Supporting Information

Secondary Metabolites with Chemical Diversity from the Marine-derived Fungus *Pseudallescheria boydii* F19-1 and Their Cytotoxic Activity

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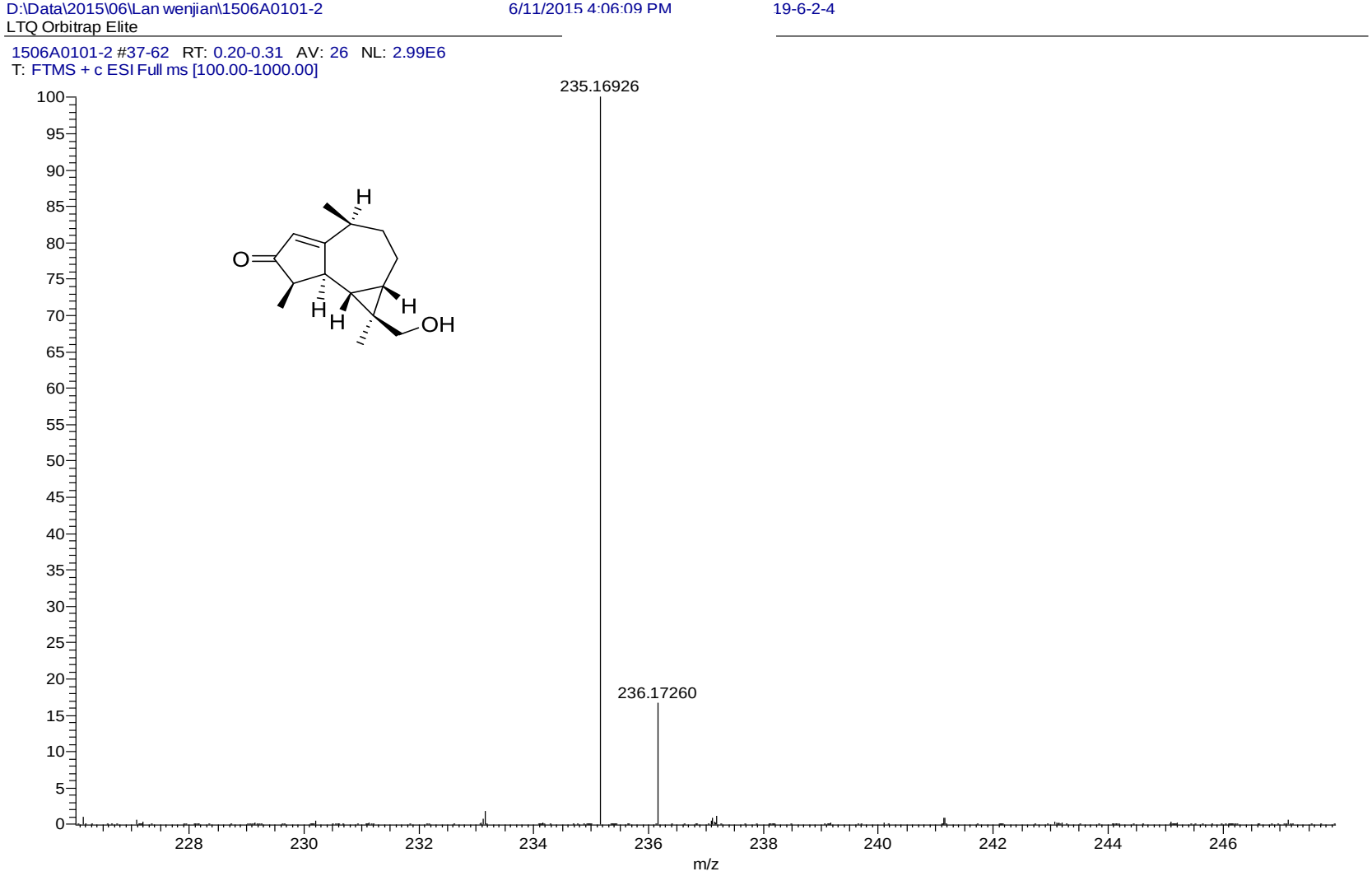


Figure S2. ^{1}H-NMR spectrum of pseuboydone A **(1)** in $CDCl_3$ (400MHz)

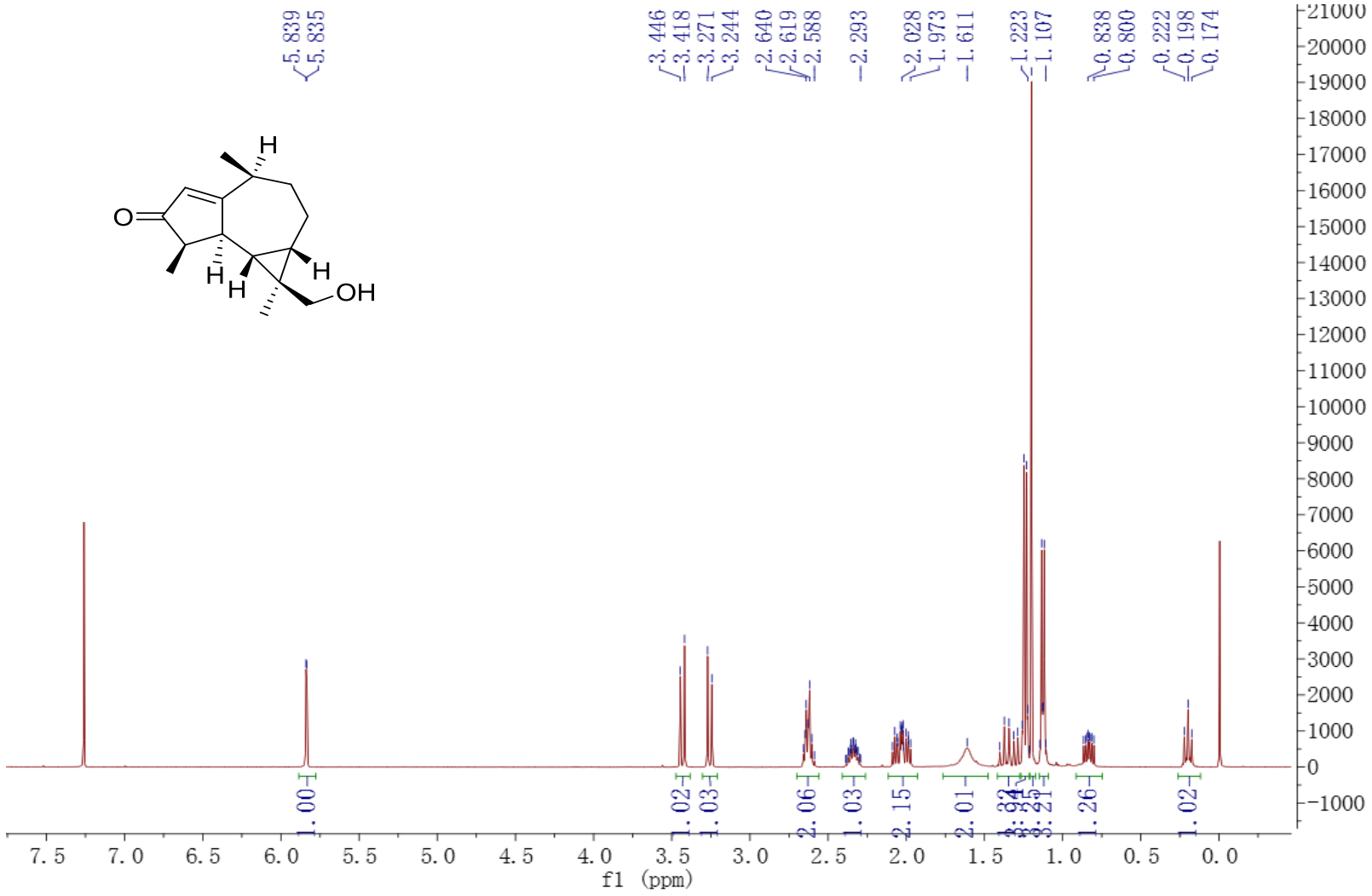


Figure S3. ^{13}C NMR and DEPT spectra of pseuboydone A **(1)** in $CDCl_3$ (100MHz)

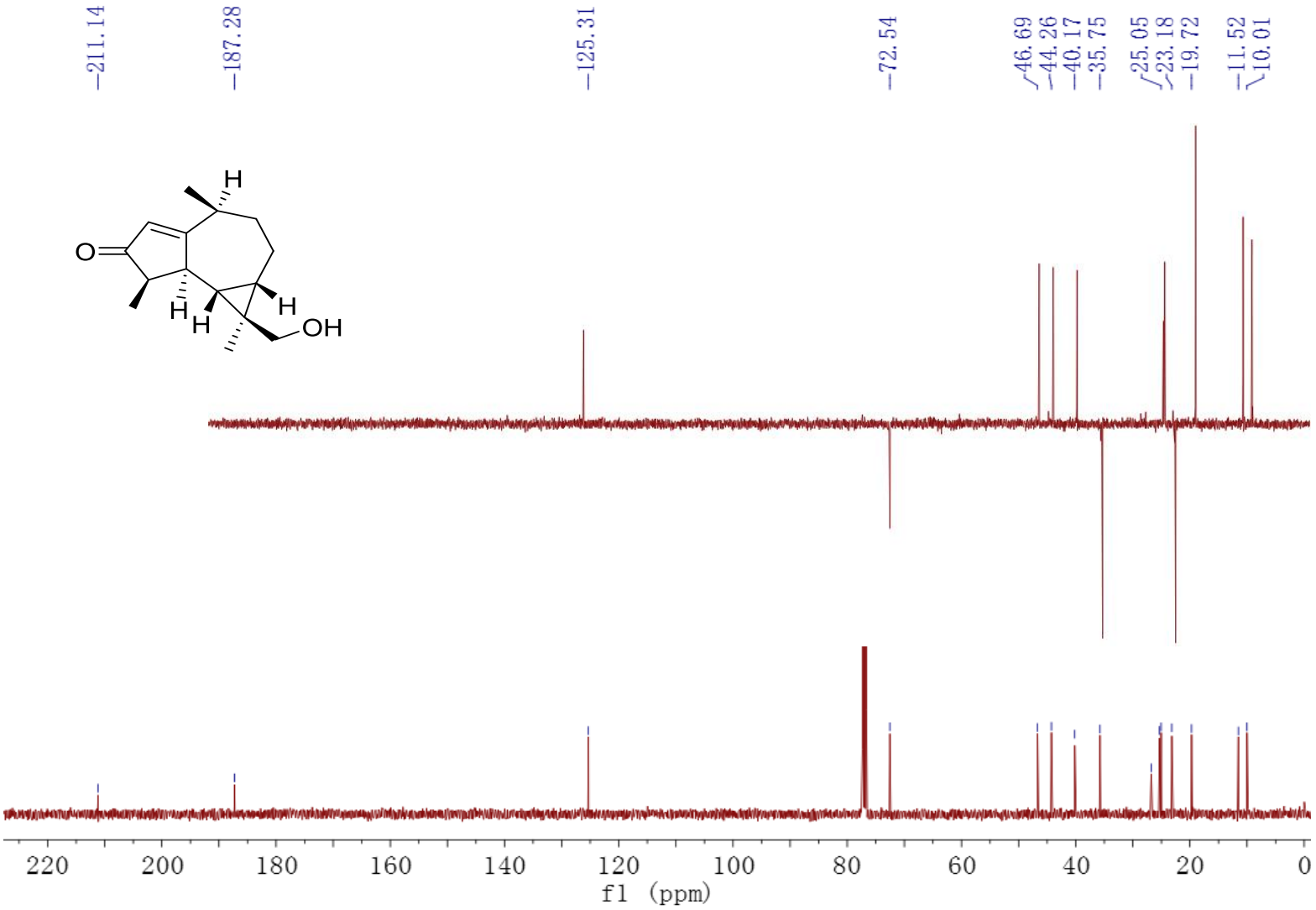


Figure S4. HMQC spectrum of pseuboydone A **(1)** in $CDCl_3$

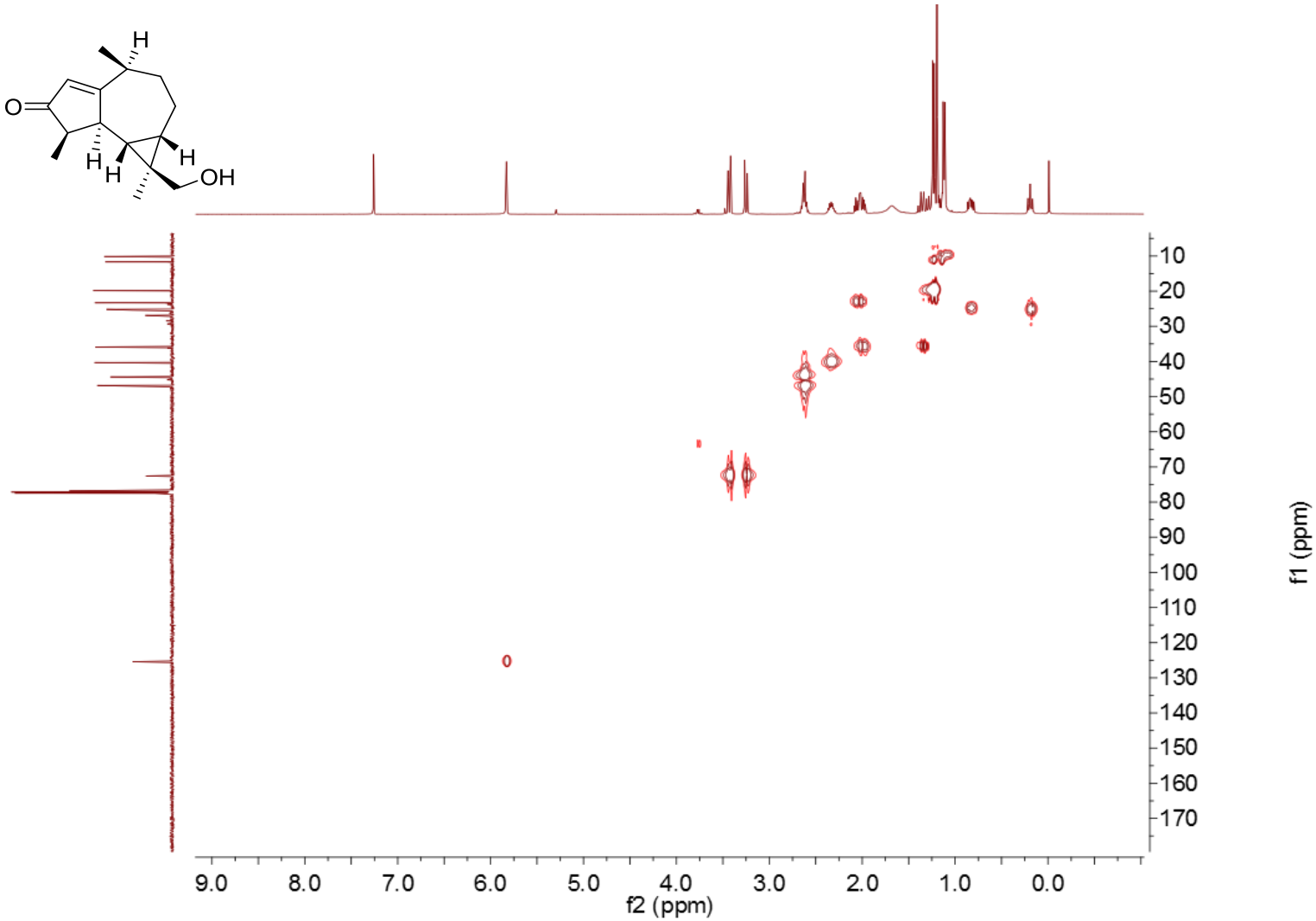


Figure S5. ^{1}H-^{1}H COSY spectrum of pseuboydone A **(1)** in $CDCl_3$

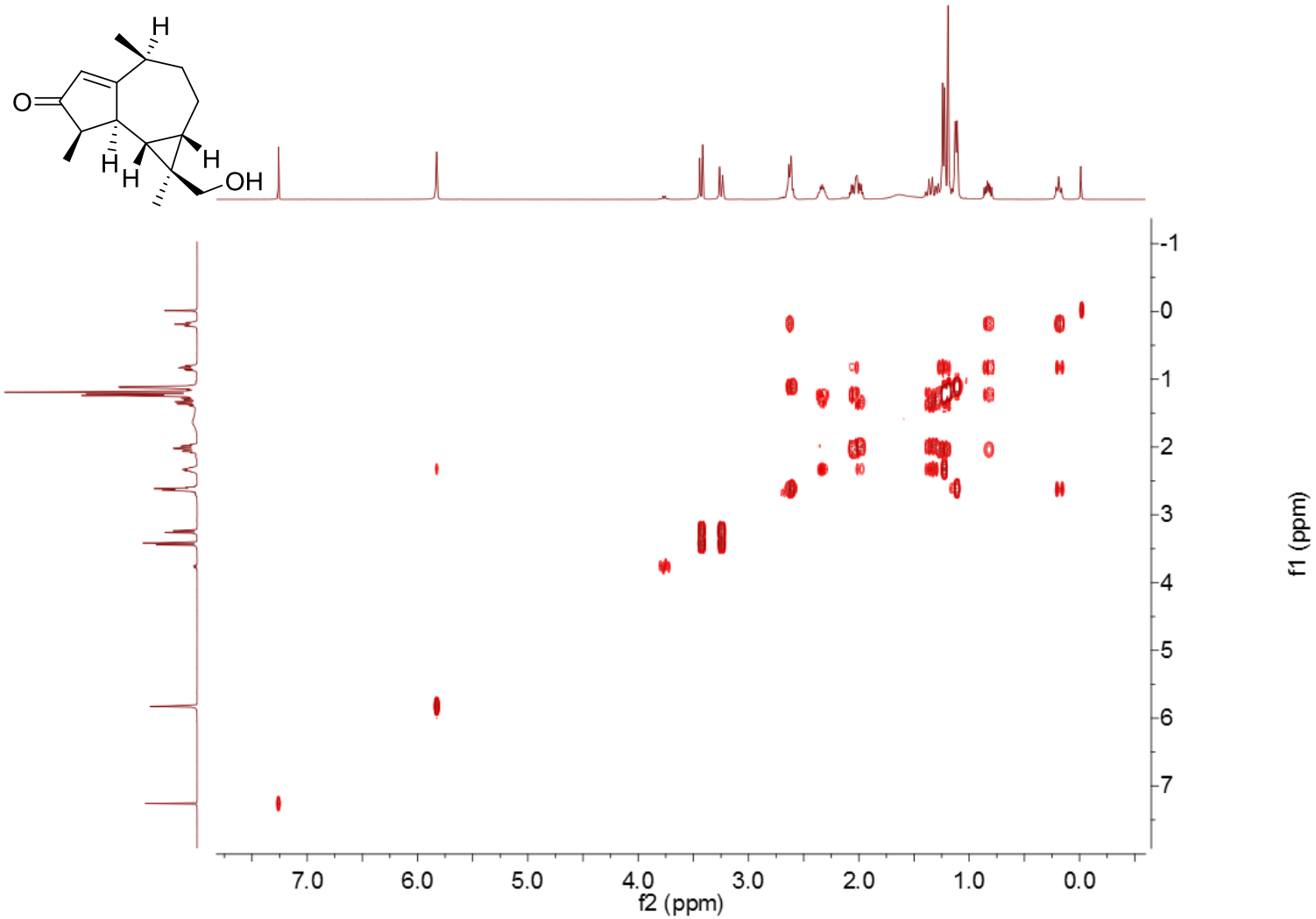


Figure S6. HMBC spectrum of pseuboydone A **(1)** in $CDCl_3$

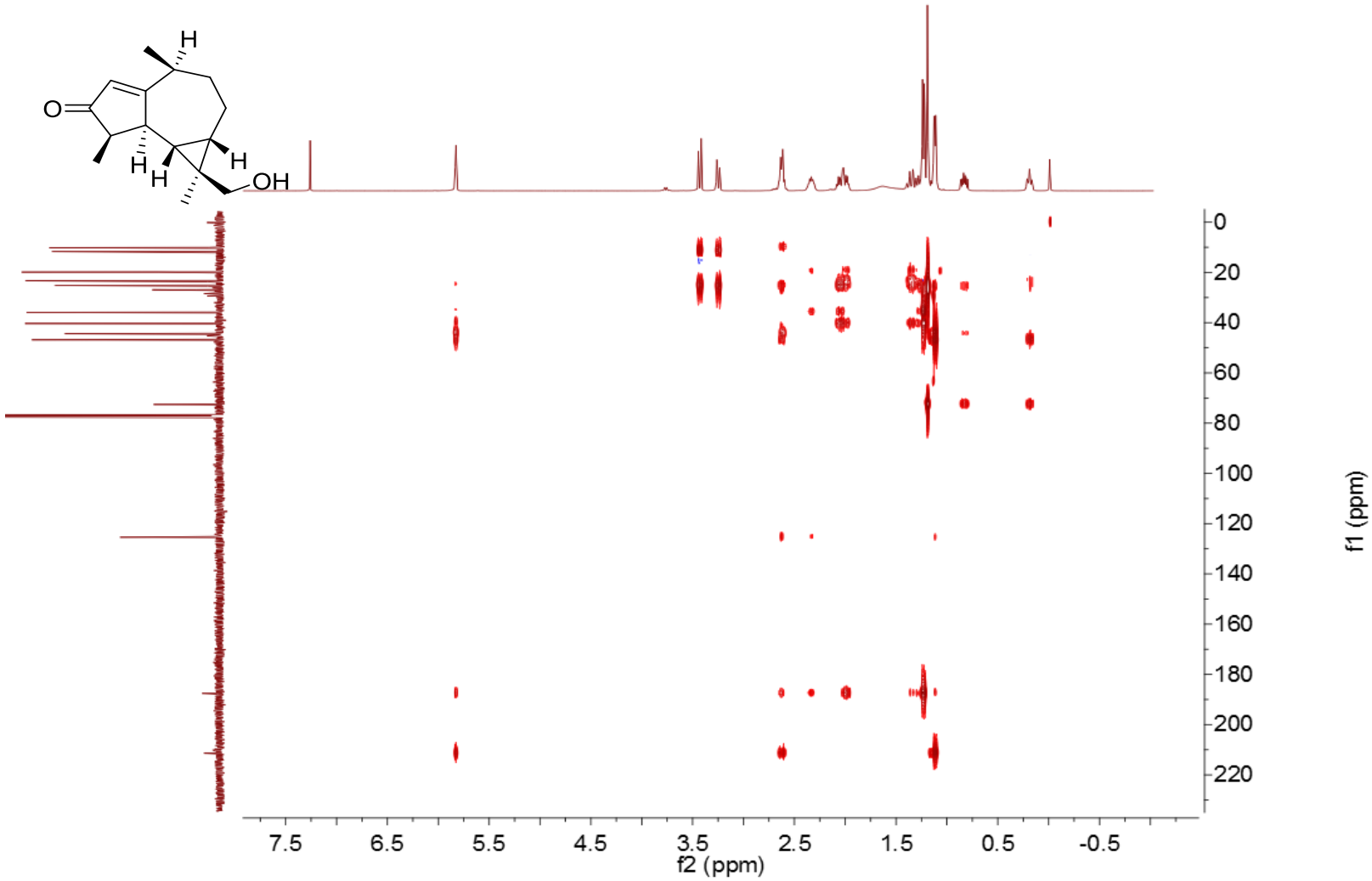


Figure S7. NOESY spectrum of pseuboydone A **(1)** in $CDCl_3$

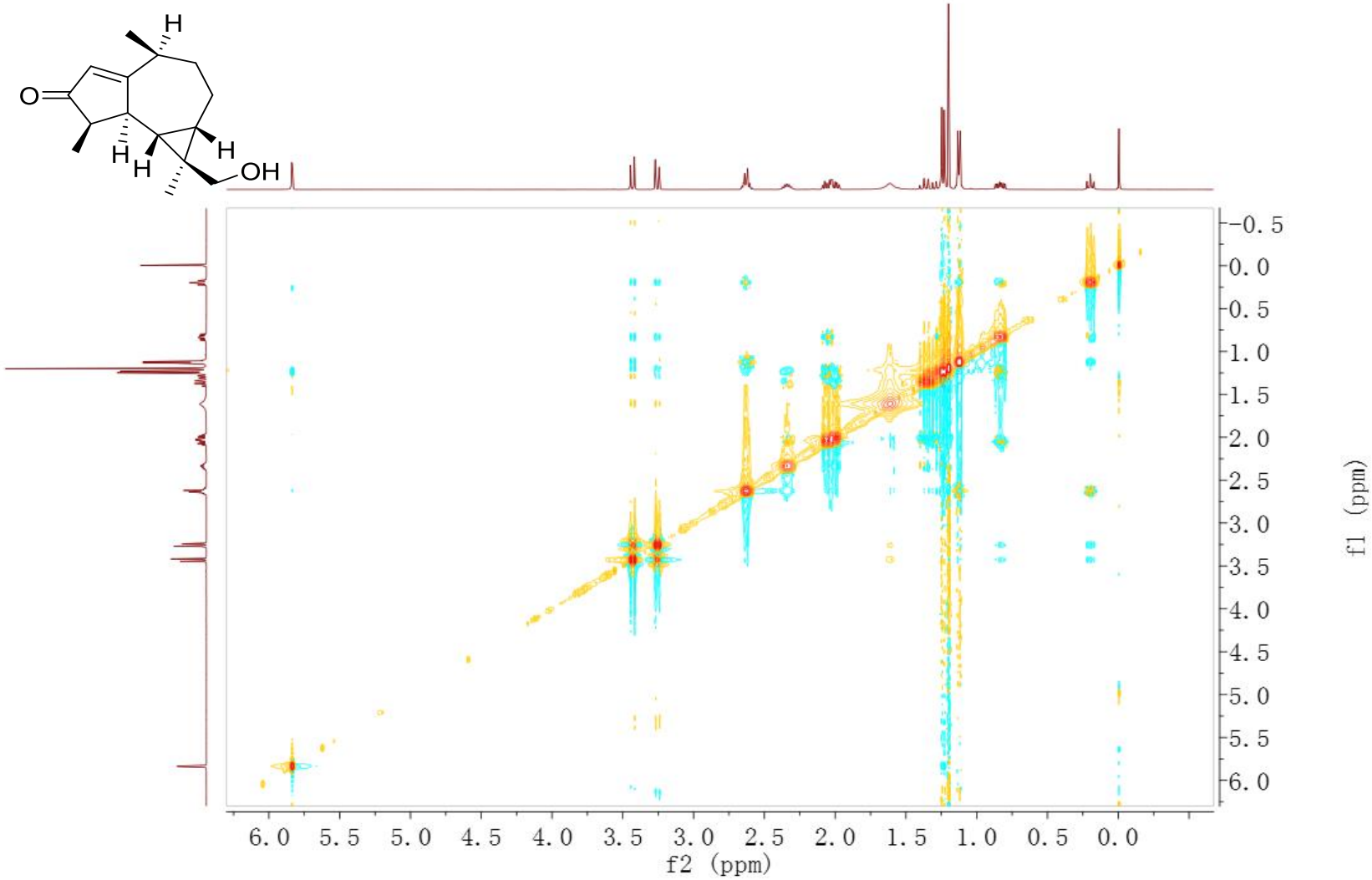


Figure S8. HR-ESI-MS spectrum of pseuboydone B **(2)**

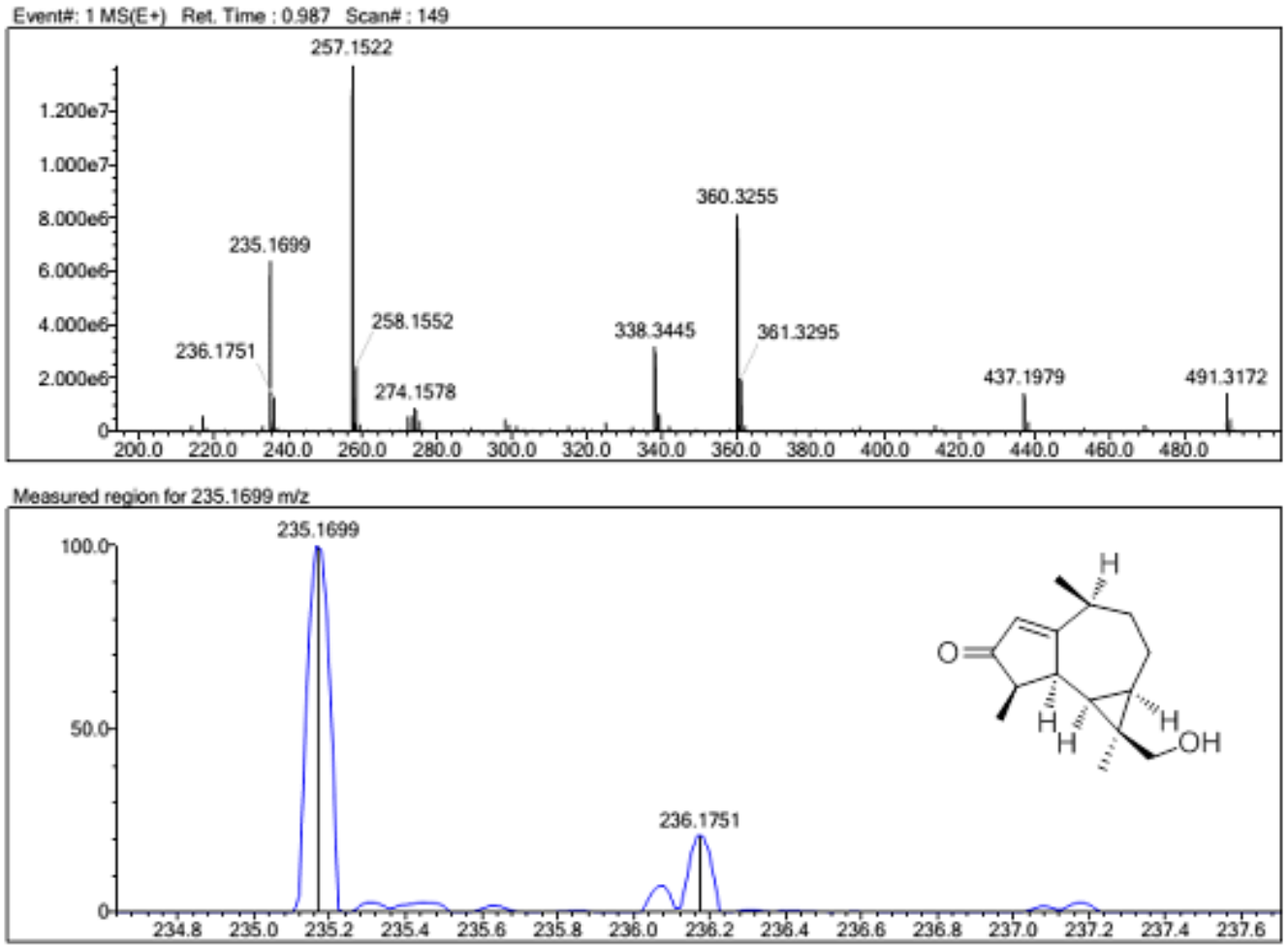


Figure S9. ^{1}H-NMR spectrum of pseuboydone B **(2)** in $CDCl_3$ (400MHz)

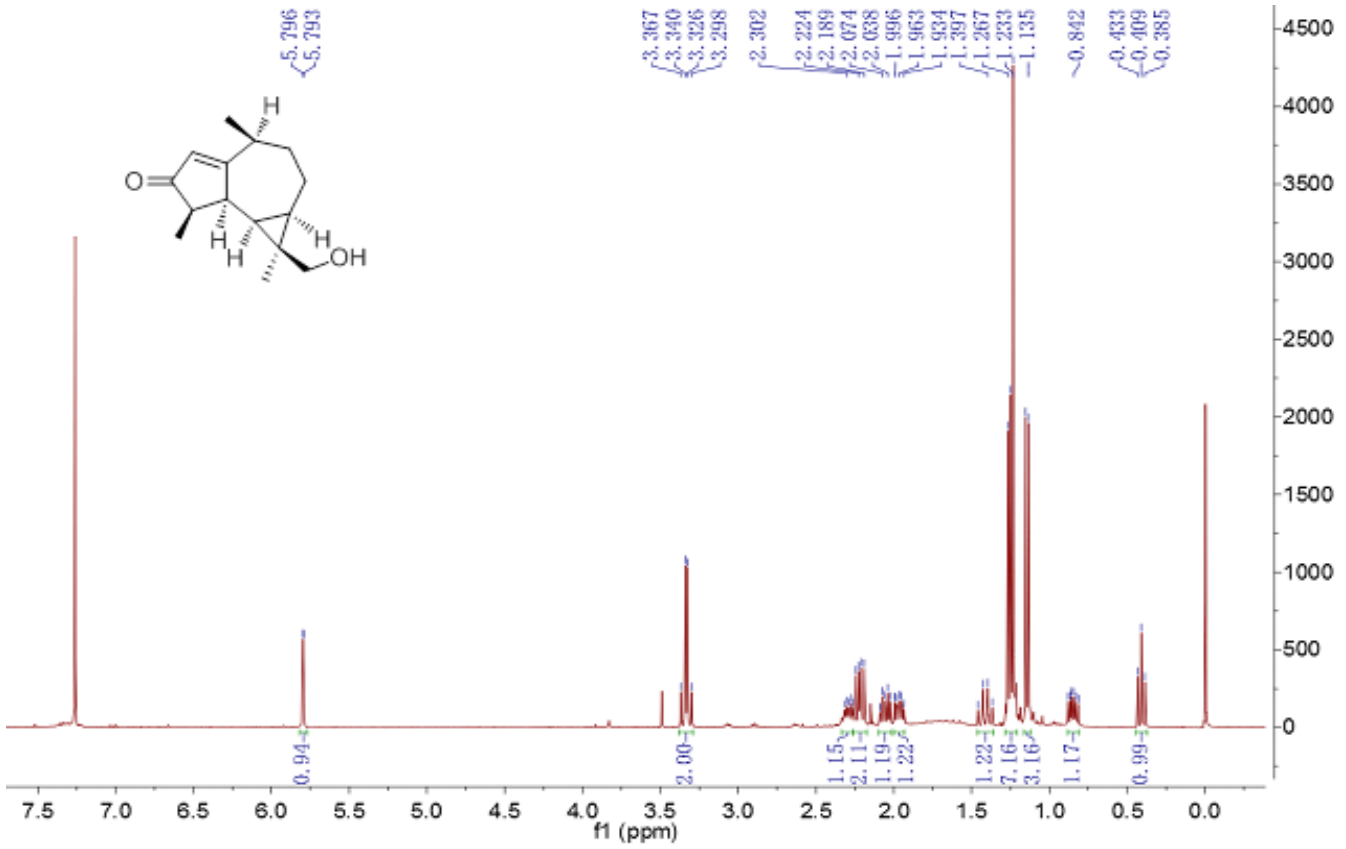
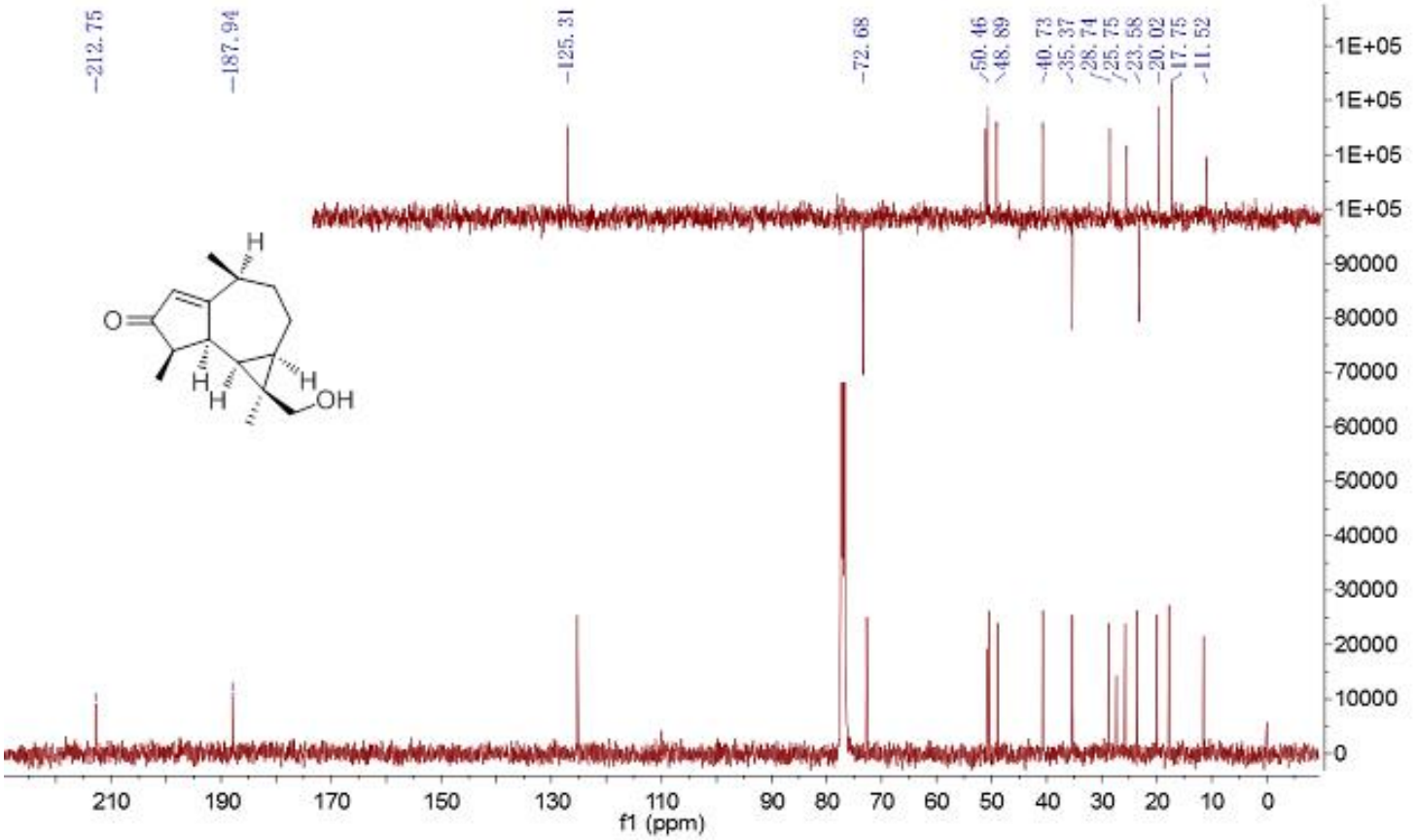


Figure S10. ^{13}C-NMR and DEPT spectra of pseuboydone B **(2)** in $CDCl_3$ (100MHz)



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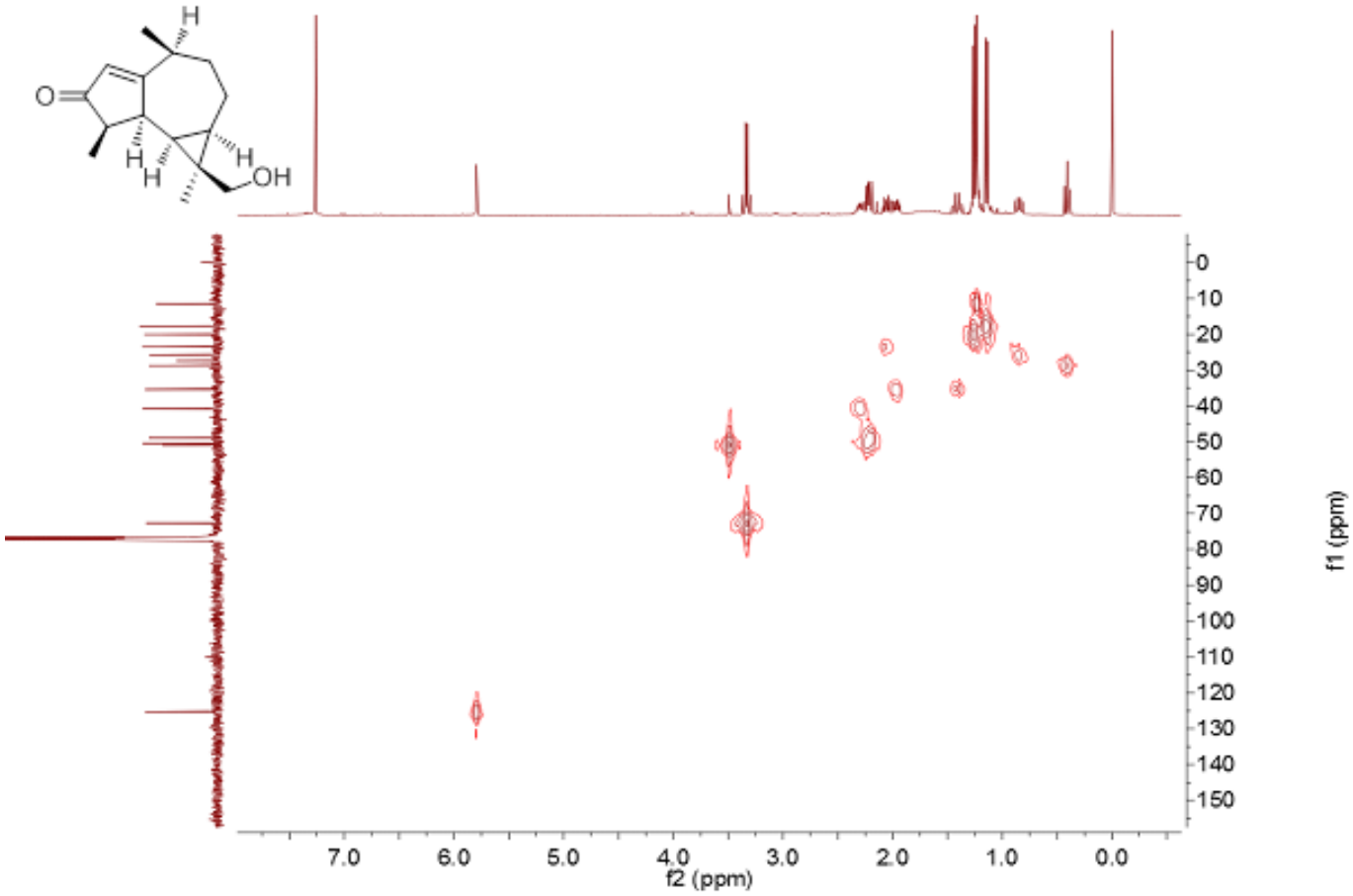

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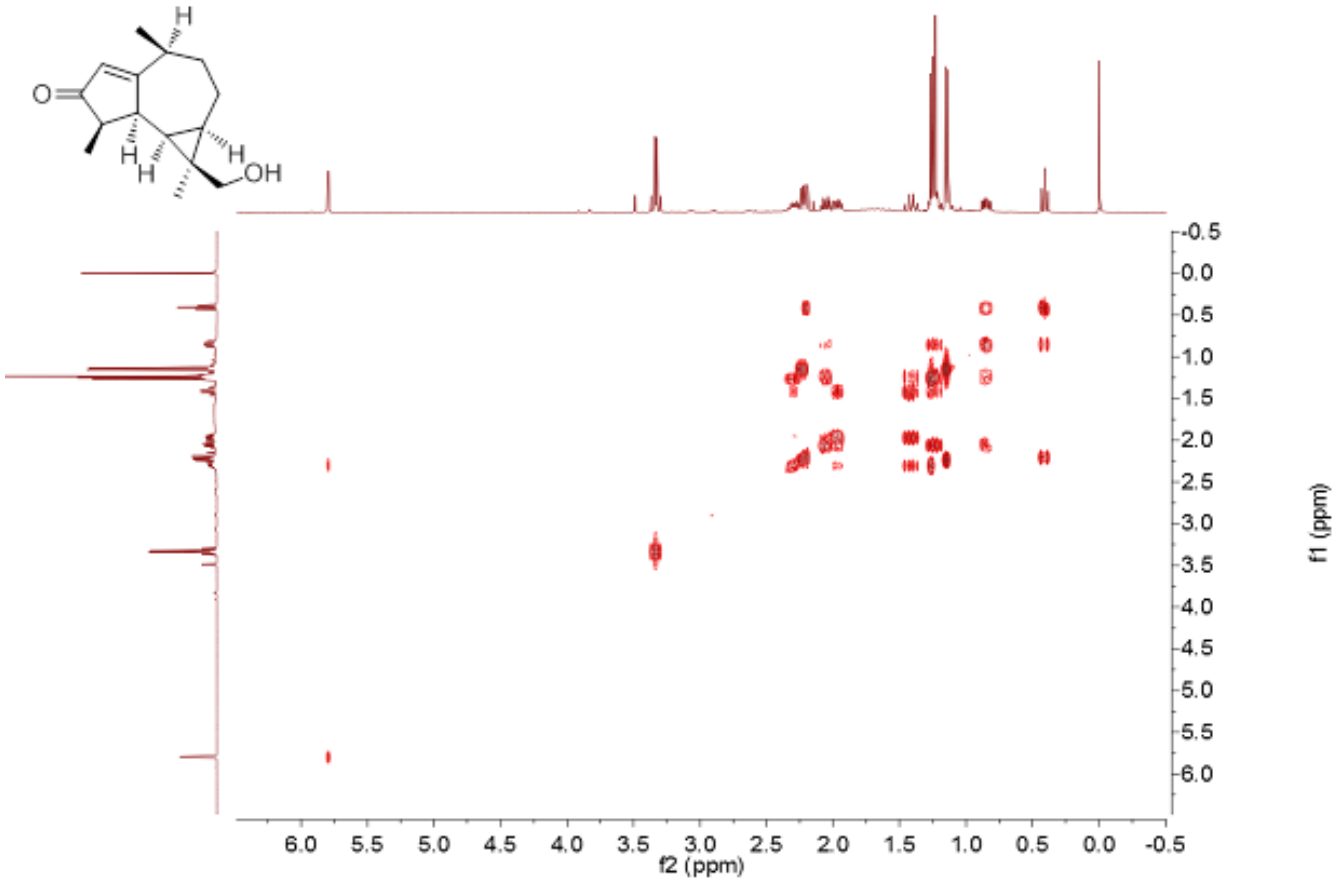

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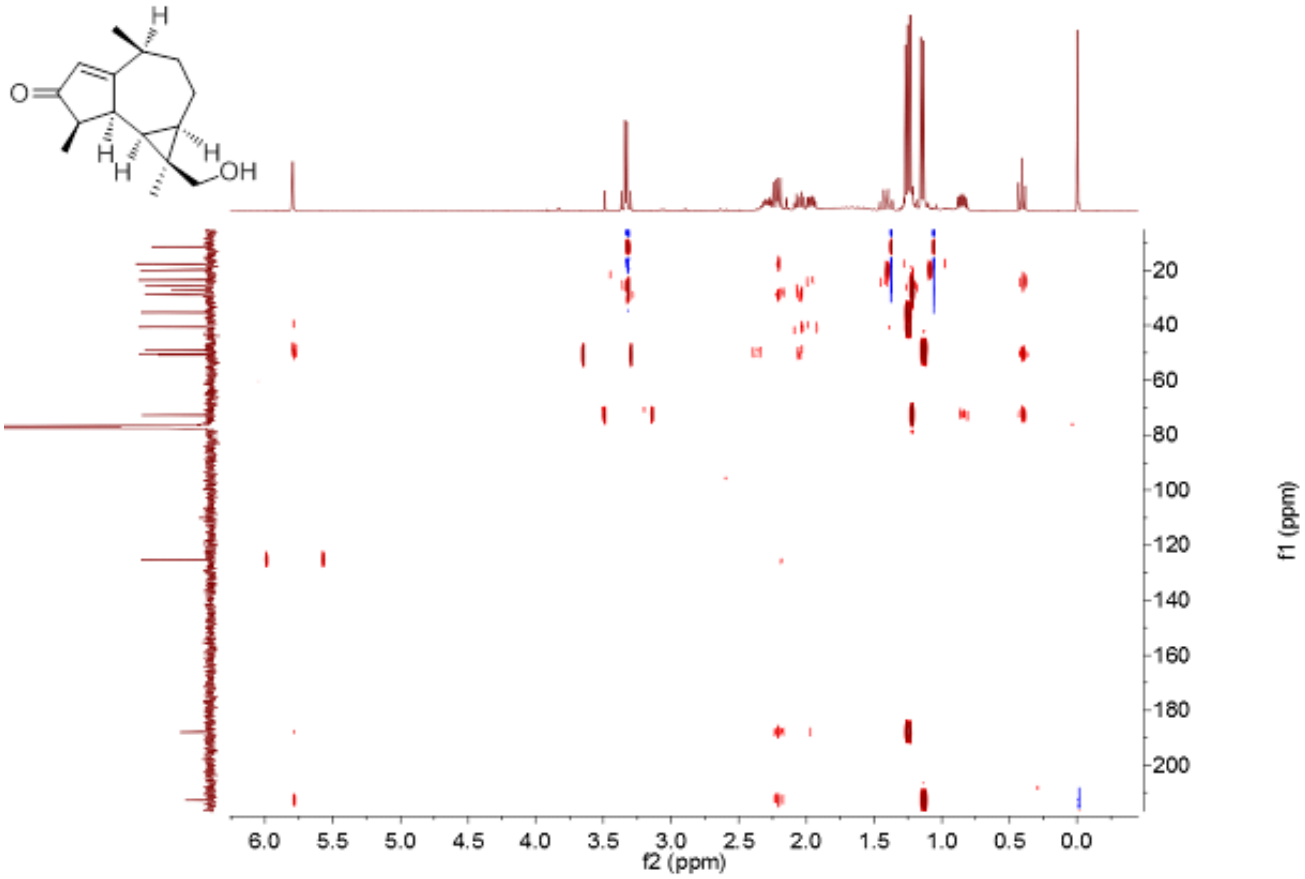

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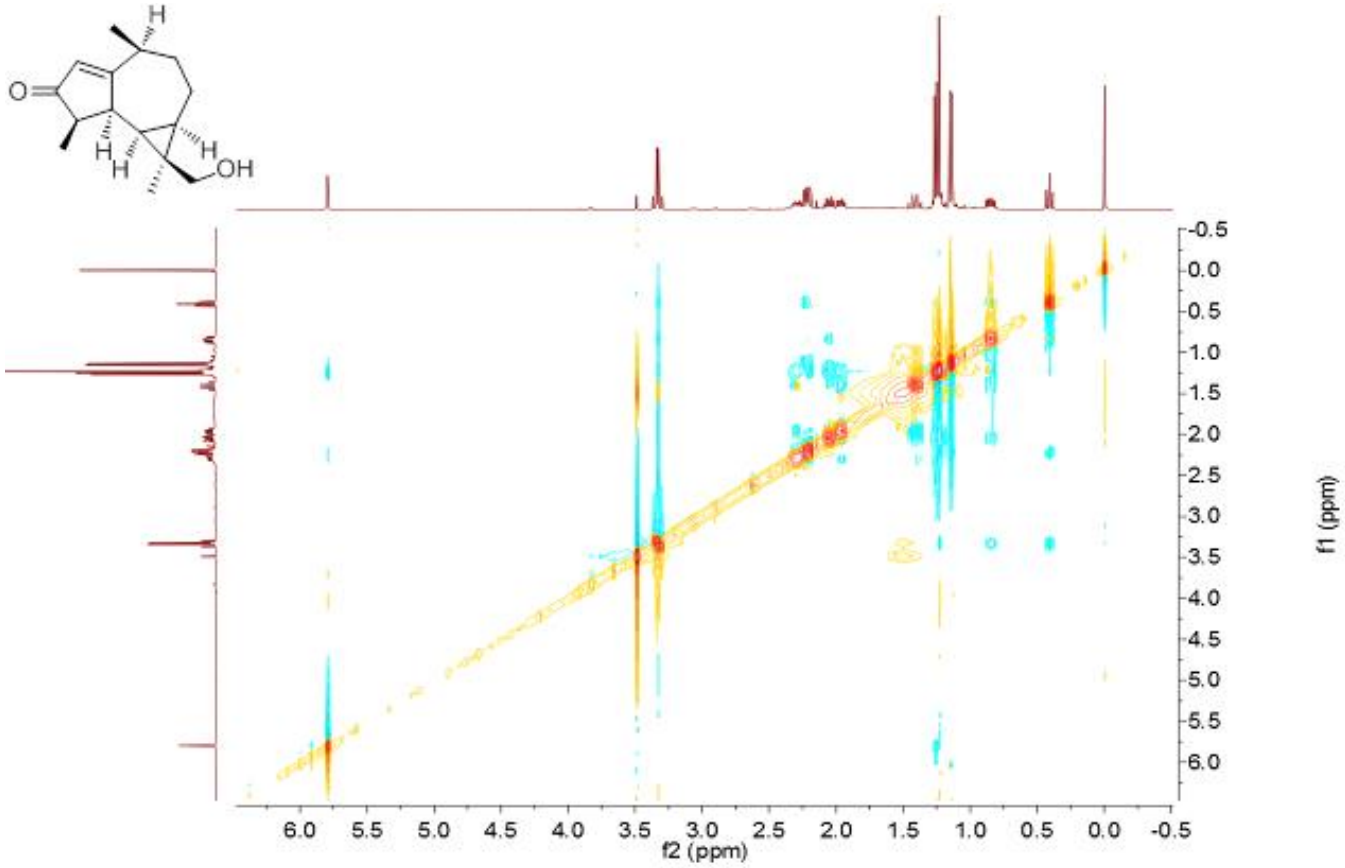
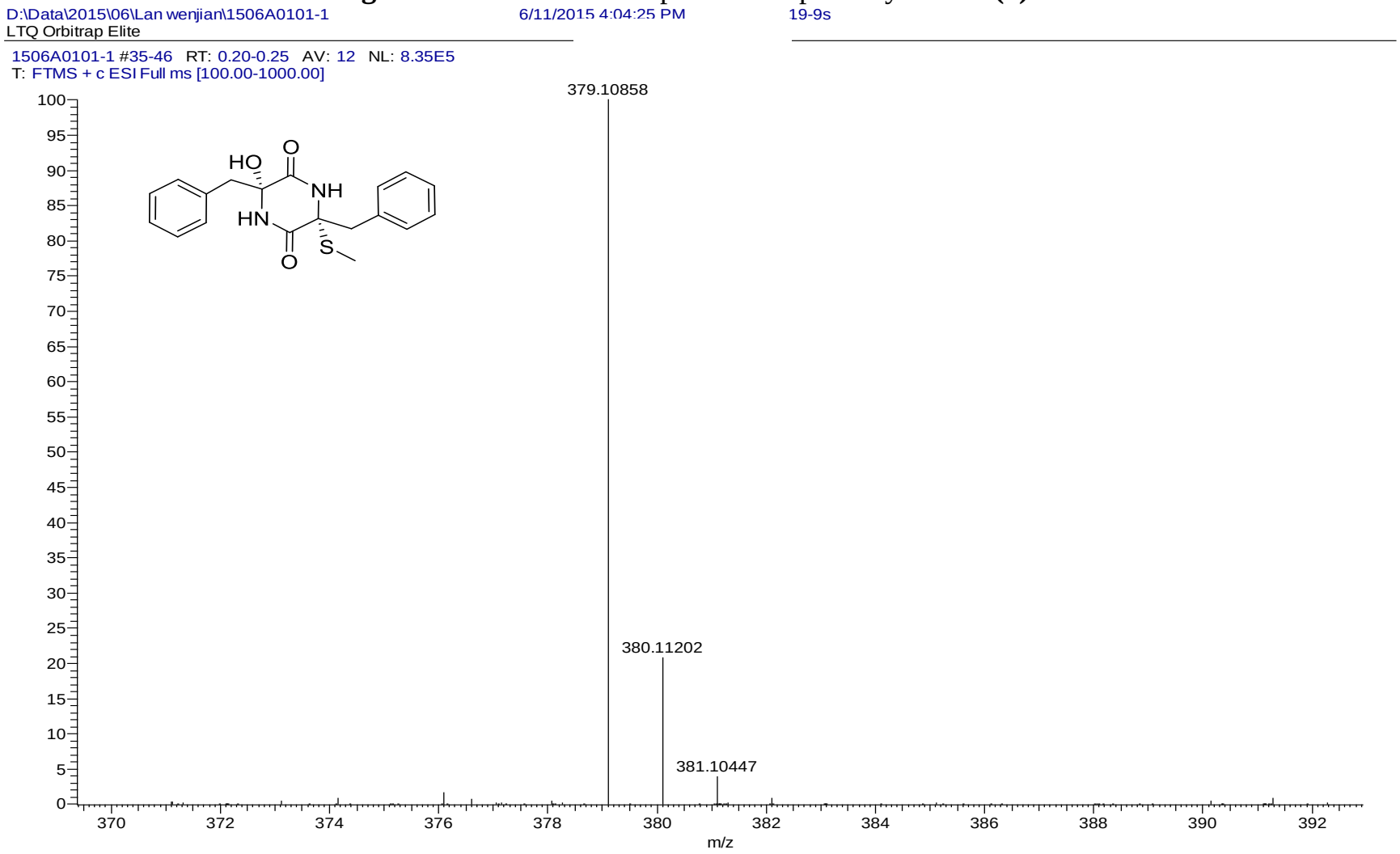


Figure S15. HR-ESI-MS spectrum of pseuboydone C **(3)**



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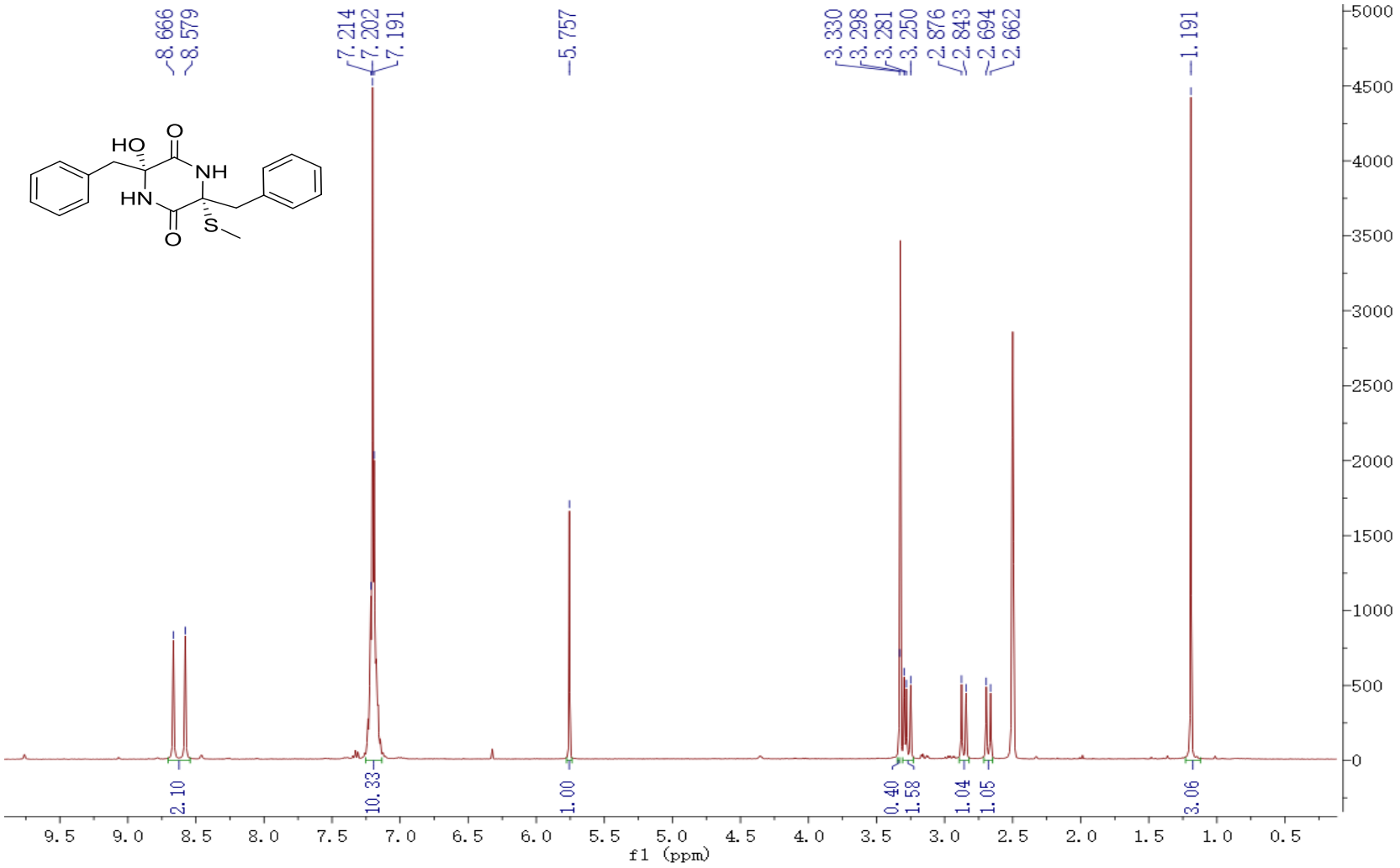

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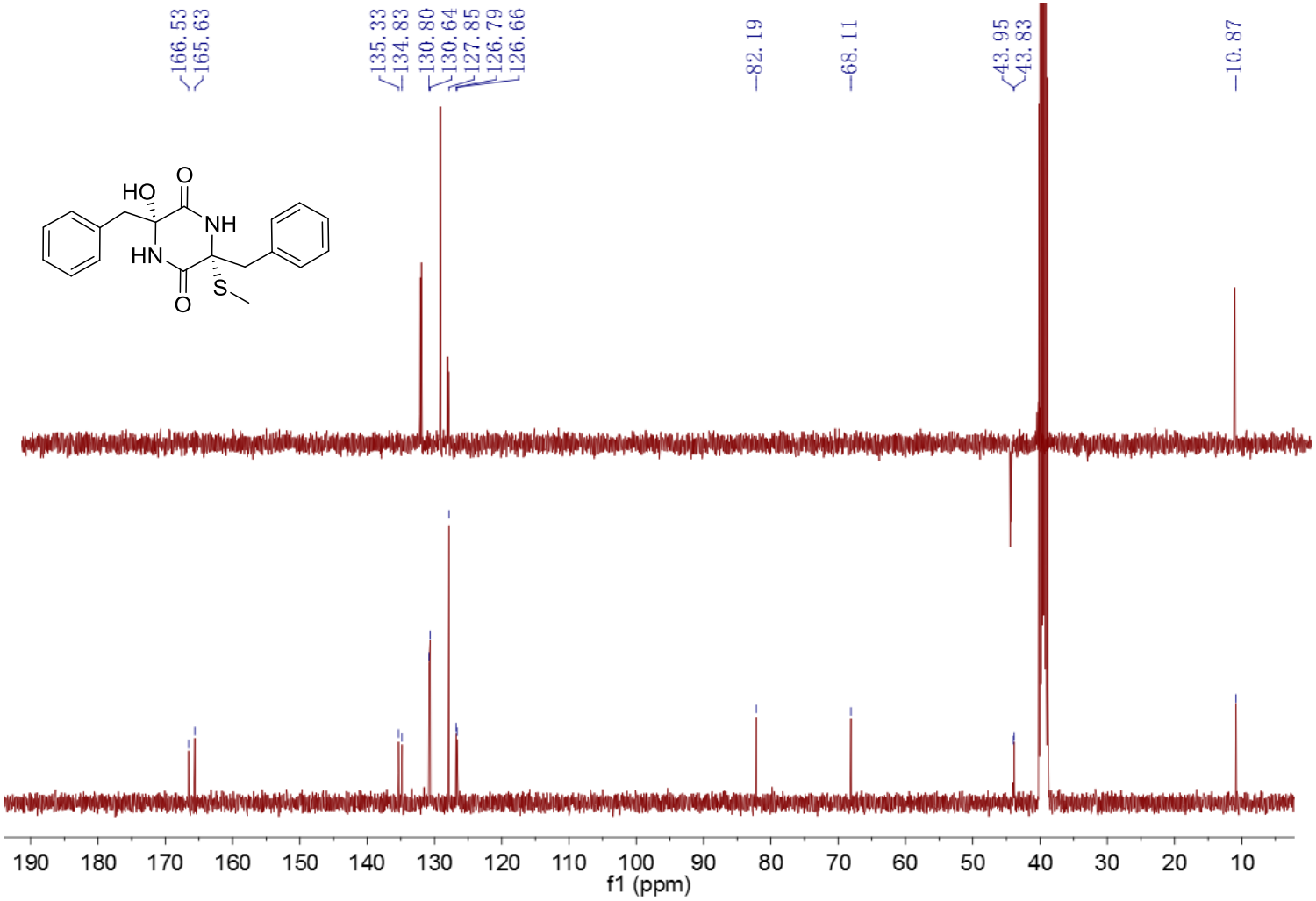

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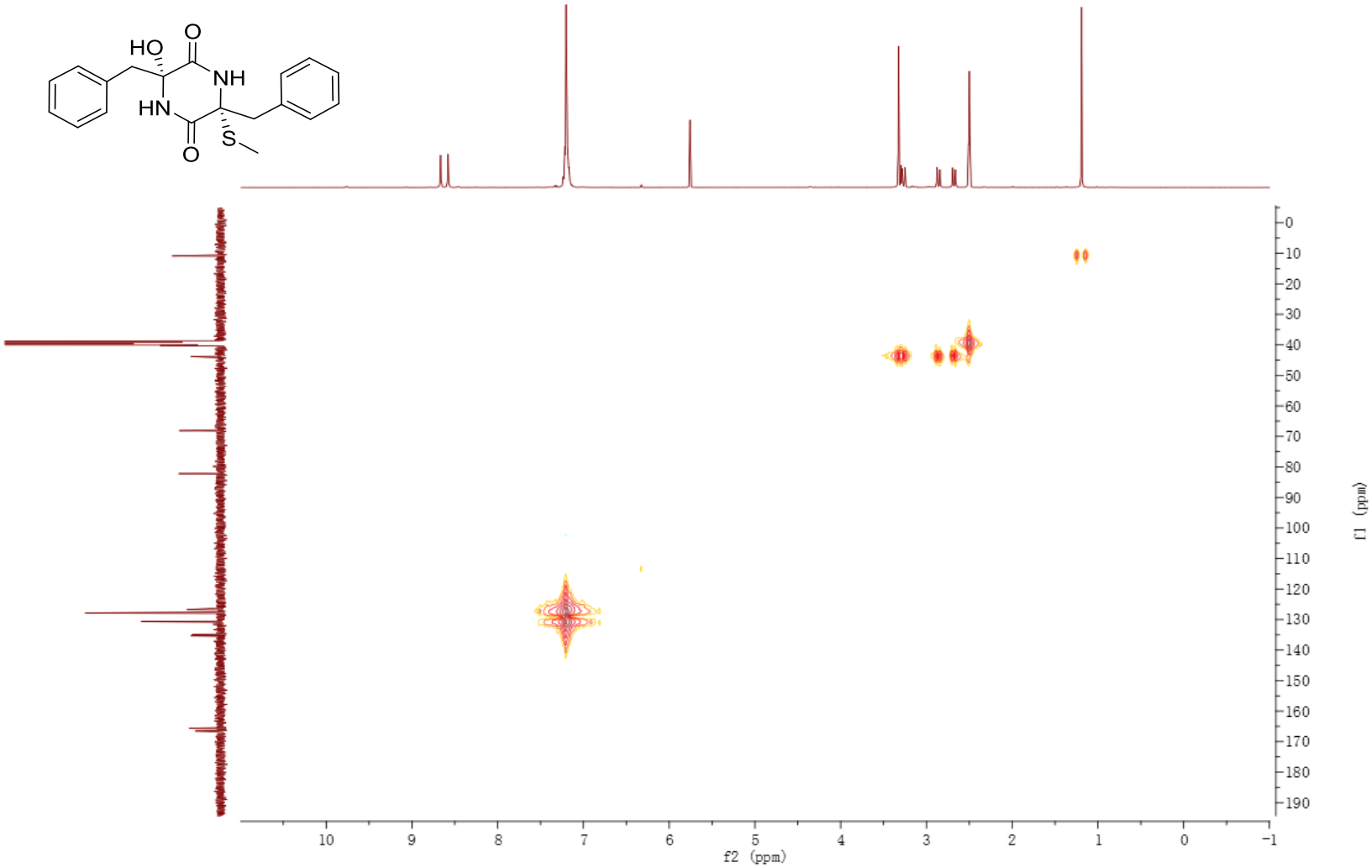

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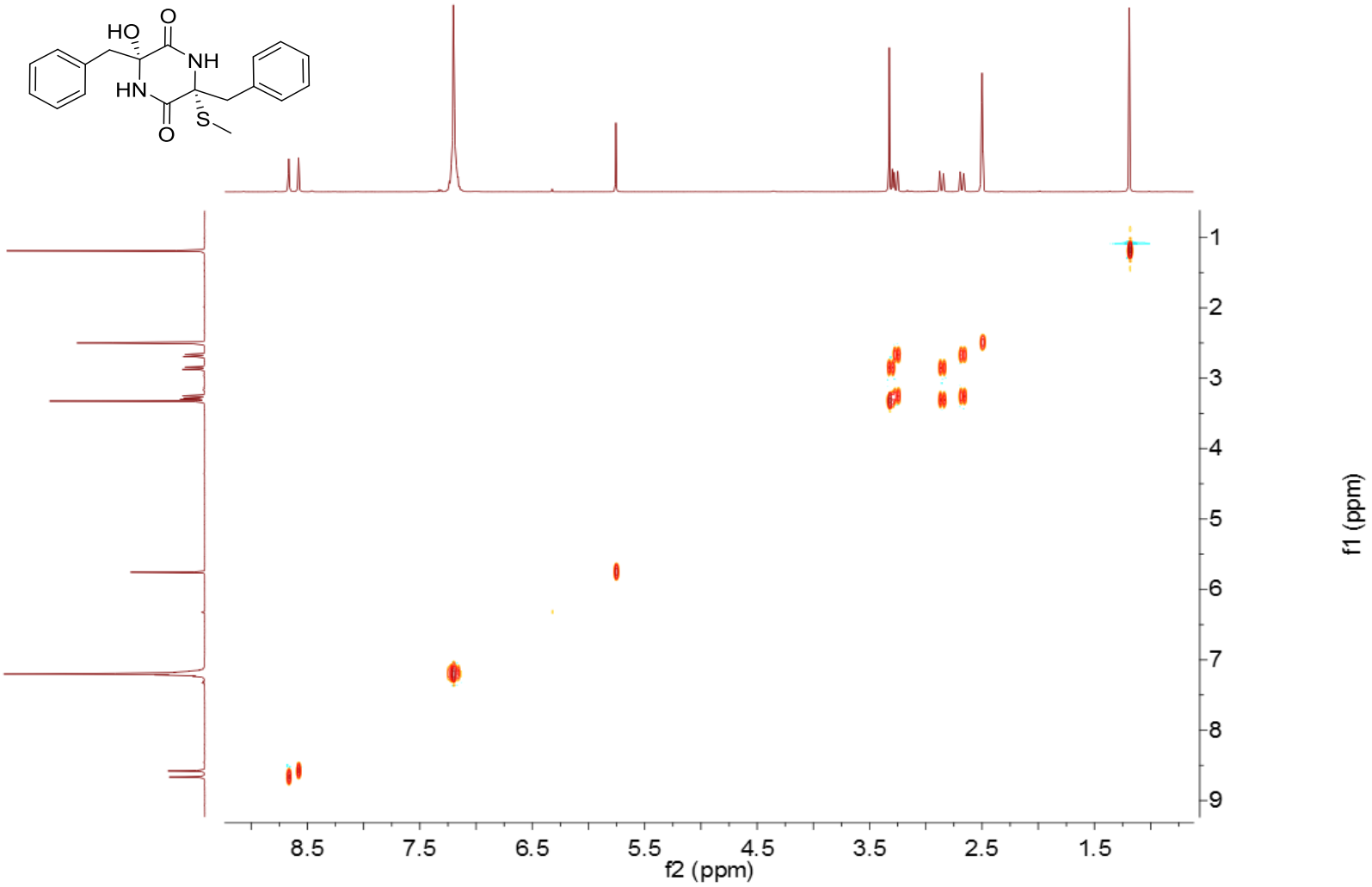

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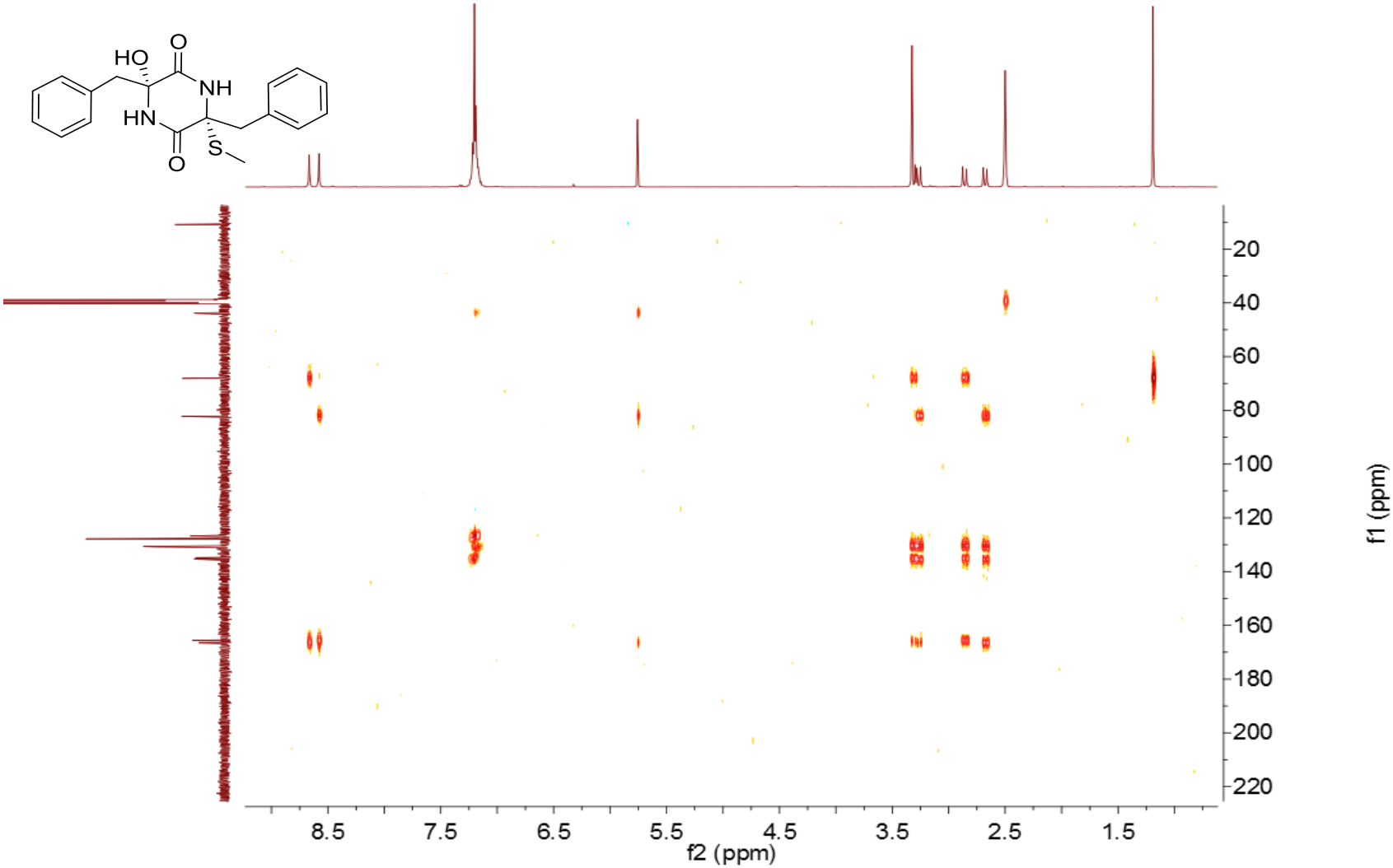

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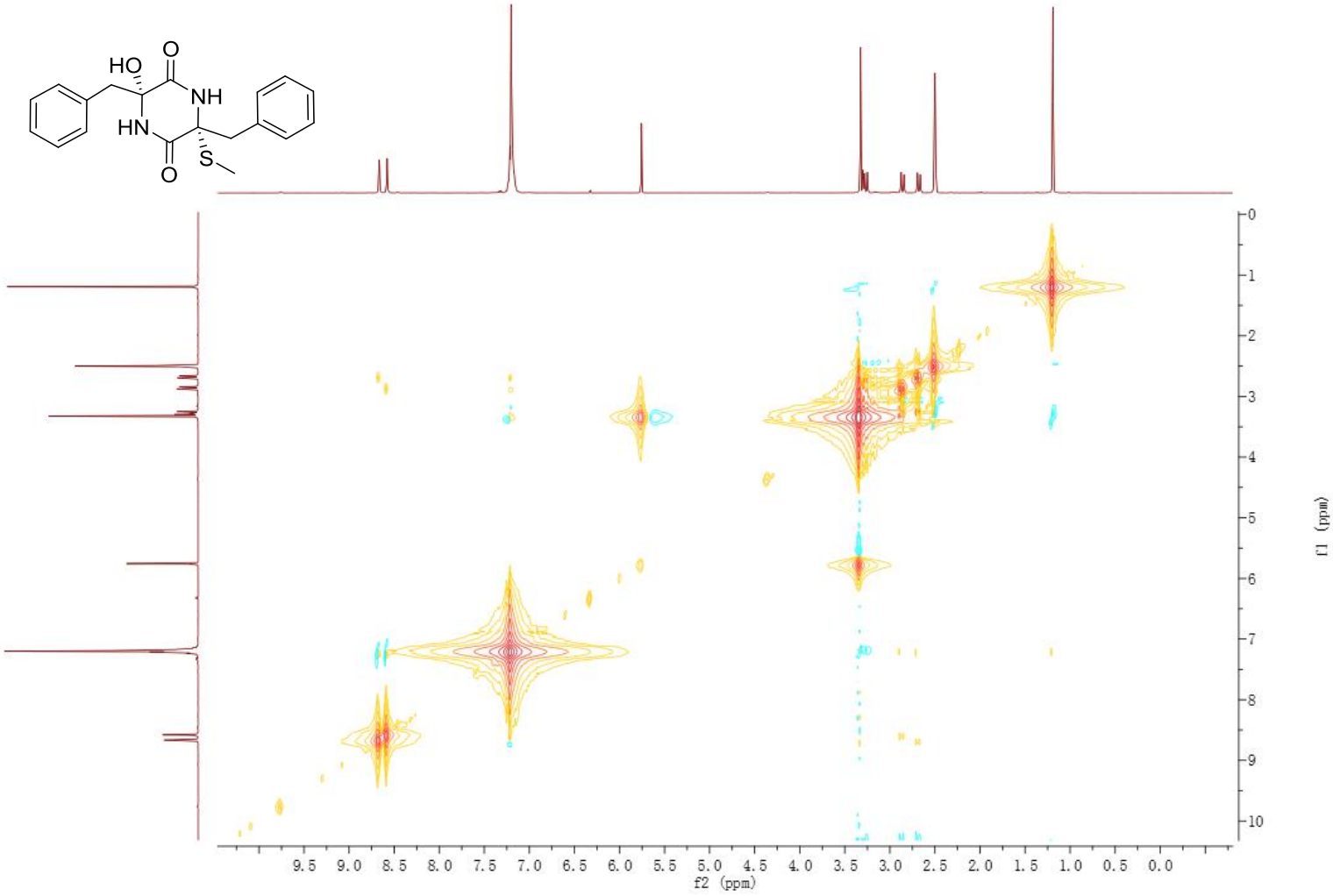
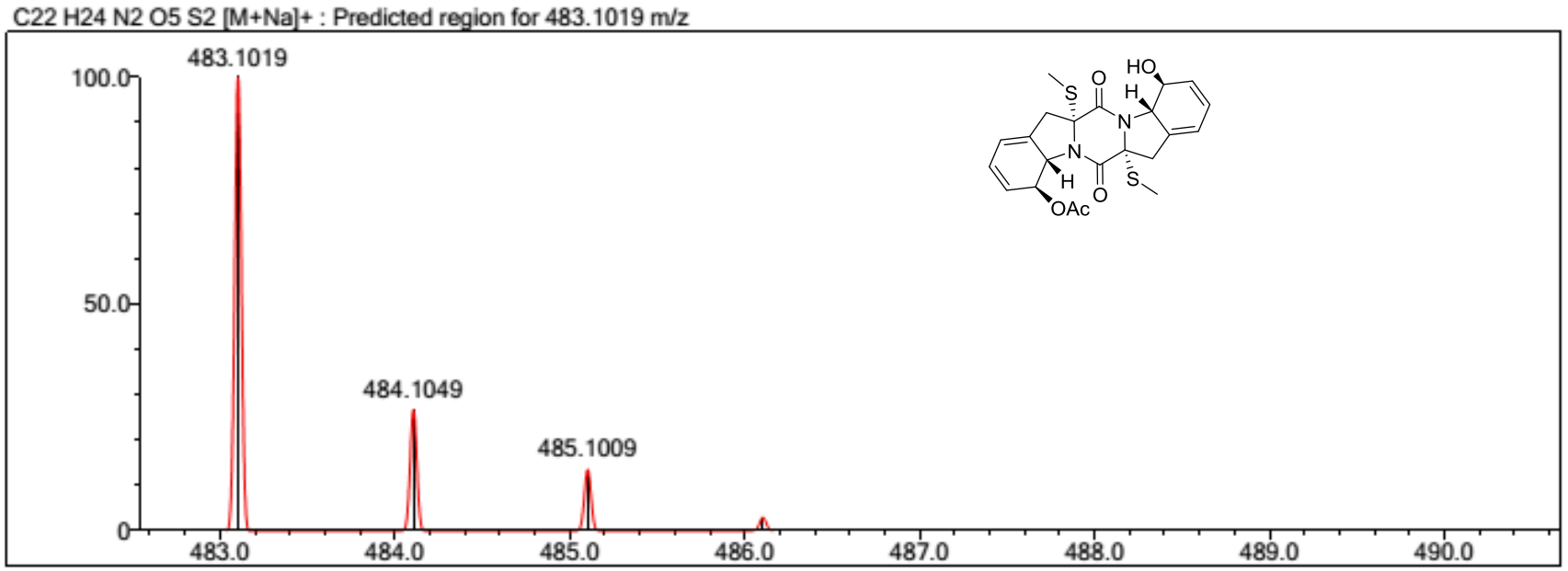


Figure S22. HR-ESI-MS spectrum of pseuboydone D **(4)**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.21	C22 H24 N2 O5 S2	[M+Na]+	483.1025	483.1019	0.6	1.24	92.76	12.0

Figure S23. ^{1}H-NMR spectrum of pseuboydoneD **(4)** in $CDCl_3$ (500MHz)

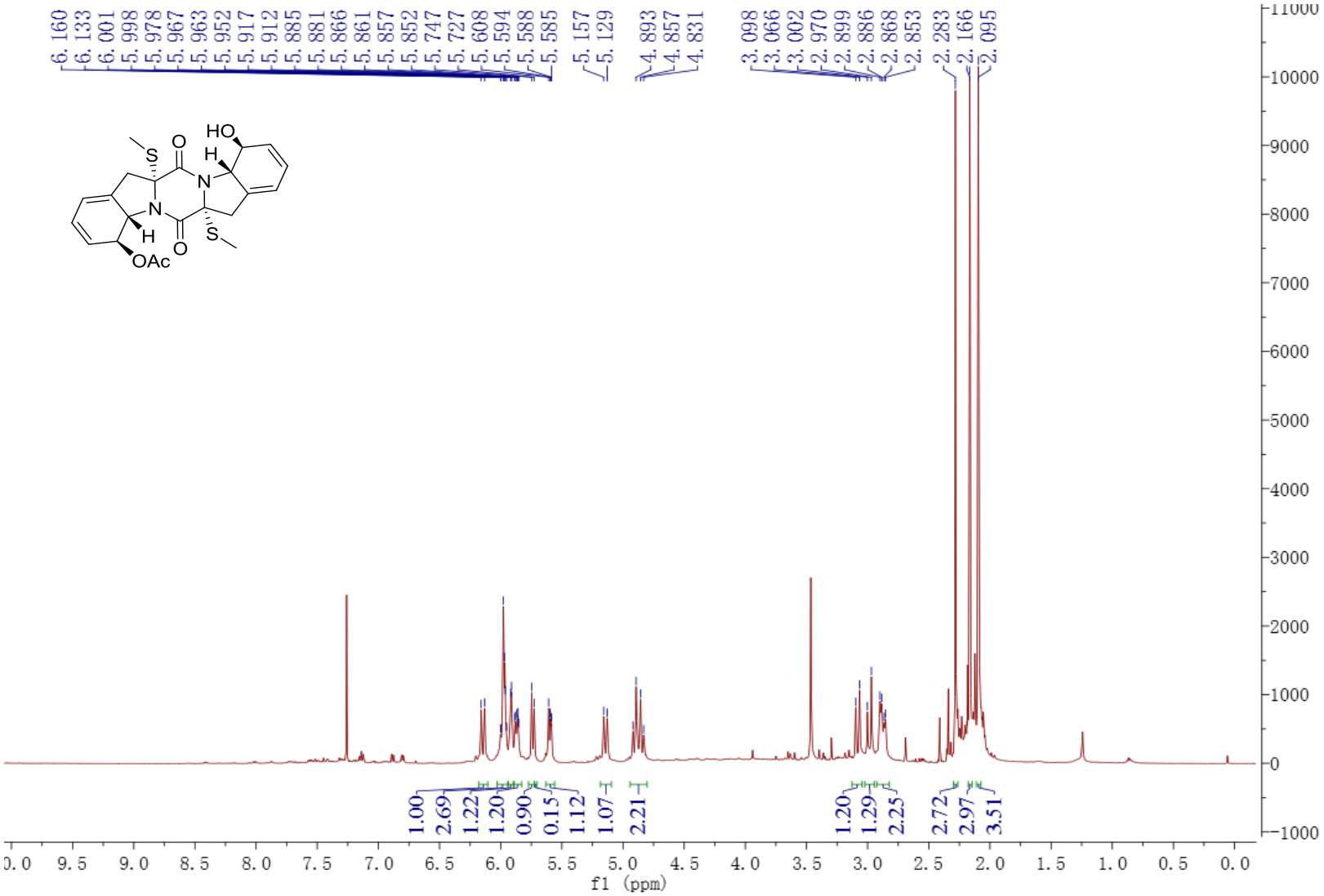


Figure S24. ^{13}C-NMR and DEPT spectra of pseuboydone D **(4)** in $CDCl_3$ (125MHz)

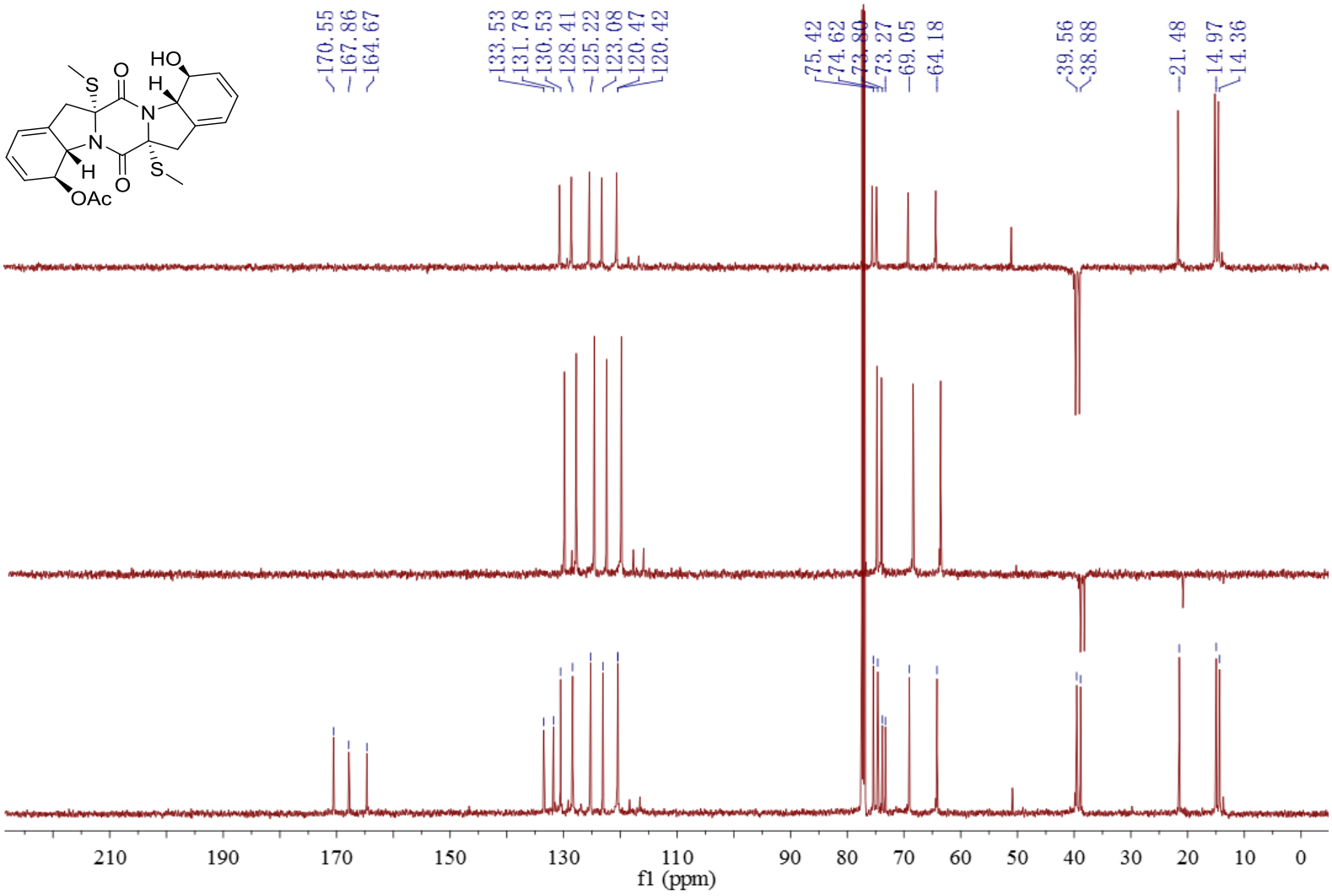


Figure S25. HMQC spectrum of pseuboydone D **(4)** in $CDCl_3$

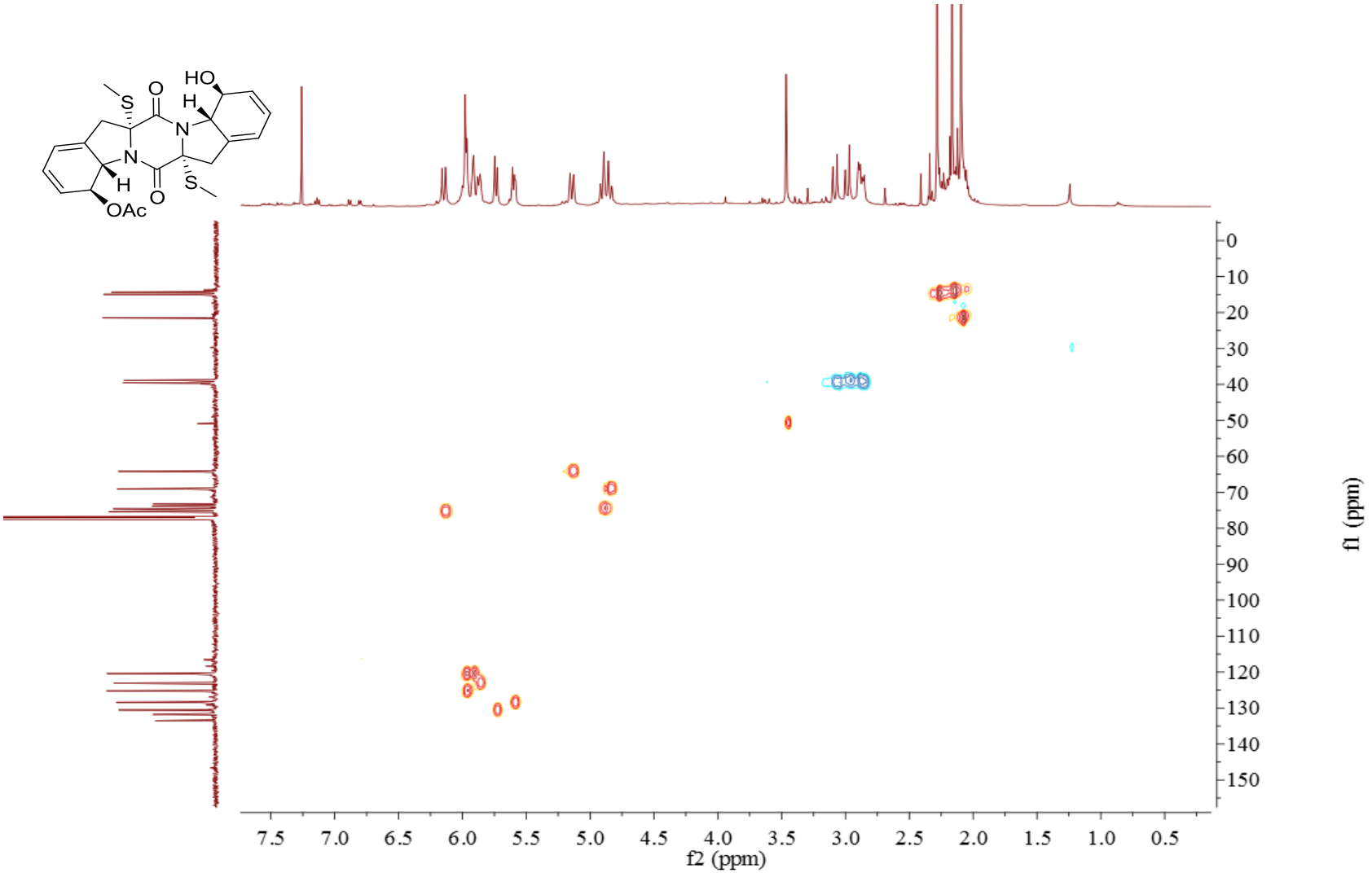


Figure S26. ^{1}H-^{1}H COSY spectrum of pseuboydone D **(4)** in $CDCl_3$

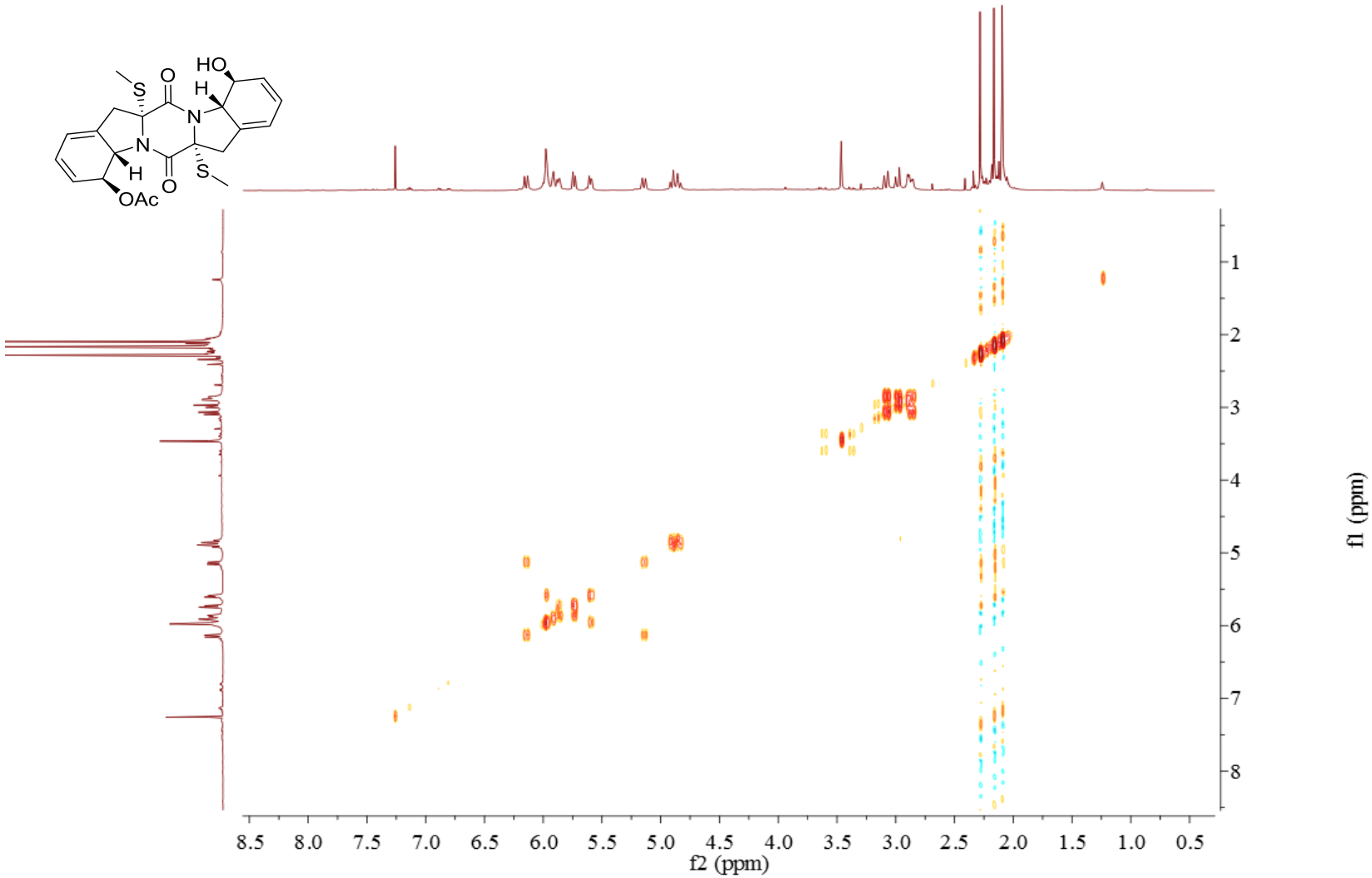


Figure S27. HMBC spectrum of pseuboydone D **(4)** in $CDCl_3$

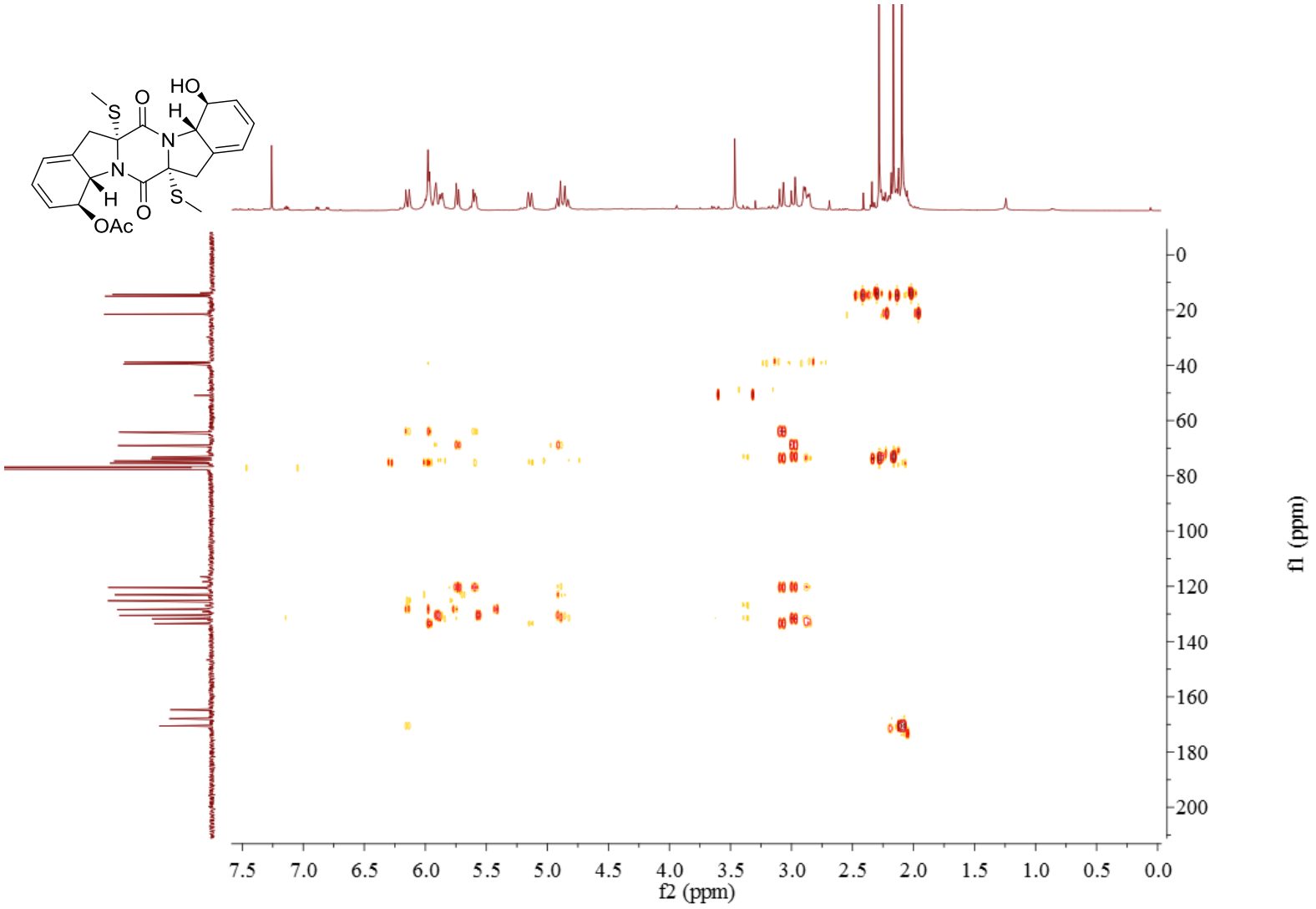


Figure S28. LR-ESI-MS spectrum of haematocin **(5)** in $CDCl_3$

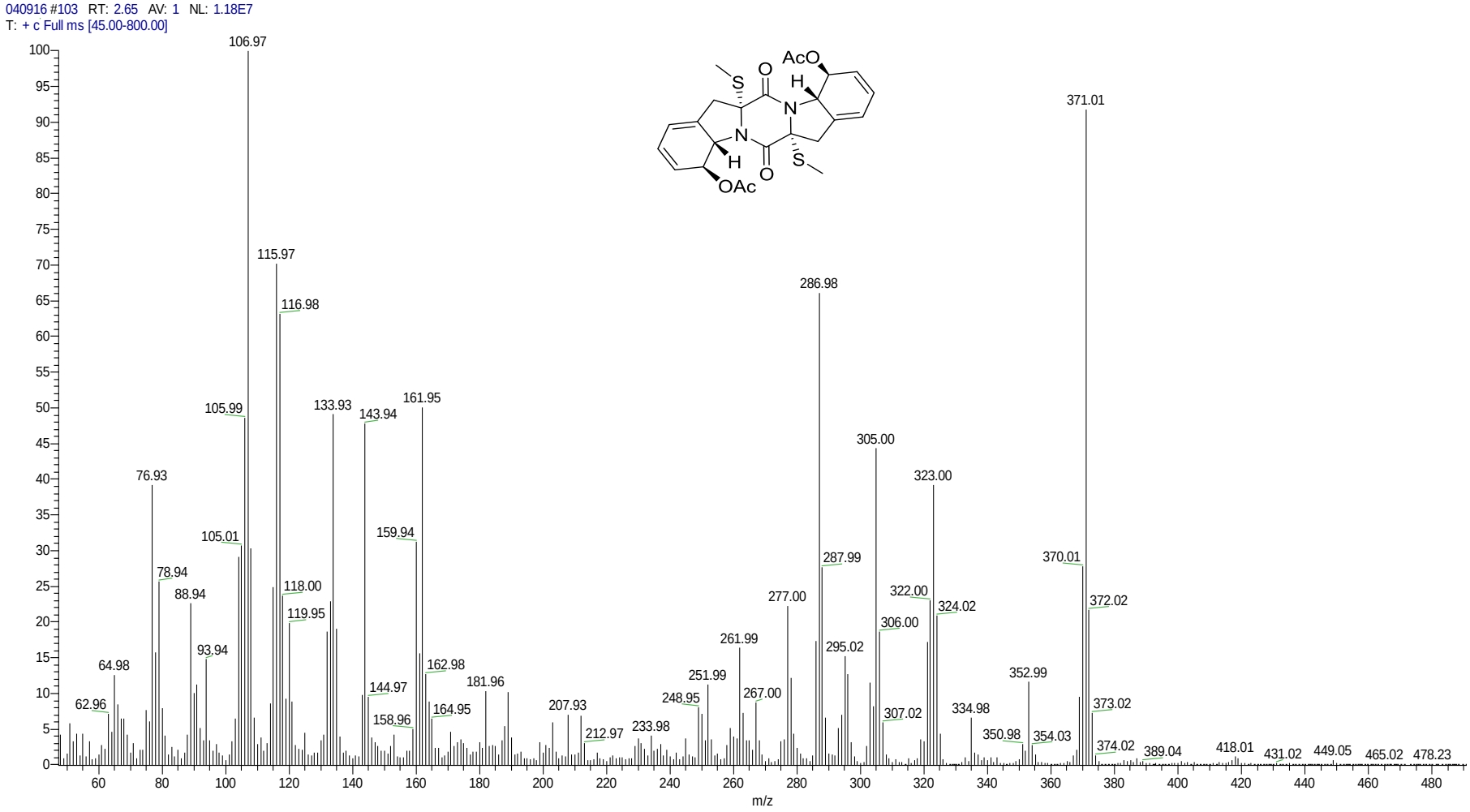


Figure S29. ^{1}H-NMR spectrum of haematocin **(5)** in $CDCl_3$

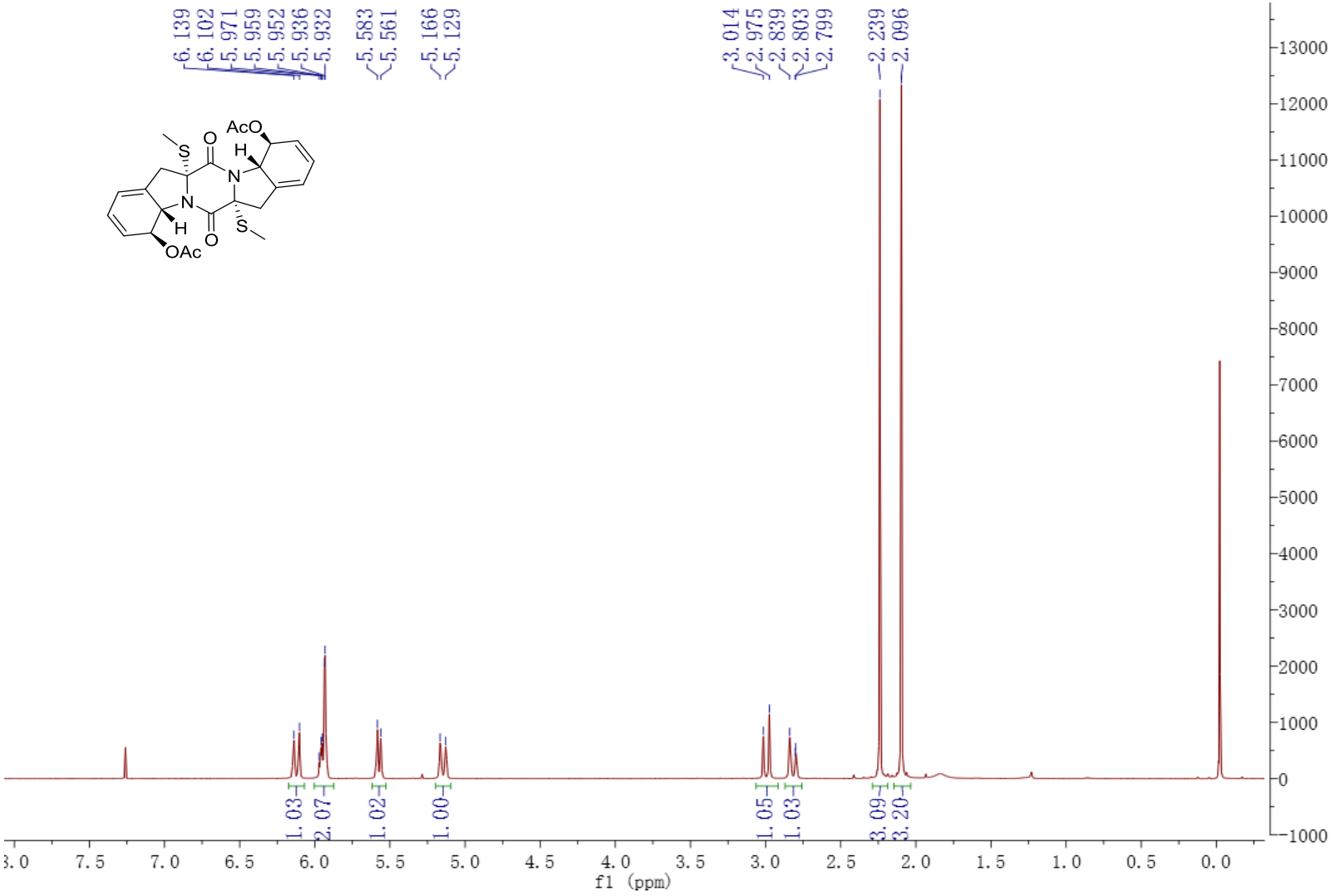


Figure S30. ^{13}C-NMR and DEPT spectra of haematocin **(5)**

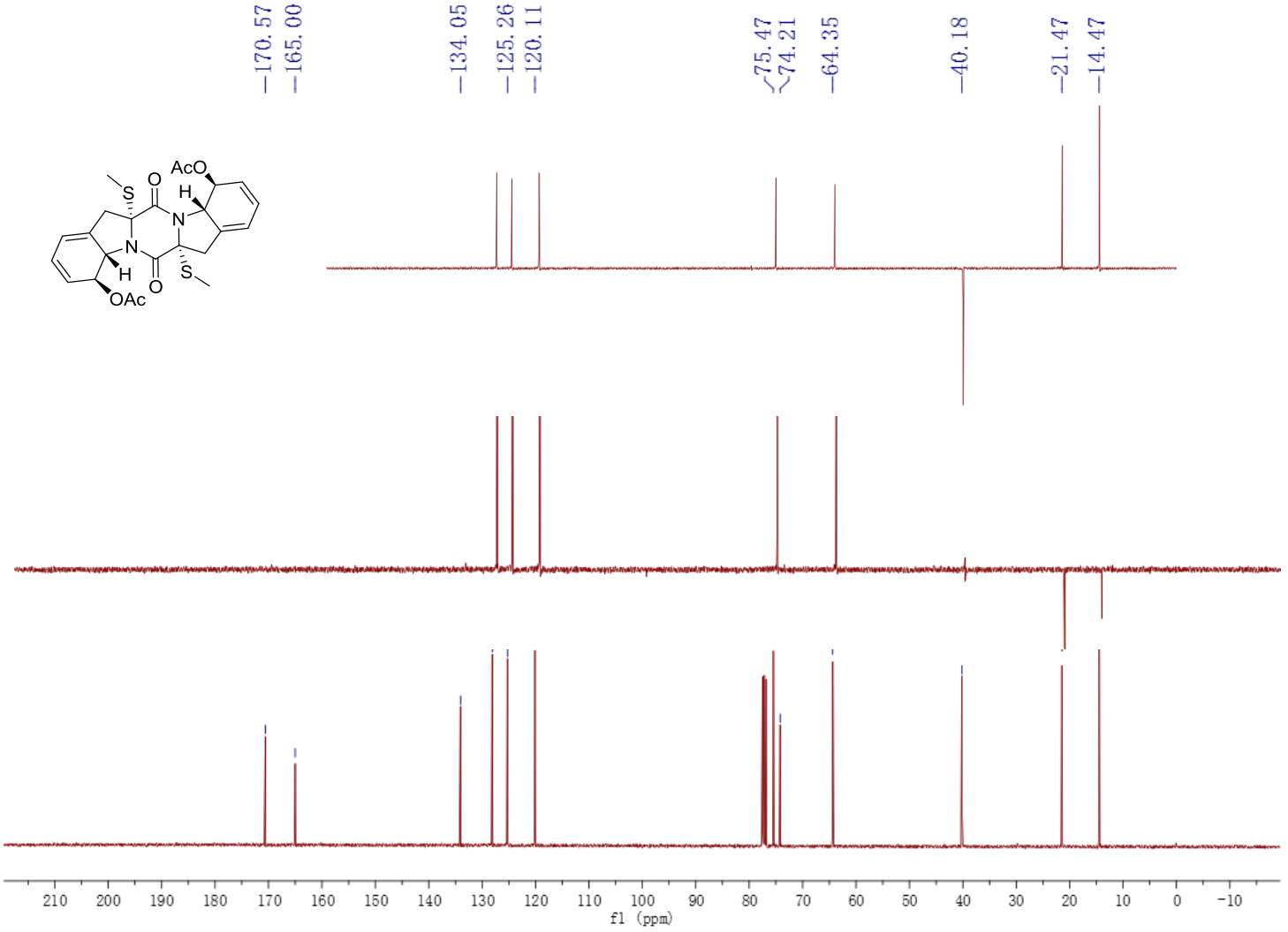


Figure S31. HMQC spectrum of haematocin **(5)** in $CDCl_3$

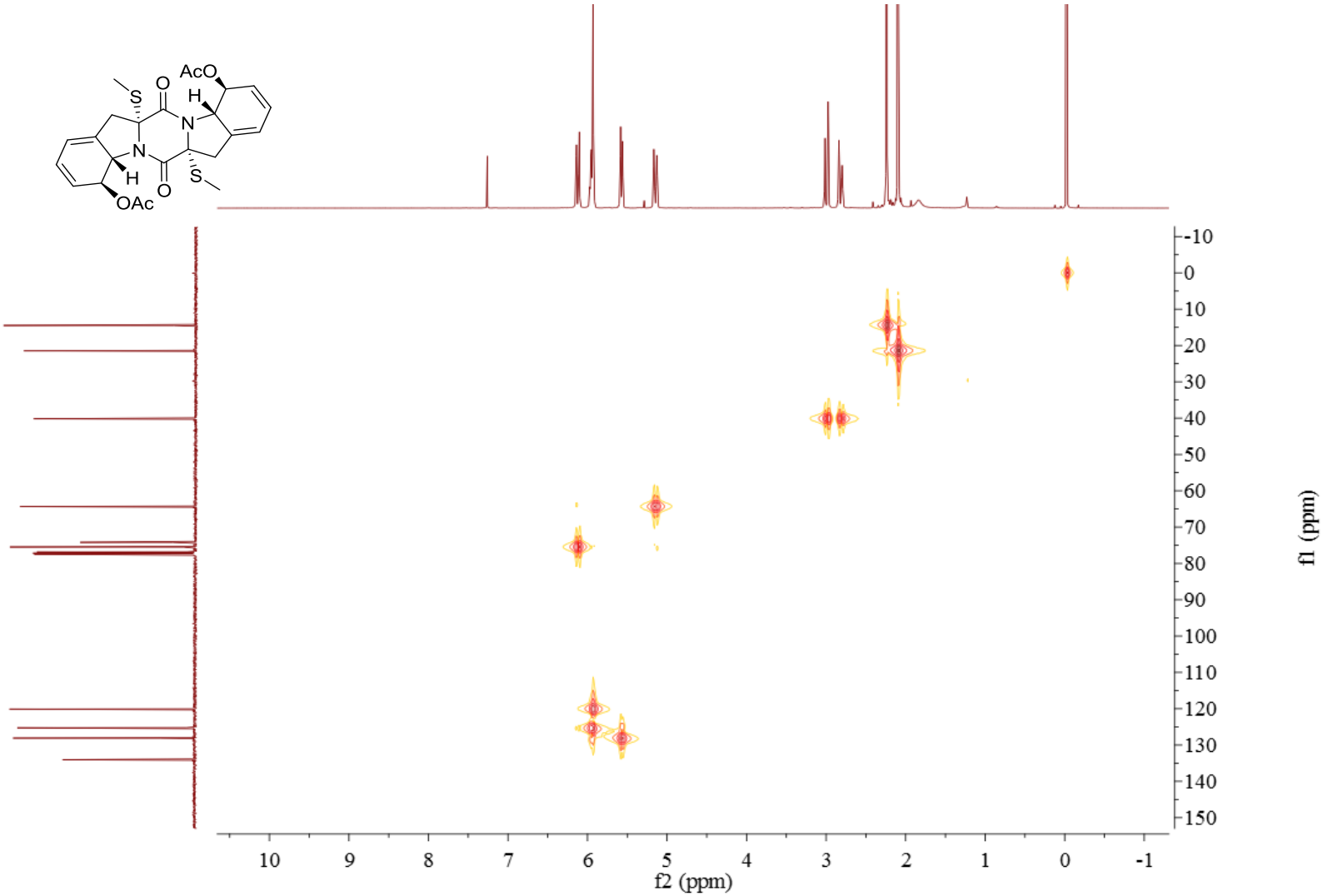


Figure S32. ^{1}H-^{1}H COSY spectrum of haematocin **(5)** in $CDCl_3$

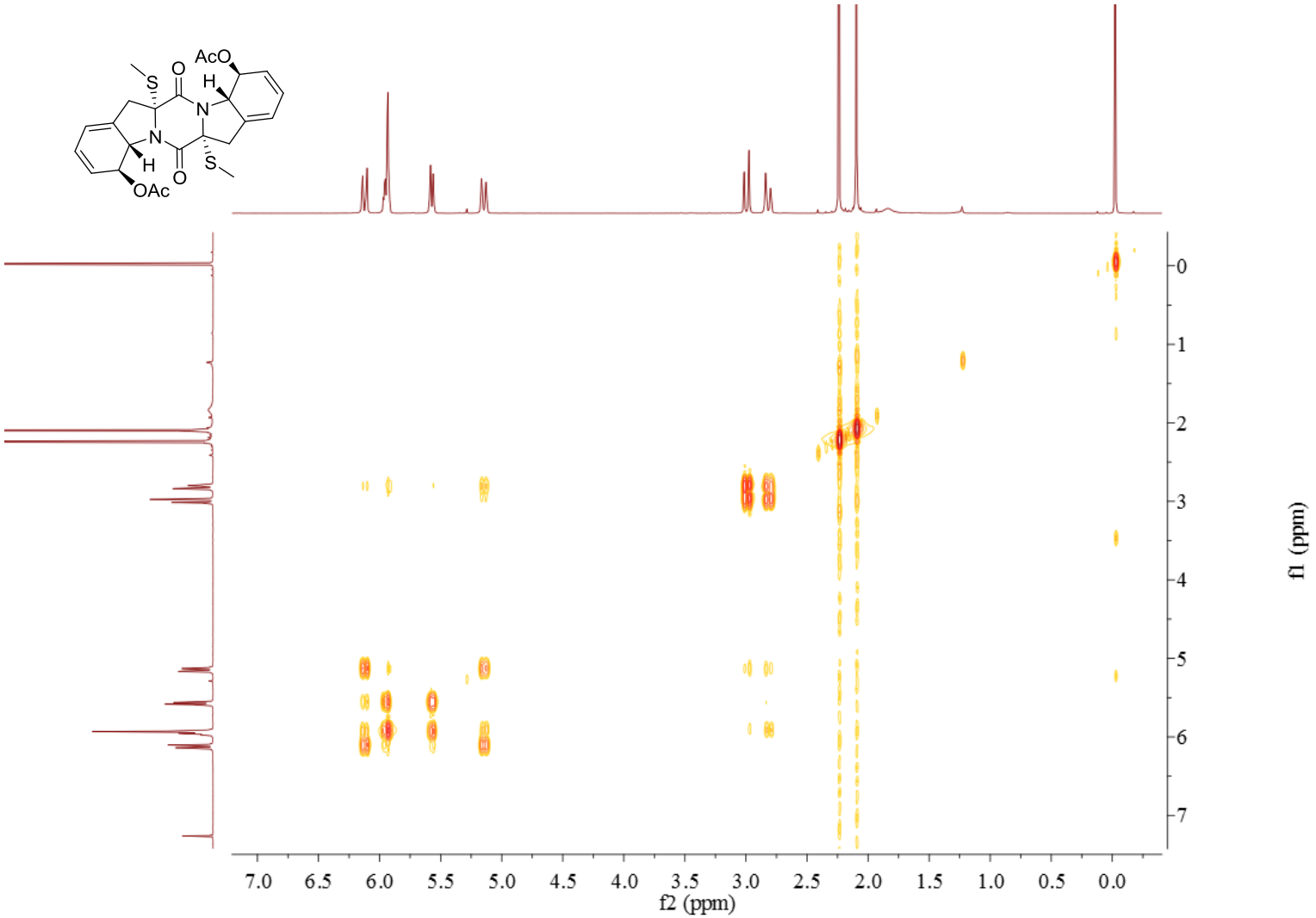


Figure S33. HMBC spectrum of haematocin **(5)** in $CDCl_3$

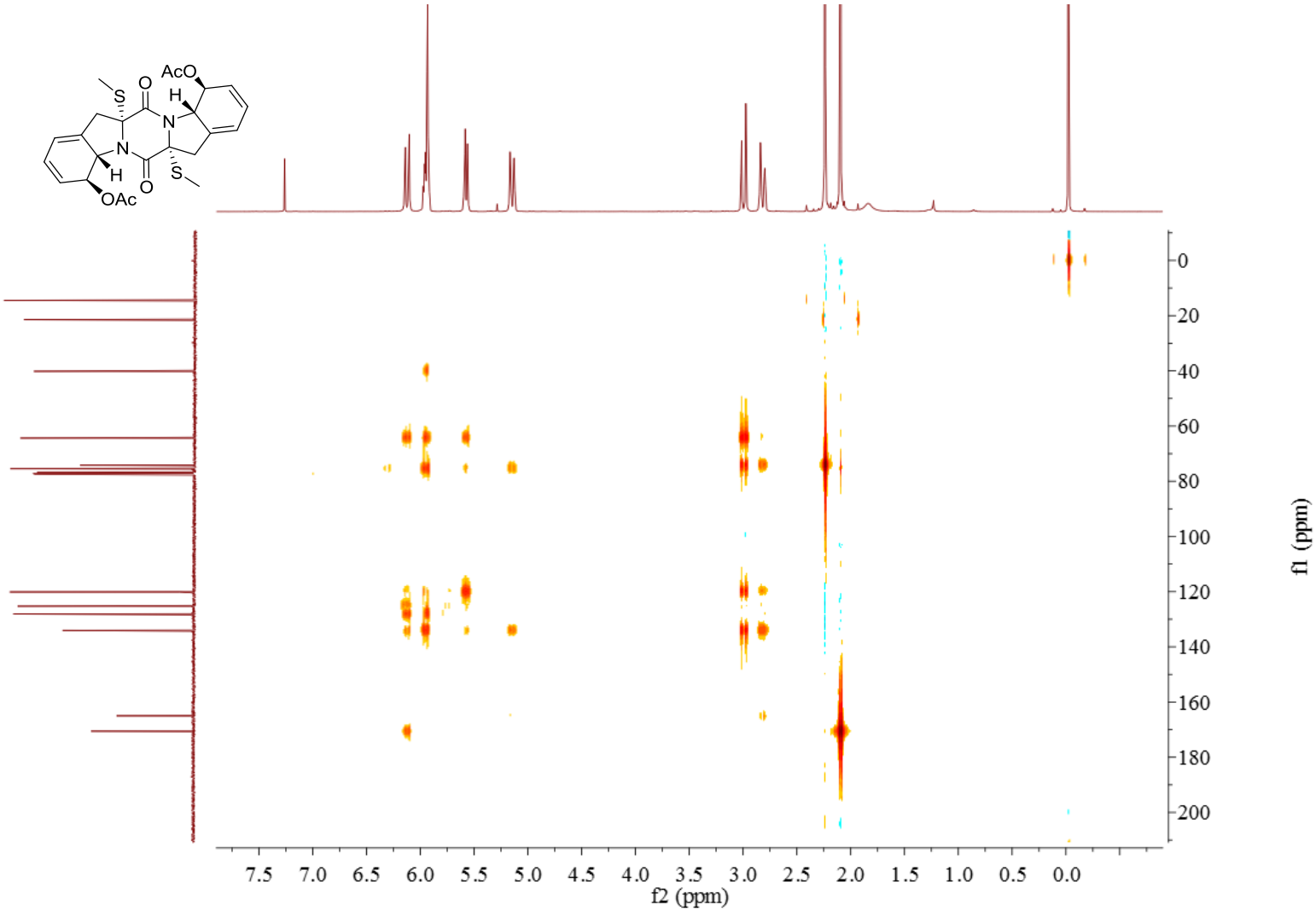


Figure S34. NOESY spectrum of haematocin (**5**) in CDCl3

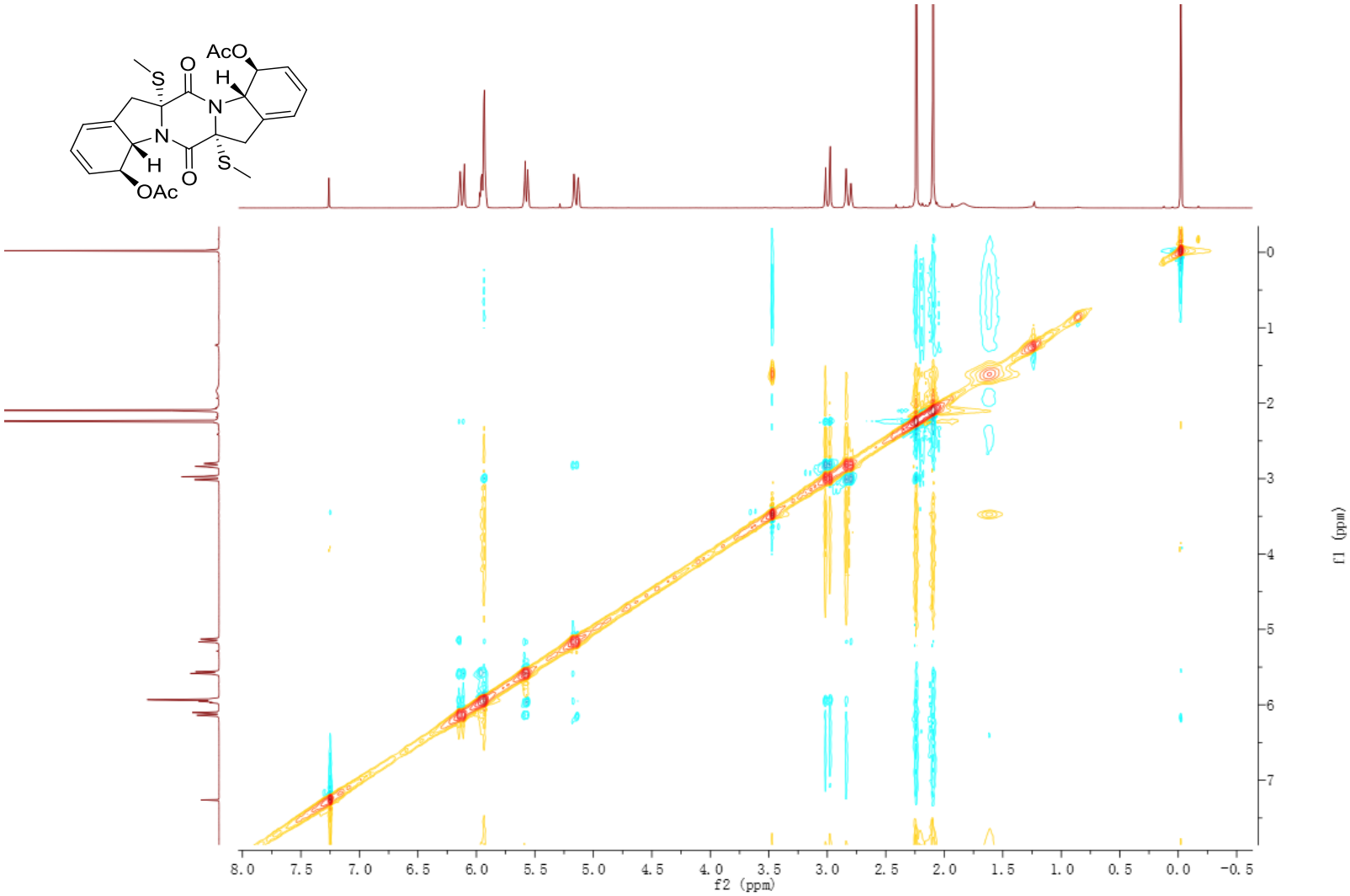


Figure S35. LR-ESI-MS spectrum of boydine A **(6)**

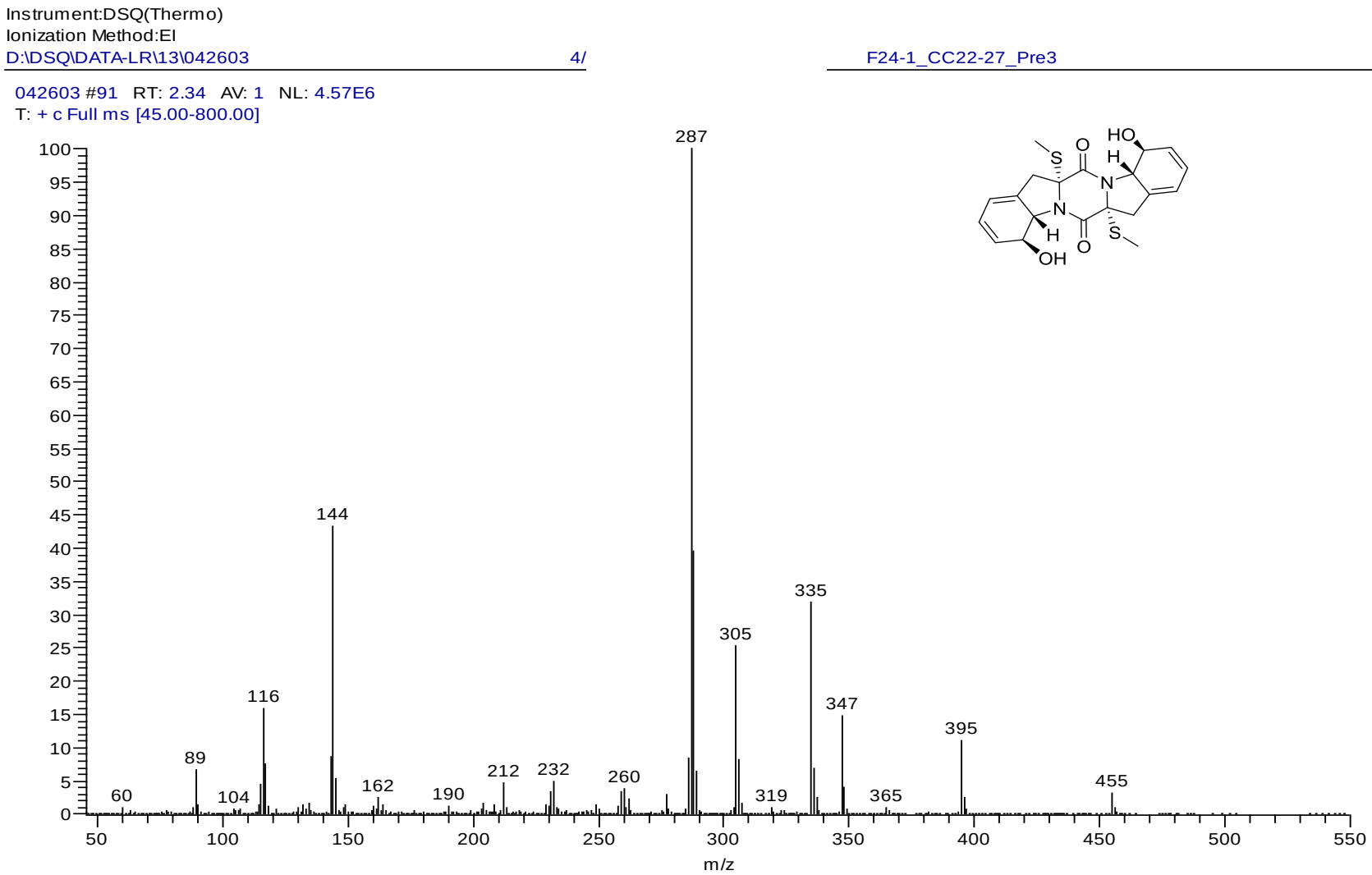


Figure S36. ^{1}H-NMR spectrum of boydine A **(6)** in $CDCl_3$ (400MHz)

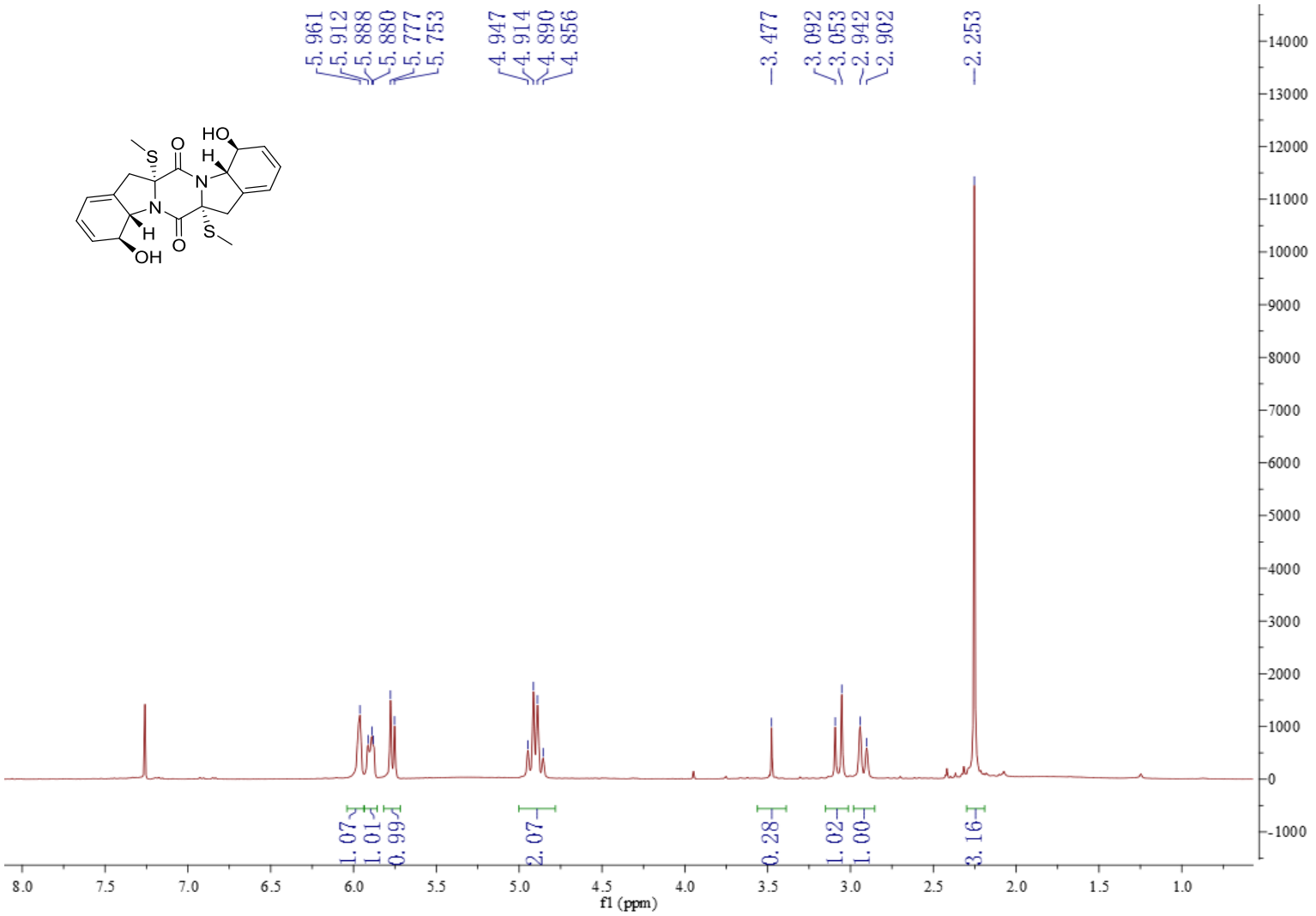


Figure S37. ^{13}C-NMR and DEPT spectra of boydine A **(6)** in $CDCl_3$ (100MHz)

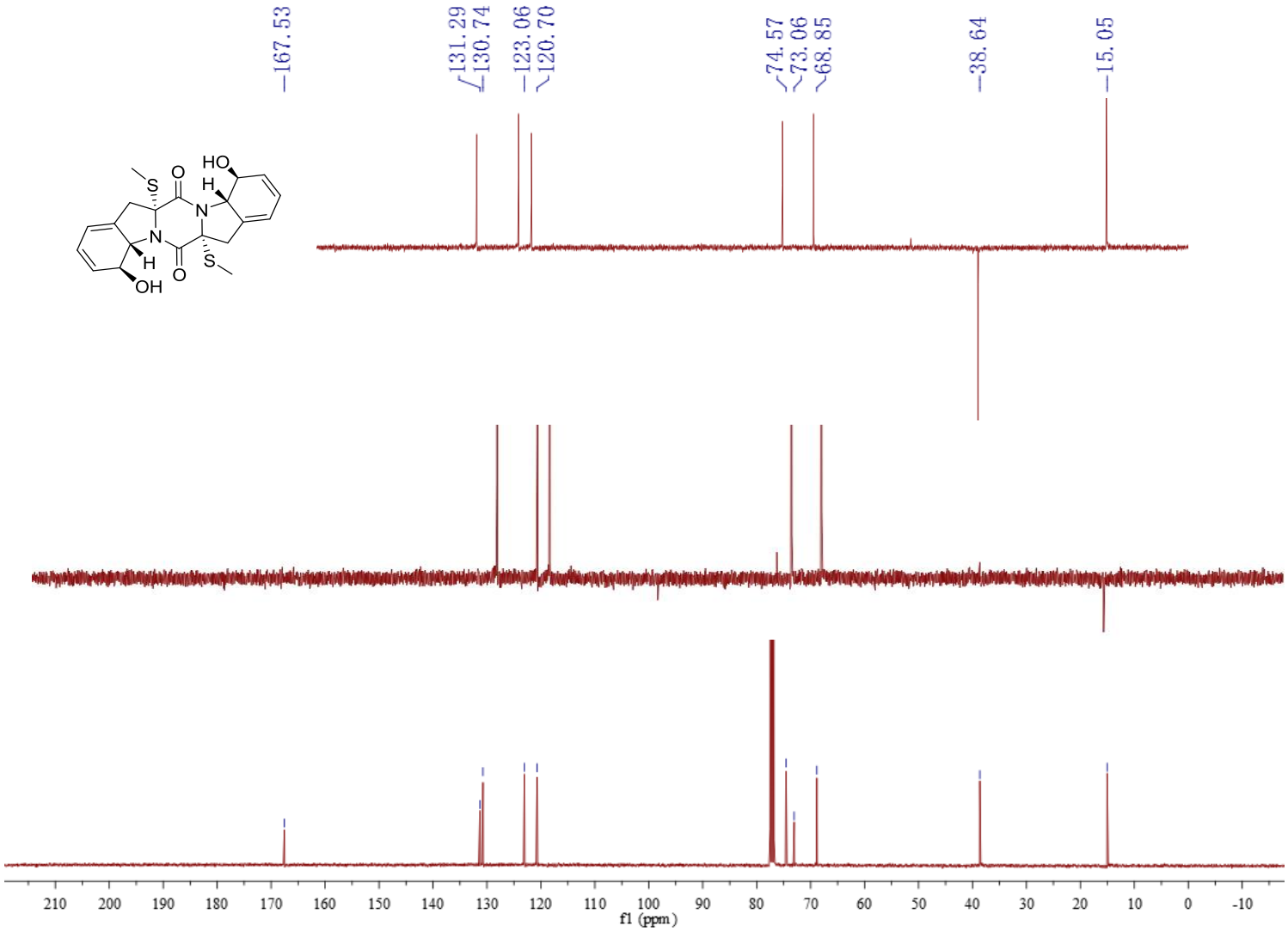


Figure S38. HMQC spectrum of boydine A **(6)** in $CDCl_3$

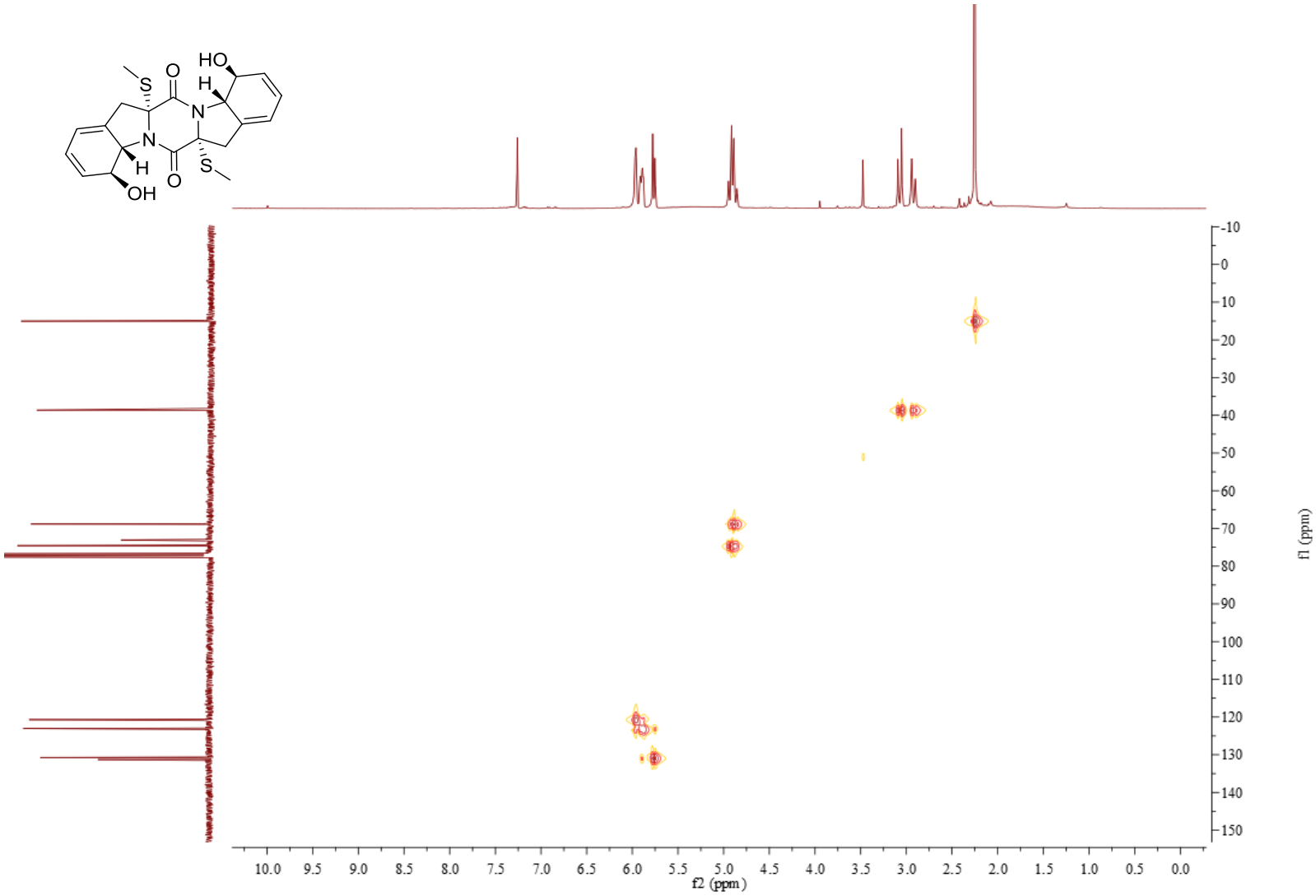


Figure S39. ^{1}H-^{1}H COSY spectrum of boydine A **(6)** in $CDCl_3$

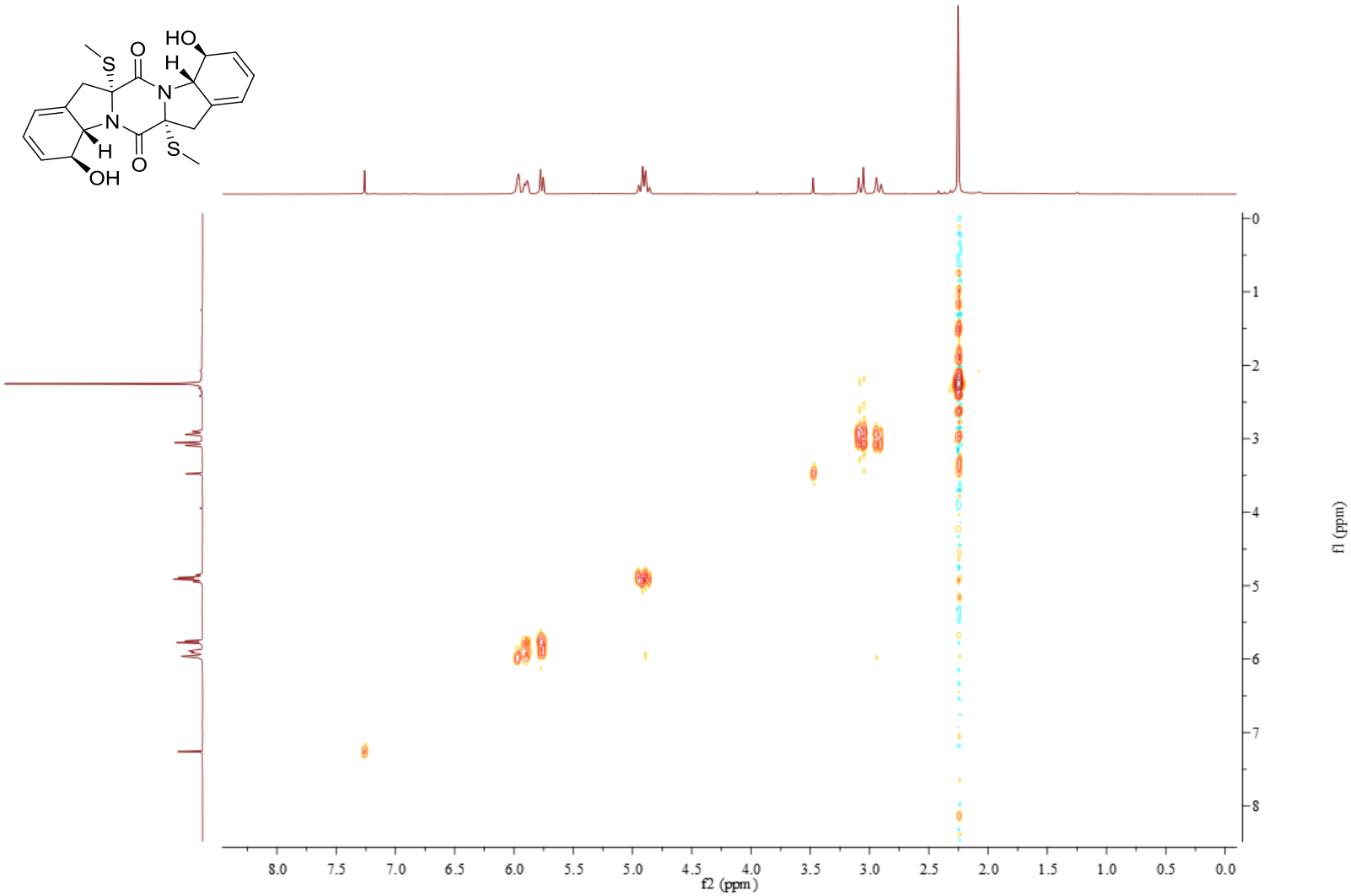


Figure S40. HMBC spectrum of boydine A **(6)** in $CDCl_3$

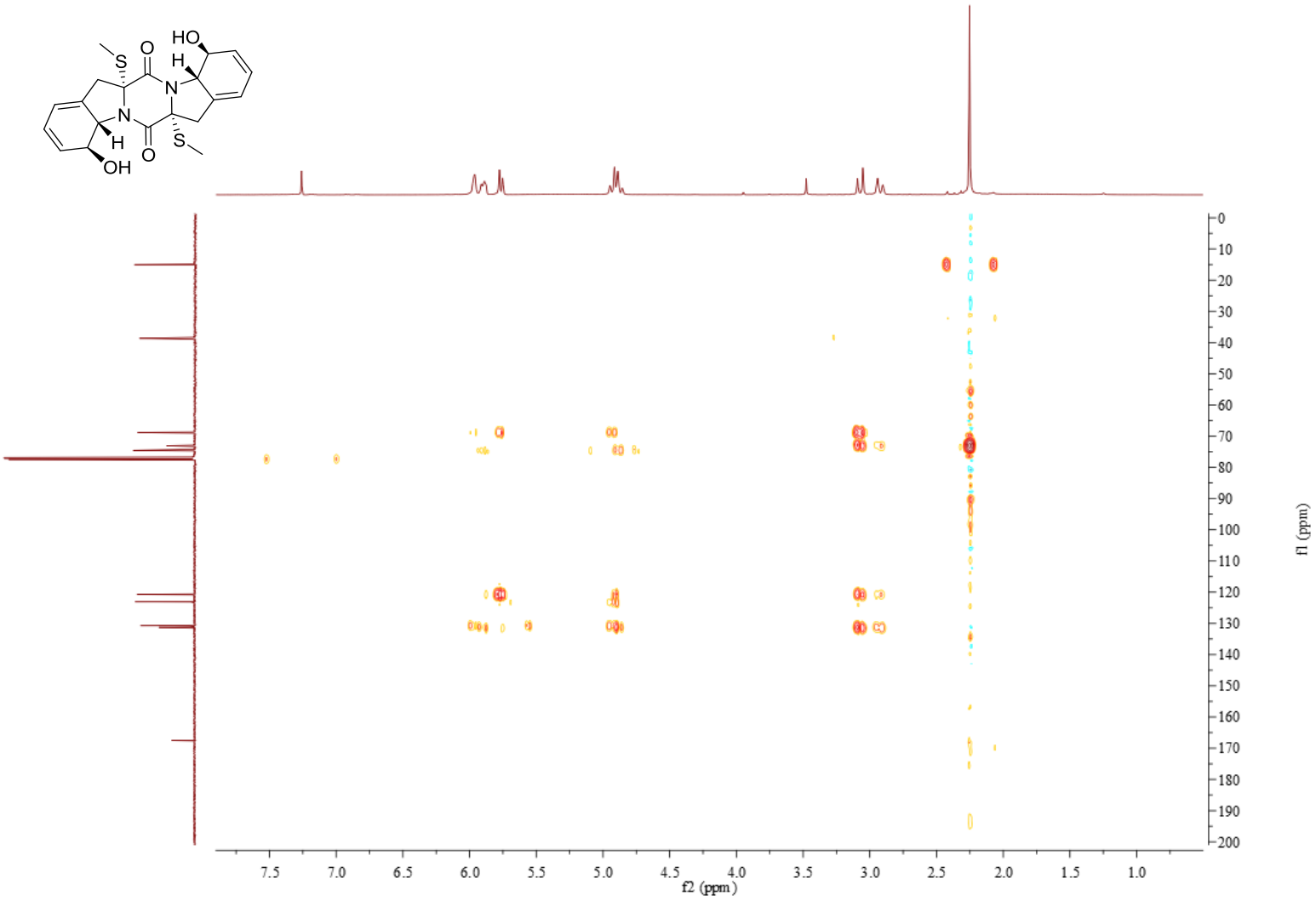


Figure S41. NOESY spectrum of boydine A **(6)** in $CDCl_3$

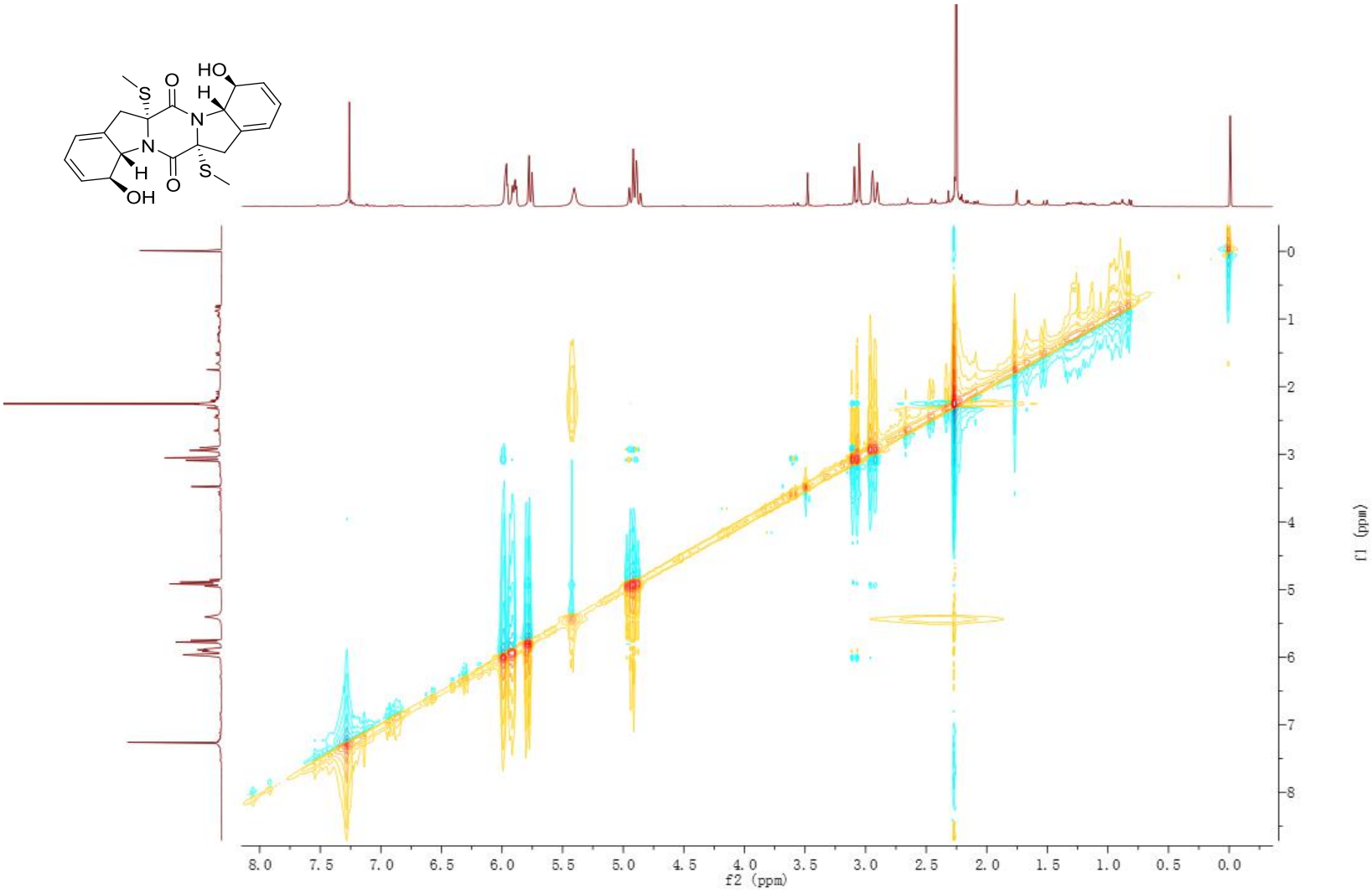


Figure S42. LR-ESI-MS spectrum of boydine B **(7)**

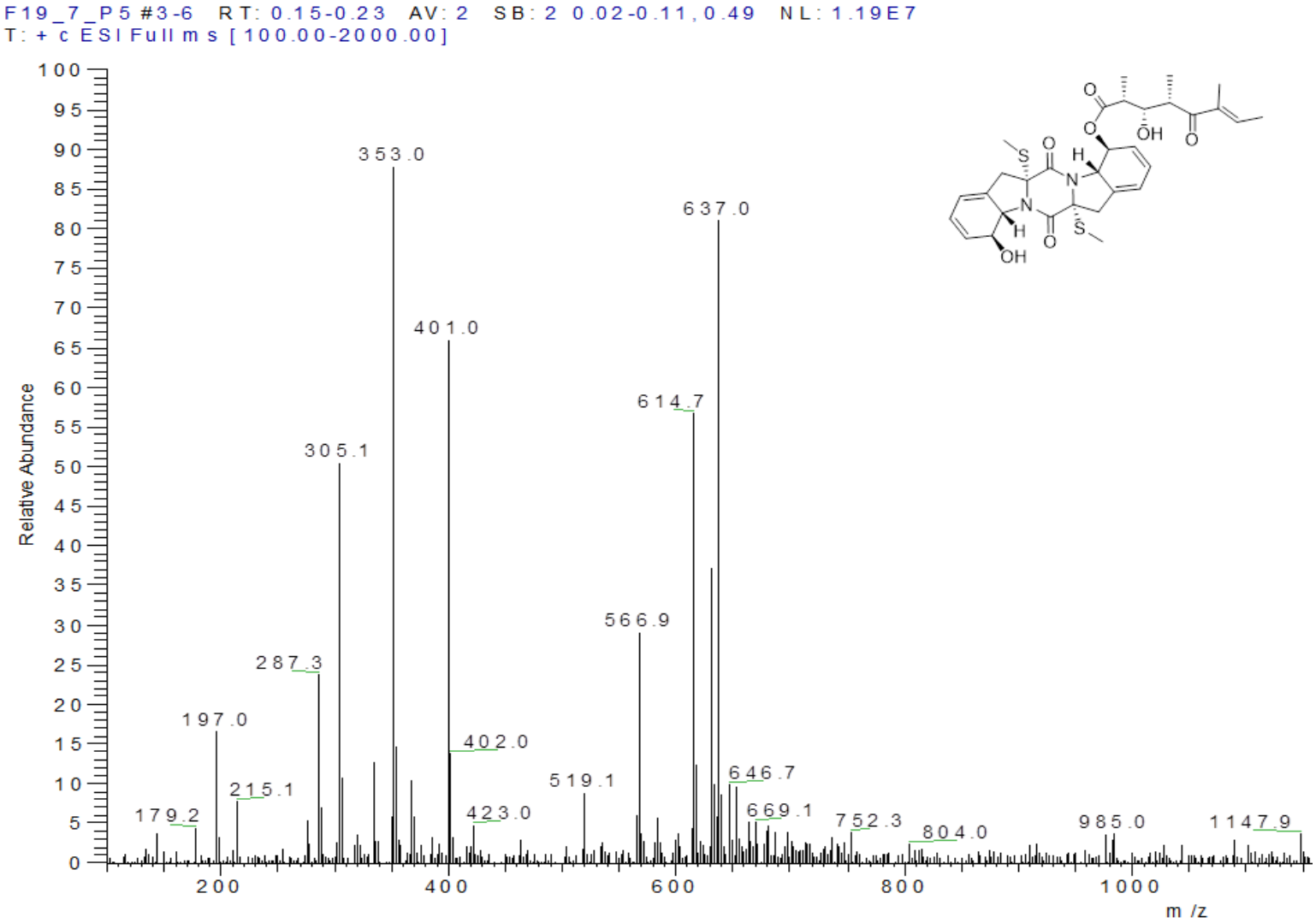


Figure S43. ^{1}H-NMR spectrum of boydine B **(7)** in $CDCl_3$ (400MHz)

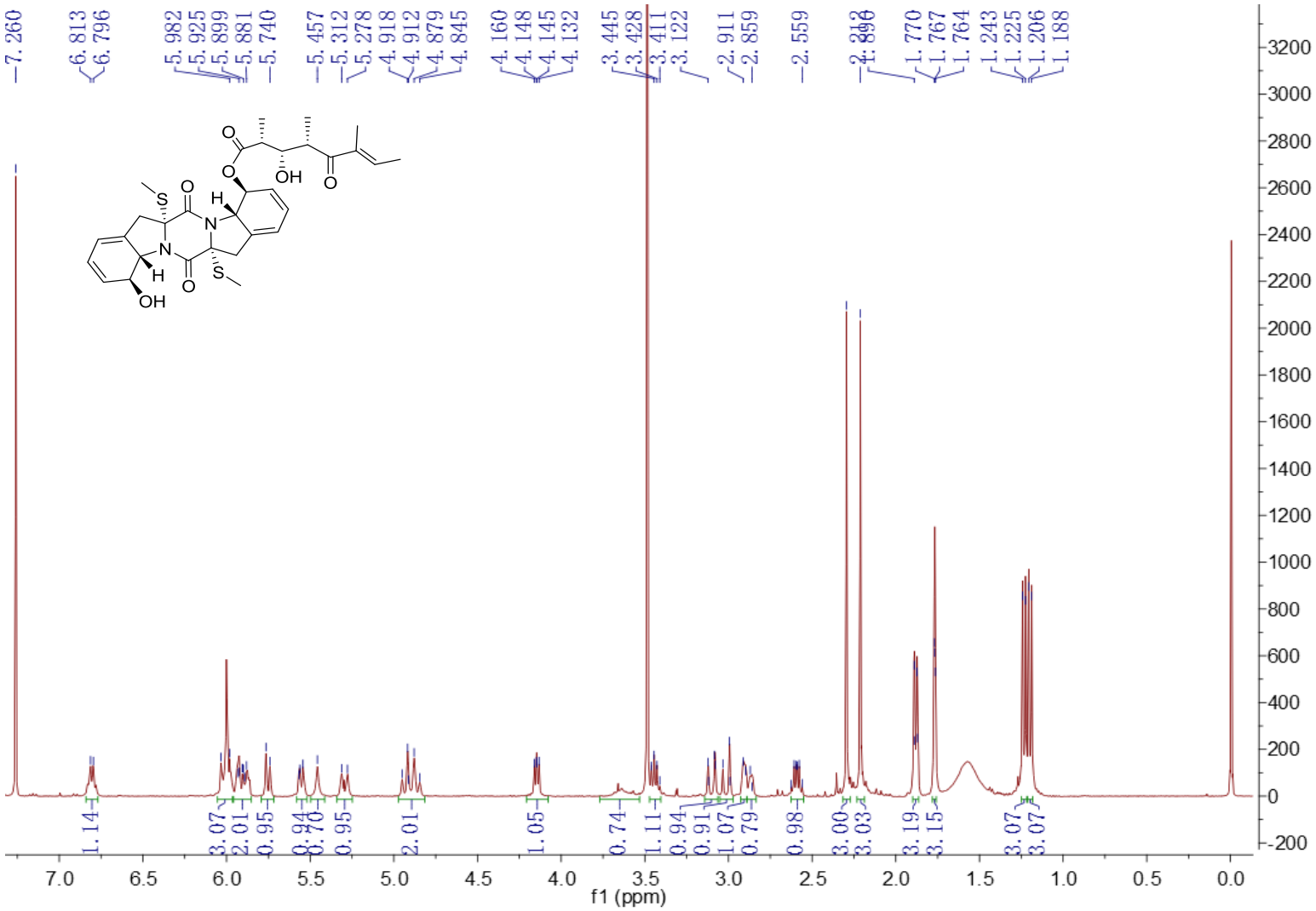


Figure S44. ^{13}C-NMR spectrum of boydine B **(7)** in $CDCl_3$ (100MHz)

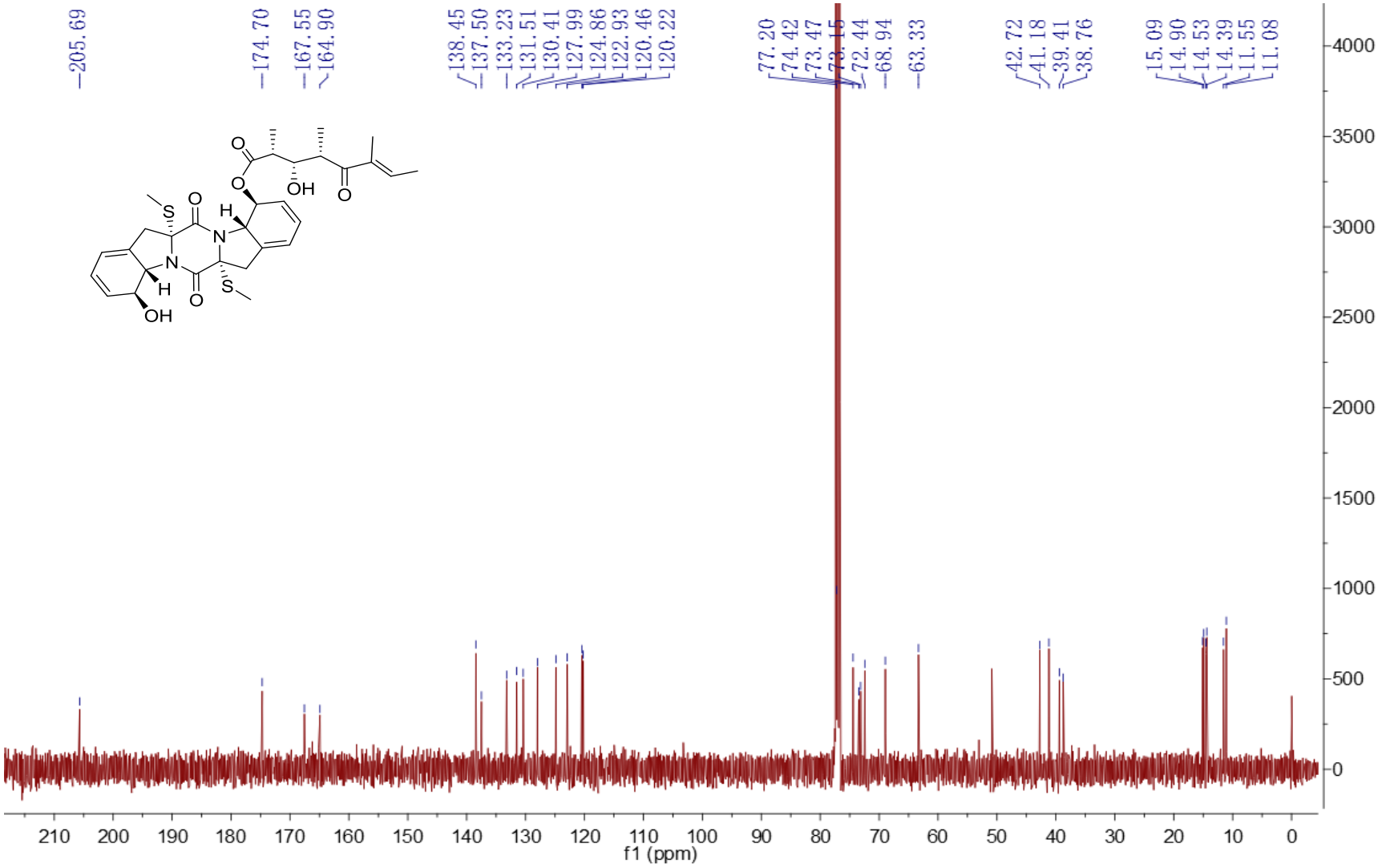


Figure S45. ^{1}H-NMR spectrum of phomazine B **(8)** in $CDCl_3$ (400MHz)

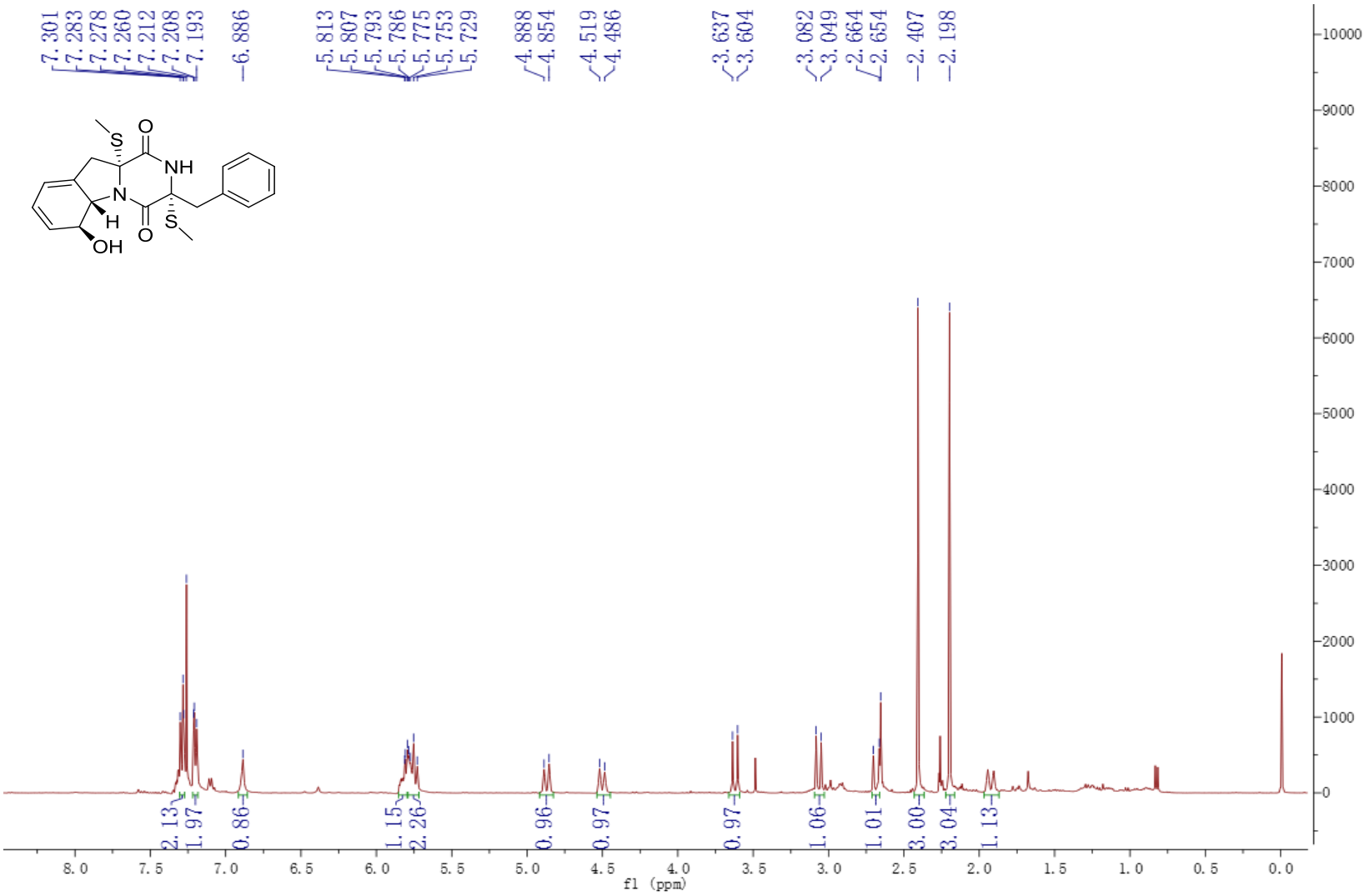


Figure S46. ^{13}C-NMR and DEPT spectra of phomazine B **(8)** in $CDCl_3$ (100MHz)

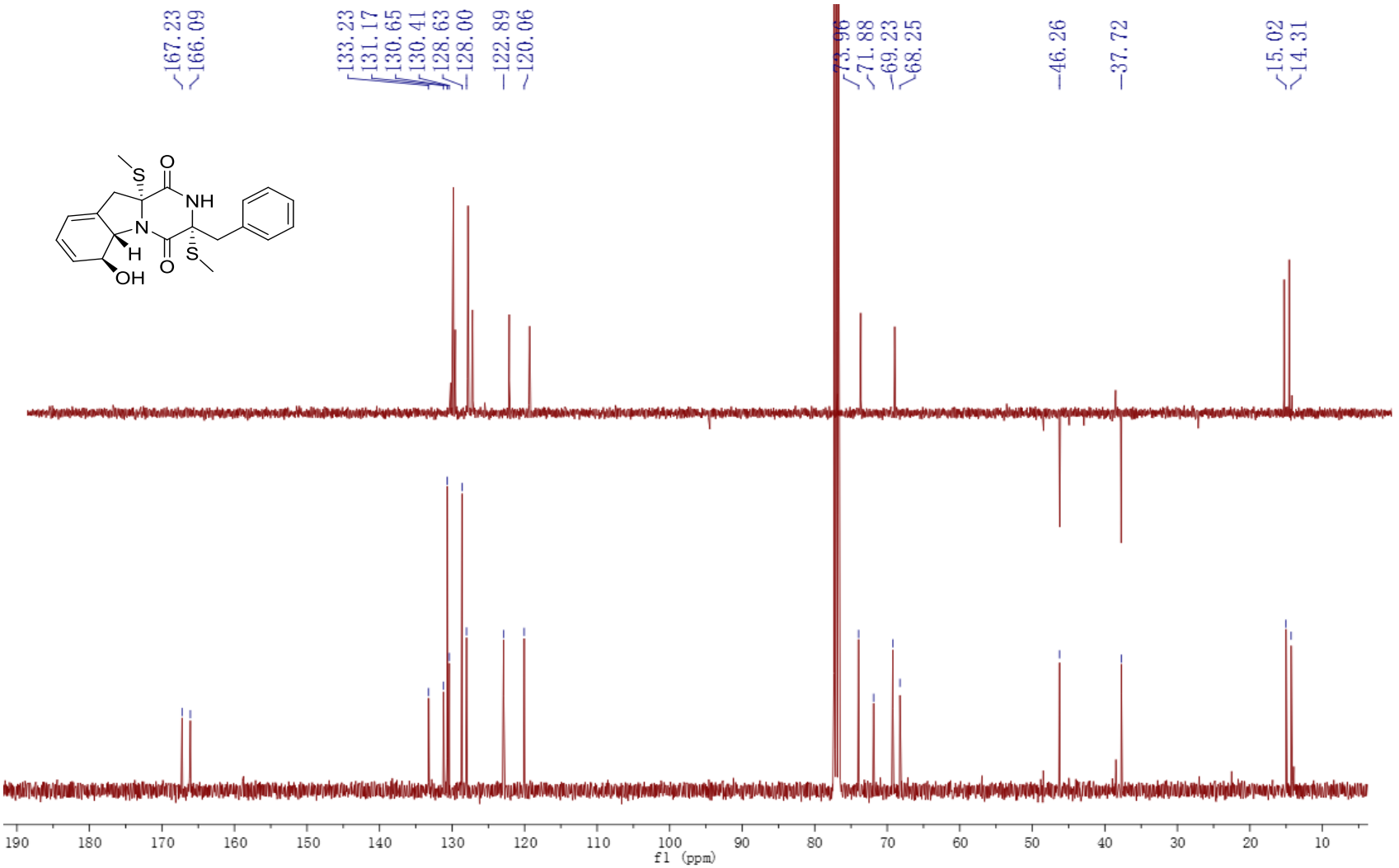


Figure S47. HMQC spectrum of phomazine B **(8)** in $CDCl_3$

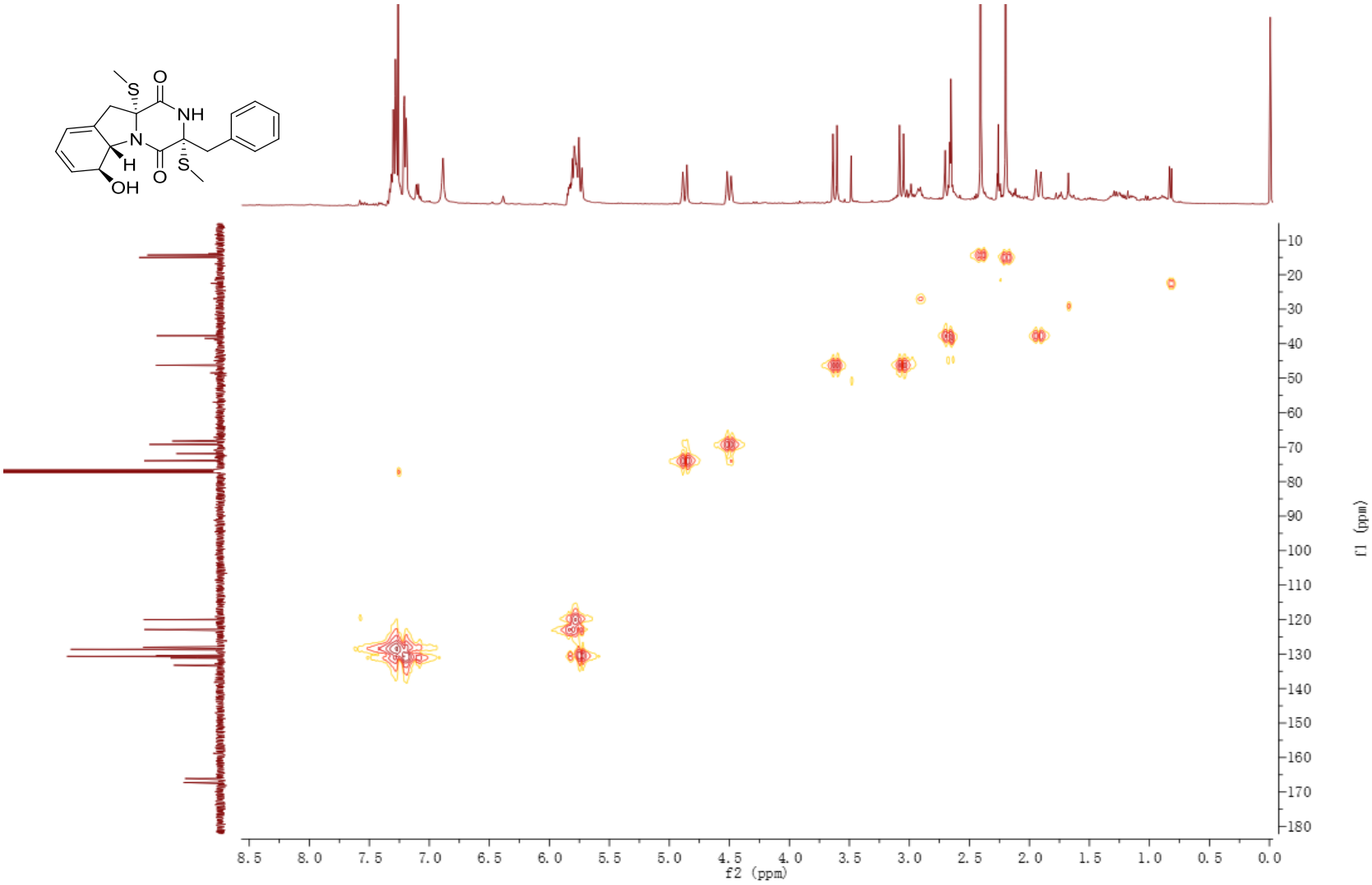


Figure S48. HMBC spectrum of phomazine B **(8)** in $CDCl_3$

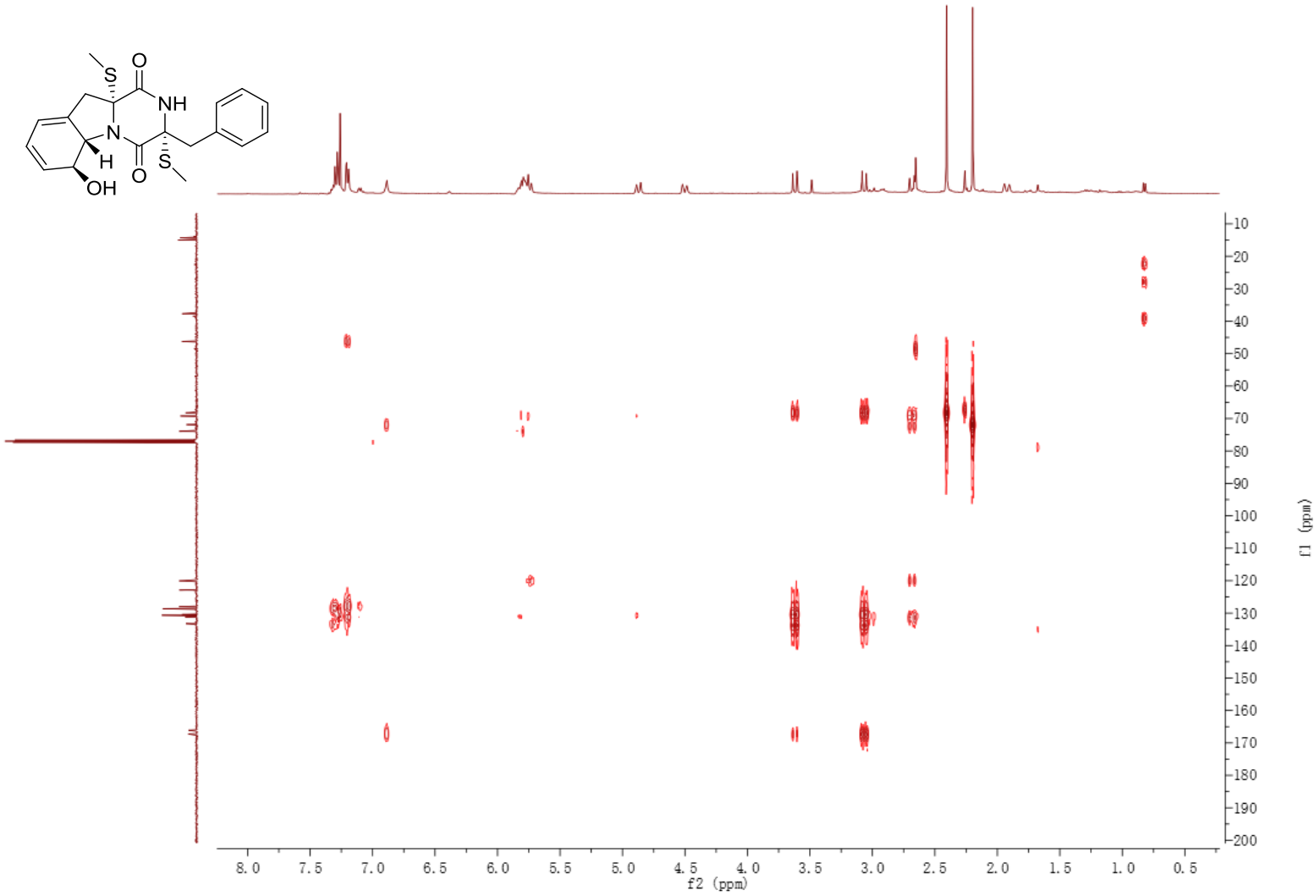


Figure S49. NOESY spectrum of phomazine B **(8)** in $CDCl_3$

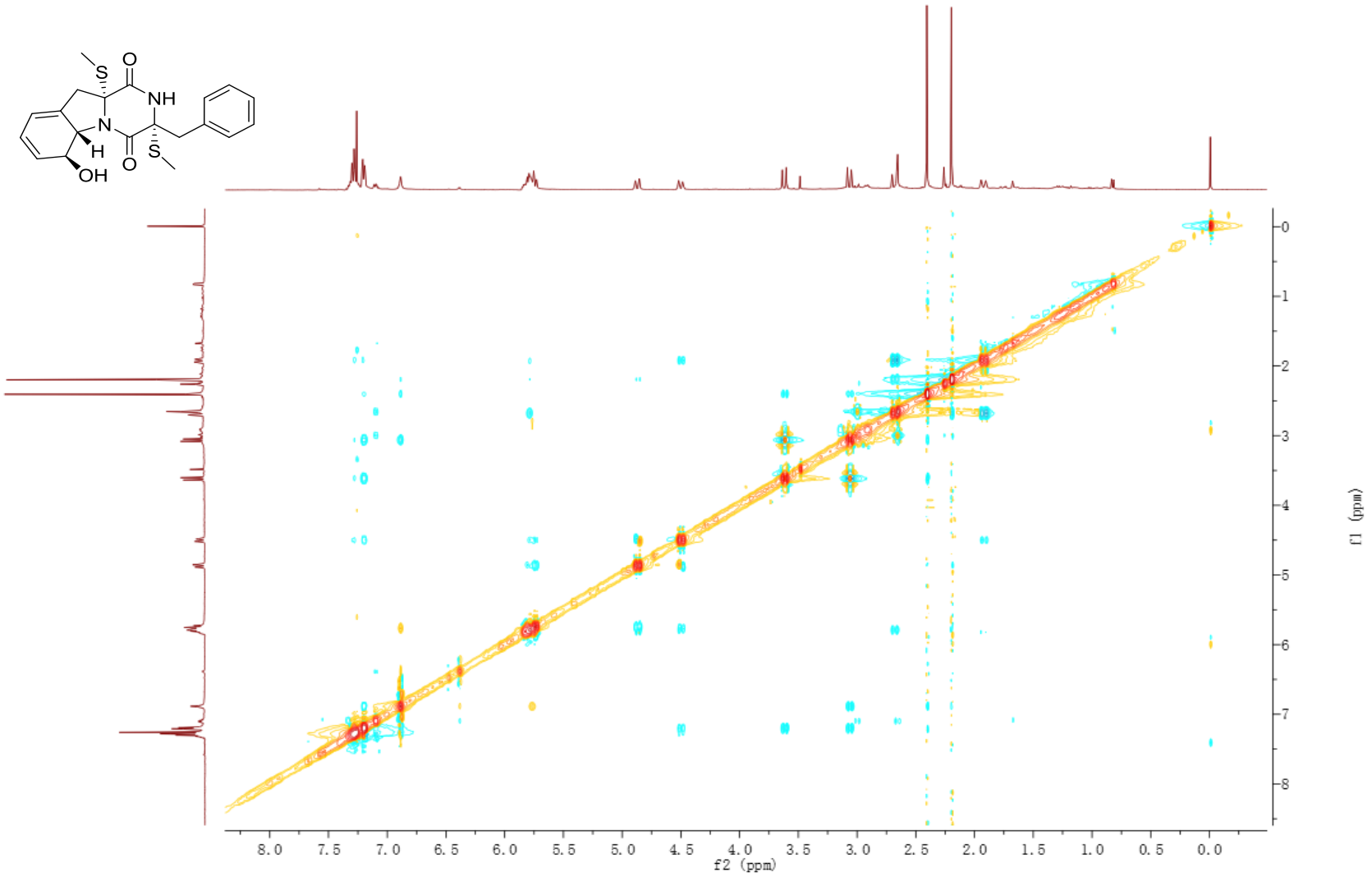


Figure S50. ^{1}H-NMR spectrum of bisdethiobis (methylthio) gliotoxin **(9)** in $CDCl_3$ (400MHz)

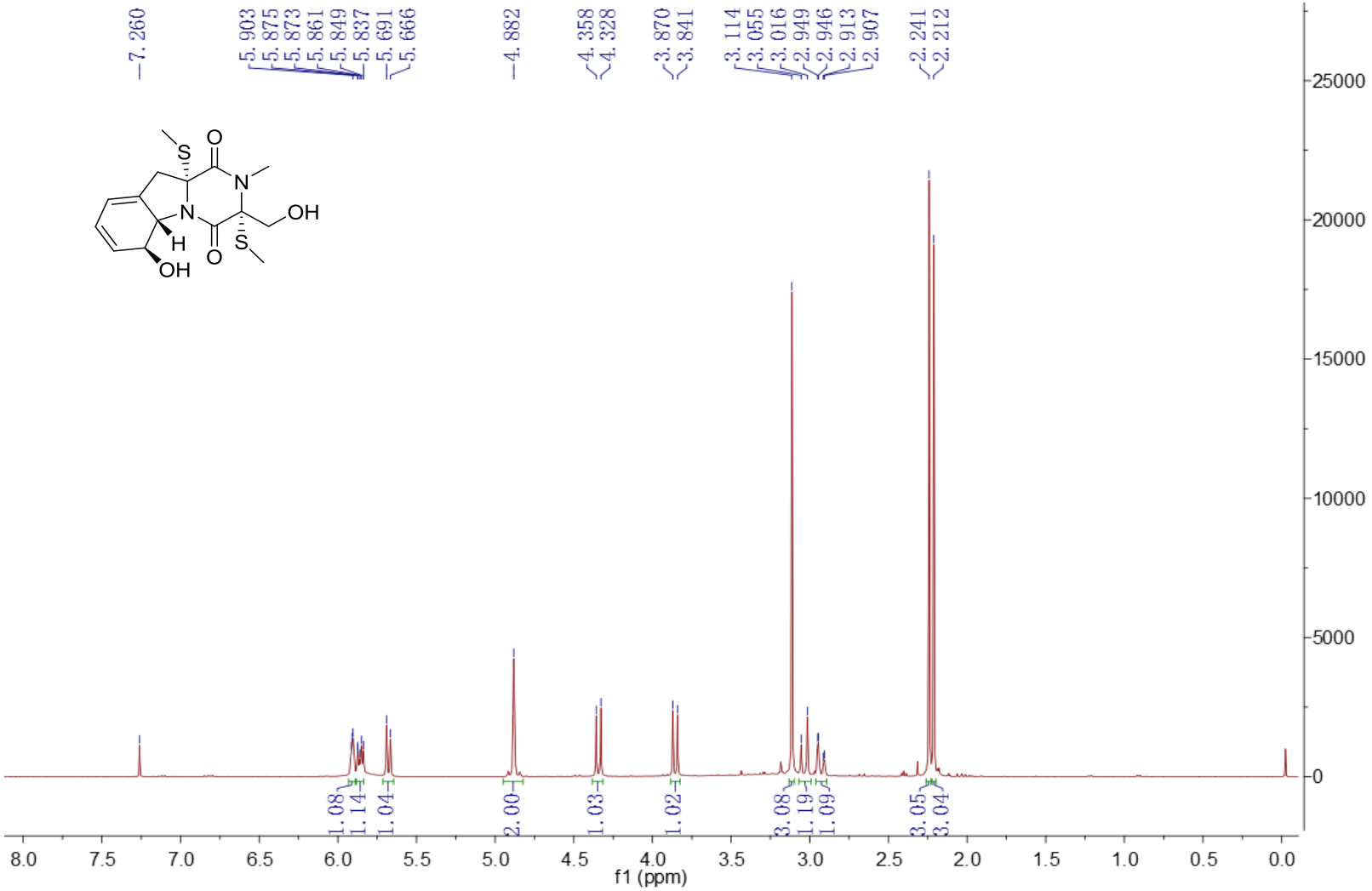


Figure S51. ^{13}C-NMR spectrum of bisdethiobis (methylthio) gliotoxin **(9)** in $CDCl_3$ (100MHz)

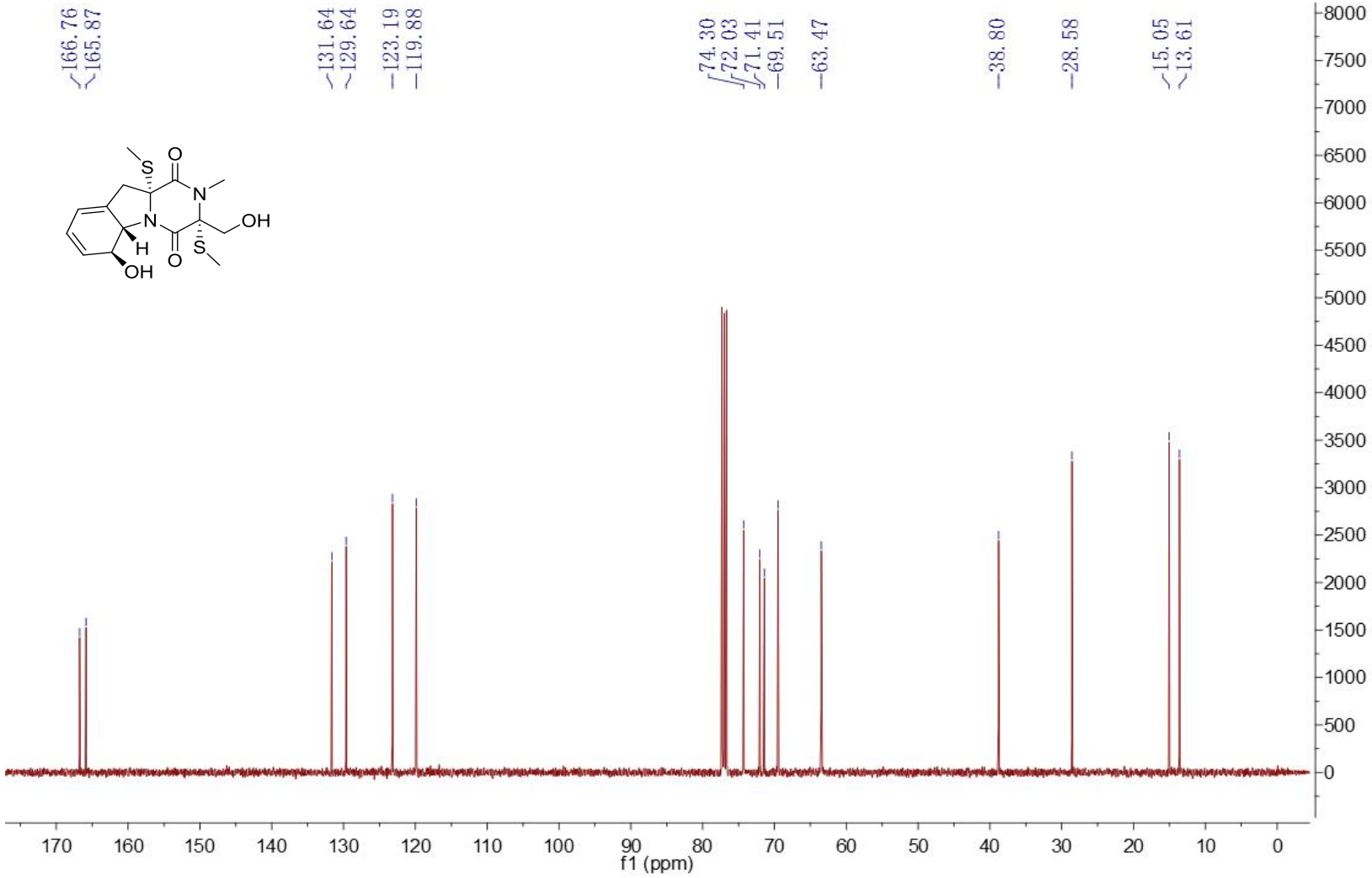


Figure S52. [1]H-NMR spectrum of cyclo-(2, 2′-dimethylthio-Phe-Phe (**10**) in DMSO-d_6 (400MHz)

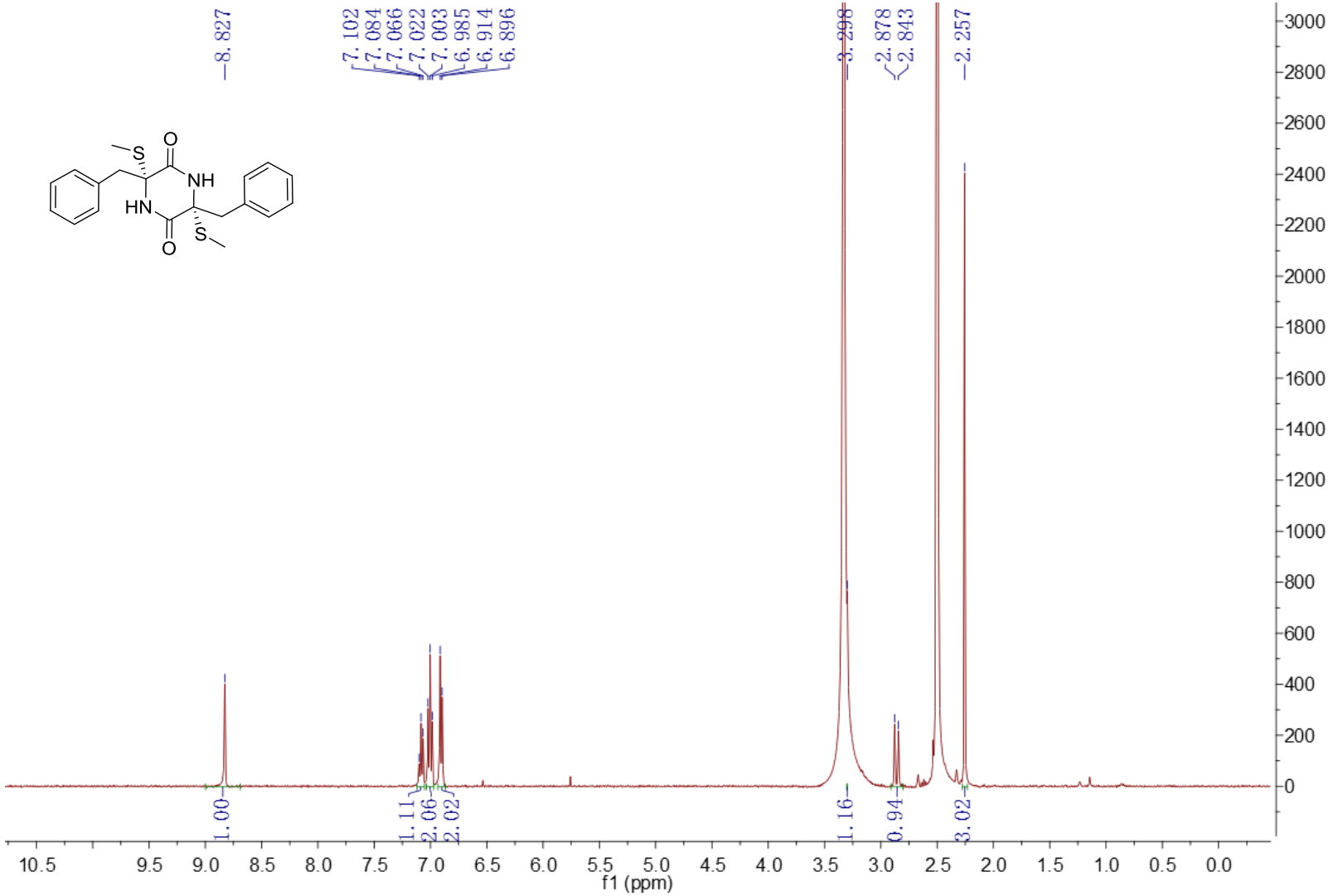


Figure S53. ^{1}H-NMR spectrum of cyclo-(Phe-Phe) (**11**) in DMSO-d_6 (400MHz)

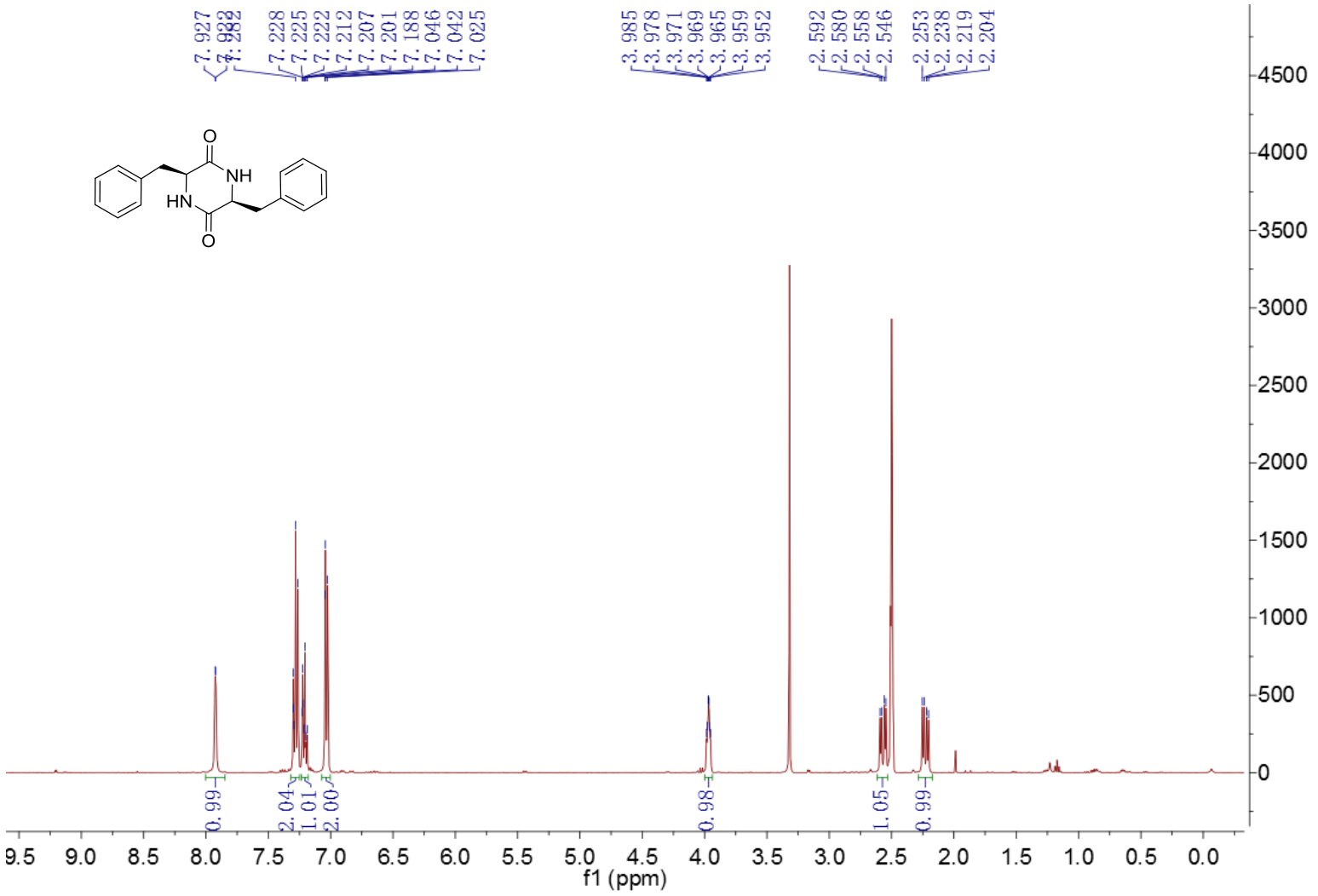


Figure S54. ^{13}C-NMR and DEPT spectra of cyclo-(Phe-Phe) (**11**) in DMSO-d_6 (100MHz)

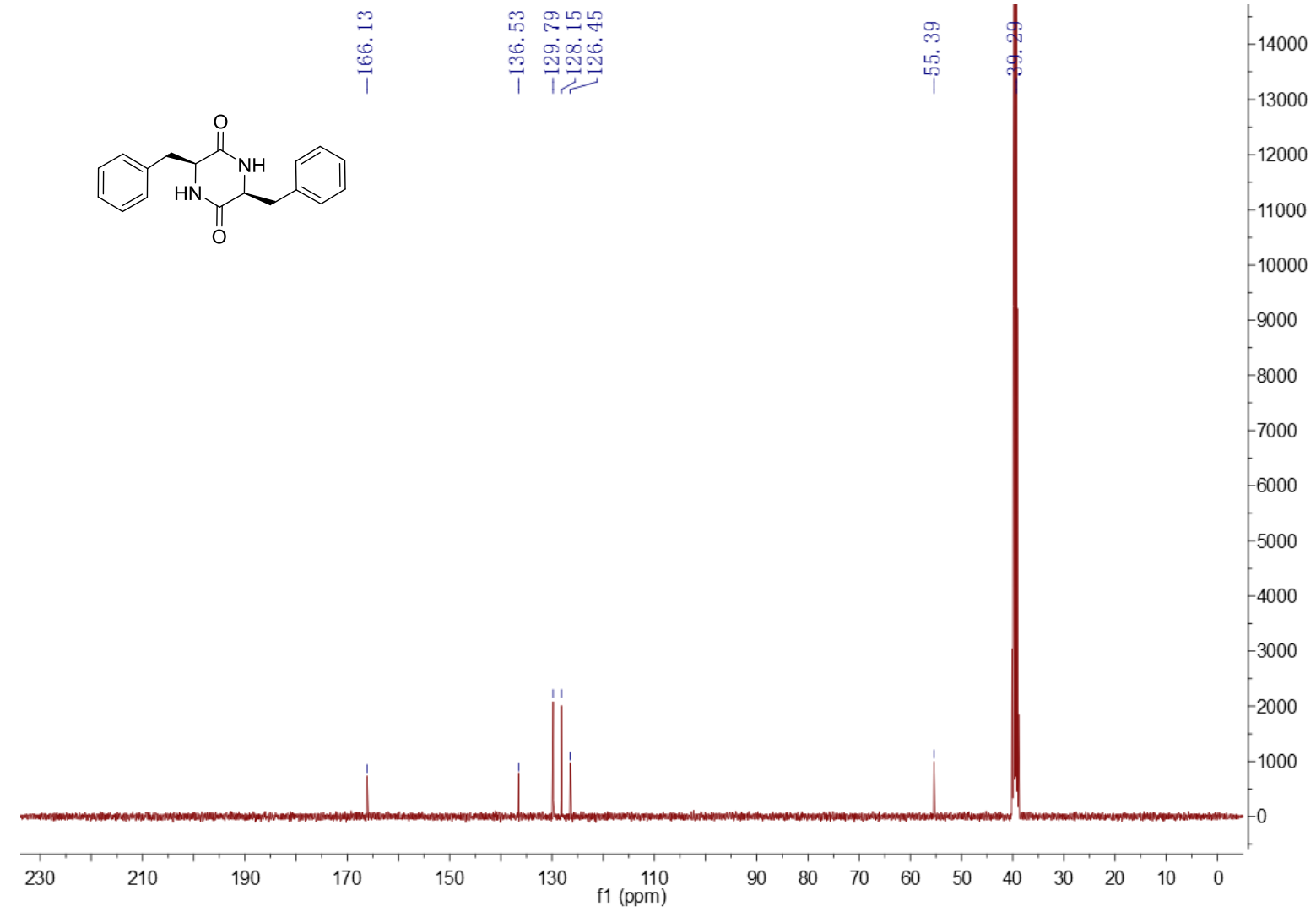


Figure S55. LR-ESI-MS spectrum of ditryptophenaline (**12**)

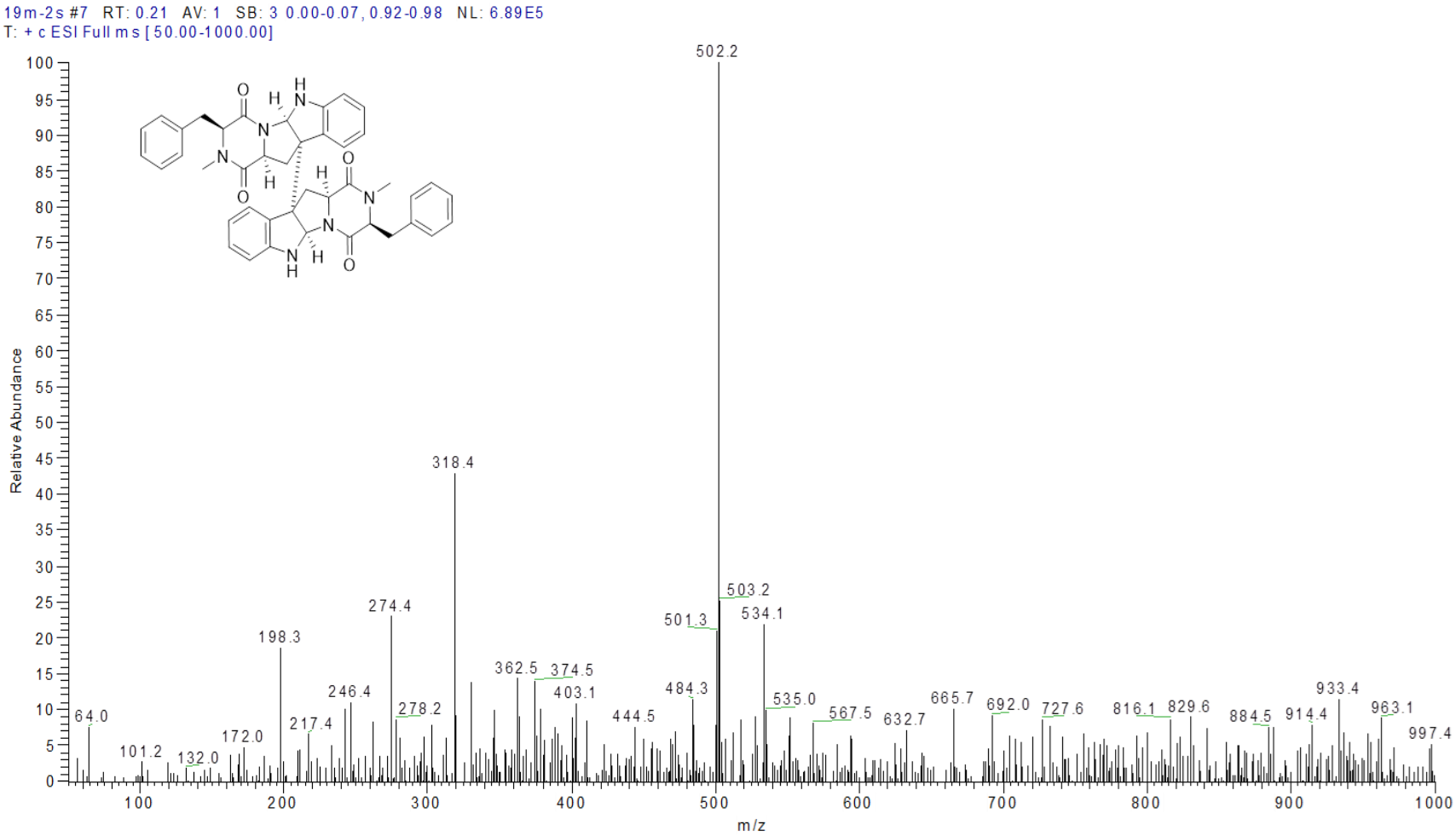


Figure S56. ^{1}H-NMR spectrum of ditryptophenaline (**12**) in $CDCl_3$ (400MHz)

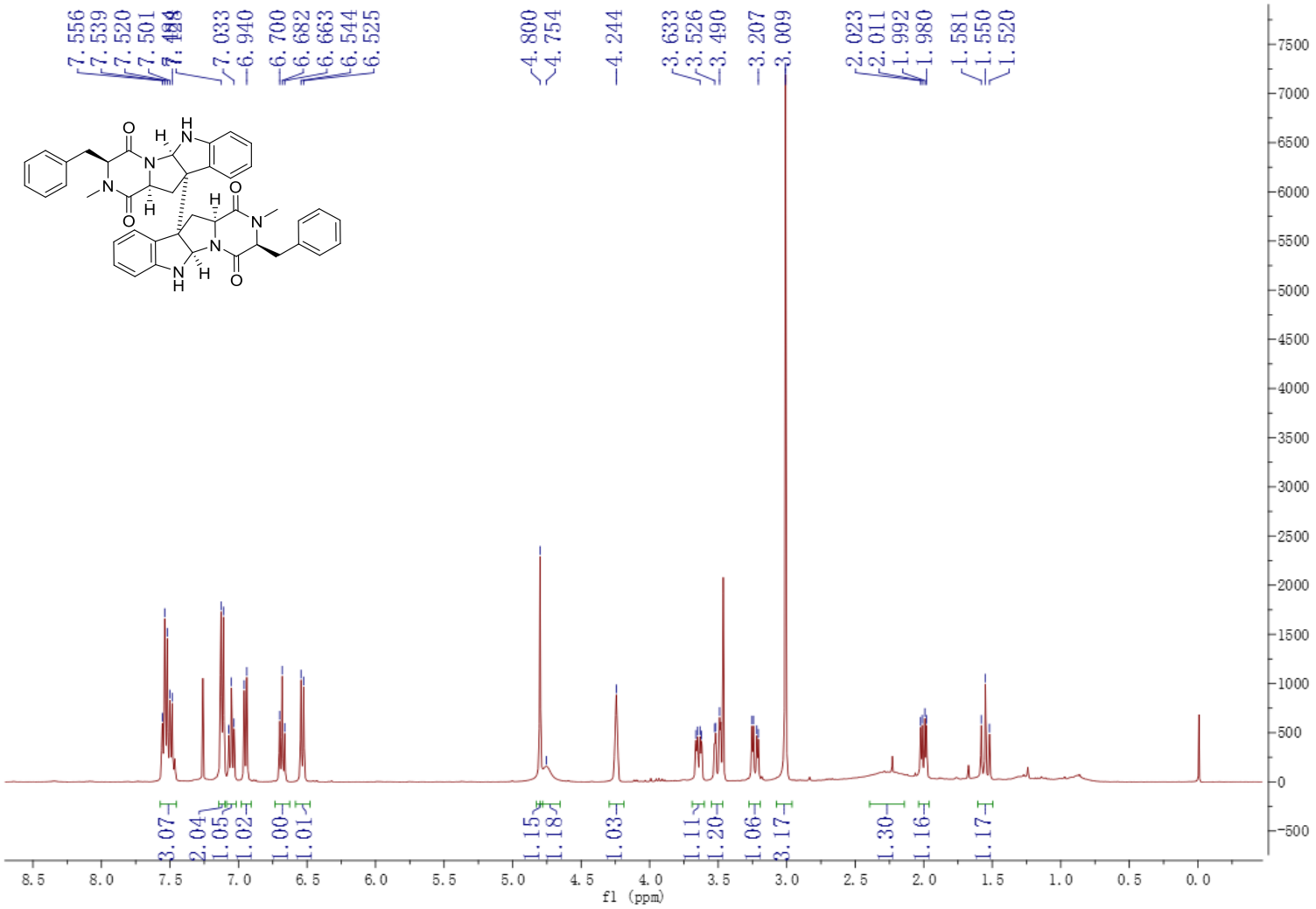


Figure S57. ^{13}C-NMR and DEPT spectra of ditryptophenaline (**12**) in $CDCl_3$ (100MHz)

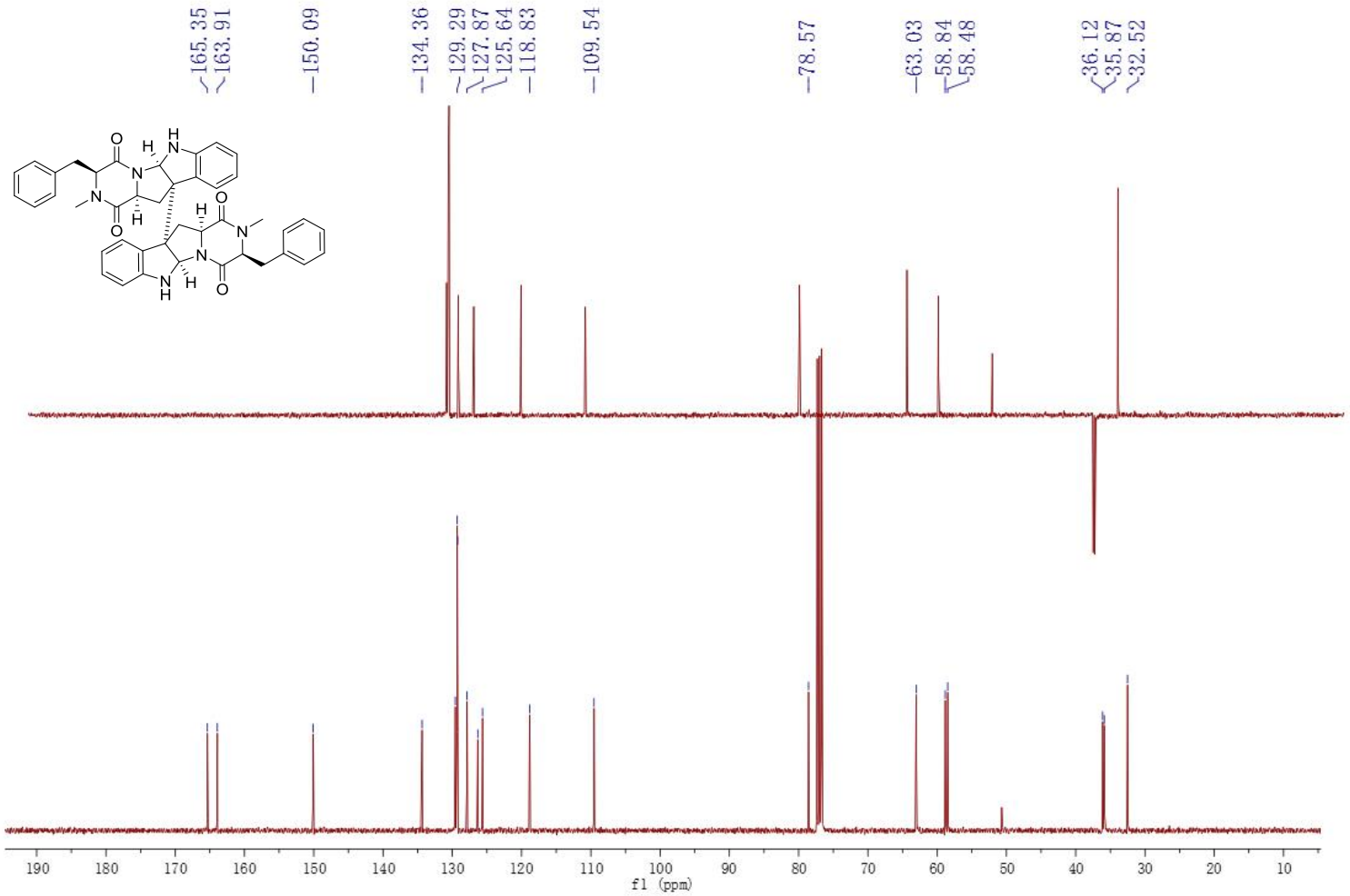


Figure S58. NOESY spectrum of ditryptophenaline (**12**) in $CDCl_3$

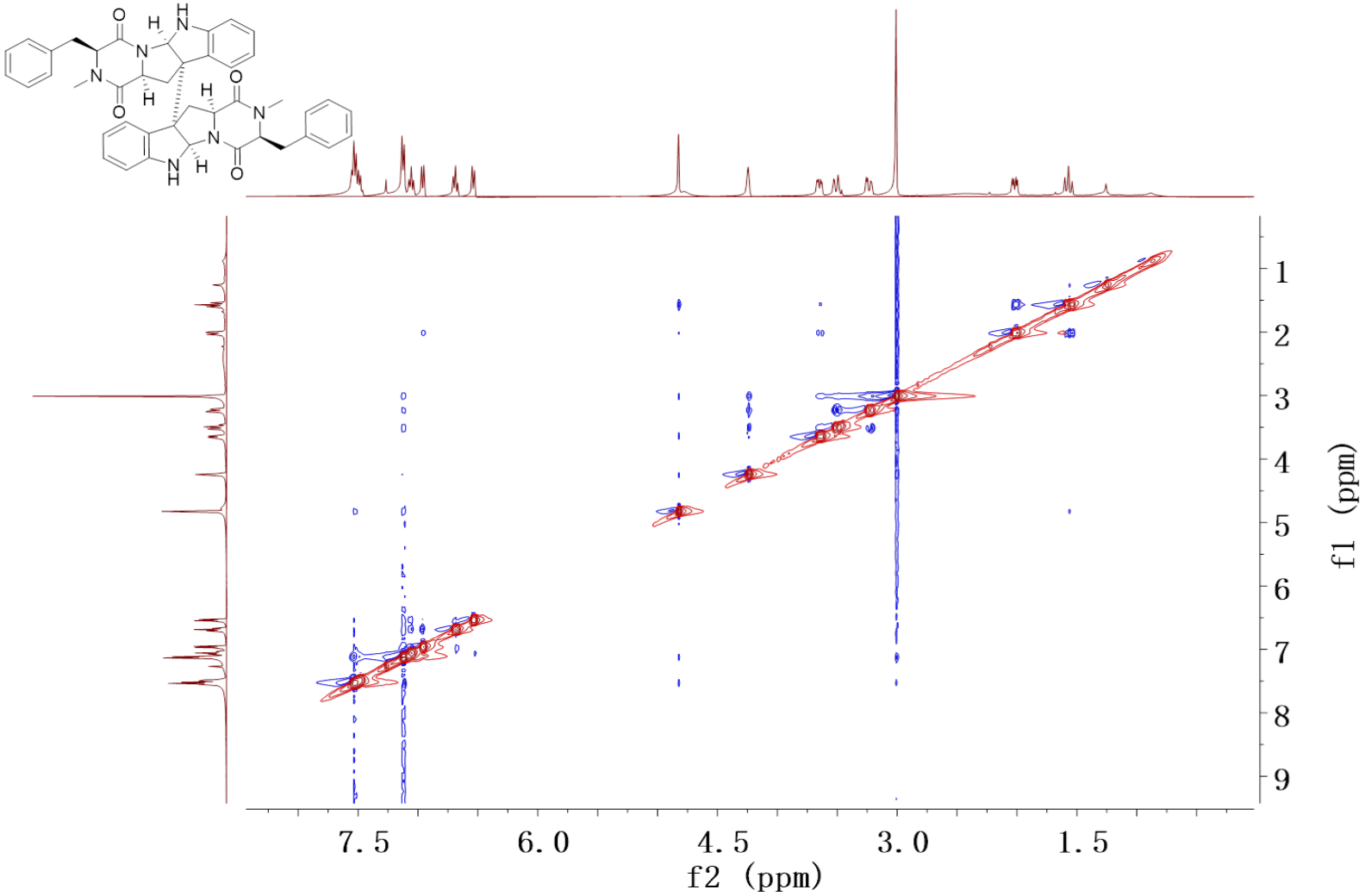


Figure S59. HR-ESI-MS spectrum of pseuboydone E **(13)**

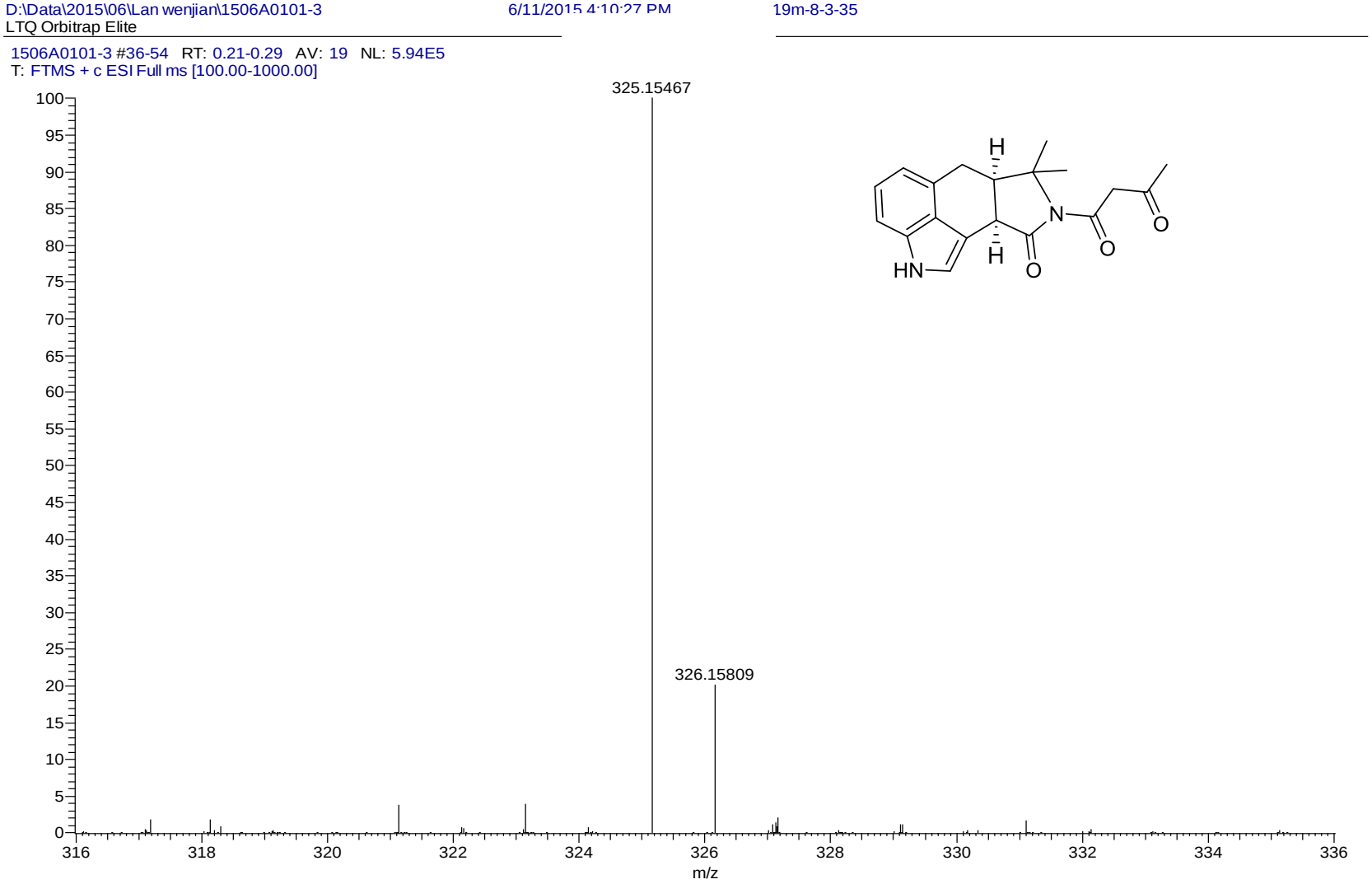


Figure S60. ^{1}H-NMR spectrum of pseuboydone E **(13)** in $CDCl_3$ (400MHz)

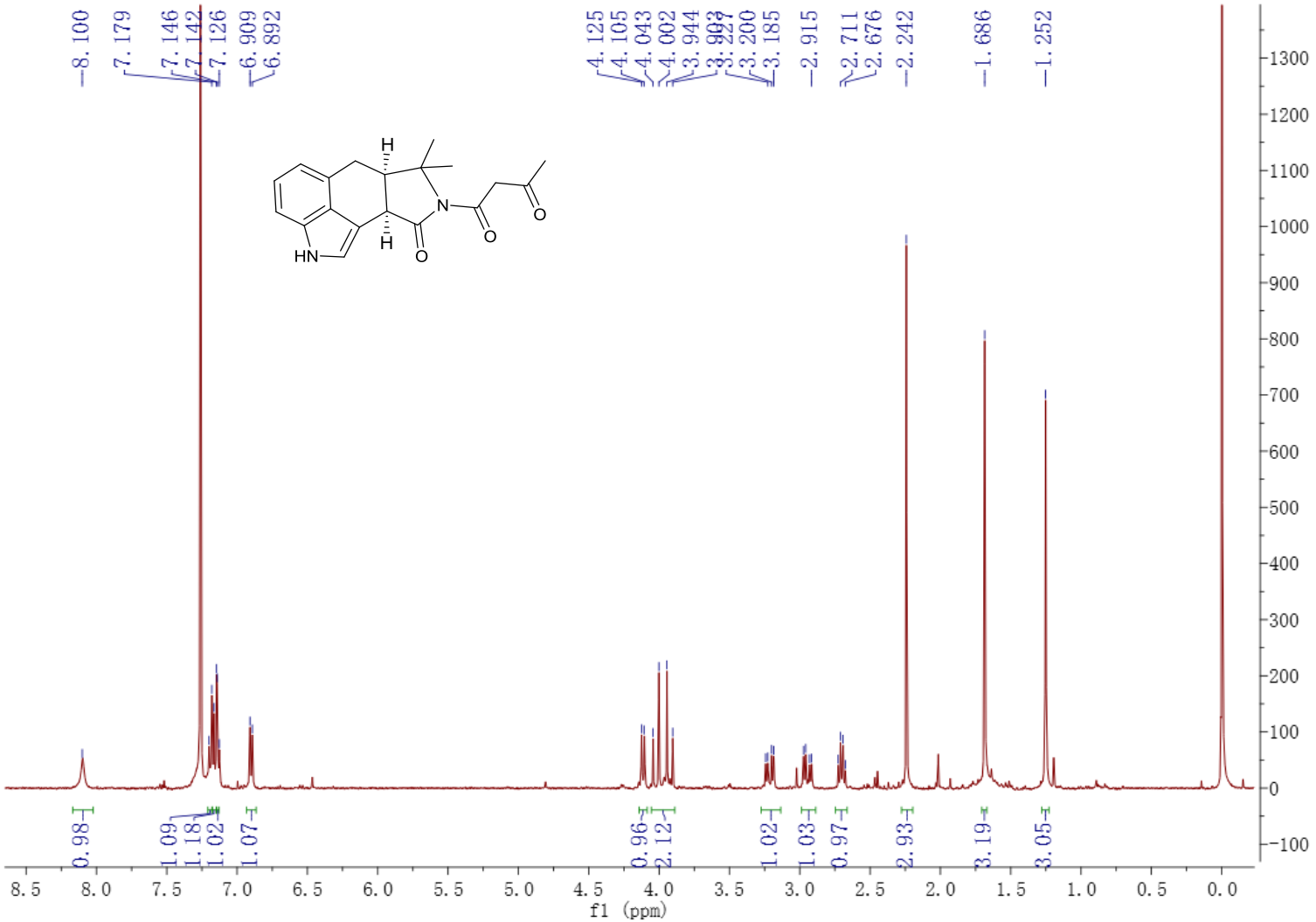


Figure S61. ^{13}C NMR and DEPT spectra of pseuboydone E **(13)** in $CDCl_3$ (100MHz)

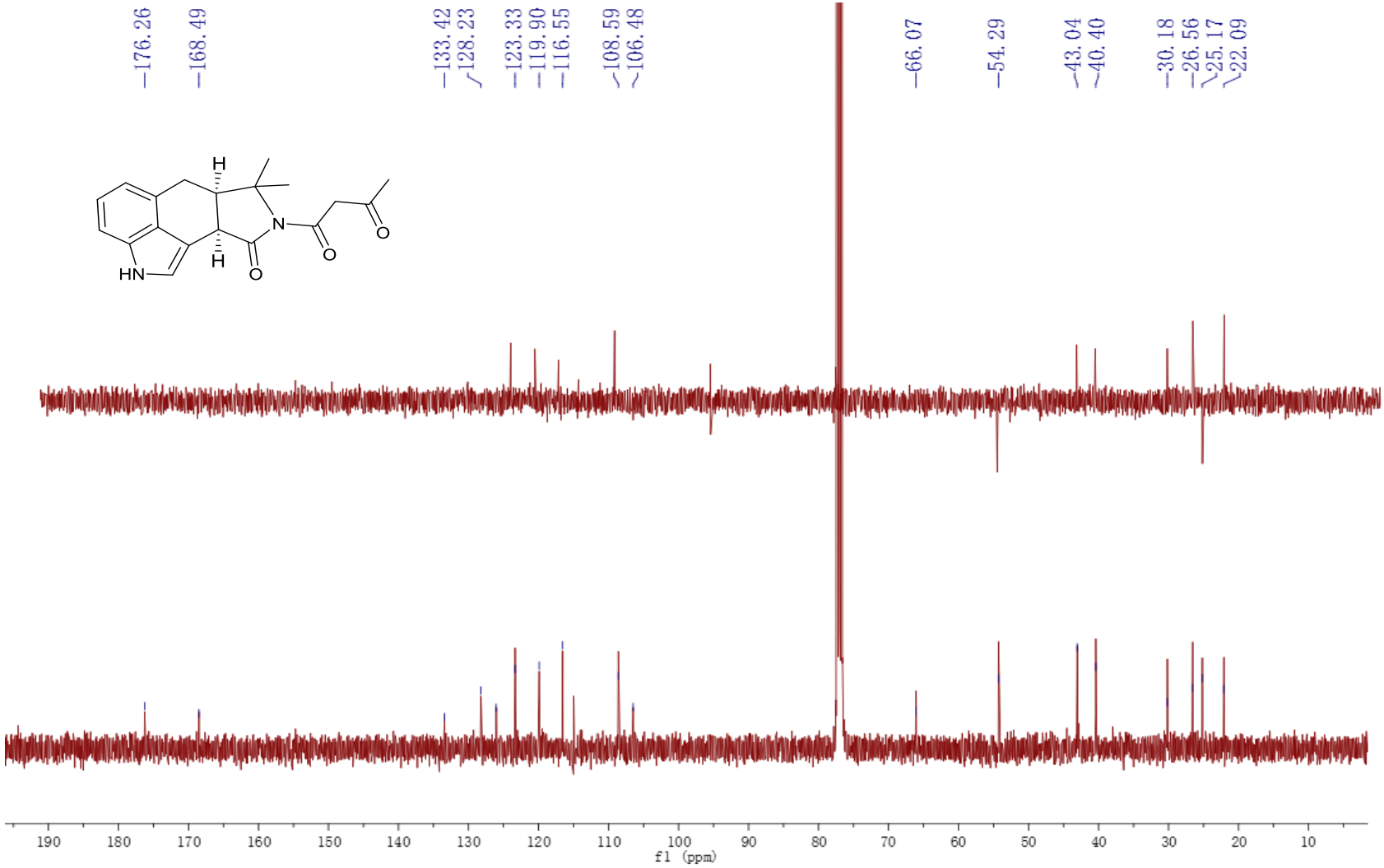


Figure S62. HMQC spectrum of pseuboydone E **(13)** in $CDCl_3$

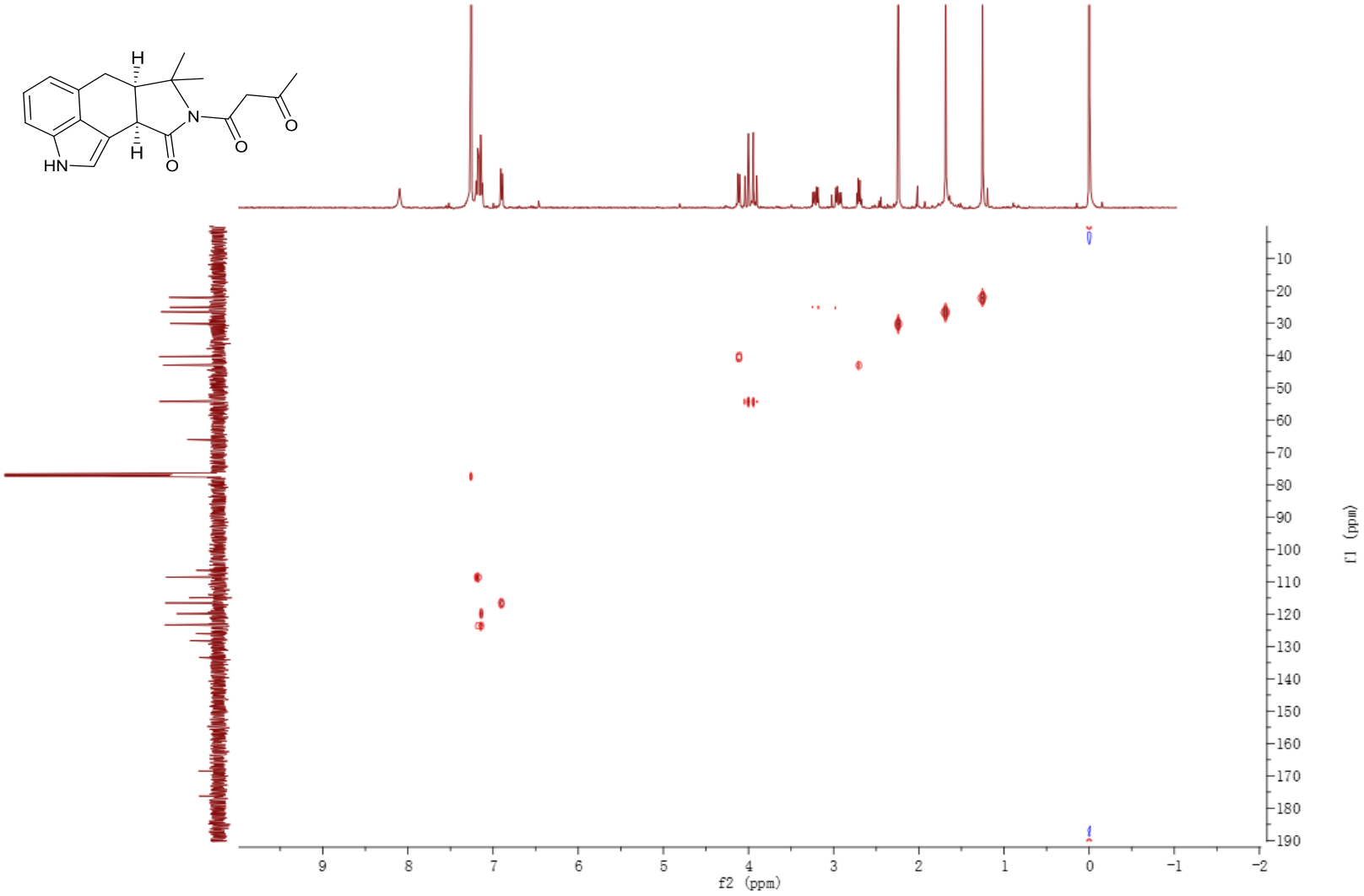


Figure S63. ^{1}H-^{1}H COSY spectrum of pseuboydone E **(13)** in $CDCl_3$

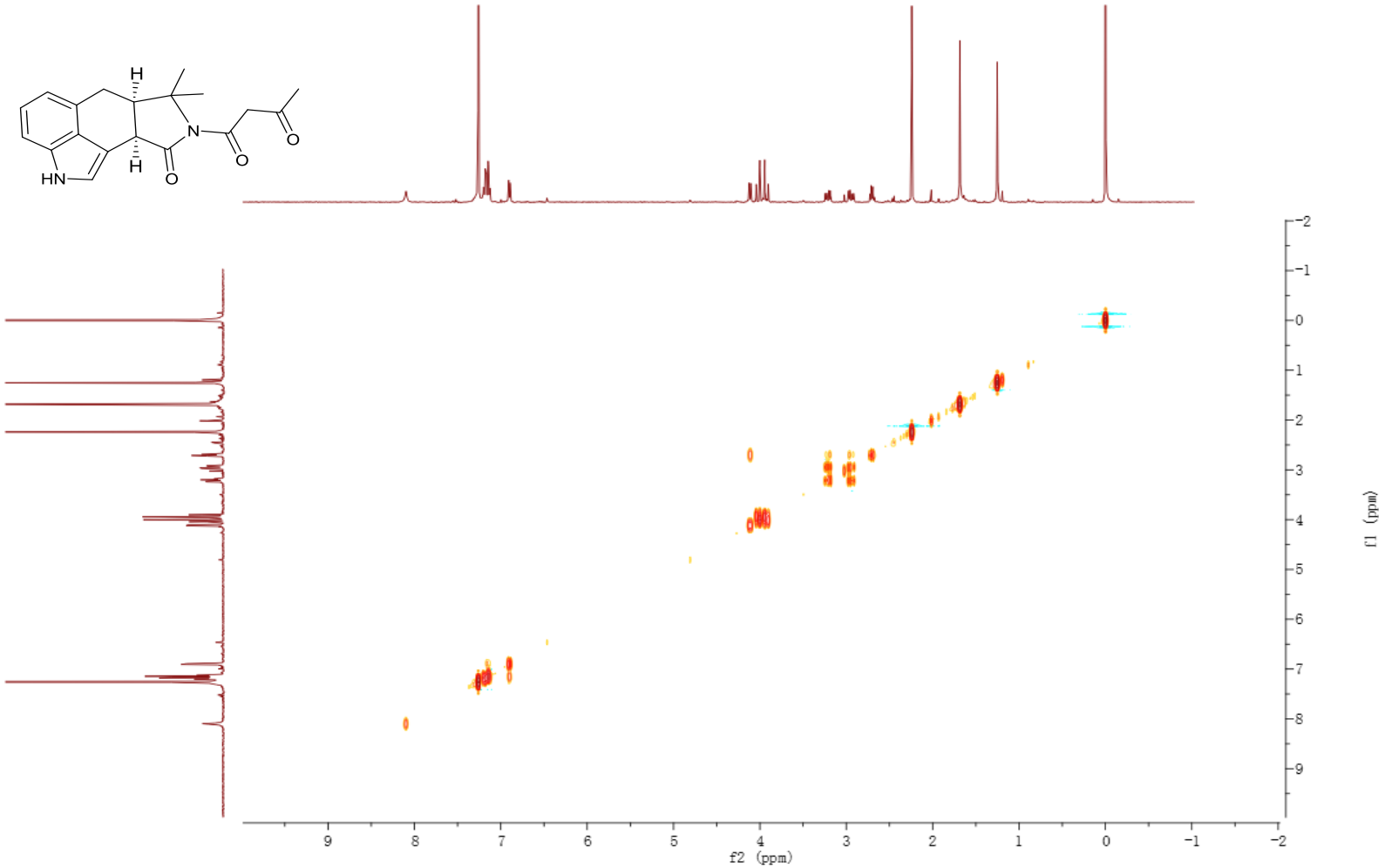


Figure S64. HMBC spectrum of pseuboydone E **(13)** in $CDCl_3$

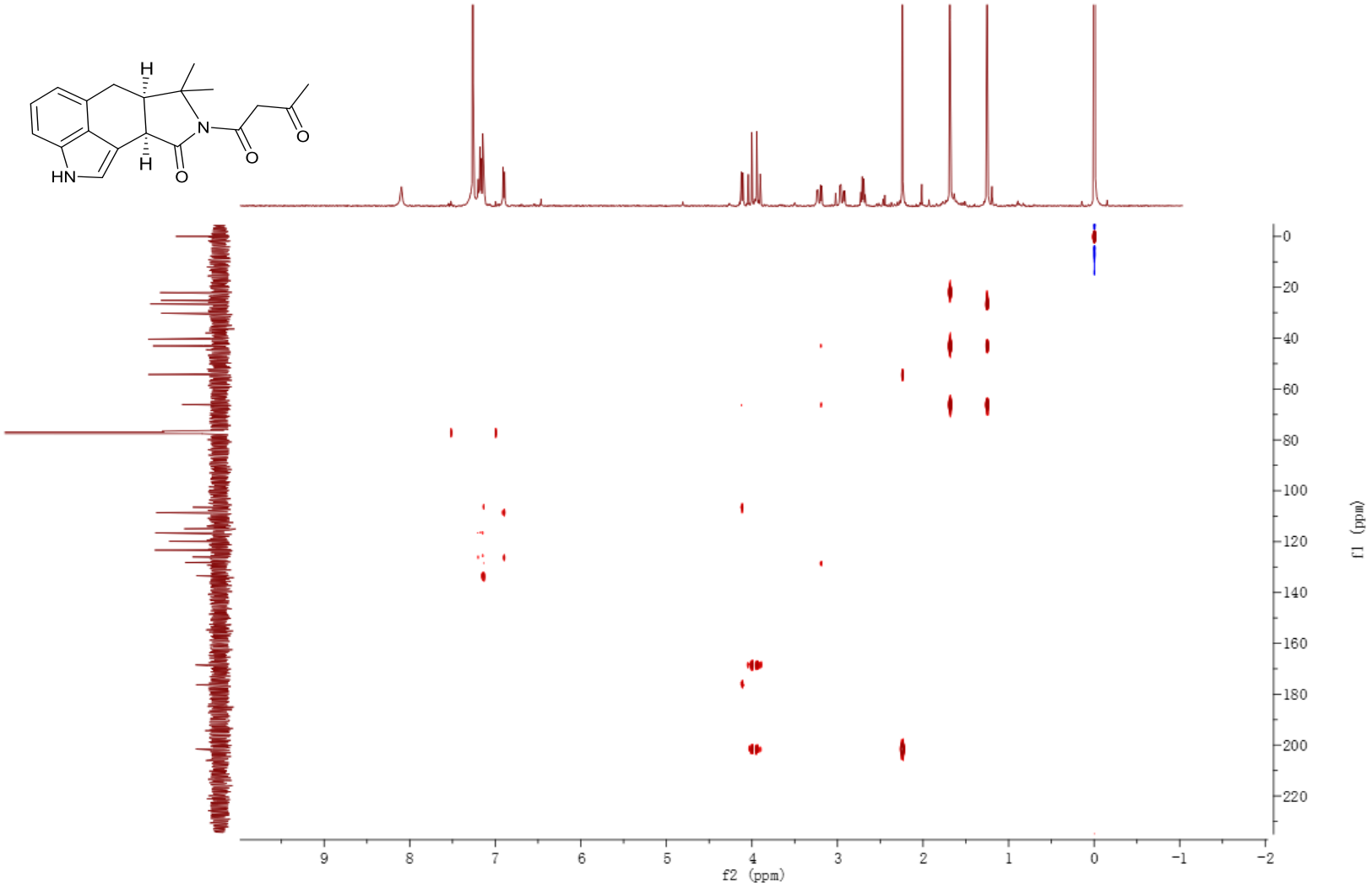


Figure S65. NOESY spectrum of pseuboydone E **(13)** in $CDCl_3$

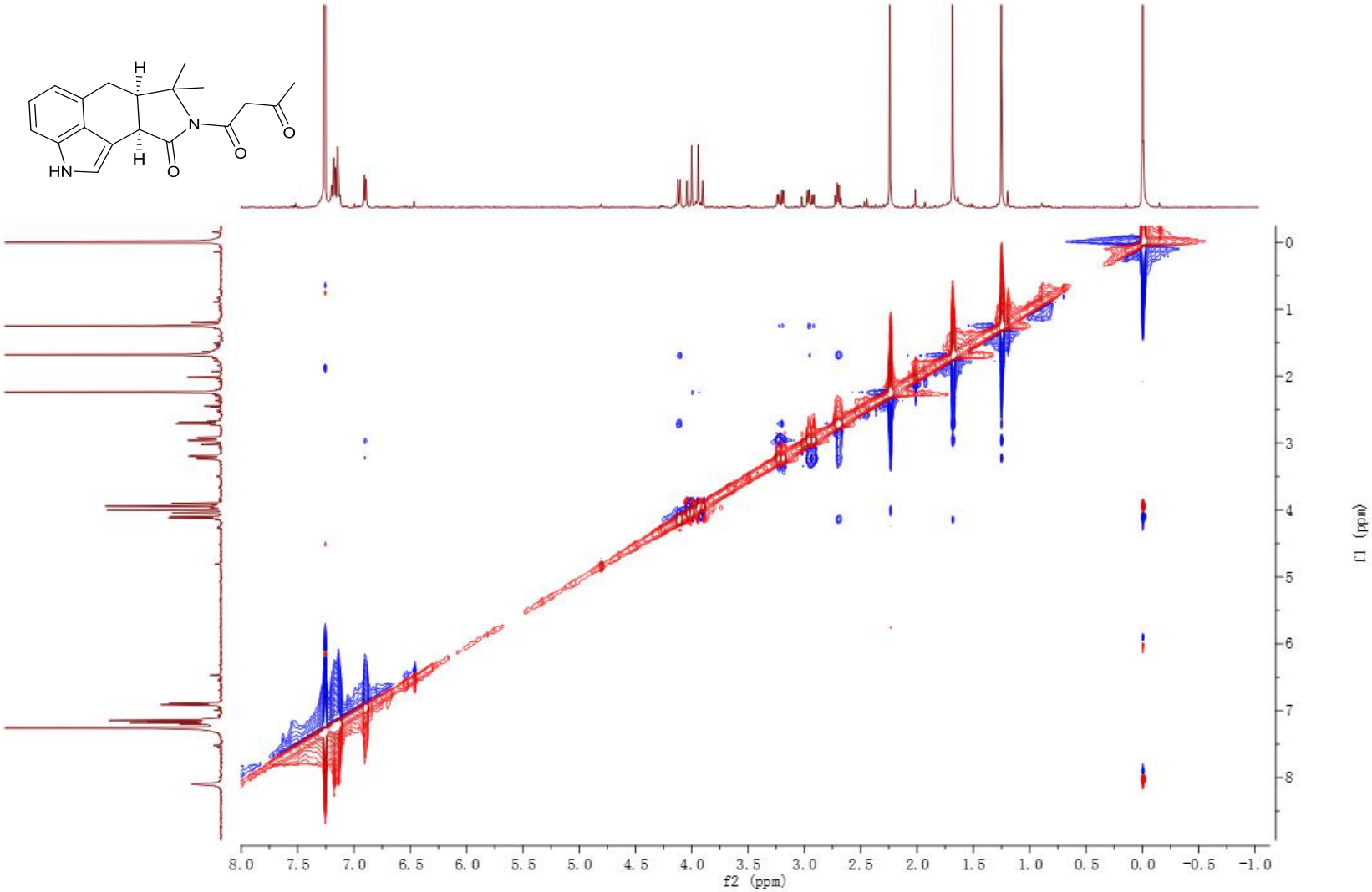


Figure S66. ^{1}H-NMR spectrum of speradine C **(14)** in $CDCl_3$ (400MHz)

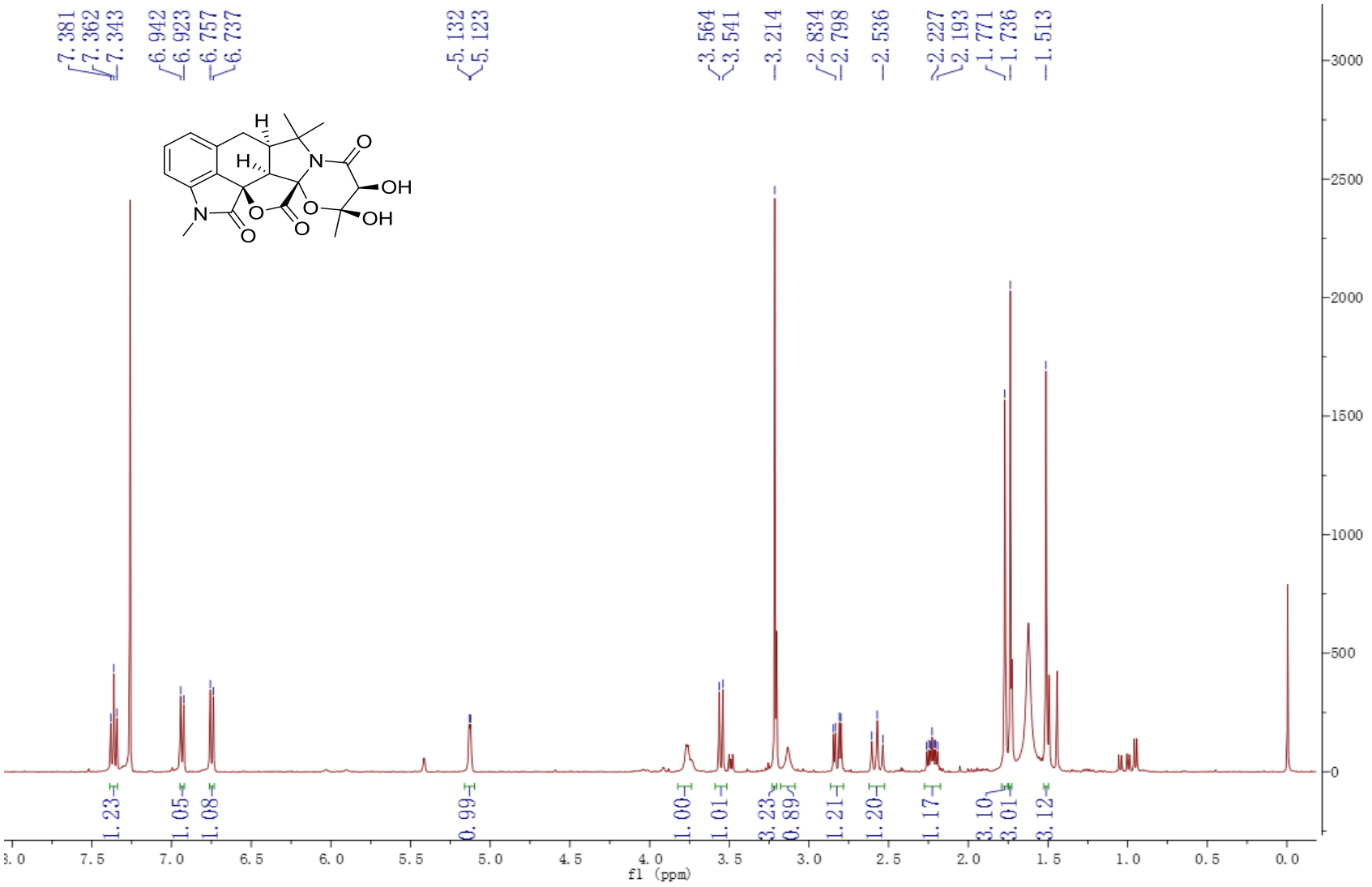


Figure S67. ^{13}C-NMR spectrum of speradine C **(14)** in $CDCl_3$ (100MHz)

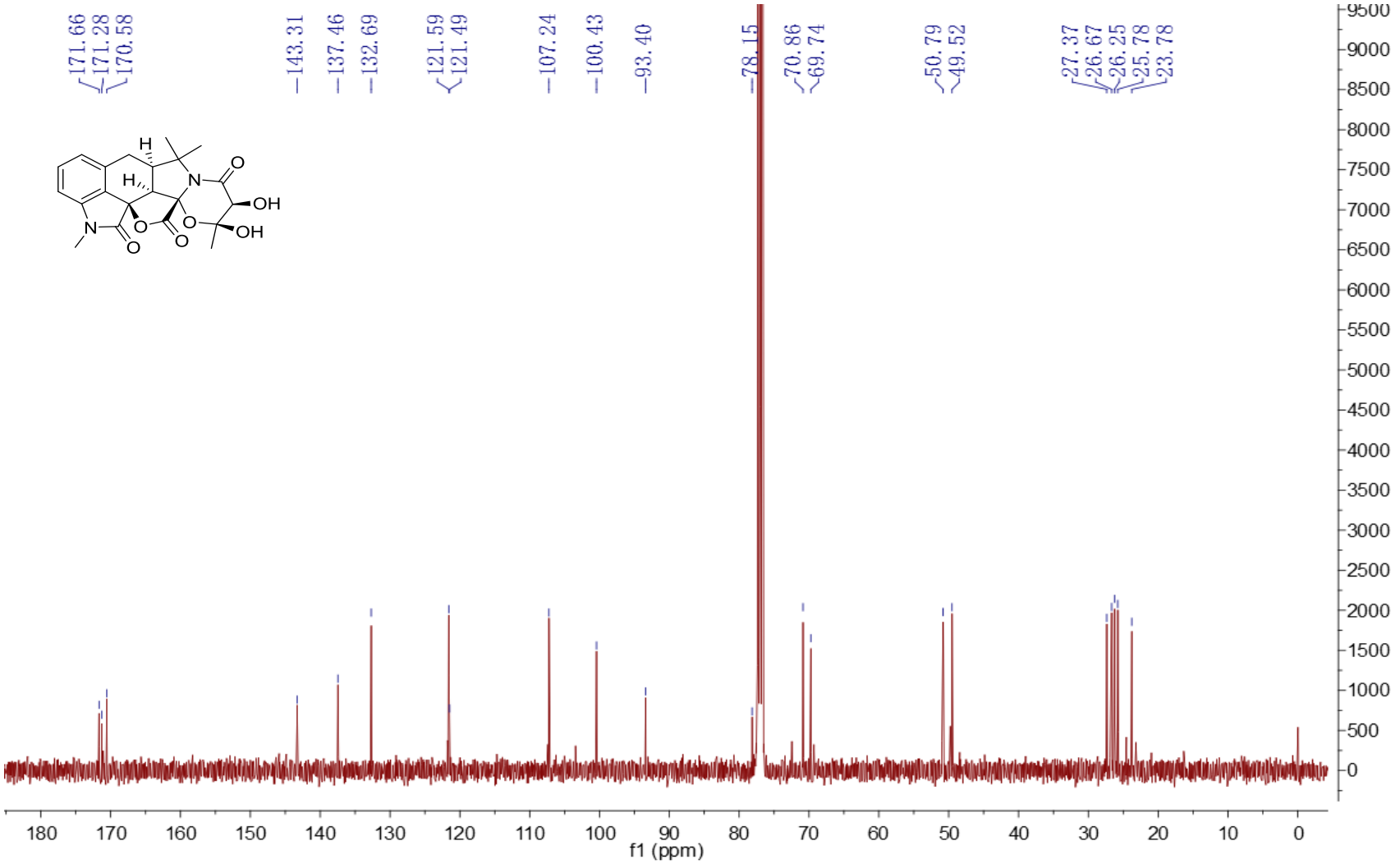


Figure S68. NOESY spectrum of speradine C **(14)** in $CDCl_3$

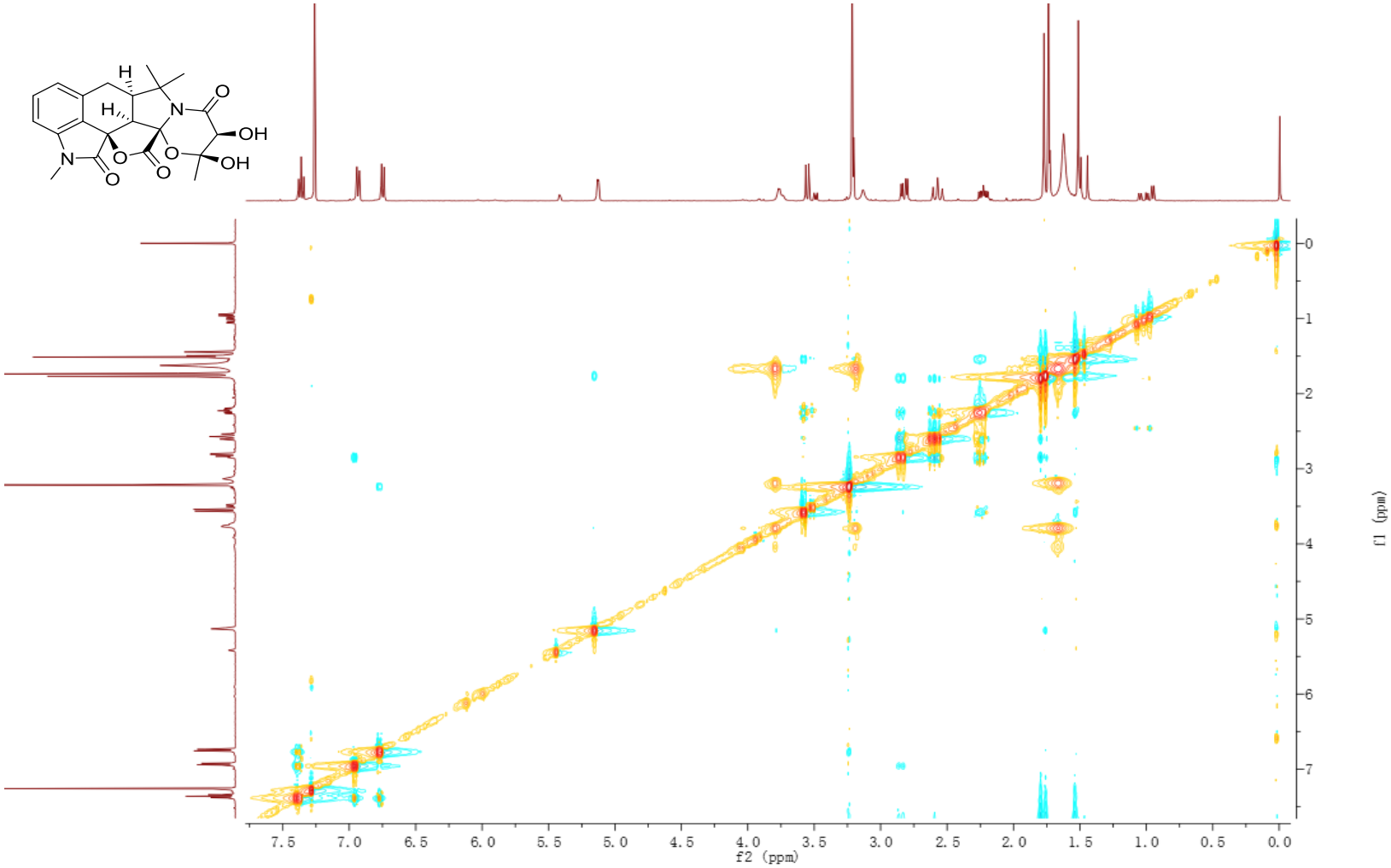


Figure S69. ^{1}H-NMR spectrum of speradine **B (15)** in $CDCl_3$ (400MHz)

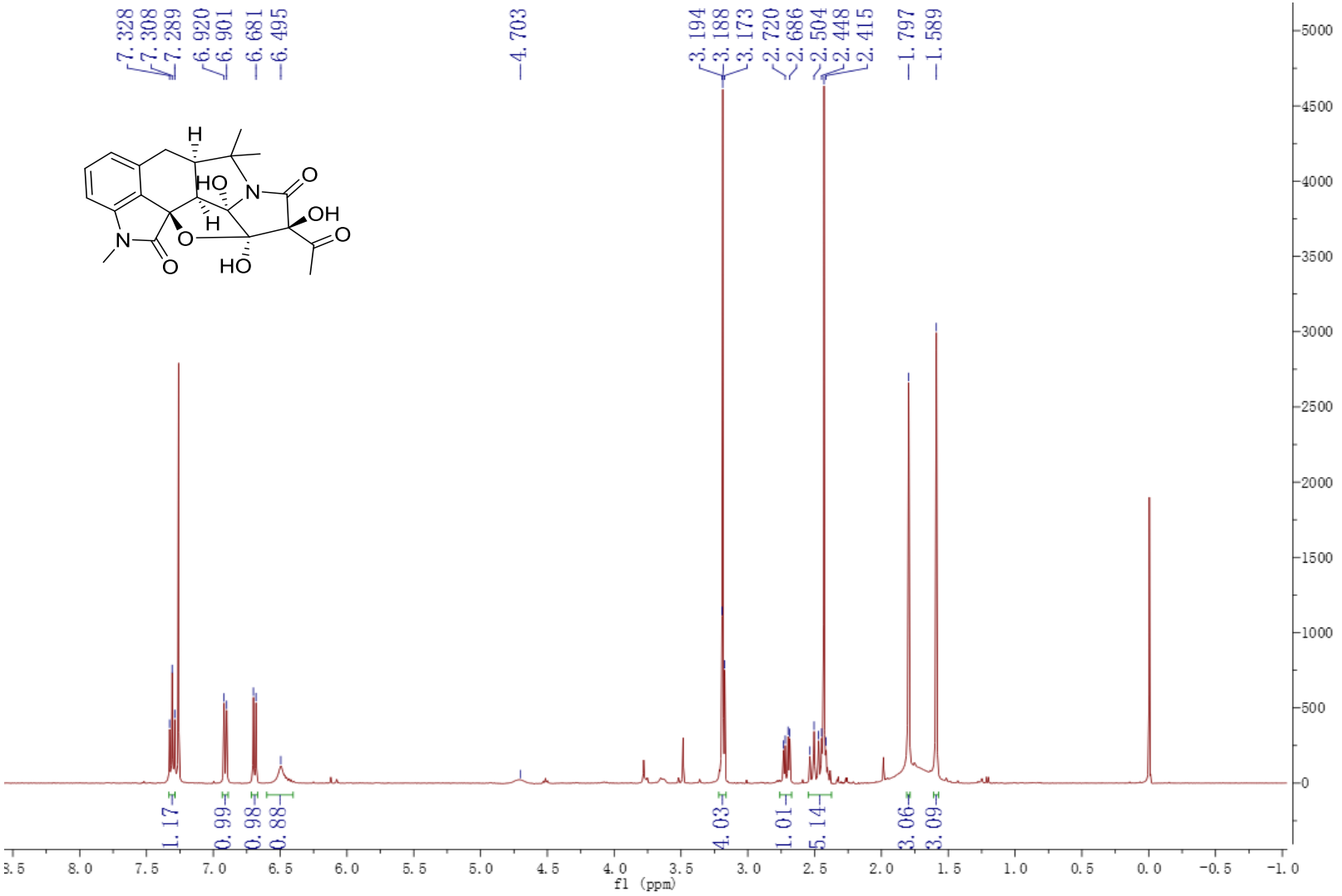


Figure S70. ^{13}C-NMR spectrum of speradine **B (15)** in $CDCl_3$ (100MHz)

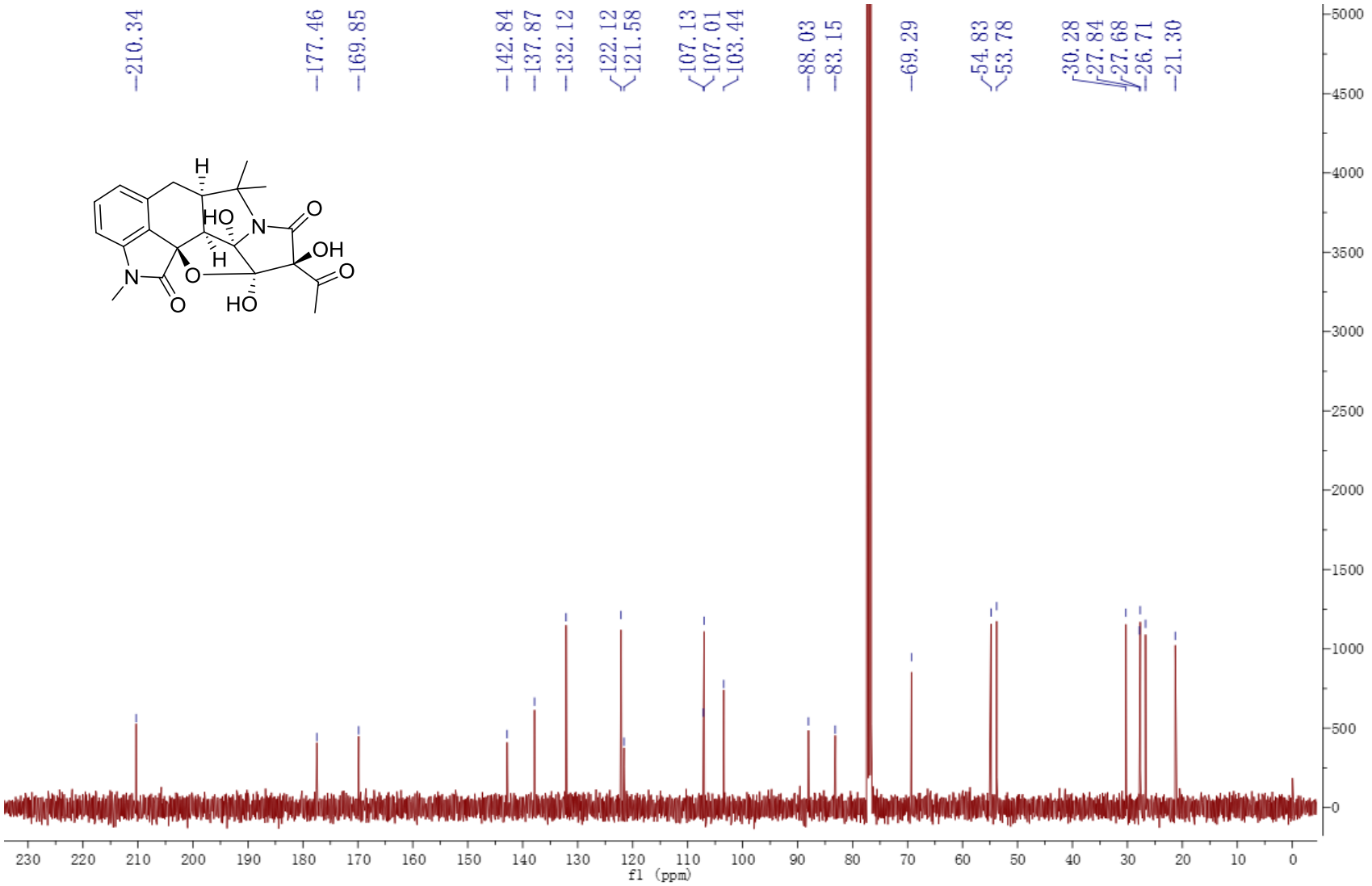


Figure S71. HMQC spectrum of speradine **B (15)** in $CDCl_3$

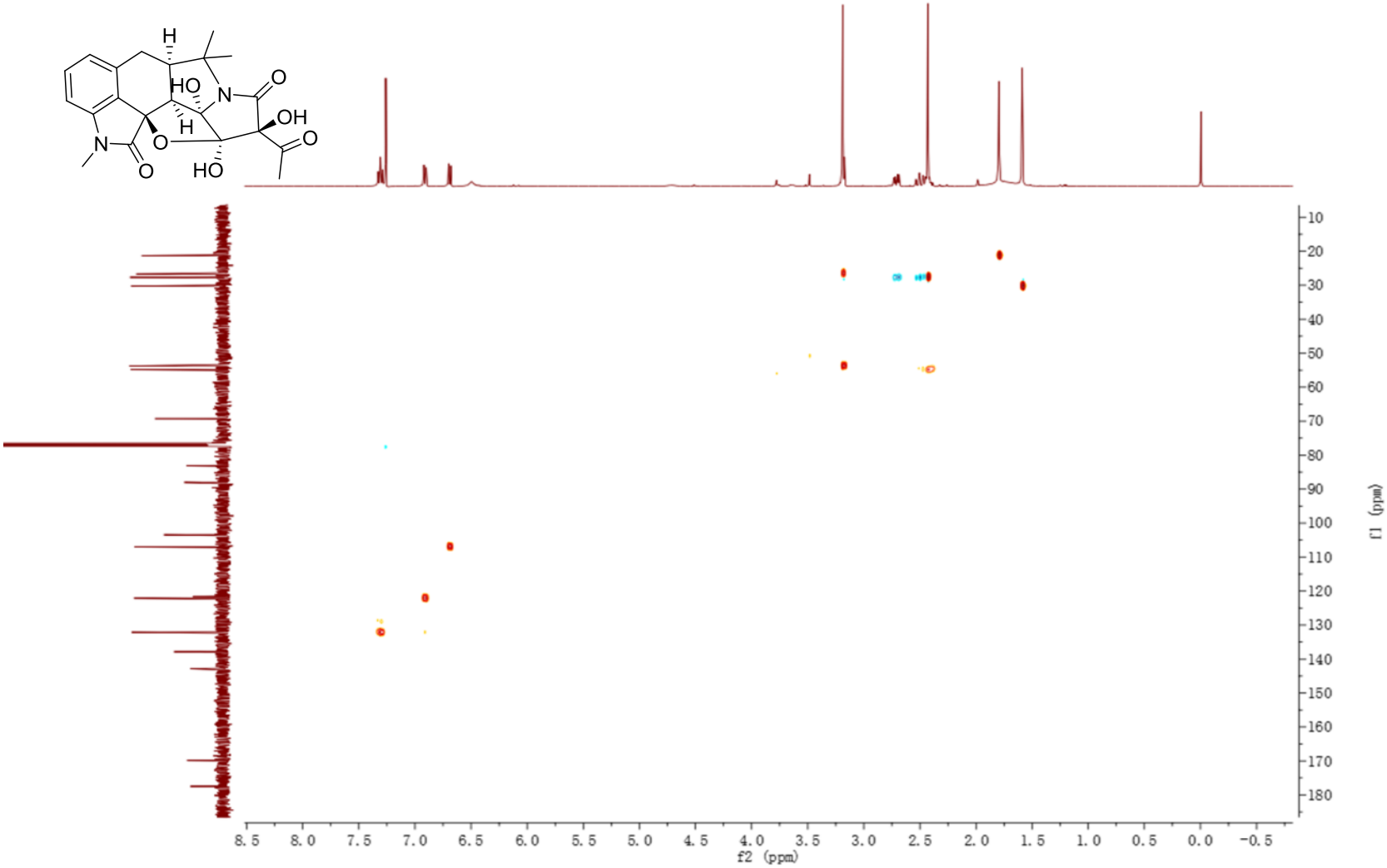


Figure S72. HMBC spectrum of speradine **B (15)** in $CDCl_3$

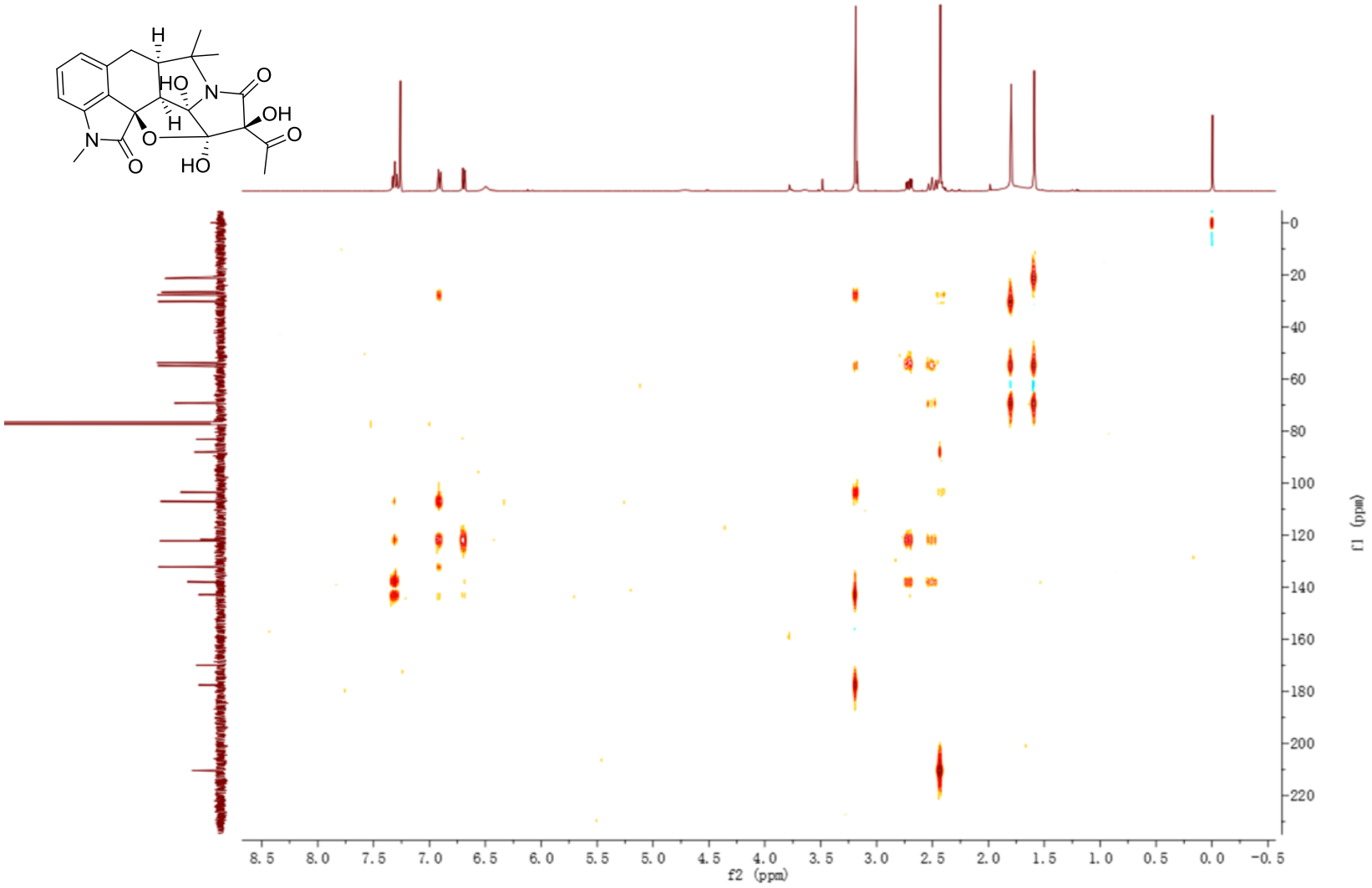


Figure S73. ^{1}H-NMR spectrum of cyclopiamide E (**16**) in $CDCl_3$ (400MHz)

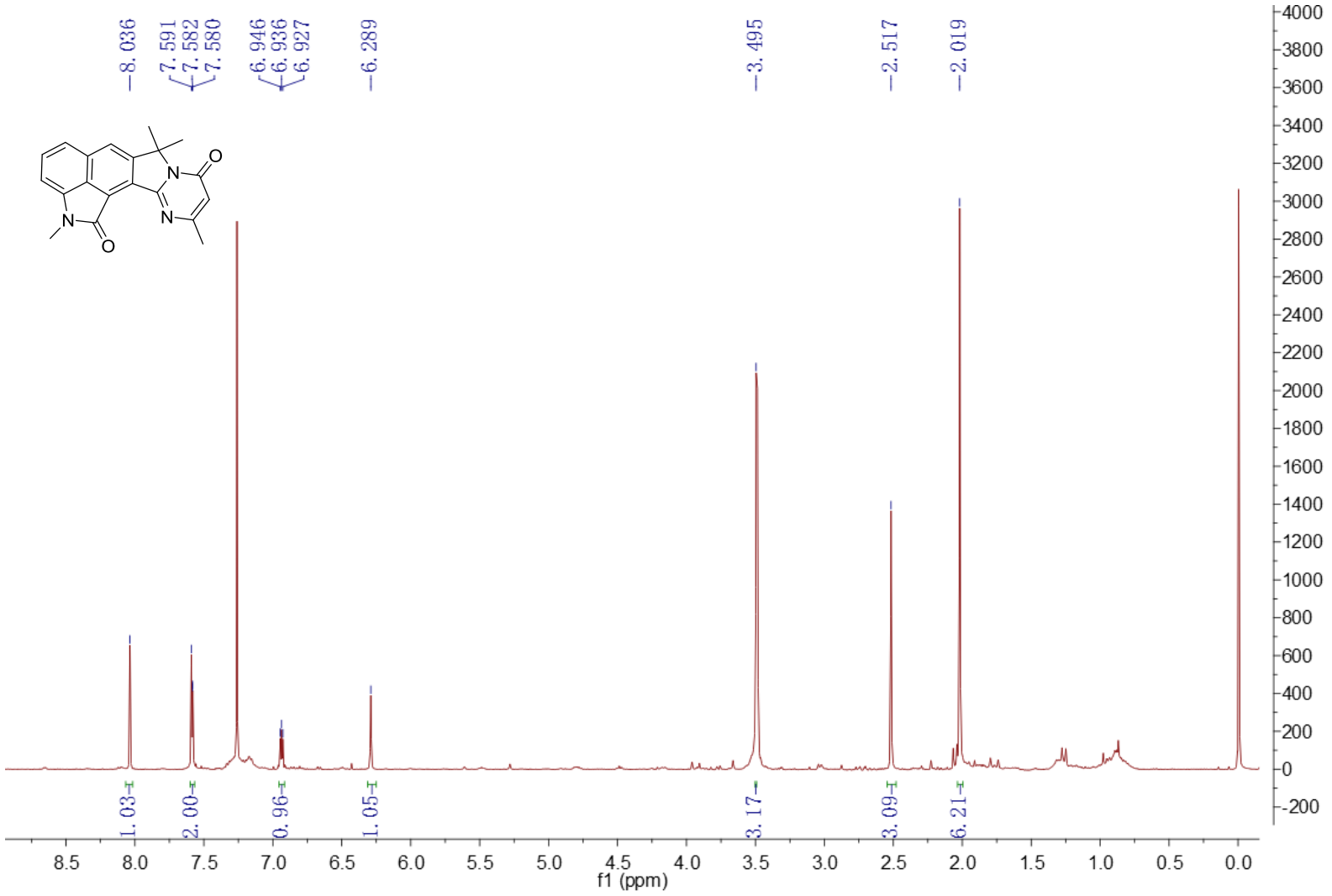


Figure S74. ^{13}C NMR and DEPT spectra of cyclopiamide E (**16**) in $CDCl_3$ (100MHz)

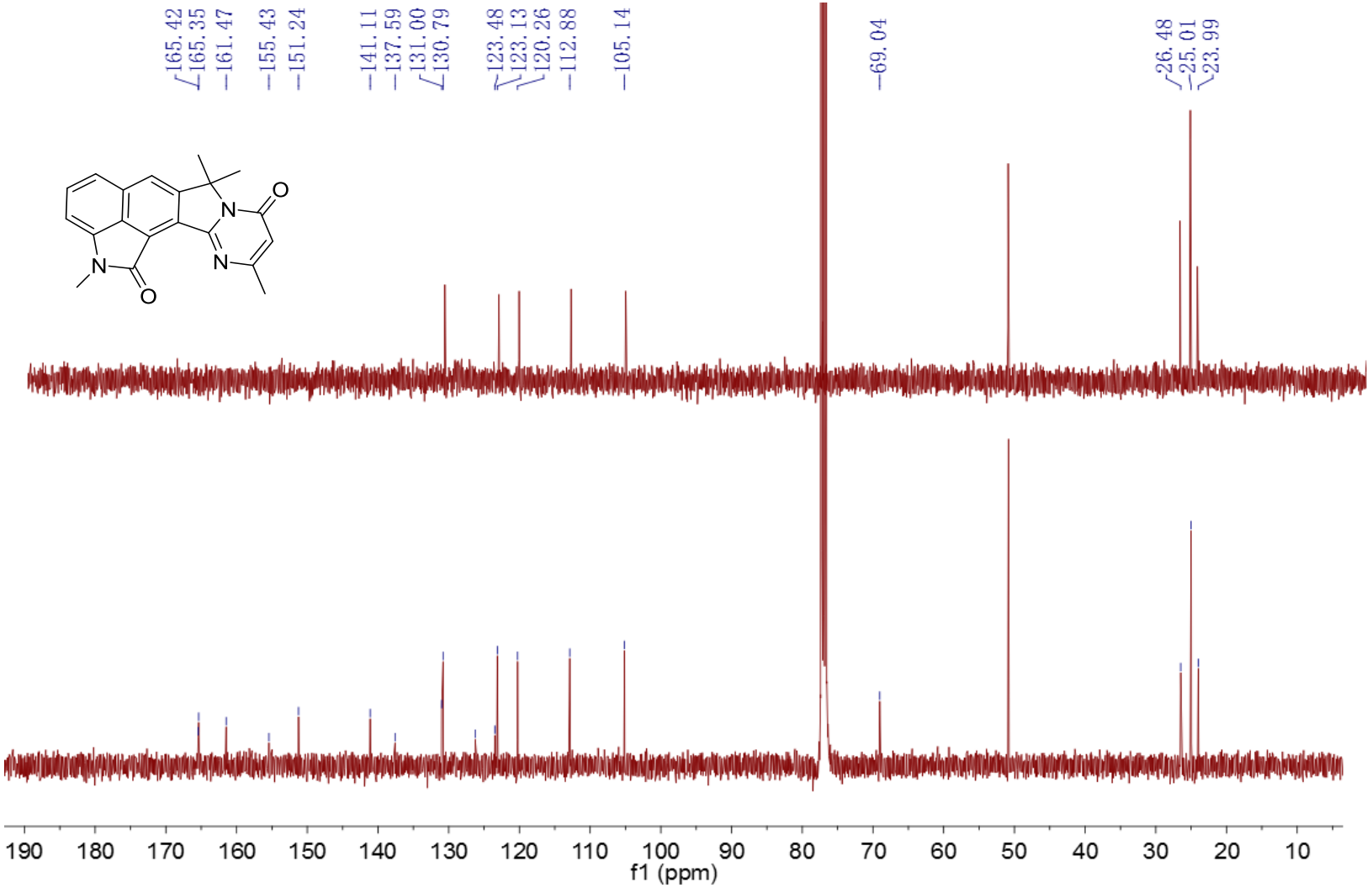


Figure S75. HMQC spectrum of cyclopiamide E (**16**) in $CDCl_3$

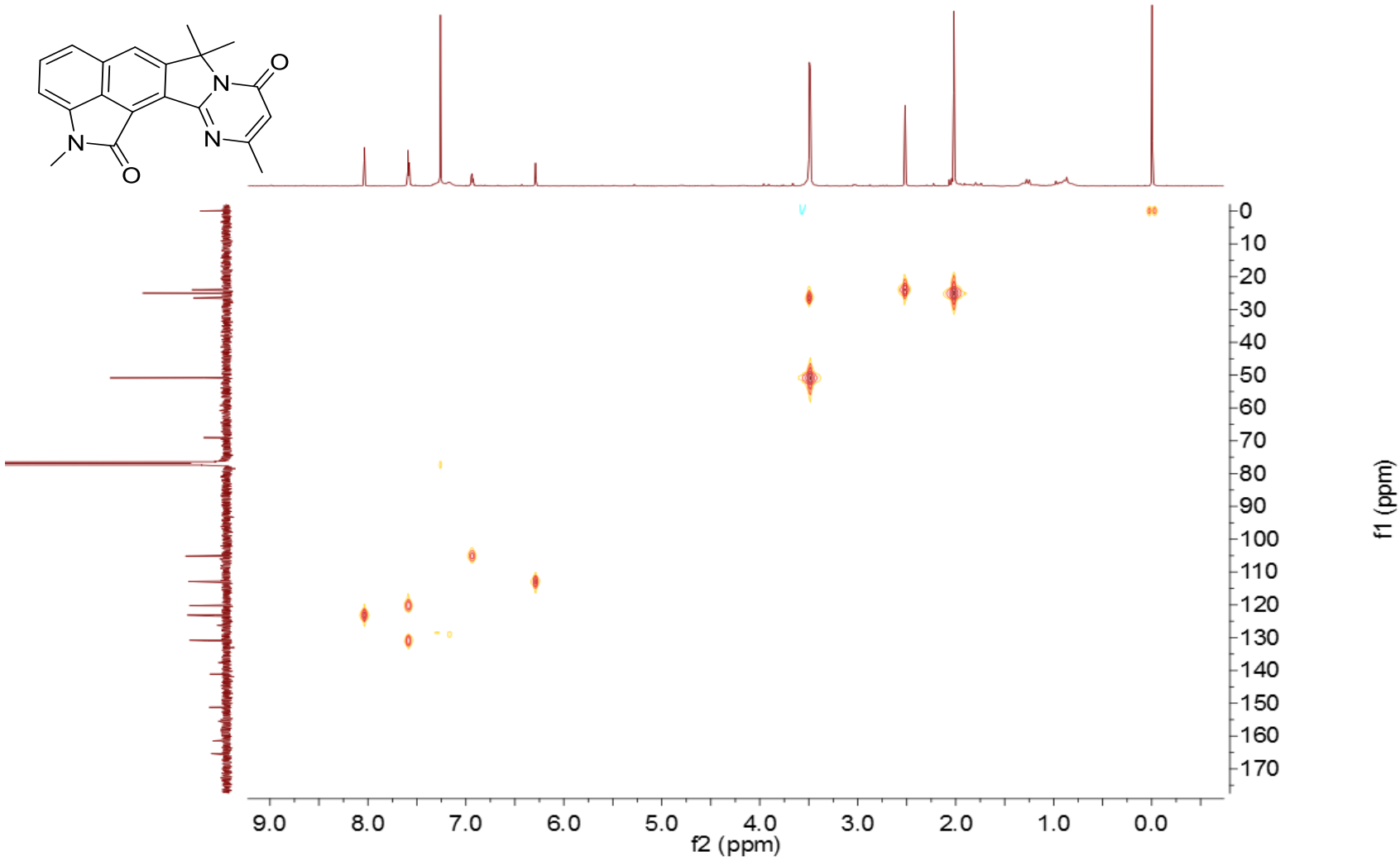


Figure S76. HMBC spectrum of cyclopiamide E (**16**) in $CDCl_3$

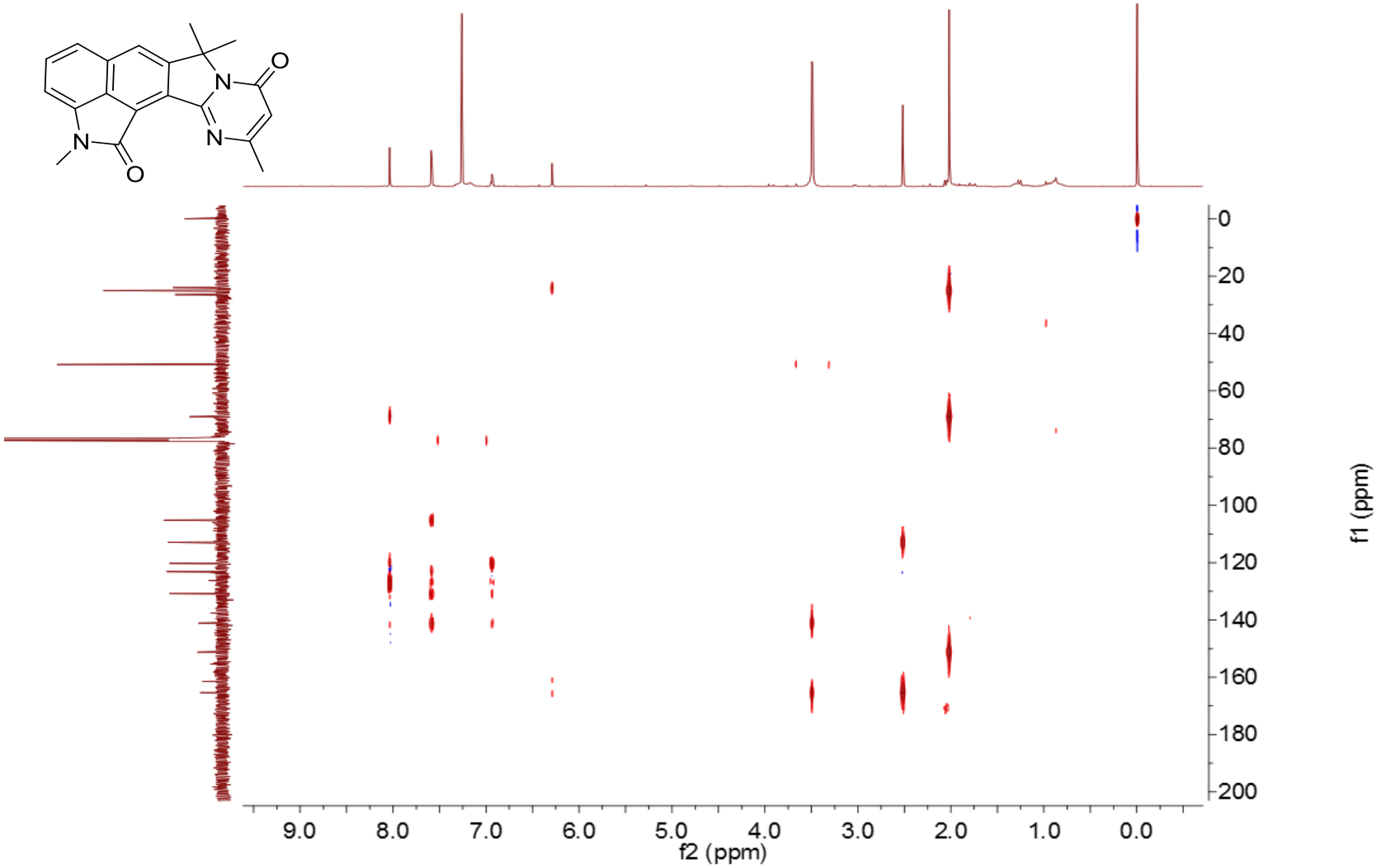


Figure S77. NOESY spectrum of cyclopiamide E (**16**) in $CDCl_3$

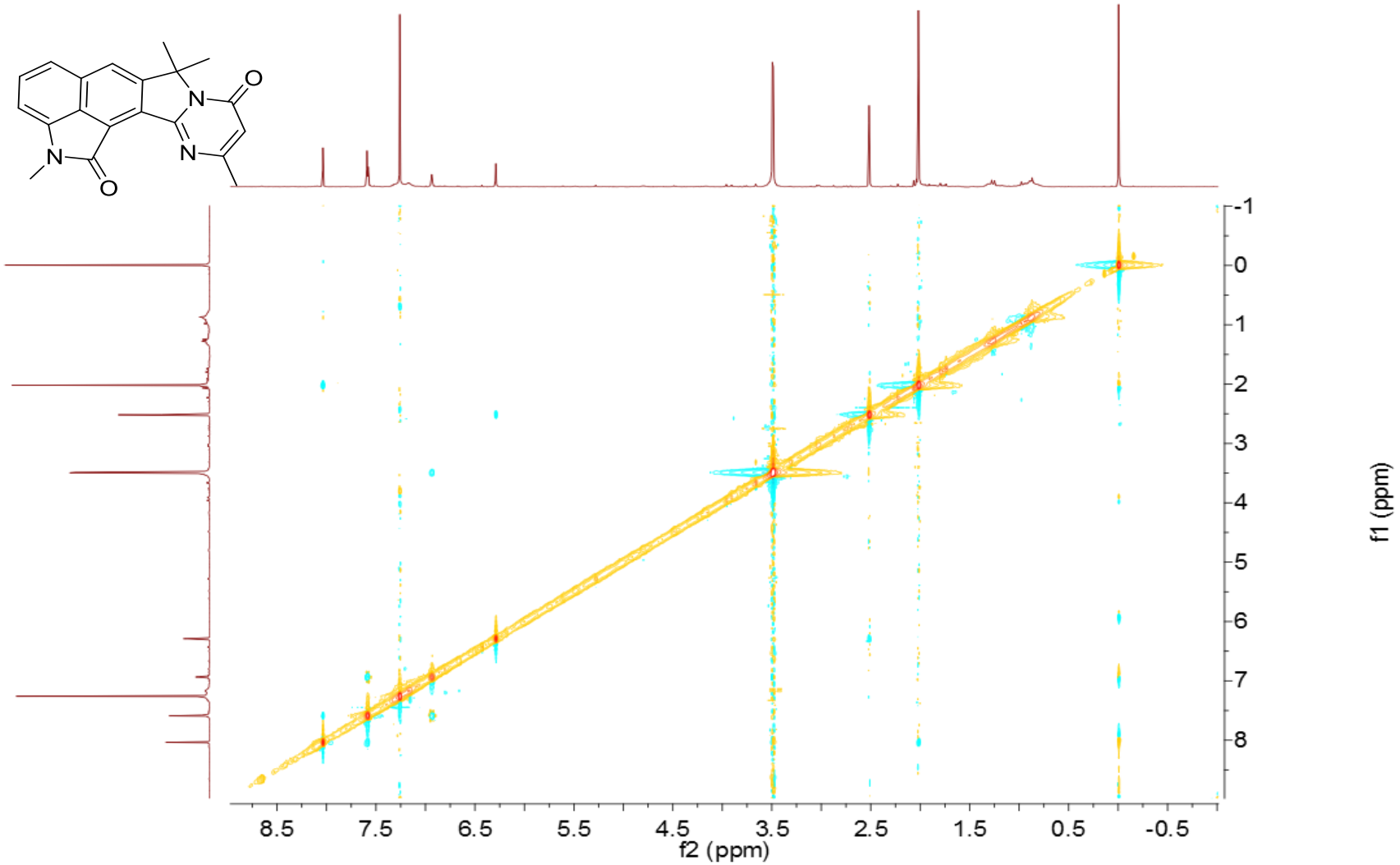


Figure S78. ^{1}H-NMR spectrum of 24, 25-dehydro-10, 11-dihydro-20-hydroxyaflavinin **(17)** in $CDCl_3$ (400MHz)

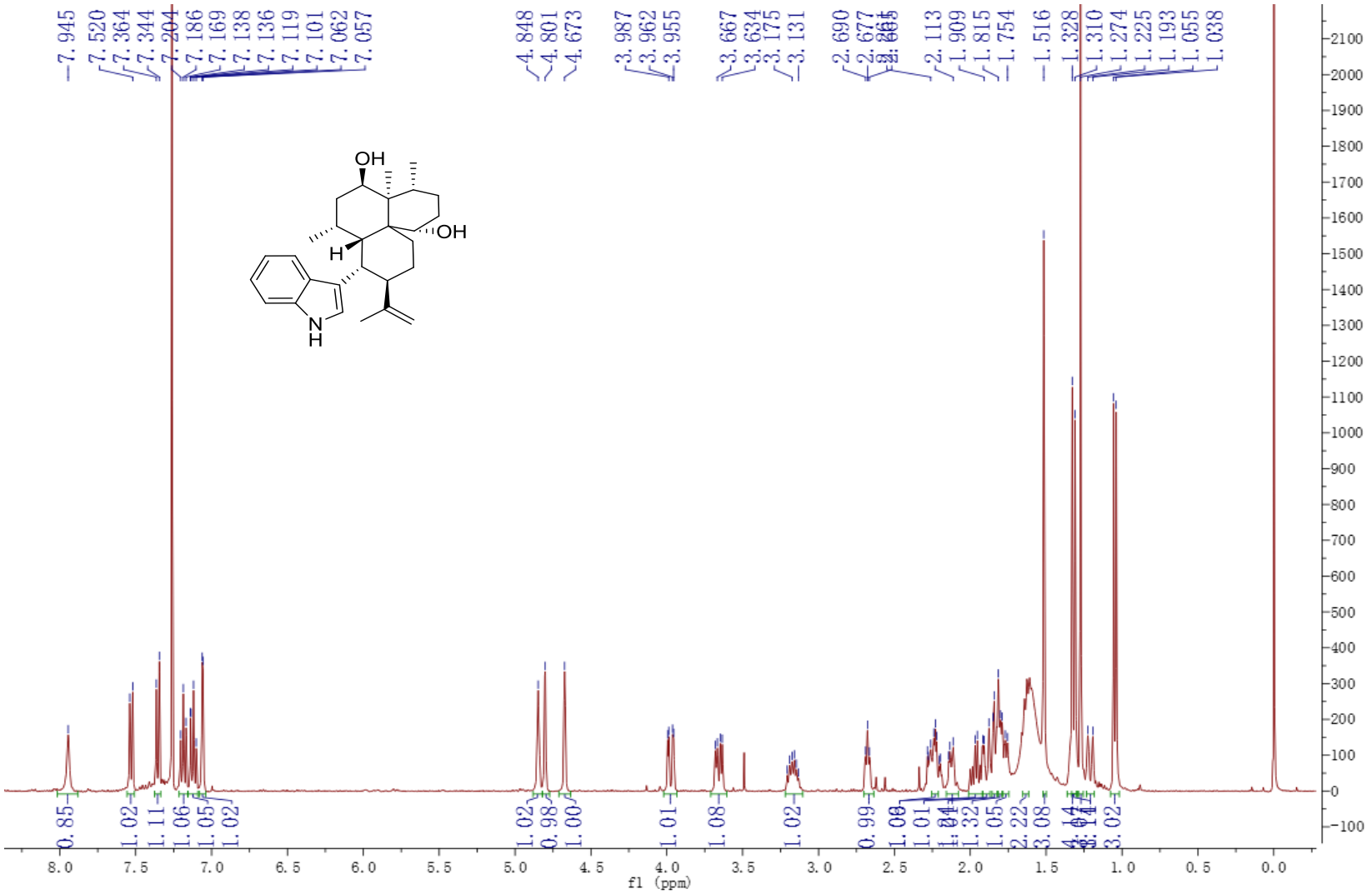


Figure S79. ^{13}C-NMR spectrum of 24, 25-dehydro-10,11-dihydro-20-hydroxyaflavinin **(17)** in $CDCl_3$ (100MHz)

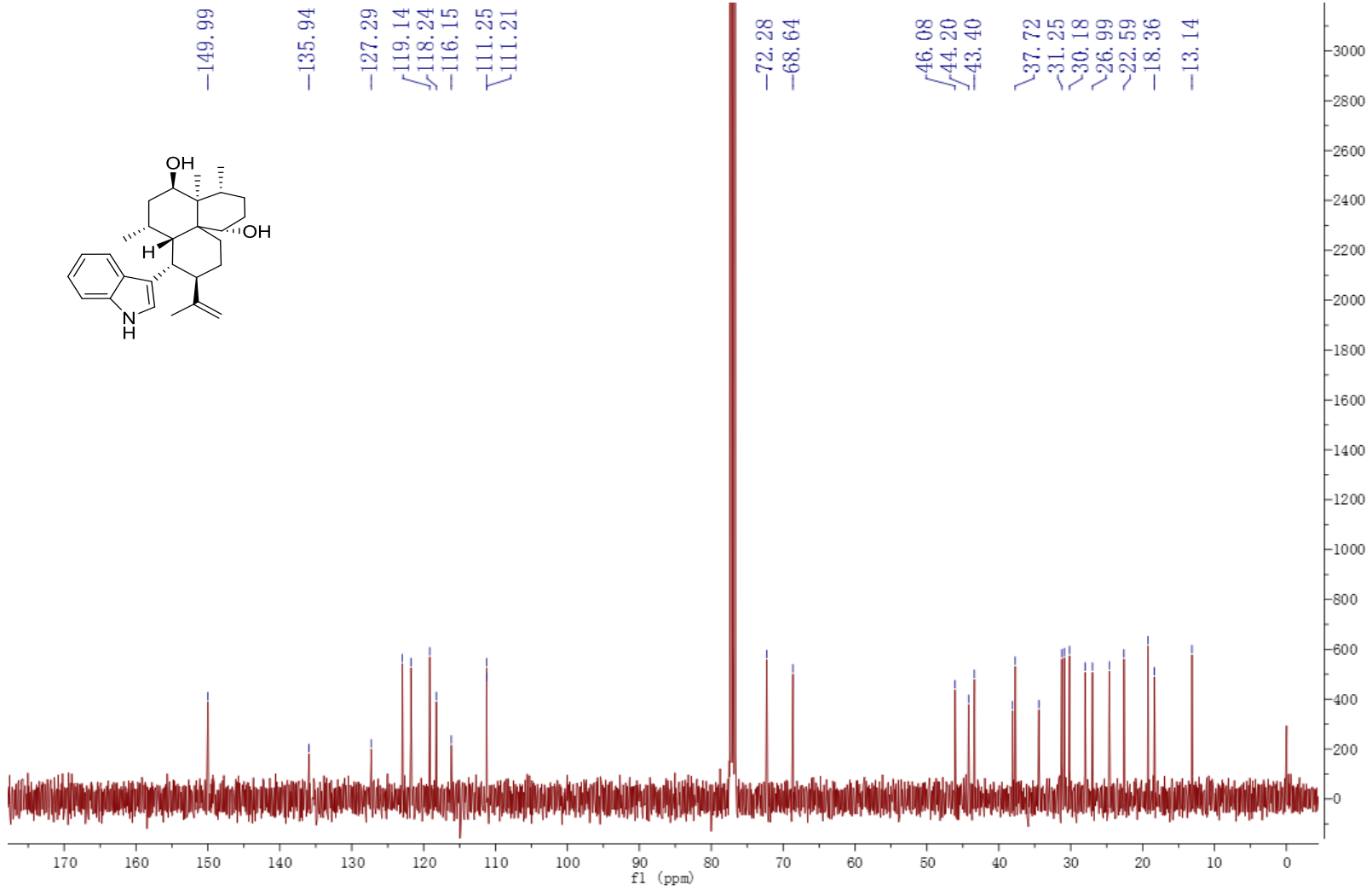


Figure S80. NOESY spectrum of 24, 25-dehydro-10, 11-dihydro-20-hydroxyaflavinin **(17)** in $CDCl_3$

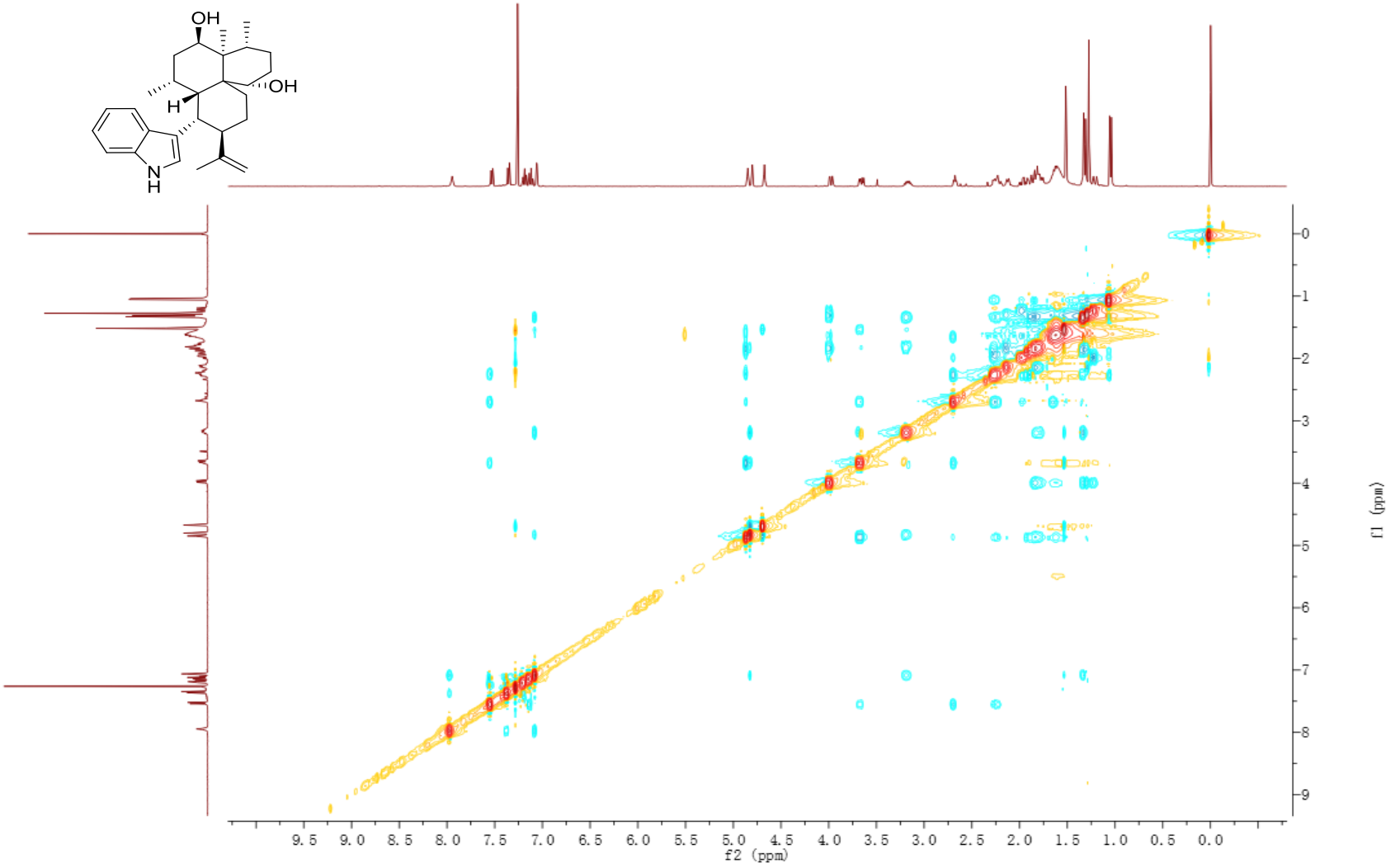


Figure S81. ^{1}H-NMR spectrum of aflavinine **(18)** in $CDCl_3$ (400MHz)

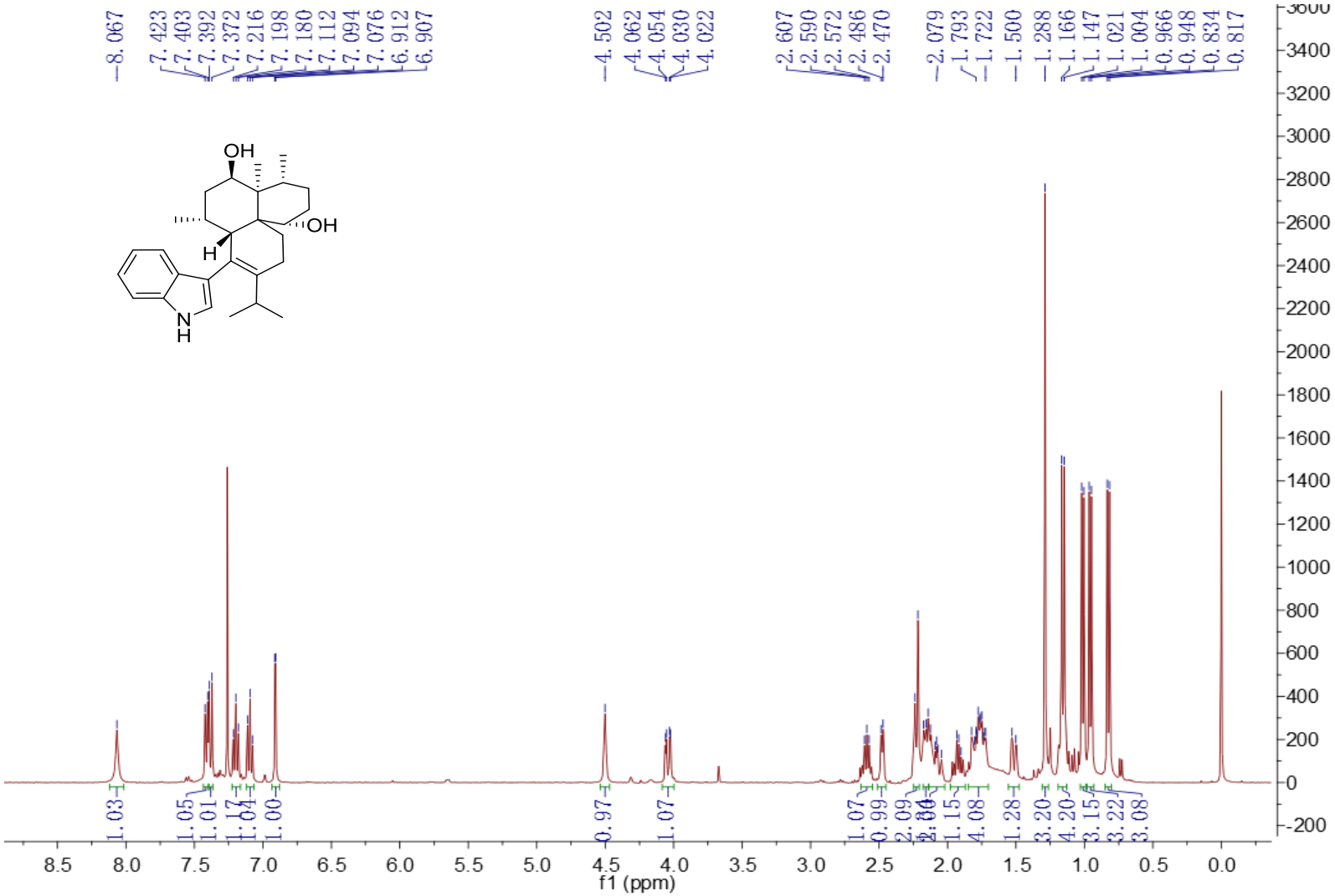


Figure S82. ^{13}C-NMR and DEPT spectra of aflavinine **(18)** in $CDCl_3$ (100MHz)

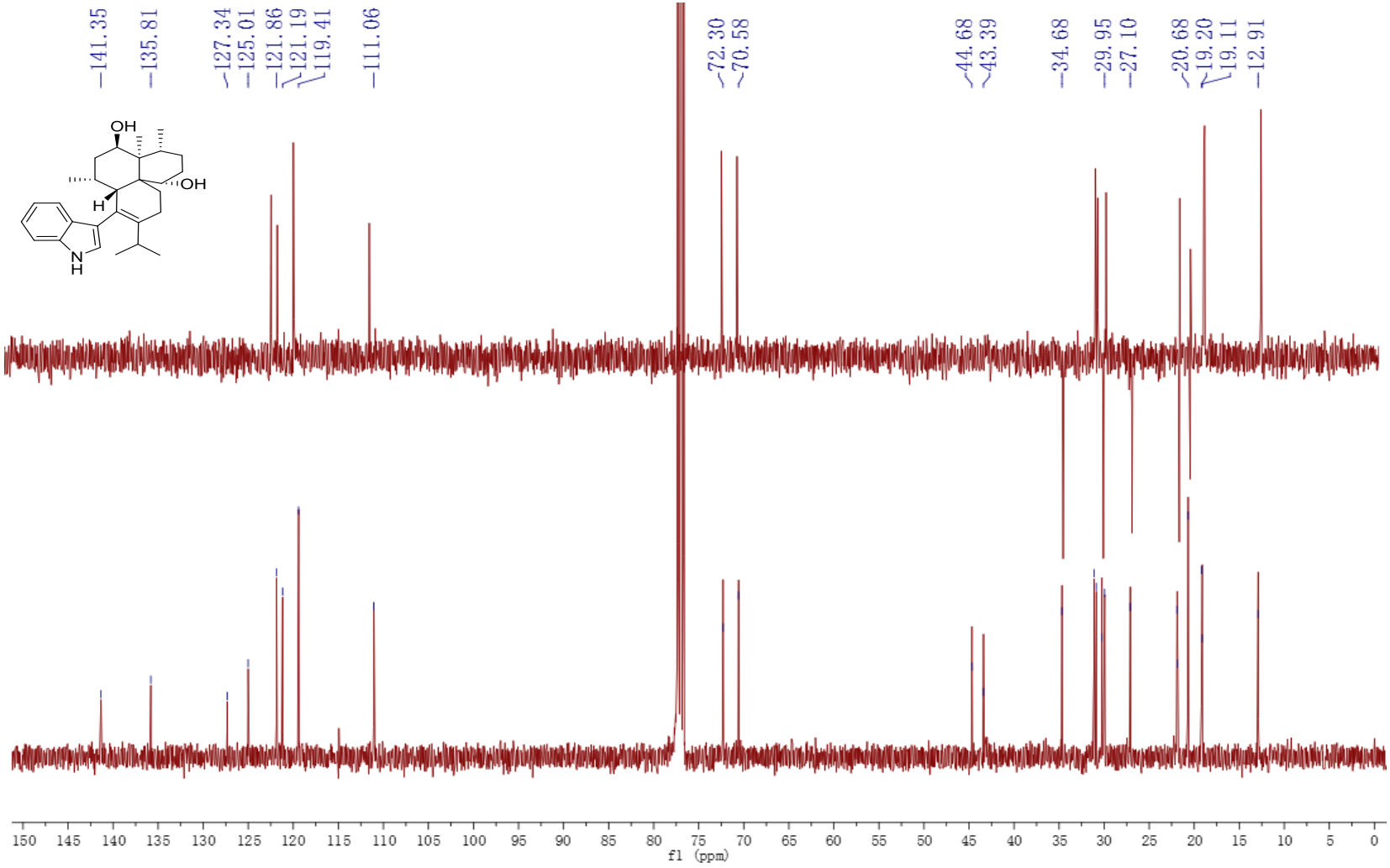


Figure S83. HMQC spectrum of aflavinine **(18)** in $CDCl_3$

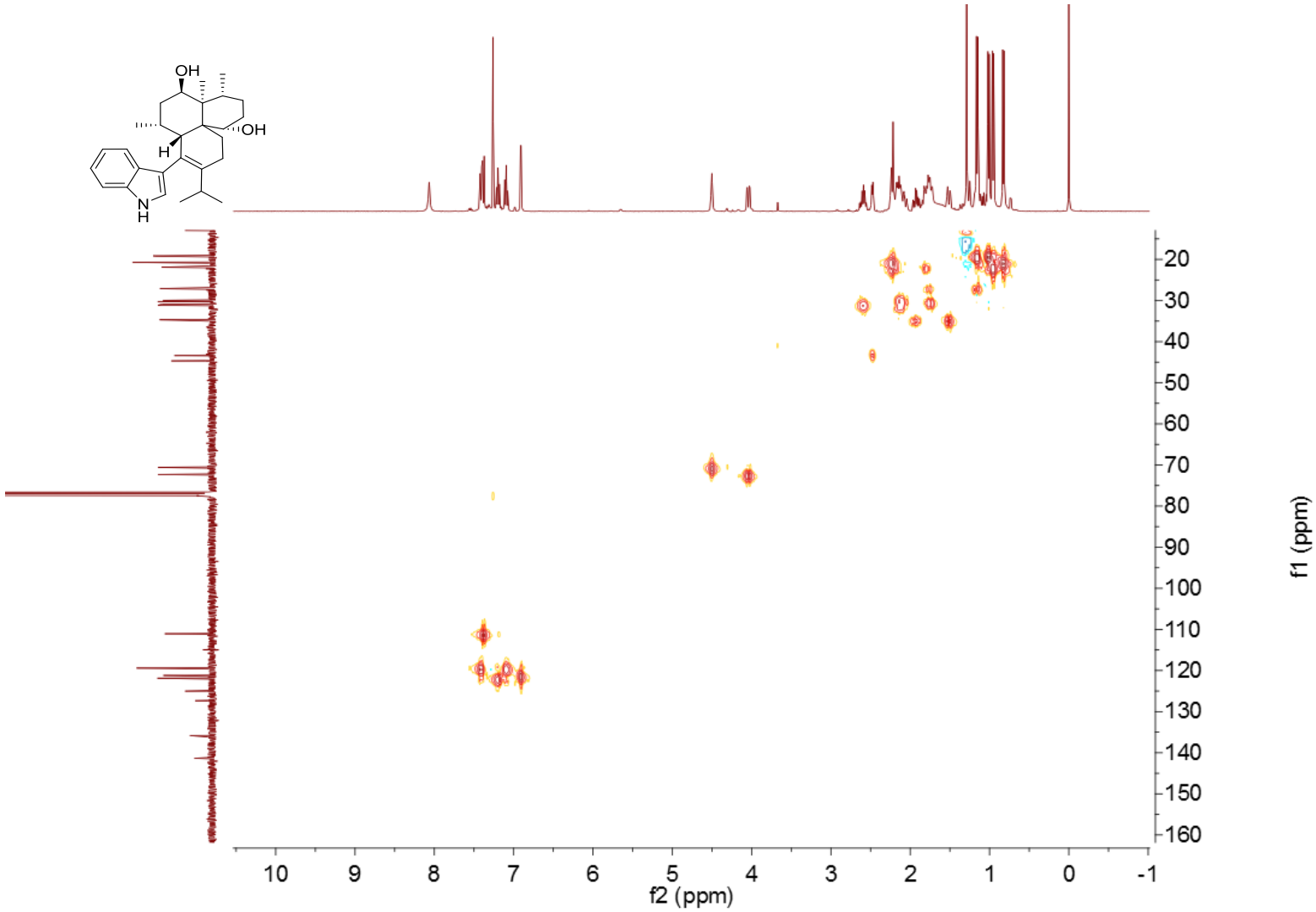


Figure S84. ^{1}H-^{1}H COSY spectrum of aflavinine **(18)** in $CDCl_3$

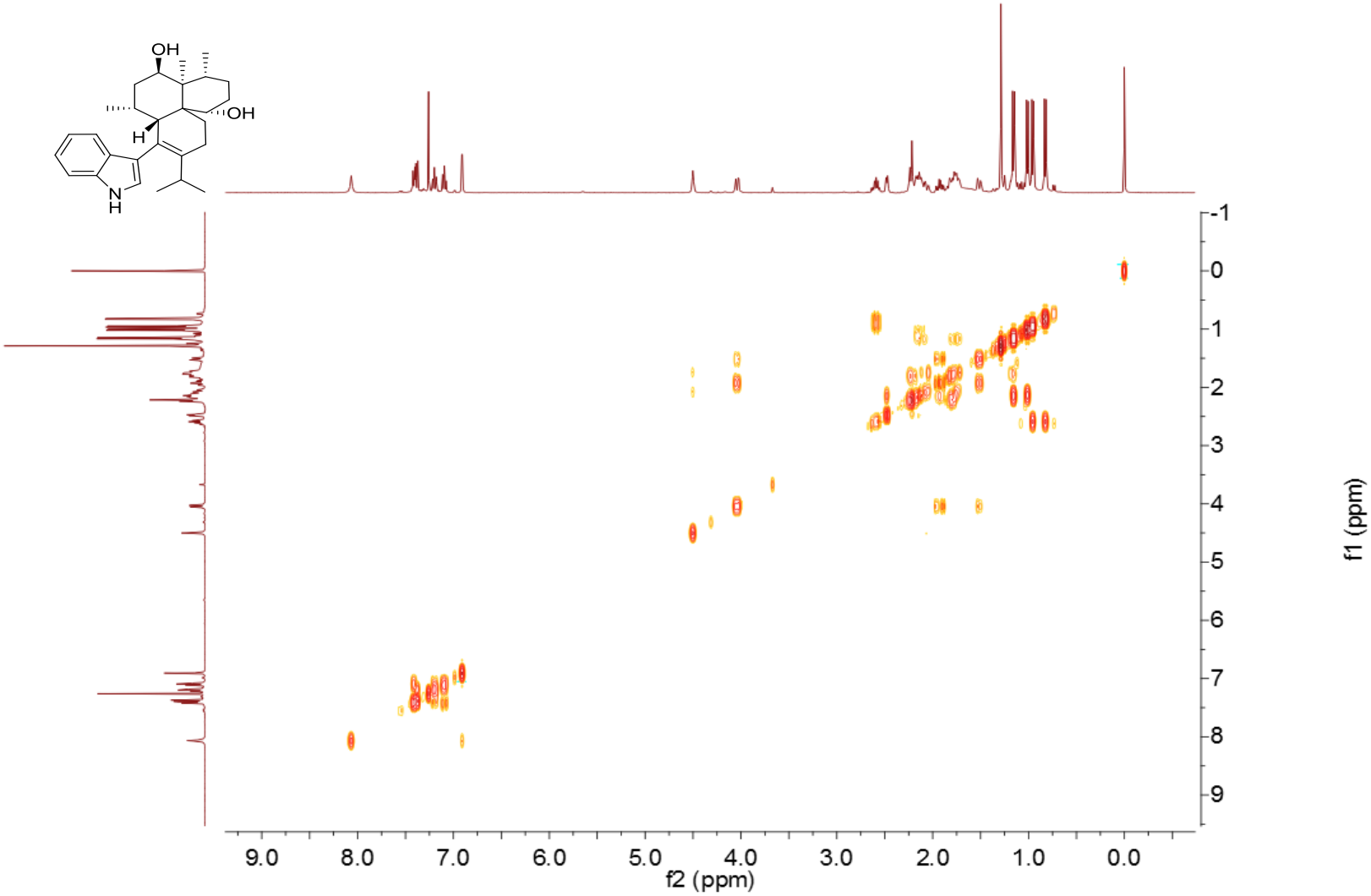


Figure S85. HMBC spectrum of aflavinine **(18)** in $CDCl_3$

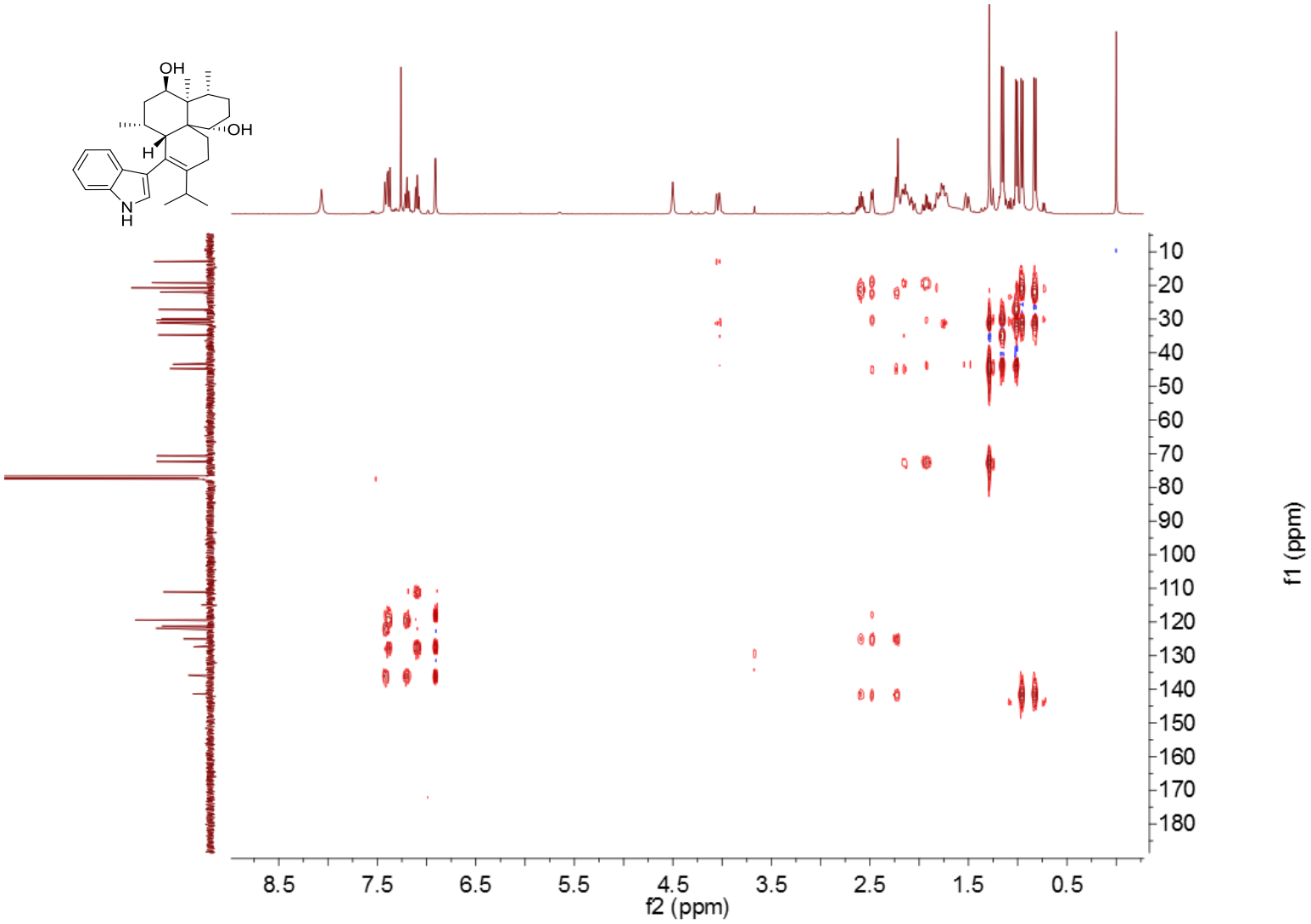


Figure S86. NOESY spectrum of aflavinine **(18)** in $CDCl_3$

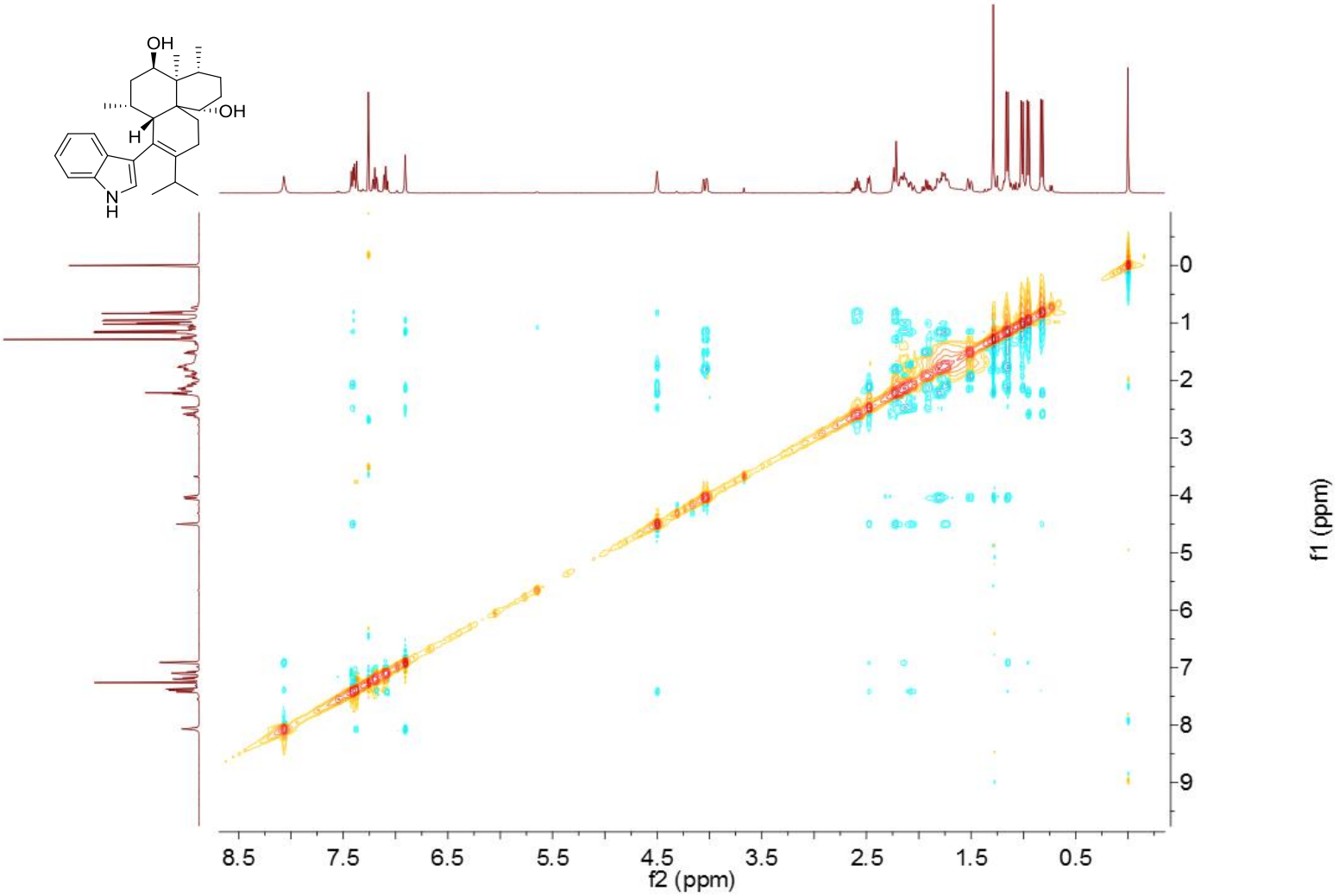


Figure **S87.** ^{1}H-NMR spectrum of β-aflatrem (**19**) in DMSO-d_6 (400MHz)

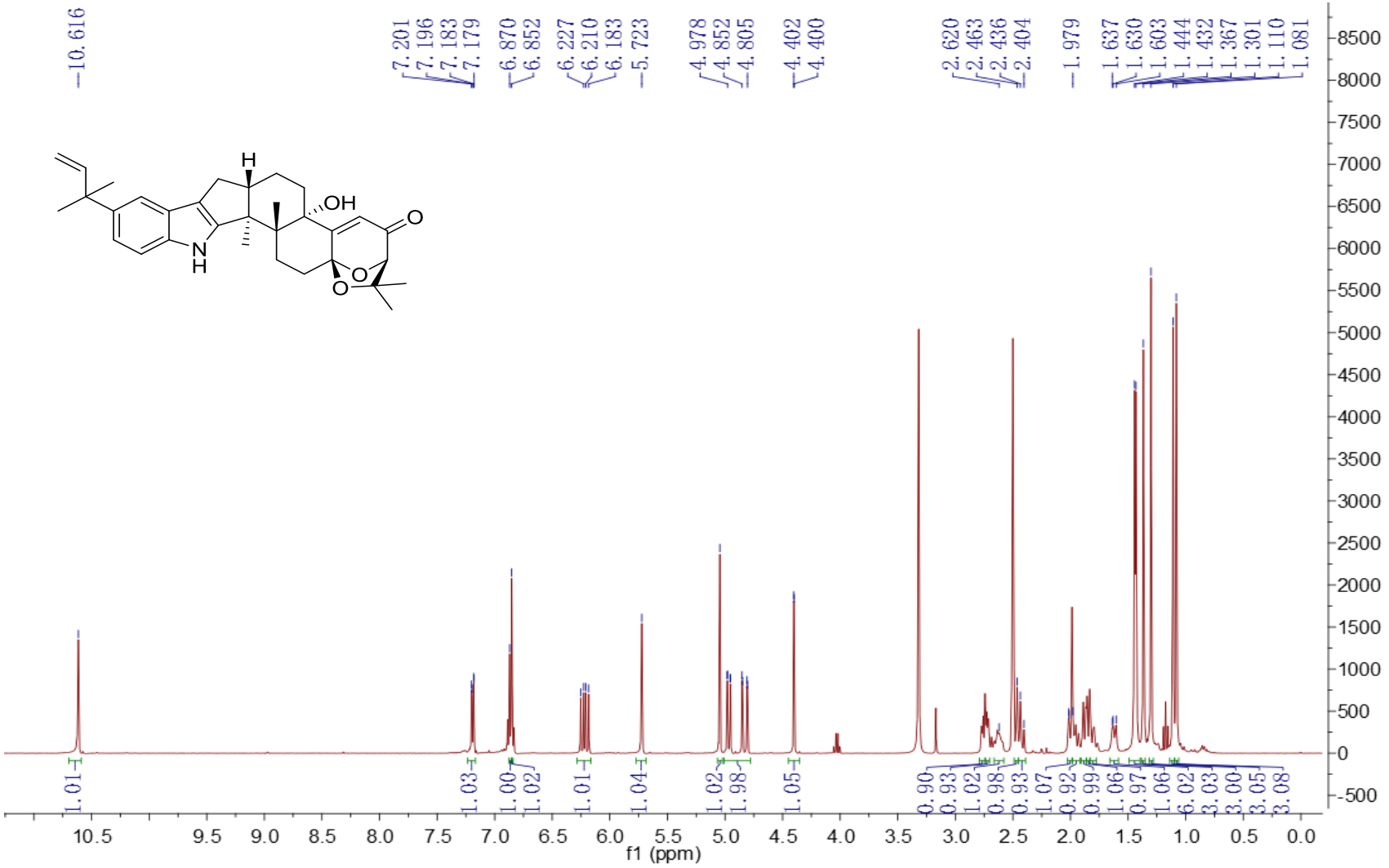


Figure S88. ^{13}C-NMR and DEPT spectra of β-aflatrem (**19**) in DMSO-d_6

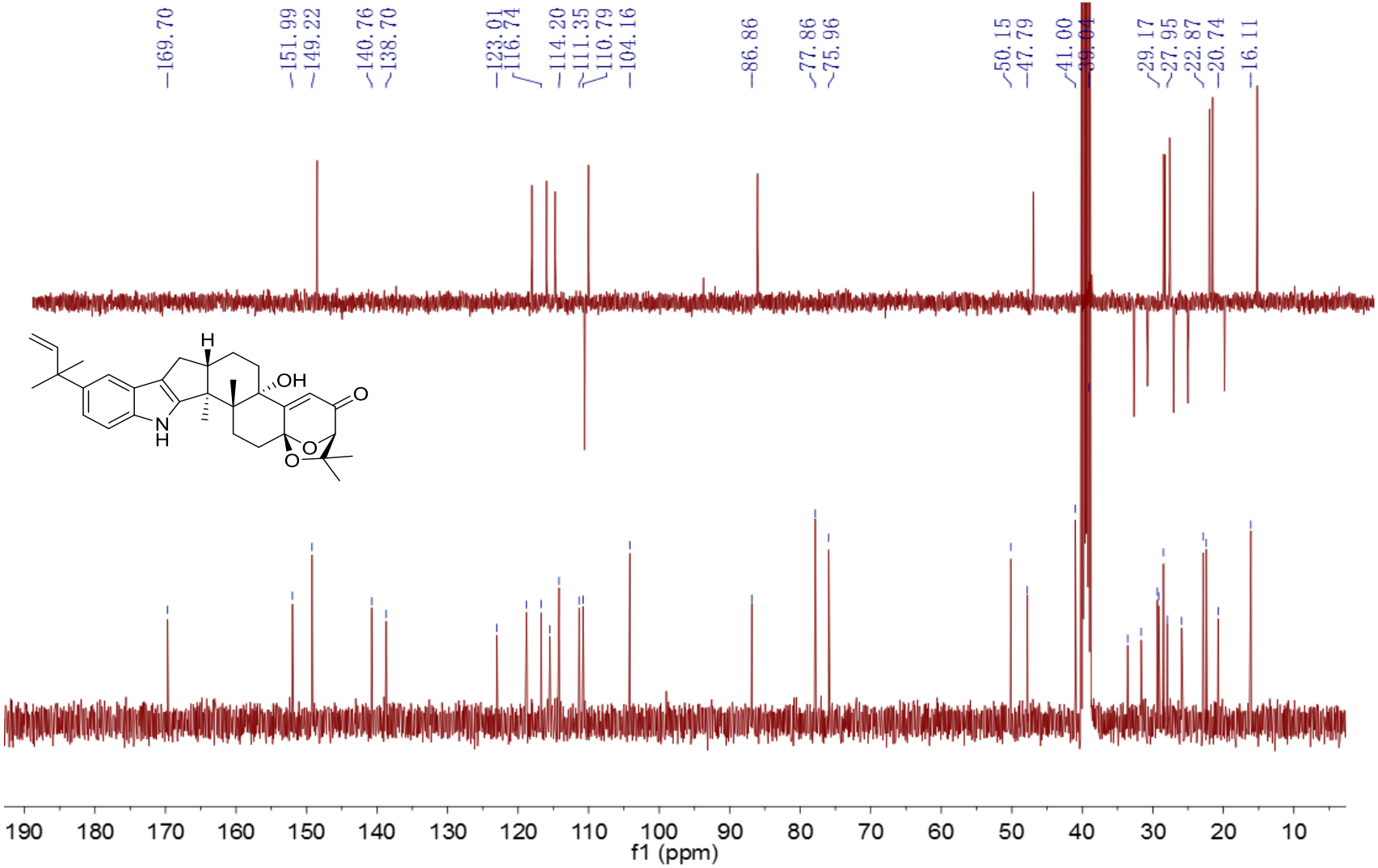


Figure S89. NOESY spectrum of β-aflatrem (**19**) in DMSO-d_6

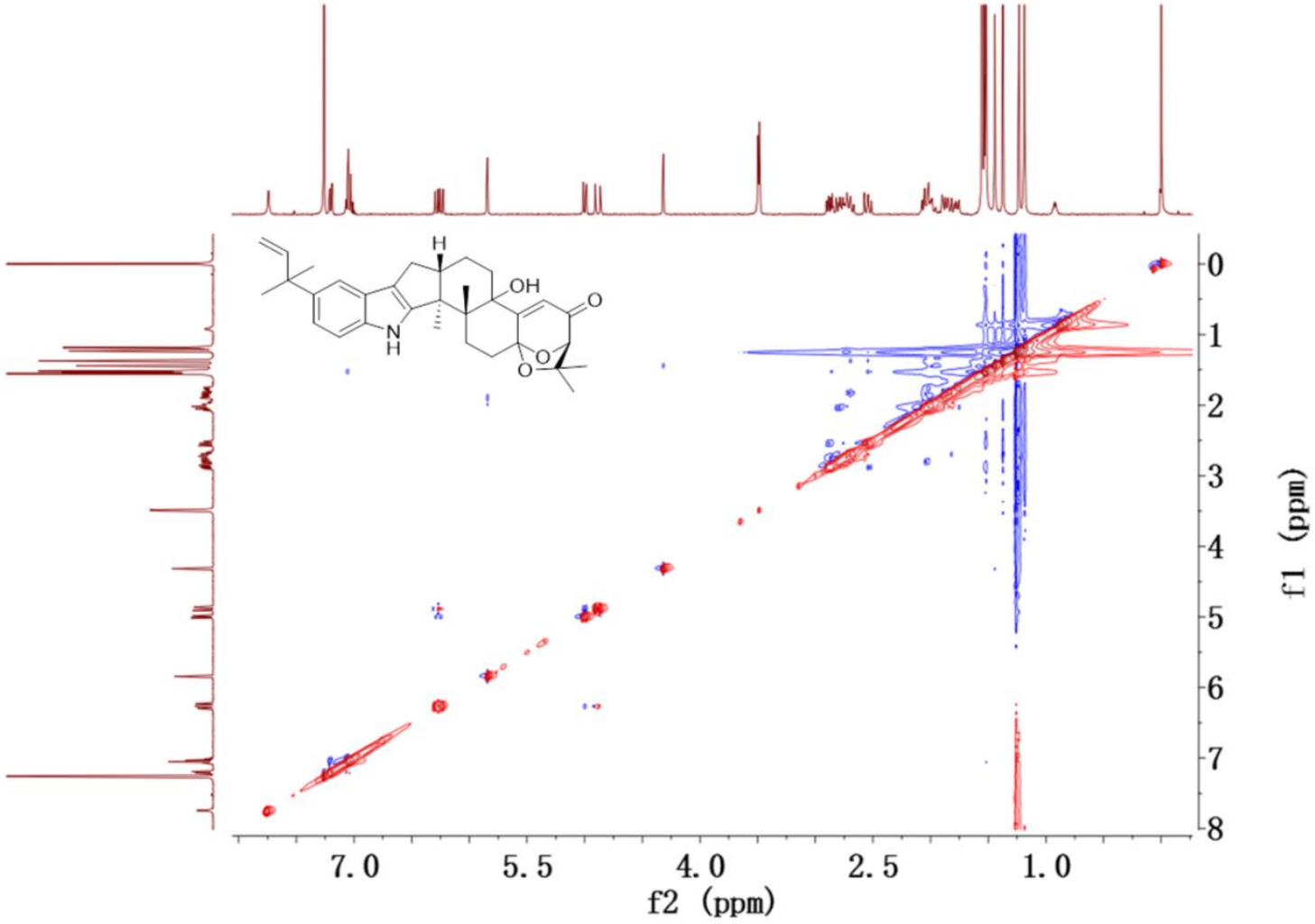


Figure S90. ^{1}H-NMR spectrum of pyripyropene A (**20**) in $CDCl_3$ (400MHz)

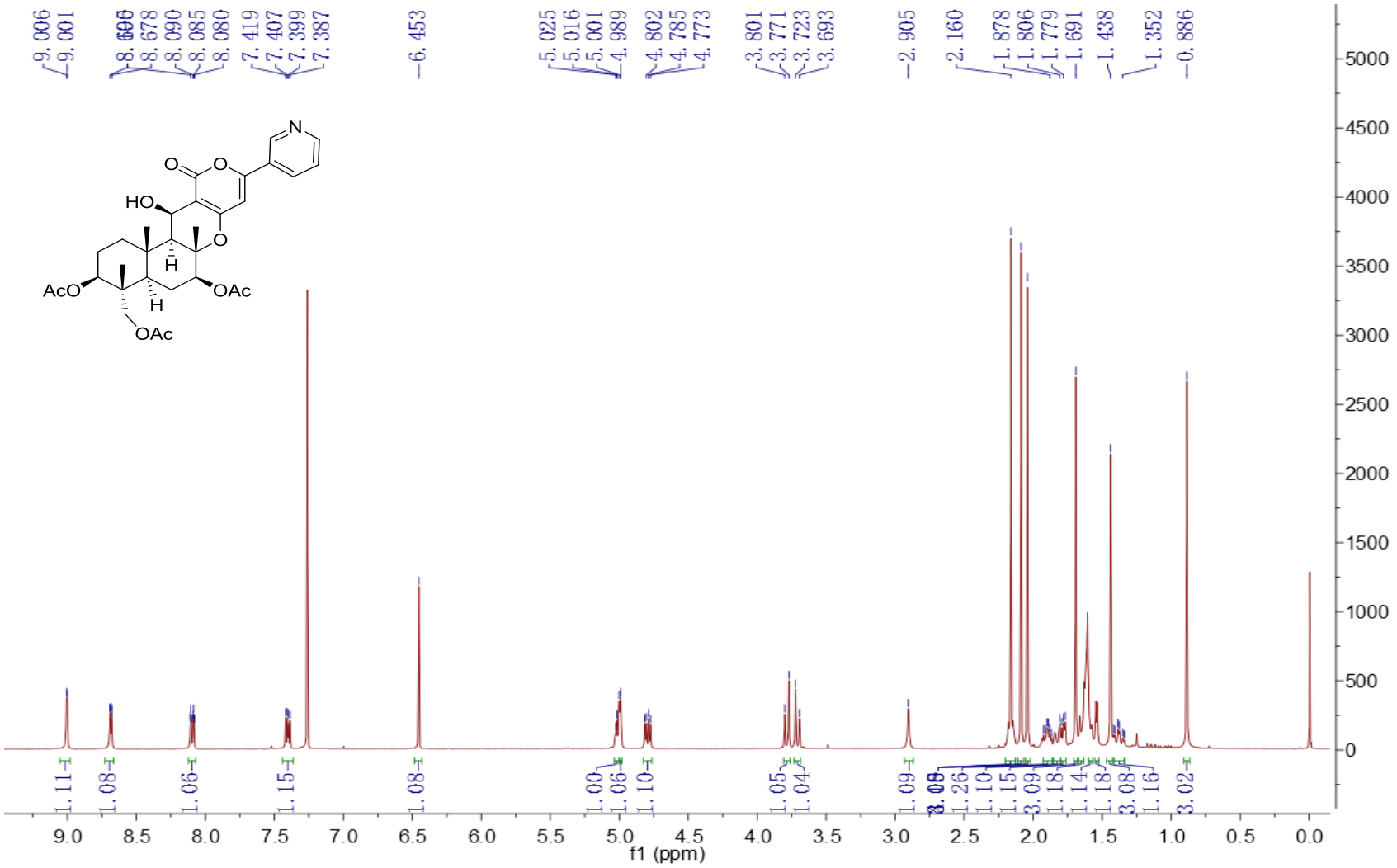


Figure S91. ^{13}C-NMR spectrum of pyripyropene A (**20**) in $CDCl_3$ (100MHz)

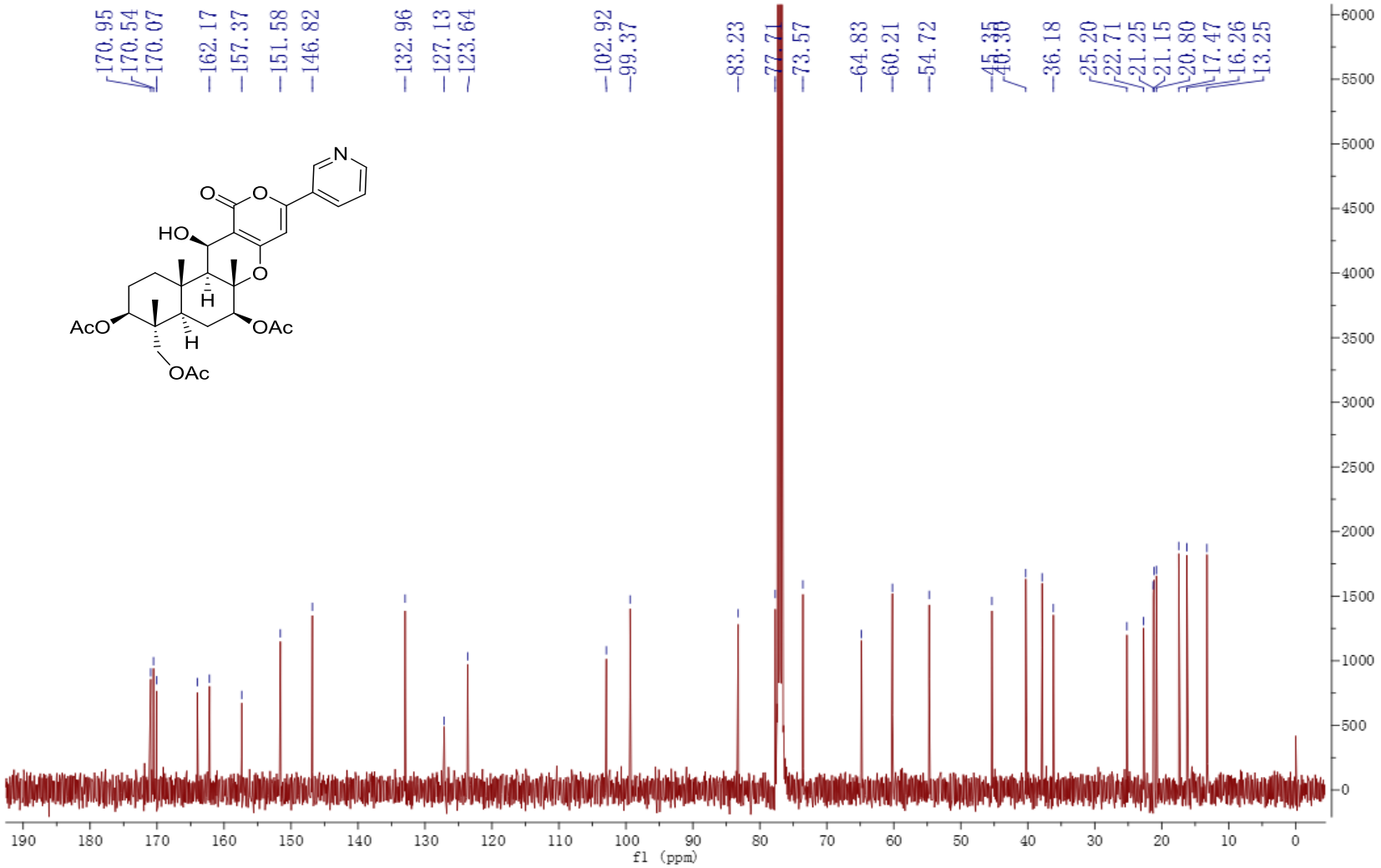


Figure S92. NOESY spectrum of pyripyropene A (**20**) in $CDCl_3$

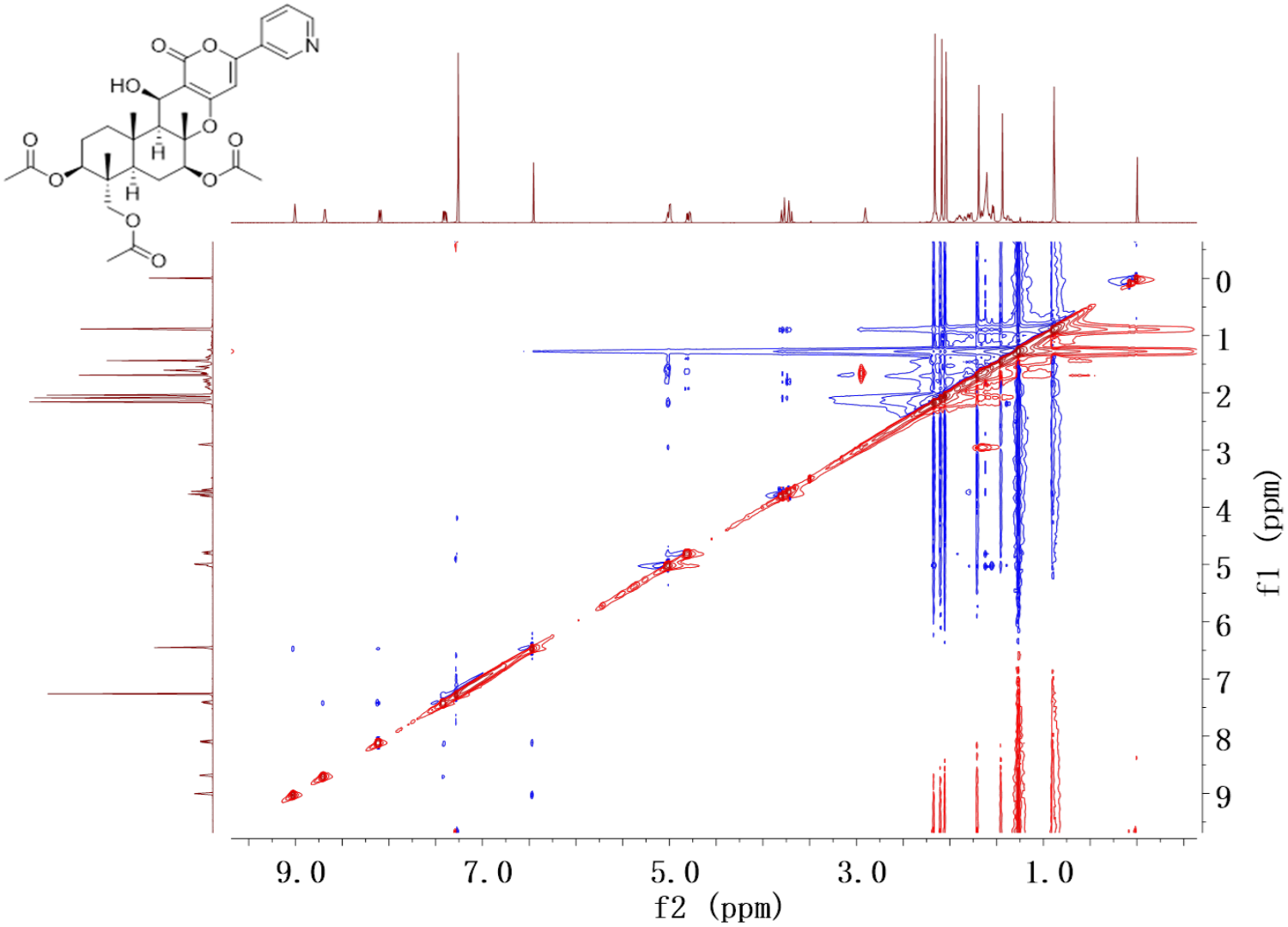
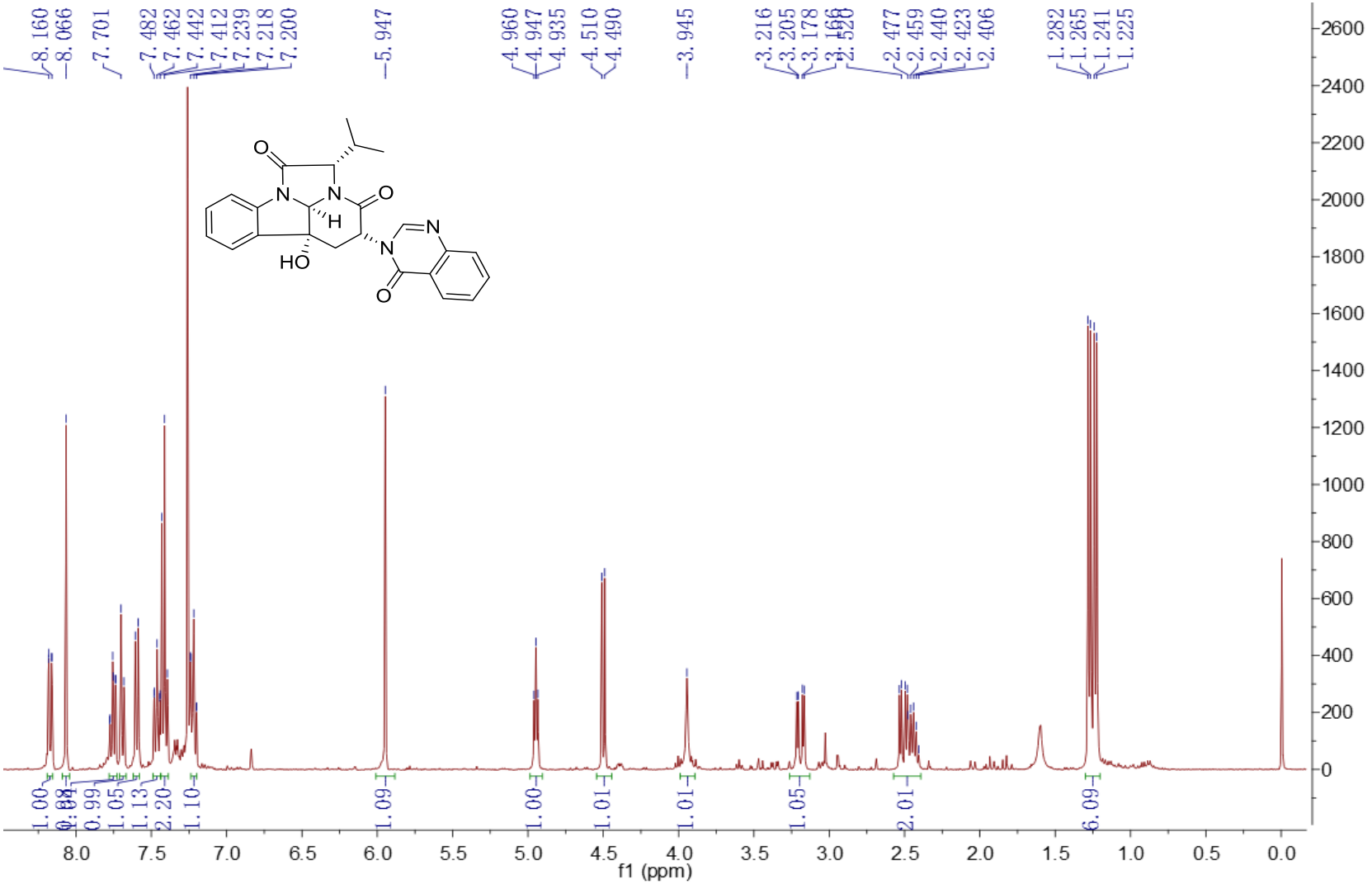


Figure S93. ^{1}H-NMR spectrum of pseudofischerine (**21**) in $CDCl_3$ (400MHz)



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

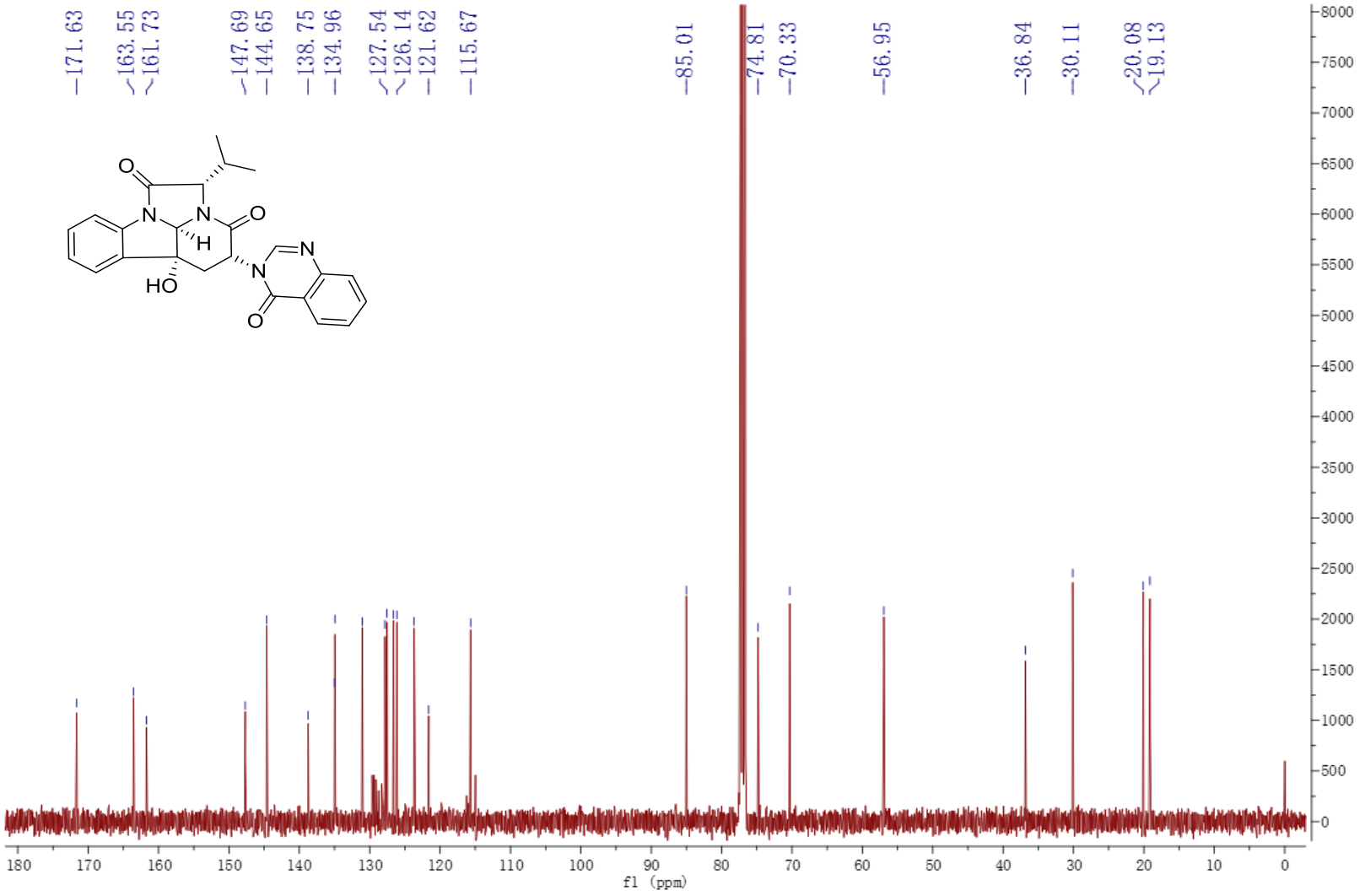


Figure S95. HMQC spectrum of pseudofischerine (**21**) in $CDCl_3$

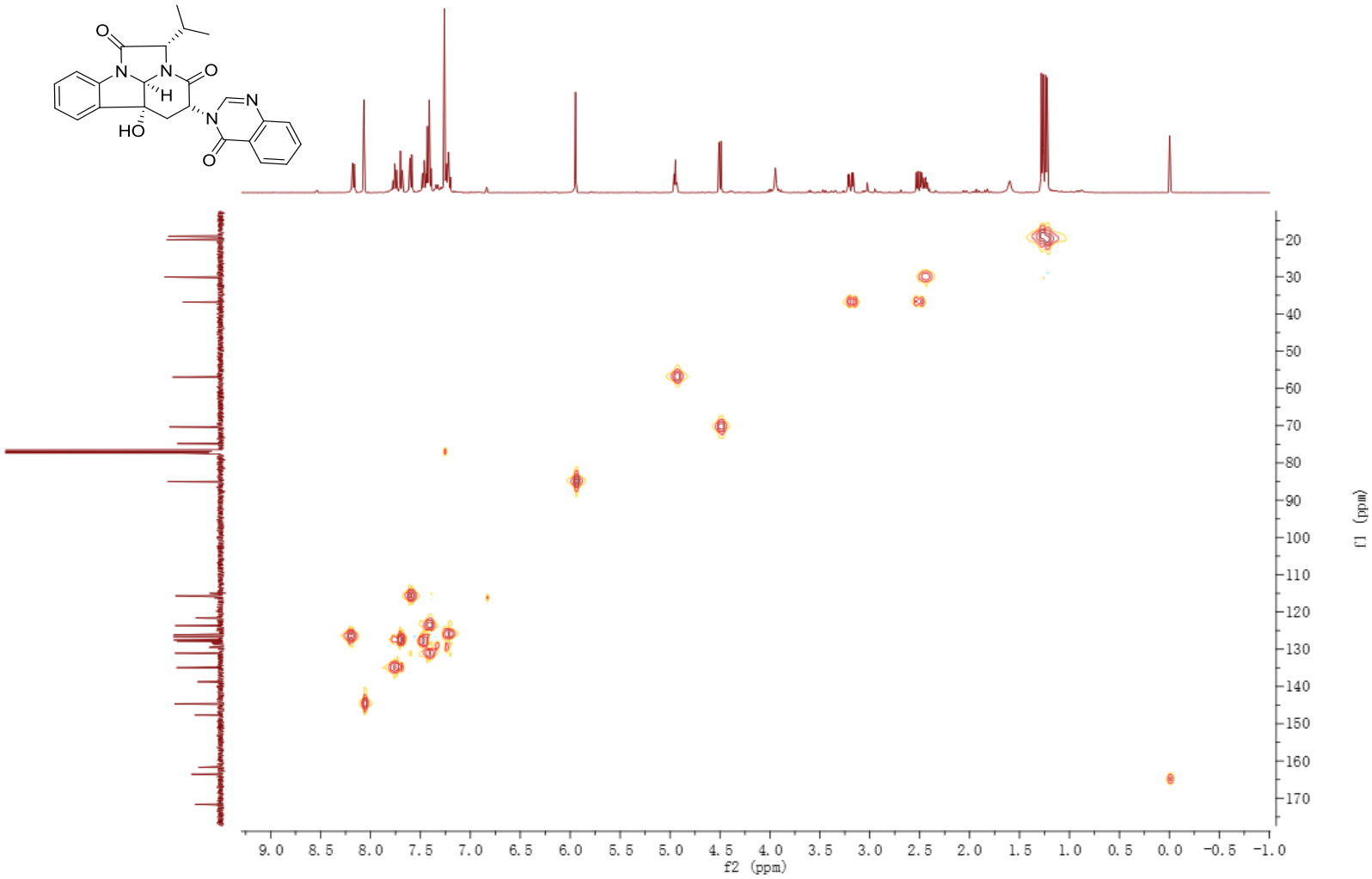


Figure S96. ^{1}H-^{1}H COSY spectrum of pseudofischerine (**21**) in $CDCl_3$

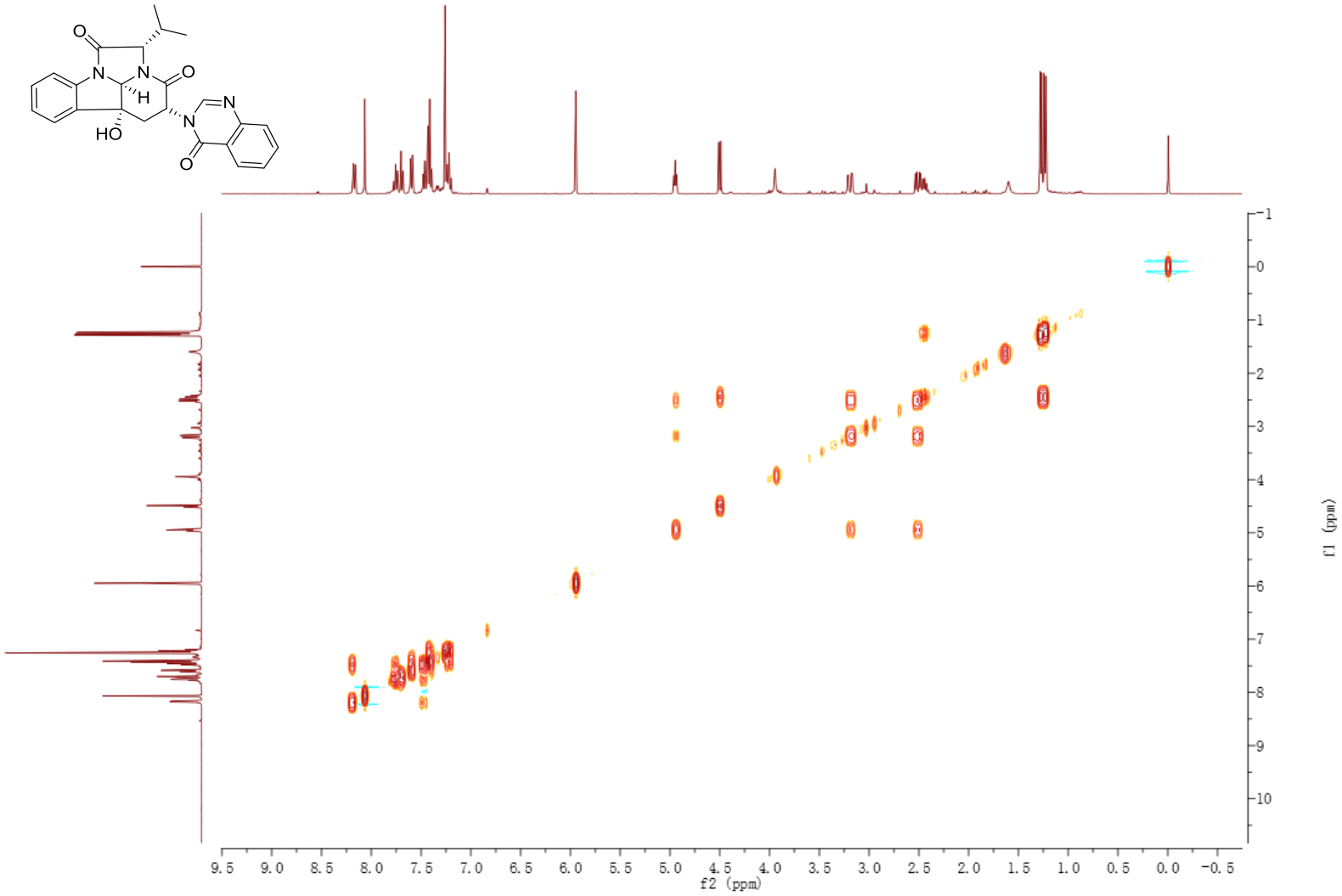


Figure S97. HMBC spectrum of pseudofischerine (**21**) in $CDCl_3$

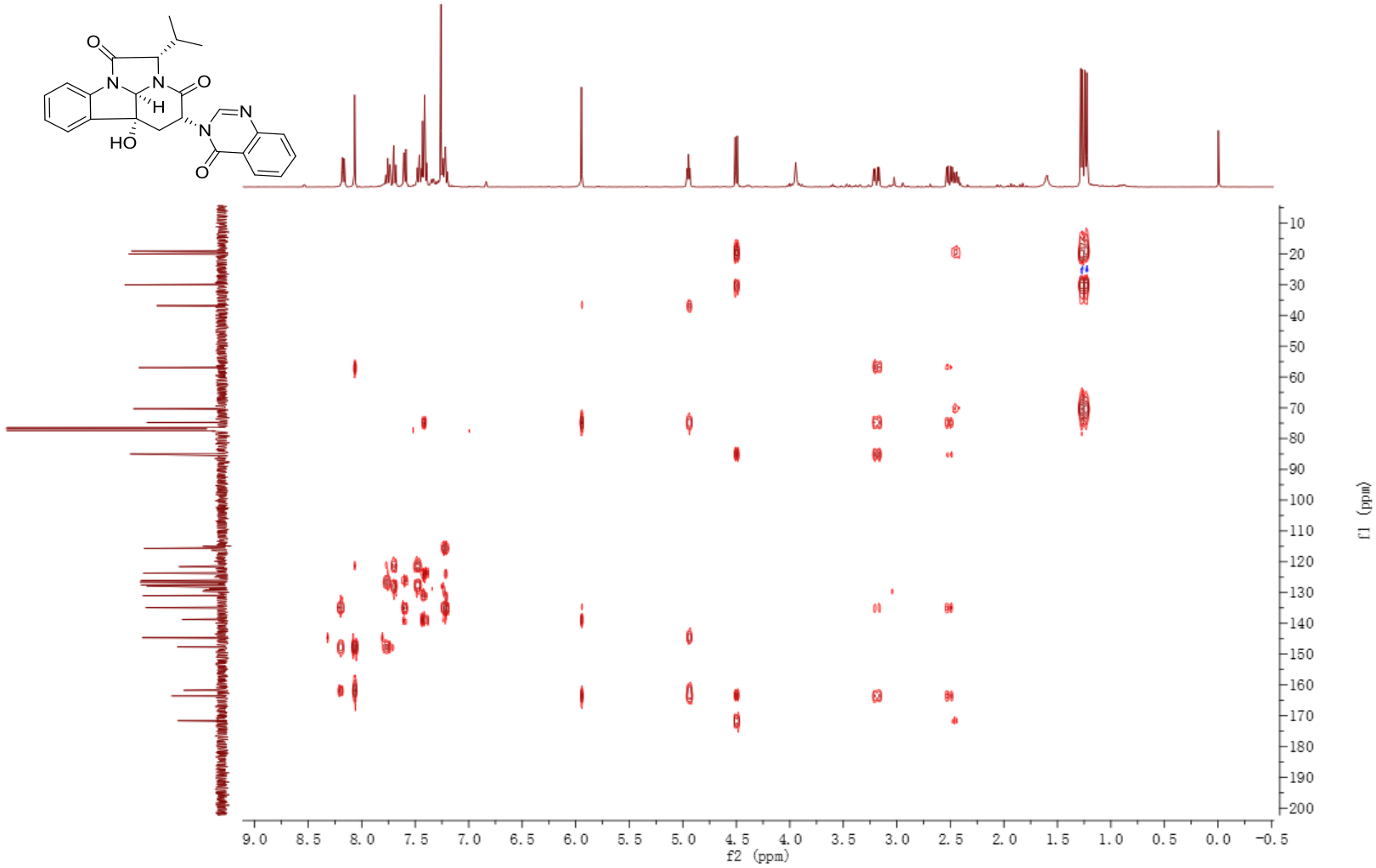


Figure S98. NOESY spectrum of pseudofischerine (**21**) in $CDCl_3$

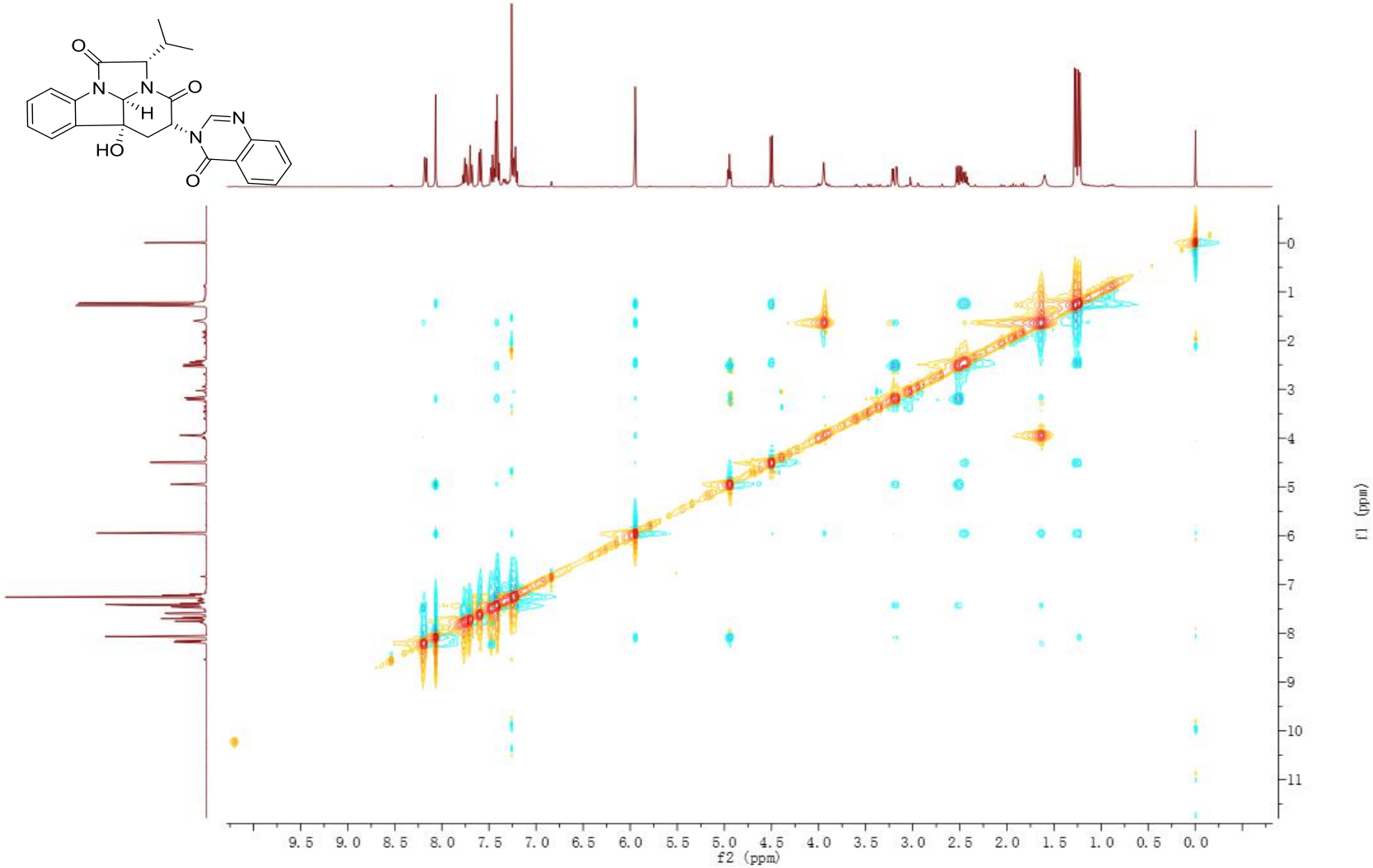


Figure S99. HR-EI-MS spectrum of 4-(1-hydroxy-1-methylpropyl)-2-isobutylpyrazin-2(1H)-one (**22**) in $CDCl_3$

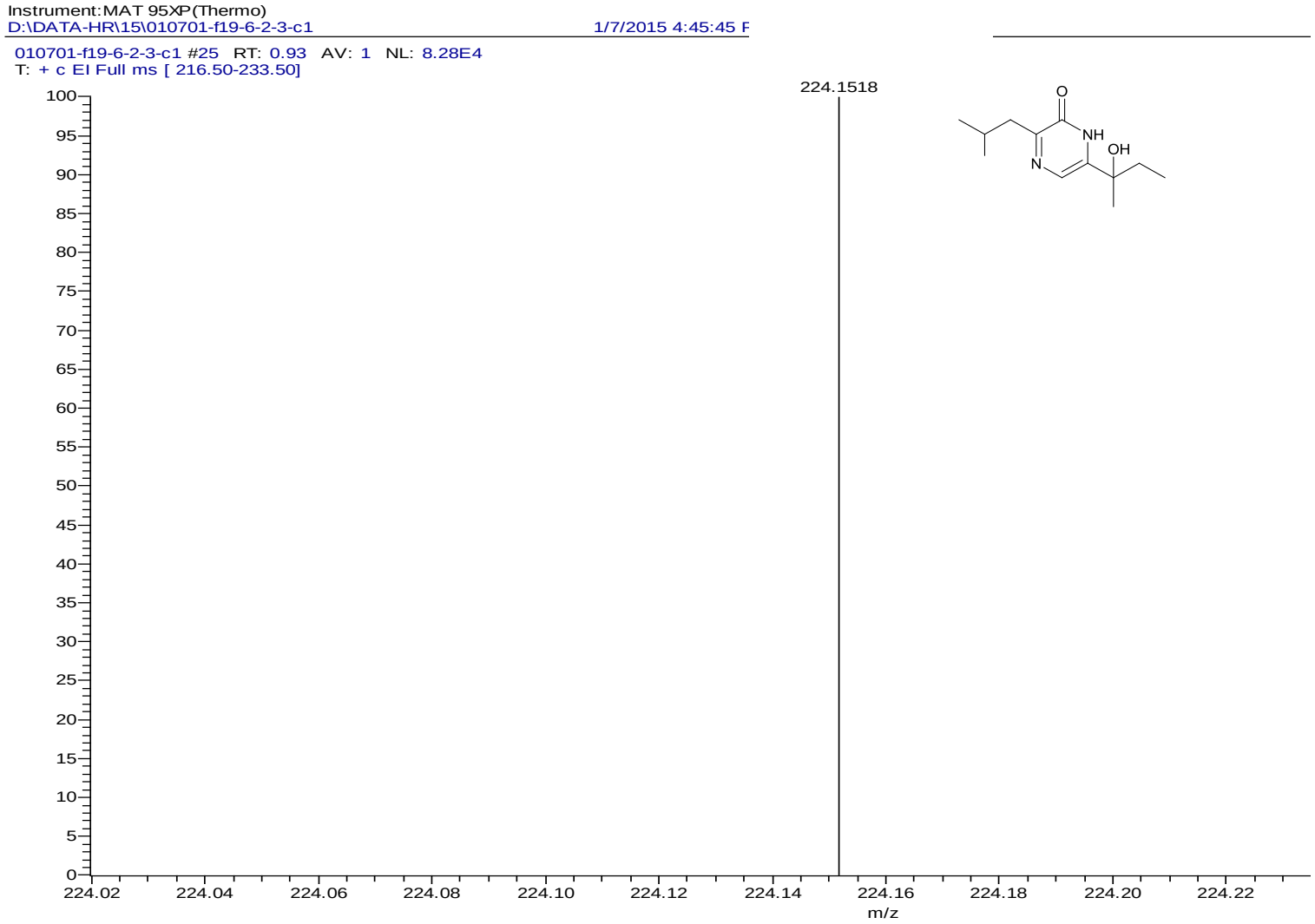


Figure S100. ^{1}H-NMR spectrum of 4-(1-hydroxy-1-methylpropyl)-2-isobutylpyrazin-2(1H)-one (**22**) in $CDCl_3$ (400MHz)

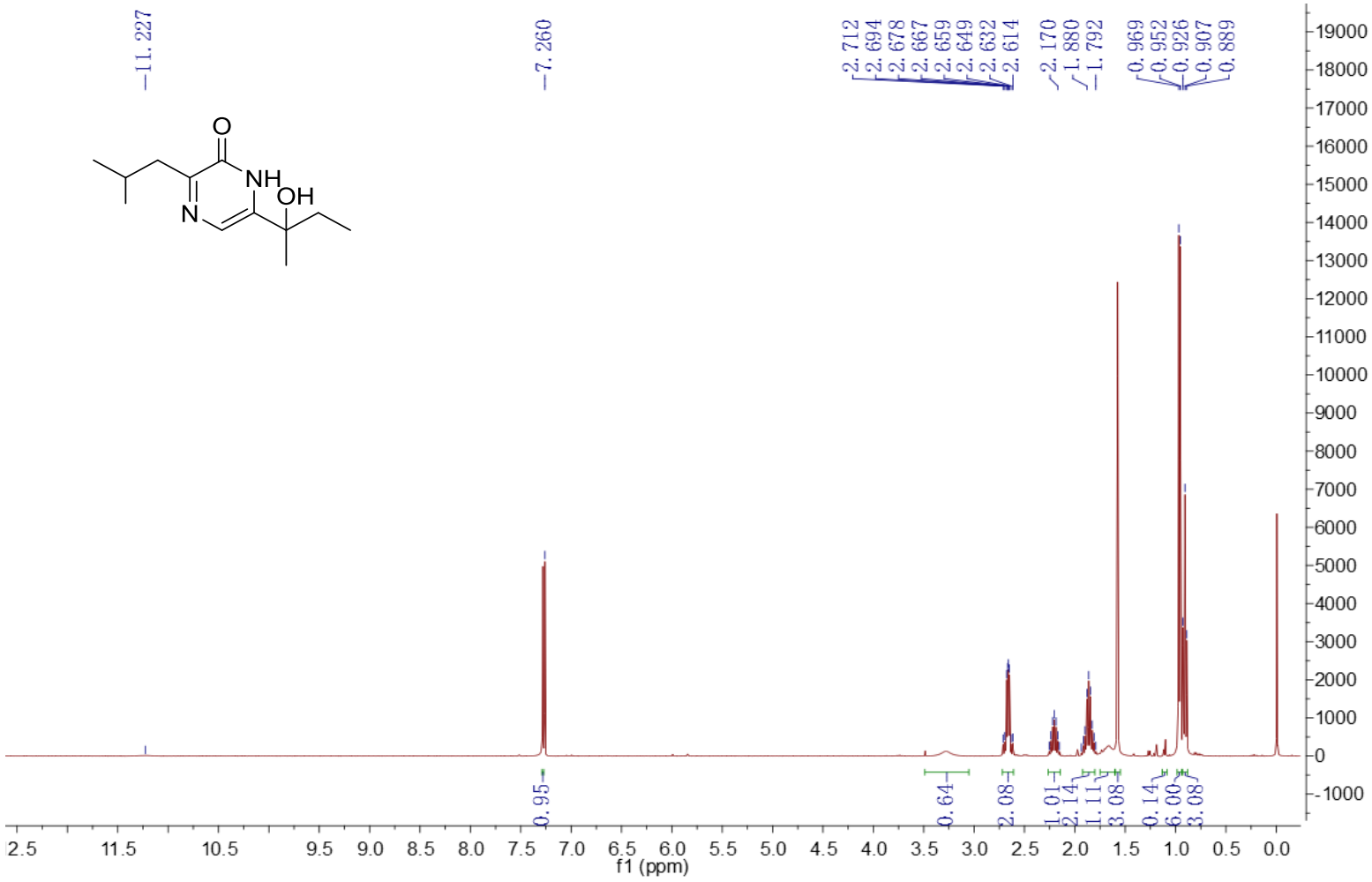


Figure S101. ^{13}C-NMR and DEPT spectra of 4-(1-hydroxy-1-methylpropyl)-2-isobutylpyrazin-2(1H)-one (**22**) in $CDCl_3$ (100MHz)

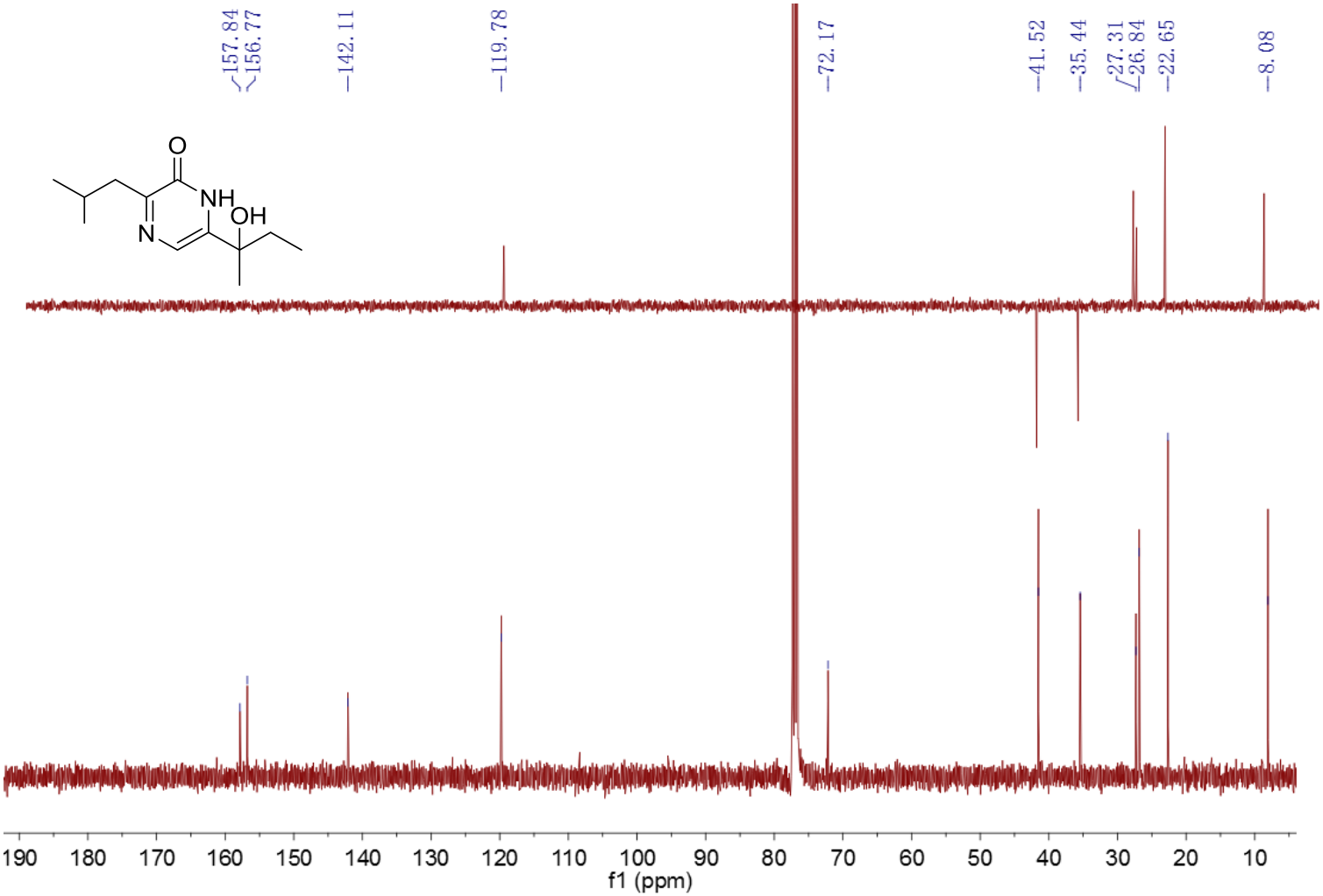


Figure S102. HR-EI-MS spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in $CDCl_3$

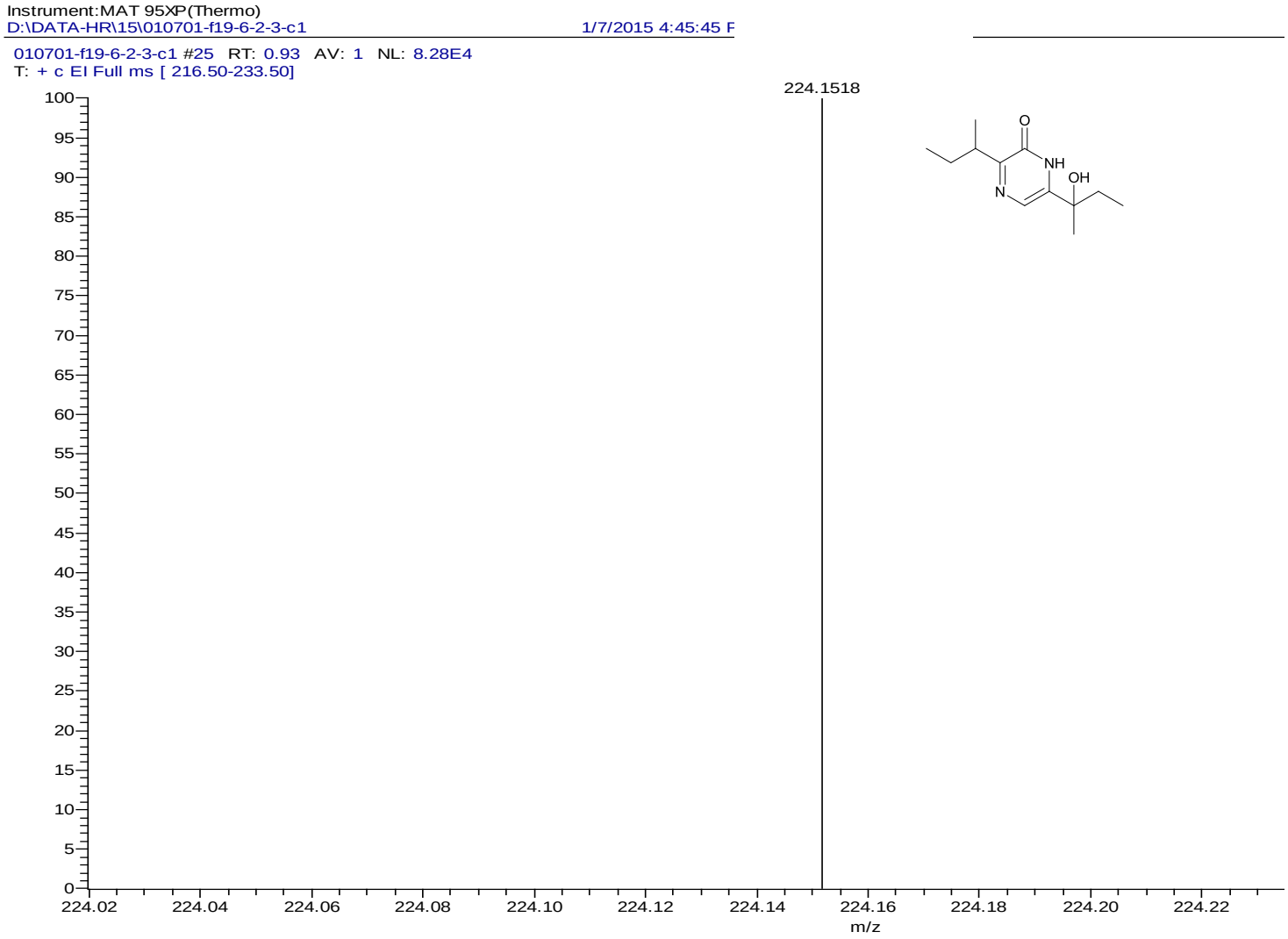


Figure S103. ^{1}H-NMR spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in $CDCl_3$ (400MHz)

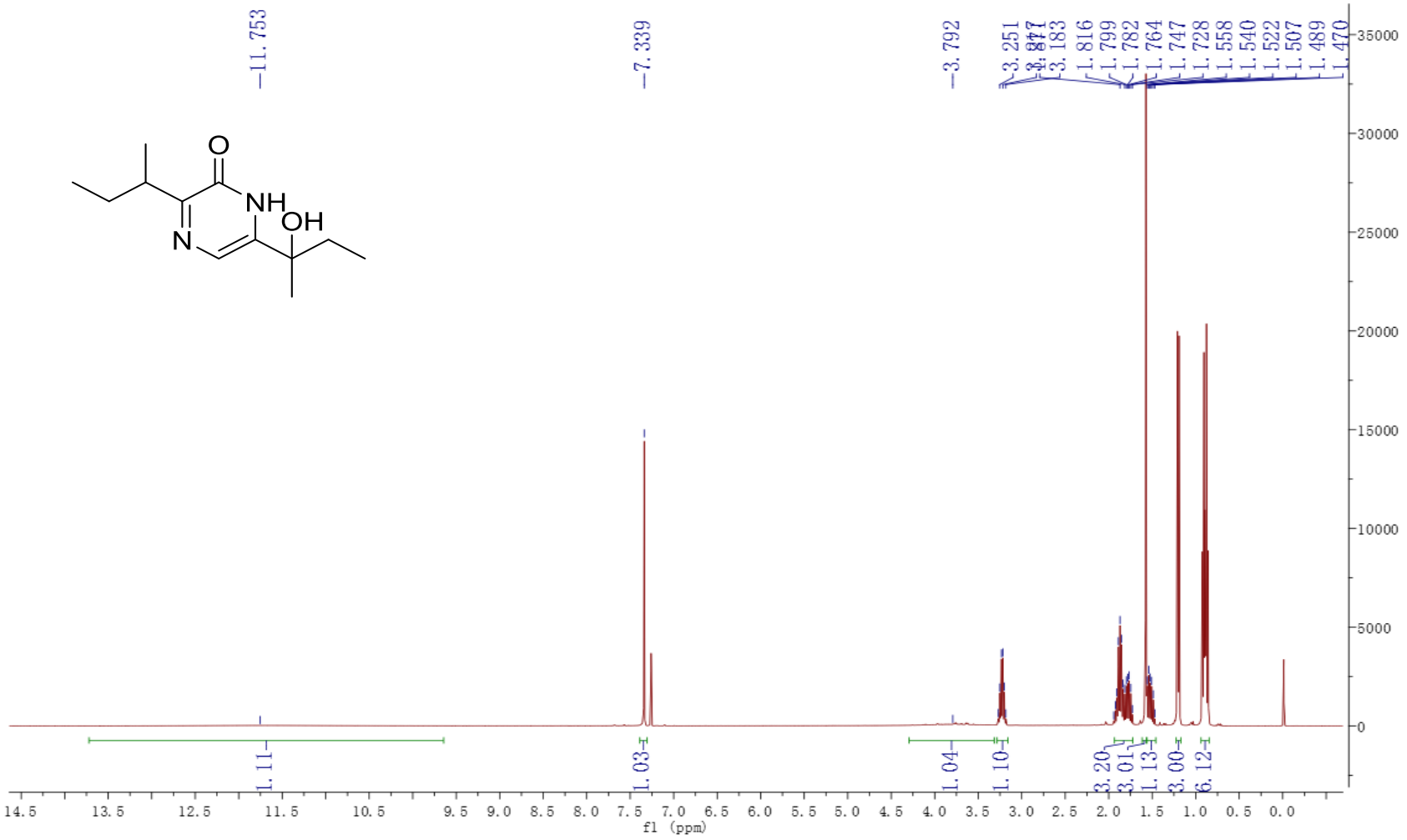


Figure S104. ^{13}C-NMR and DEPT spectra of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in $CDCl_3$ (100MHz)

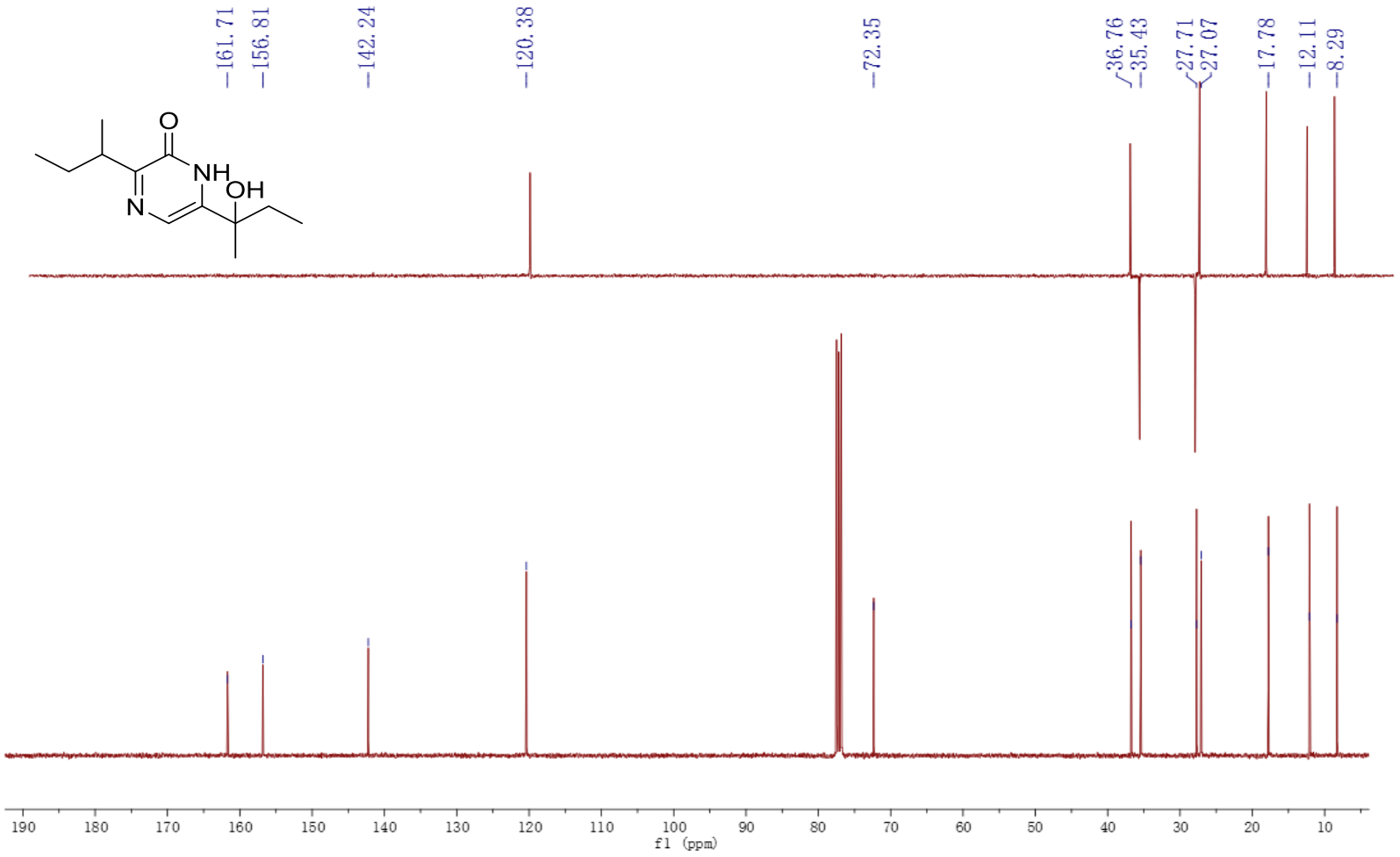


Figure S105. HMQC spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in $CDCl_3$

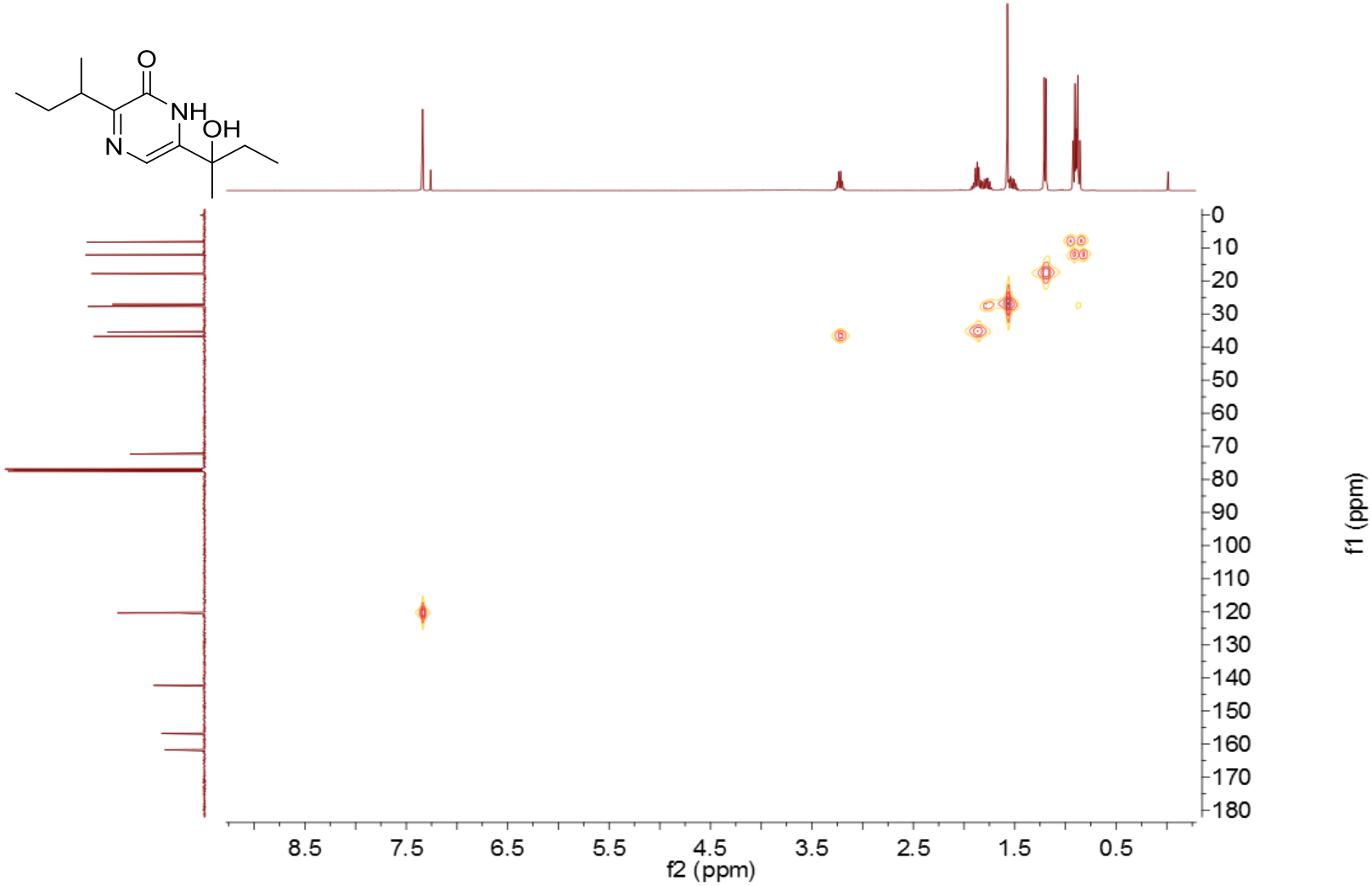


Figure S106. ^{1}H-^{1}H COSY spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in $CDCl_3$

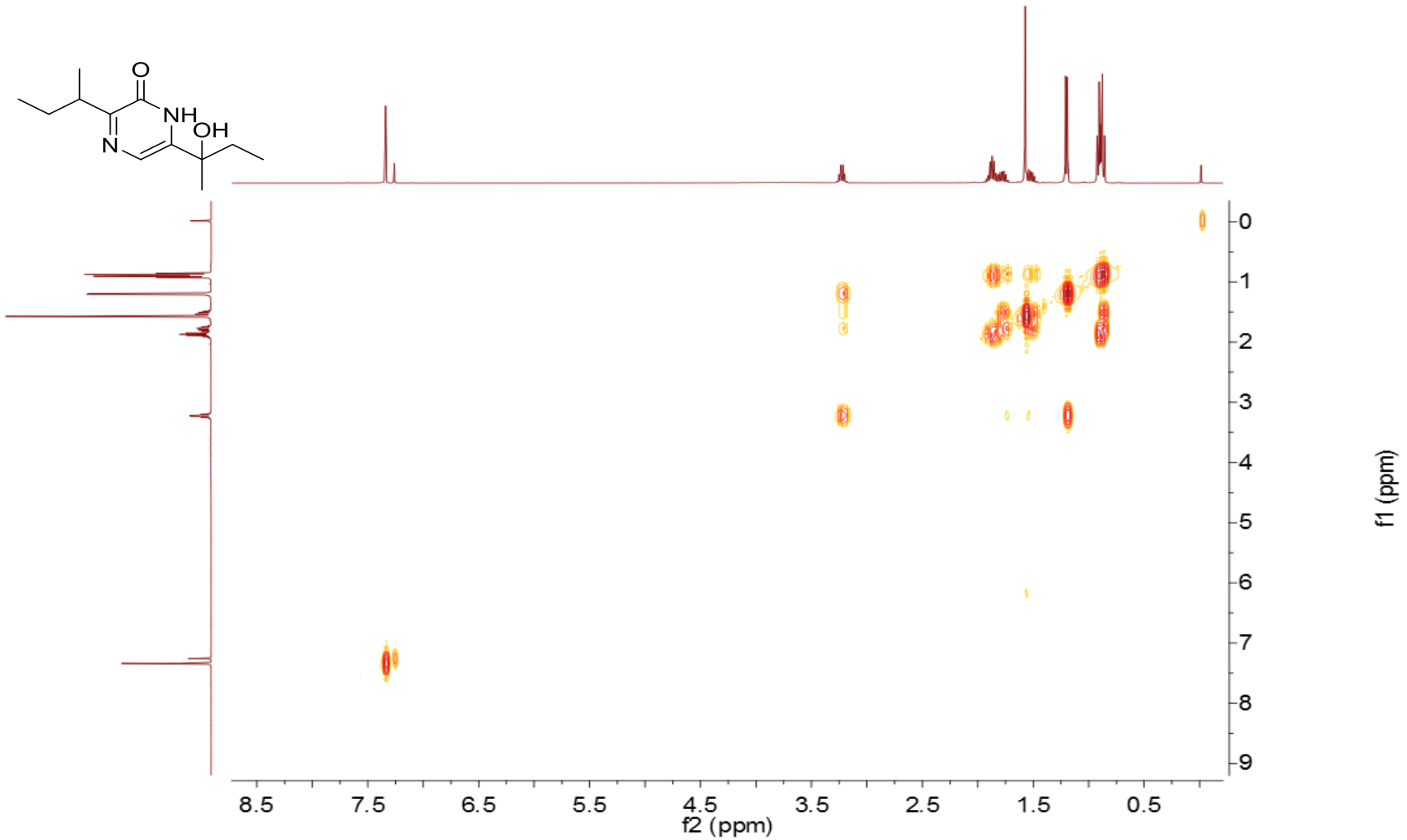


Figure S107. HMBC spectrum of 4-(1-hydroxy-1-methylpropyl)-2-secbutylpyrazin-2(1H)-one (**23**) in $CDCl_3$

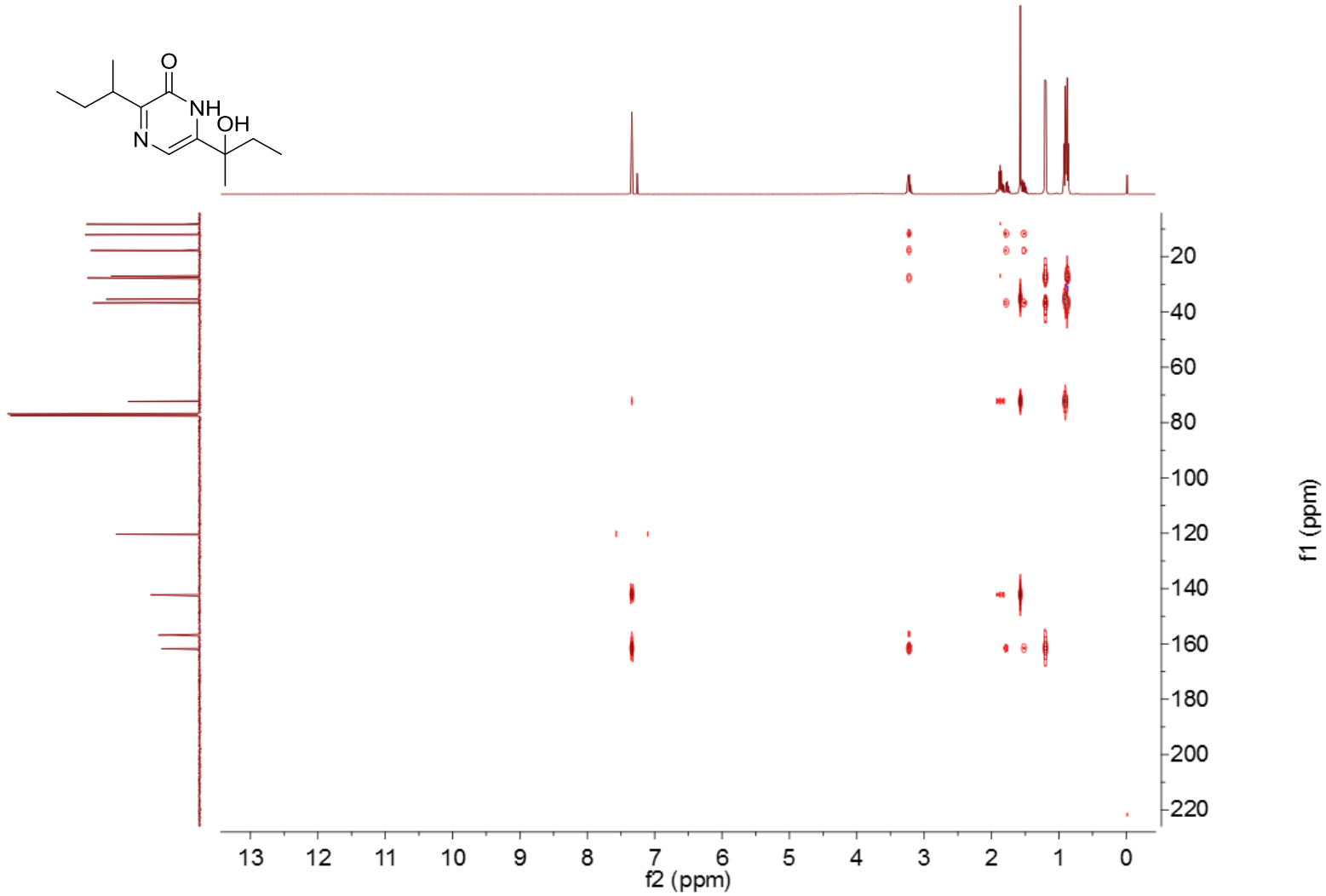


Figure S108. ^{1}H-NMR spectrum of O-methylsterigmatocystin (**24**) in $CDCl_3$ (400MHz)

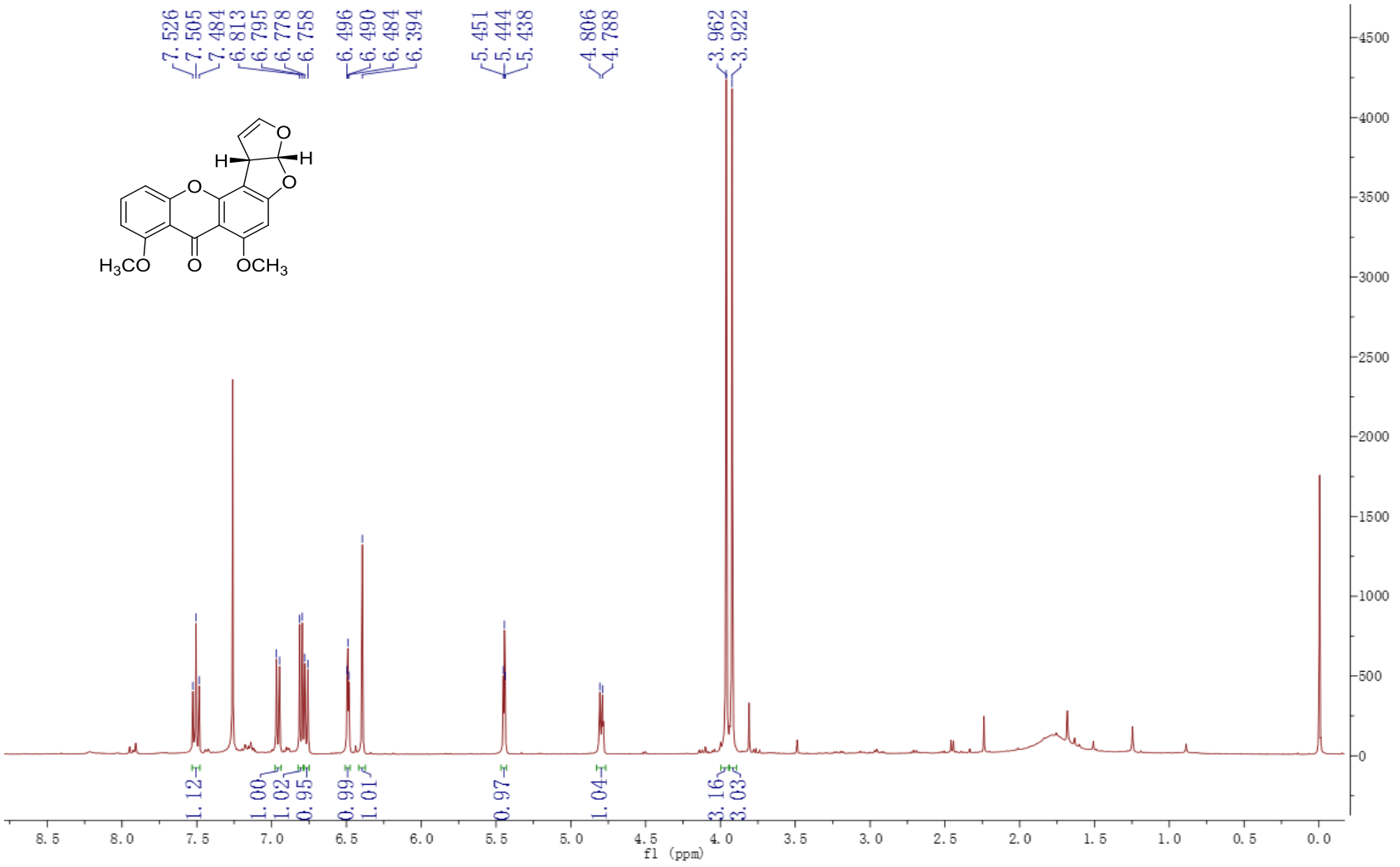


Figure S109. ^{13}C-NMR spectrum of O-methylsterigmatocystin (**24**) in $CDCl_3$ (100MHz)

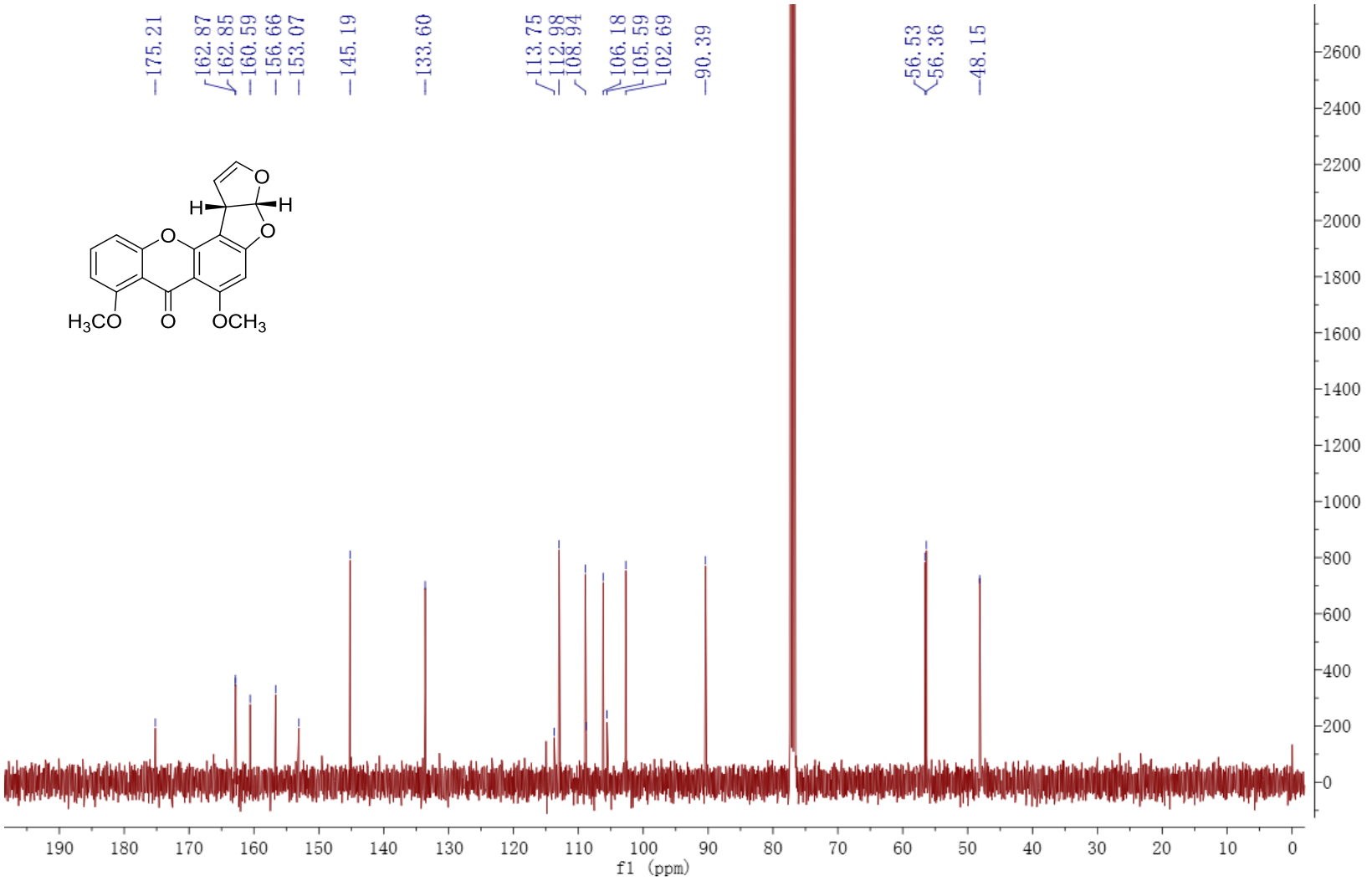


Figure S110. NOESY spectrum of O-methylsterigmatocystin (**24**) in $CDCl_3$

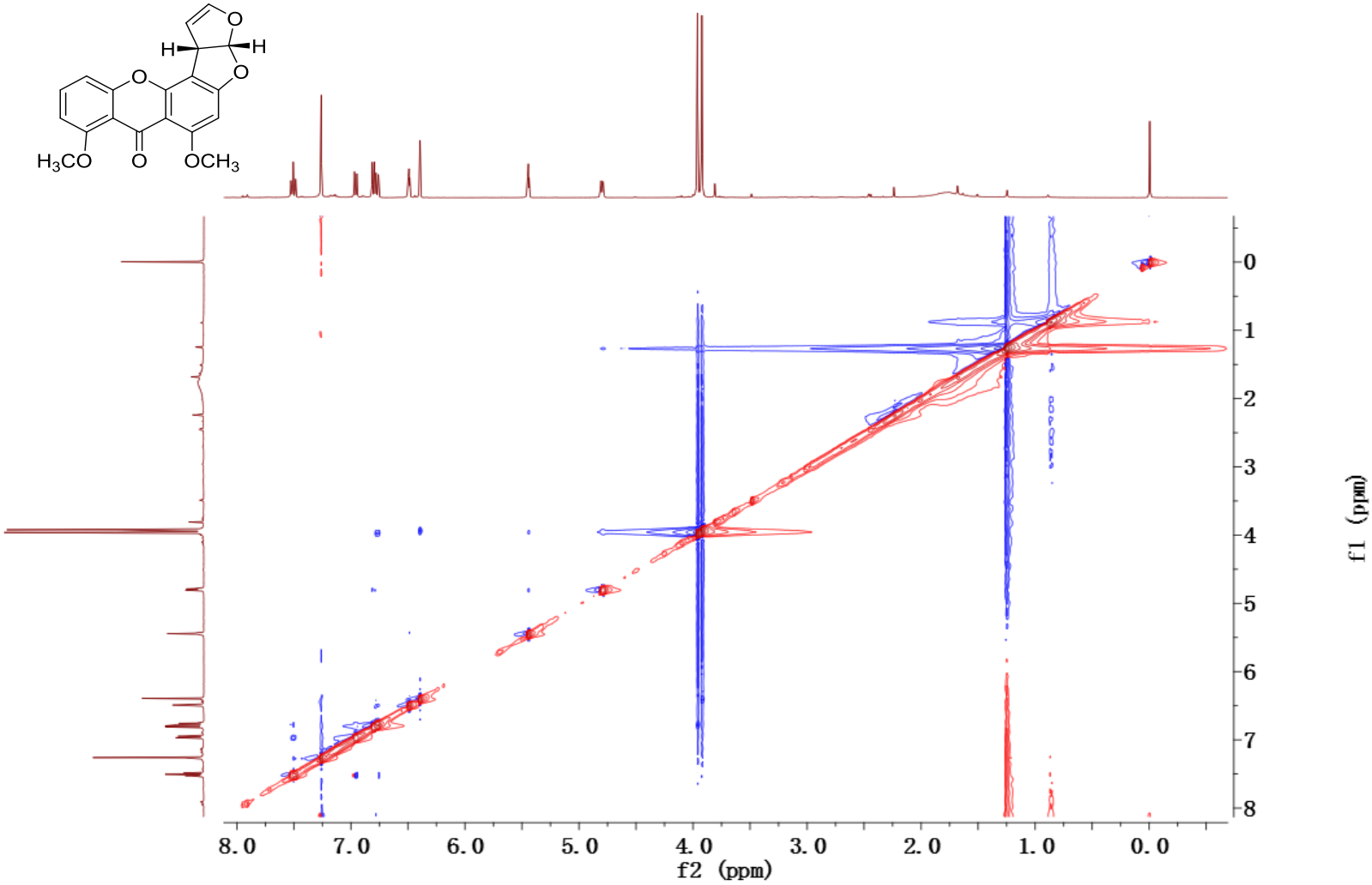


Figure S111. ^{1}H-NMR spectrum of asperfuran (**25**) in $CDCl_3$ (400MHz)

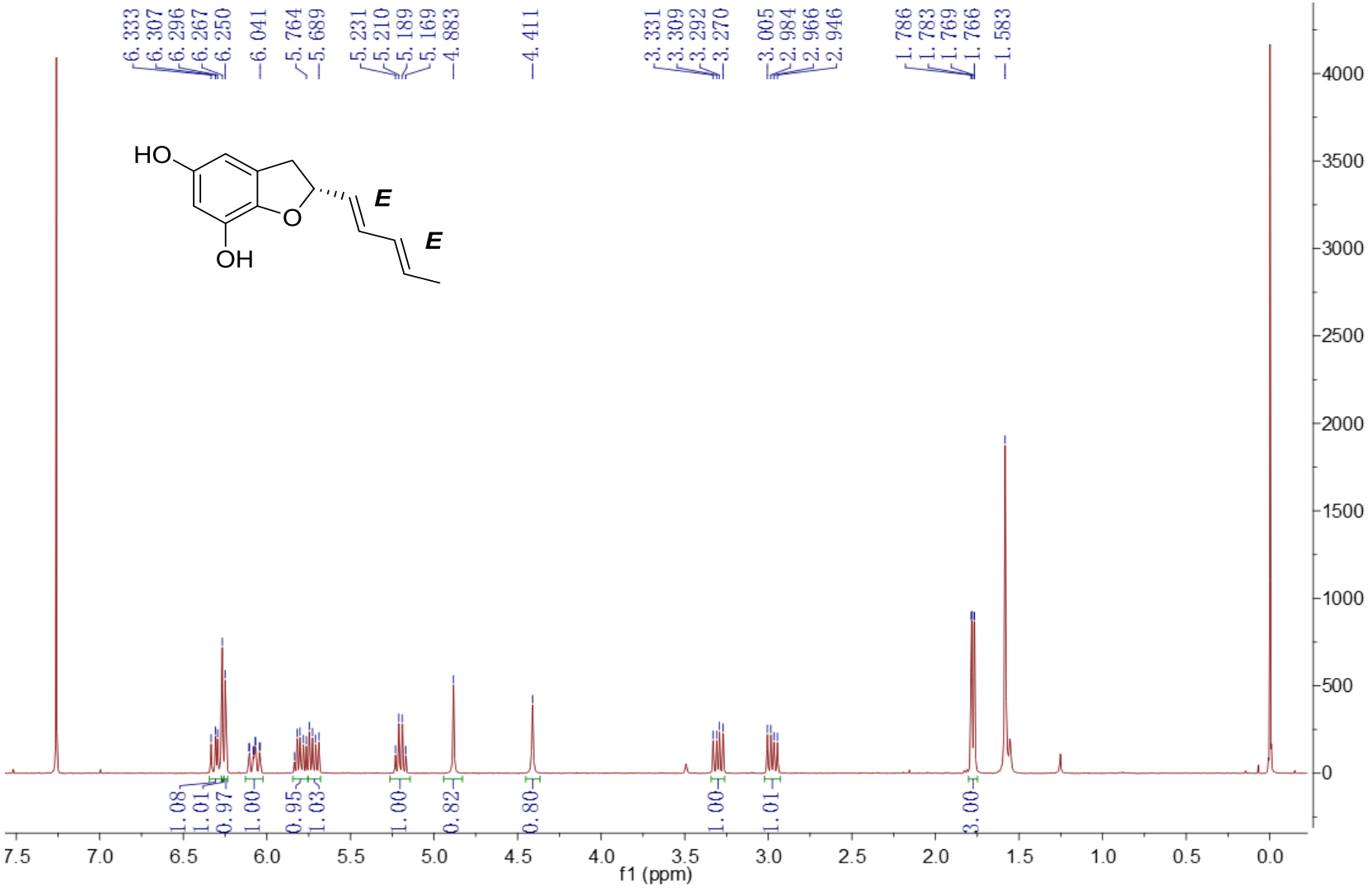


Figure S112. ^{13}C-NMR spectrum of asperfuran (**25**) in $CDCl_3$ (100MHz)