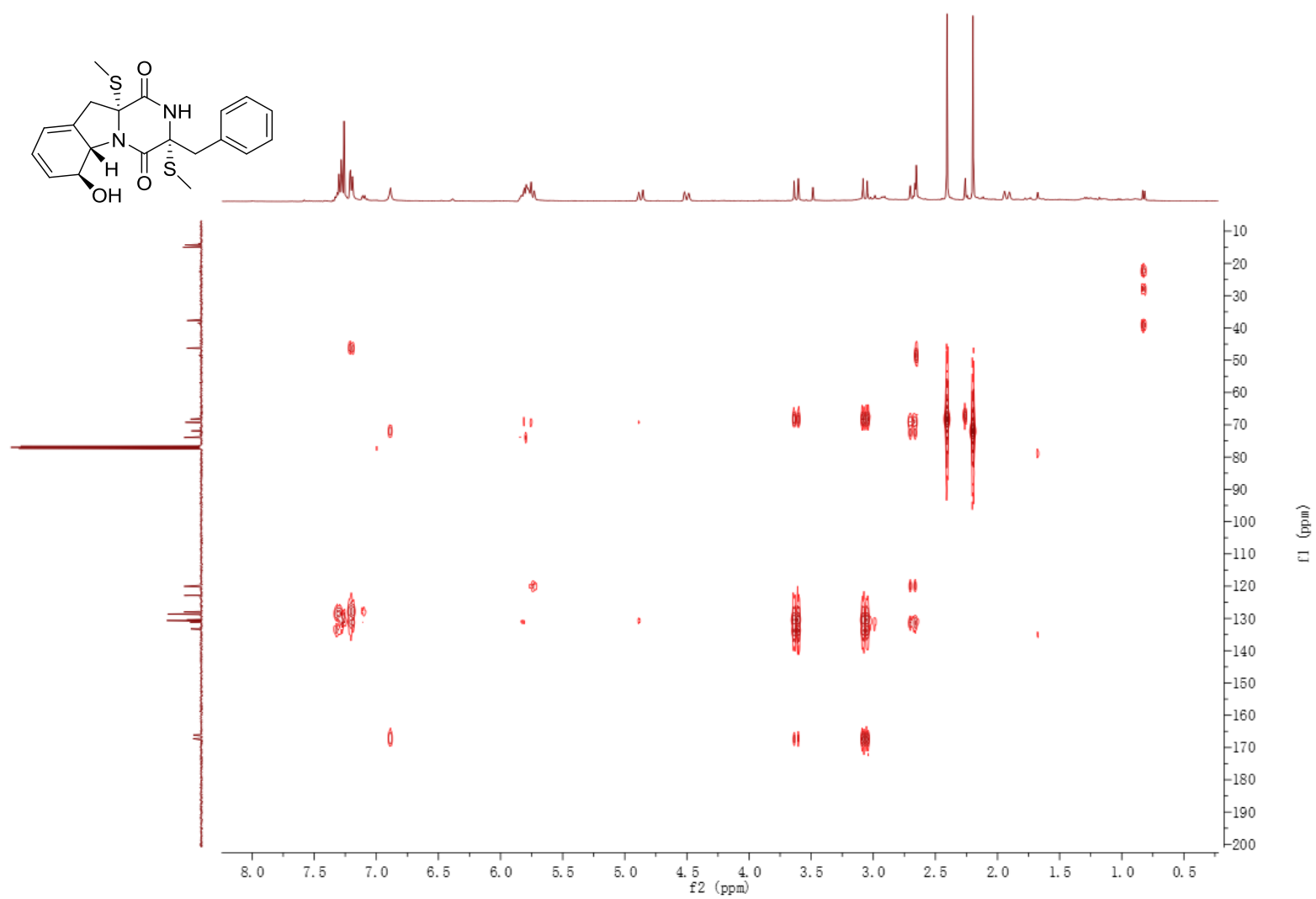


Figure S49. NOESY spectrum of phomazine B (**8**) in CDCl₃

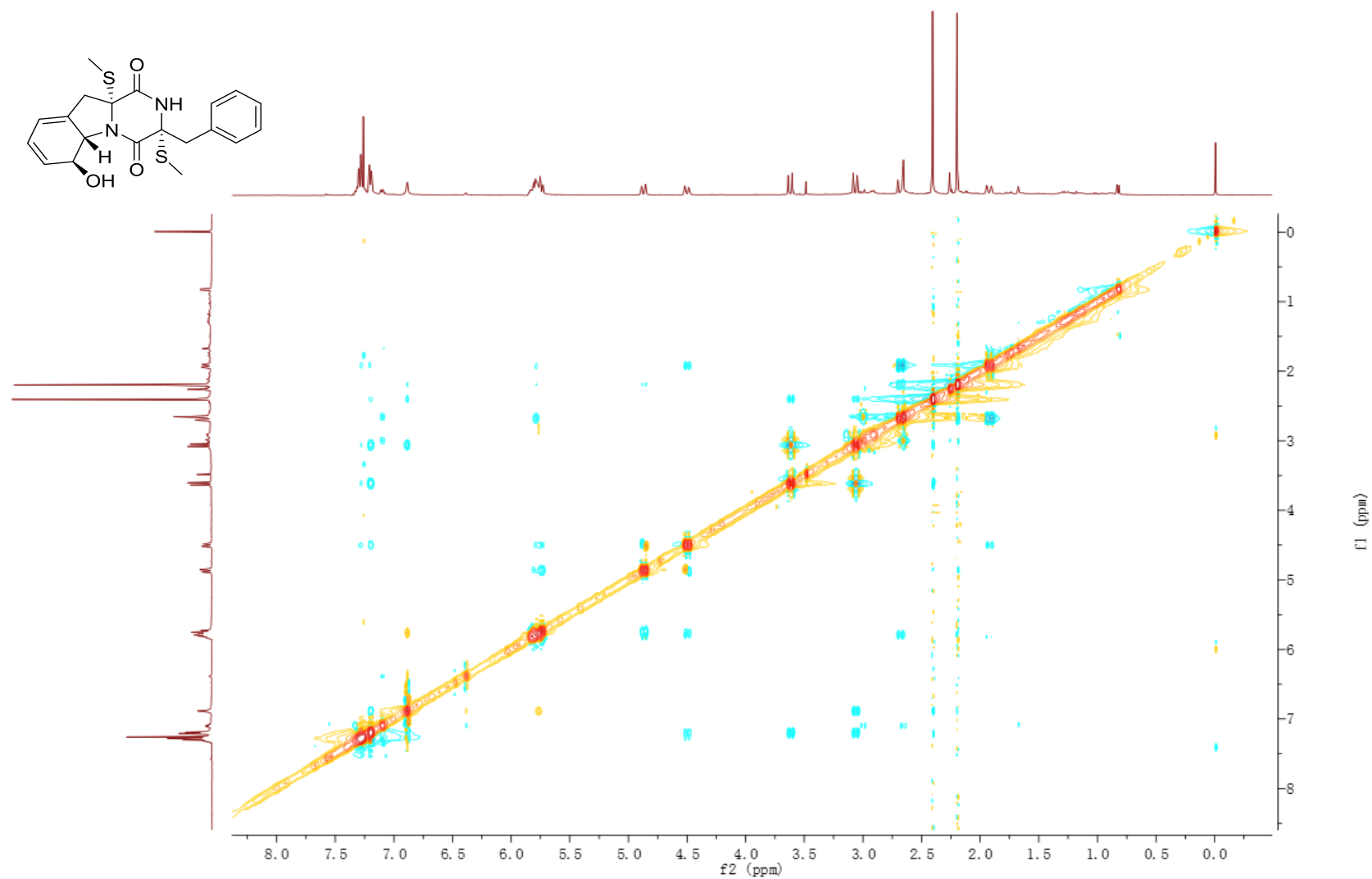


Figure S50. ^1H -NMR spectrum of bisdethiobis (methylthio) gliotoxin (**9**) in CDCl_3 (400MHz)

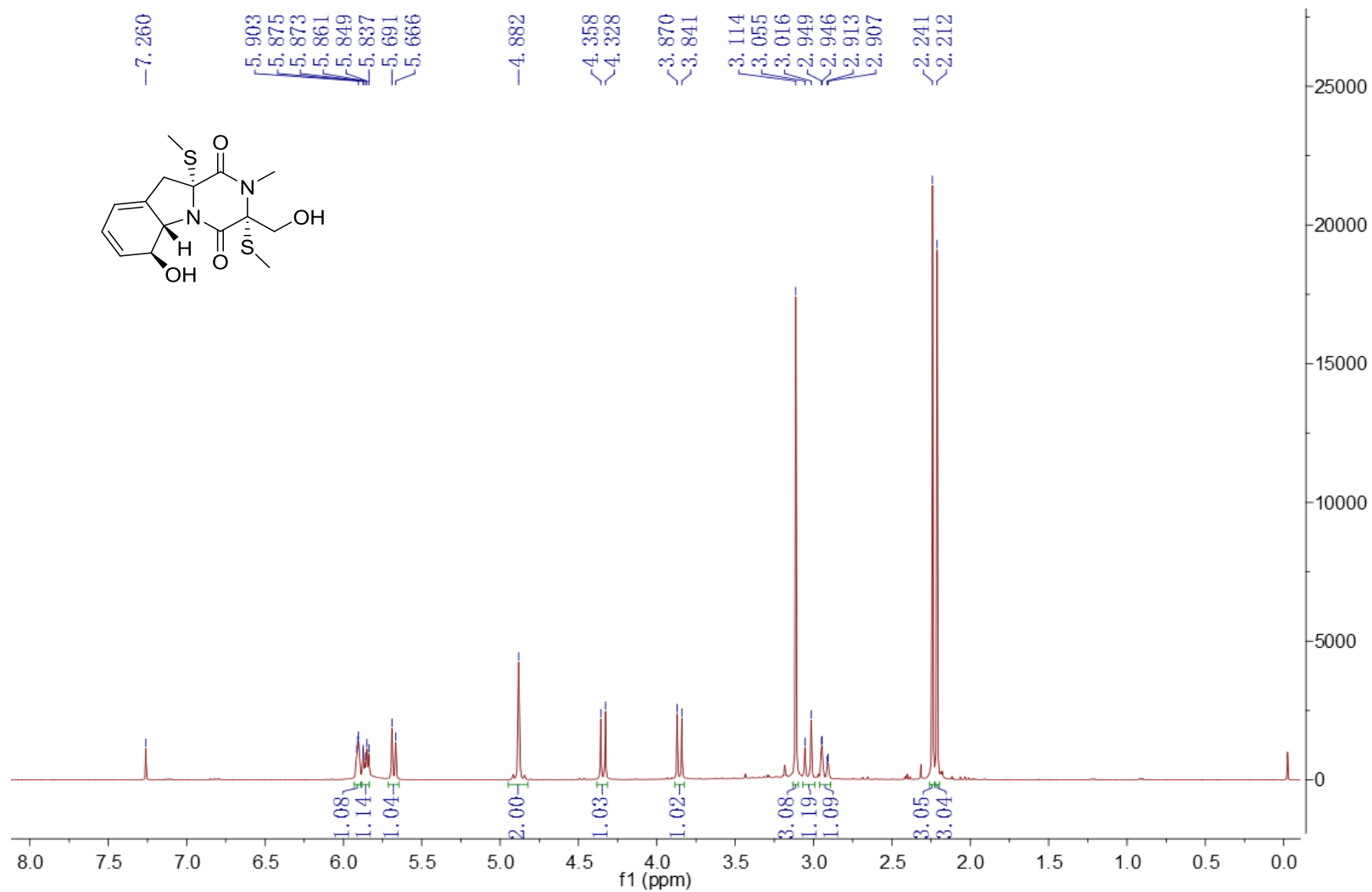


Figure S51. ^{13}C -NMR spectrum of bisdethiobis (methylthio) gliotoxin (**9**) in CDCl_3 (100MHz)

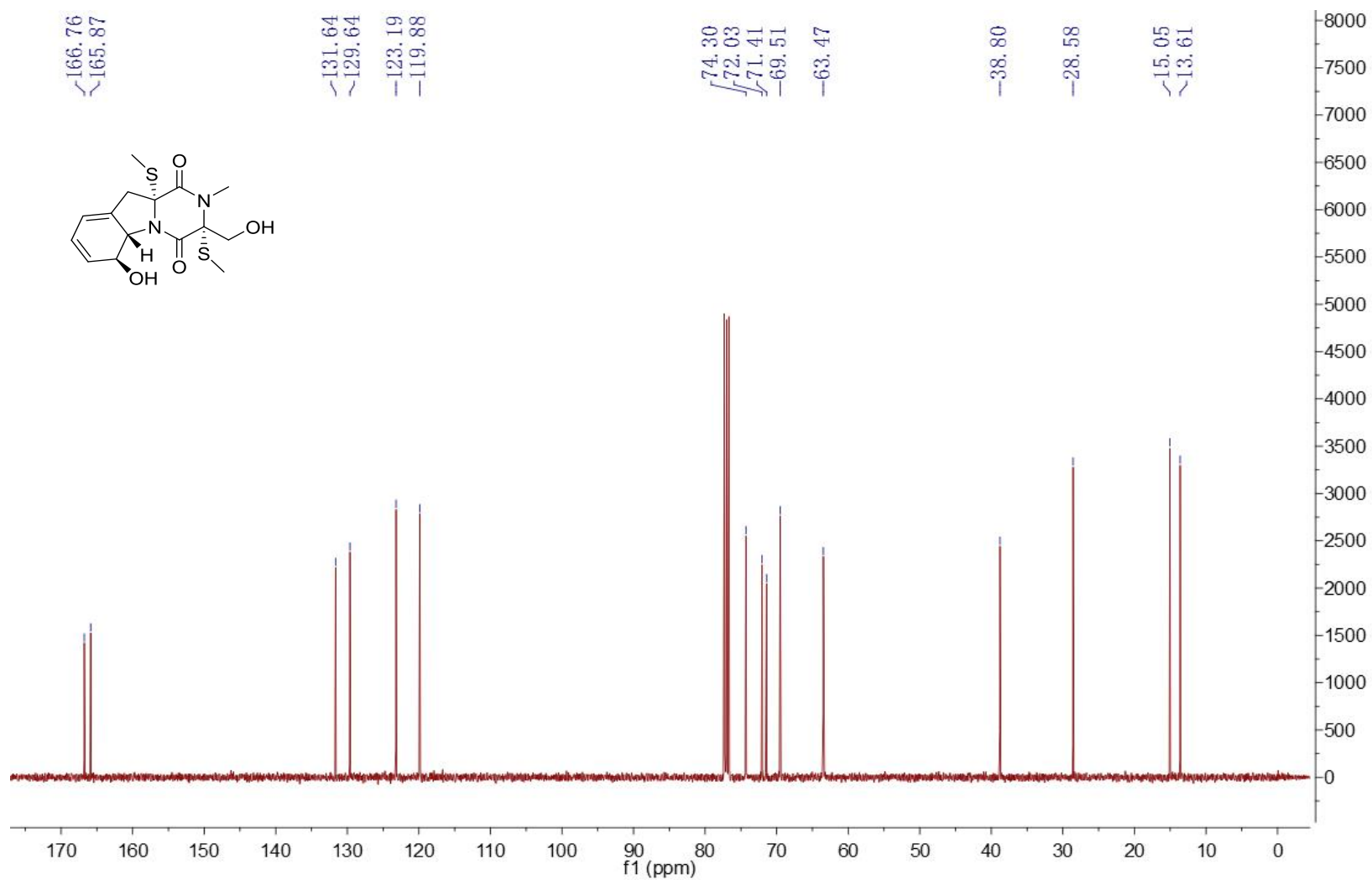


Figure S52. ^1H -NMR spectrum of cyclo-(2, 2'-dimethylthio-Phe-Phe (**10**) in $\text{DMSO}-d_6$ (400MHz)

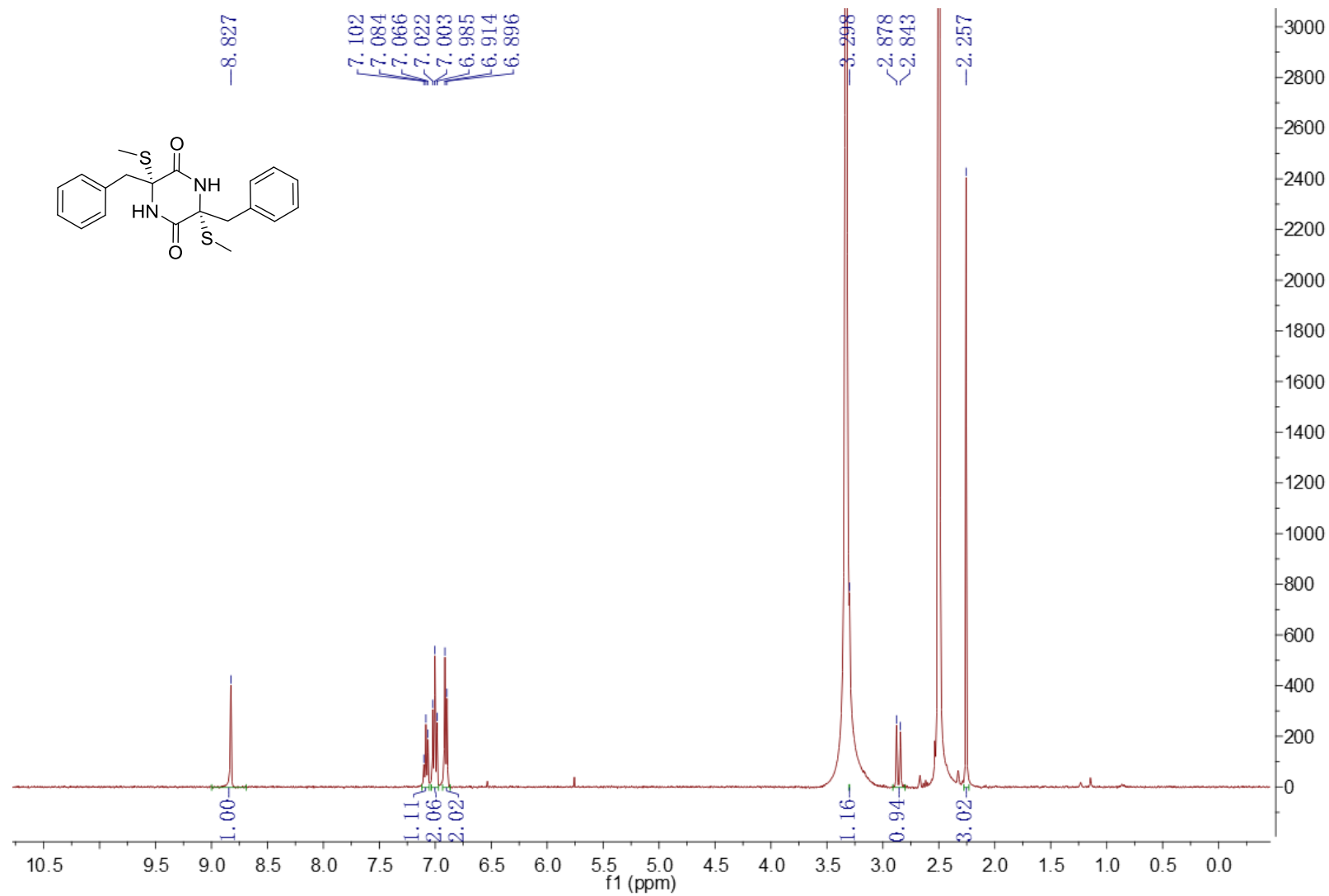


Figure S53. ^1H -NMR spectrum of cyclo-(Phe-Phe) (**11**) in $\text{DMSO-}d_6$ (400MHz)

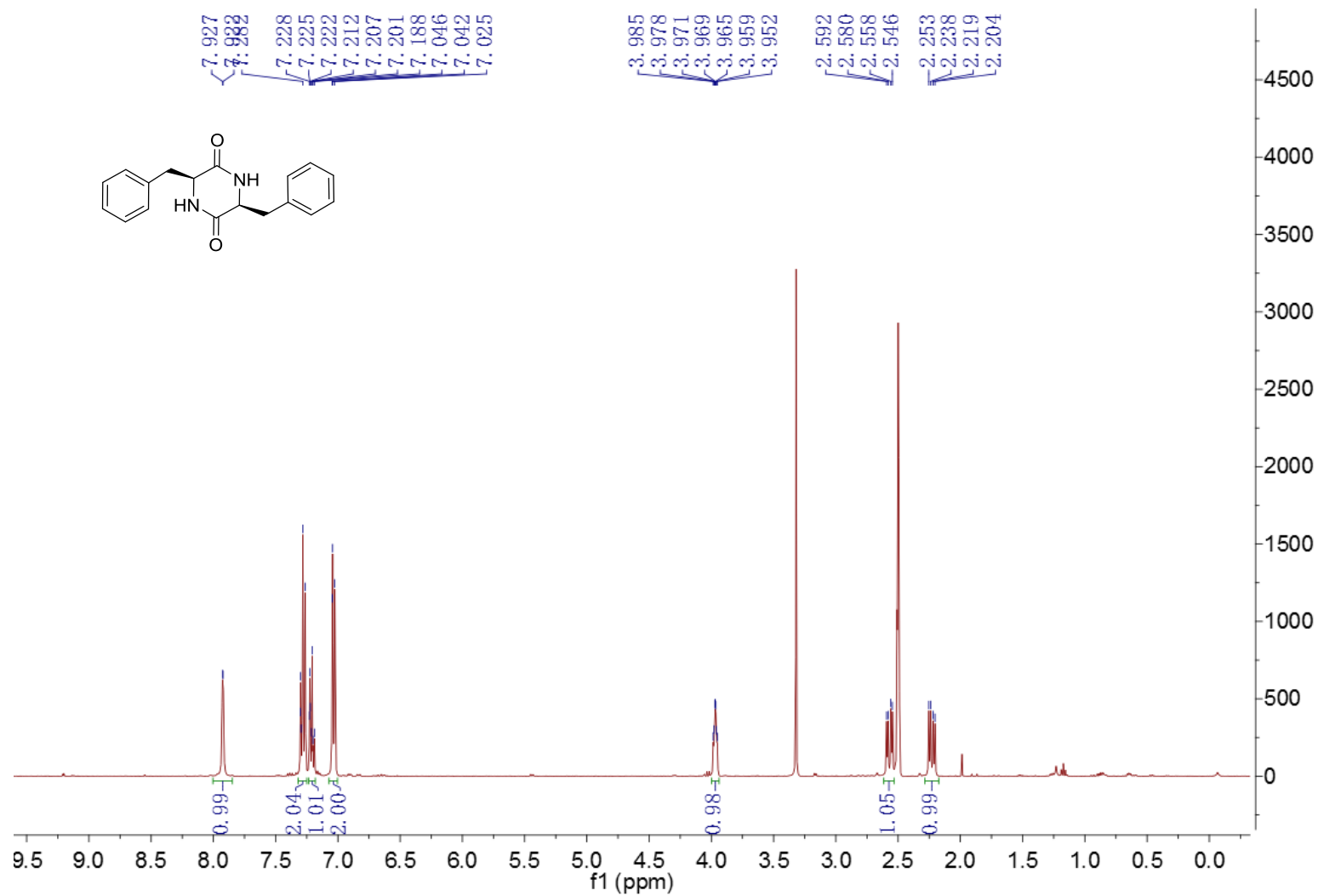


Figure S54. ^{13}C -NMR and DEPT spectra of cyclo-(Phe-Phe) (**11**) in $\text{DMSO-}d_6$ (100MHz)

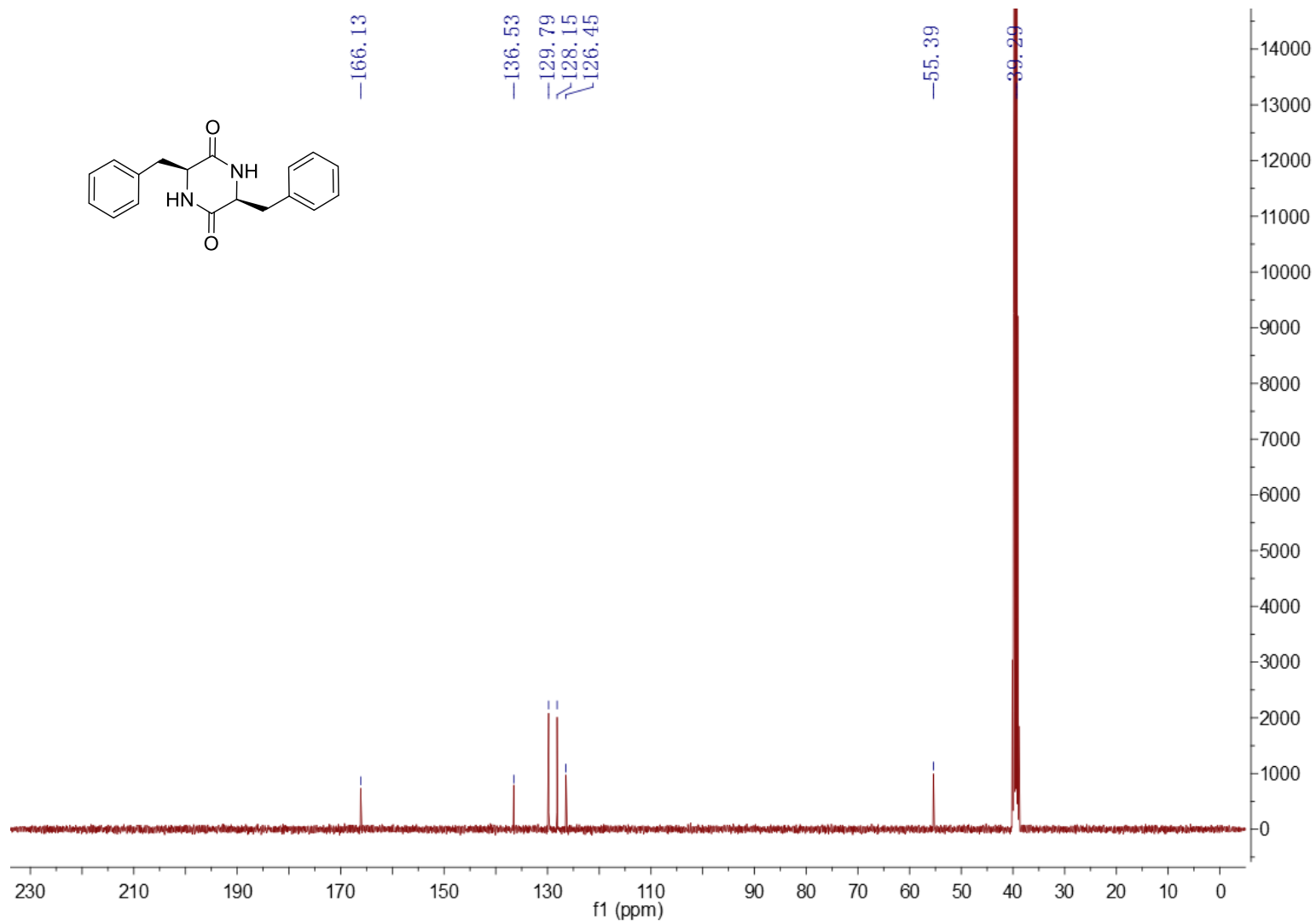


Figure S55. LR-ESI-MS spectrum of ditryptophenaline (**12**)

19m-2s #7 RT: 0.21 AV: 1 SB: 3 0.00-0.07, 0.92-0.98 NL: 6.89E5
T: + c ESI Full ms [50.00-1000.00]

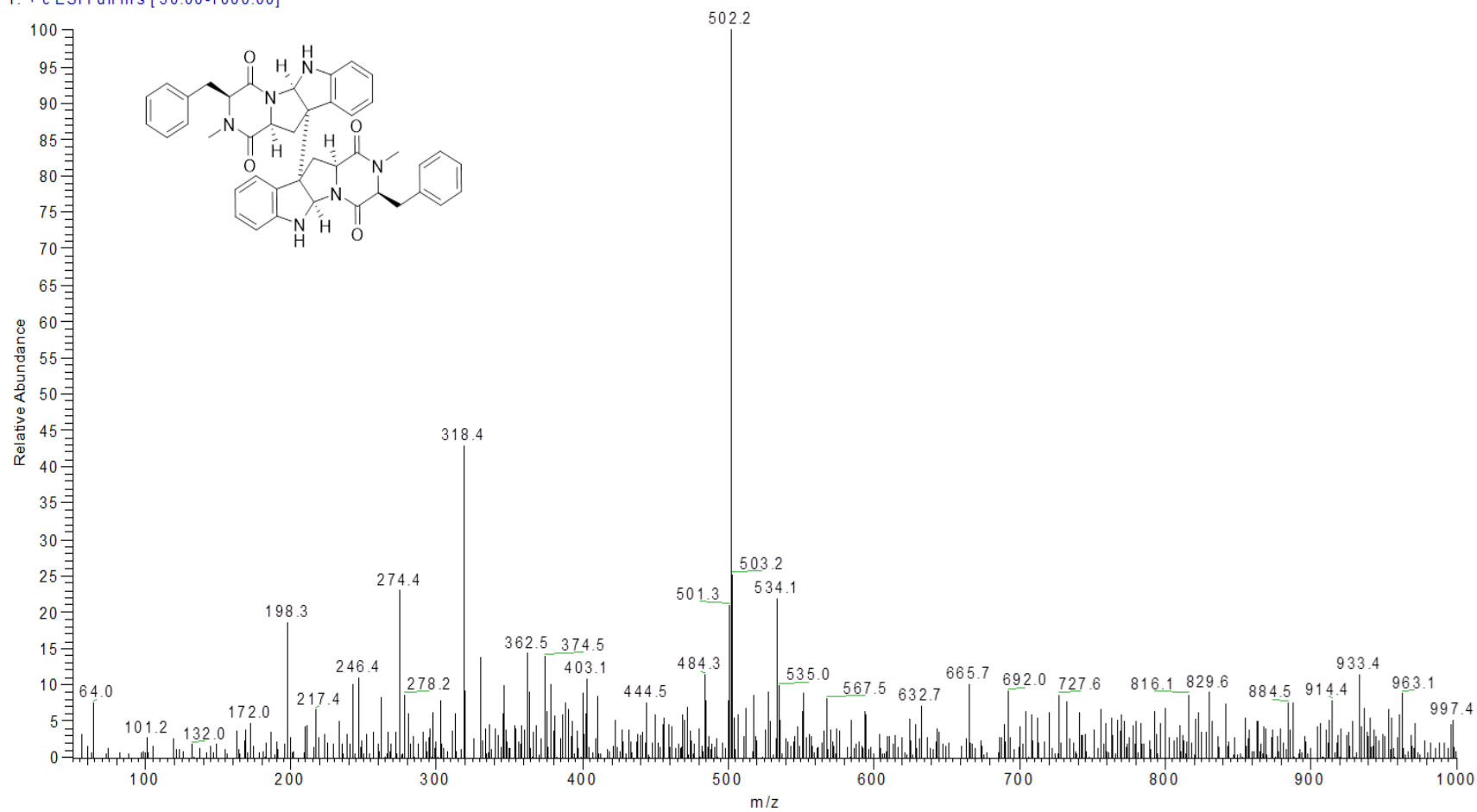


Figure S56. ^1H -NMR spectrum of ditryptophenaline (**12**) in CDCl_3 (400MHz)

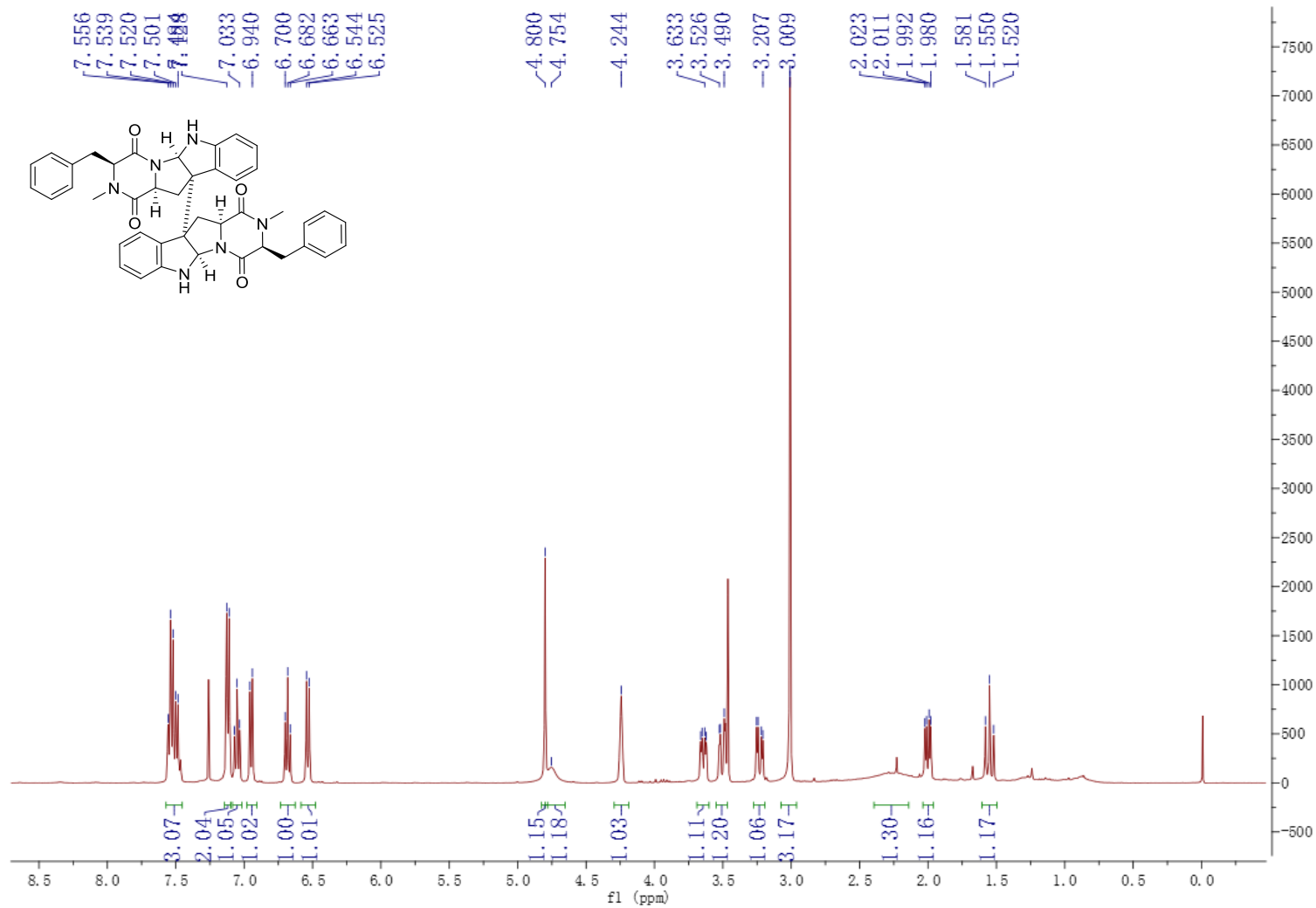


Figure S57. ^{13}C -NMR and DEPT spectra of ditryptophenaline (**12**) in CDCl_3 (100MHz)

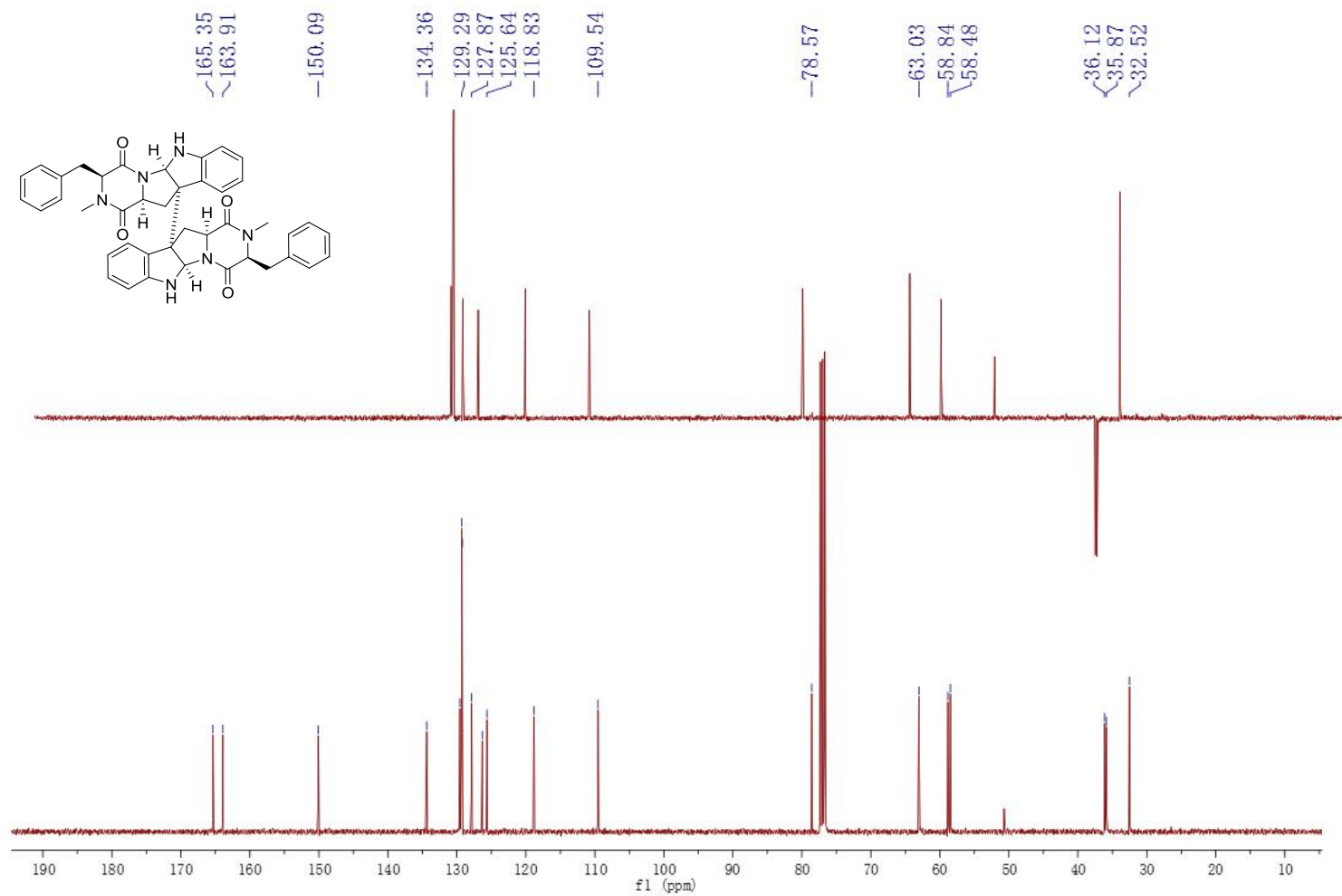


Figure S58. NOESY spectrum of ditryptophenaline (**12**) in CDCl₃

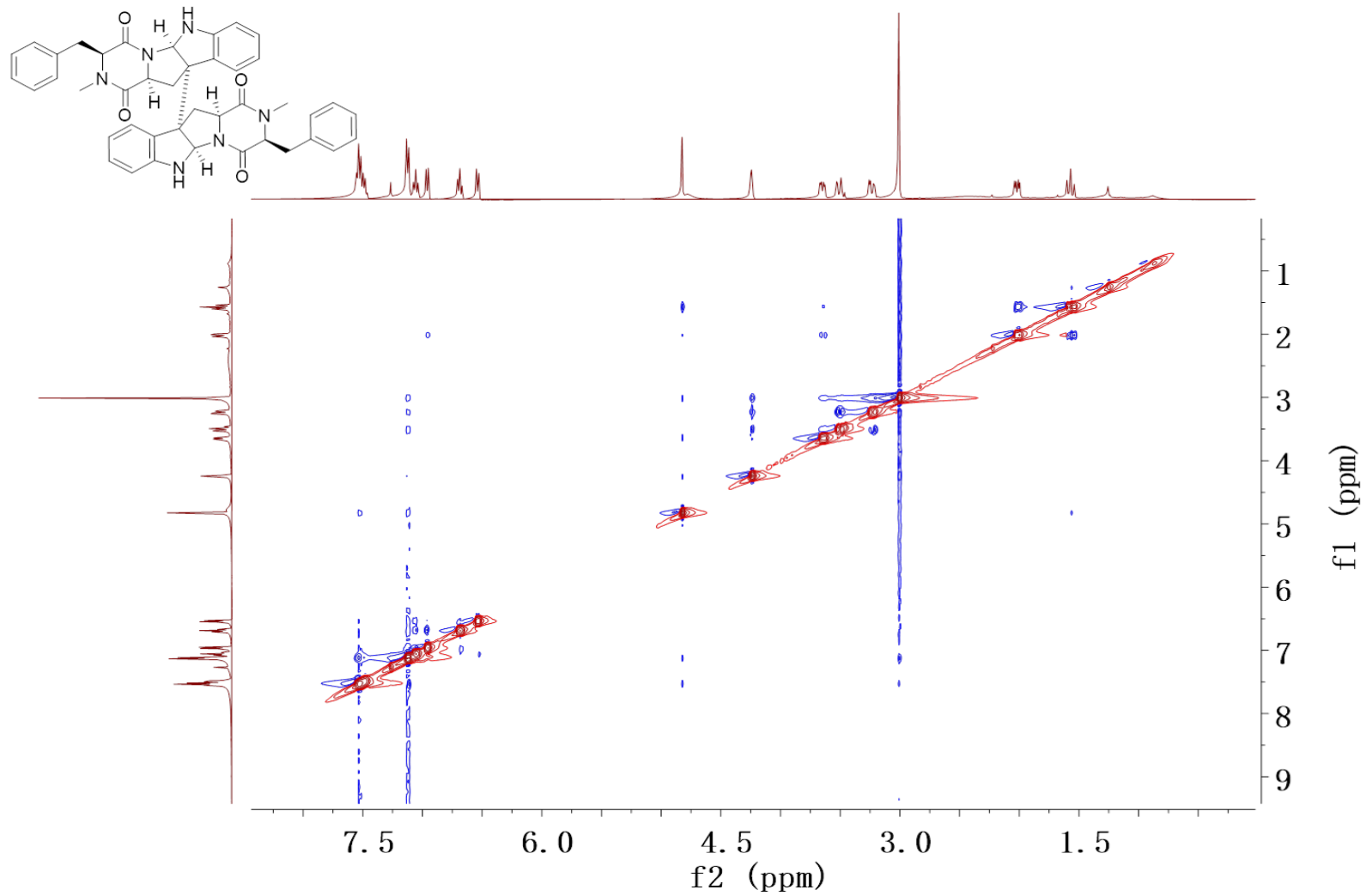


Figure S59. HR-ESI-MS spectrum of pseuboydone E (**13**)

D:\Data\2015\06\Lan wenjian\1506A0101-3
LTQ Orbitrap Elite

6/11/2015 4:10:27 PM

19m-8-3-35

1506A0101-3 #36-54 RT: 0.21-0.29 AV: 19 NL: 5.94E5
T: FTMS + c ESI Full ms [100.00-1000.00]

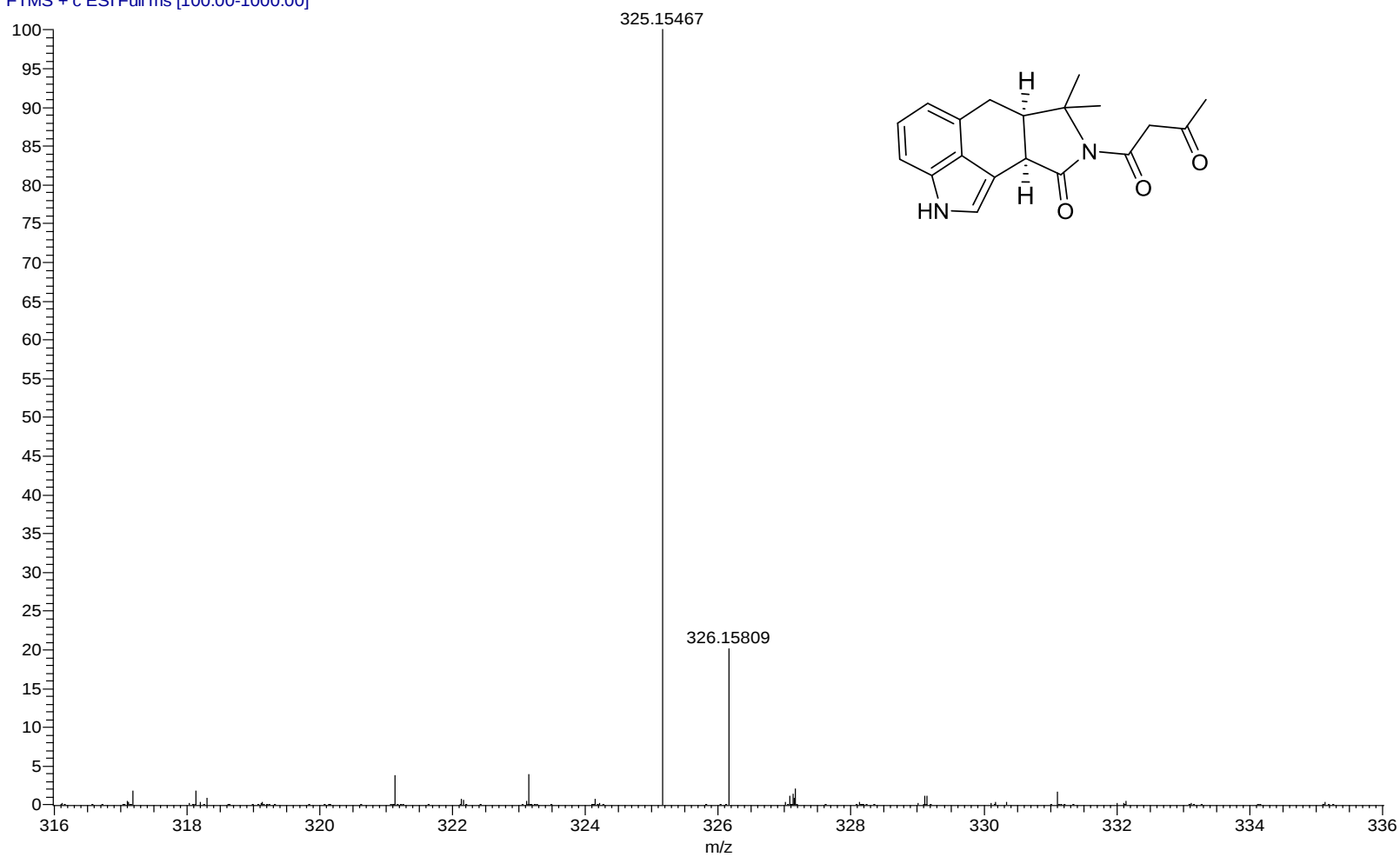


Figure S60. ^1H -NMR spectrum of pseuboydone E (**13**) in CDCl_3 (400MHz)

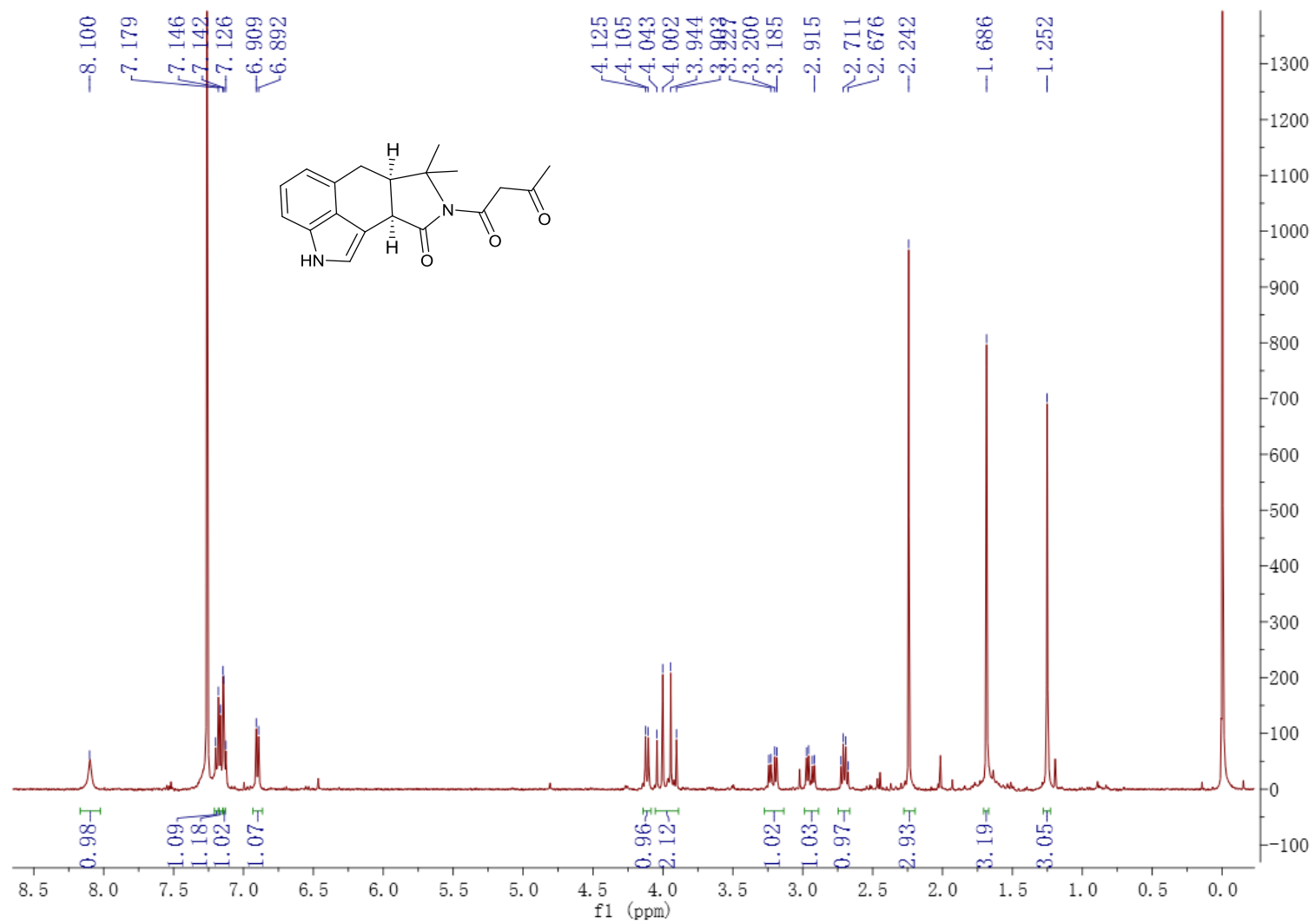


Figure S61. ^{13}C NMR and DEPT spectra of pseuboydone E (**13**) in CDCl_3 (100MHz)

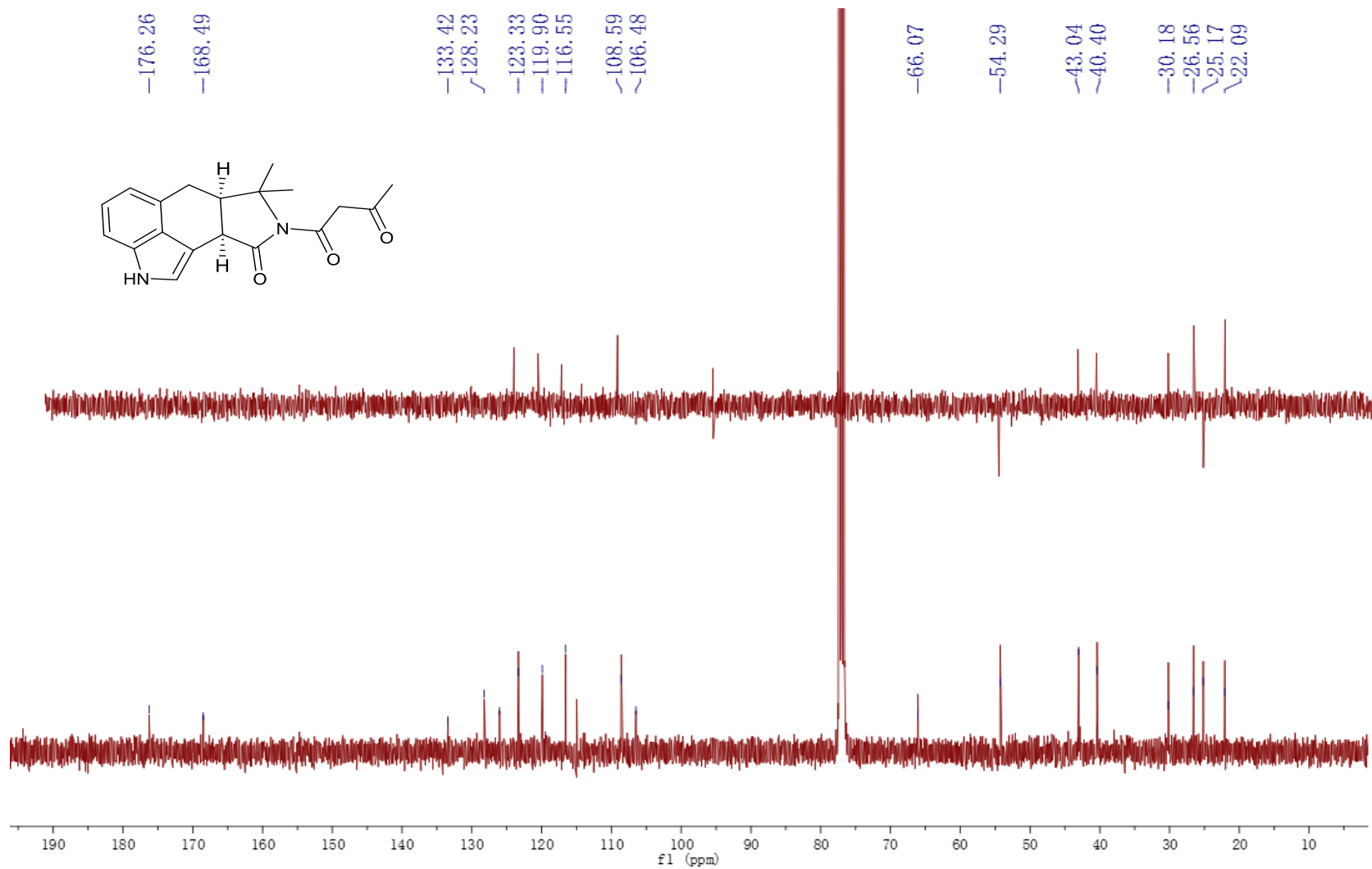


Figure S62. HMQC spectrum of pseuboydone E (**13**) in CDCl₃

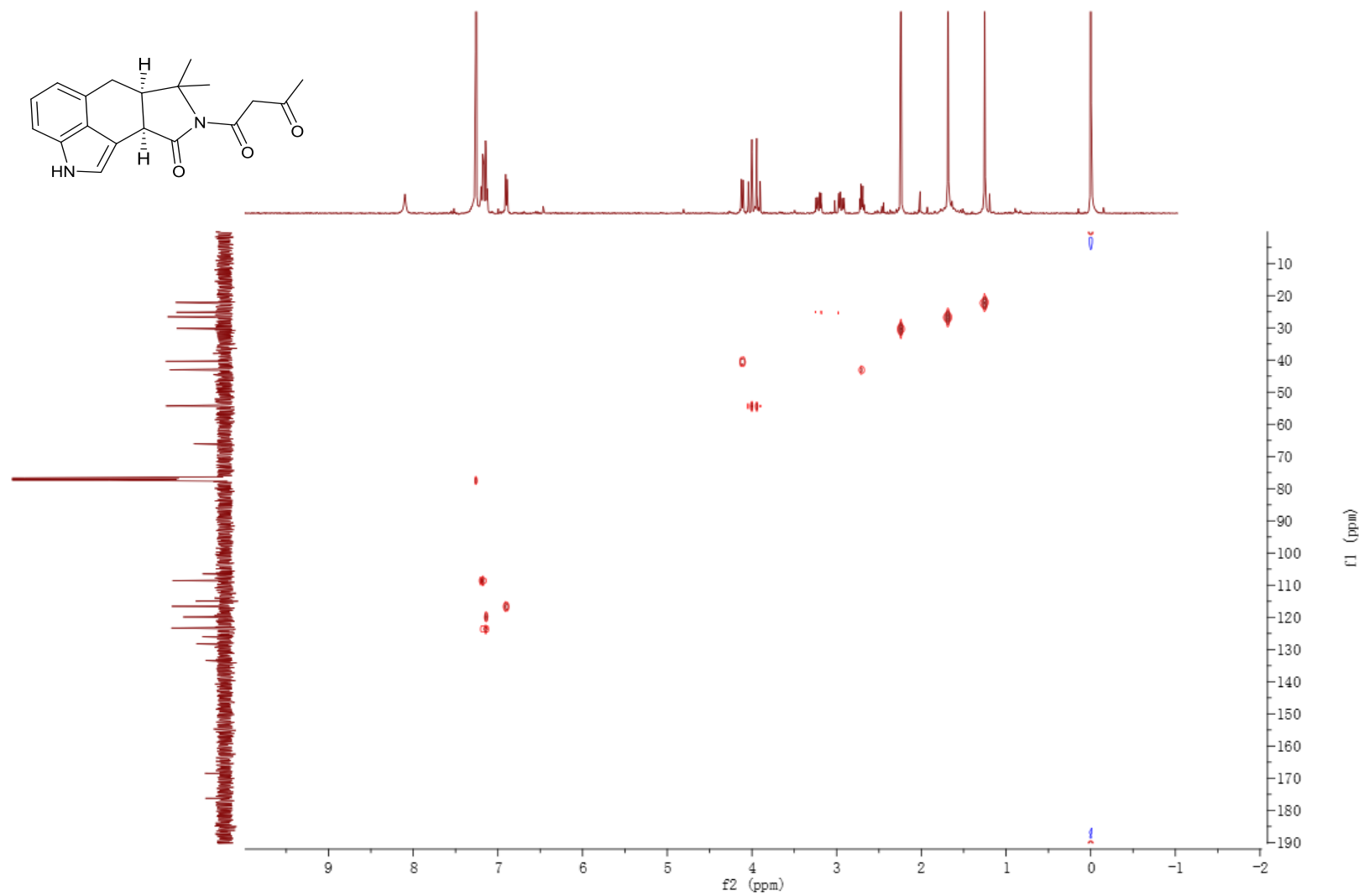


Figure S63. ^1H - ^1H COSY spectrum of pseuboydone E (**13**) in CDCl_3

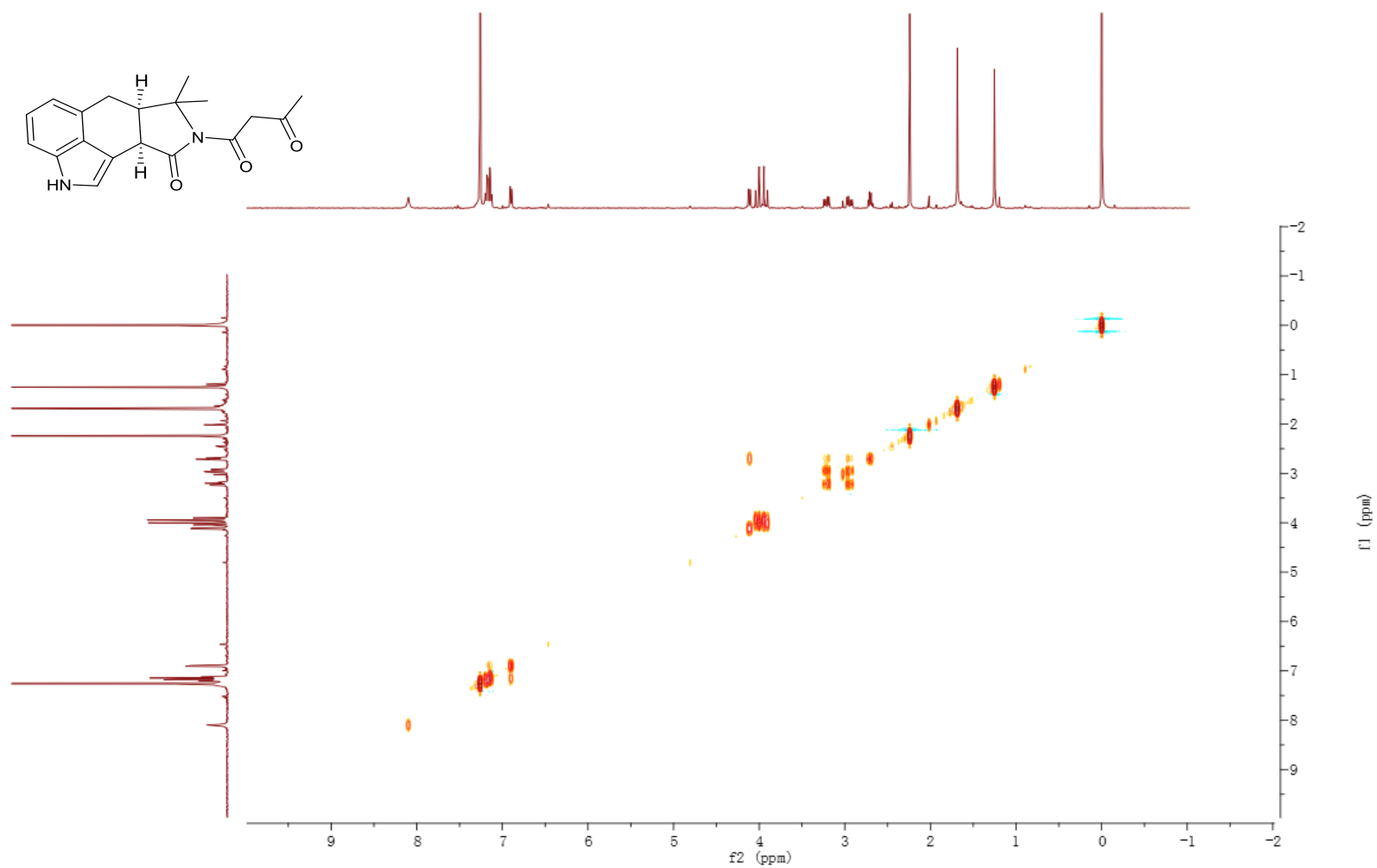


Figure S64. HMBC spectrum of pseuboydone E (**13**) in CDCl₃

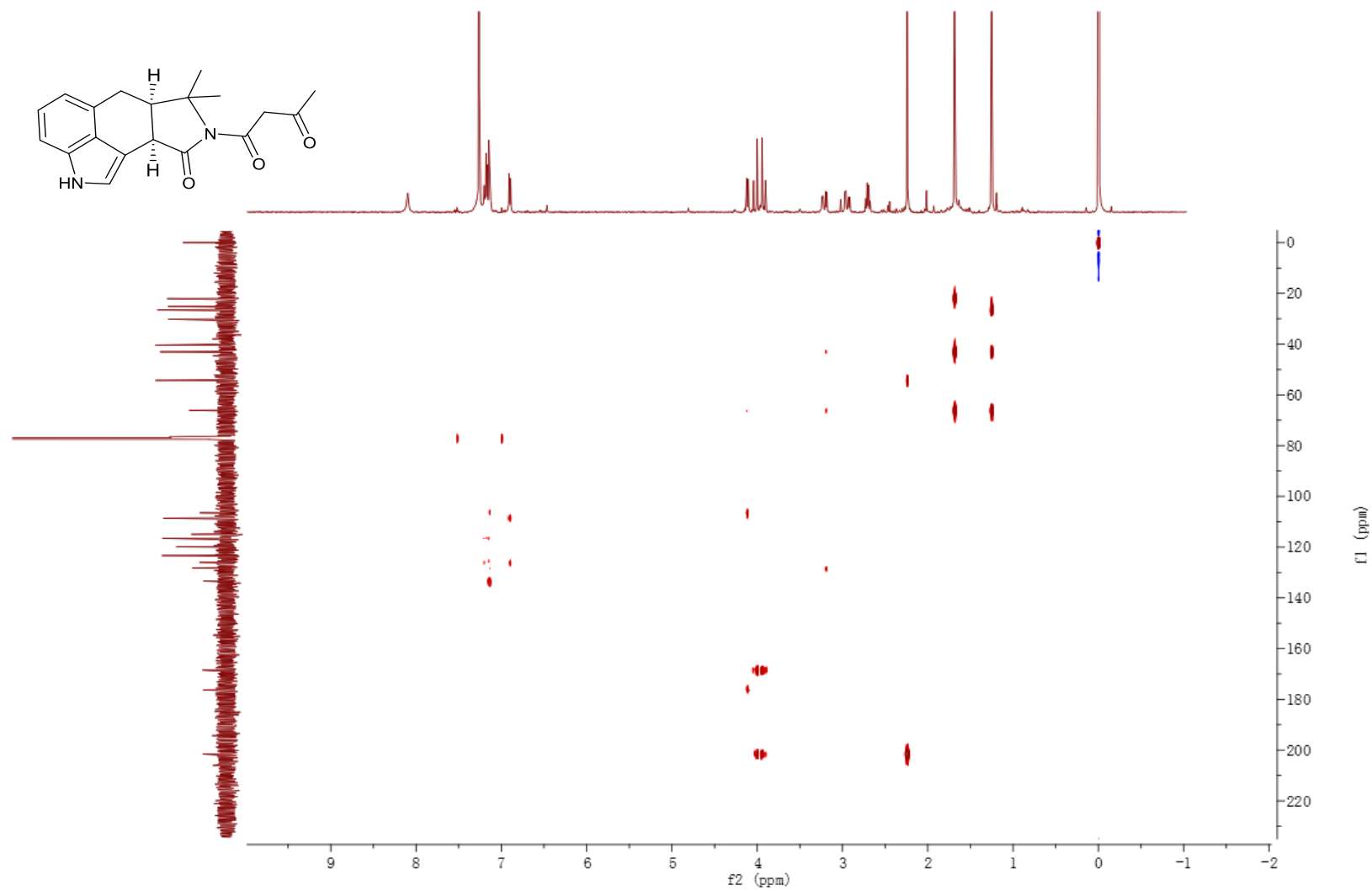


Figure S65. NOESY spectrum of pseuboydone E (**13**) in CDCl₃

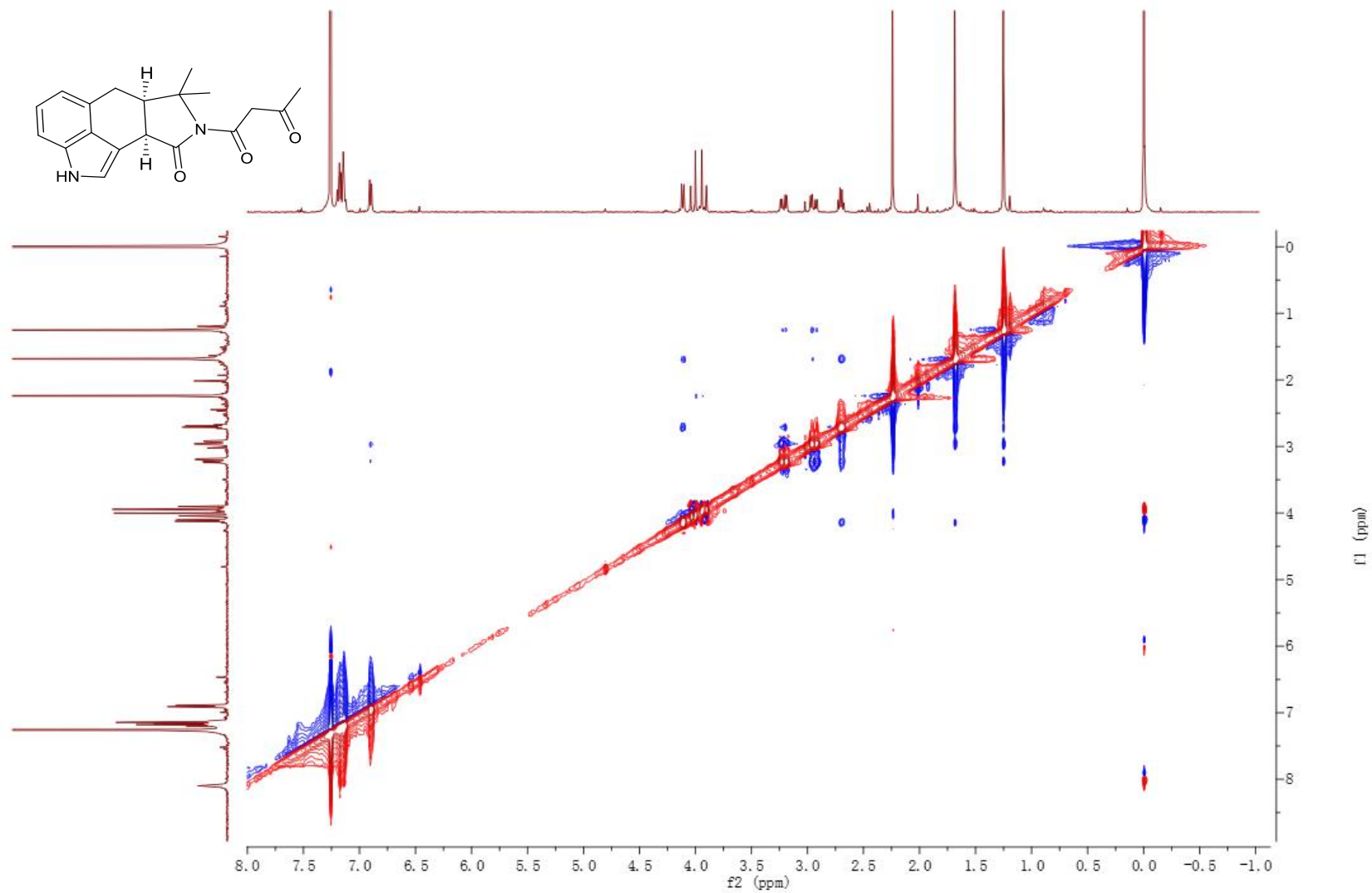


Figure S66. ^1H -NMR spectrum of speradine C (**14**) in CDCl_3 (400MHz)

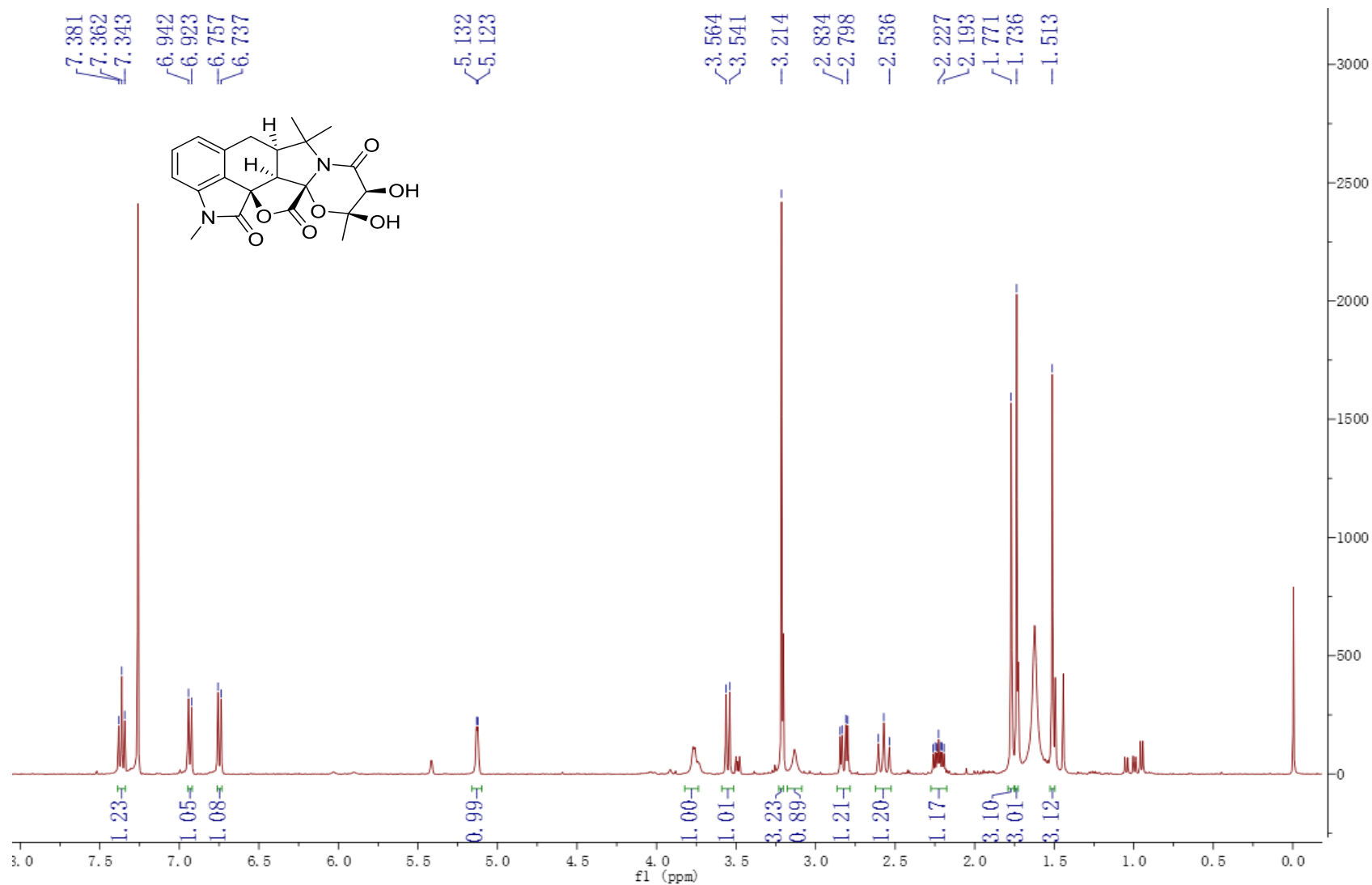


Figure S67. ^{13}C -NMR spectrum of speradine C (**14**) in CDCl_3 (100MHz)

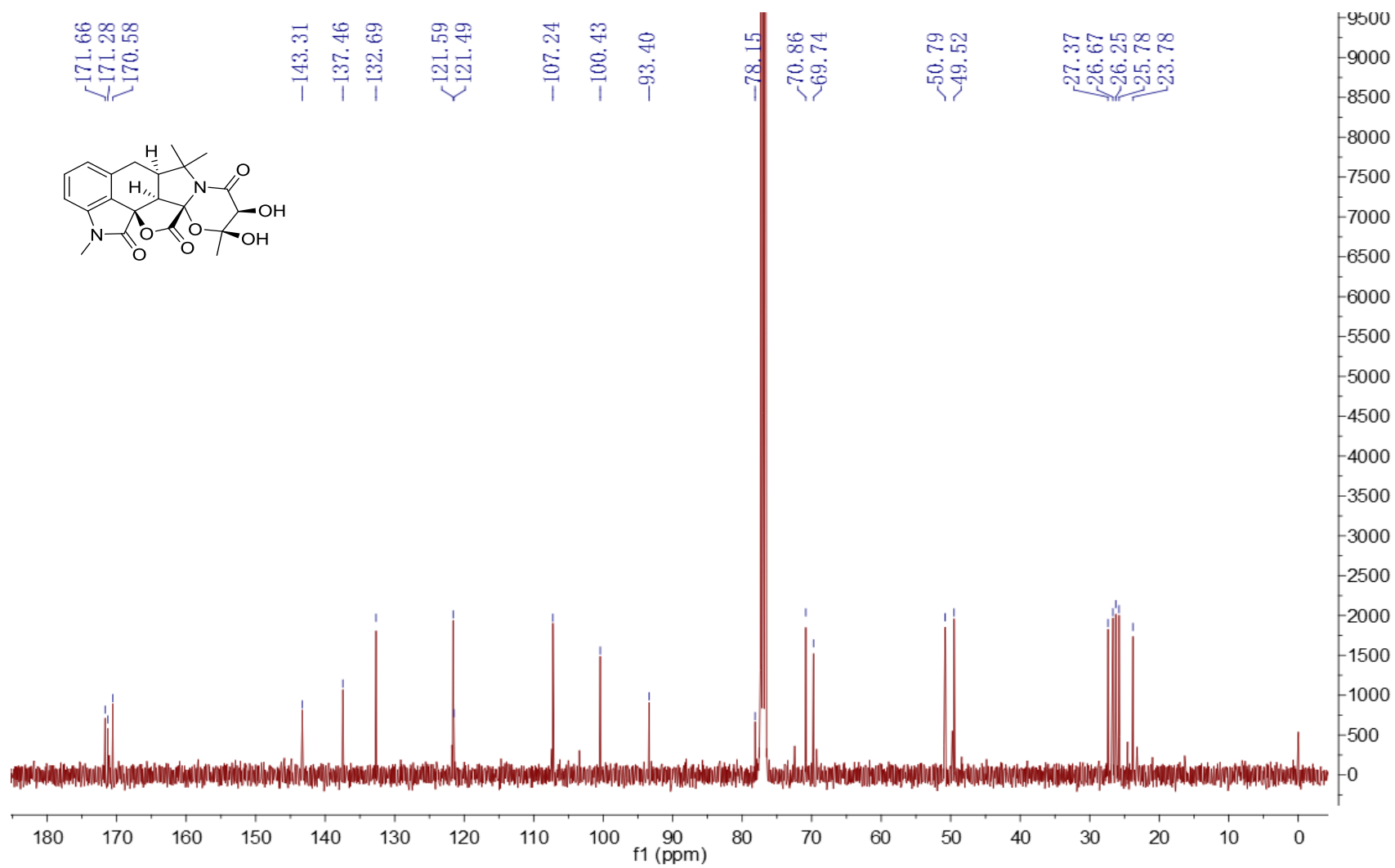


Figure S68. NOESY spectrum of speradine C (**14**) in CDCl₃

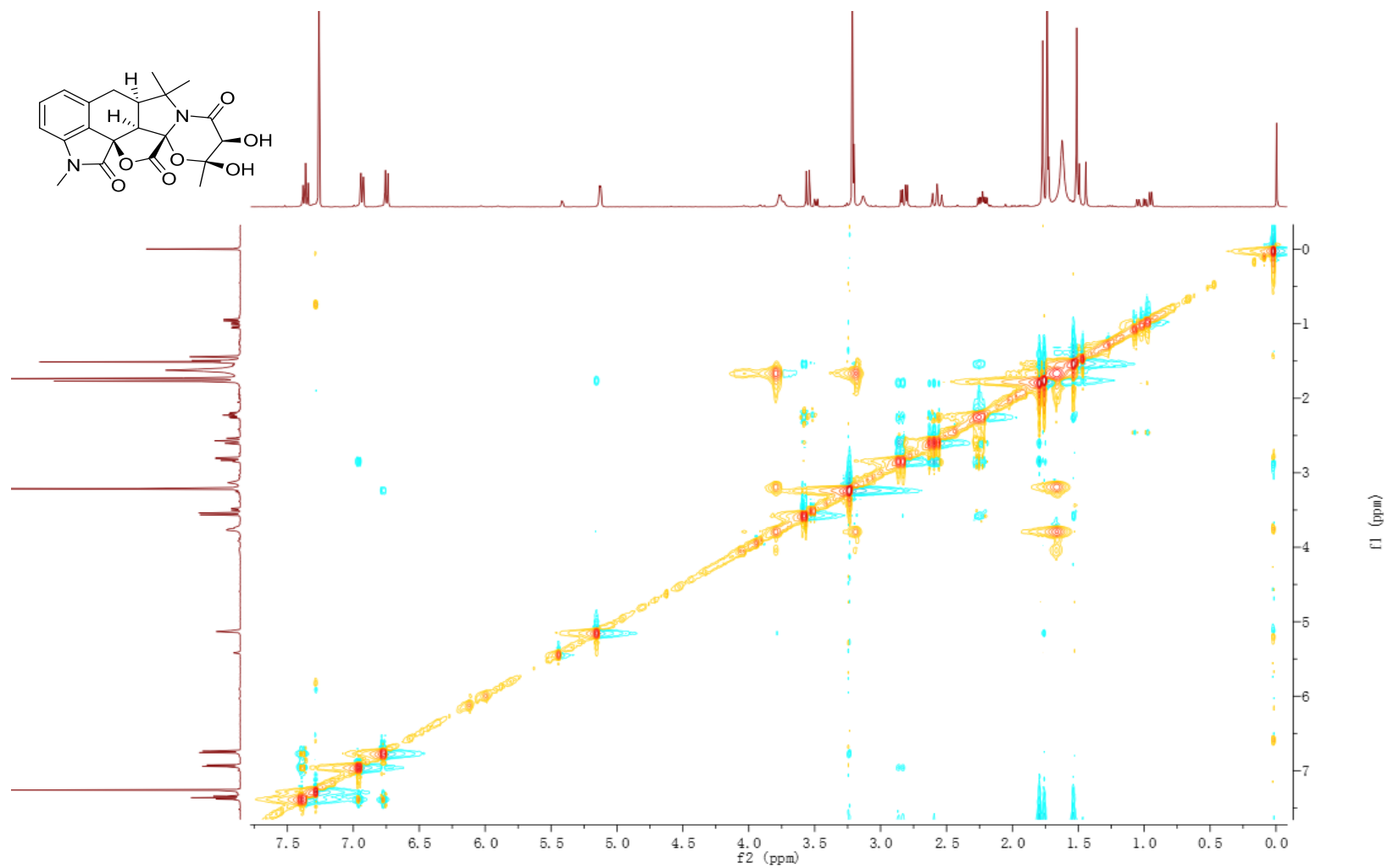


Figure S69. ^1H -NMR spectrum of speradine **B** (**15**) in CDCl_3 (400MHz)

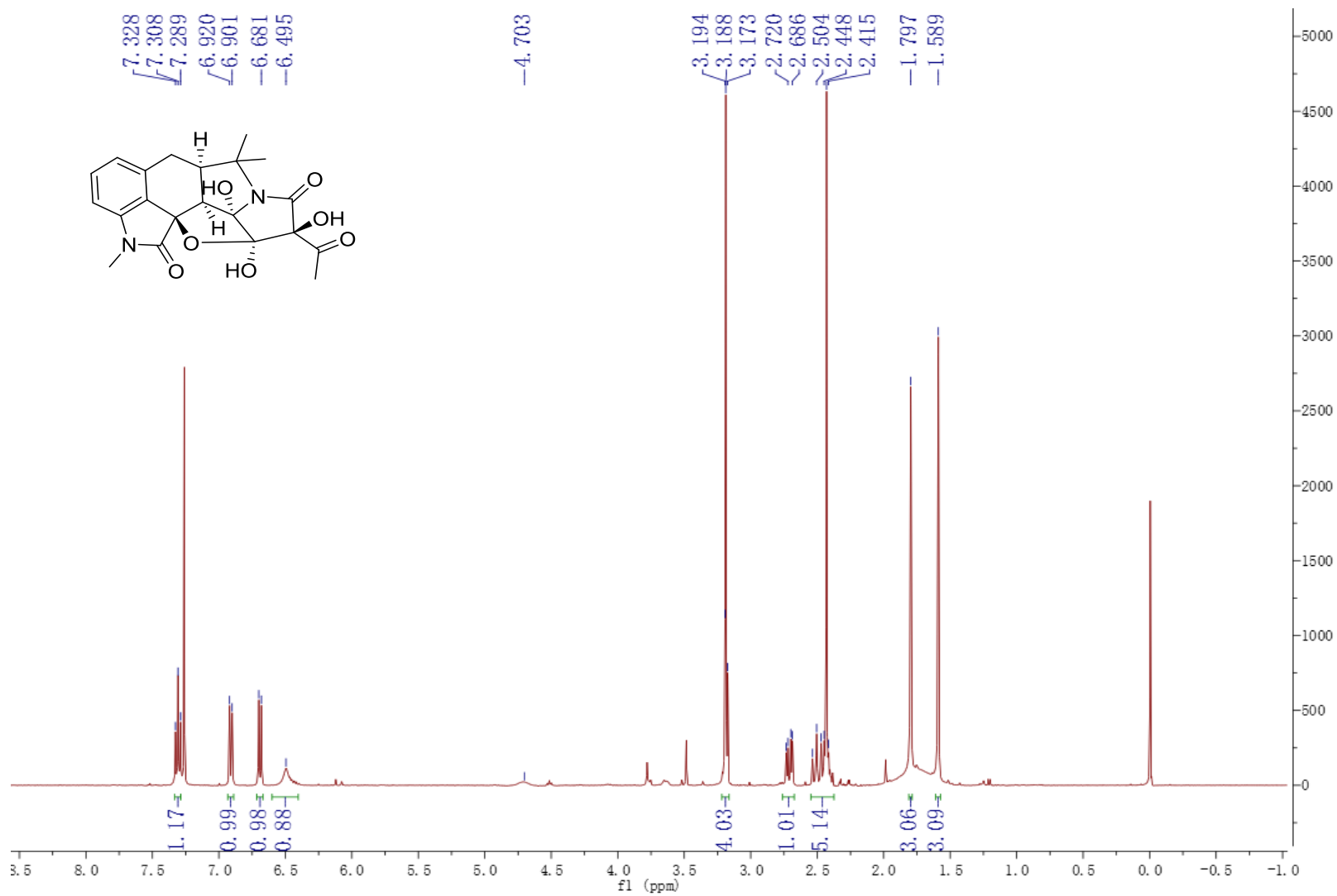


Figure S70. ^{13}C -NMR spectrum of speradine **B** (**15**) in CDCl_3 (100MHz)

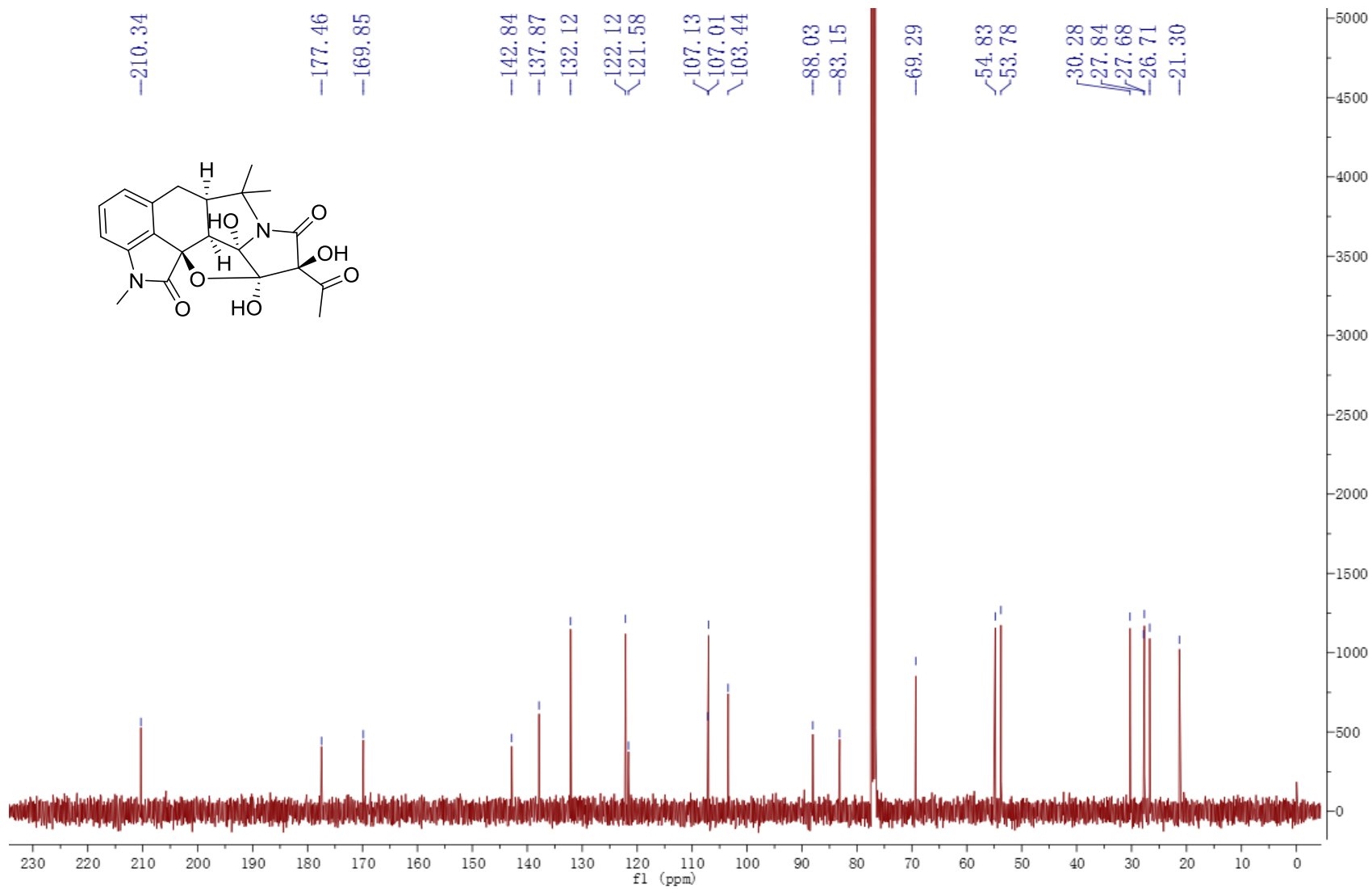


Figure S71. HMQC spectrum of speradine **B** (15) in CDCl₃

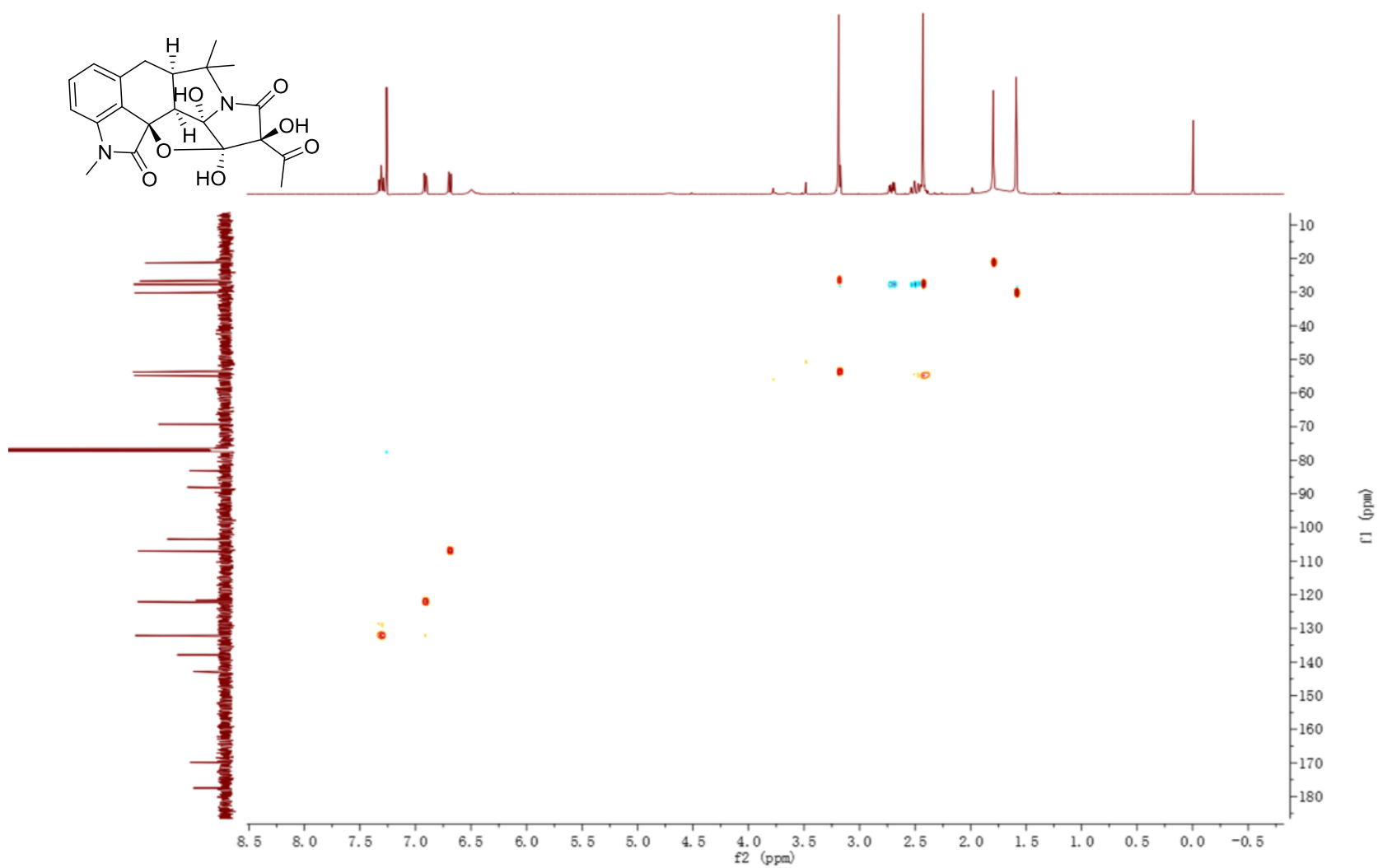


Figure S72. HMBC spectrum of speradine **B** (15) in CDCl₃

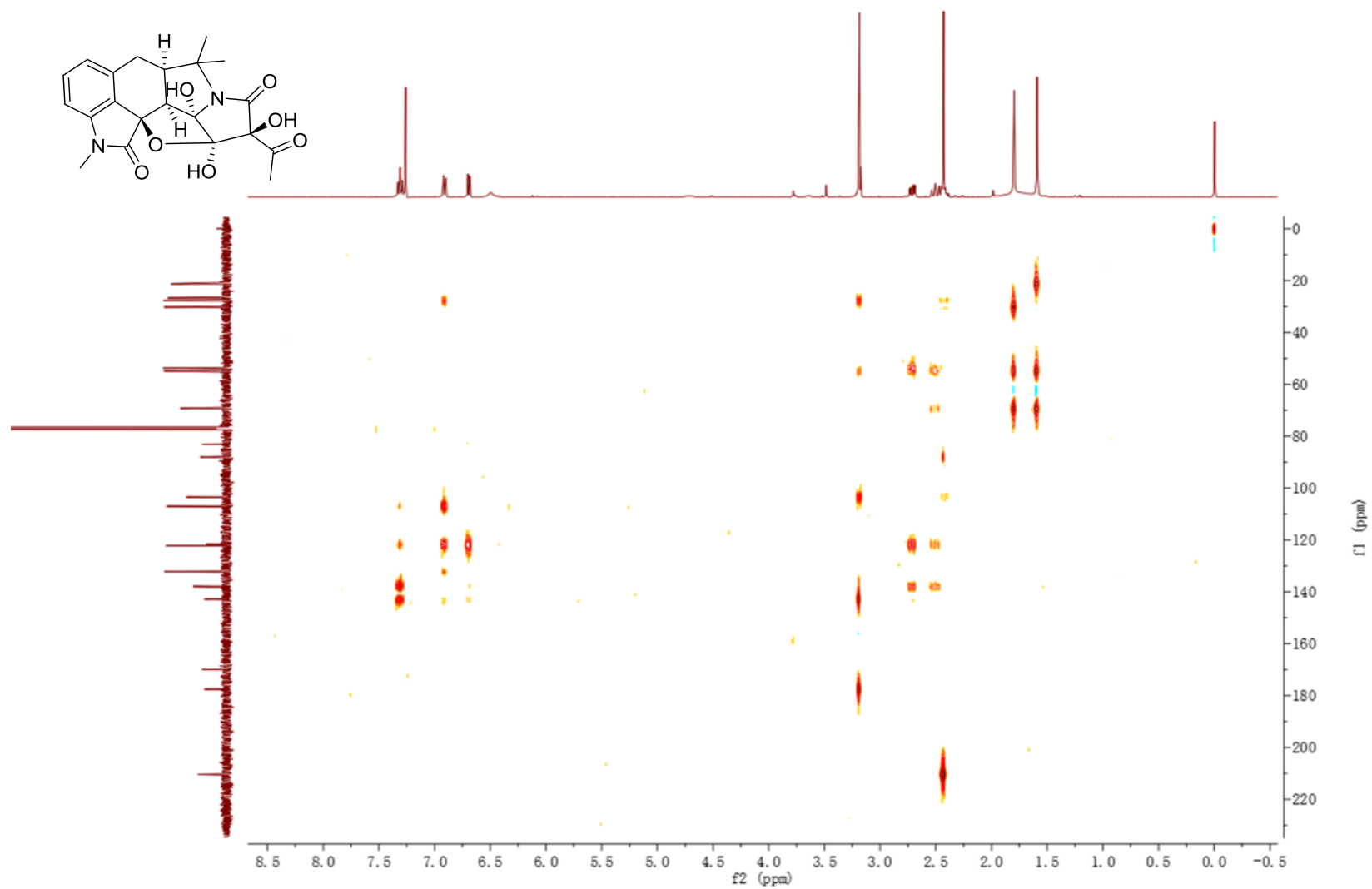


Figure S73. ^1H -NMR spectrum of cyclopiamide E (**16**) in CDCl_3 (400MHz)

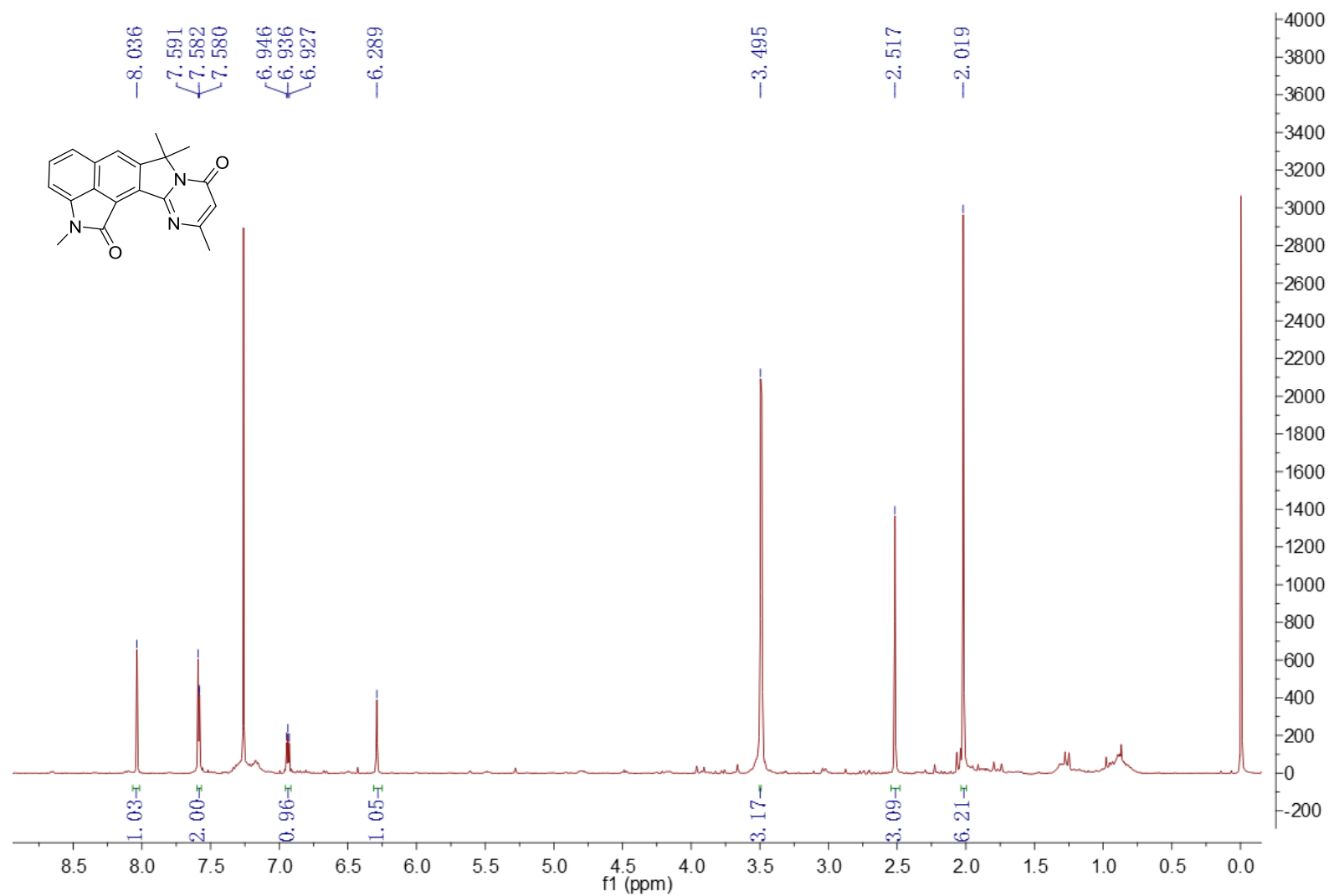


Figure S74. ^{13}C NMR and DEPT spectra of cyclopiamide E (**16**) in CDCl_3 (100MHz)

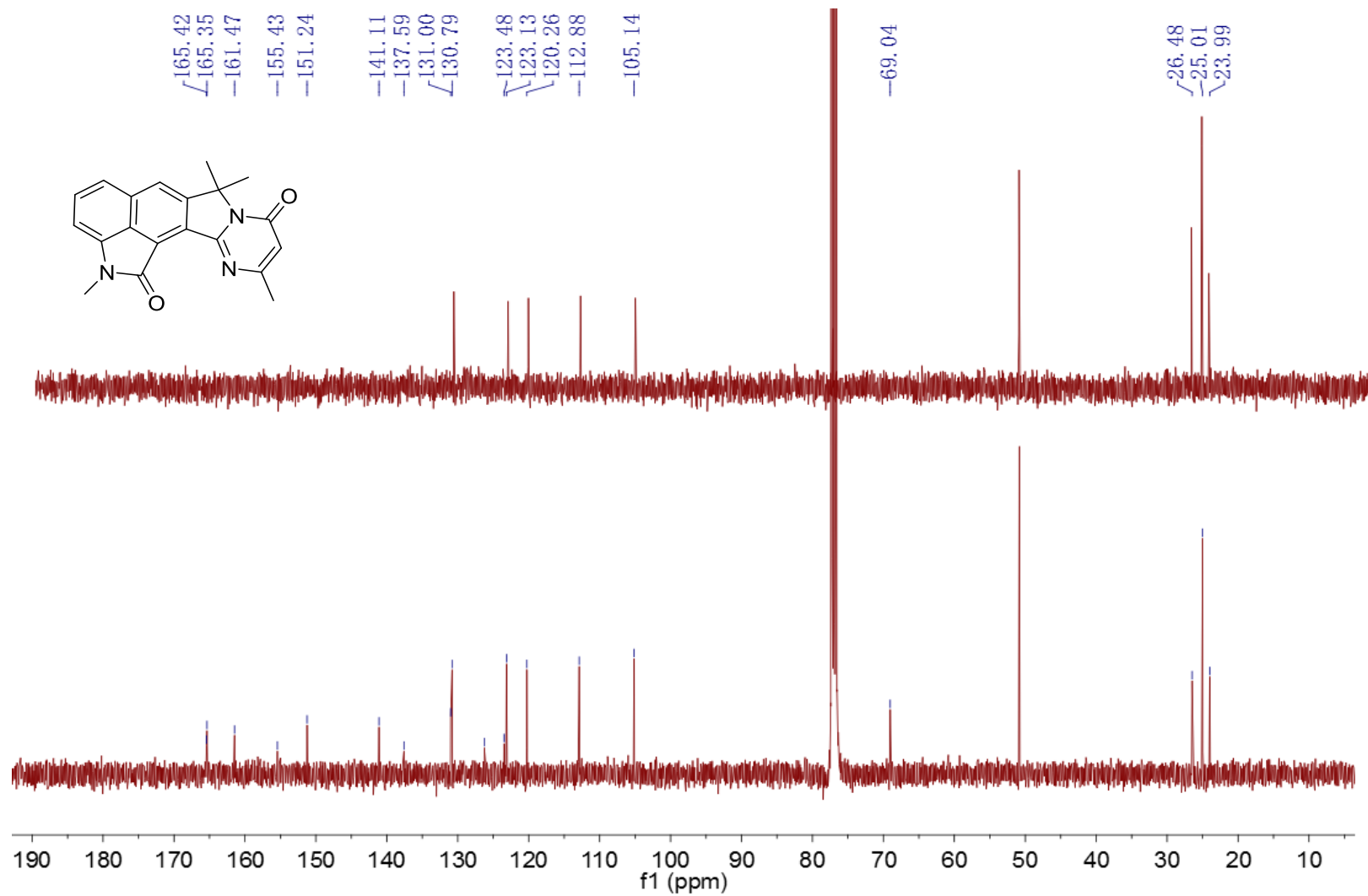


Figure S75. HMQC spectrum of cyclopamide E (**16**) in CDCl₃

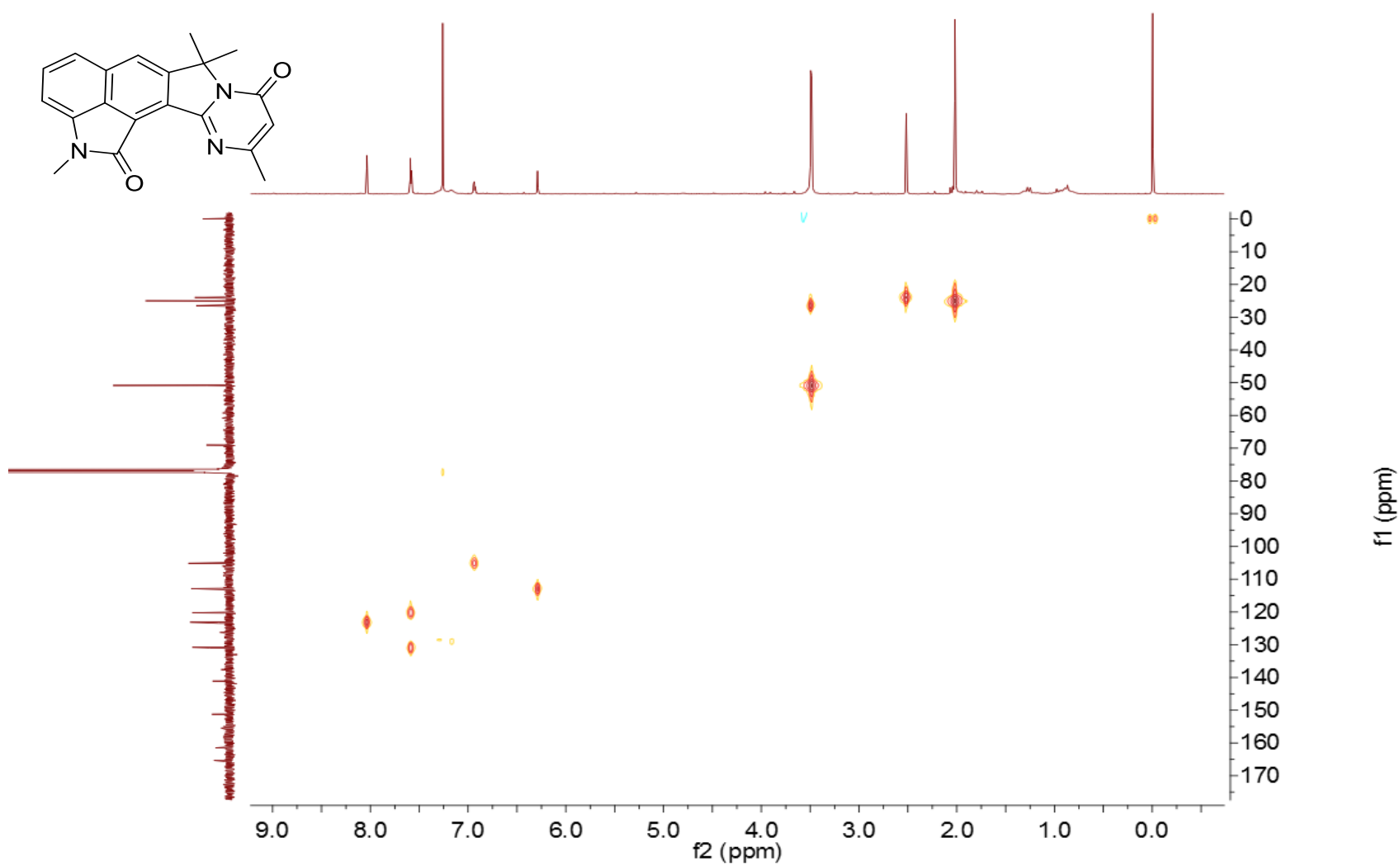


Figure S76. HMBC spectrum of cyclopamide E (**16**) in CDCl₃

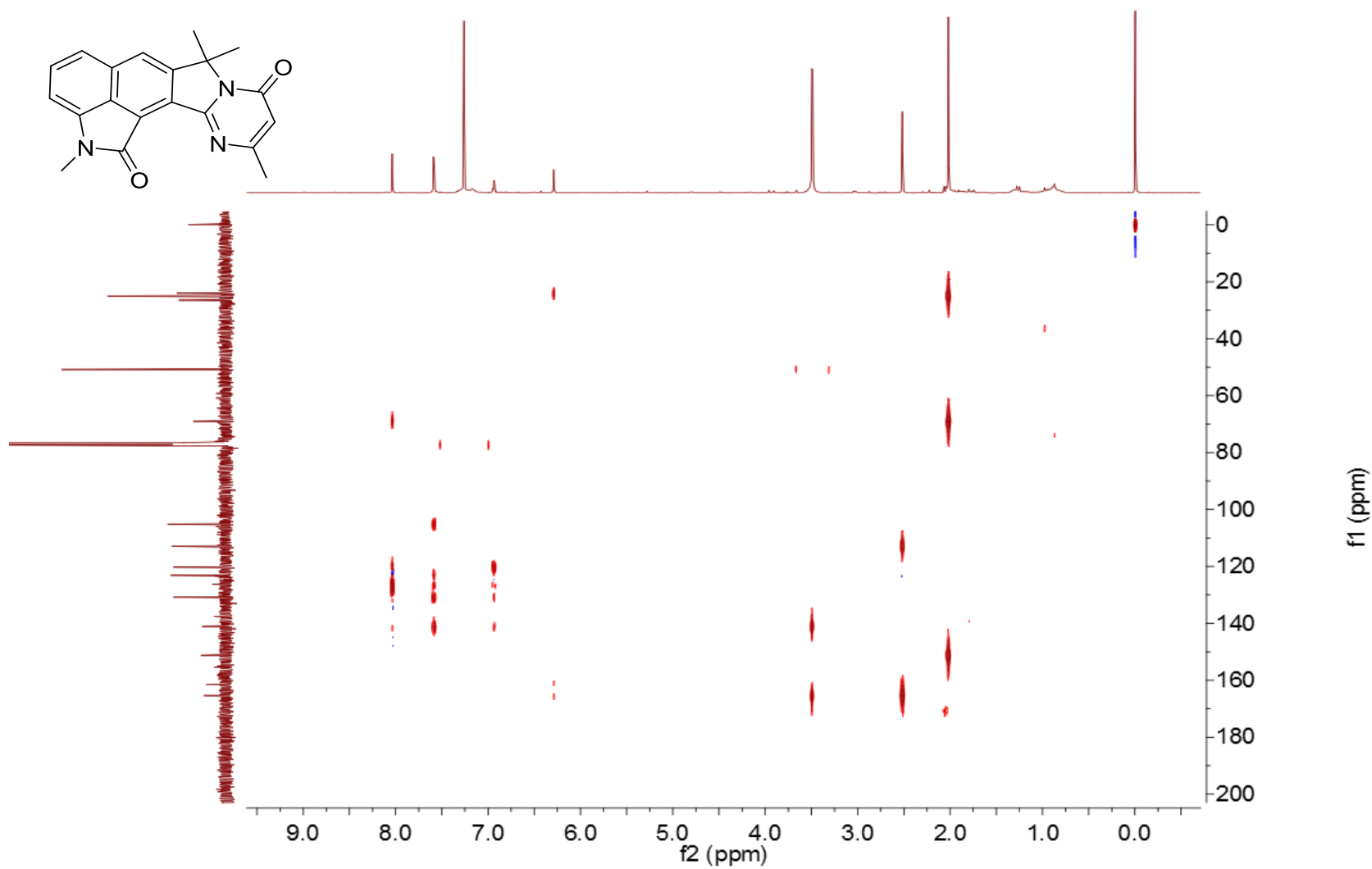


Figure S77. NOESY spectrum of cyclopiamide E (**16**) in CDCl₃

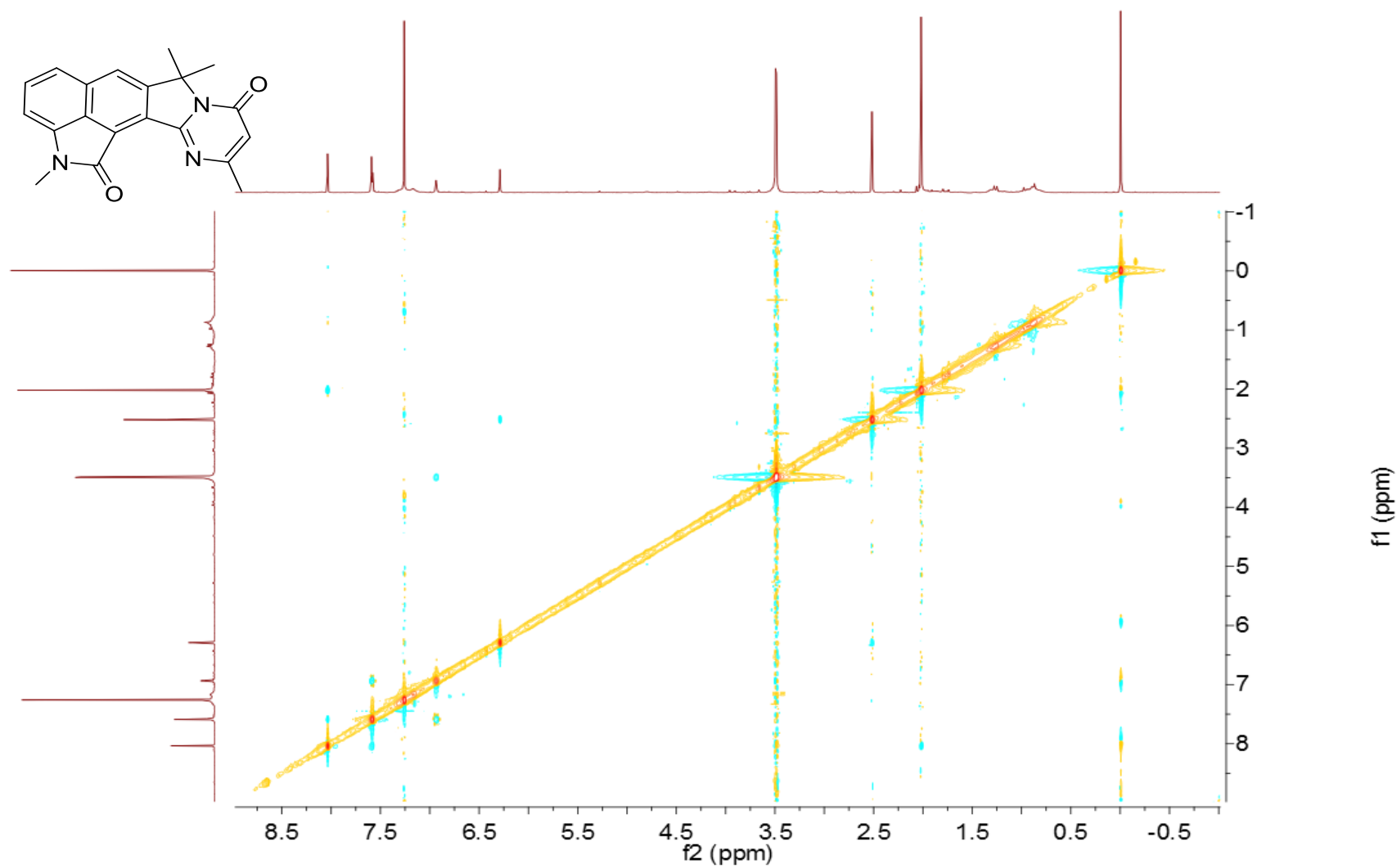


Figure S78. ^1H -NMR spectrum of 24, 25-dehydro-10, 11-dihydro-20-hydroxyaflavinin (**17**) in CDCl_3 (400MHz)

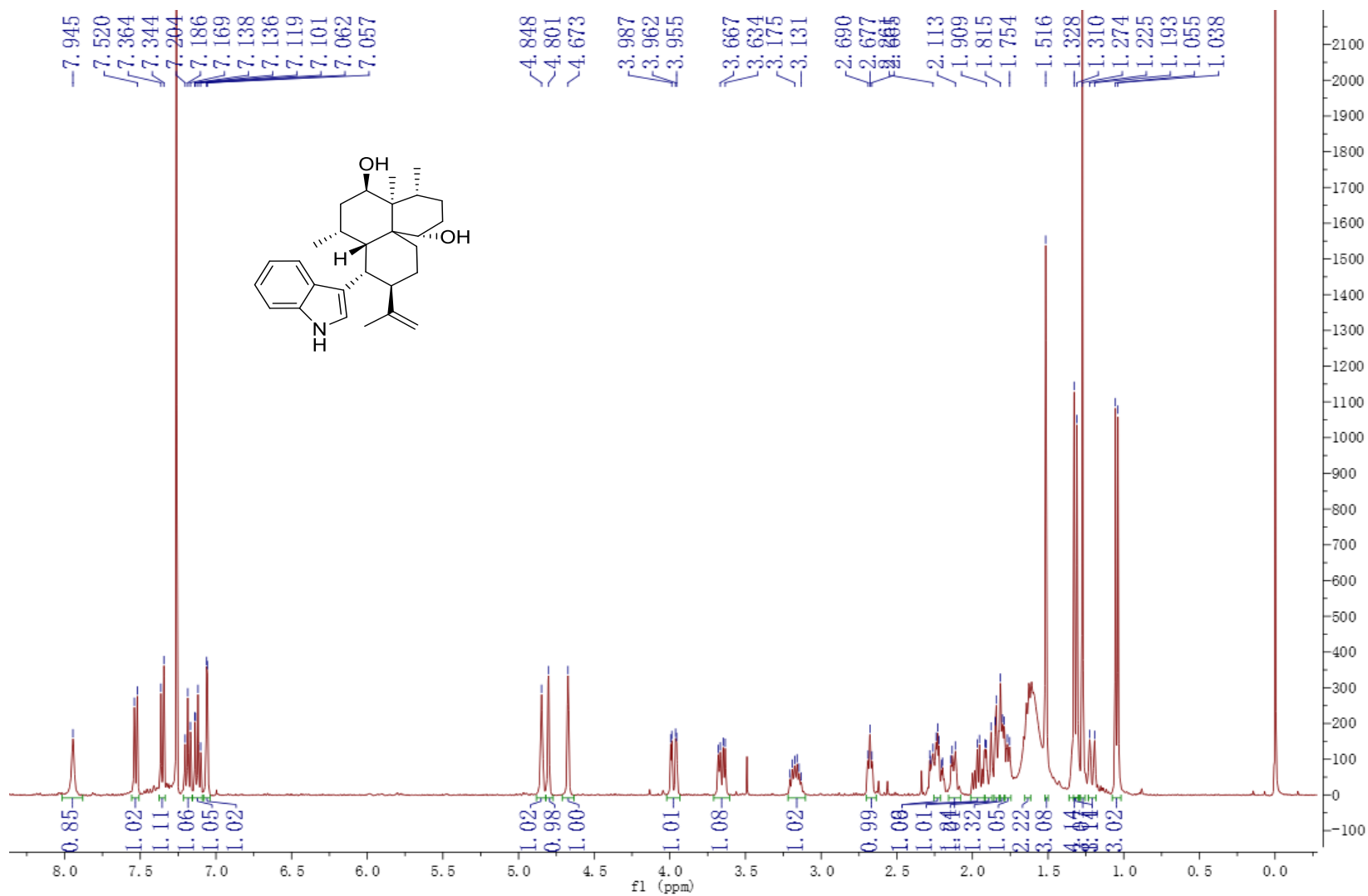


Figure S79. ^{13}C -NMR spectrum of 24, 25-dehydro-10,11-dihydro-20-hydroxyaflavinin (**17**) in CDCl_3 (100MHz)

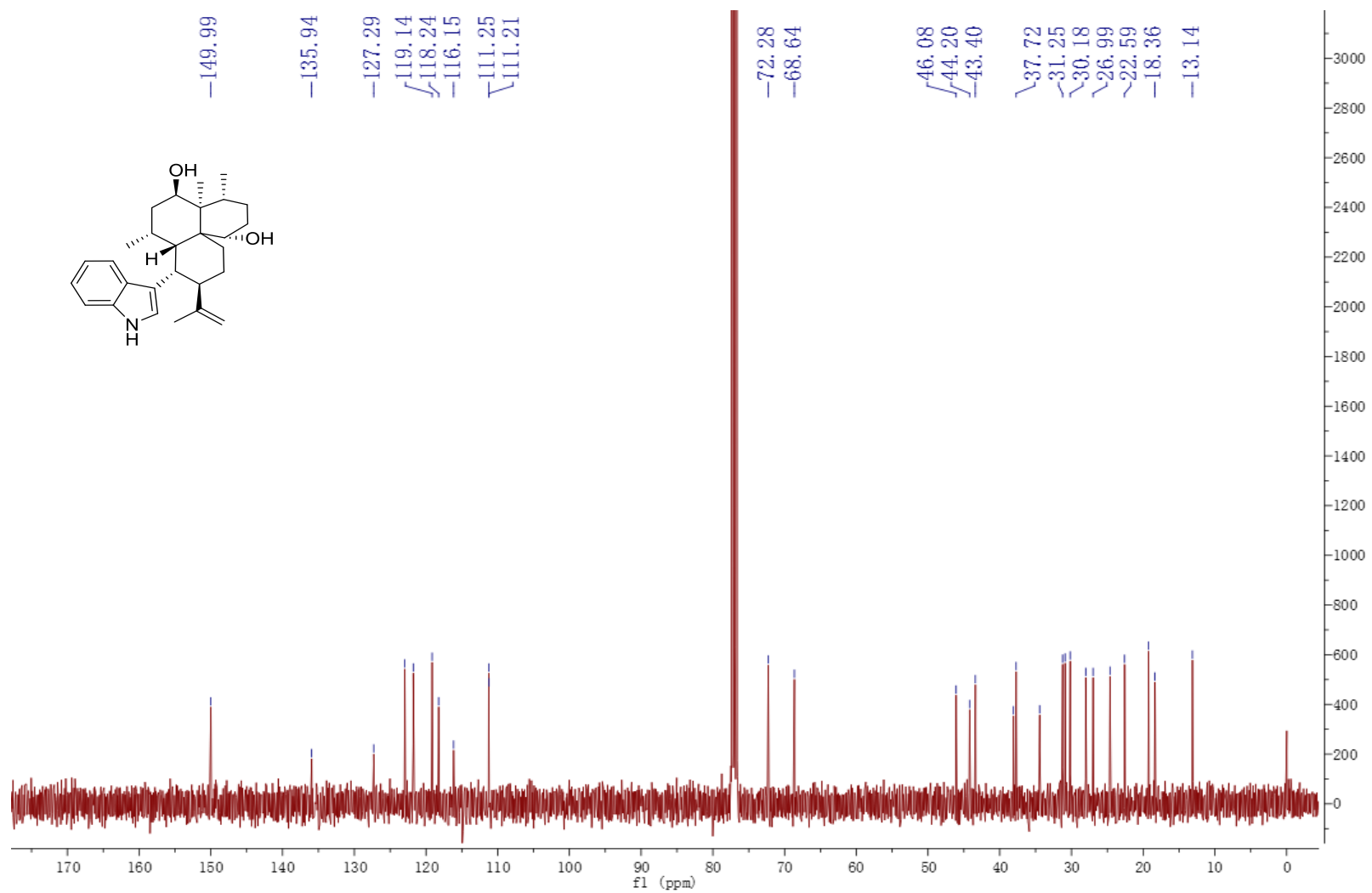


Figure S80. NOESY spectrum of 24, 25-dehydro-10, 11-dihydro-20-hydroxyaflavinin (**17**) in CDCl₃

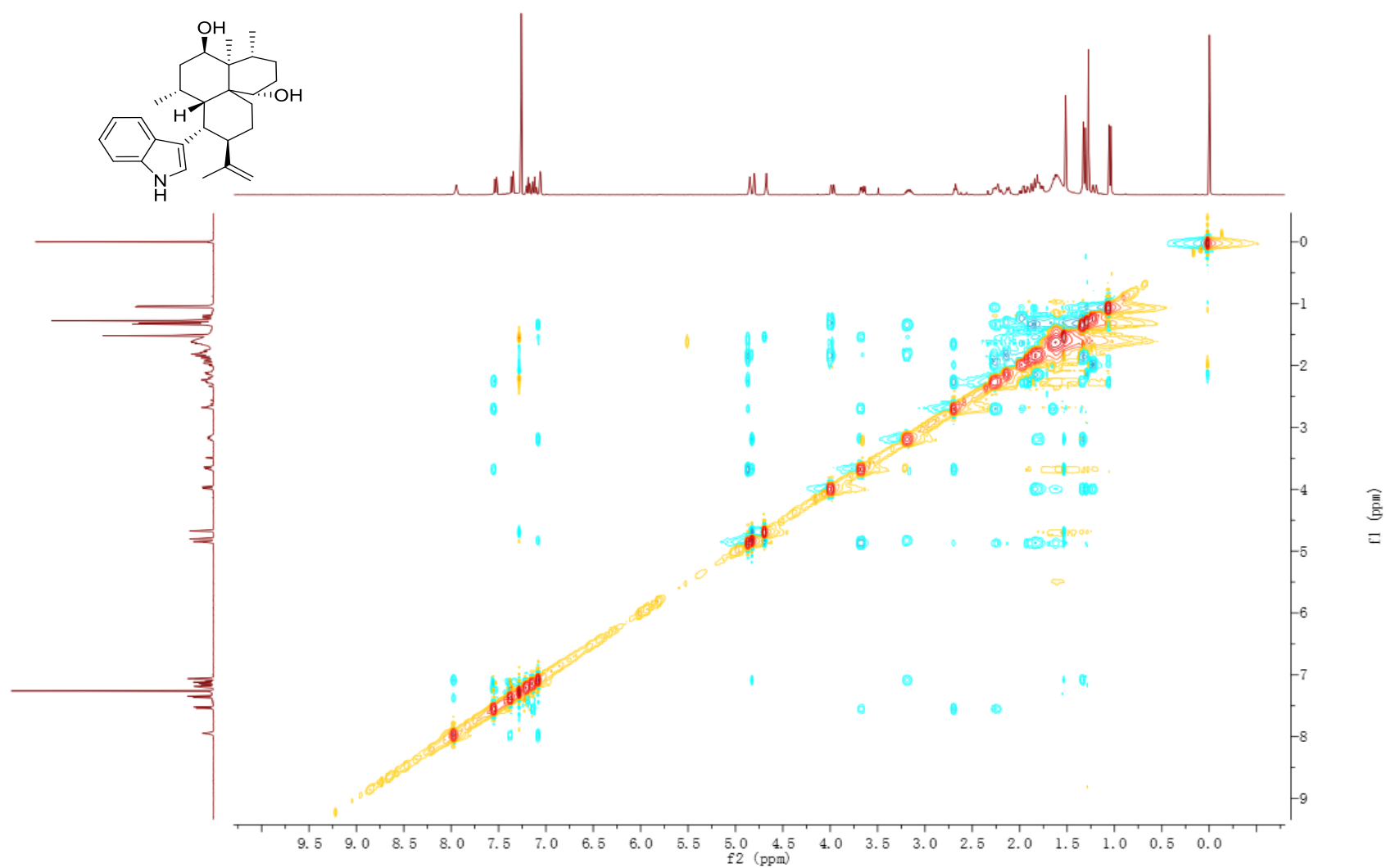
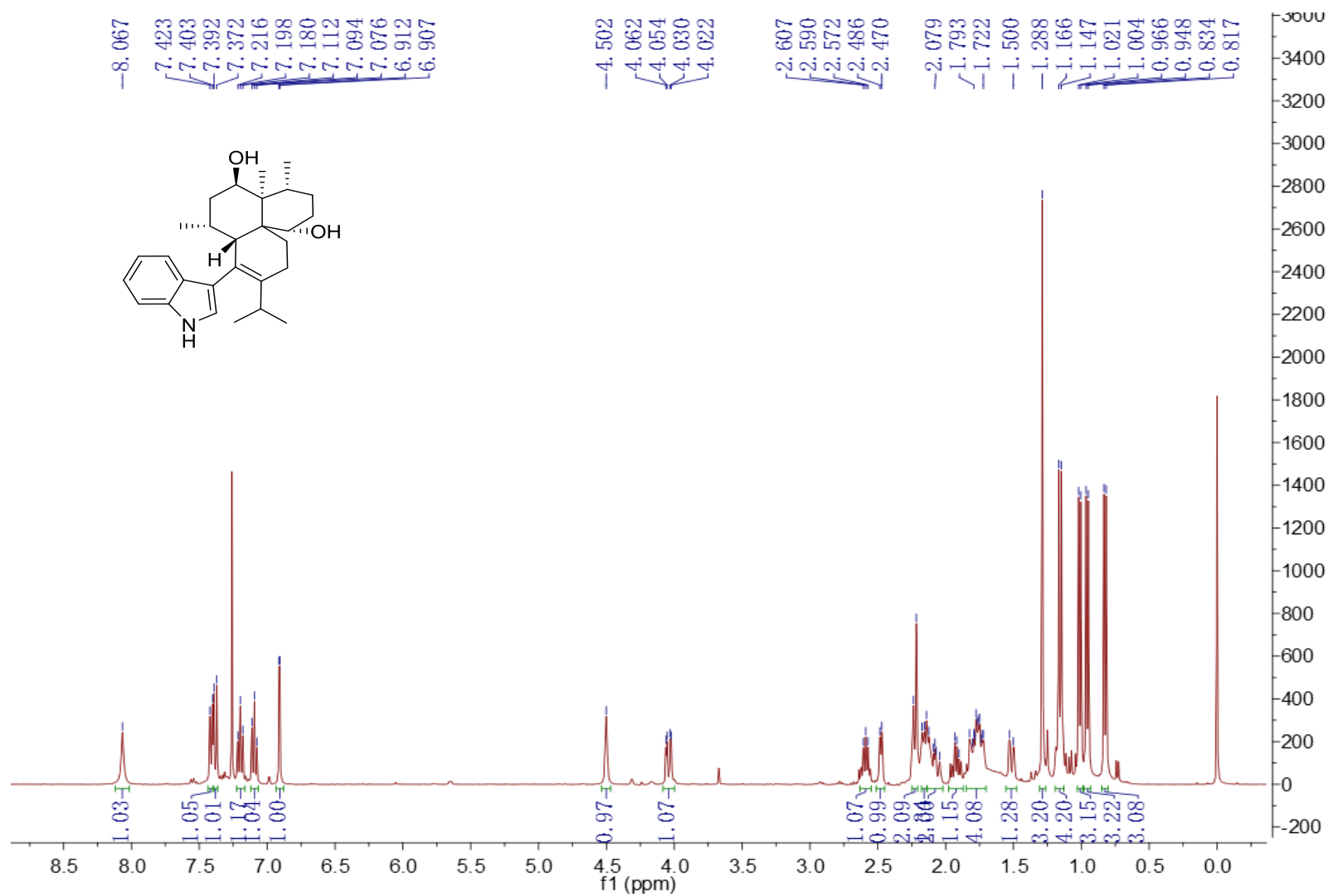


Figure S81. ^1H -NMR spectrum of aflavinine (**18**) in CDCl_3 (400MHz)



Chemical structure of compound 10a is shown in the top left corner. The ¹³C NMR spectrum (CDCl₃) is displayed below the structure, with peaks labeled with their chemical shifts (ppm):

- 141.35
- 135.81
- 127.34
- 125.01
- 121.86
- 121.19
- 119.41
- 111.06
- 72.30
- 70.58
- 44.68
- 43.39
- 34.68
- 29.95
- 27.10
- 20.68
- 19.20
- 19.11
- 12.91

Figure S83. HMQC spectrum of aflavinine (**18**) in CDCl₃

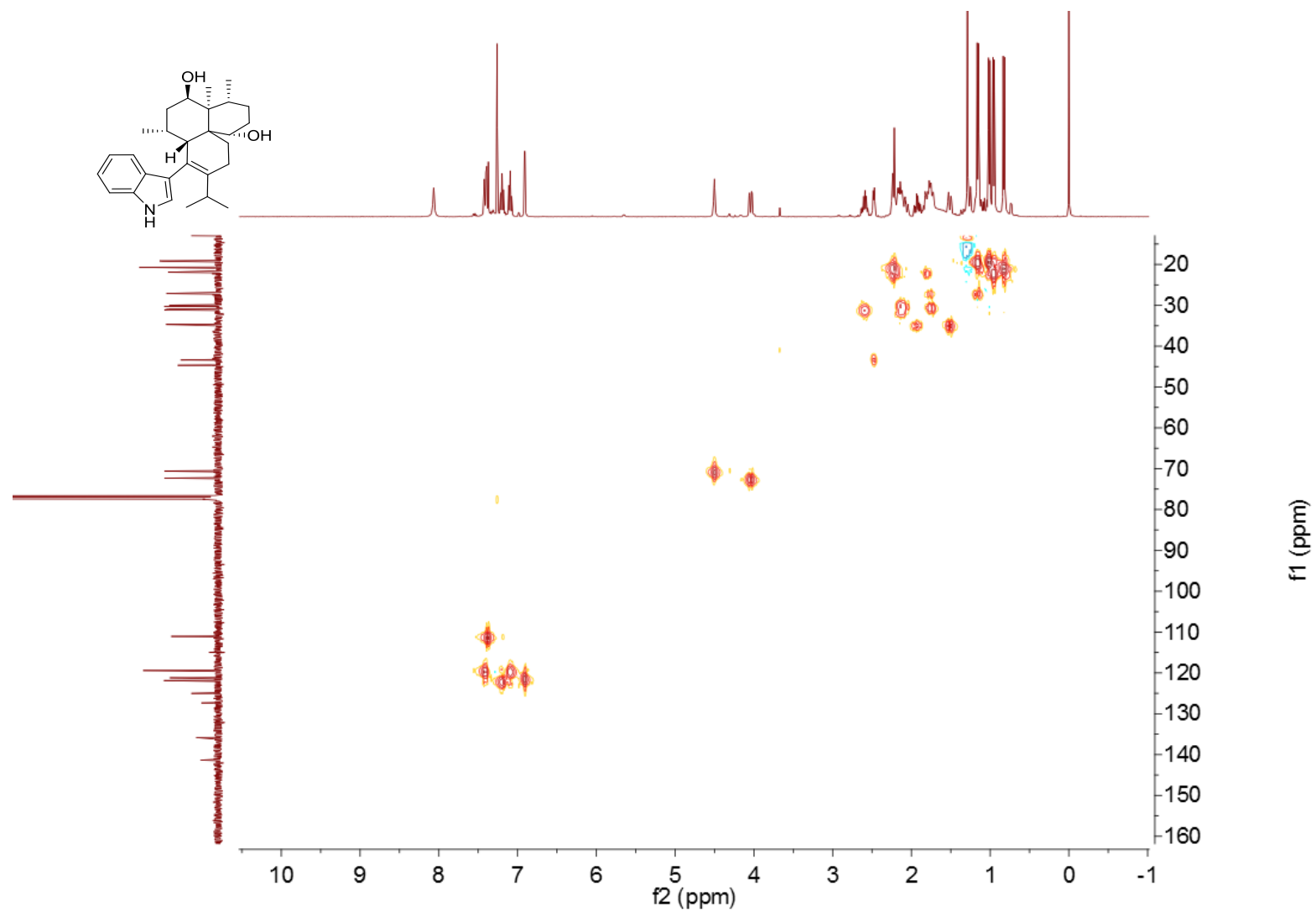


Figure S84. ^1H - ^1H COSY spectrum of aflavinine (**18**) in CDCl_3

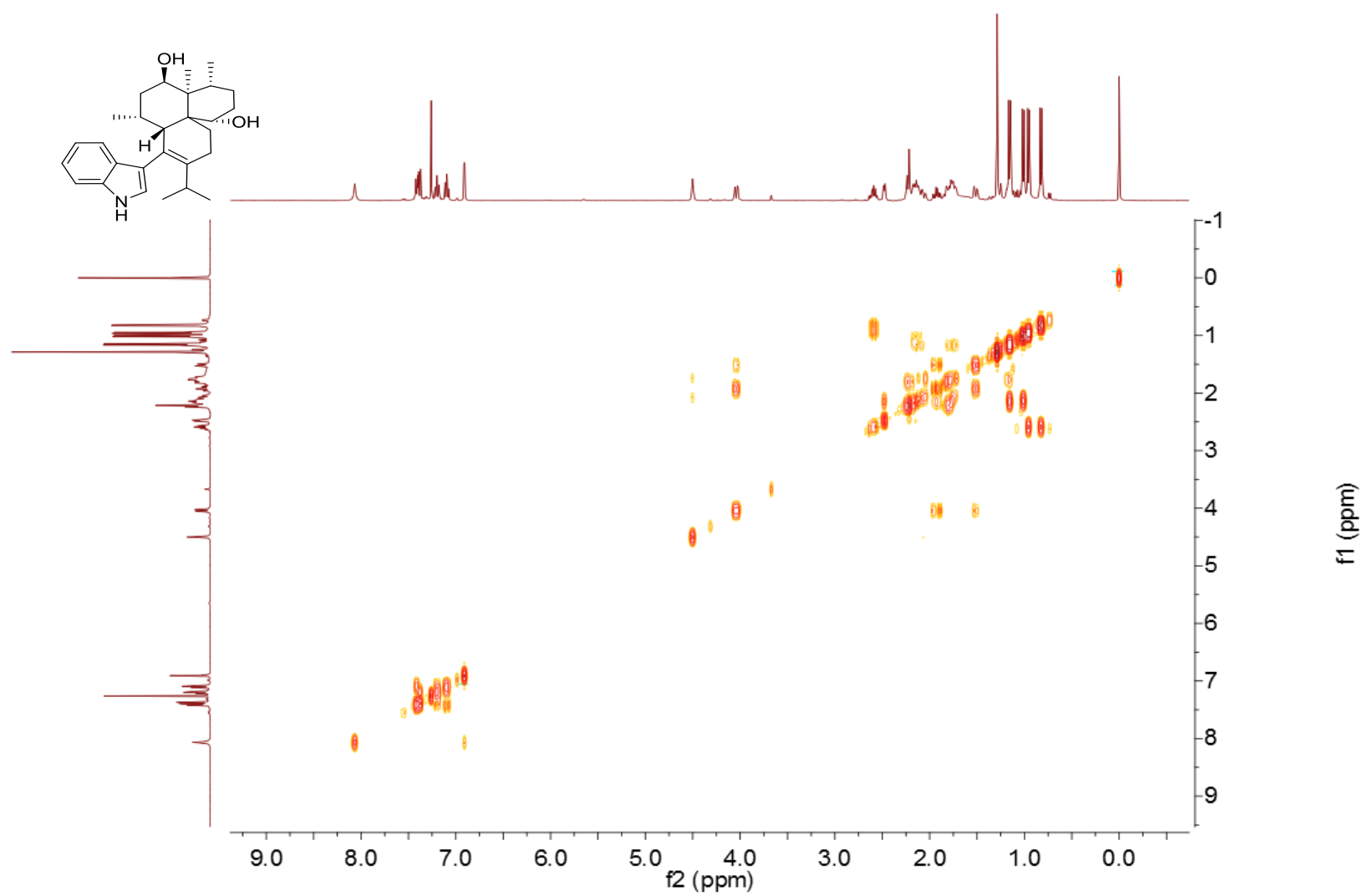


Figure S85. HMBC spectrum of aflavinine (**18**) in CDCl₃

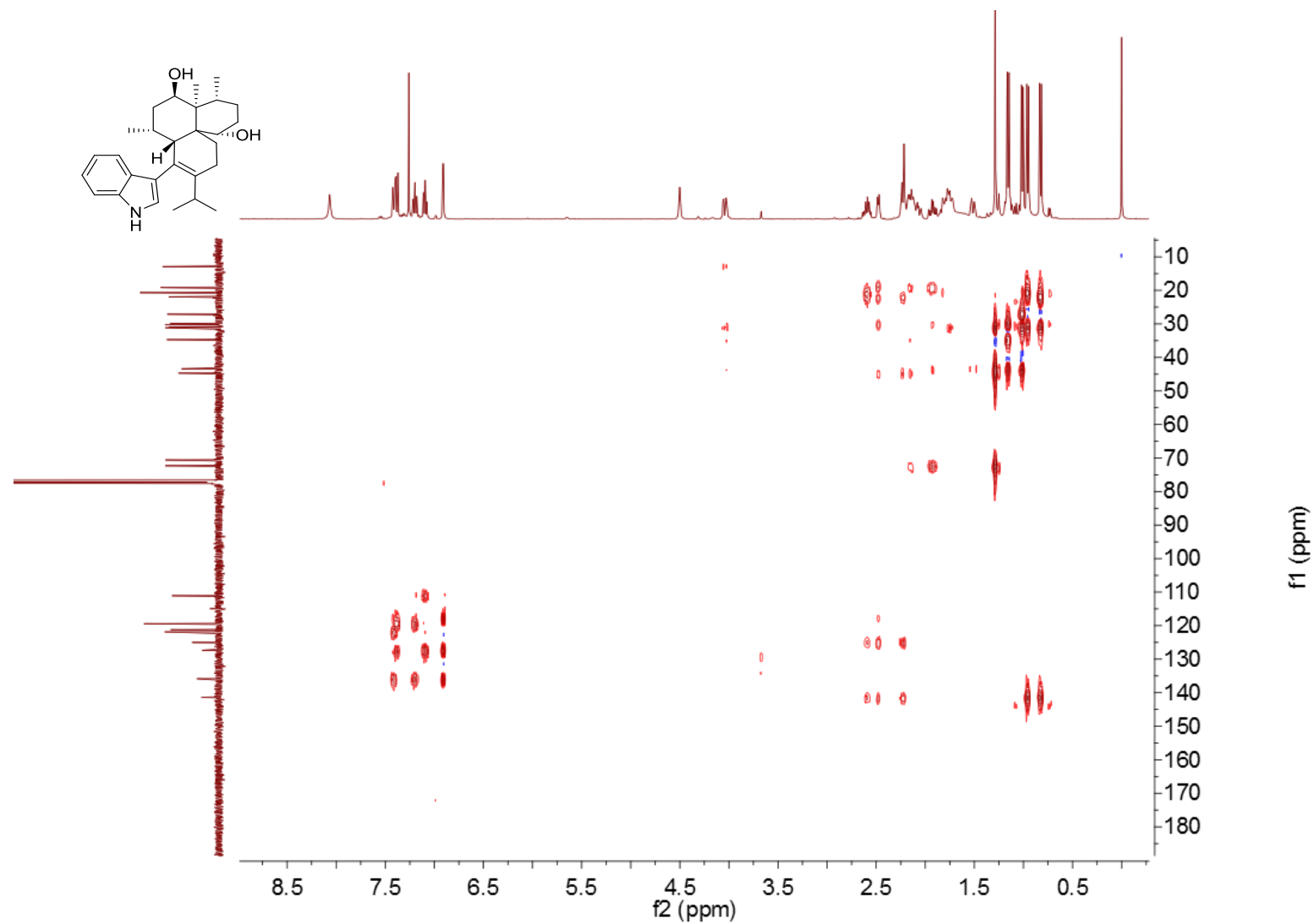


Figure S86. NOESY spectrum of aflavinine (**18**) in CDCl₃

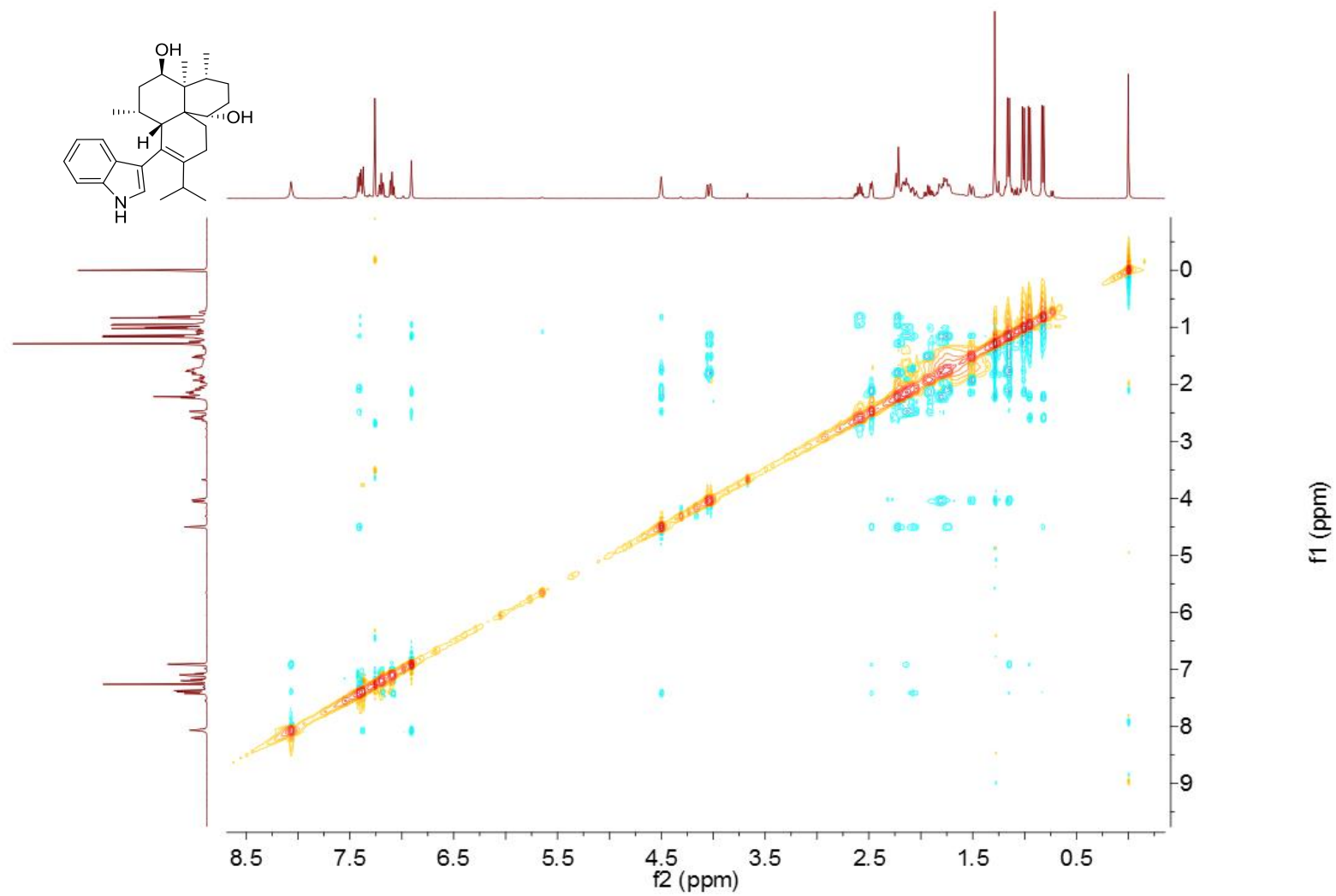


Figure S87. ^1H -NMR spectrum of β -aflatrem (**19**) in $\text{DMSO}-d_6$ (400MHz)

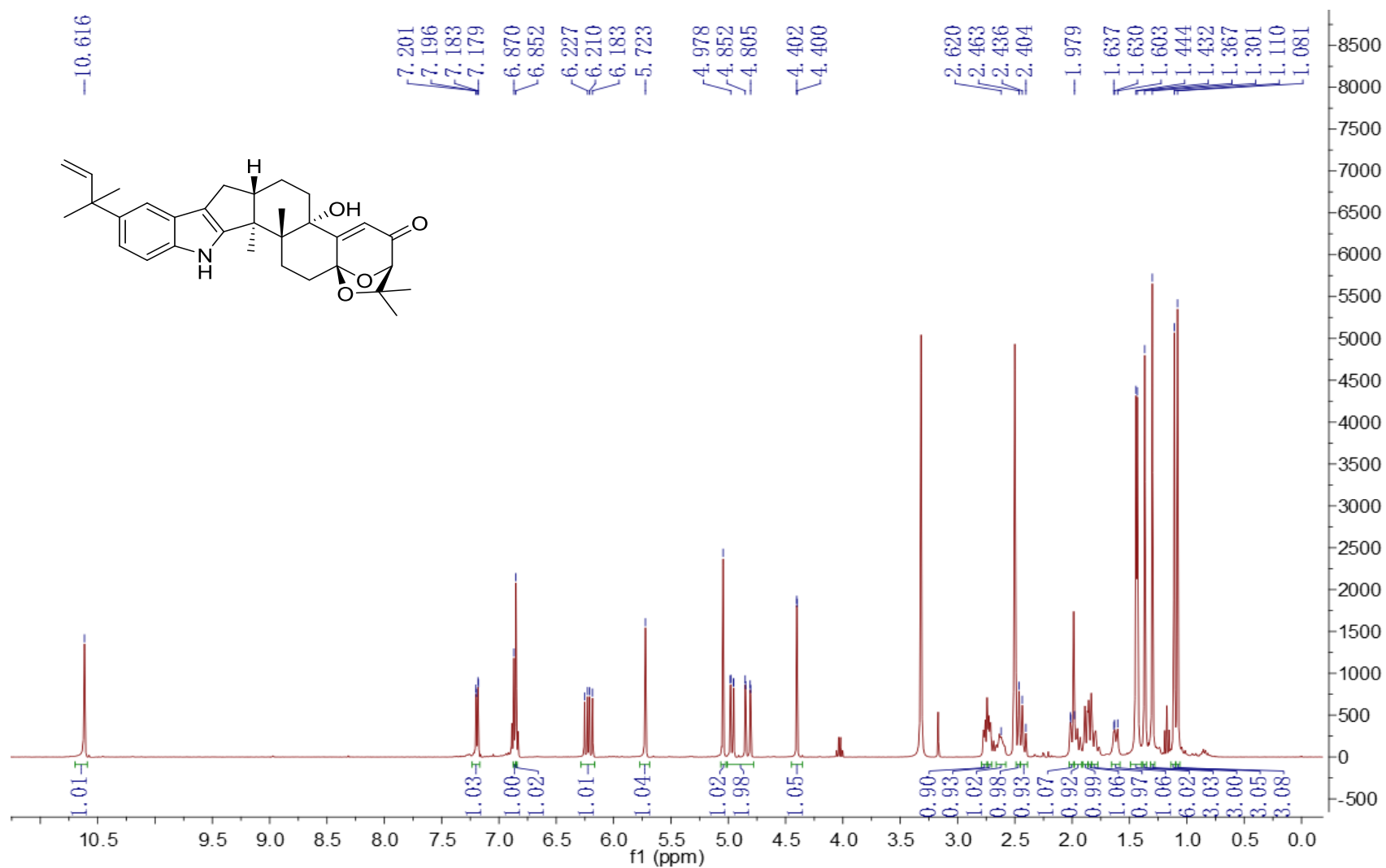


Figure S88. ^{13}C -NMR and DEPT spectra of β -aflatrem (**19**) in $\text{DMSO-}d_6$

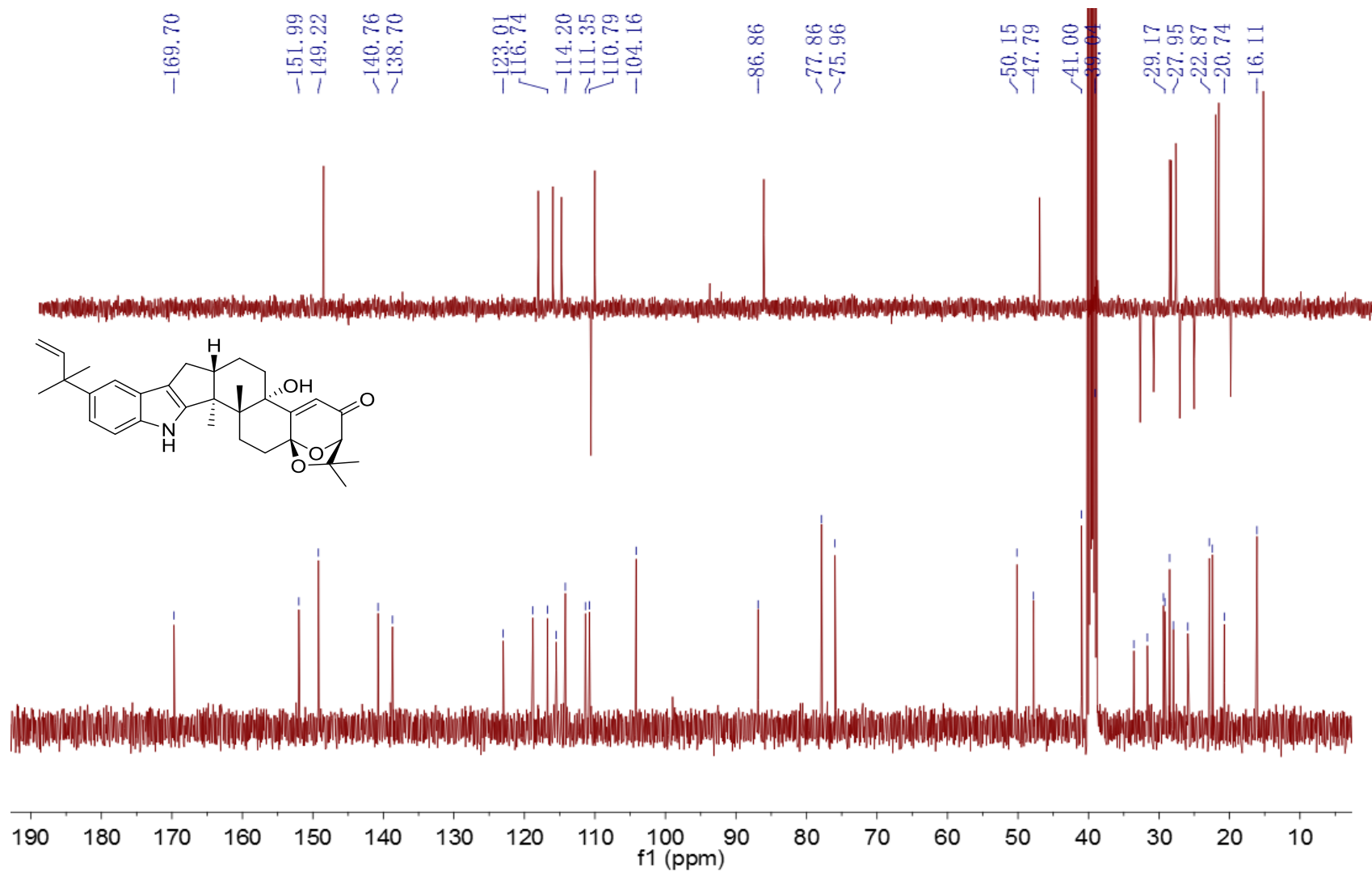


Figure S89. NOESY spectrum of β -aflatrem (**19**) in DMSO- d_6

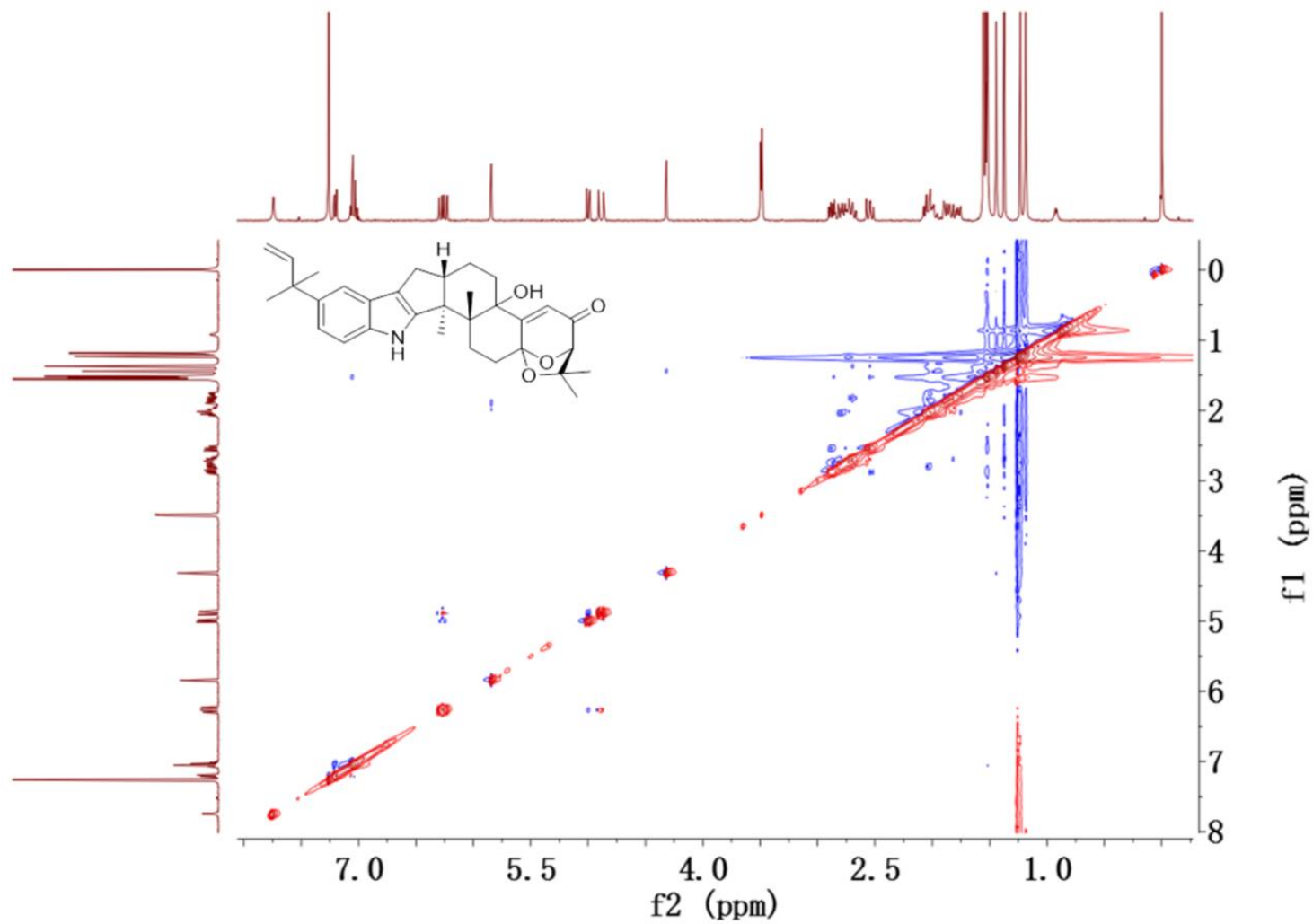


Figure S90. ^1H -NMR spectrum of pyripyropene A (**20**) in CDCl_3 (400MHz)

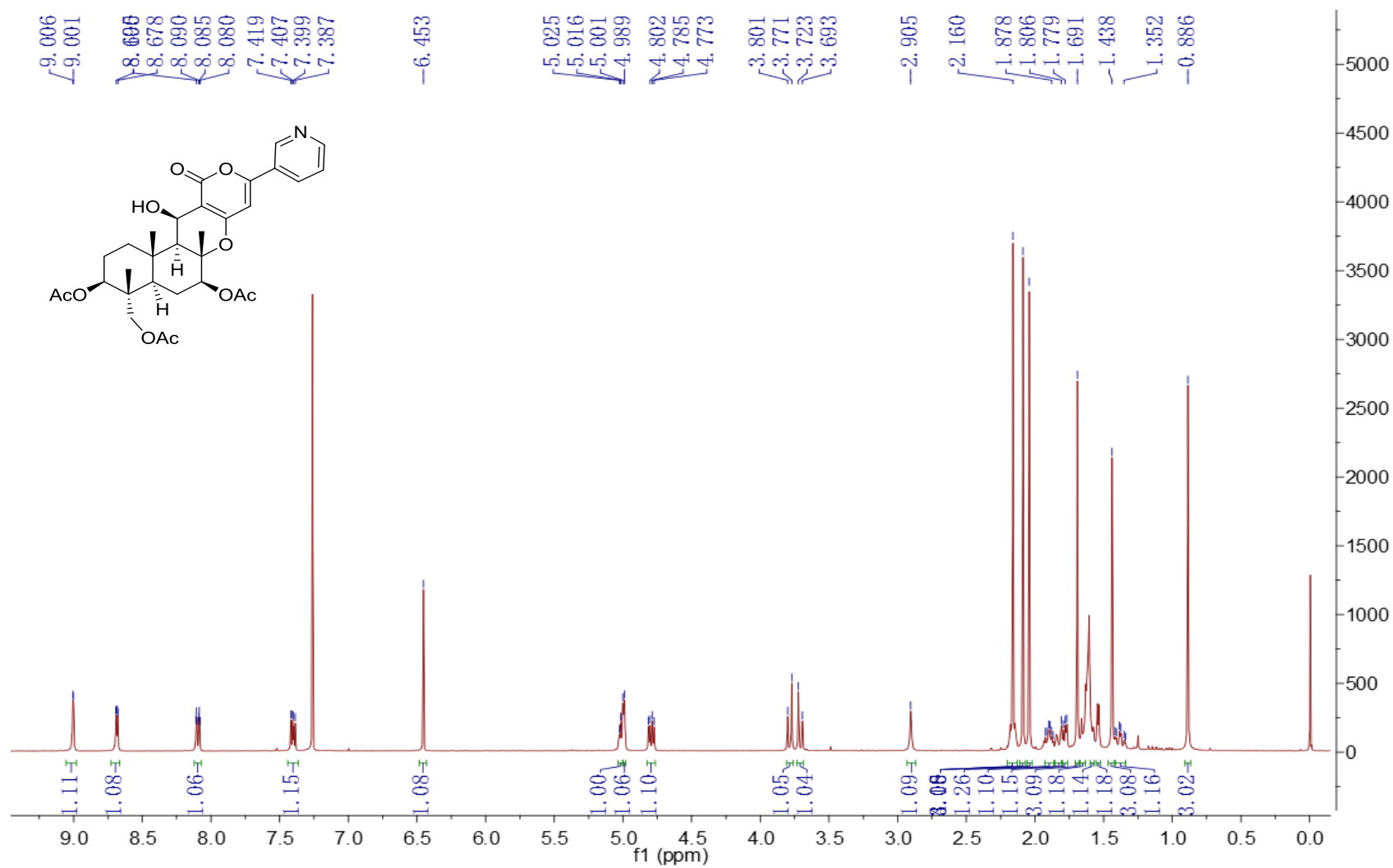


Figure S91. ^{13}C -NMR spectrum of pyripyropene A (**20**) in CDCl_3 (100MHz)

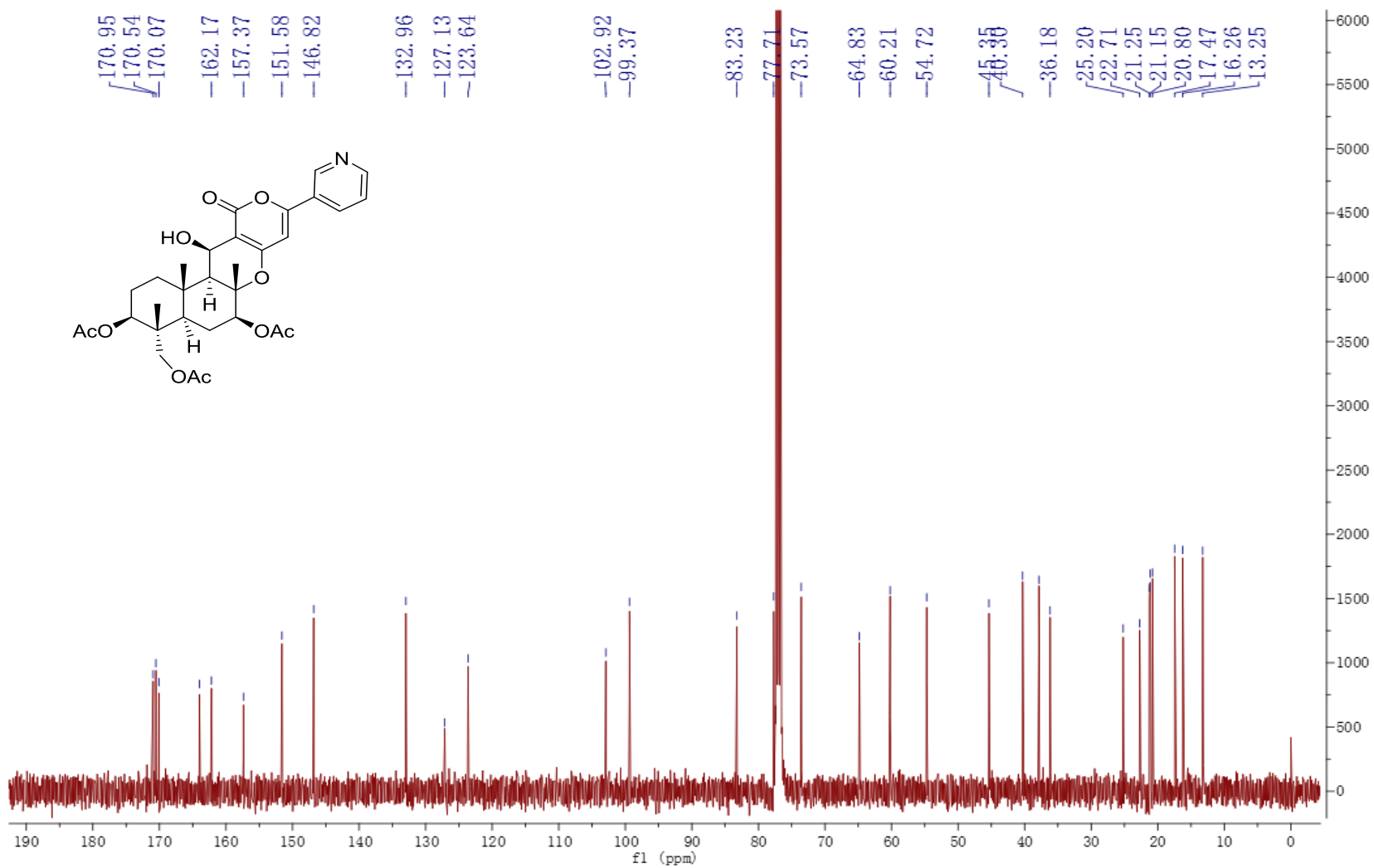


Figure S92. NOESY spectrum of pyripyropene A (**20**) in CDCl₃

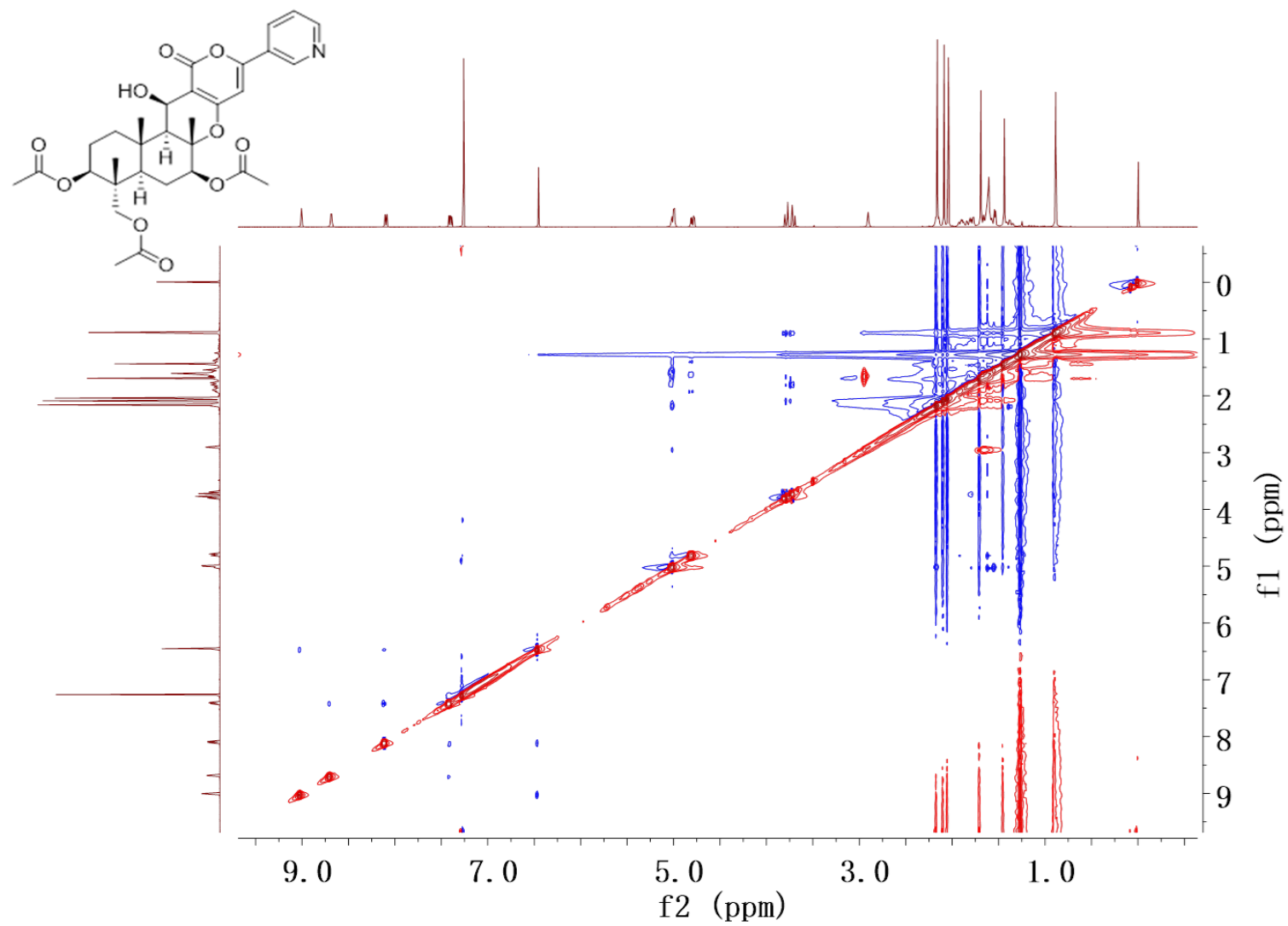
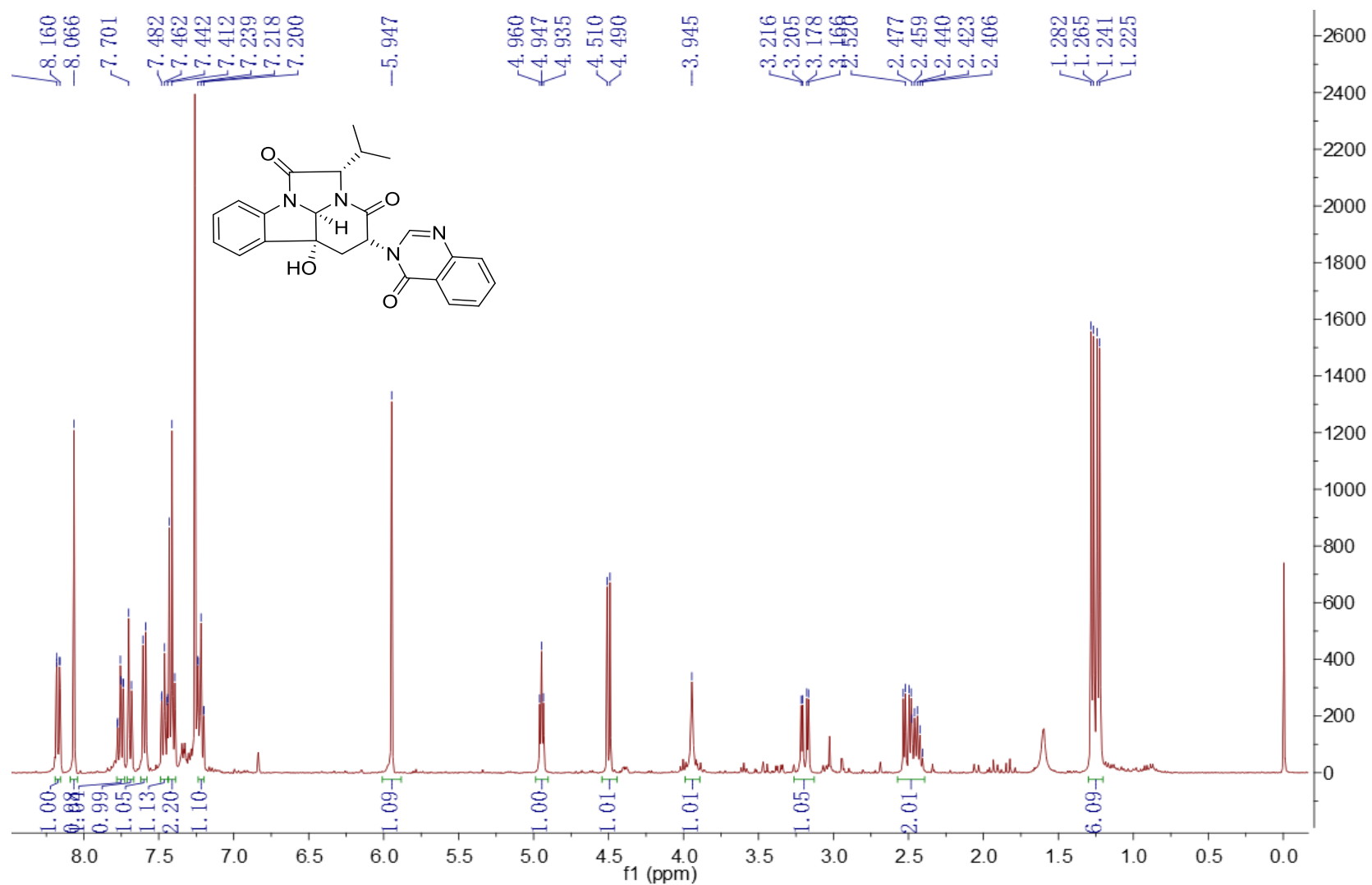


Figure S93. ^1H -NMR spectrum of pseudofischerine (**21**) in CDCl_3 (400MHz)



FigureS94. ^{13}C -NMR spectrum of pseudofischerine (**21**) in CDCl_3 (100MHz)

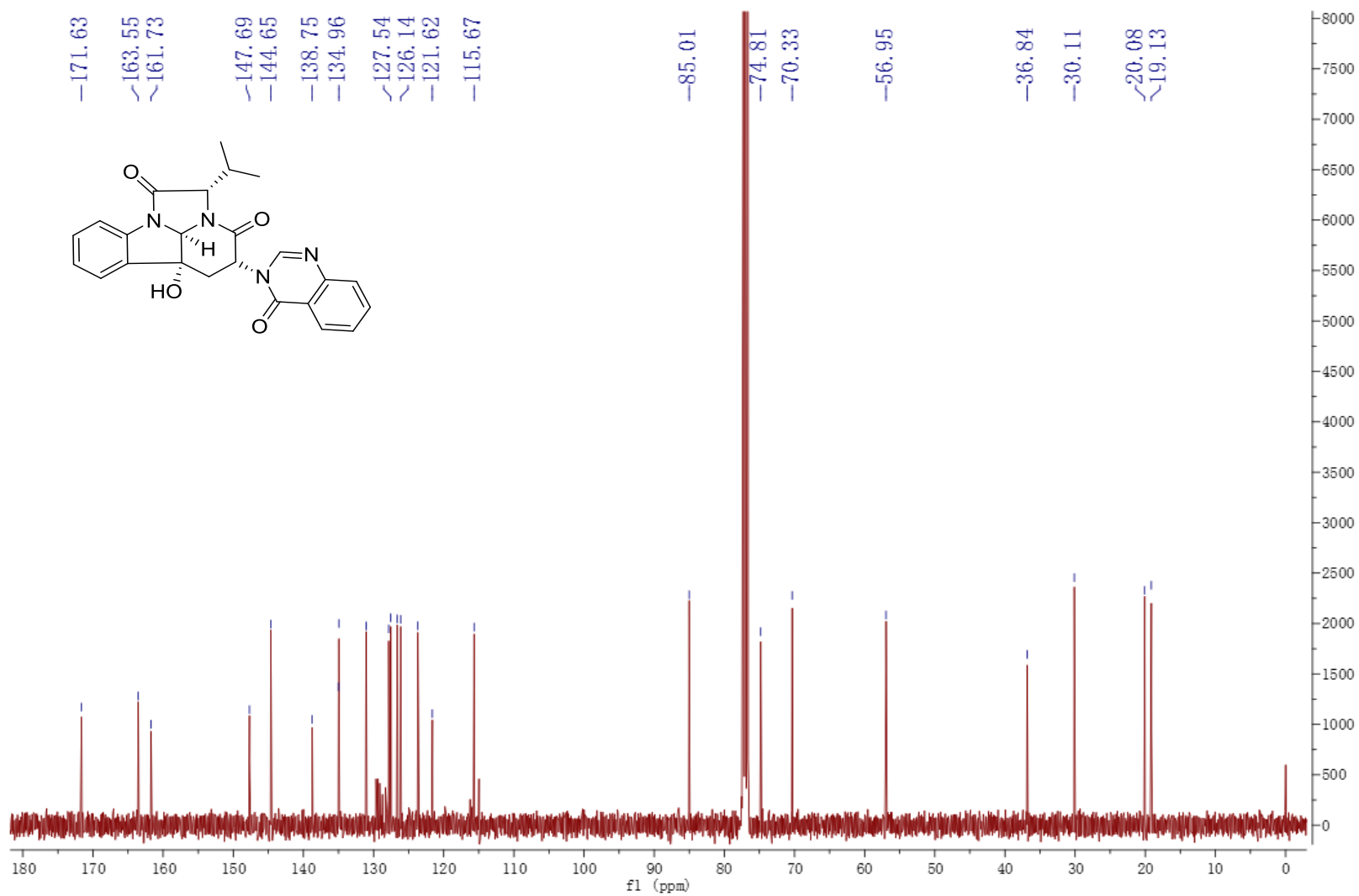


Figure S95. HMQC spectrum of pseudofischerine (**21**) in CDCl₃

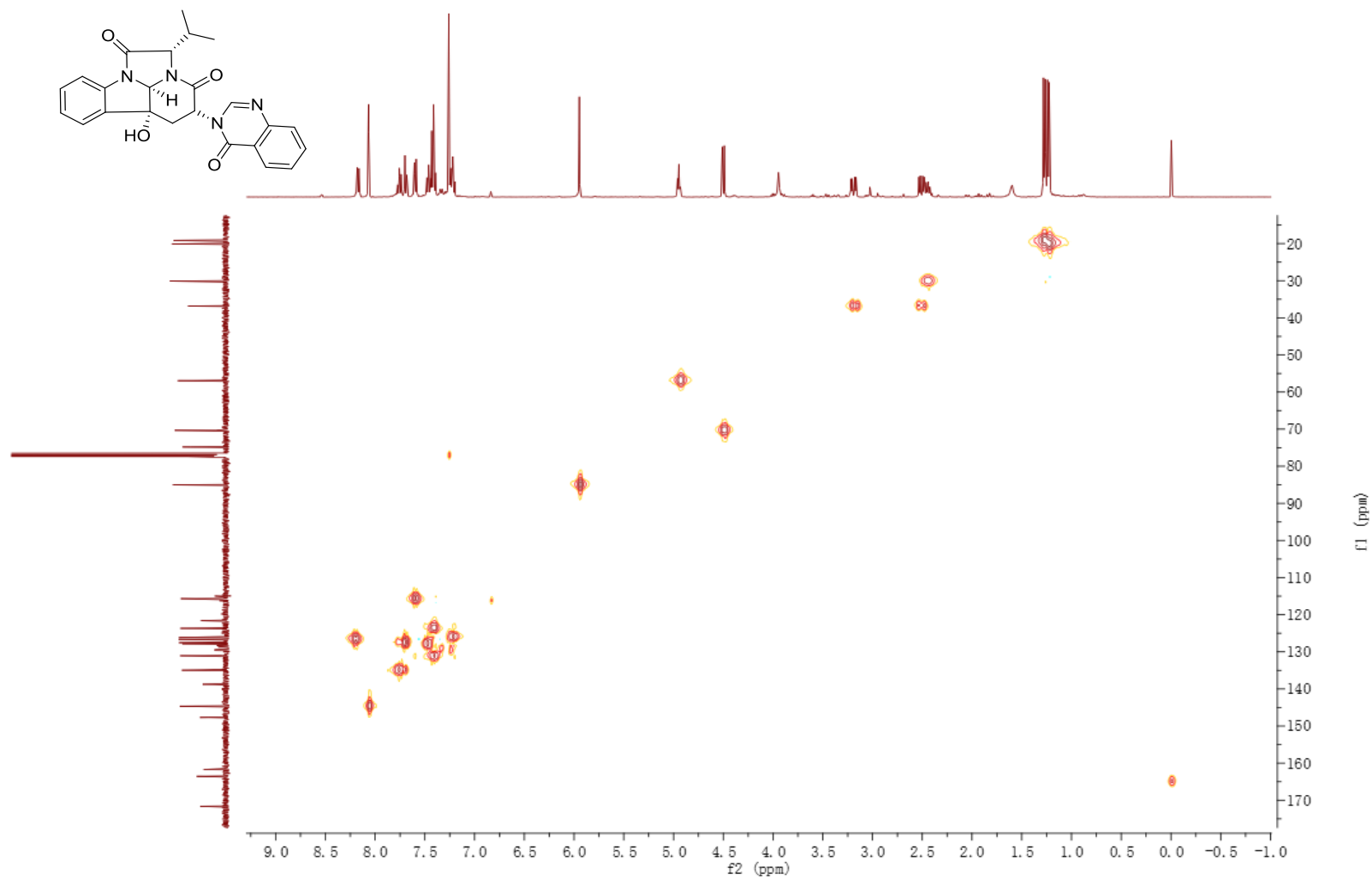


Figure S96. ^1H - ^1H COSY spectrum of pseudofischerine (**21**) in CDCl_3

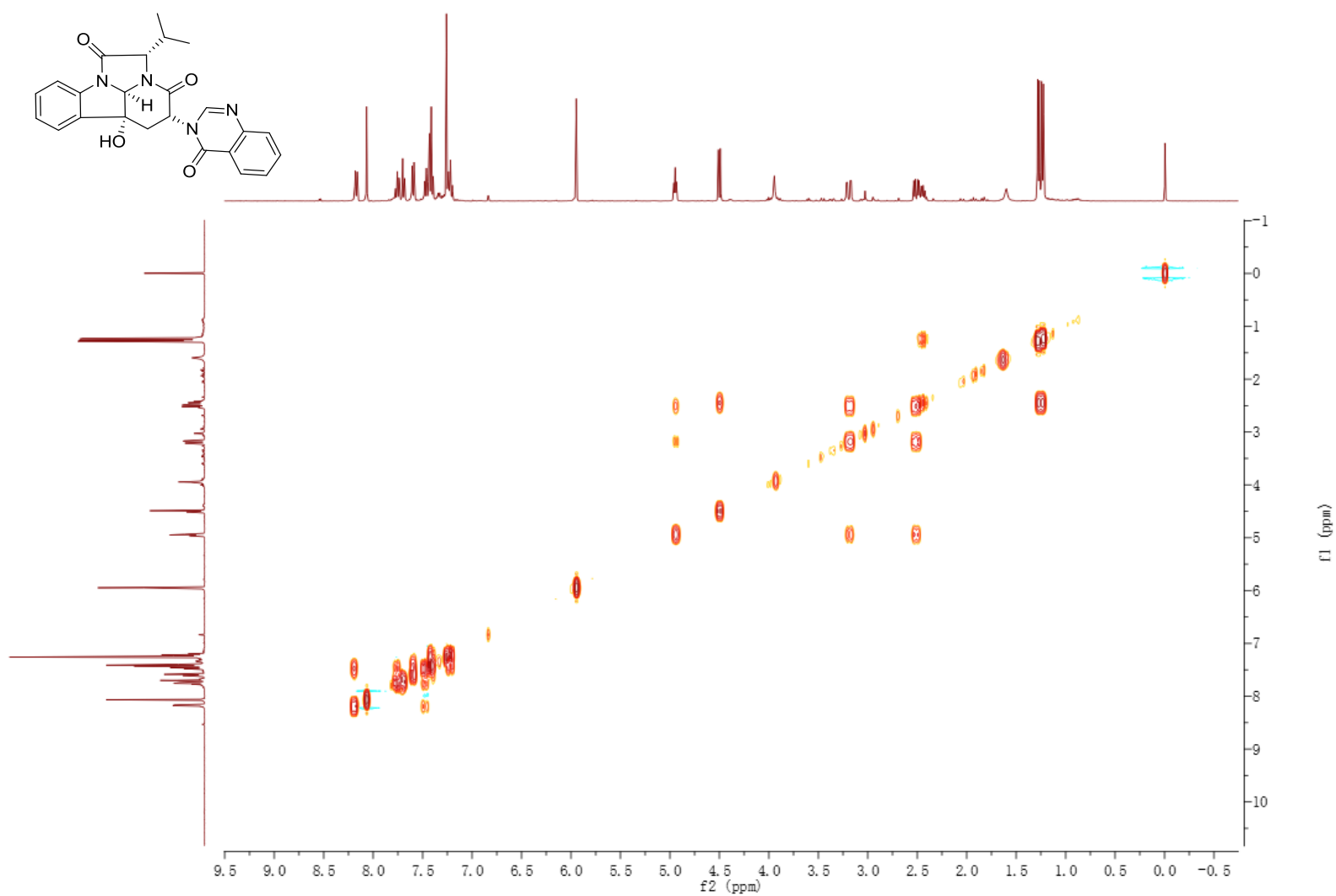


Figure S97. HMBC spectrum of pseudofischerine (**21**) in CDCl₃

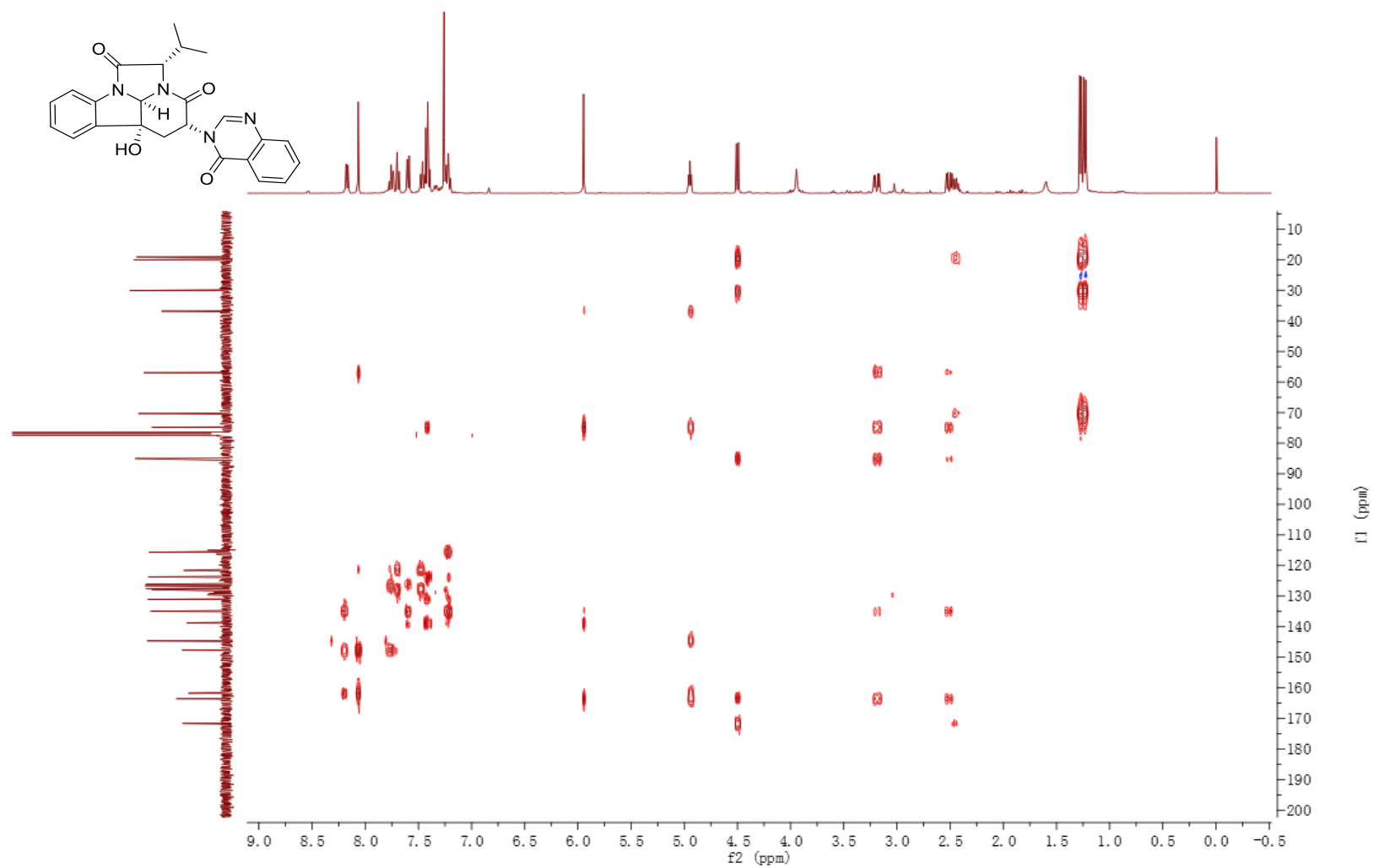


Figure S98. NOESY spectrum of pseudofischerine (**21**) in CDCl₃

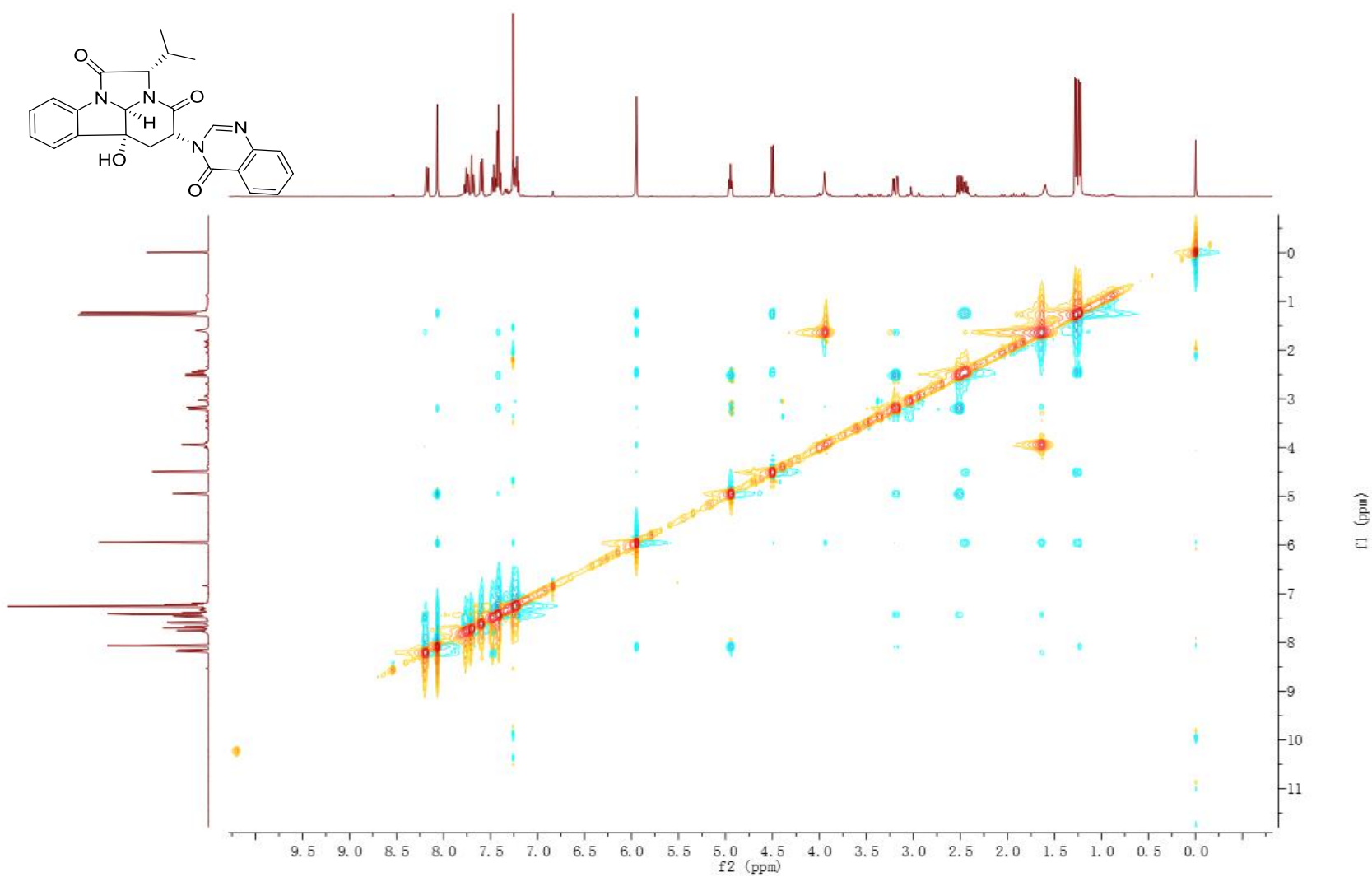


Figure S99. HR-EI-MS spectrum of 4-(1-hydroxy-1-methylpropyl)-2-isobutylpyrazin-2(1H)-one (**22**) in CDCl₃

Instrument: MAT 95XP (Thermo)

D:\DATA-HR\15\010701-f19-6-2-3-c1

1/7/2015 4:45:45 F

010701-f19-6-2-3-c1 #25 RT: 0.93 AV: 1 NL: 8.28E4

T: + c EI Full ms [216.50-233.50]



Figure S100. ^1H -NMR spectrum of 4-(1-hydroxy-1-methylpropyl)-2-isobutylpyrazin-2(1H)-one (**22**) in CDCl_3 (400MHz)

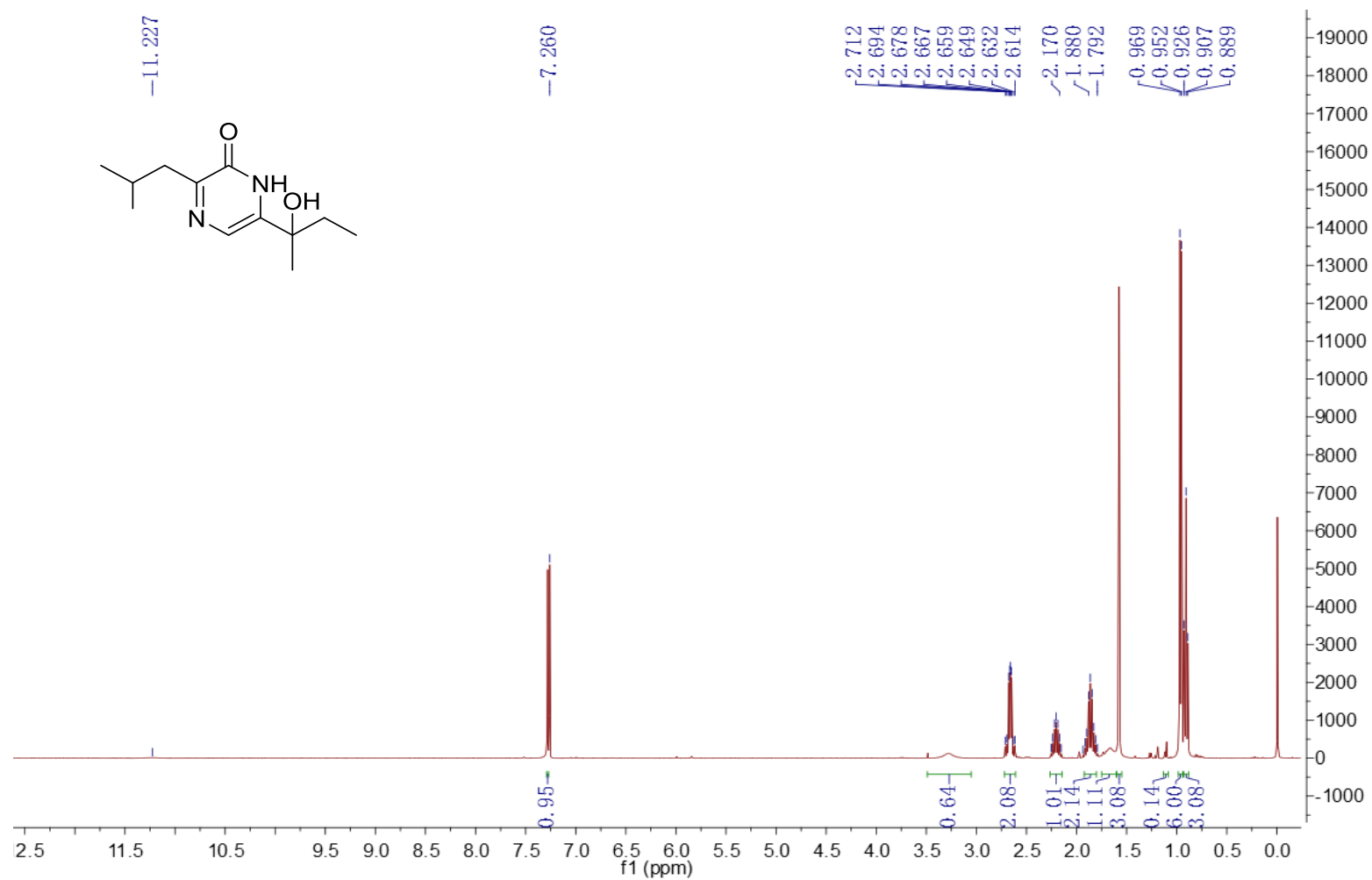


Figure S101. ^{13}C -NMR and DEPT spectra of 4-(1-hydroxy-1-methylpropyl)-2-isobutylpyrazin-2(1H)-one (**22**) in CDCl_3 (100MHz)

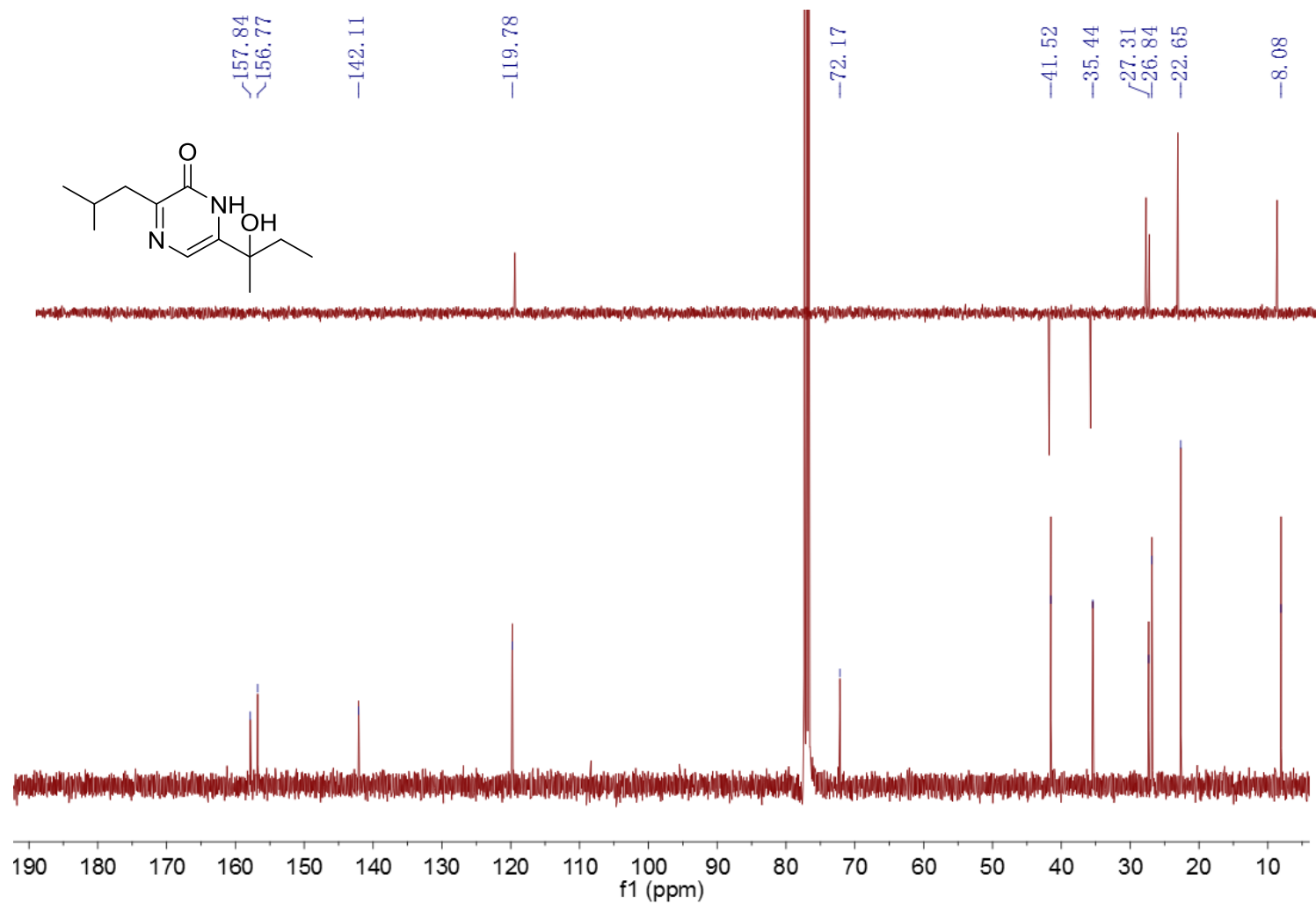


Figure S102. HR-EI-MS spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in CDCl₃

Instrument: MAT 95XP(Thermo)

D:\DATA-HR\15\010701-f19-6-2-3-c1

1/7/2015 4:45:45 F

010701-f19-6-2-3-c1 #25 RT: 0.93 AV: 1 NL: 8.28E4

T: + c EI Full ms [216.50-233.50]



Figure S103. ^1H -NMR spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in CDCl_3 (400MHz)

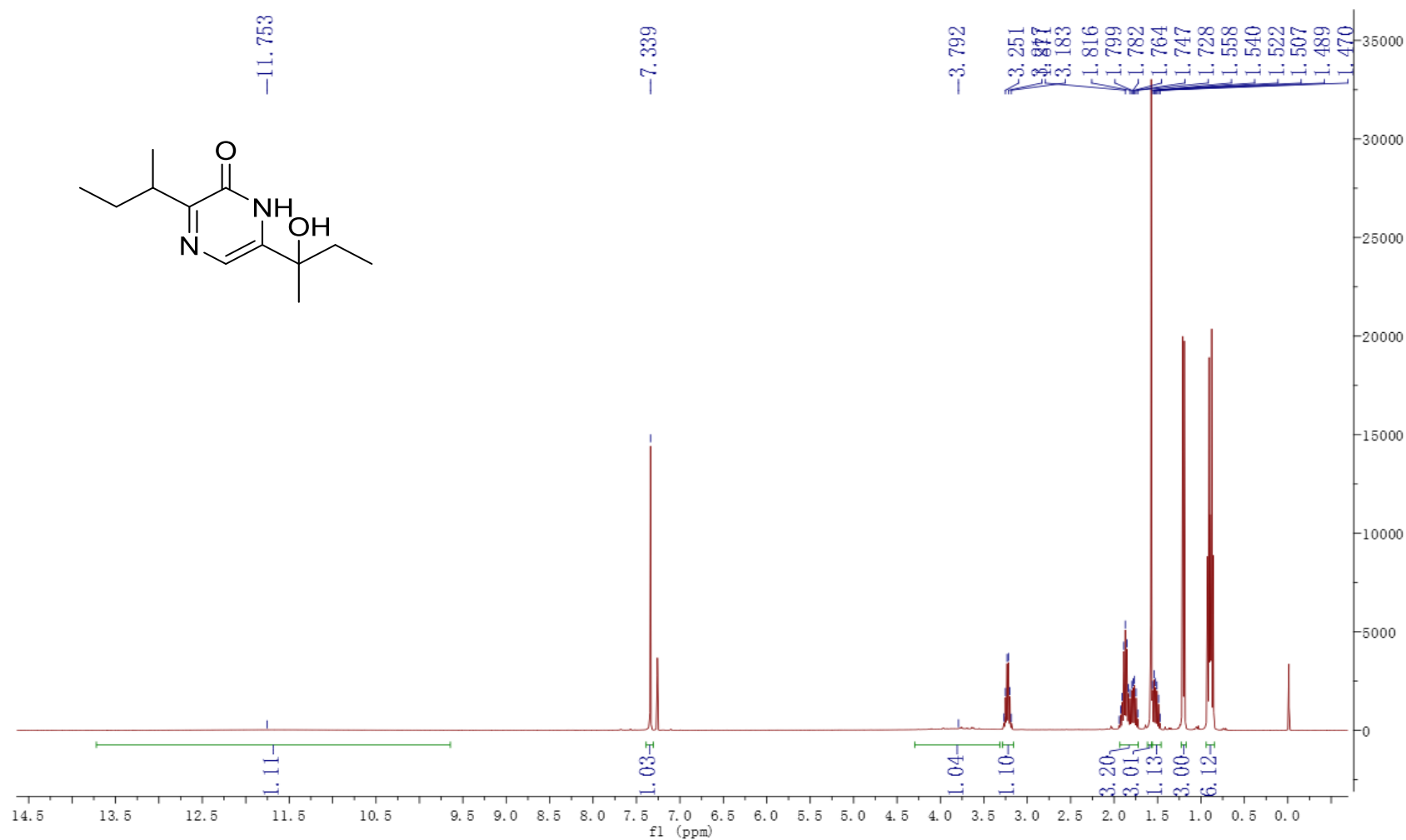


Figure S104. ^{13}C -NMR and DEPT spectra of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in CDCl_3 (100MHz)

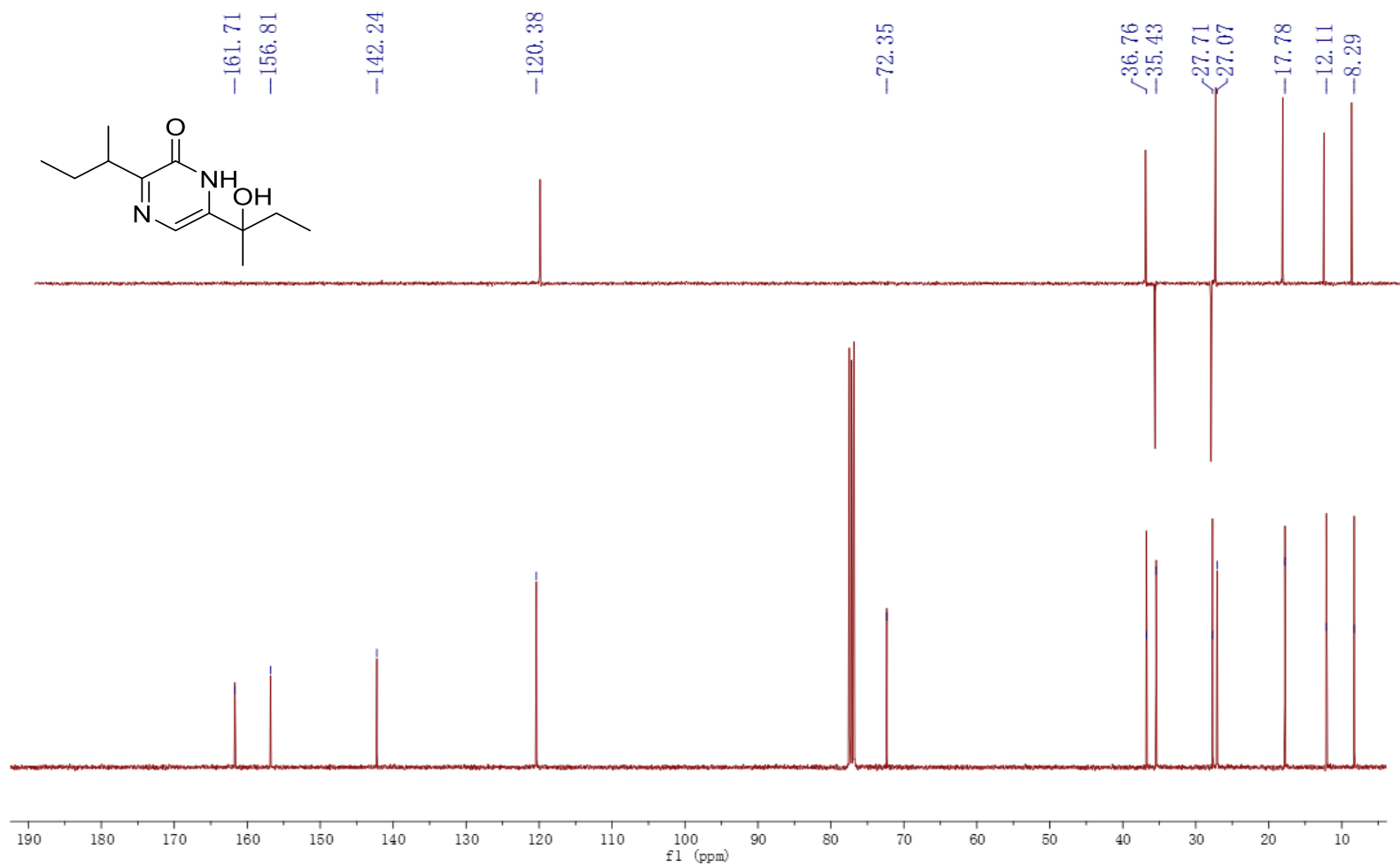


Figure S105. HMQC spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in CDCl₃

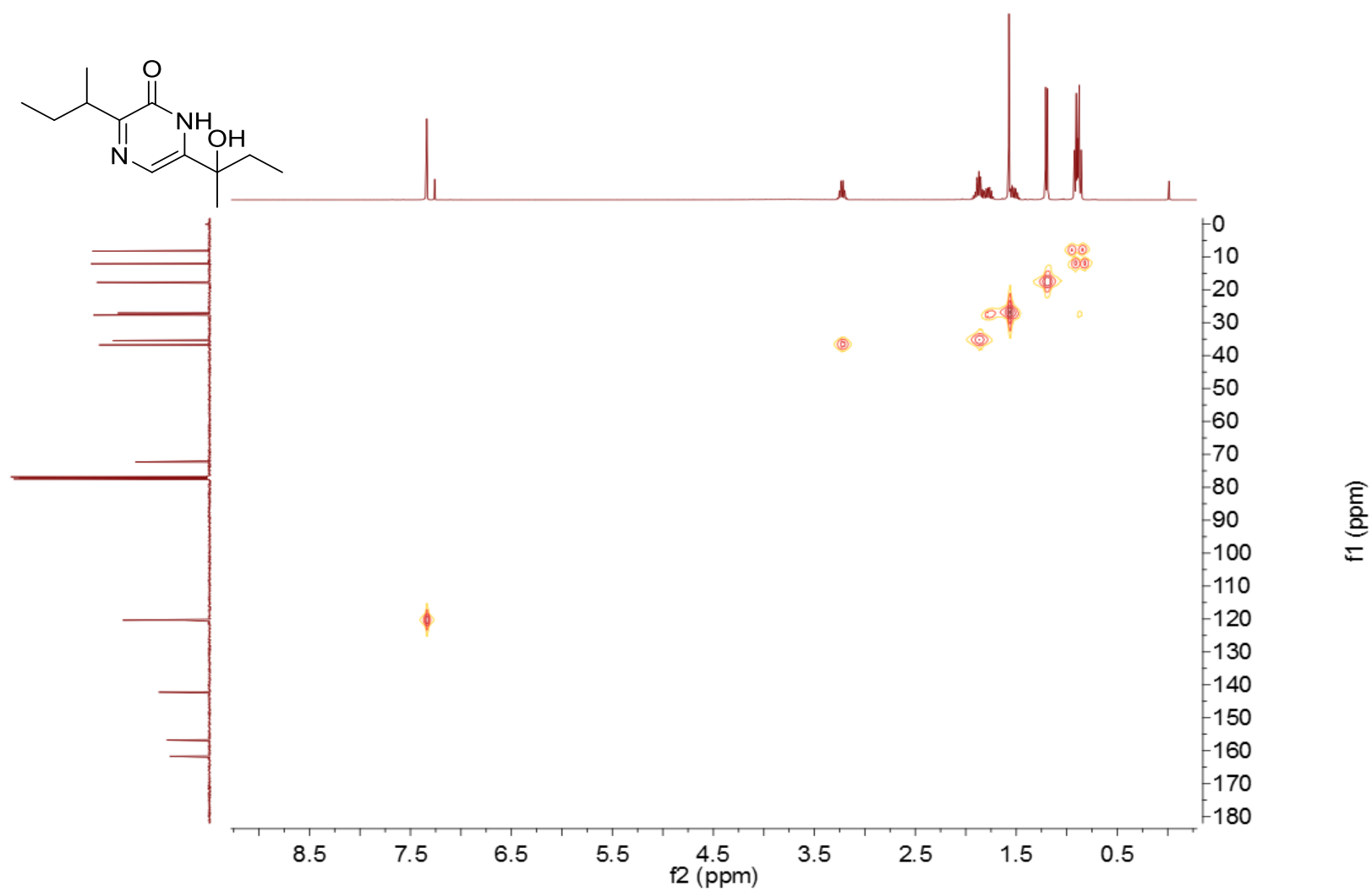


Figure S106. ^1H - ^1H COSY spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in CDCl_3

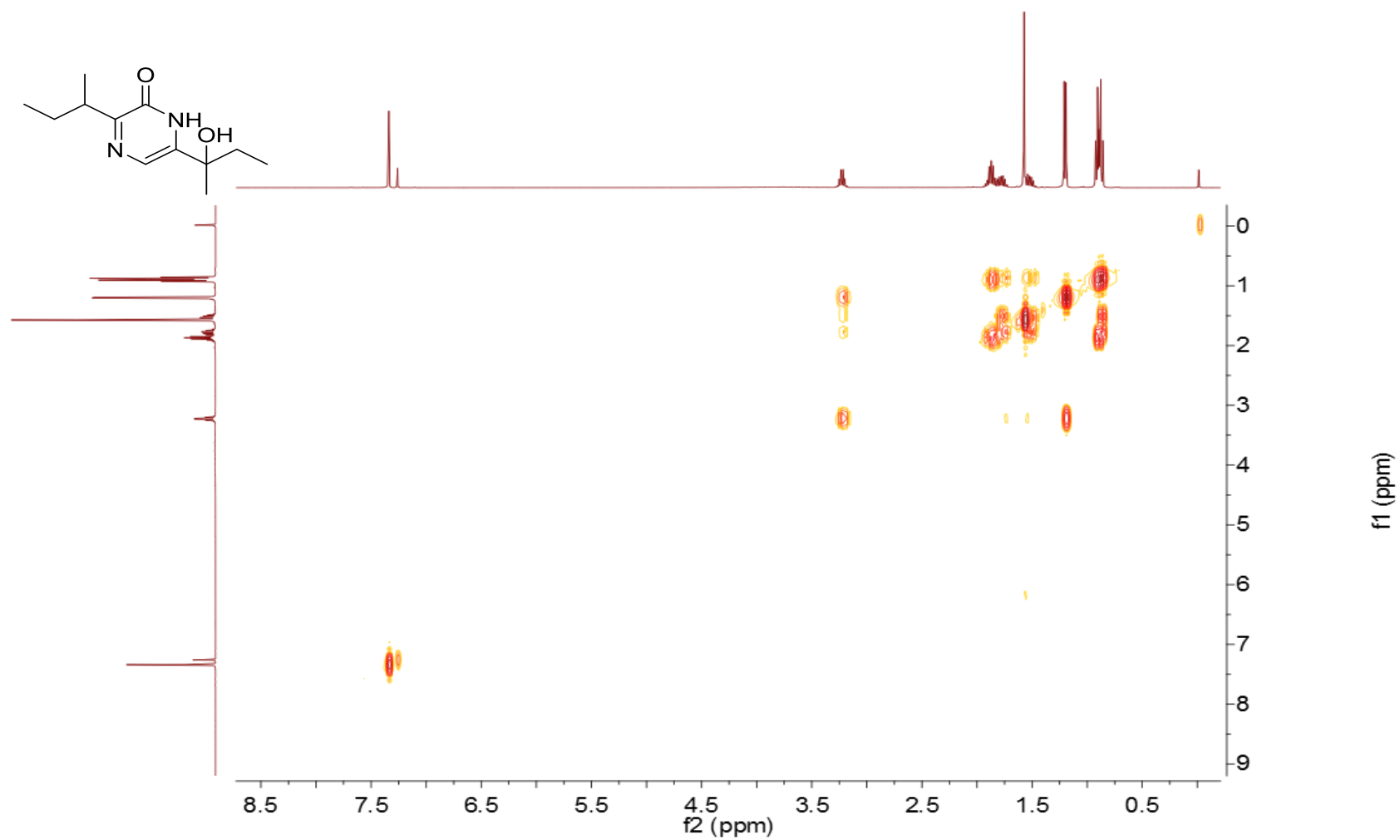


Figure S107. HMBC spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in CDCl₃

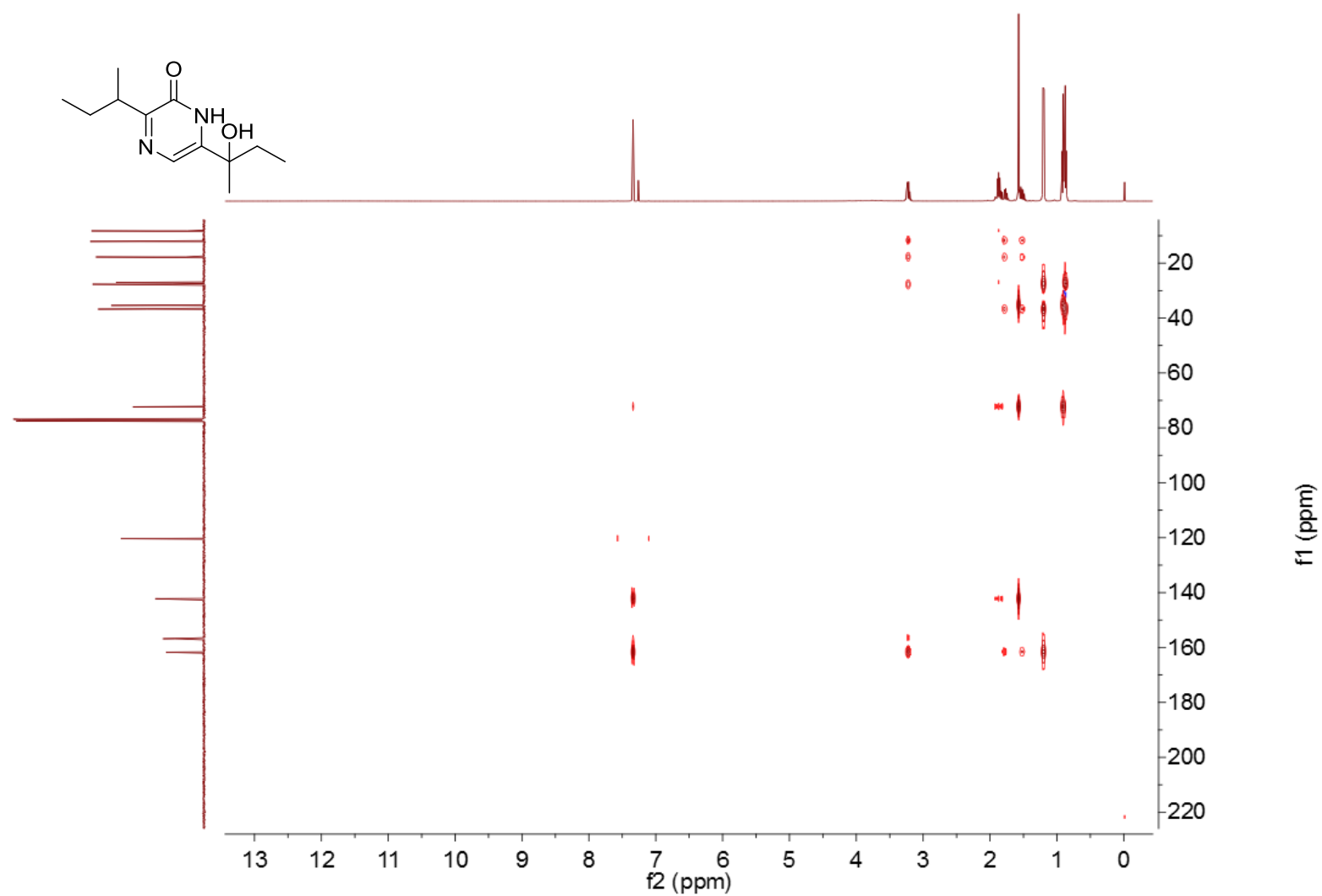


Figure S108. ^1H -NMR spectrum of O-methylsterigmatocystin (**24**) in CDCl_3 (400MHz)

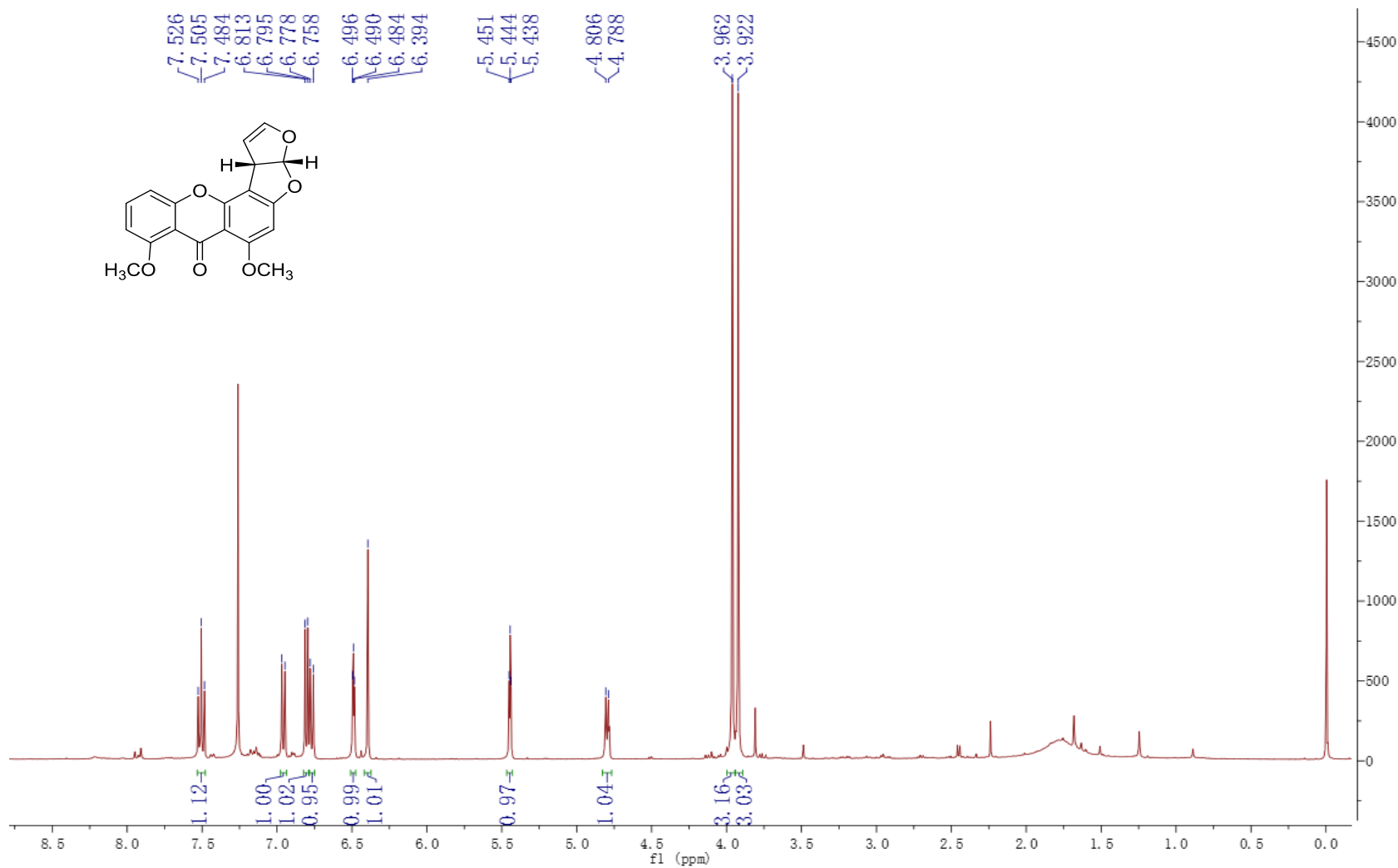


Figure S109. ^{13}C -NMR spectrum of O-methylsterigmatocystin (**24**) in CDCl_3 (100MHz)

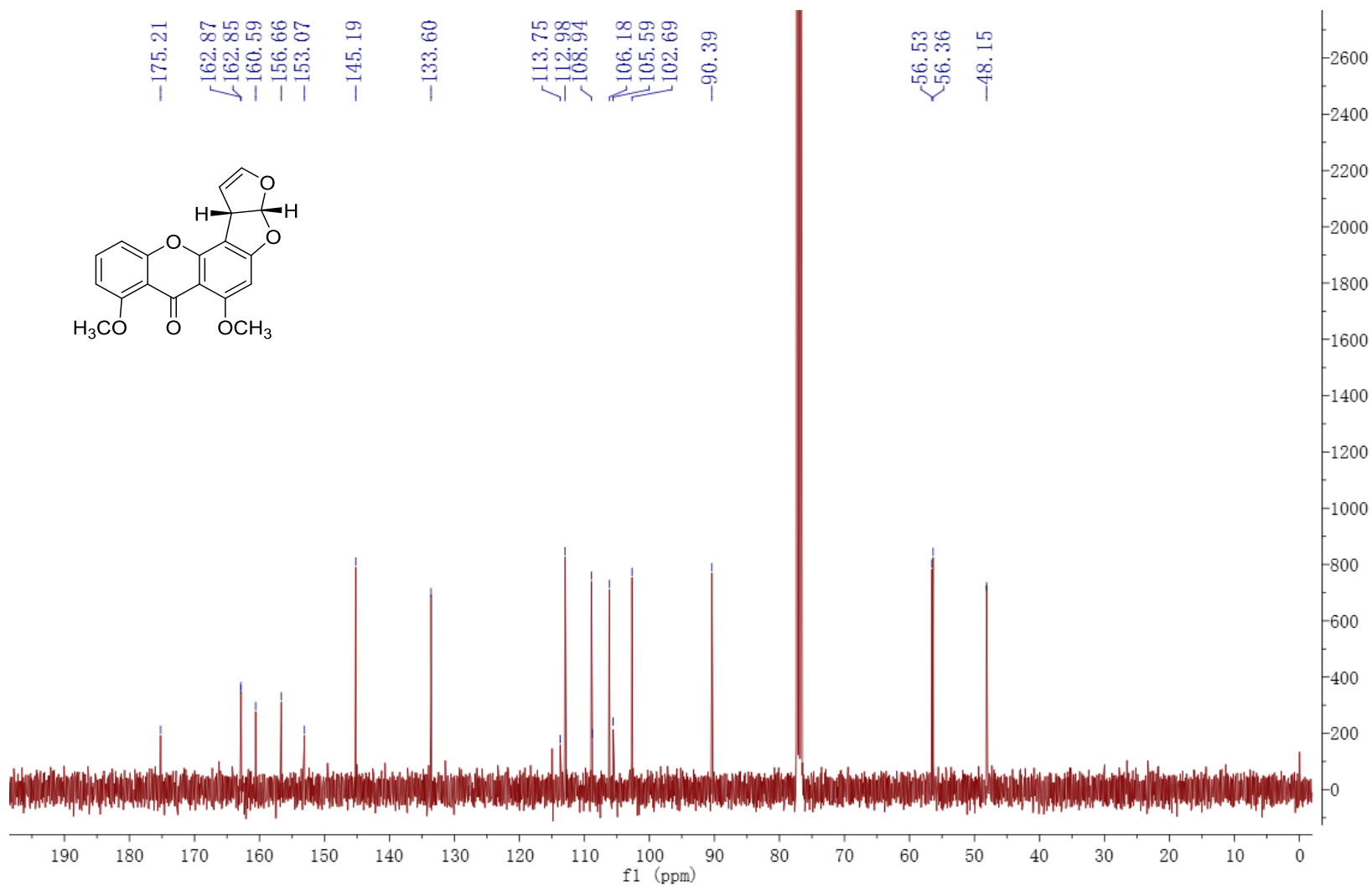


Figure S110. NOESY spectrum of O-methylsterigmatocystin (**24**) in CDCl₃

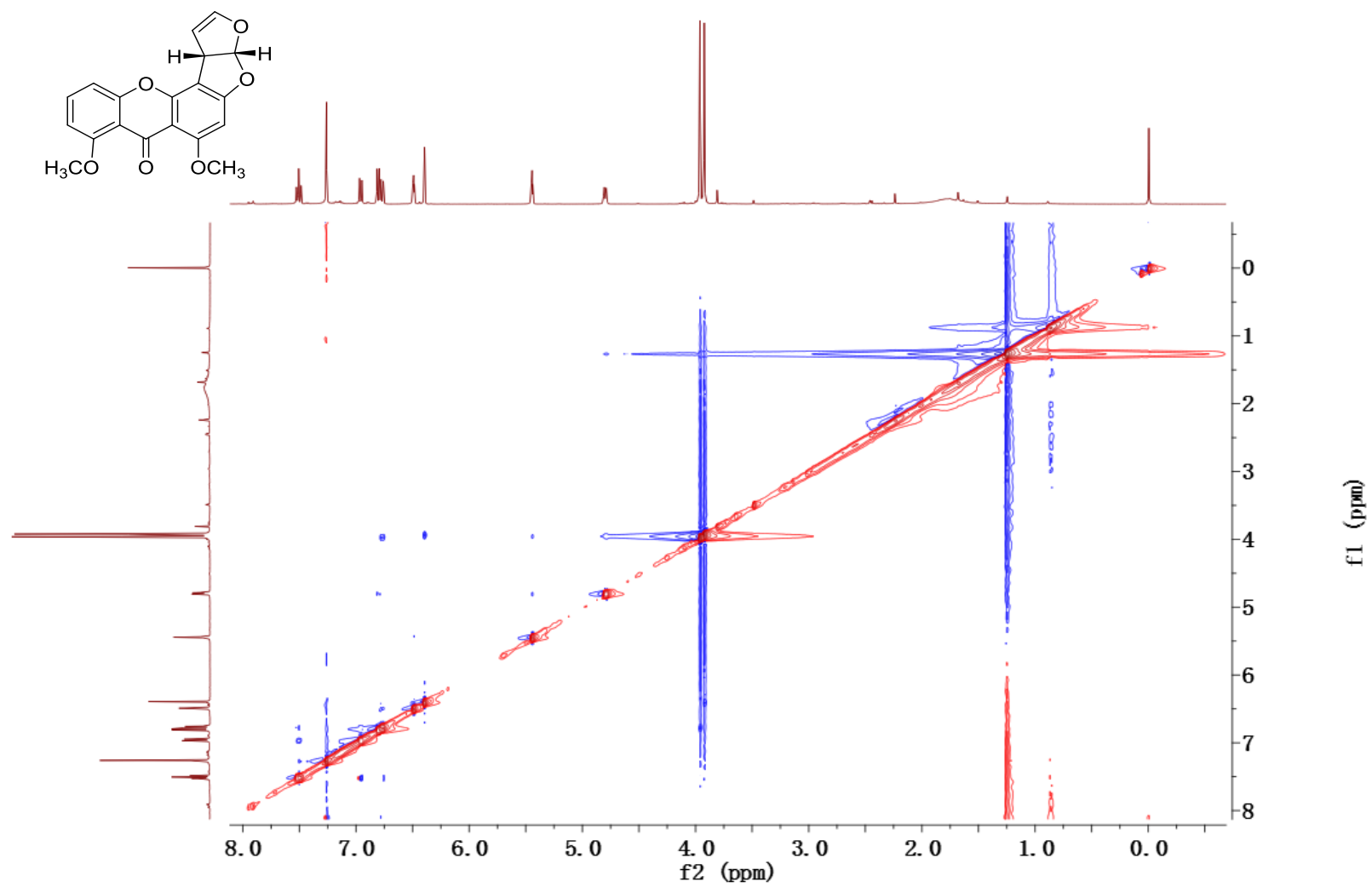


Figure S111. ^1H -NMR spectrum of asperfuran (25) in CDCl_3 (400MHz)

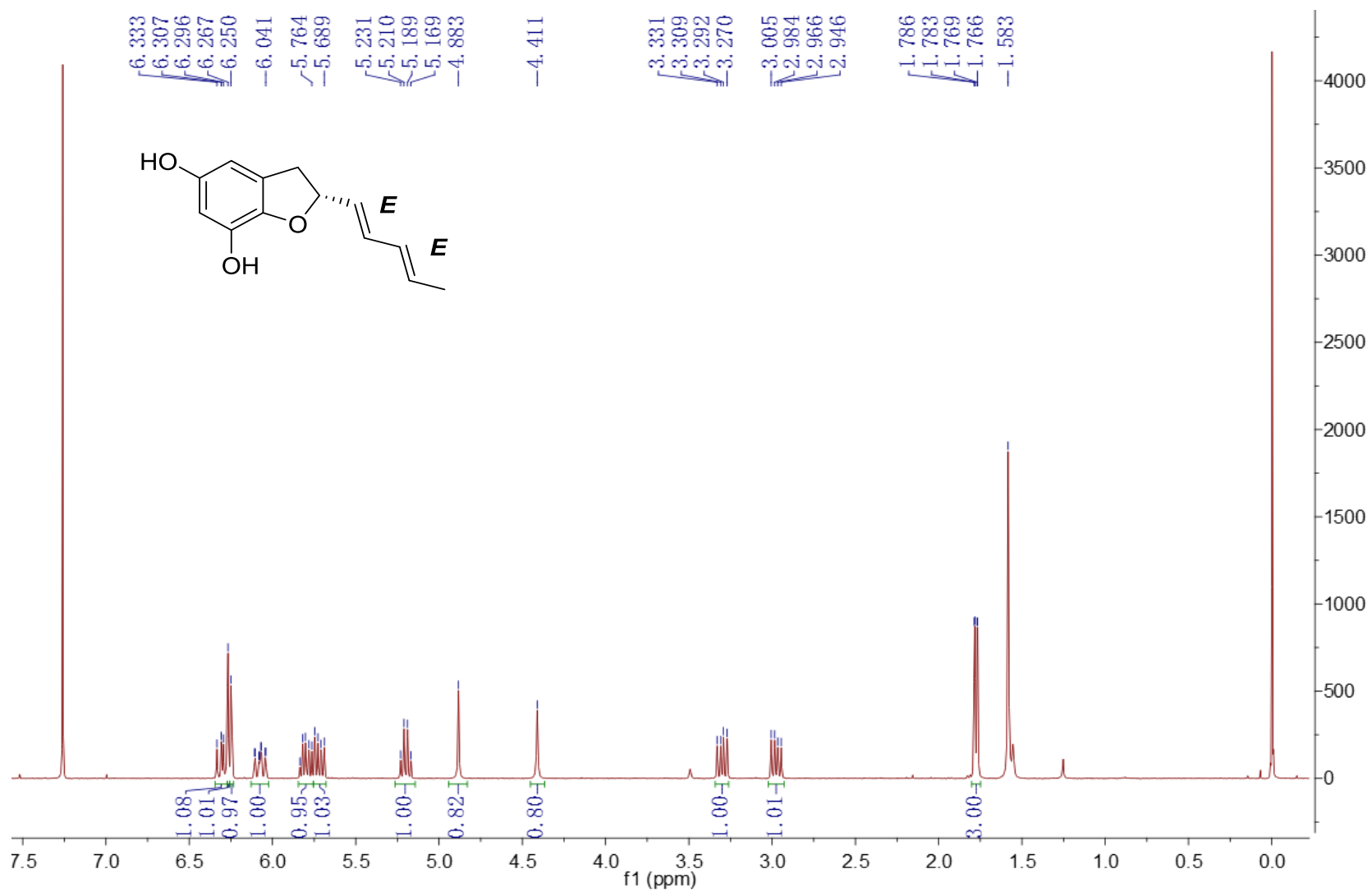


Figure S112. ^{13}C -NMR spectrum of asperfuran (25) in CDCl_3 (100MHz)

