

Supporting Information

Diverse secondary metabolites from the marine-derived fungus *Dichotomomyces cejpai* F31-1

Yan-Xiu Chen ^{1,5}, Meng-Yang Xu ¹, Hou-Jin Li ², Kun-Jiao Zeng ³, Wen-Zhe Ma ⁴,
Guo-Bao Tian ³, Jun Xu ¹, De-Po Yang ^{1,5}, Wen-Jian Lan ^{1,5,*}

- ¹ School of Pharmaceutical Sciences, Sun Yat-sen University, Guangzhou 510006, China; chenyx239@mail2.sysu.edu.cn; xumy3@mail2.sysu.edu.cn; junxu@biochemomes.com; lssydp@mail.sysu.edu.cn; lanwj@mail.sysu.edu.cn
- ² School of Chemistry, Sun Yat-sen University, Guangzhou 510275, China; ceslhj@mail.sysu.edu.cn
- ³ Zhongshan School of Medicine, Sun Yat-sen University, Guangzhou 510080, China; zkj3880@163.com; tiangb@mail.sysu.edu.cn
- ⁴ State Key Laboratory of Quality Research in Chinese Medicine, Macau Institute for Applied Research in Medicine and Health, Macau University of Science and Technology, Avenida Wai Long, Taipa 519020, Macau (SAR), China; wzma@must.edu.mo
- ⁵ Guangdong Technology Research Center for Advanced Chinese Medicine, Guangzhou 510006, China
- Correspondence: lanwj@mail.sysu.edu.cn; Tel.: +86-020-3994-3042

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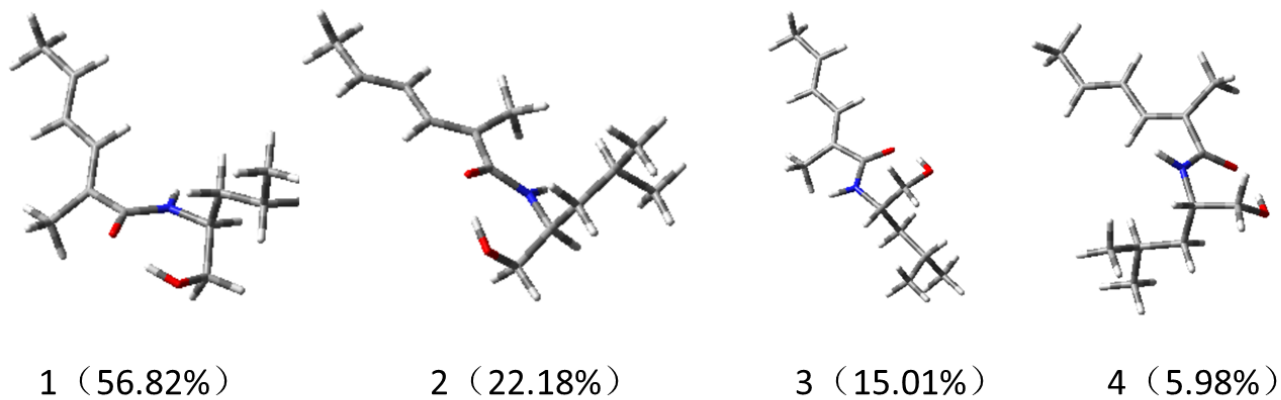
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Table S1. Comparison of the experimental optical rotation values with the calculated OR values of compounds **1–5** and **16**

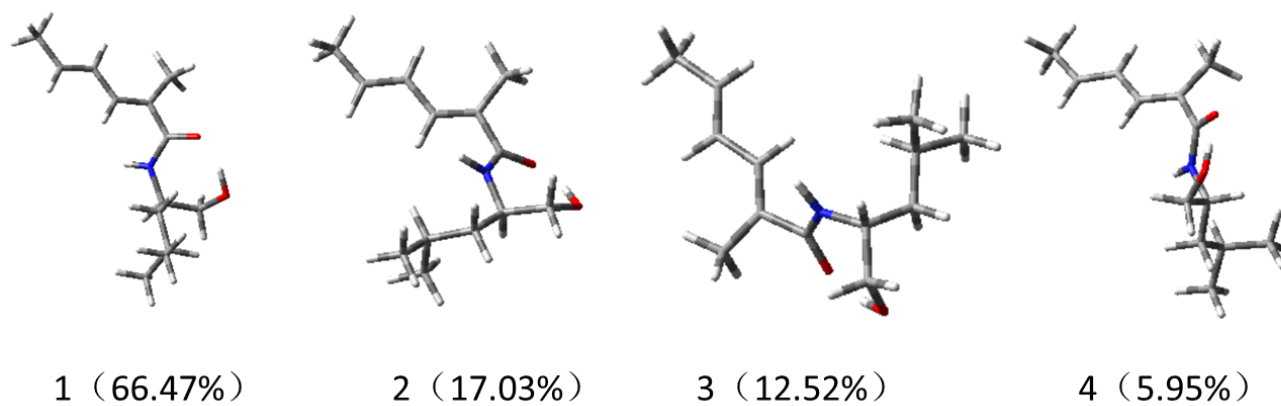
compounds	calculated OR values	experimental OR value
9S-1	-42.1	-41.9
9R-1	45.4	
9S,11R-2	-7.1	-4.4
9R,11S-2	7.4	
9S-3	-48.4	-51.6
9R-3	45.4	
9S-4	-14.5	-10.6
9R-4	14.6	
1R,2R,10R,15S-5	25.1	23.0
1S,2S,10S,15R-5	-24.5	
1R,2S,10R,15S-5	132.1	
1S,2R,10S,15R-5	-132.5	
1S,2R,10R,15S-5	52.9	
1R,2S,10S,15R-5	-50.0	
1S,2S,10R,15S-5	122.3	
1R,2R,10S,15R-5	-122.4	
3R,6S,7S,11S,13R-16	-59.6	-60.5
3S,6R,7R,11R,13S-16	56.3	
3R,6R,7R,11R,13R-16	133.3	
3S,6S,7S,11S,13S-16	160.8	
3R,6S,7S,11R,13R-16	-120.3	
3S,6R,7R,11S,13S-16	119.0	
3R,6R,7R,11S,13R-16	-78.2	
3S,6S,7S,11R,13S-16	78.6	

Figure S1. The most stable conformers of **1–5**, **16** calculated at the B3LYP/6-31+G(d) level. Relative populations are in parentheses.

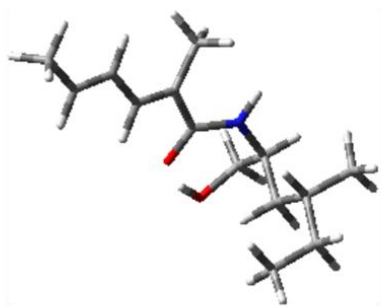
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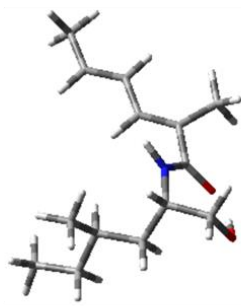
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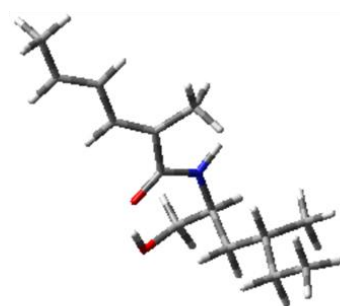
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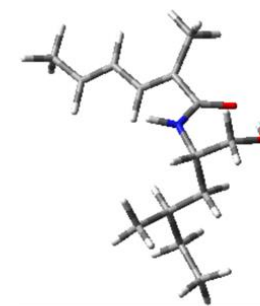
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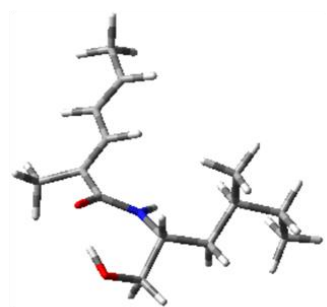


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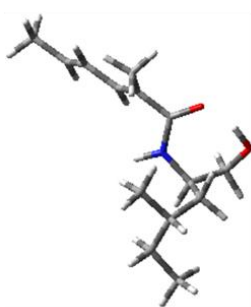


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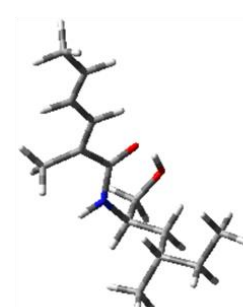
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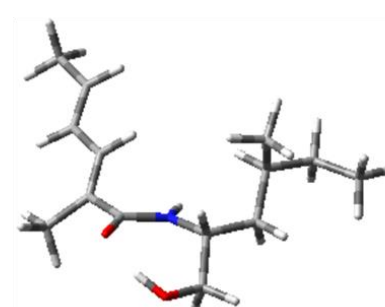
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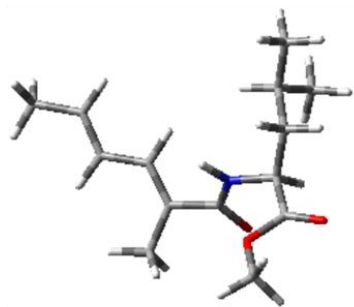


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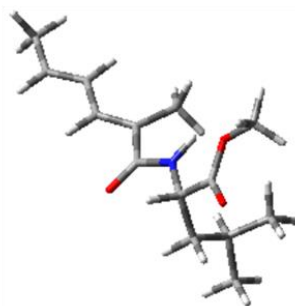


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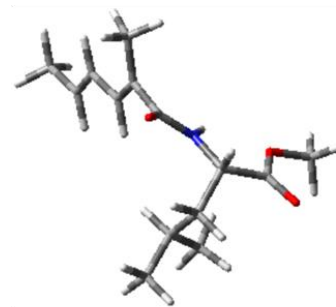
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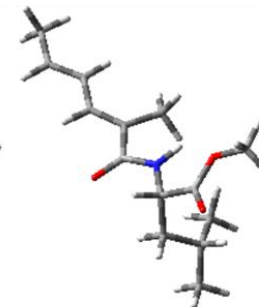
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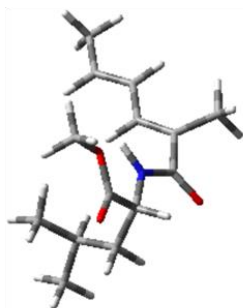


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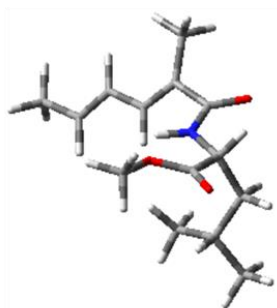


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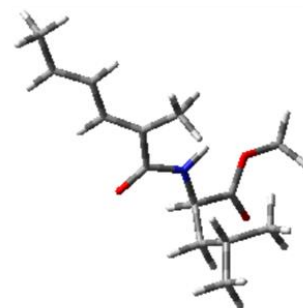
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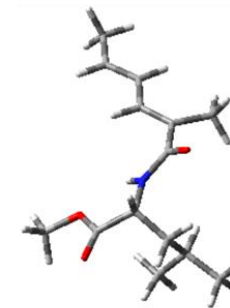
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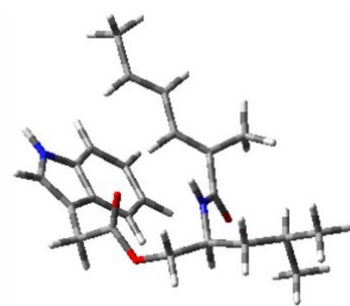


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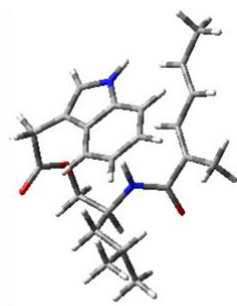


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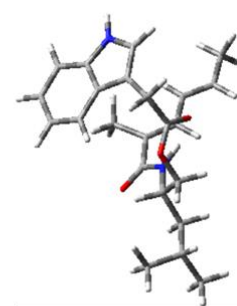
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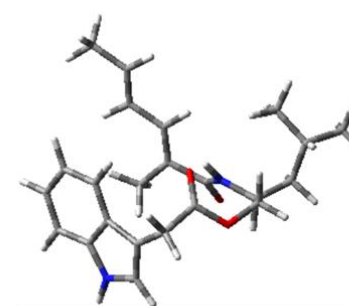
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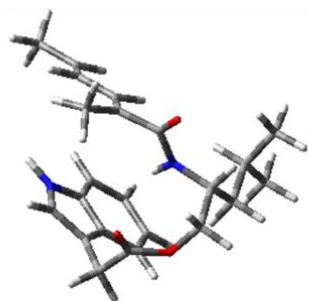


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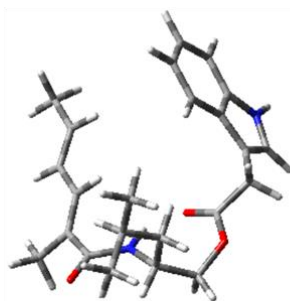


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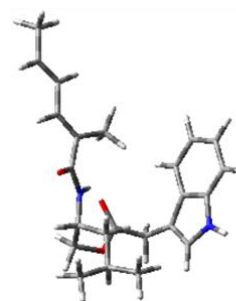
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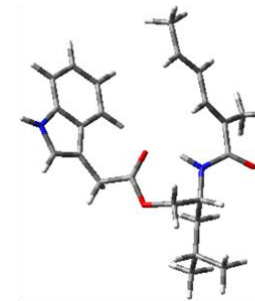
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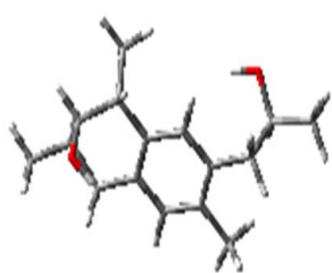


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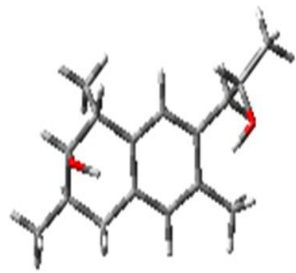


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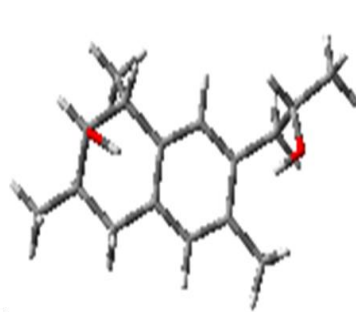
(1*R*,2*R*,10*R*,15*S*)-5



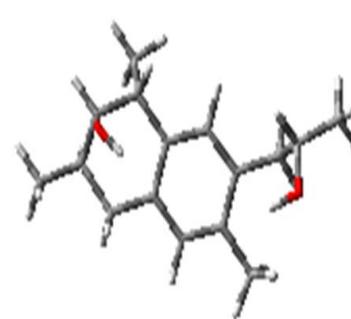
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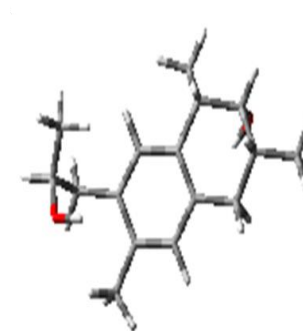
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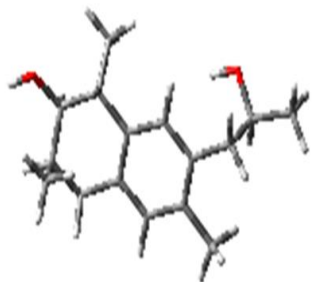
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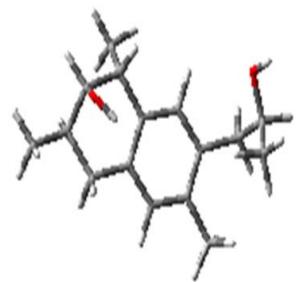
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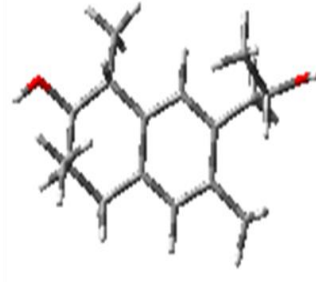
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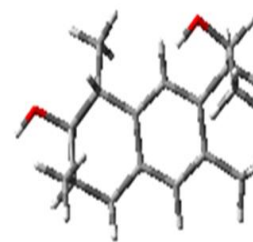
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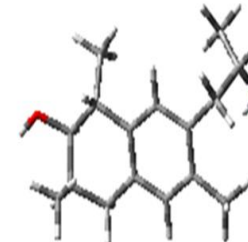
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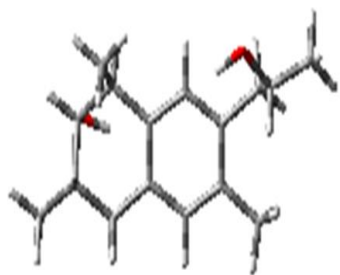


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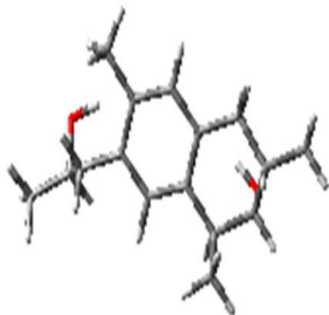


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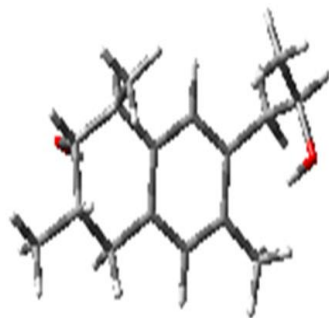
(1*S*,2*S*,10*S*,15*R*)-5



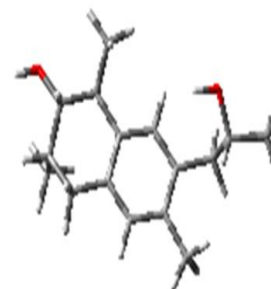
1(64.21%)



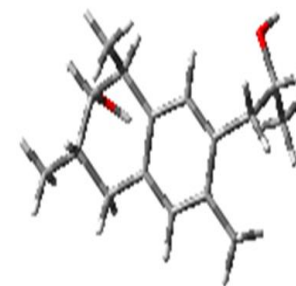
2(22.9%)



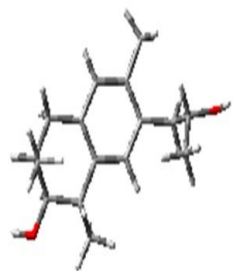
3(3.03%)



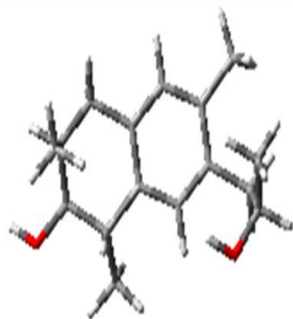
4(2.81%)



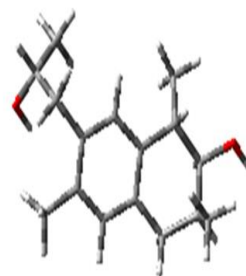
5(3.32%)



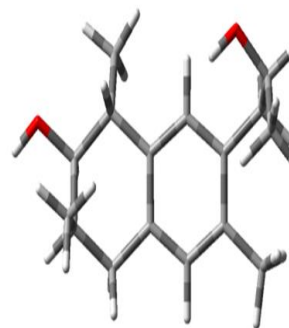
6(2.91%)



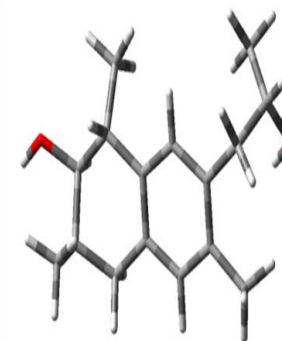
7(0.45%)



8(0.17%)



9(0.1%)

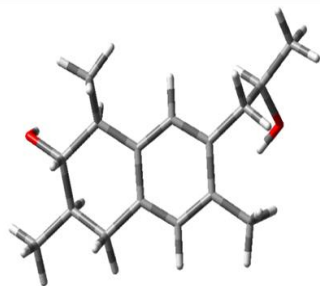


10(0.1%)

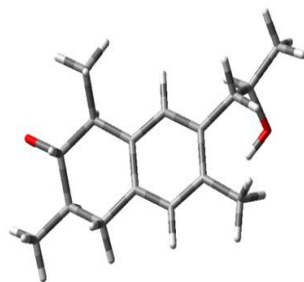
(1*R*,2*S*,10*R*,15*S*)-5



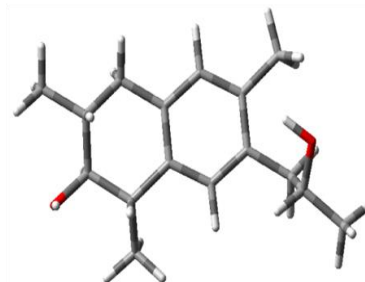
1(73.17%)



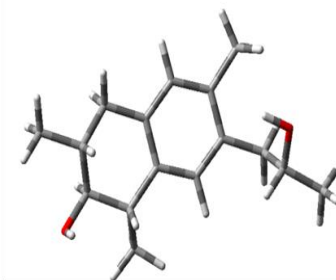
2(10.34%)



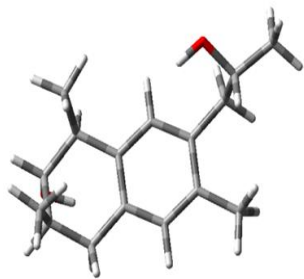
3(9.3%)



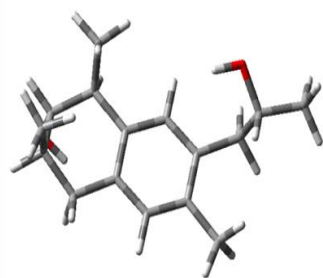
4(5.47%)



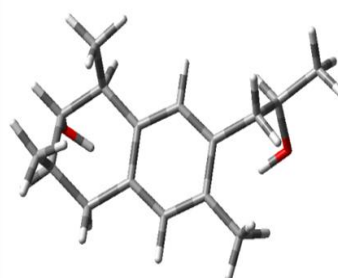
5(1.4%)



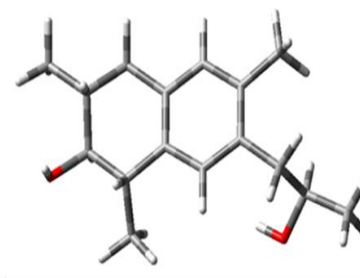
6(0.13%)



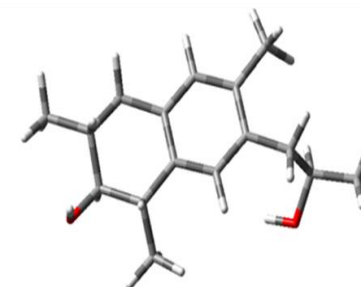
7(0.11%)



8(0.06%)

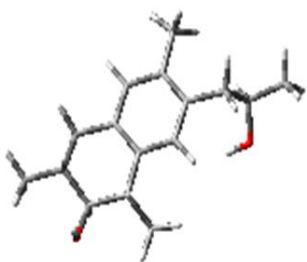


9(0.01%)

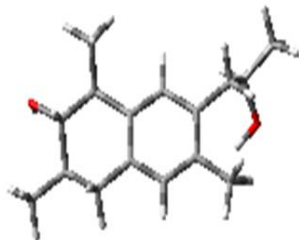


10(0.01%)

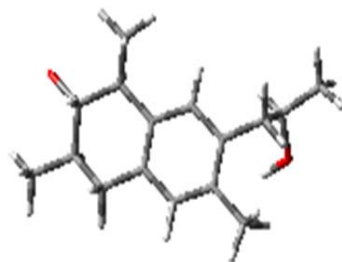
(1*S*,2*R*,10*S*,15*R*)-5



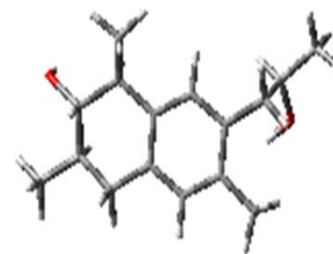
1(71%)



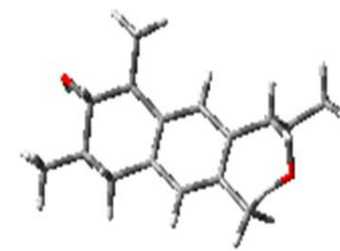
2(9.31%)



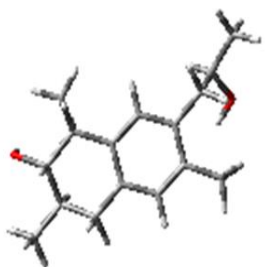
3(8.02%)



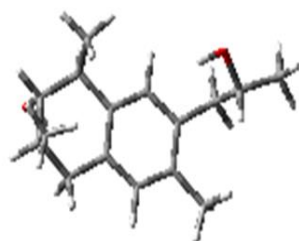
4(7.6%)



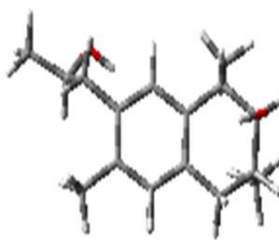
5(3.43%)



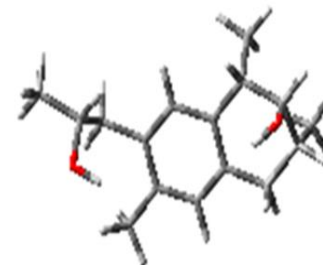
6(0.35%)



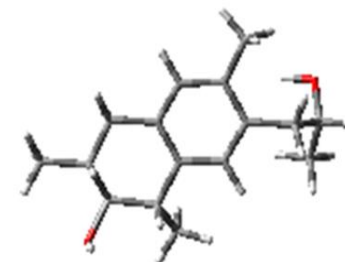
7(0.14%)



8(0.1%)

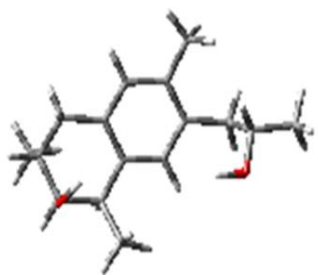


9(0.04%)

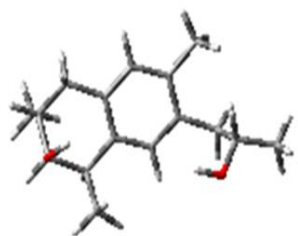


10(0.01%)

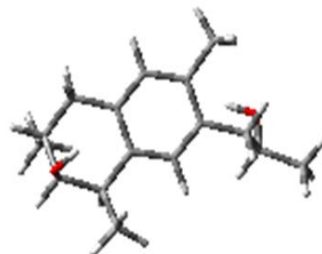
(1*S*,2*R*,10*R*,15*S*)-5



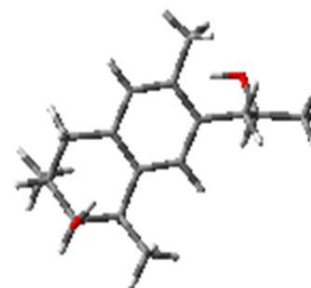
1(50.65%)



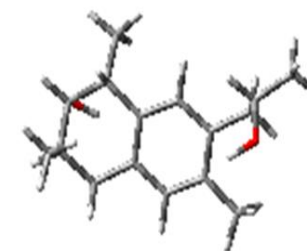
2(41.39%)



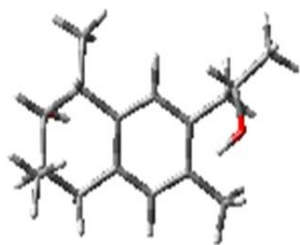
3(4%)



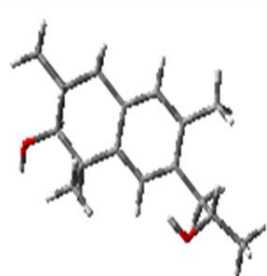
4(1.14%)



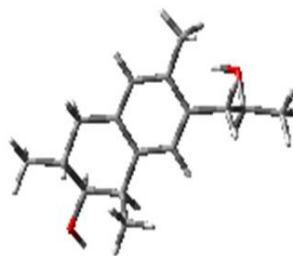
5(0.93%)



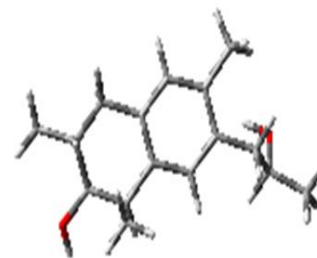
6(0.84%)



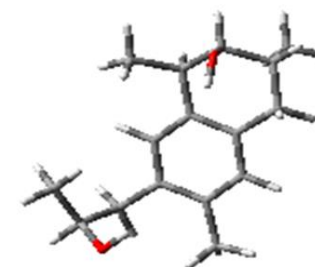
7(0.41%)



8(0.29%)

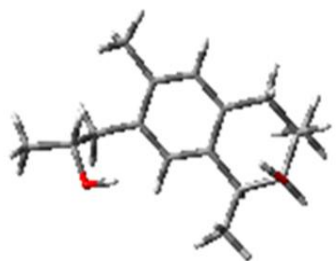


9(0.25%)

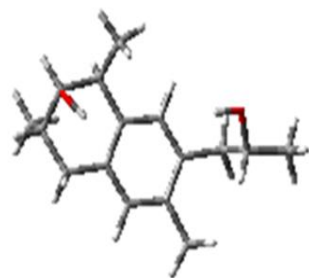


10(0.01%)

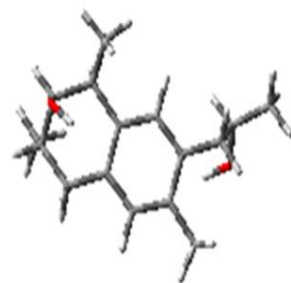
(1*R*,2*S*,10*S*,15*R*)-5



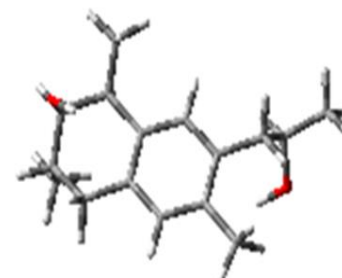
1(75.37%)



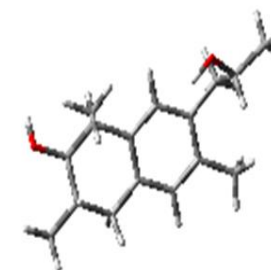
2(13.2%)



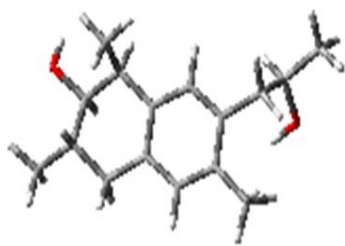
3(7.64%)



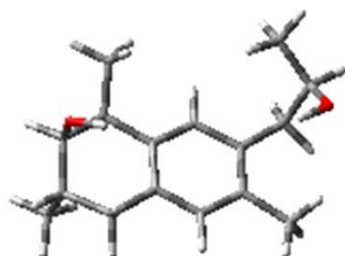
4(2.68%)



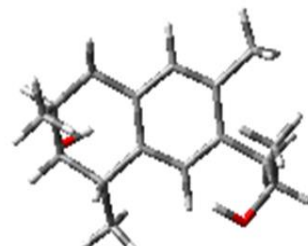
5(0.58%)



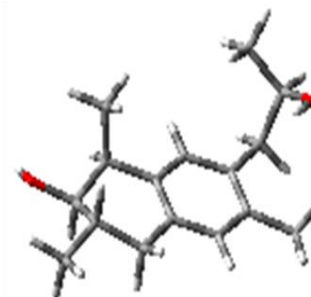
6(0.27%)



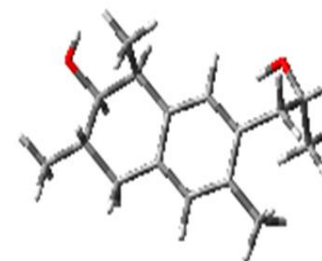
7(0.16%)



8(0.08%)

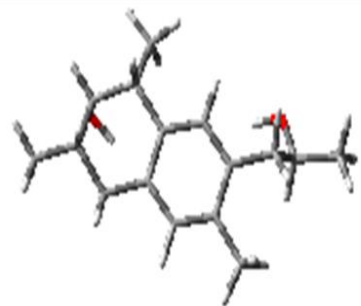


9(0.01%)

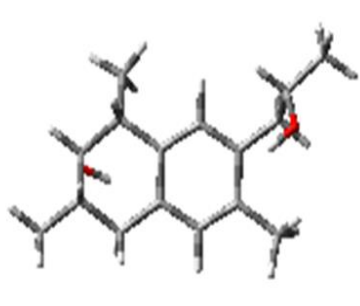


10(0.01%)

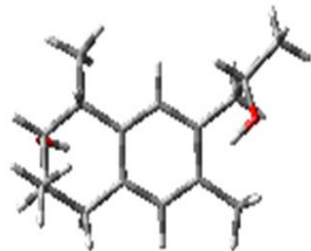
(1*S*,2*S*,10*R*,15*S*)-5



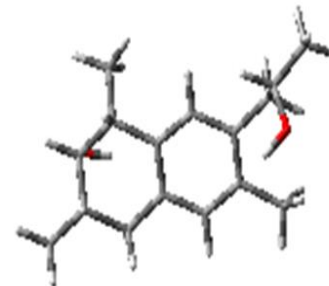
1(59.46%)



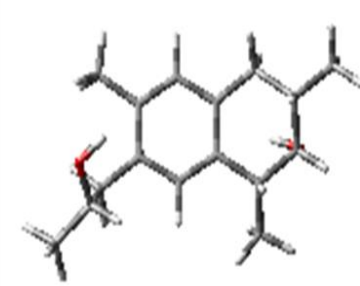
2(26.21%)



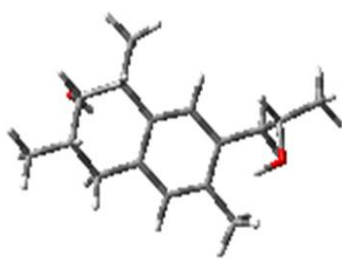
3(3.96%)



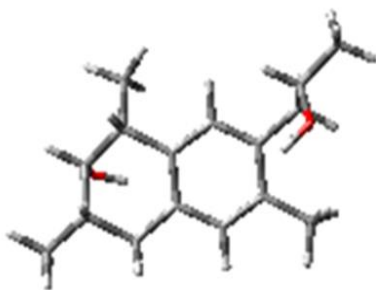
4(2.44%)



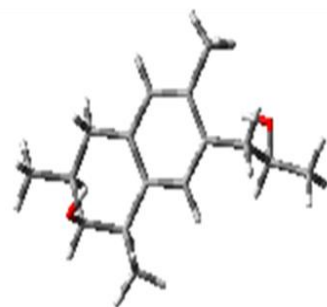
5(4.38%)



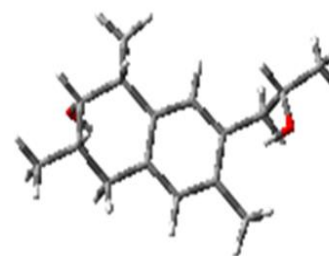
6(2.71%)



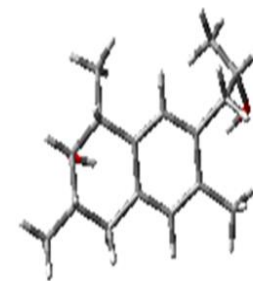
7(0.43%)



8(0.33%)

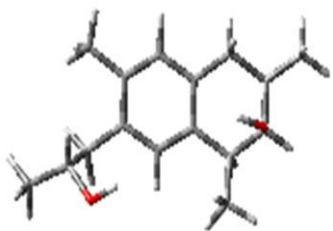


9(0.07%)

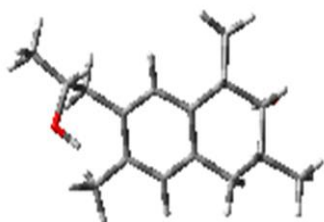


10(0.01%)

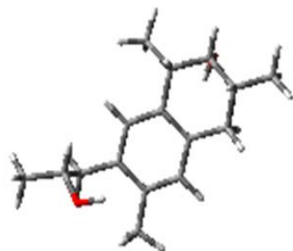
(1*R*,2*R*,10*S*,15*R*)-5



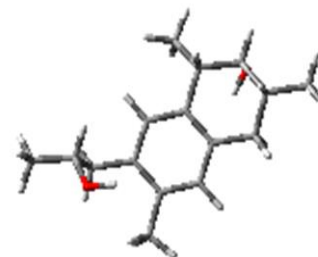
1(61.33%)



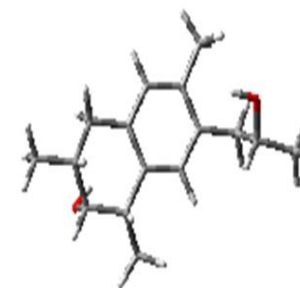
2(24.34%)



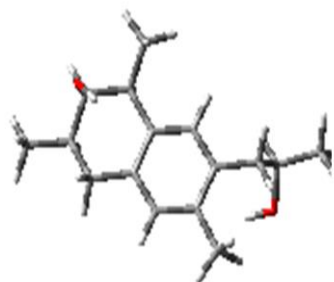
3(5.83%)



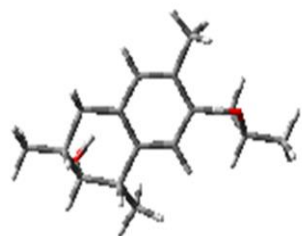
4(4.25%)



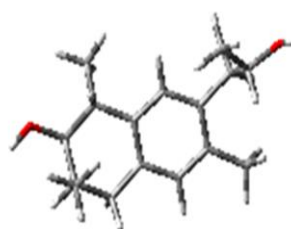
5(2.51%)



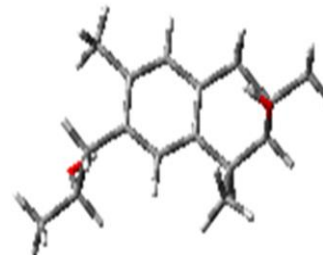
6(0.84%)



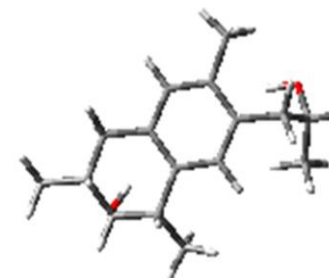
7(0.55%)



8(0.21%)

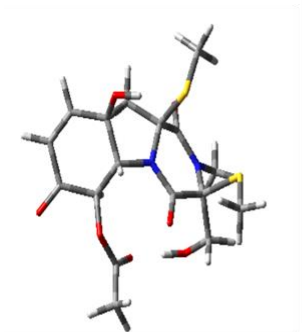


9(0.09%)

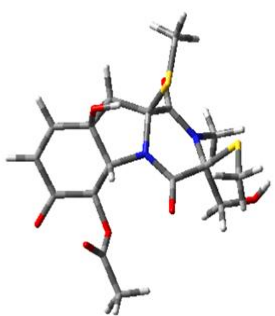


10(0.05%)

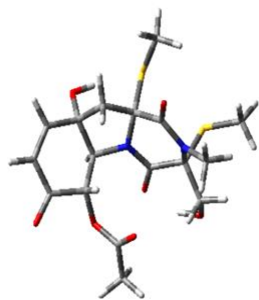
(3*R*,6*S*,7*S*,11*S*,13*R*)-16



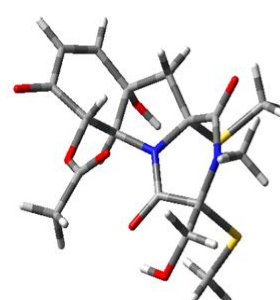
1(48.26%)



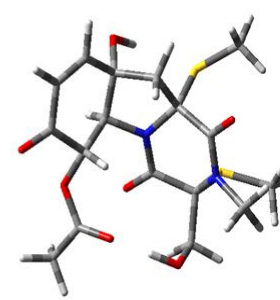
2(41.99%)



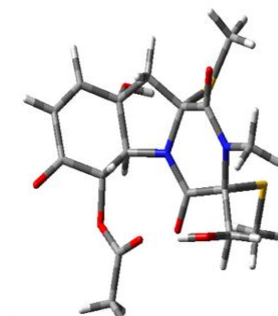
3(5.03%)



4(3.94%)

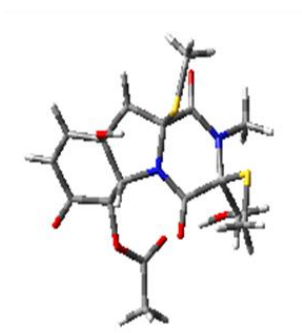


5(0.71%)

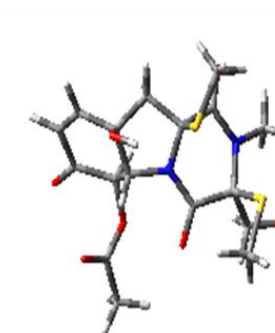


6(0.07%)

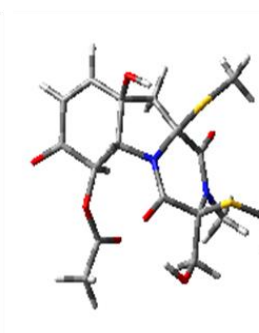
(3*S*,6*R*,7*R*,11*R*,13*S*)-16



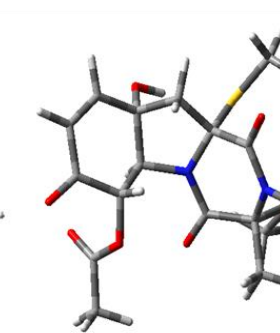
1(49.12%)



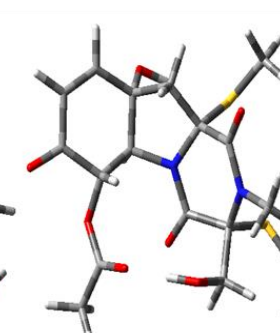
2(42.85%)



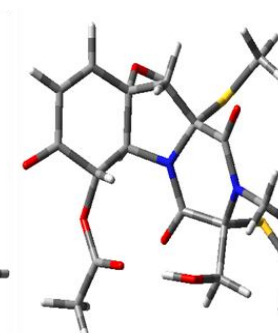
3(4.17%)



4(3.08%)

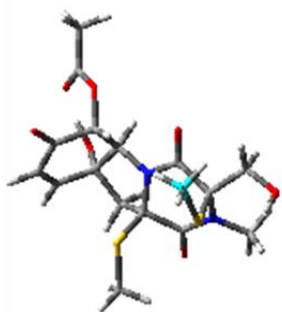


5(0.57%)

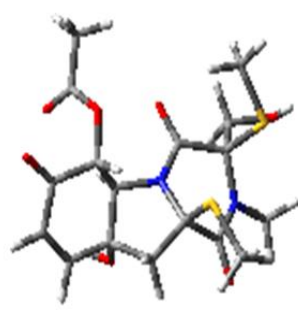


6(0.21%)

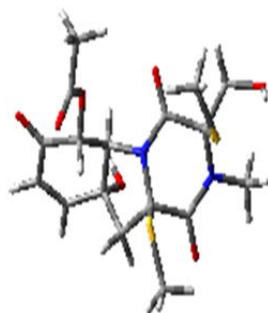
(3*R*,6*R*,7*R*,11*R*,13*R*)-16



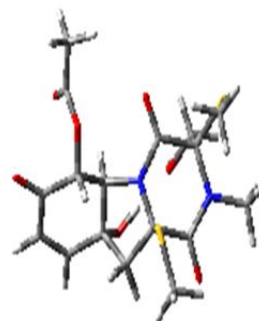
1(49.52%)



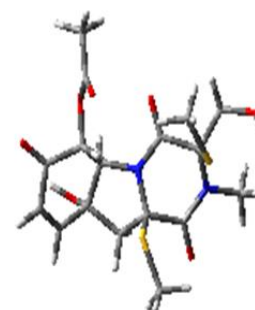
2(45.31%)



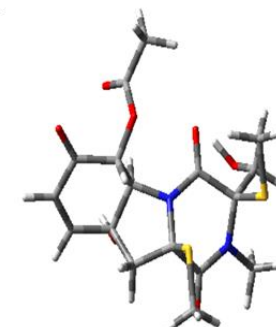
3(3.44%)



4(1.24%)

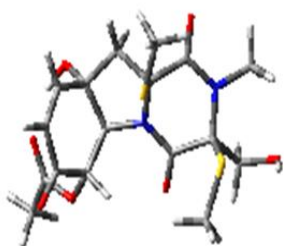


5(0.41%)

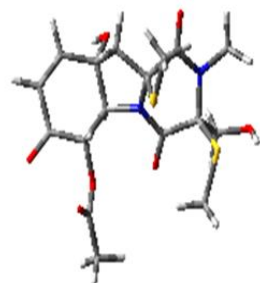


6(0.08%)

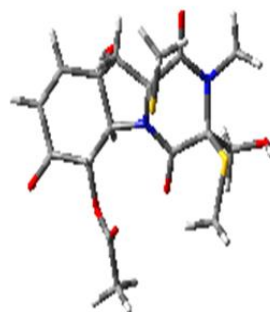
(3*S*,6*S*,7*S*,11*S*,13*S*)-16



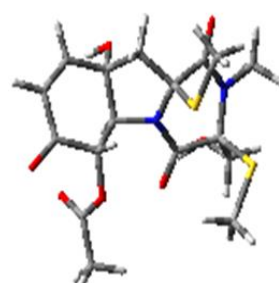
1(50.21%)



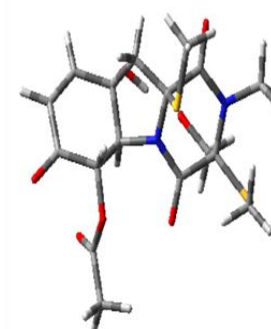
2(43.00%)



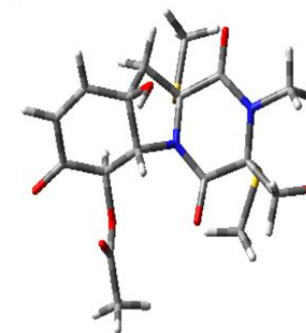
3(4.44%)



4(1.45%)

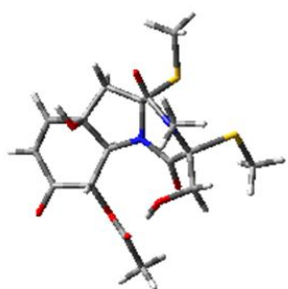


5(0.62%)

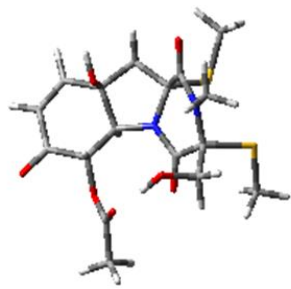


6(0.28%)

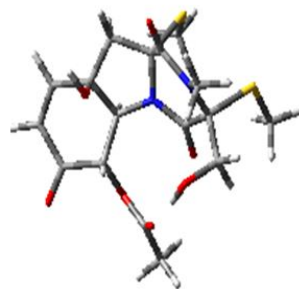
(3*R*,6*S*,7*S*,11*R*,13*R*)-16



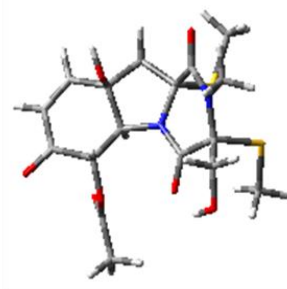
1(49.64%)



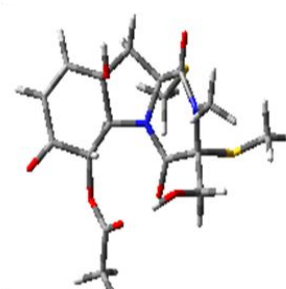
2(45.19%)



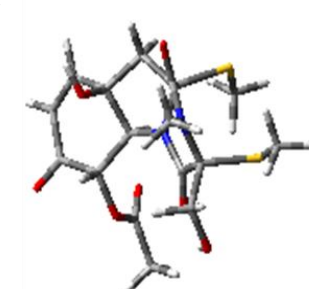
3(3.56%)



4(1.12%)

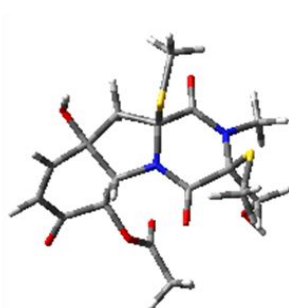


5(0.51%)

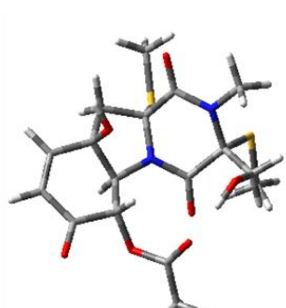


6(0.02%)

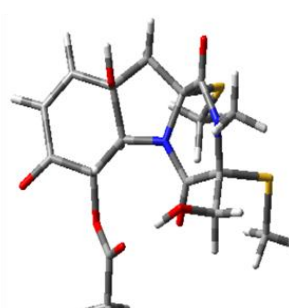
(3*S*,6*R*,7*R*,11*S*,13*S*)-16



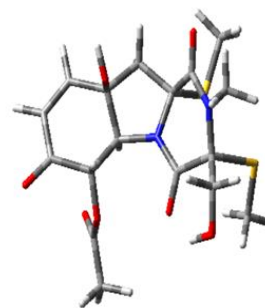
1(47.53%)



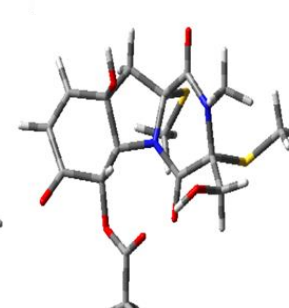
2(47.38%)



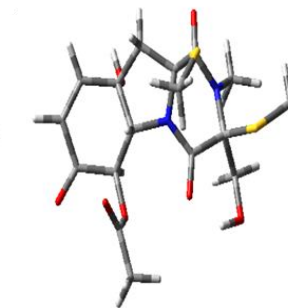
3(2.58%)



4(2.58%)

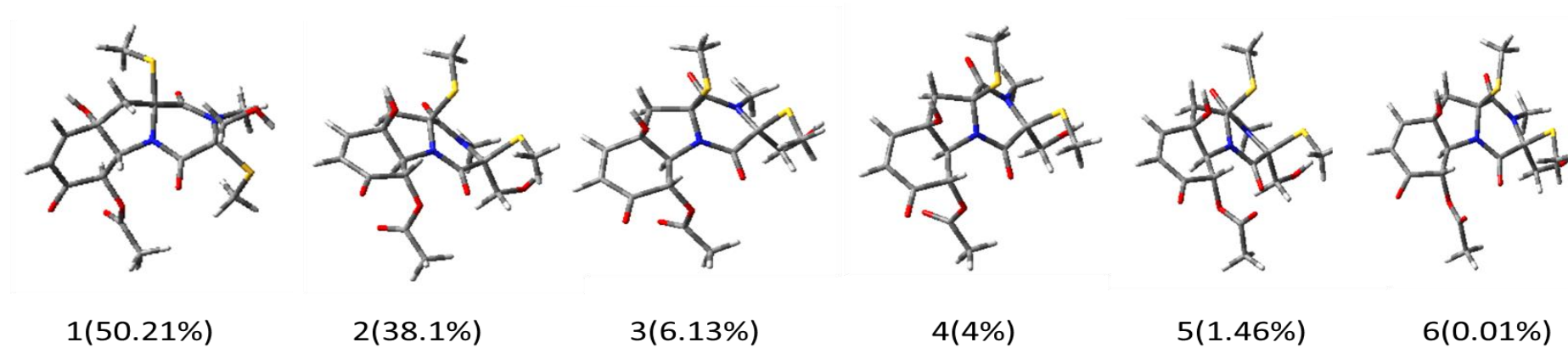


5(0.81%)



6(0.61%)

(3*R*,6*R*,7*R*,11*S*,13*R*)-16



(3*S*,6*S*,7*S*,11*R*,13*S*)-16

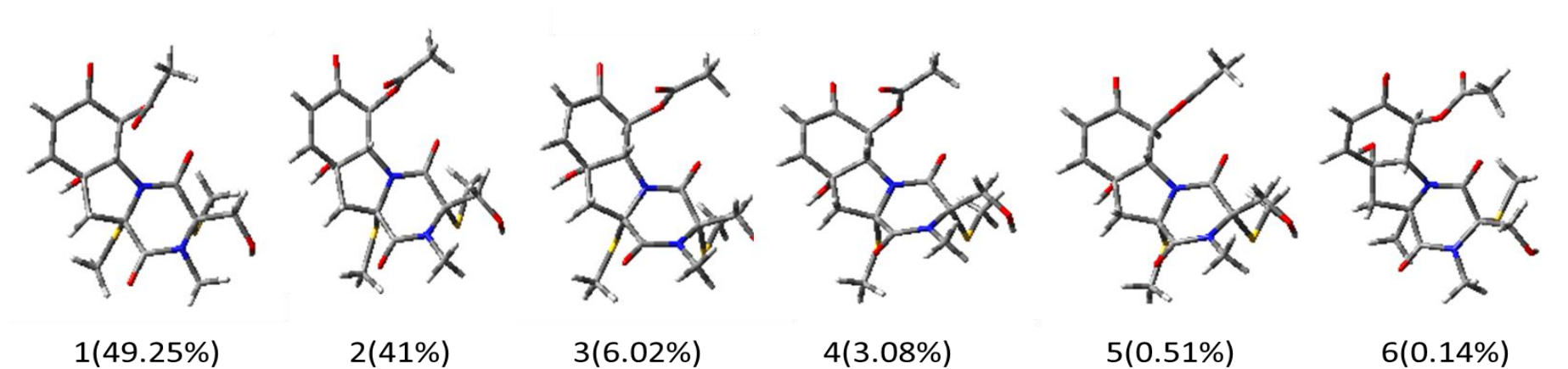


Figure S2. HR-ESI-MS spectrum of dichotomocej A (1)

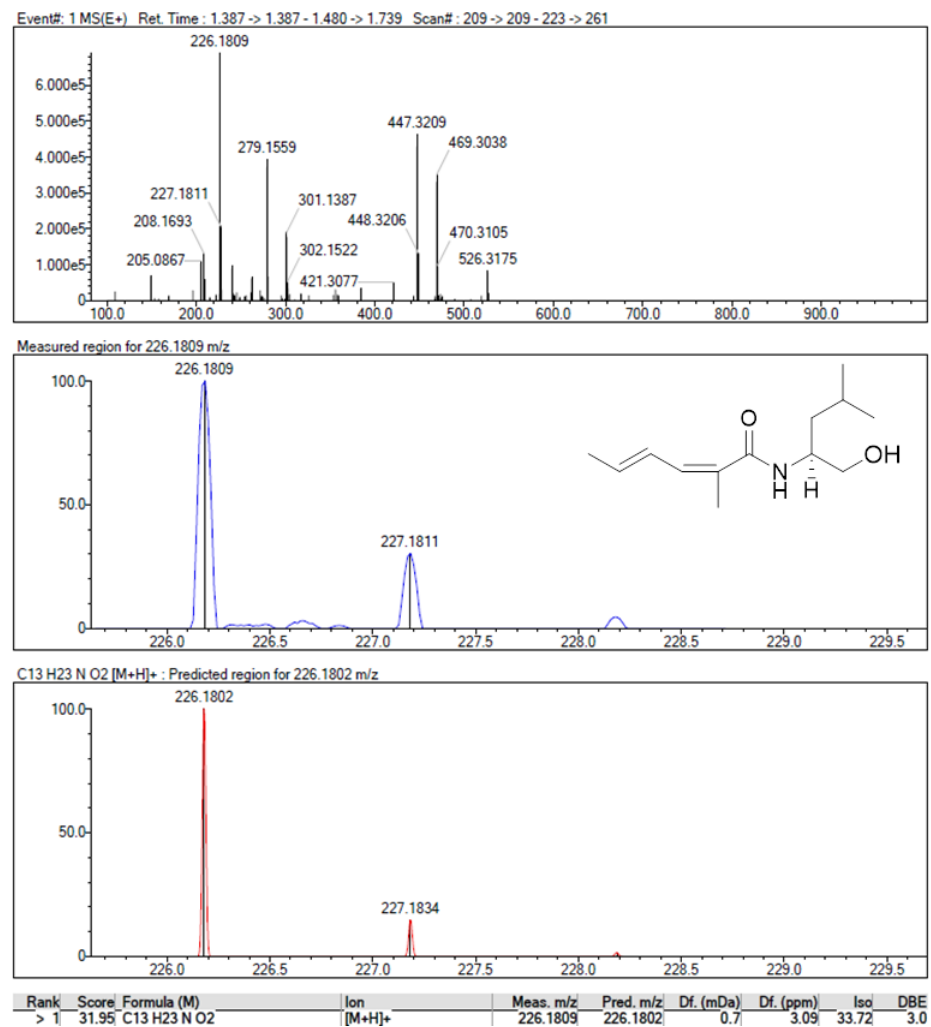


Figure S3. ^1H NMR spectrum of dichotomocej A (1) in CDCl_3 (400MHz)

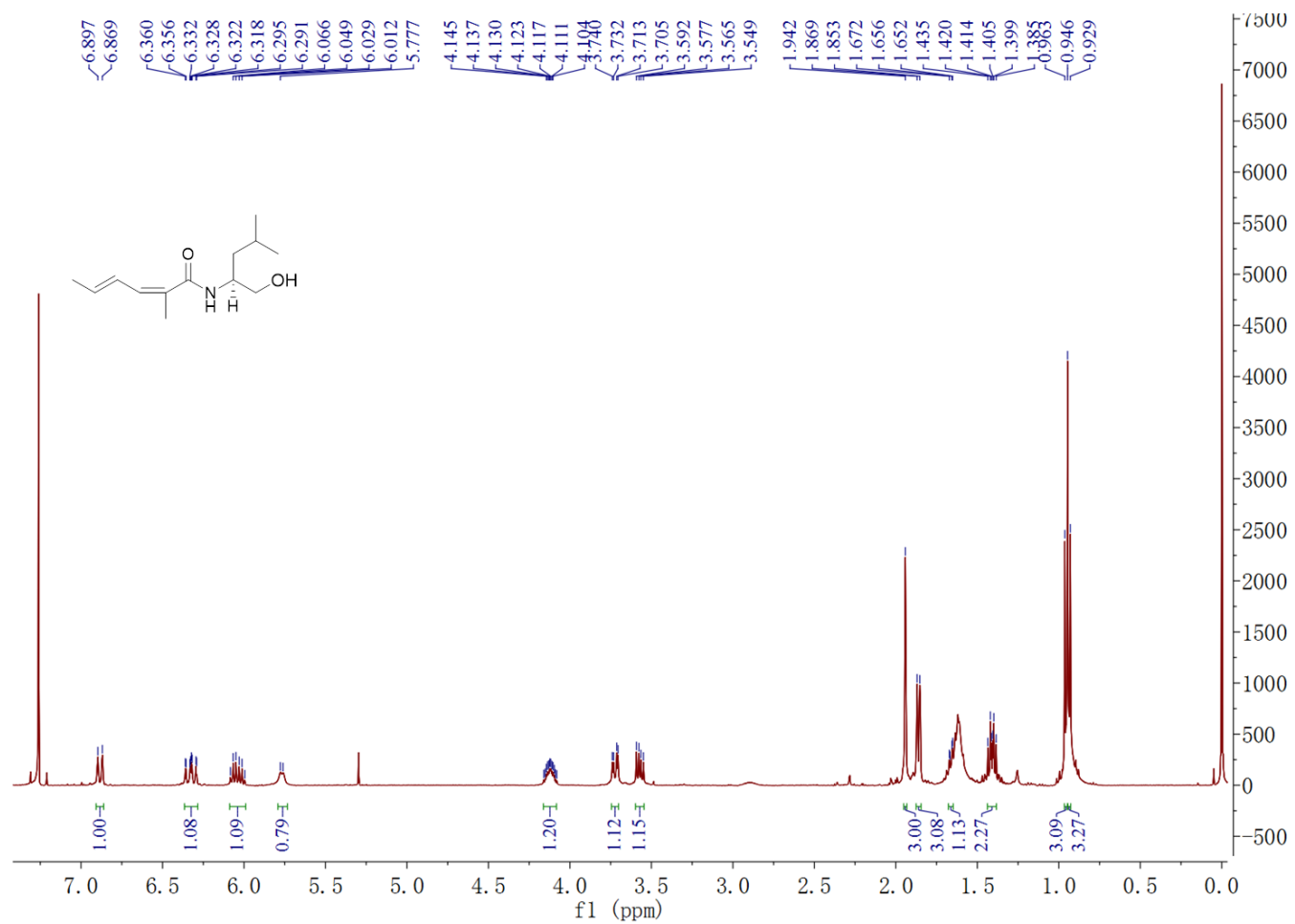


Figure S4. ^{13}C NMR spectrum of dichotomocej A (**1**) in CDCl_3 (100MHz)

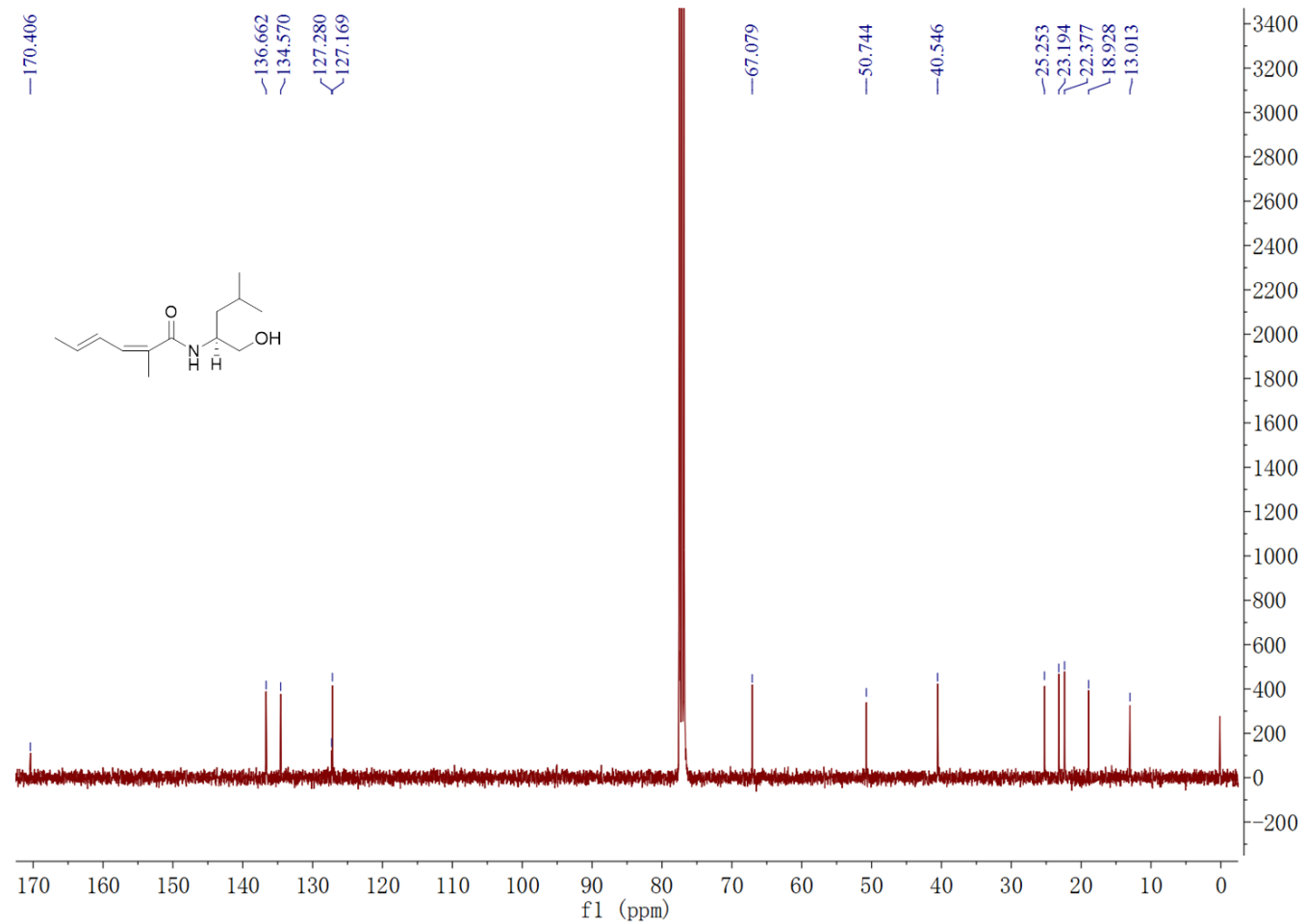


Figure S5. HMQC spectrum of dichotomej A (1) in CDCl₃

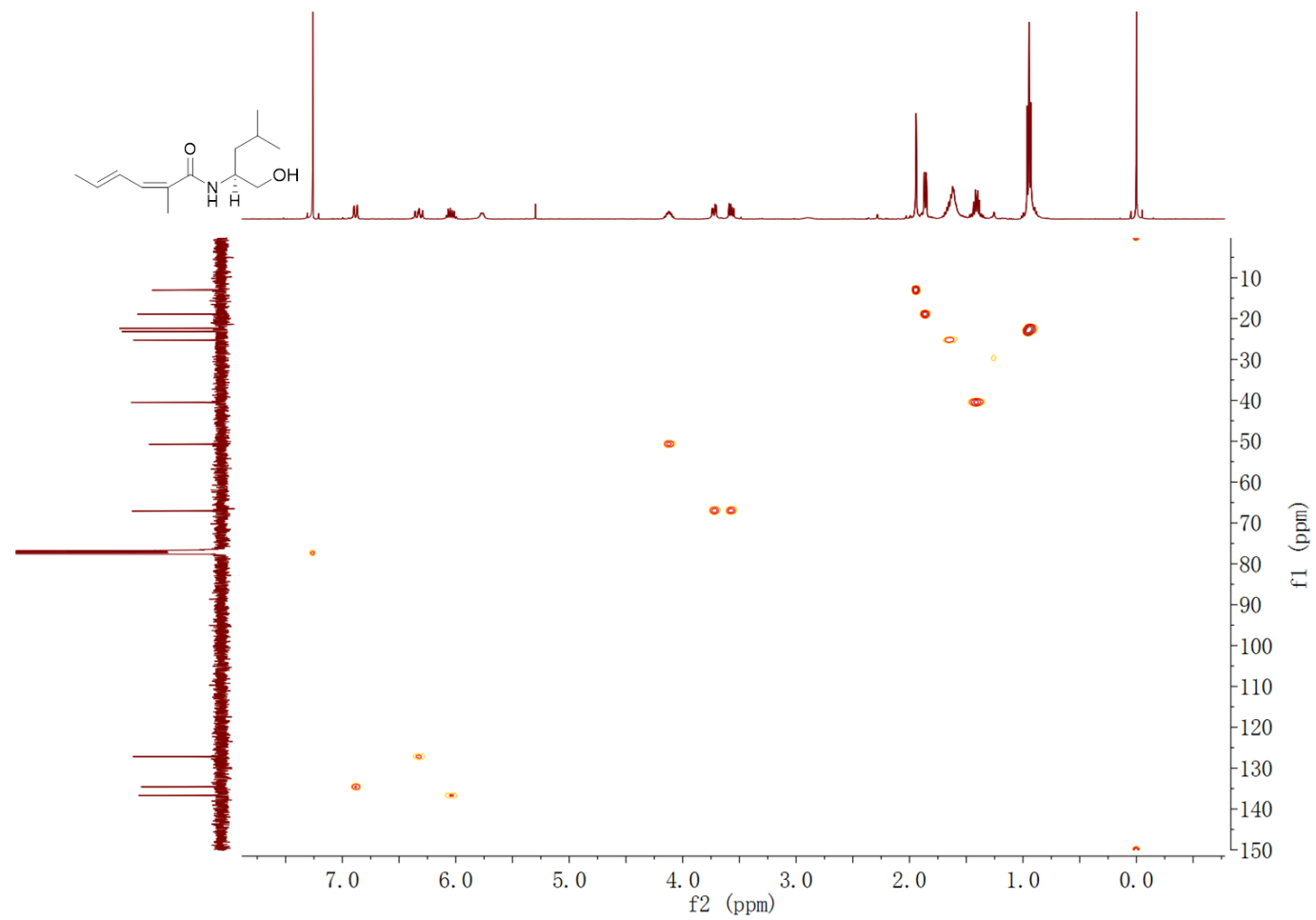


Figure S6. ^1H - ^1H COSY spectrum of dichotomej A (**1**) in CDCl_3

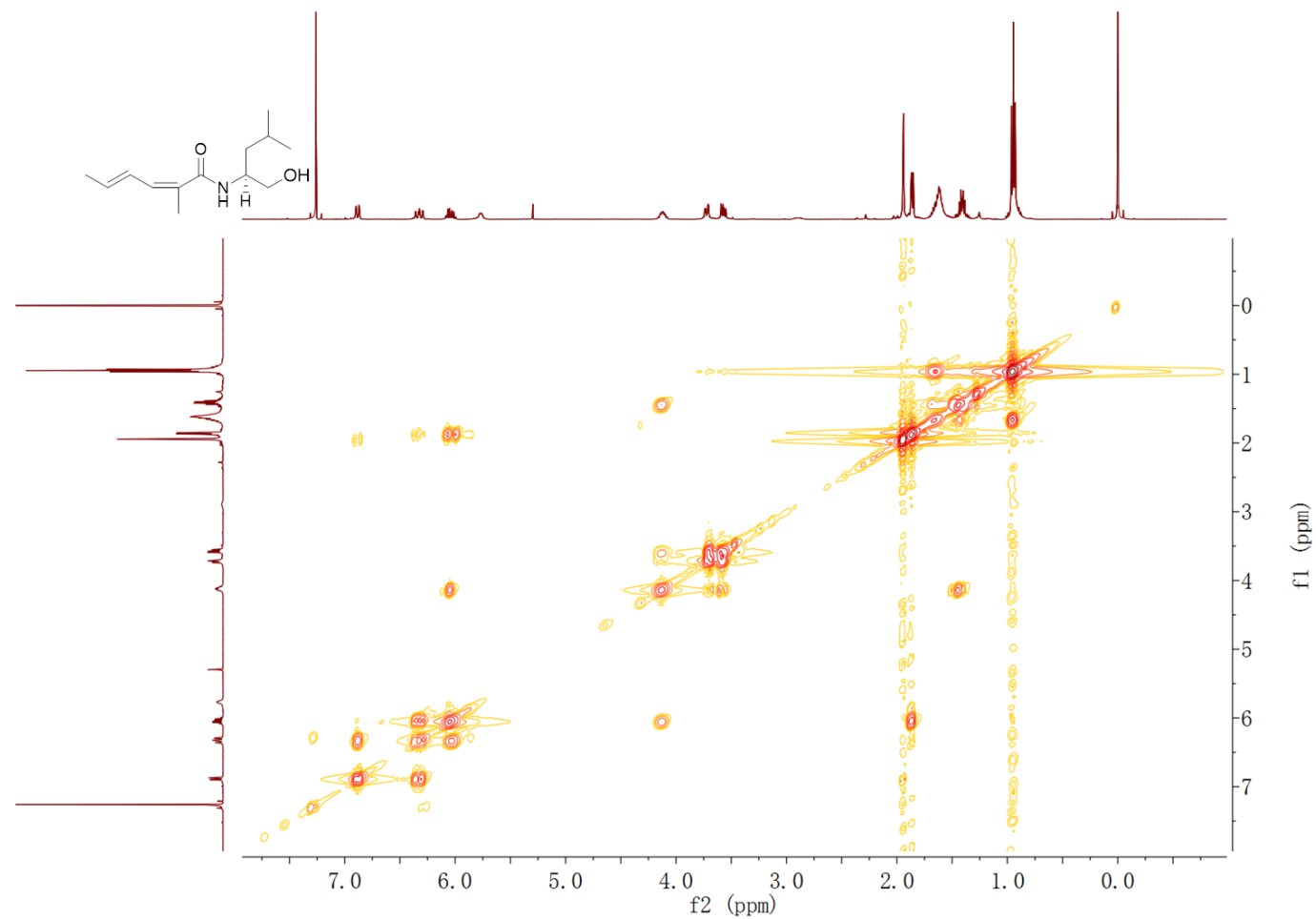


Figure S7. HMBC spectrum of dichotomej A (1) in CDCl₃

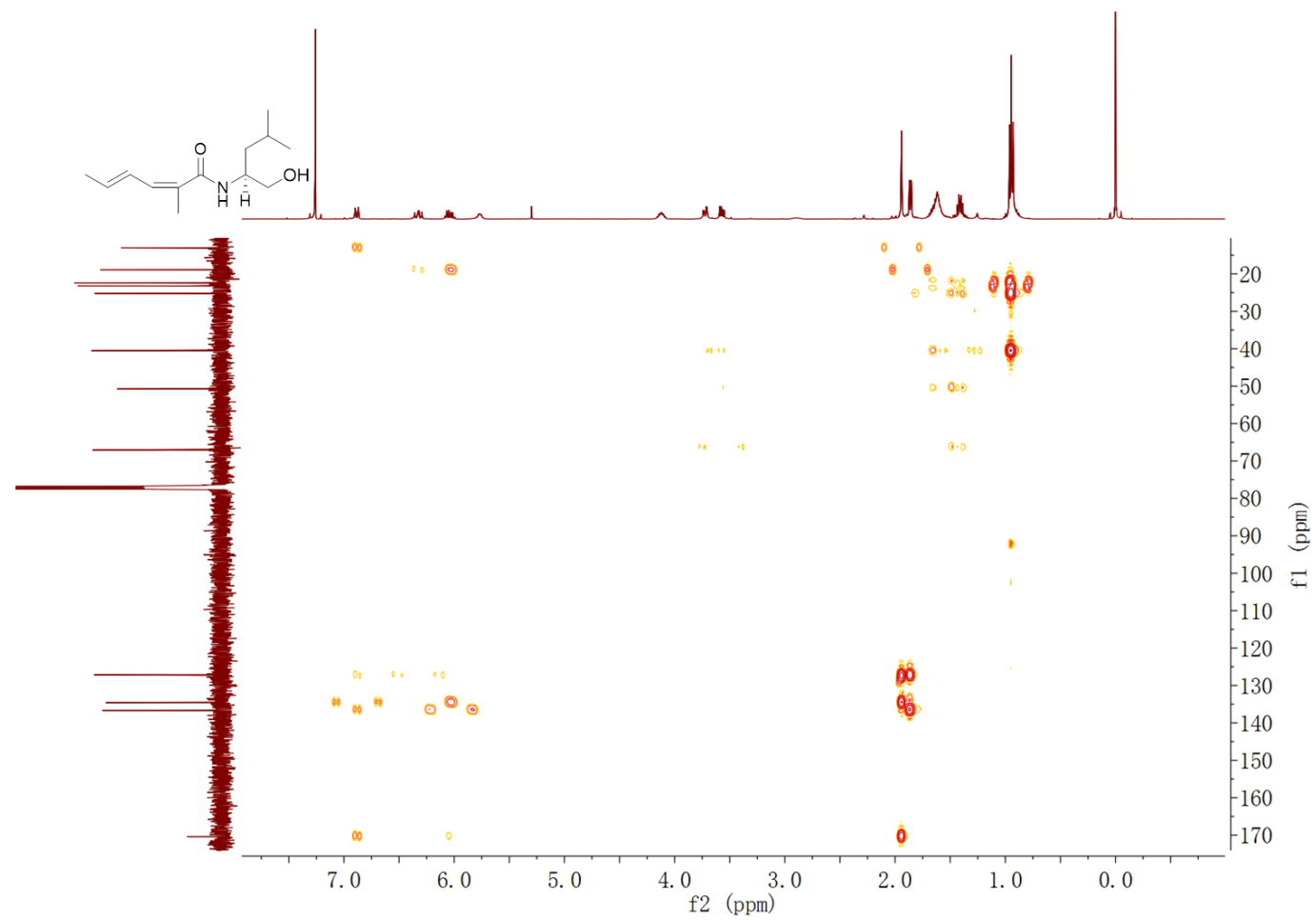


Figure S8. NOESY spectrum of dichotomeoj A (1) in CDCl₃

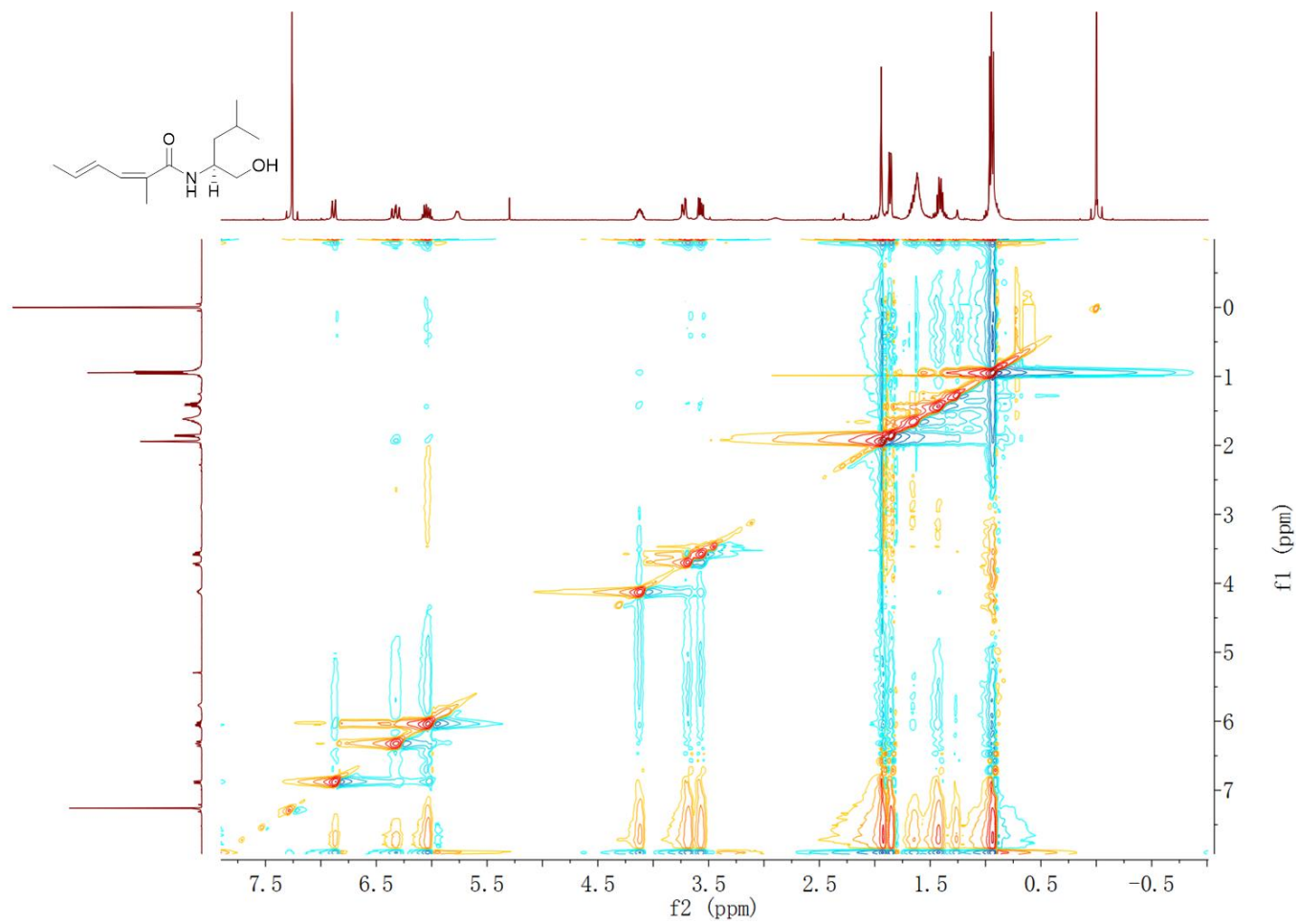


Figure S9. HR-ESI-MS spectrum of dichotomocej B (2)

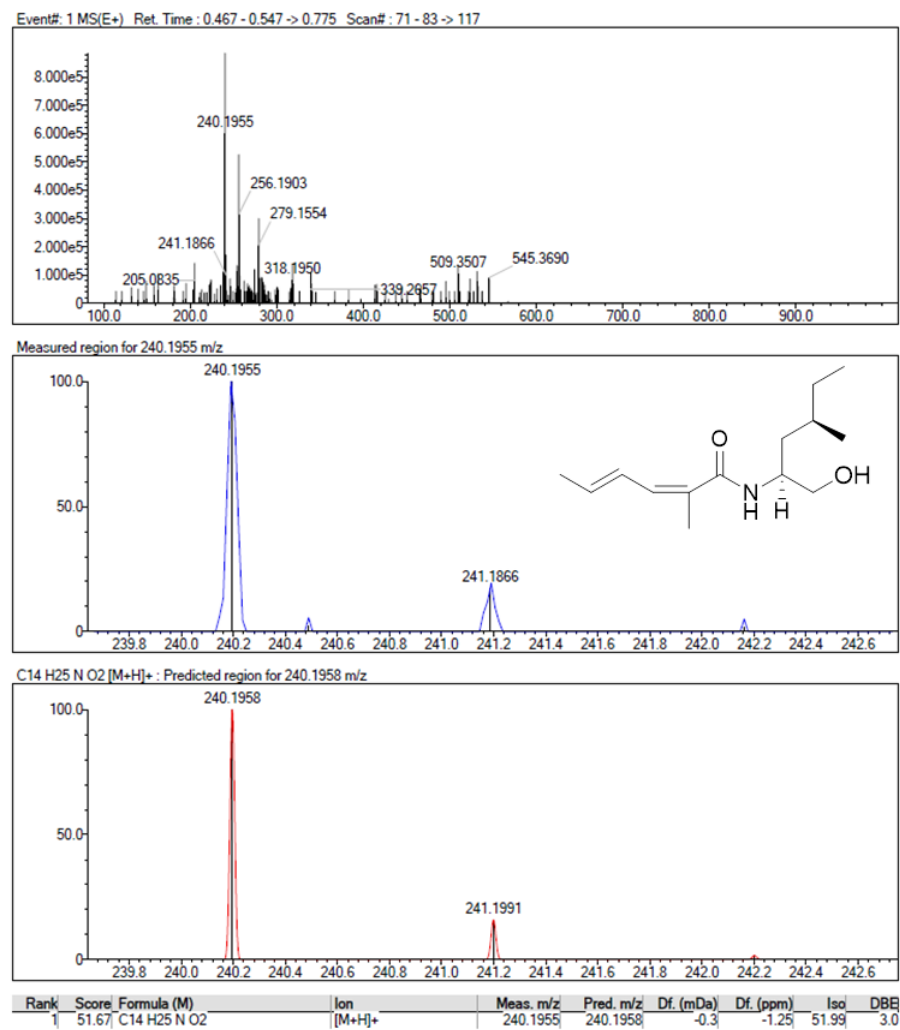


Figure S10. ^1H NMR spectrum of dichotomocej B (**2**) in CDCl_3 (400MHz)

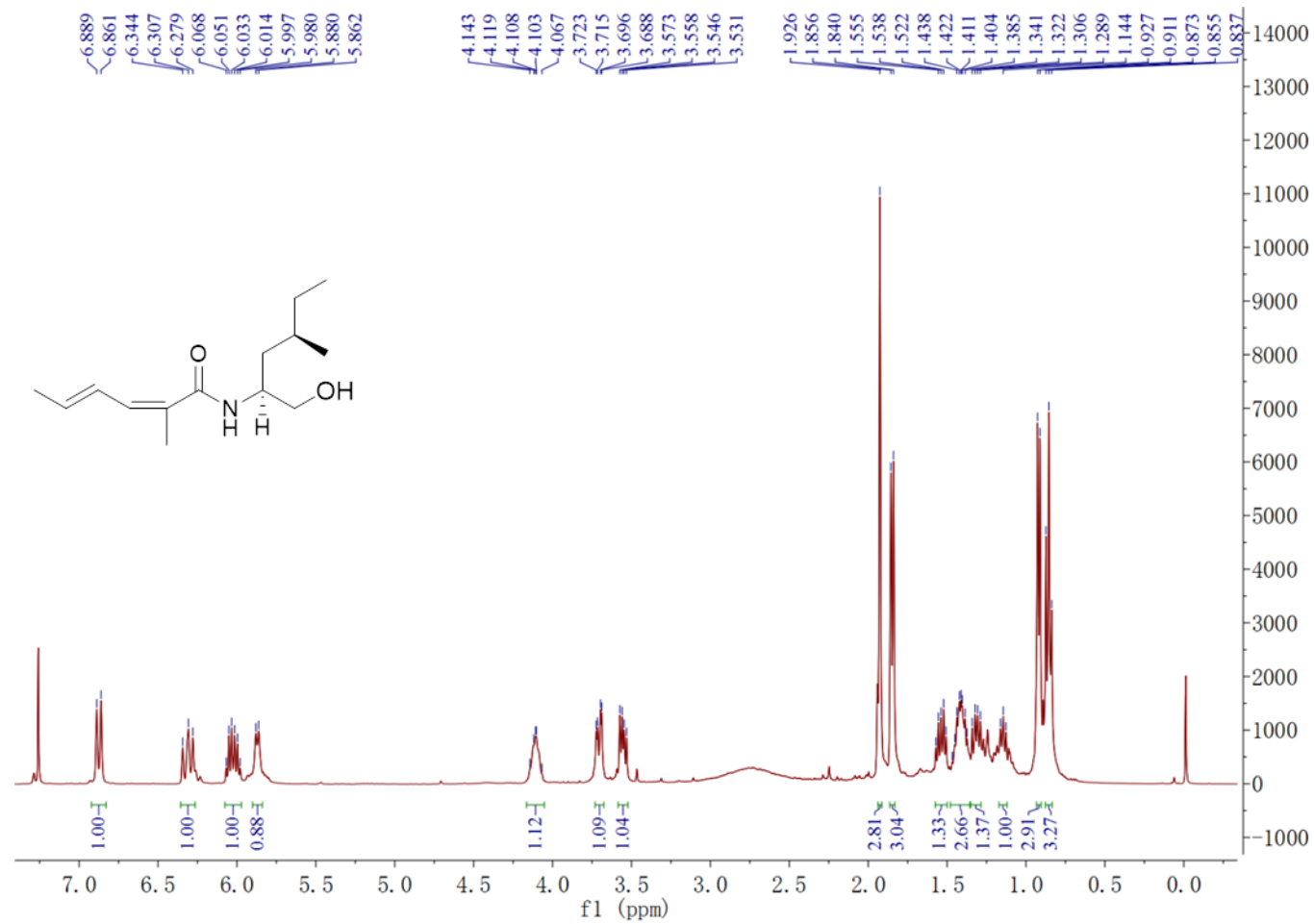


Figure S11. ^{13}C NMR spectrum of dichotomocej B (**2**) in CDCl_3 (100MHz)

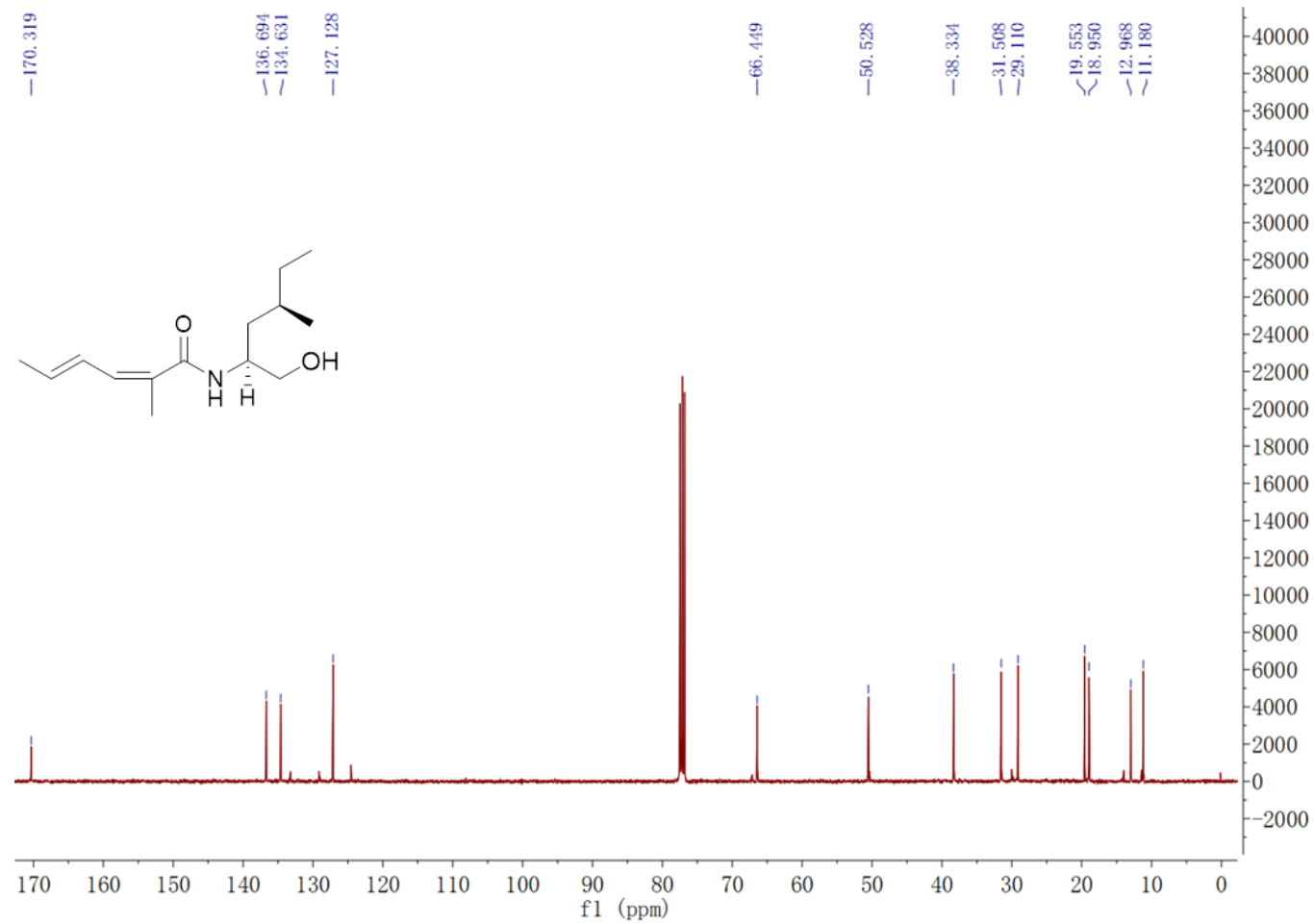


Figure S12. DEPT 135 spectrum of dichotomej B (**2**) in CDCl₃ (100MHz)

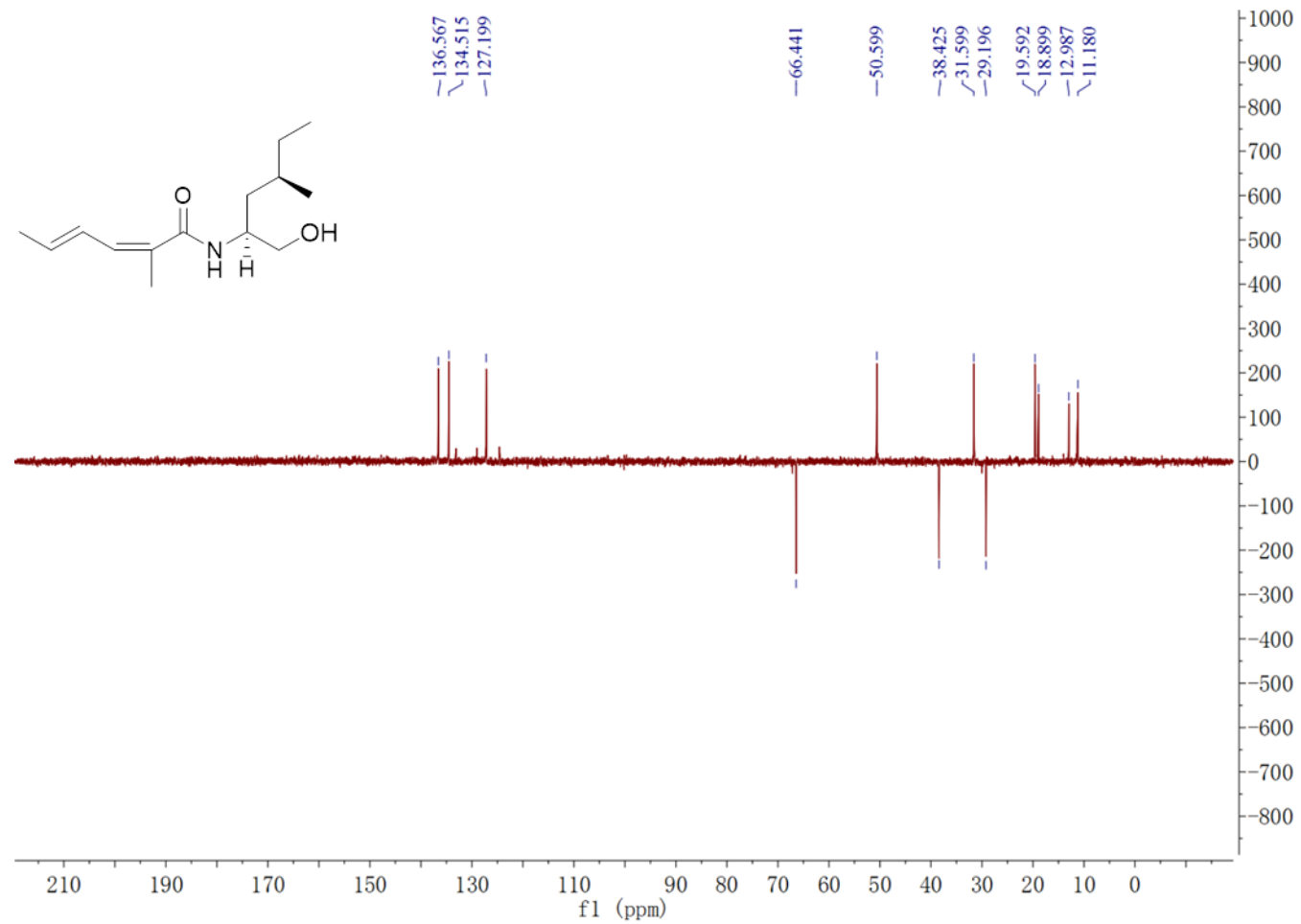


Figure S13. HMQC spectrum of dichotomocej B (**2**) in CDCl₃

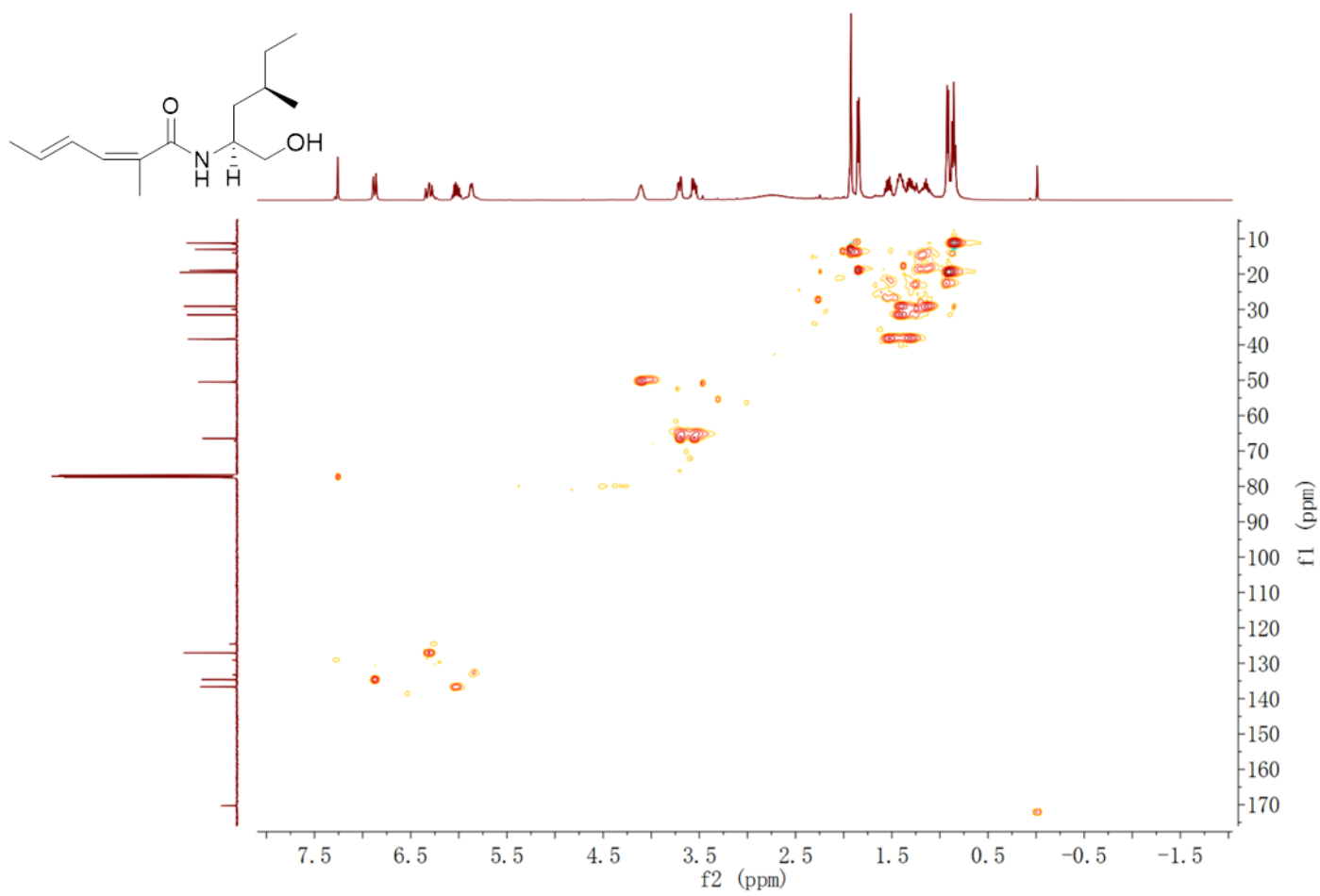


Figure S14. ^1H - ^1H COSY spectrum of dichotomocej B (**2**) in CDCl_3

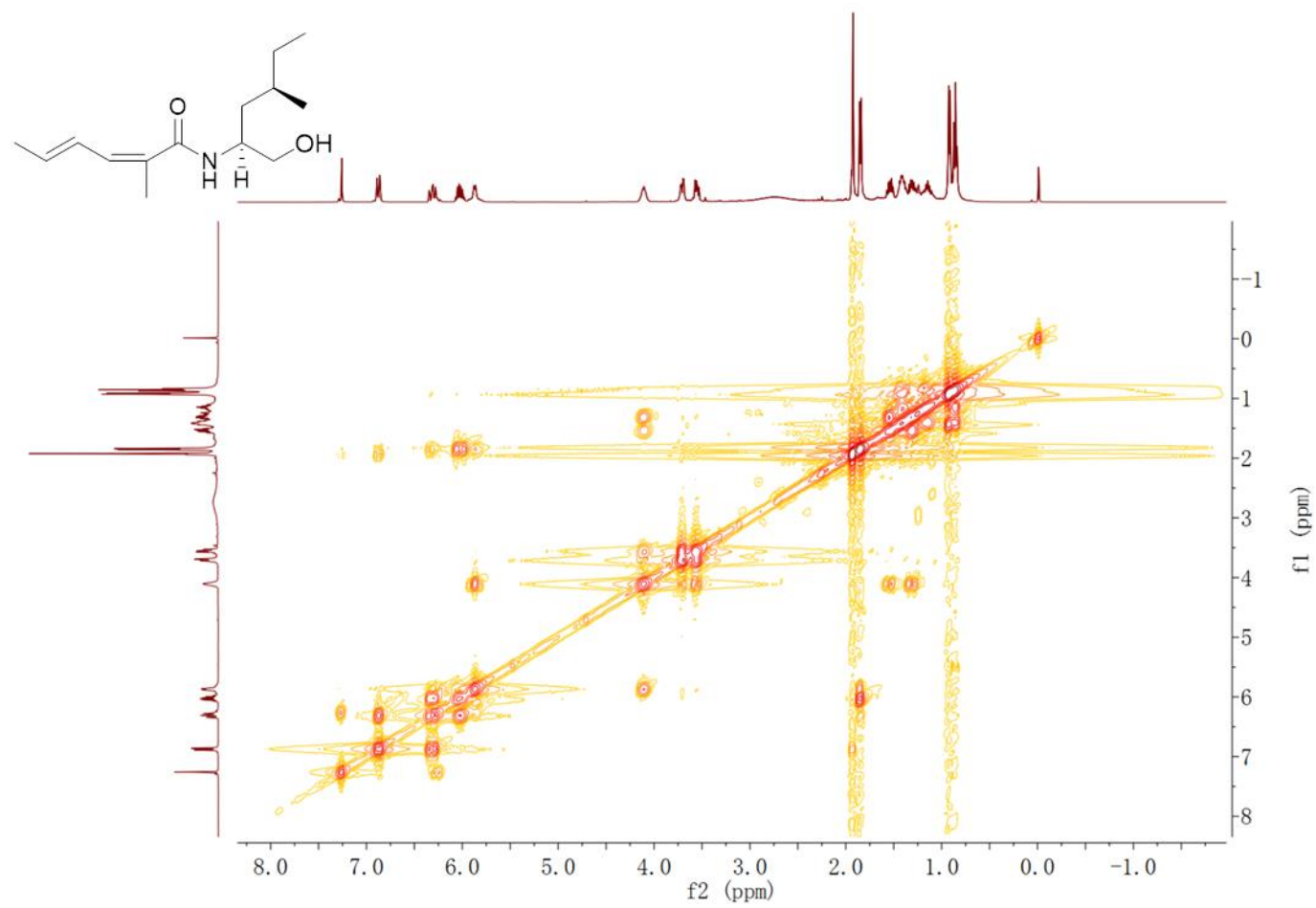


Figure S15. HMBC spectrum of dichotomocej B (2) in CDCl₃

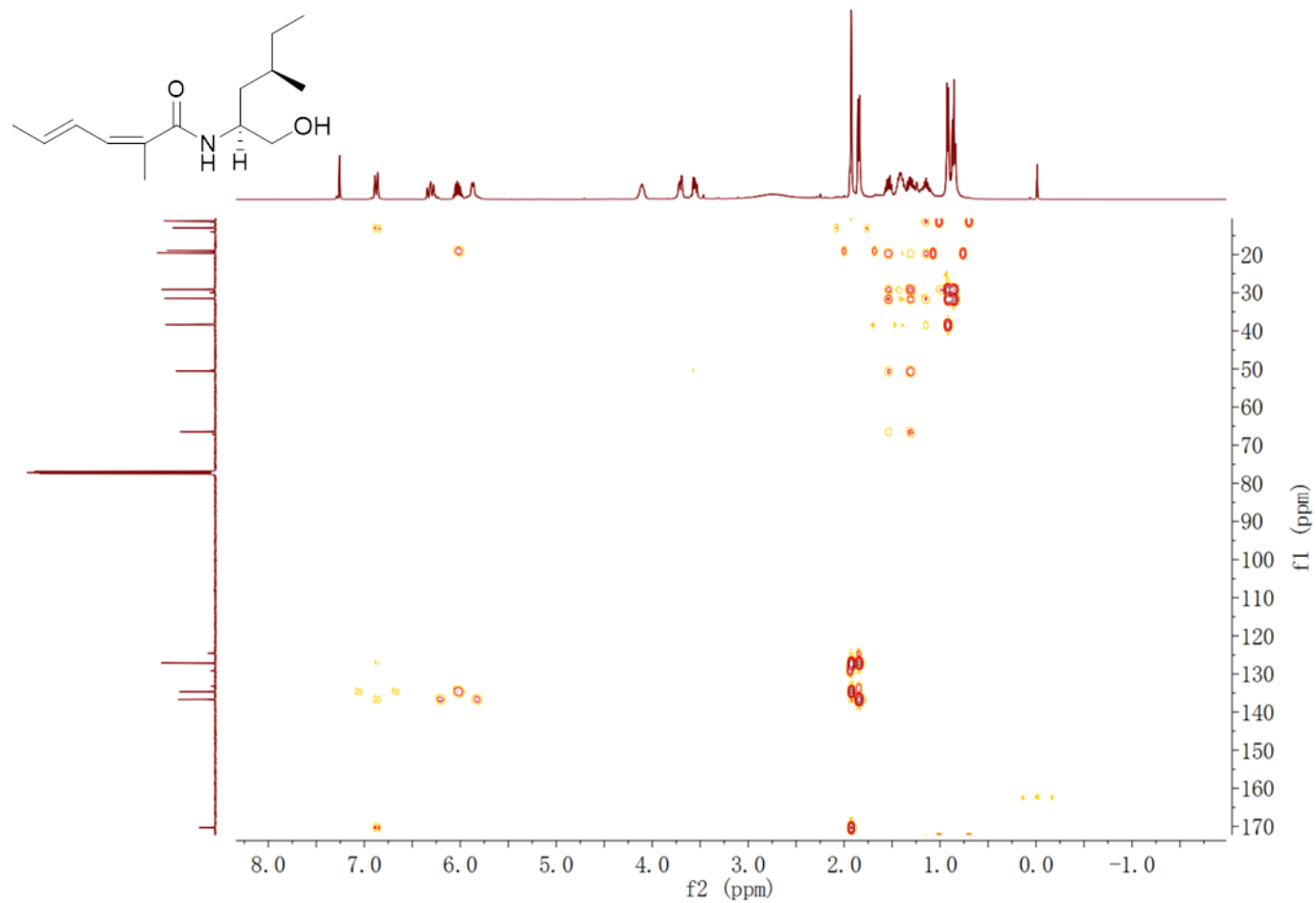


Figure S16. NOESY spectrum of dichotomej B (2) in CDCl₃

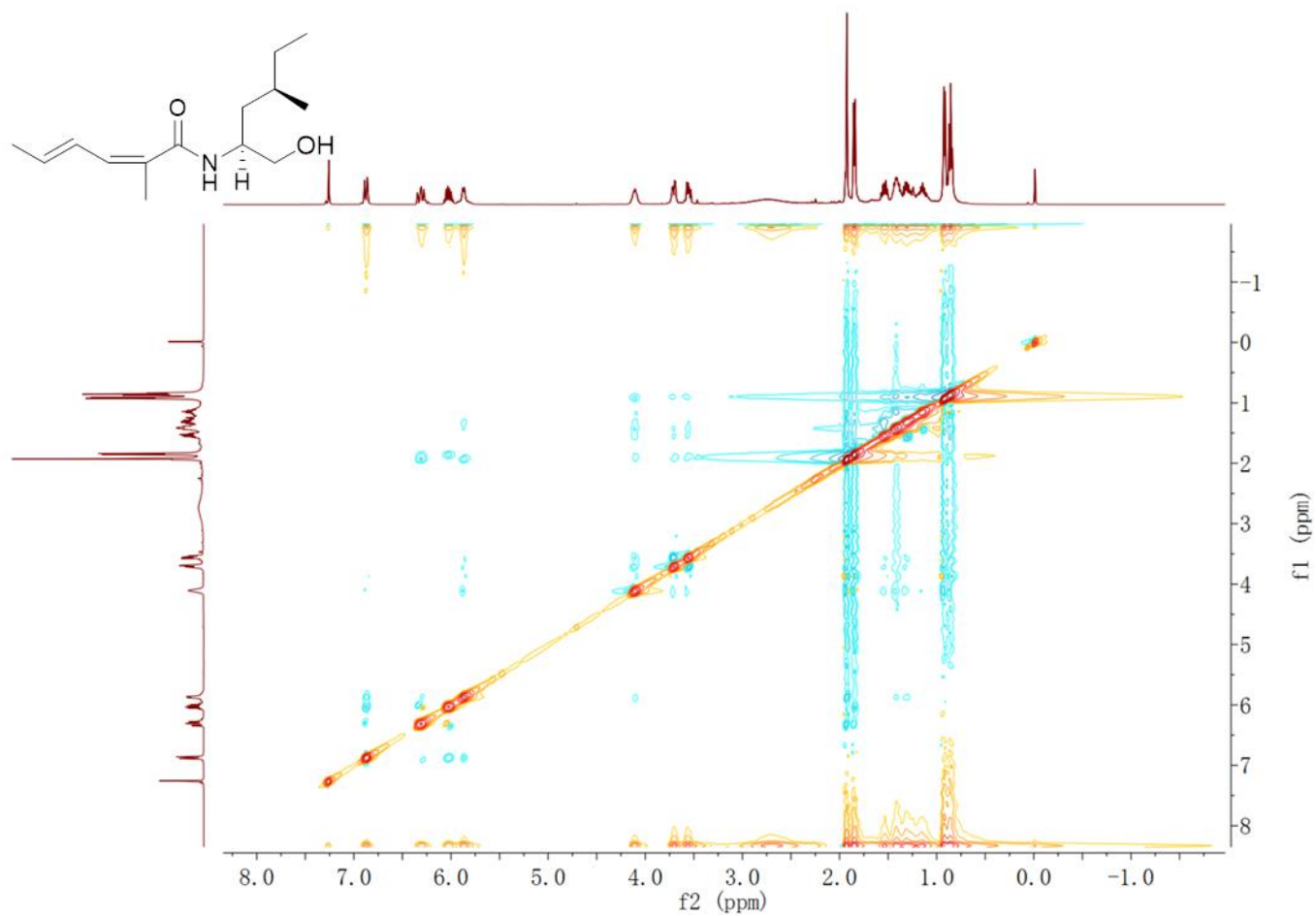


Figure S17. HR-ESI-MS spectrum of dichotomocej C (3)

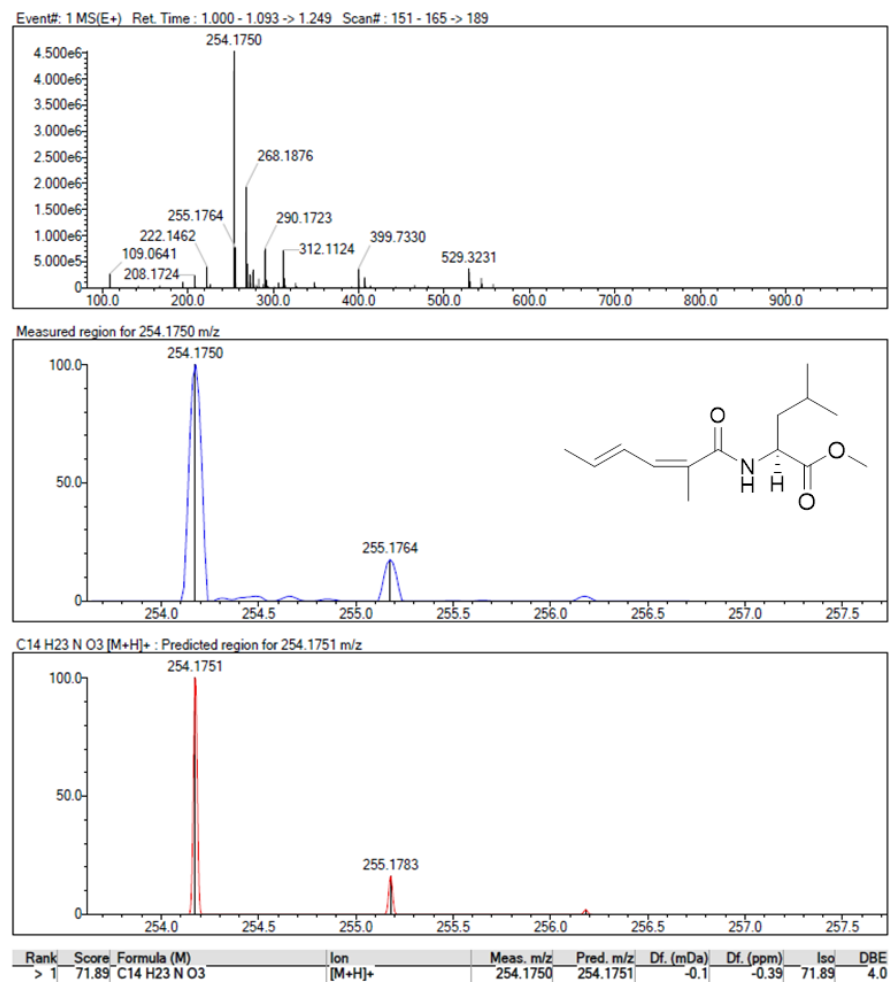


Figure S18. ^1H NMR spectrum of dichotomocej C (**3**) in CDCl_3 (400MHz)

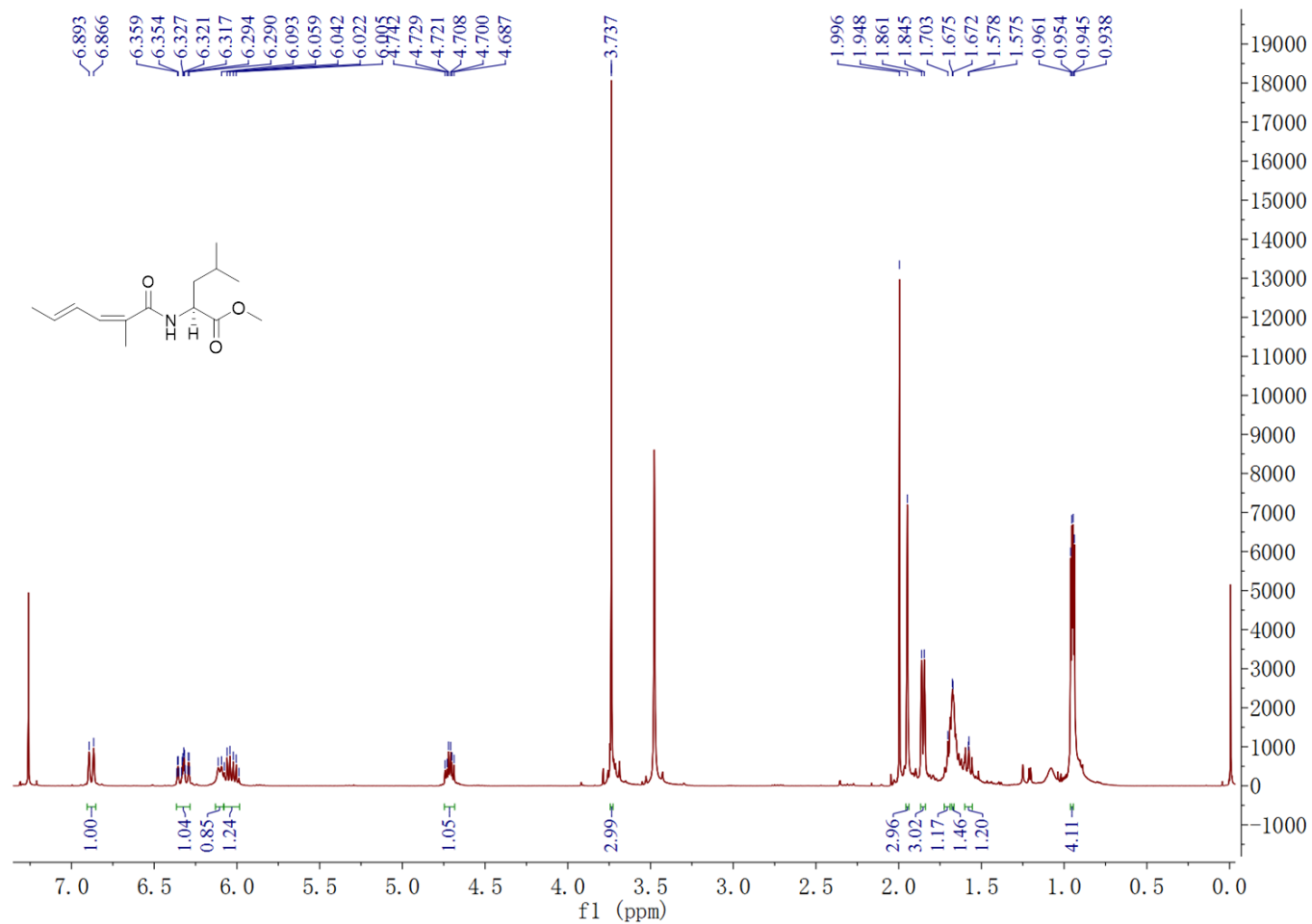


Figure S19. ^{13}C NMR spectrum of dichotomocej C (**3**) in CDCl_3 (100MHz)

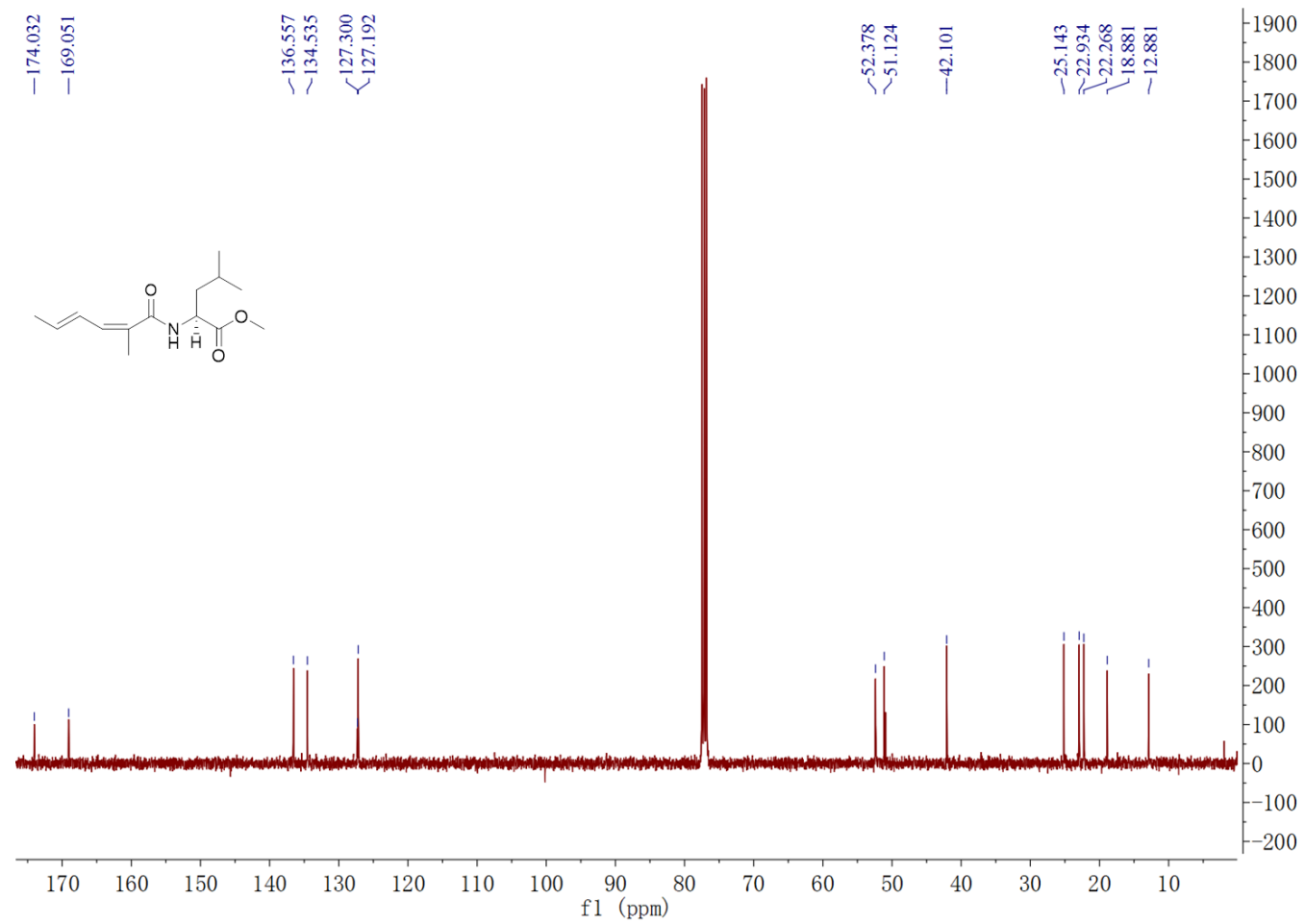


Figure S20. DEPT 135 spectrum of dichotomej C (**3**) in CDCl₃ (100MHz)

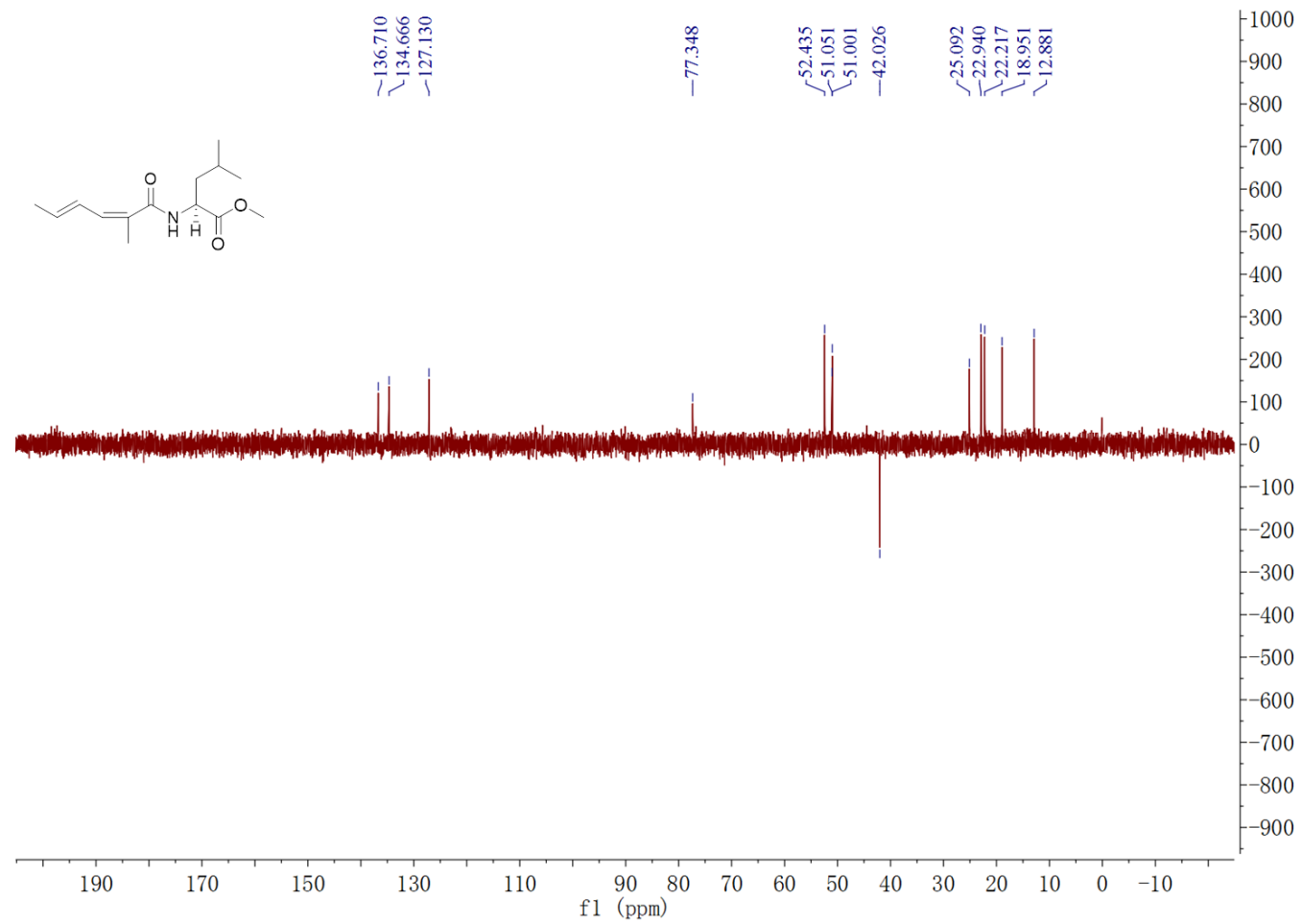


Figure S21. HMQC spectrum of dichotomocej C (**3**) in CDCl₃

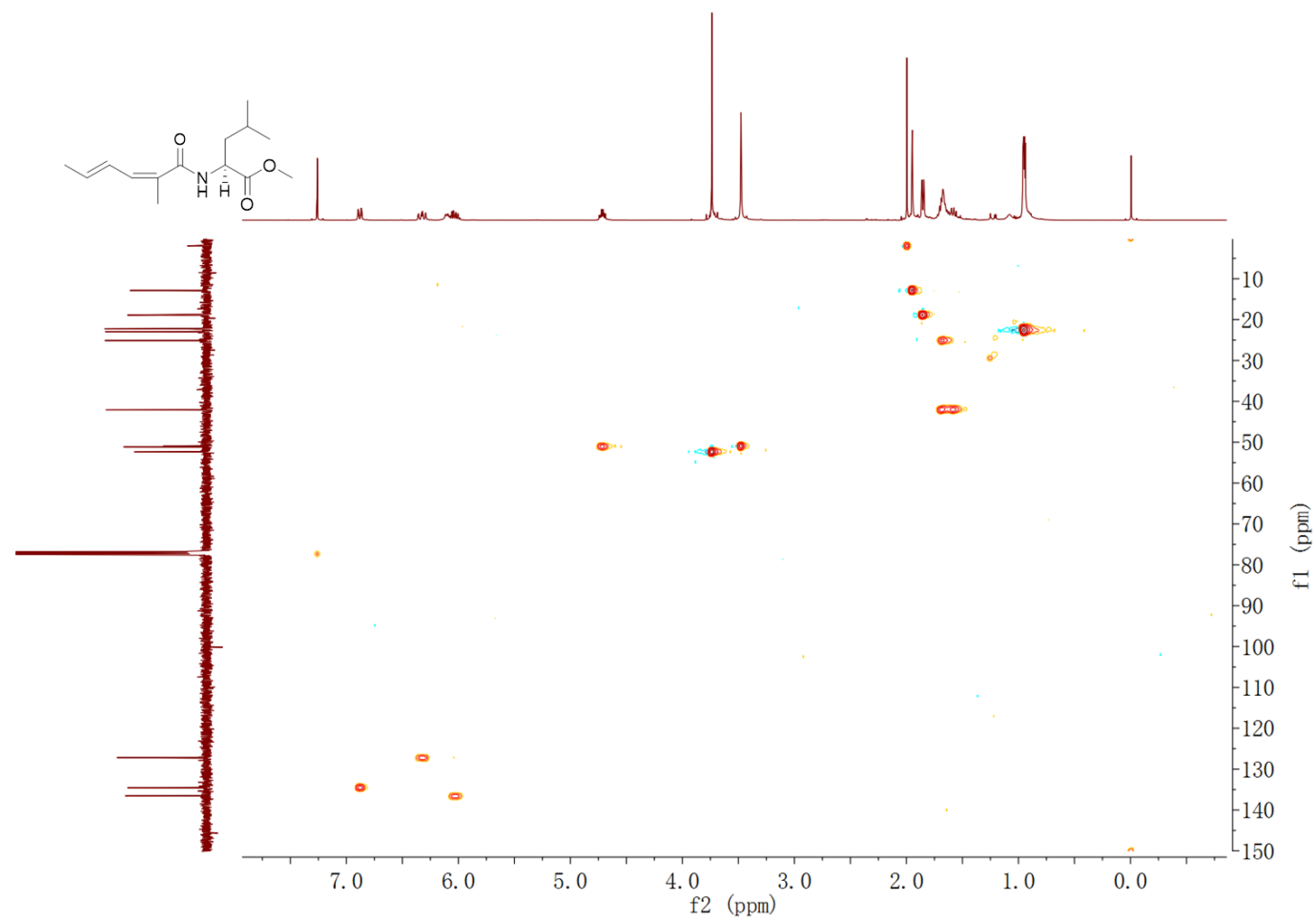


Figure S22. ^1H - ^1H COSY spectrum of dichotomocej C (**3**) in CDCl_3

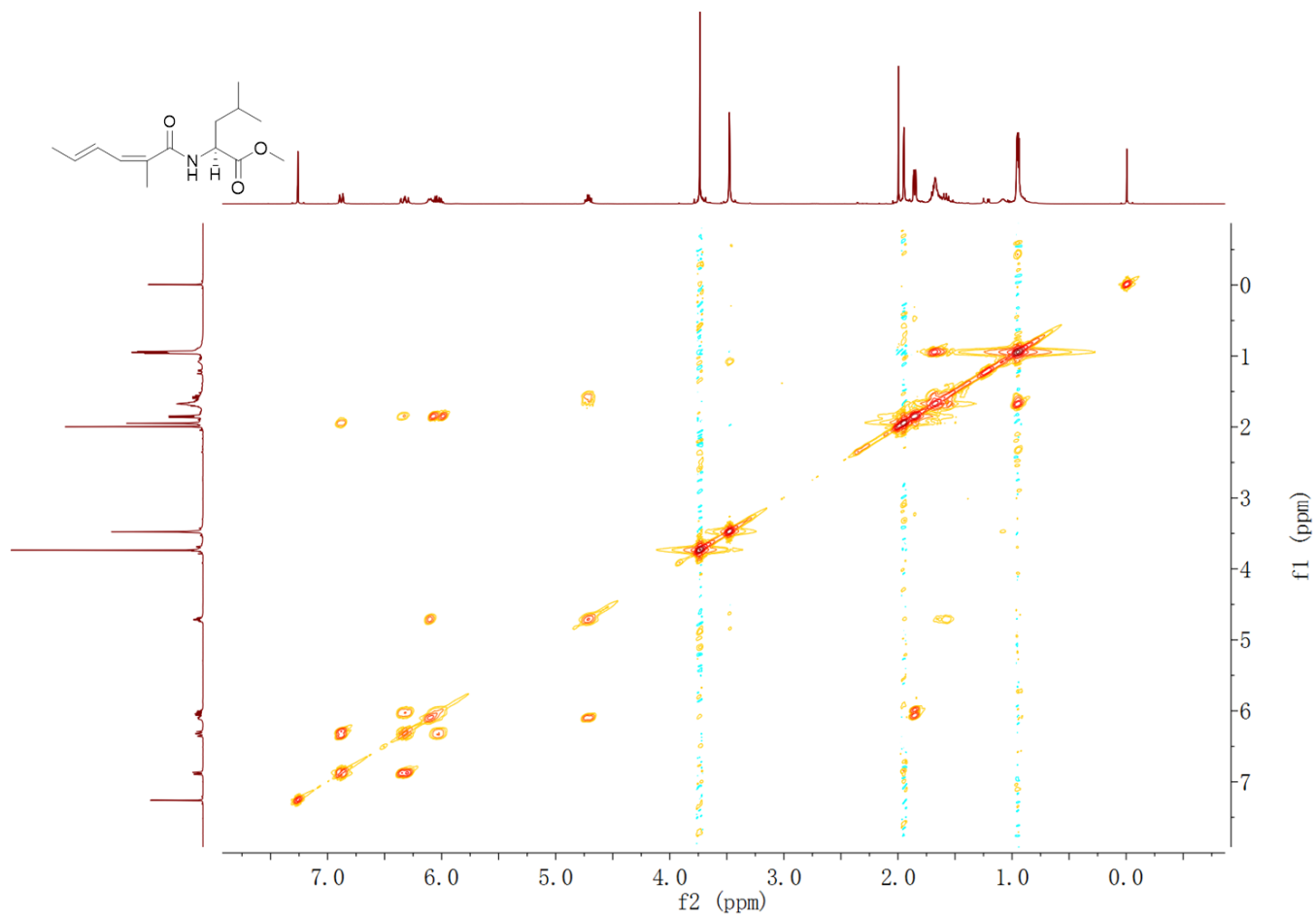


Figure S23. HMBC spectrum of dichotomocej C (**3**) in CDCl₃

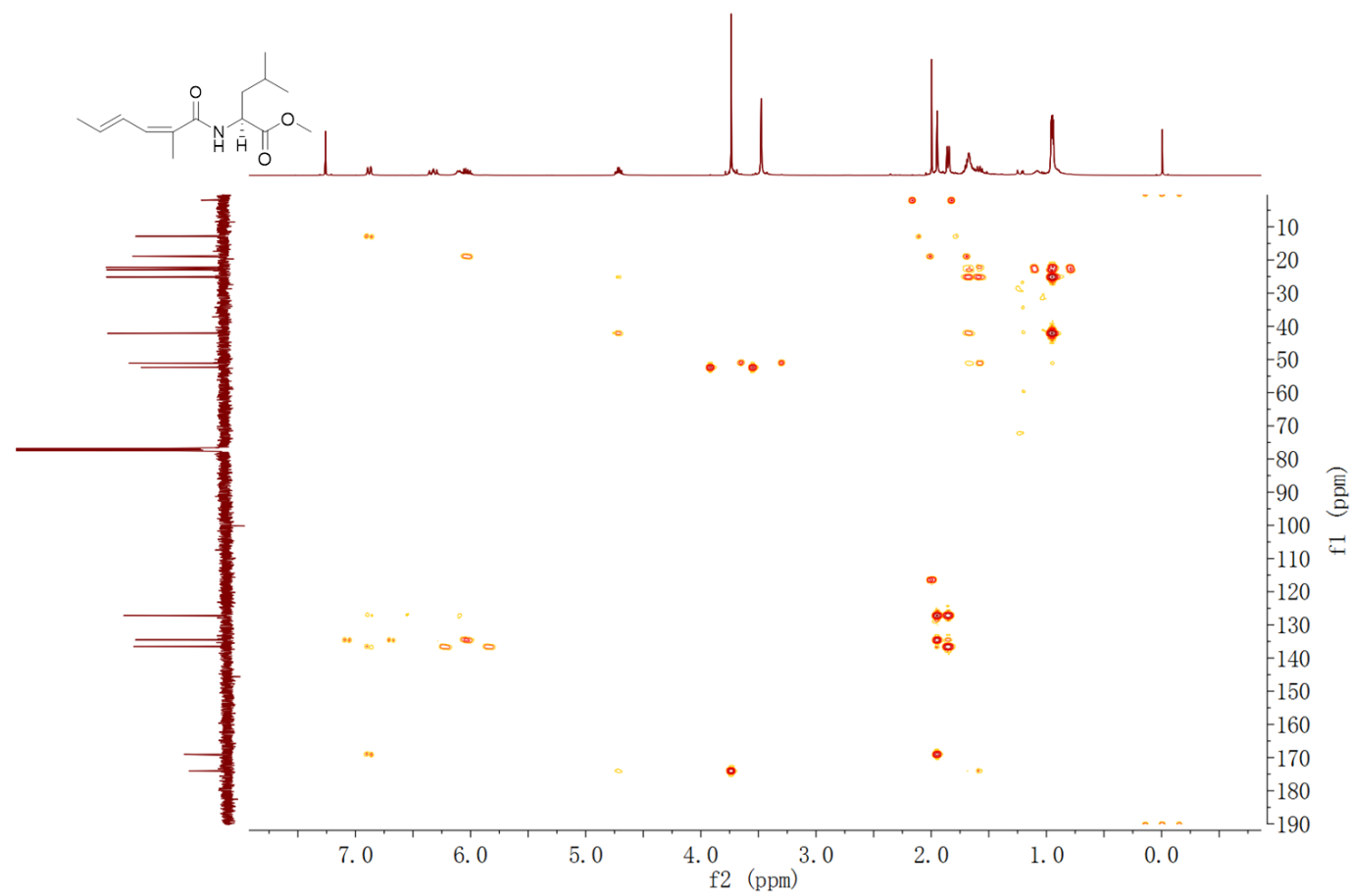


Figure S24. NOESY spectrum of dichotomocej C (**3**) in CDCl_3

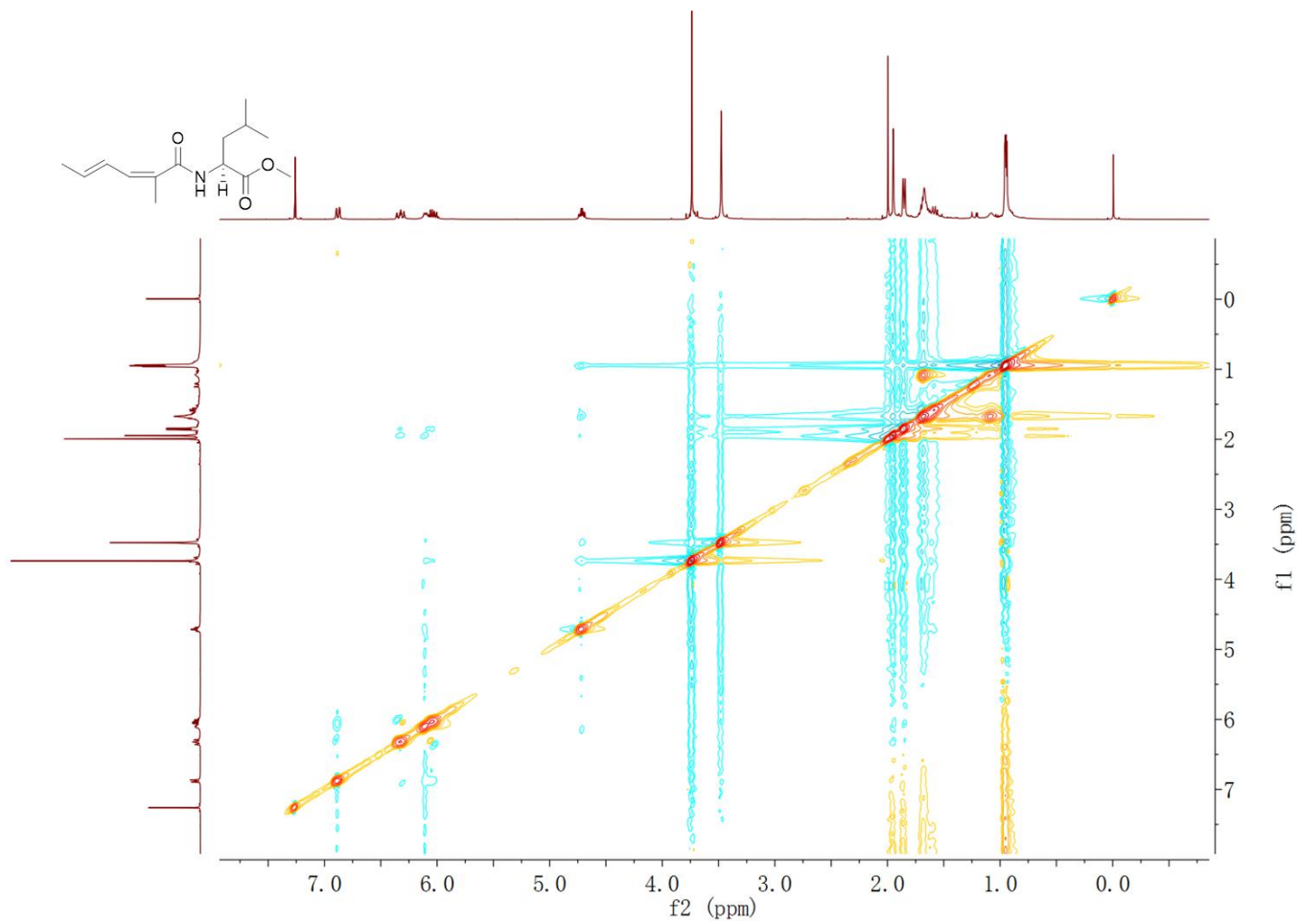


Figure S25. HR-ESI-MS spectrum of dichotomocej D (4)

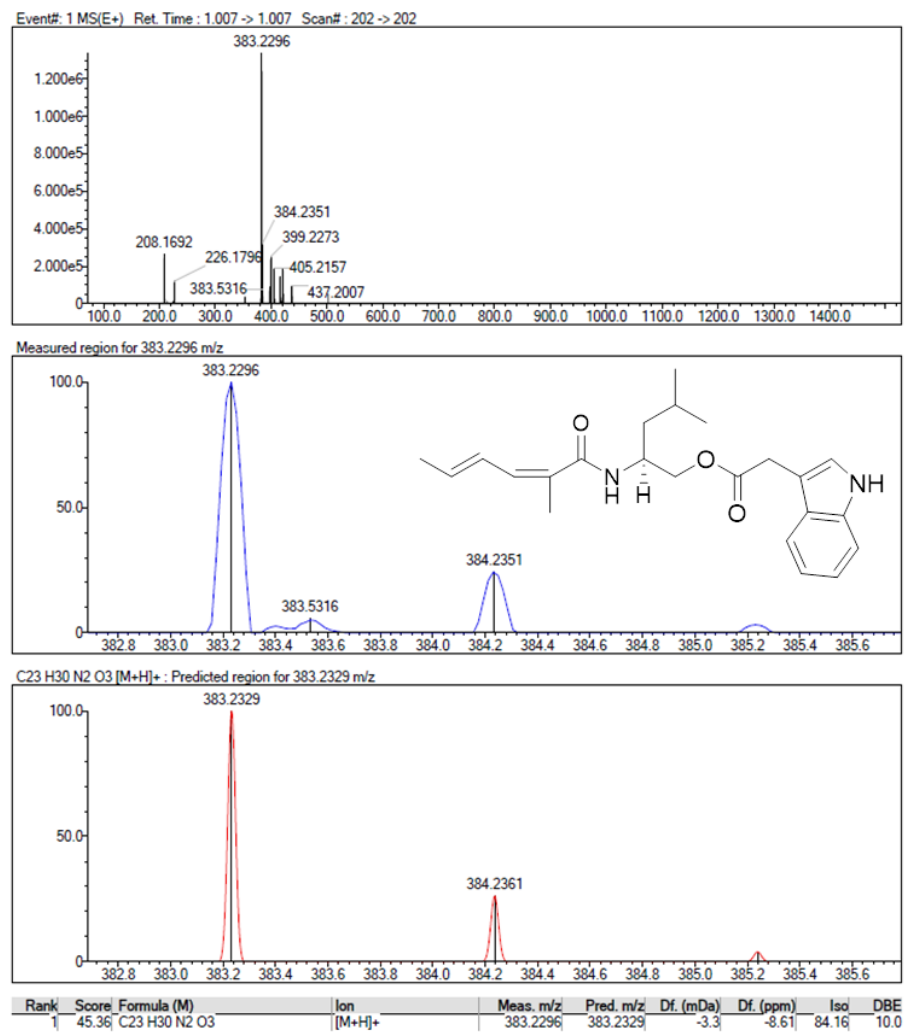


Figure S26. ¹H NMR spectrum of dichotomocej D (4) in CDCl₃ (400MHz)

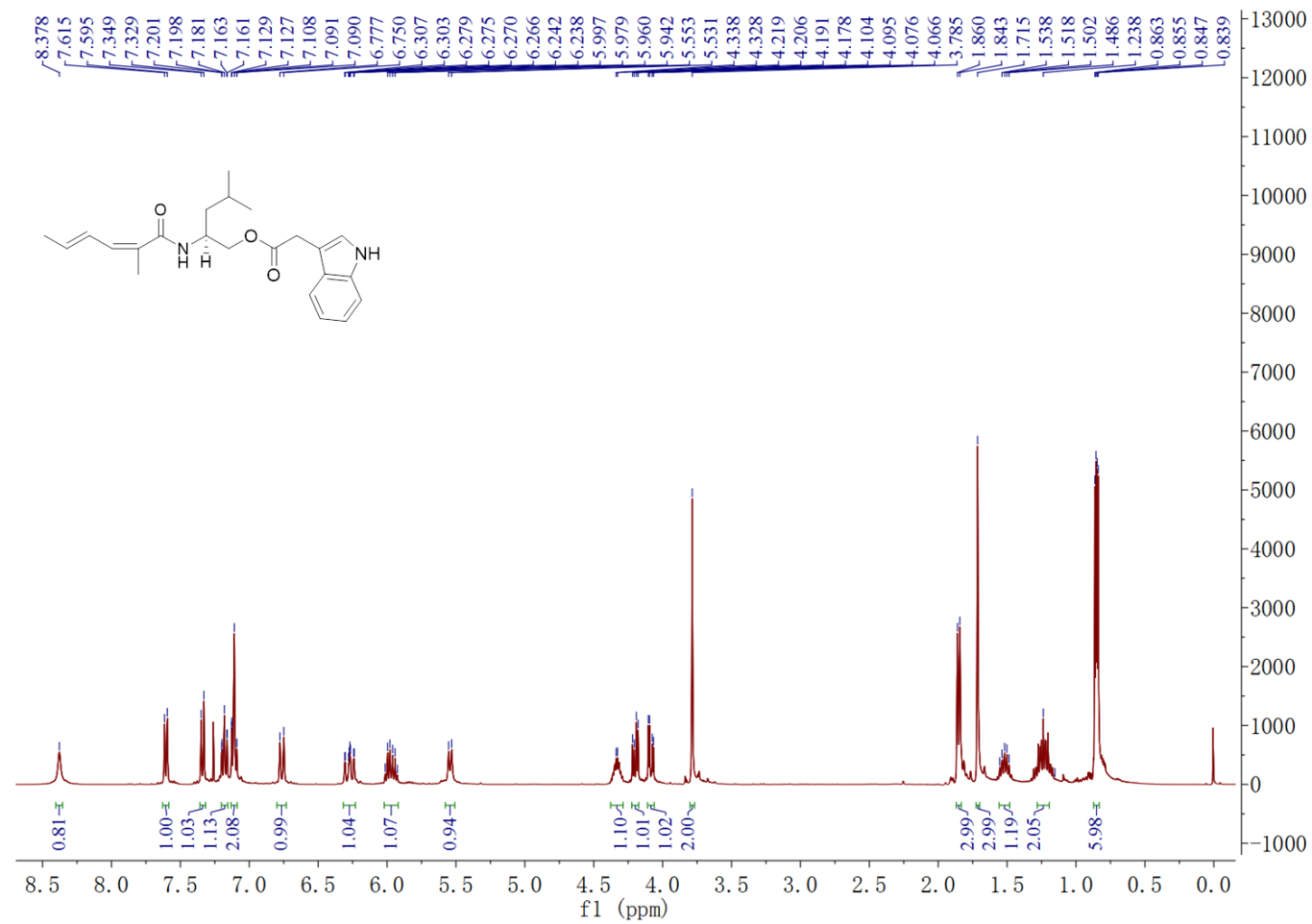


Figure S27. ^{13}C NMR spectrum of dichotomocej D (**4**) in CDCl_3 (100MHz)

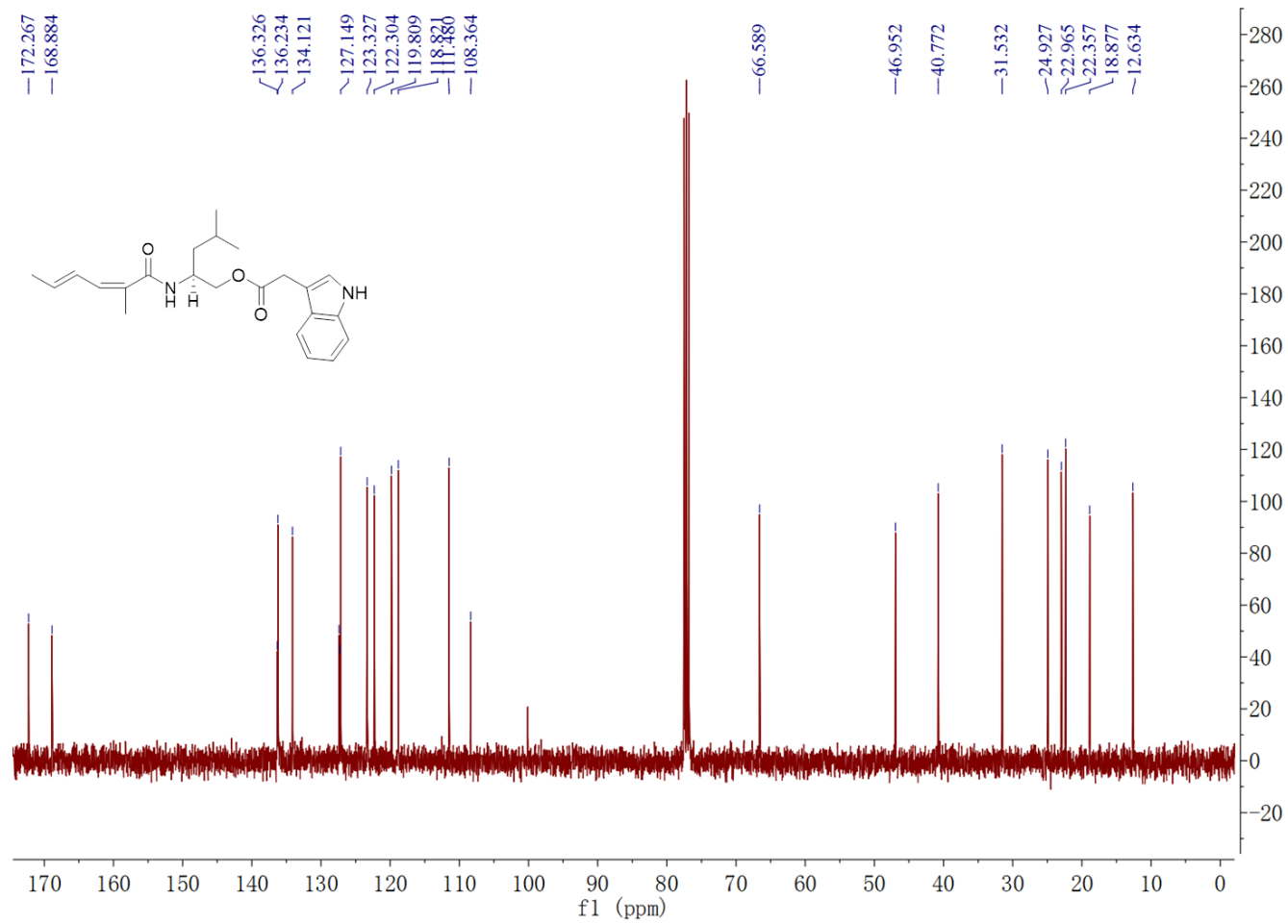


Figure S28. DEPT 135 spectrum of dichotomej D (**4**) in CDCl₃ (100MHz)

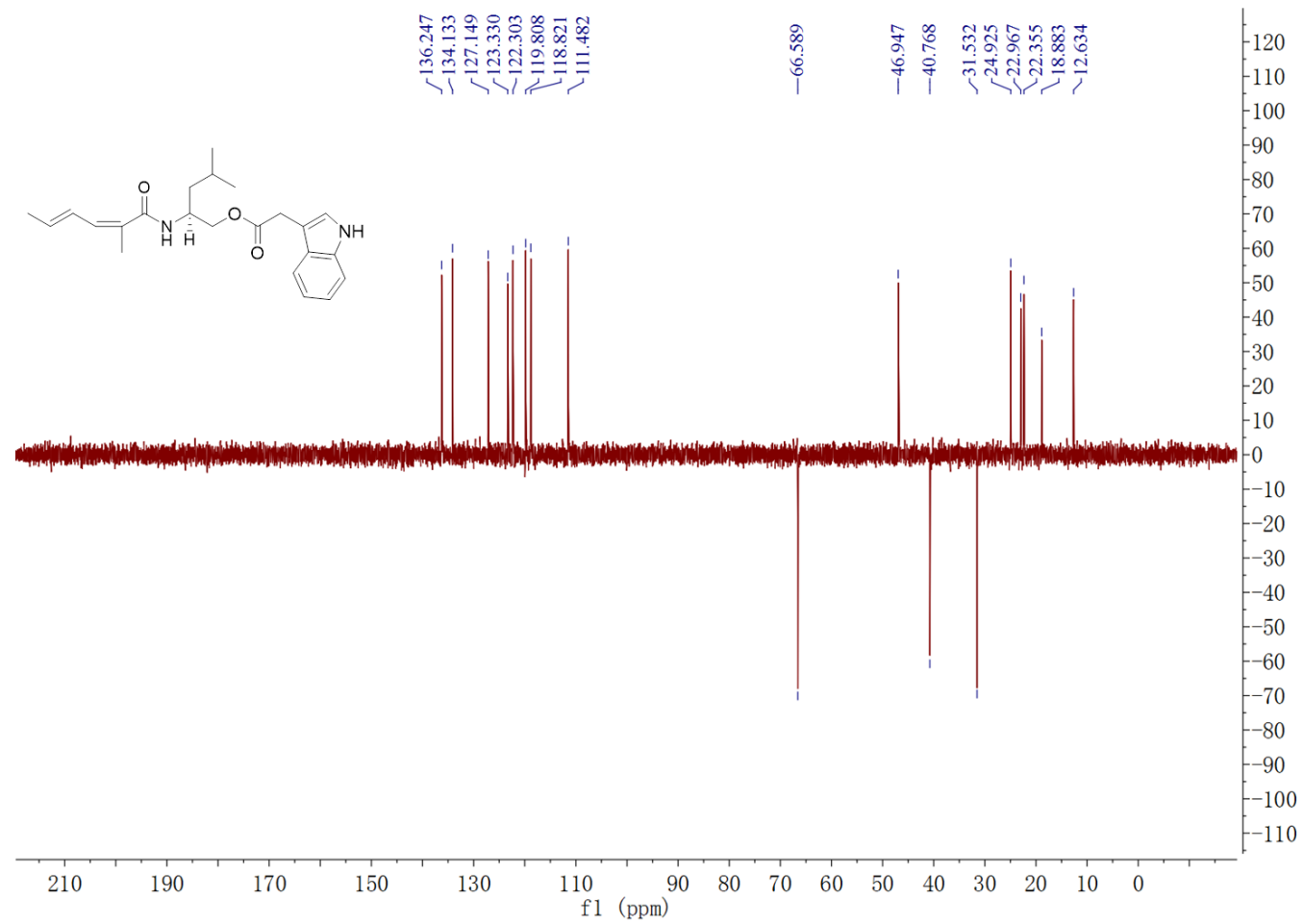


Figure S29. HMQC spectrum of dichotomocej D (**4**) in CDCl₃

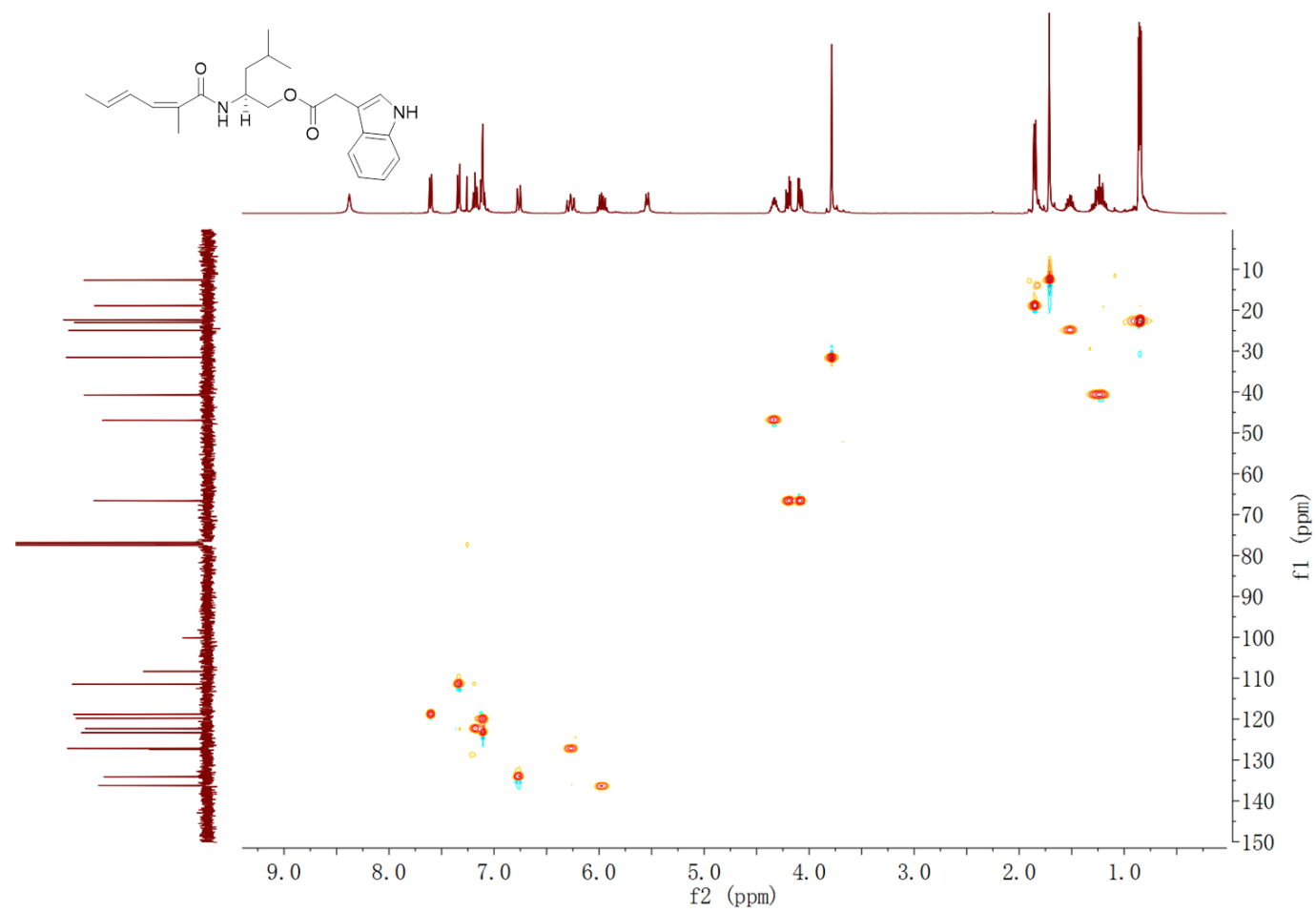


Figure S30. ^1H - ^1H COSY spectrum of dichotomocej D (**4**) in CDCl_3

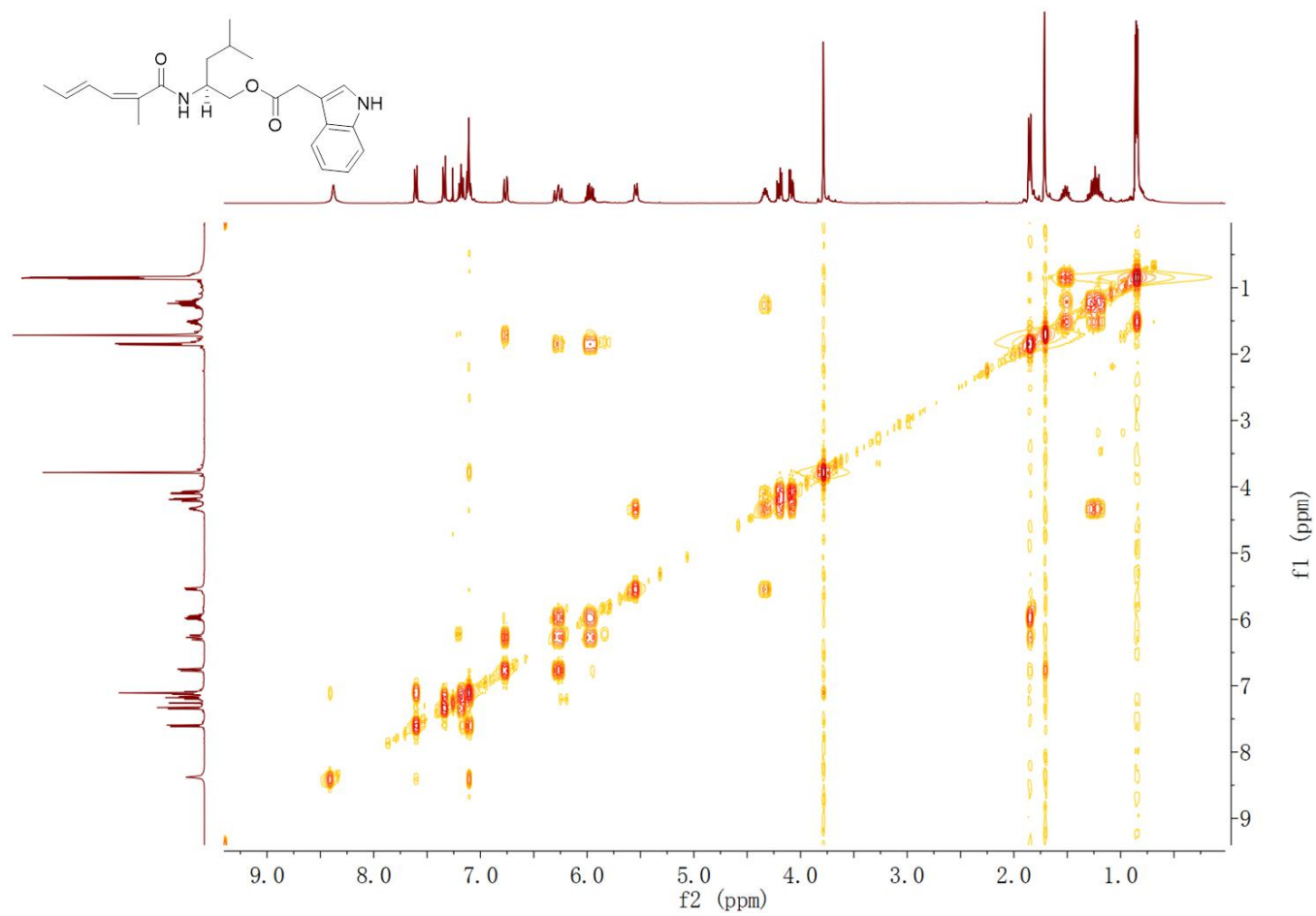


Figure S31. HMBC spectrum of dichotomocej D (**4**) in CDCl₃

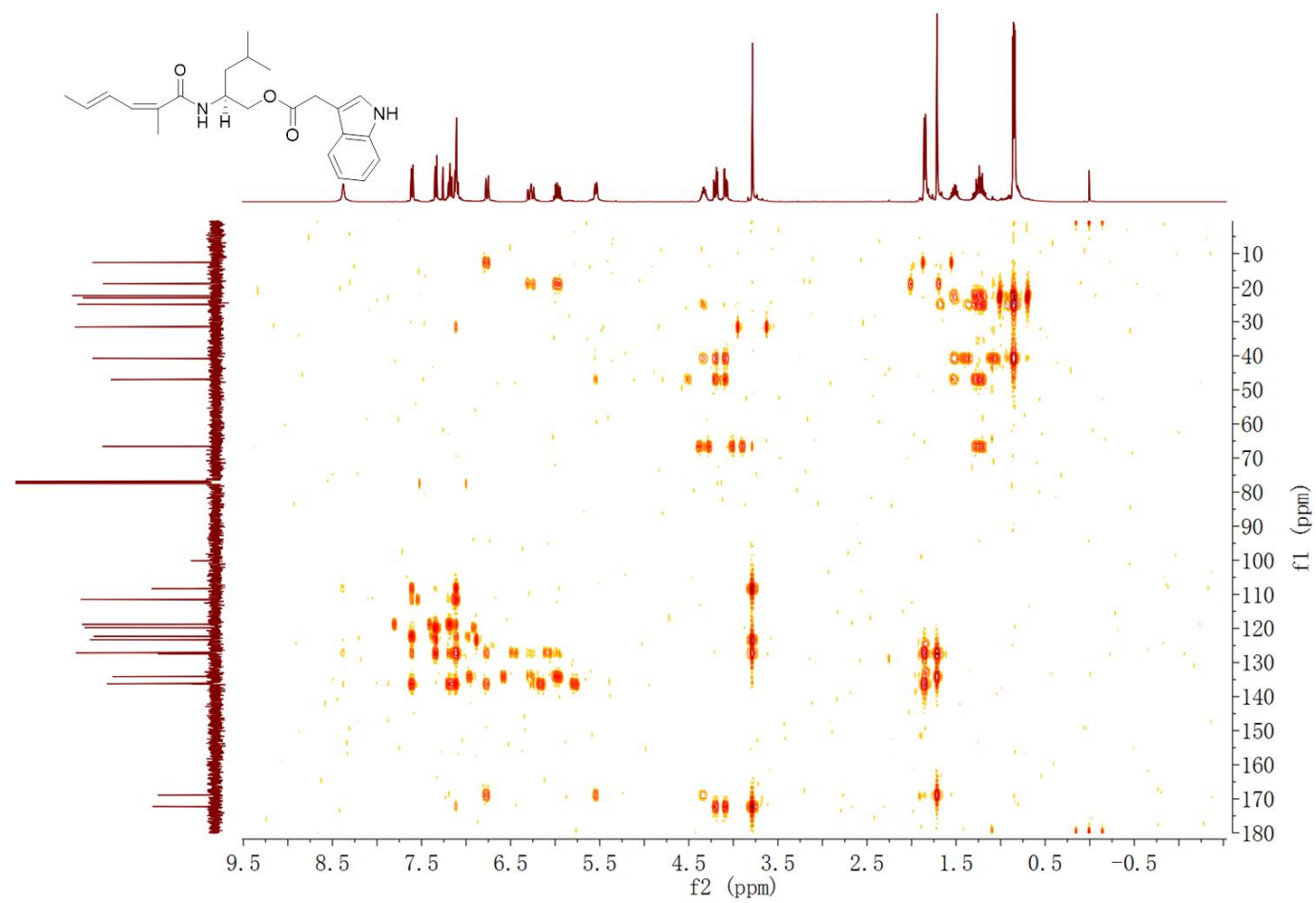


Figure S32. NOESY spectrum of dichotomej D (**4**) in CDCl₃

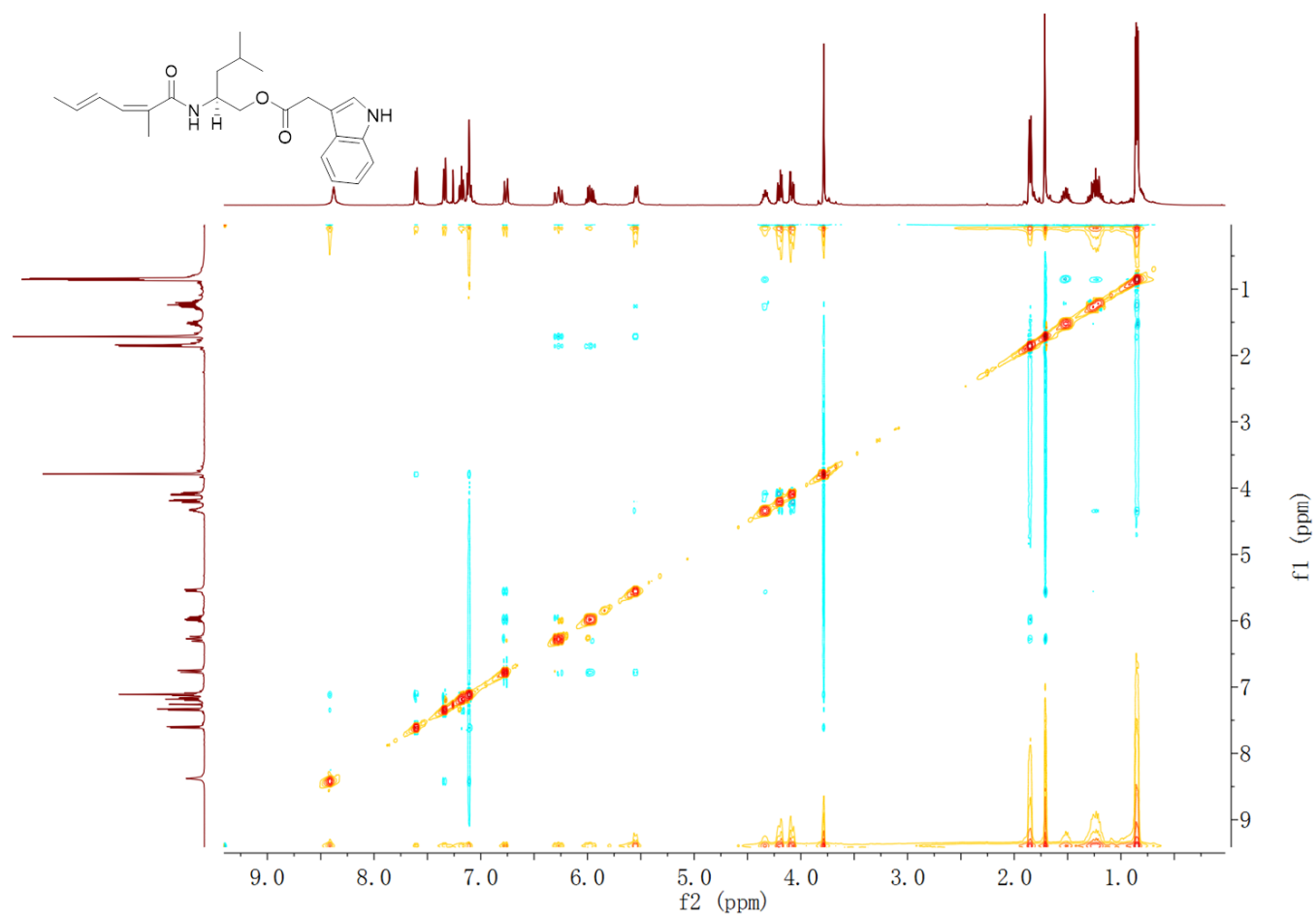


Figure S33. HR-ESI-MS spectrum of dichocetide A (**5**)

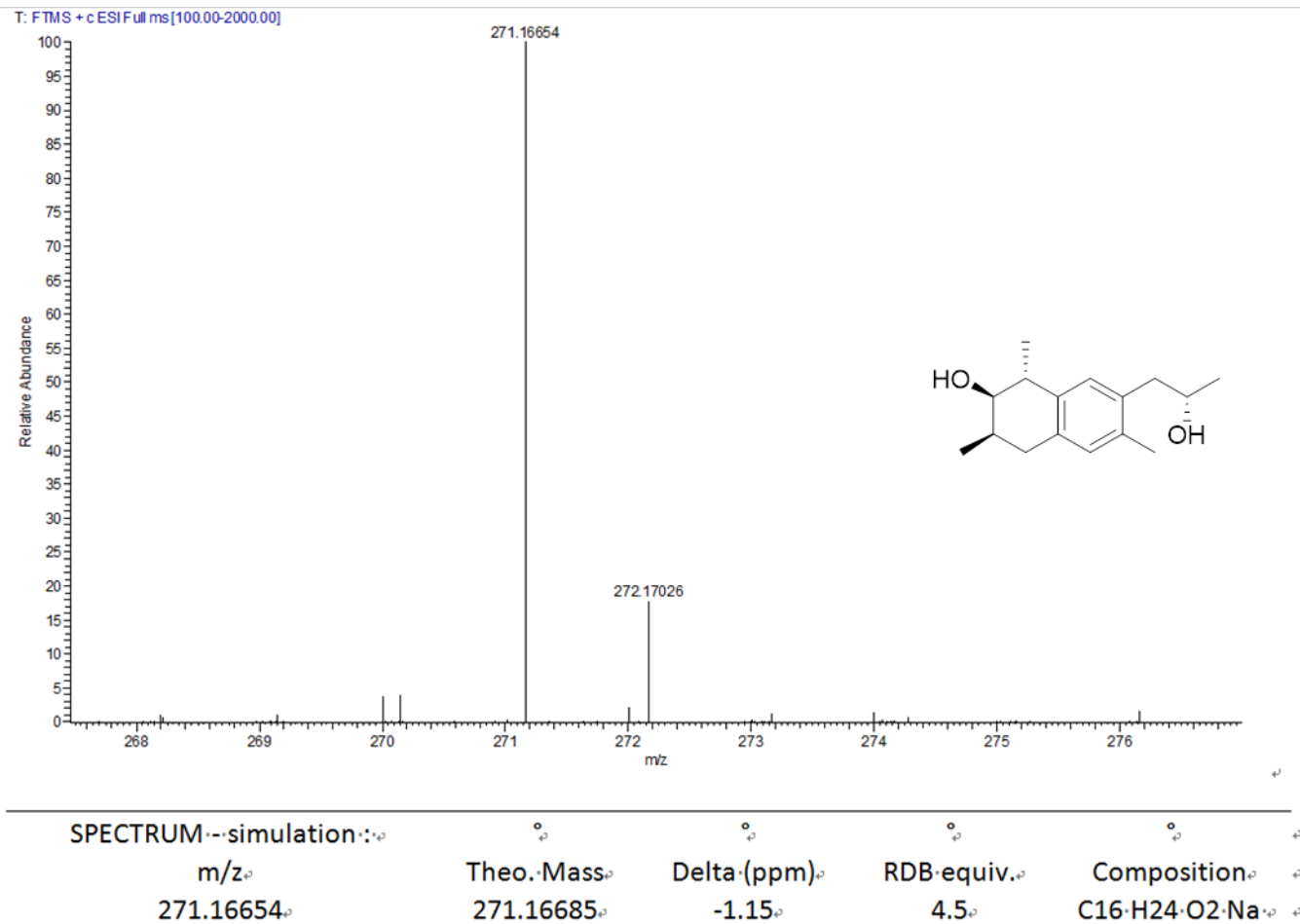


Figure S34. ^1H NMR spectrum of dichocetide A (**5**) in CDCl_3 (400MHz)

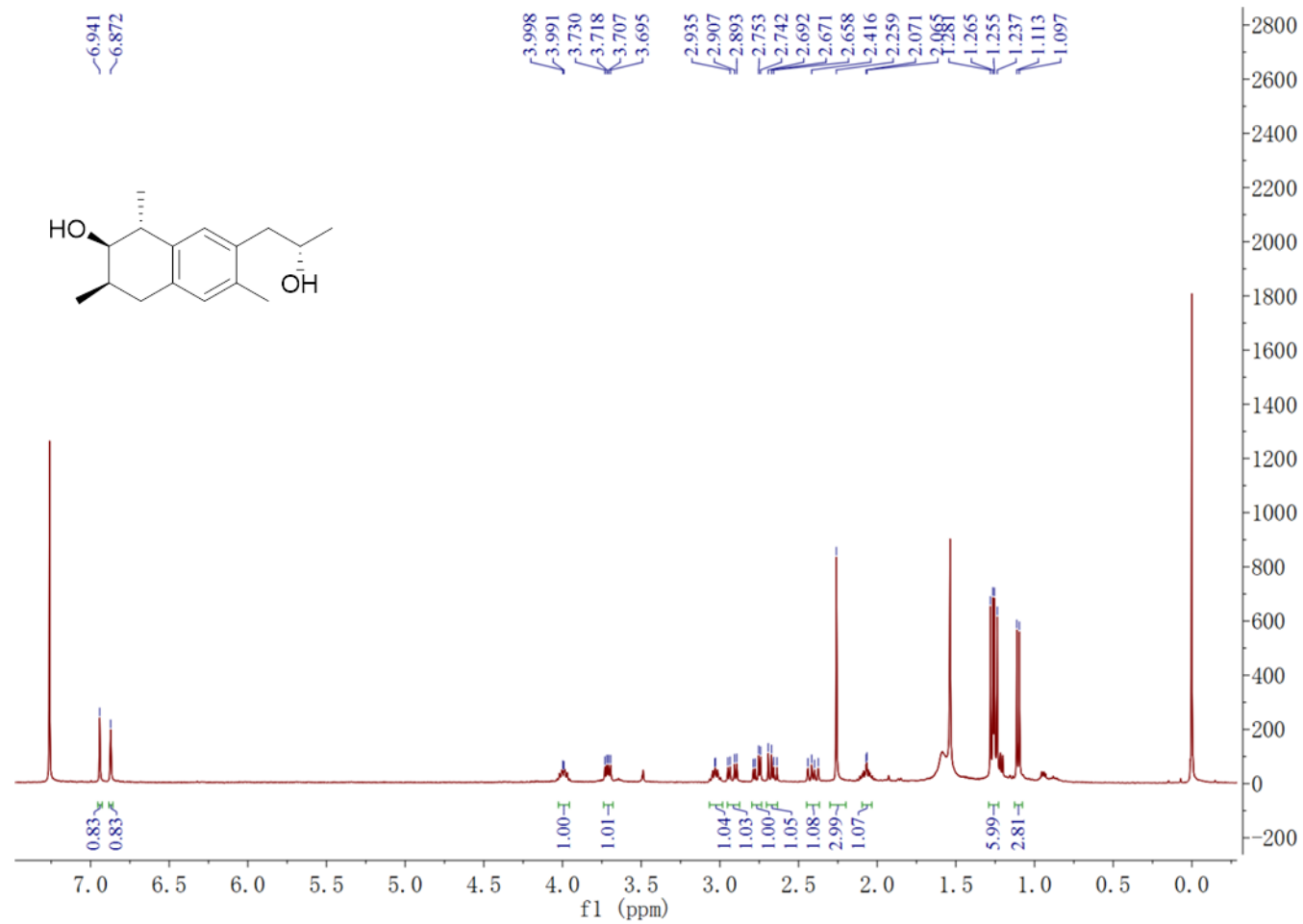


Figure S35. ^{13}C NMR spectrum of dichocetide A (**5**) in CDCl_3 (100MHz)

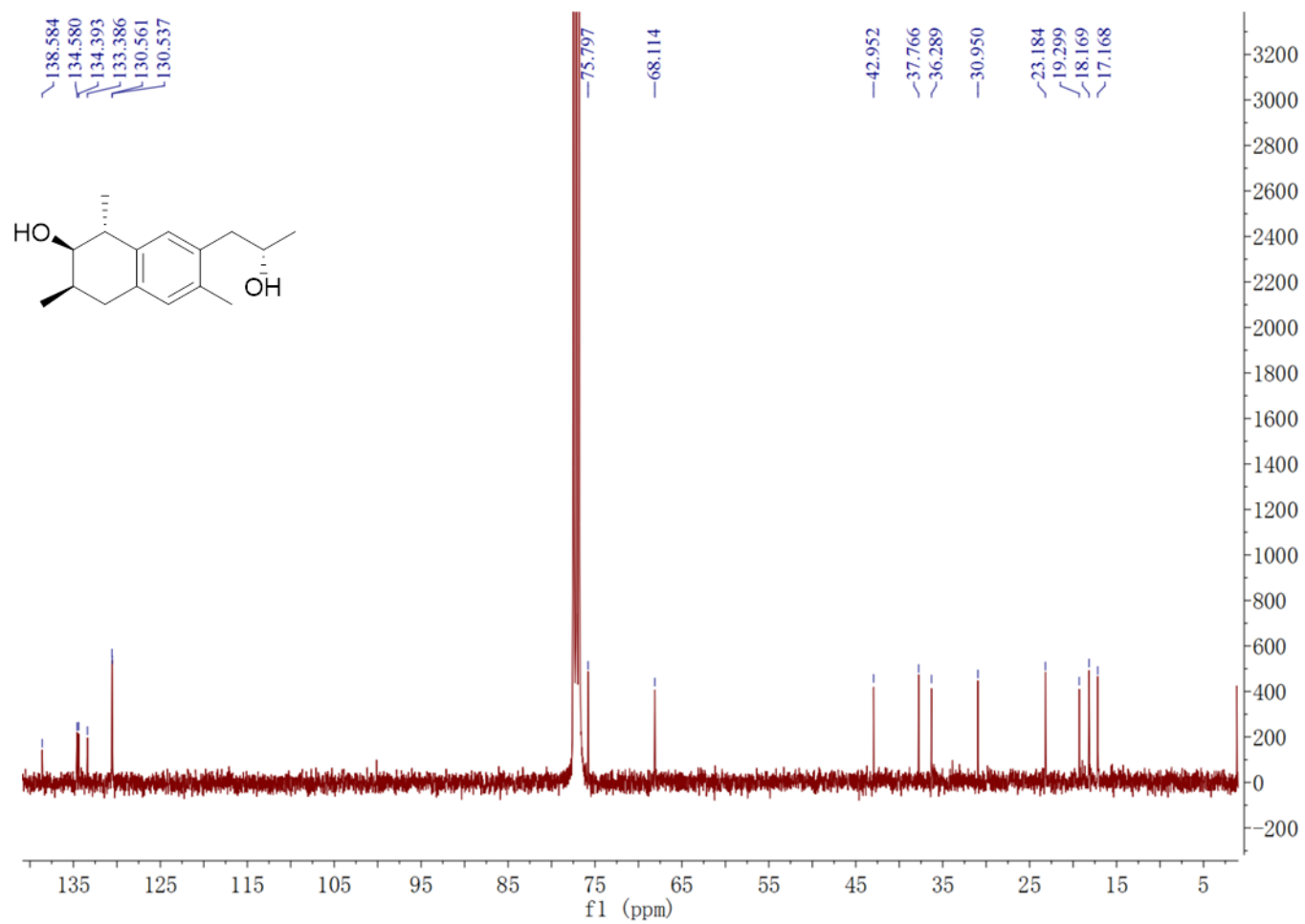


Figure S36. DEPT 135 spectrum of dichocetide A (5) in CDCl₃ (100MHz)

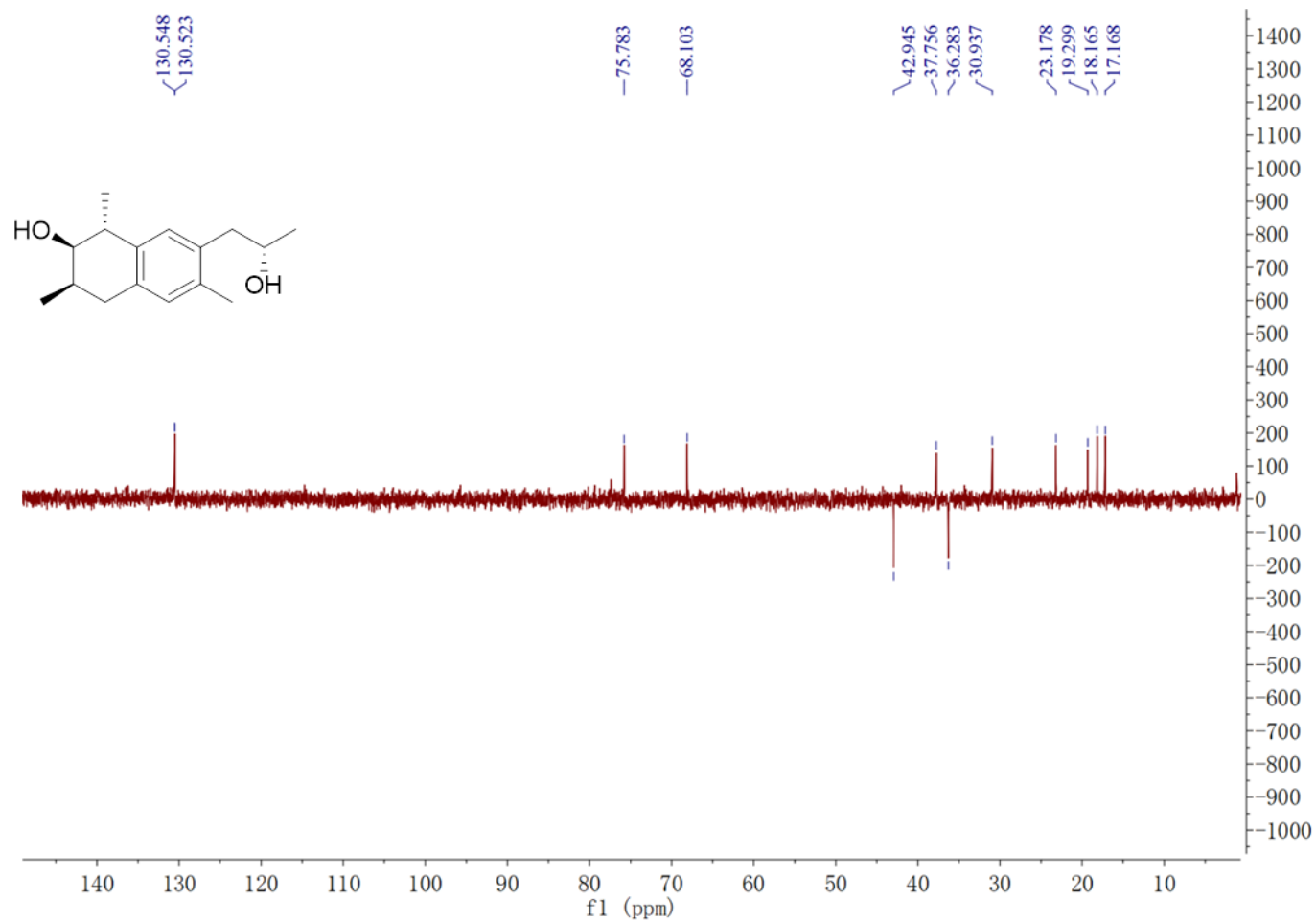


Figure S37. HMQC spectrum of dichocetide A (5) in CDCl₃

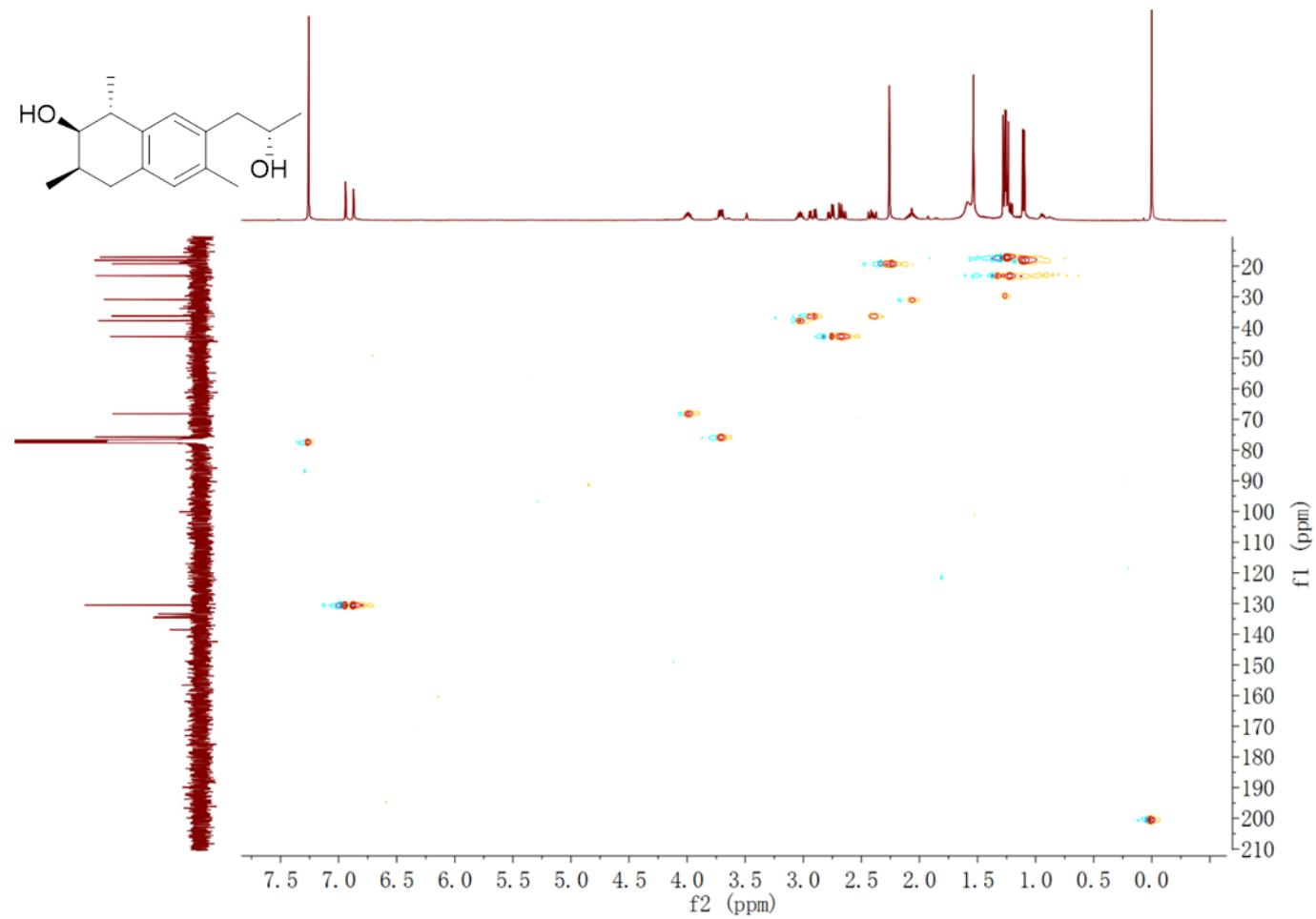


Figure S38. ^1H - ^1H COSY spectrum of dichocetide A (**5**) in CDCl_3

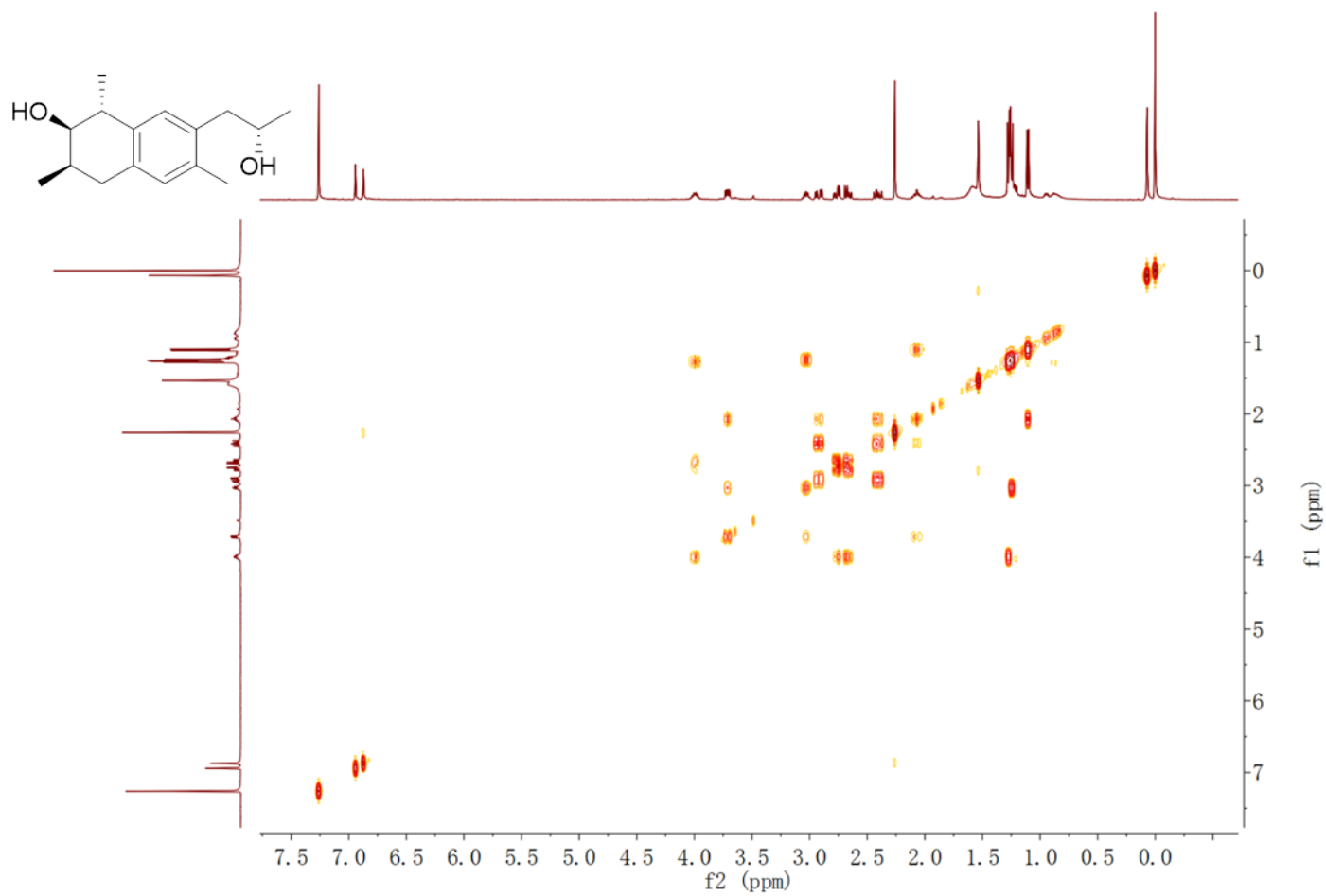


Figure S39. HMBC spectrum of dichocetide A (5) in CDCl₃

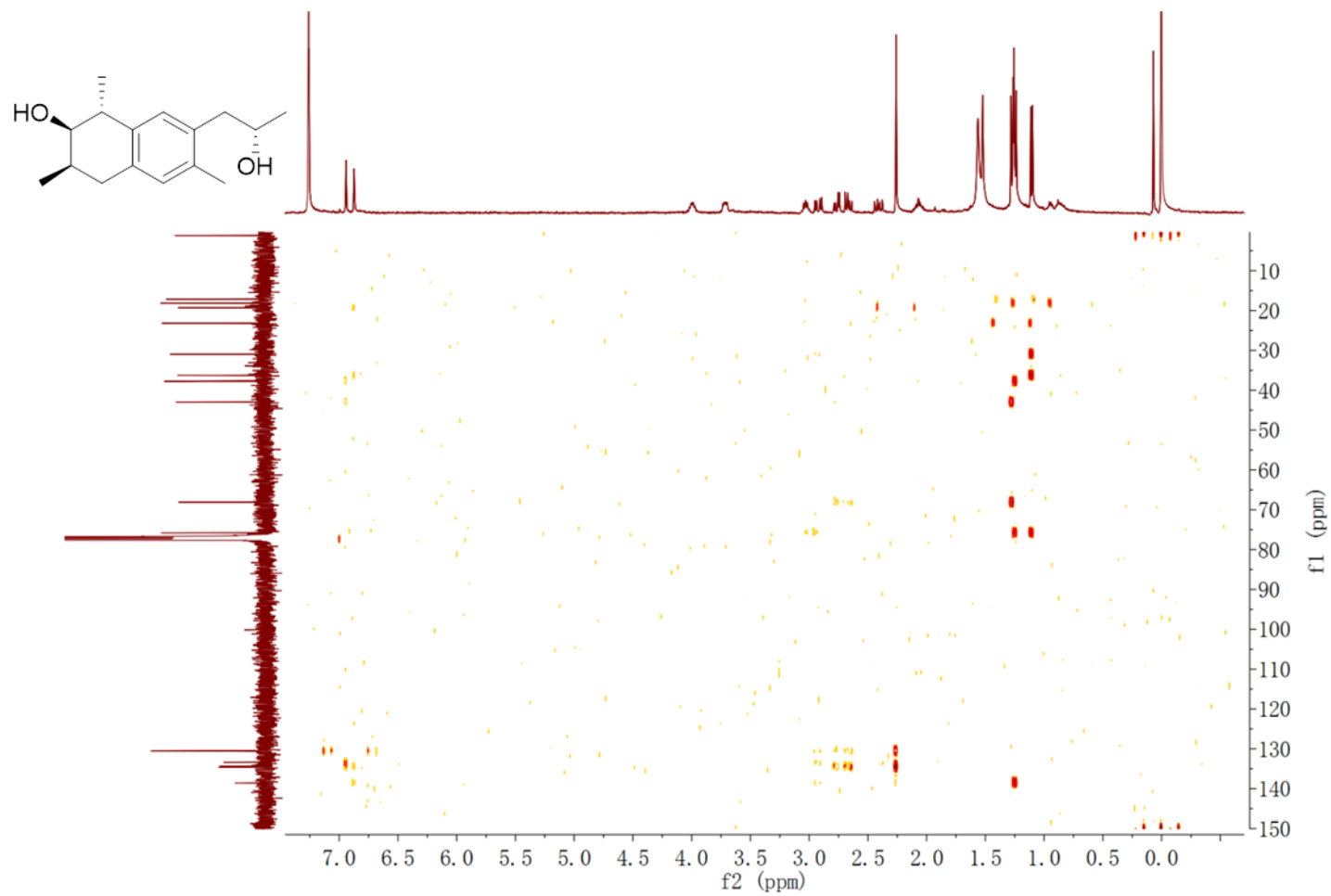


Figure S40. NOESY spectrum of dichocetide A (**5**) in CDCl₃

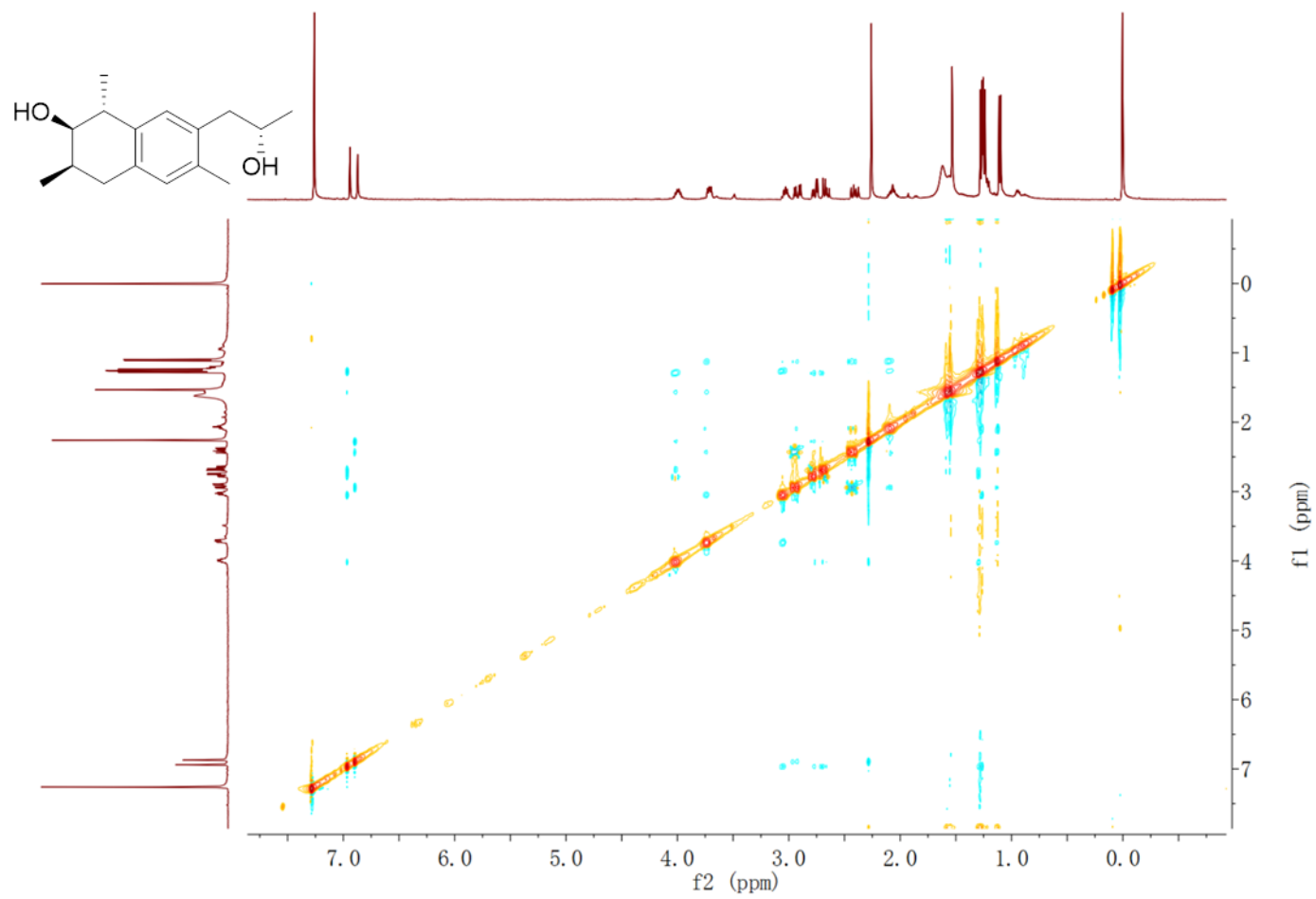


Figure S41. ^1H NMR spectrum of dichotone A (**6**) in CDCl_3 (400MHz)

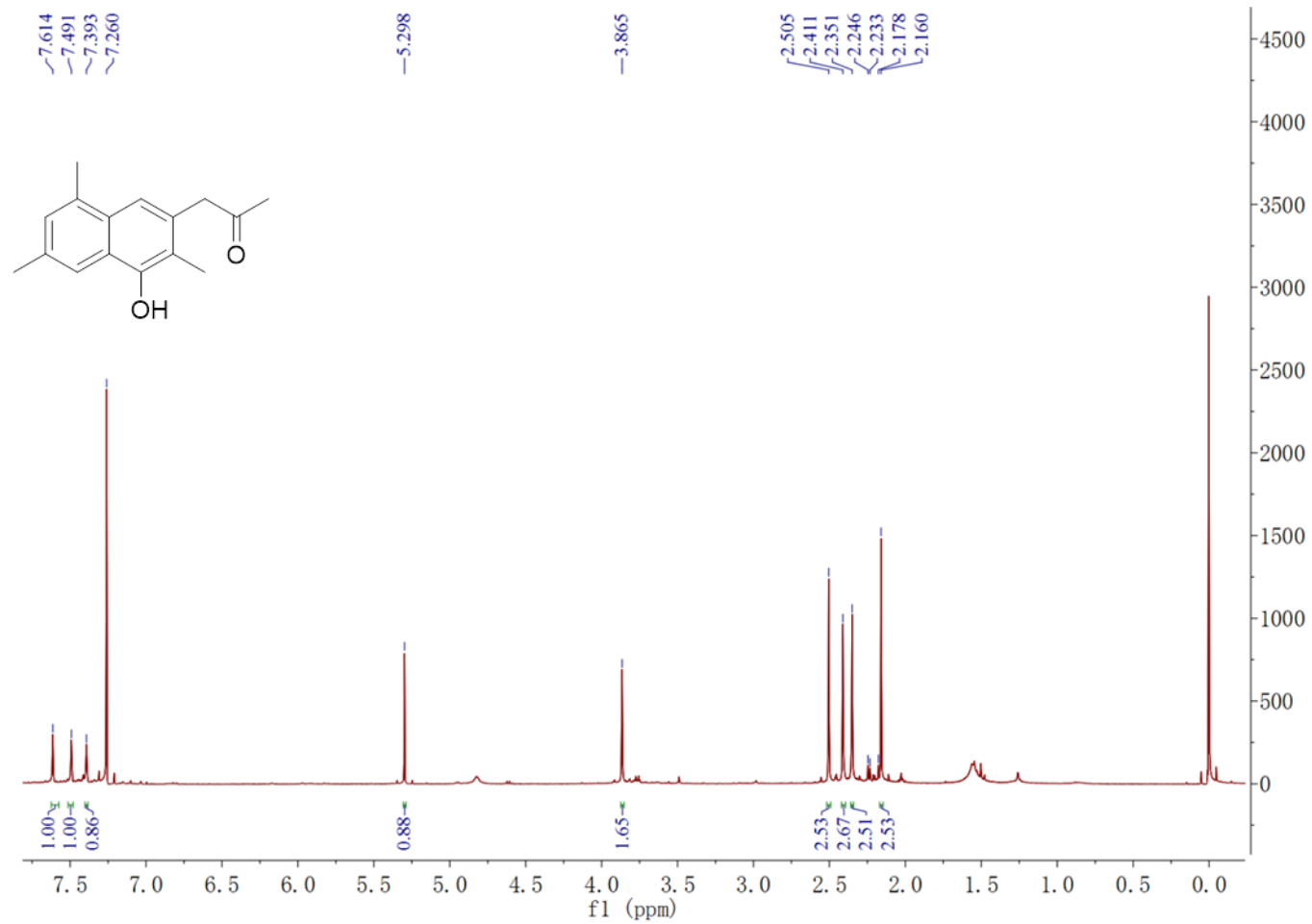


Figure S42. ^{13}C NMR spectrum of dichotone A (**6**) in CDCl_3 (100MHz)

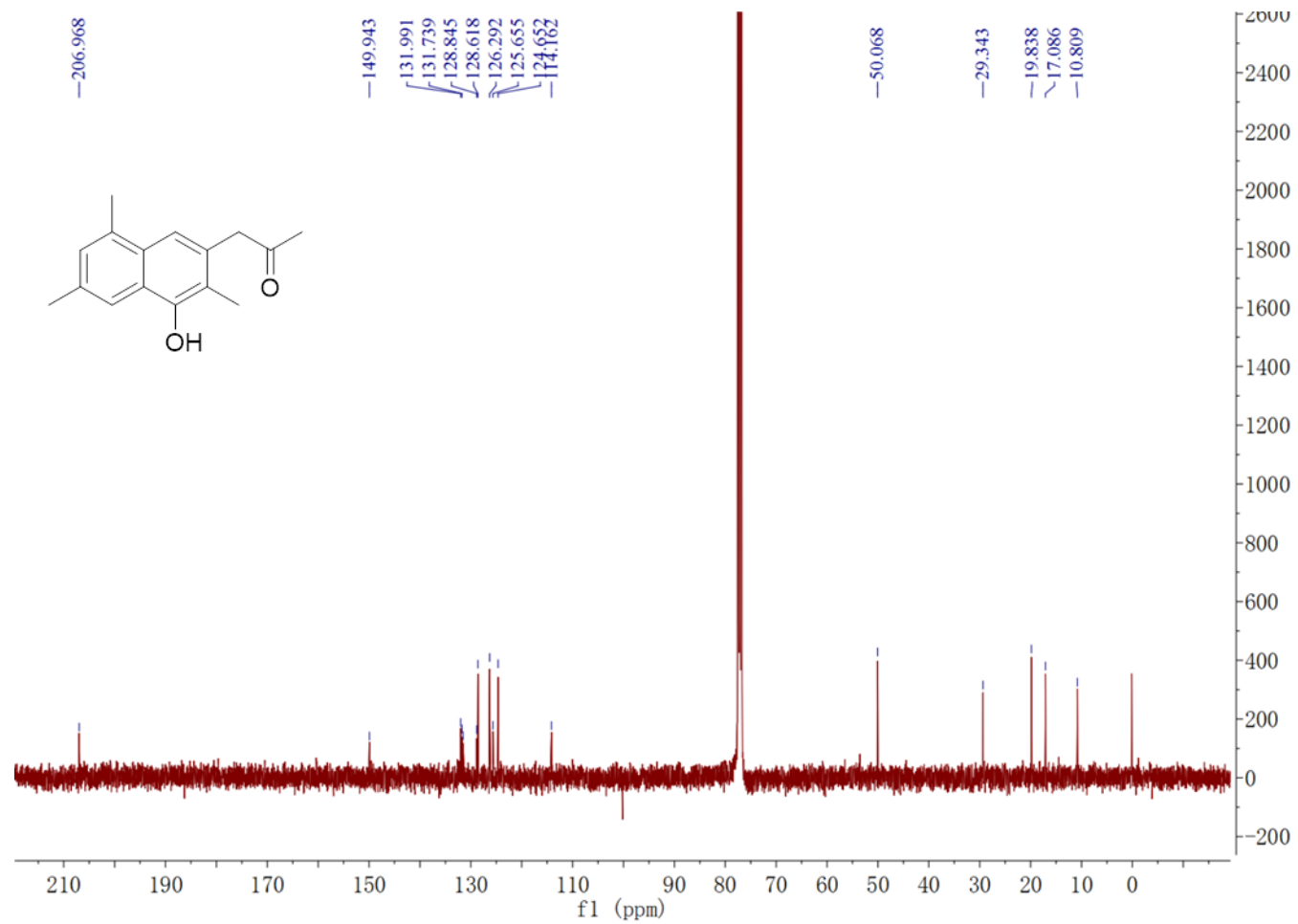


Figure S43. ^1H NMR spectrum of diorcinol (**7**) in CDCl_3 (400MHz)

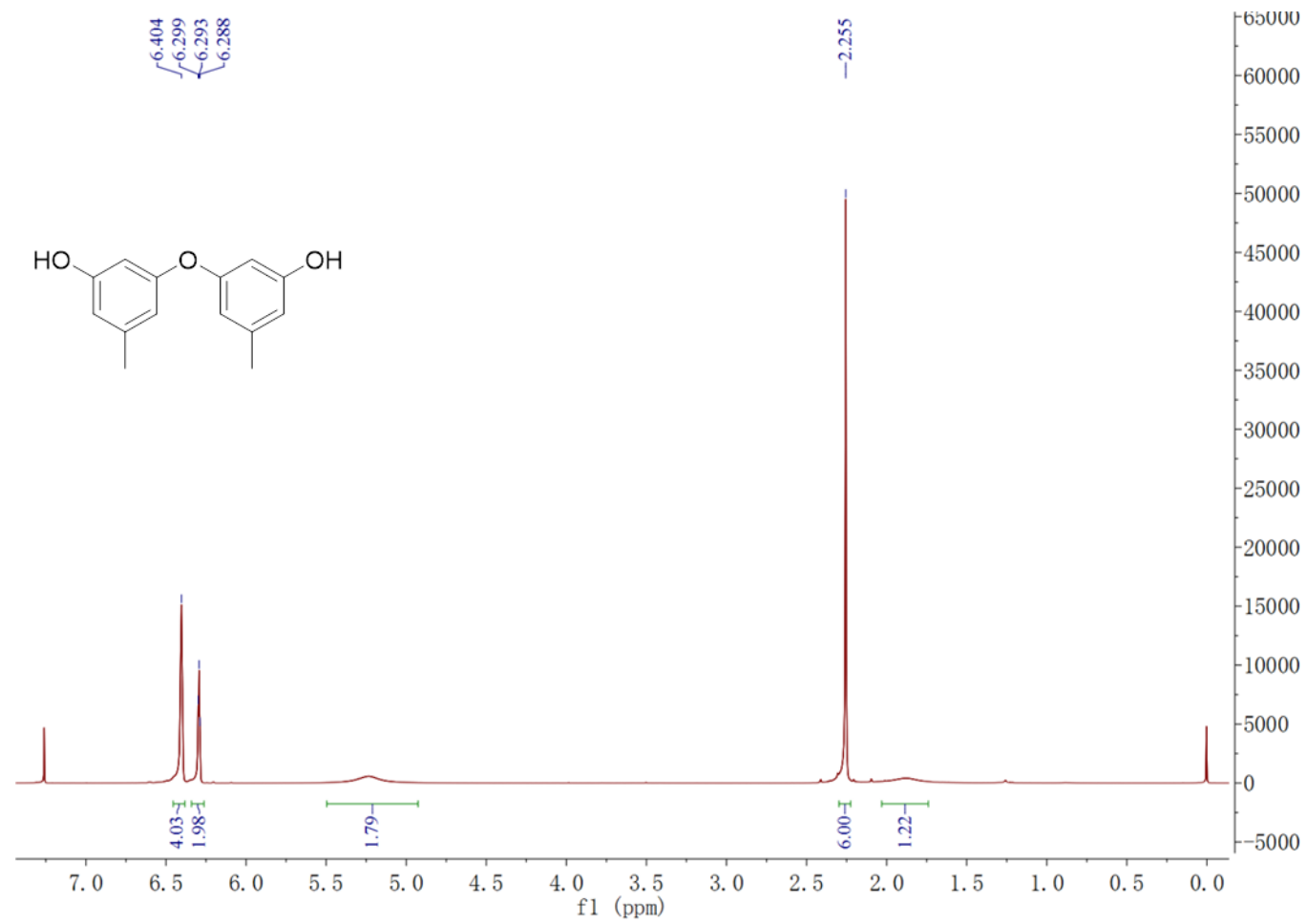


Figure S44. ^{13}C NMR spectrum of diorcinol (**7**) in CDCl_3 (100MHz)

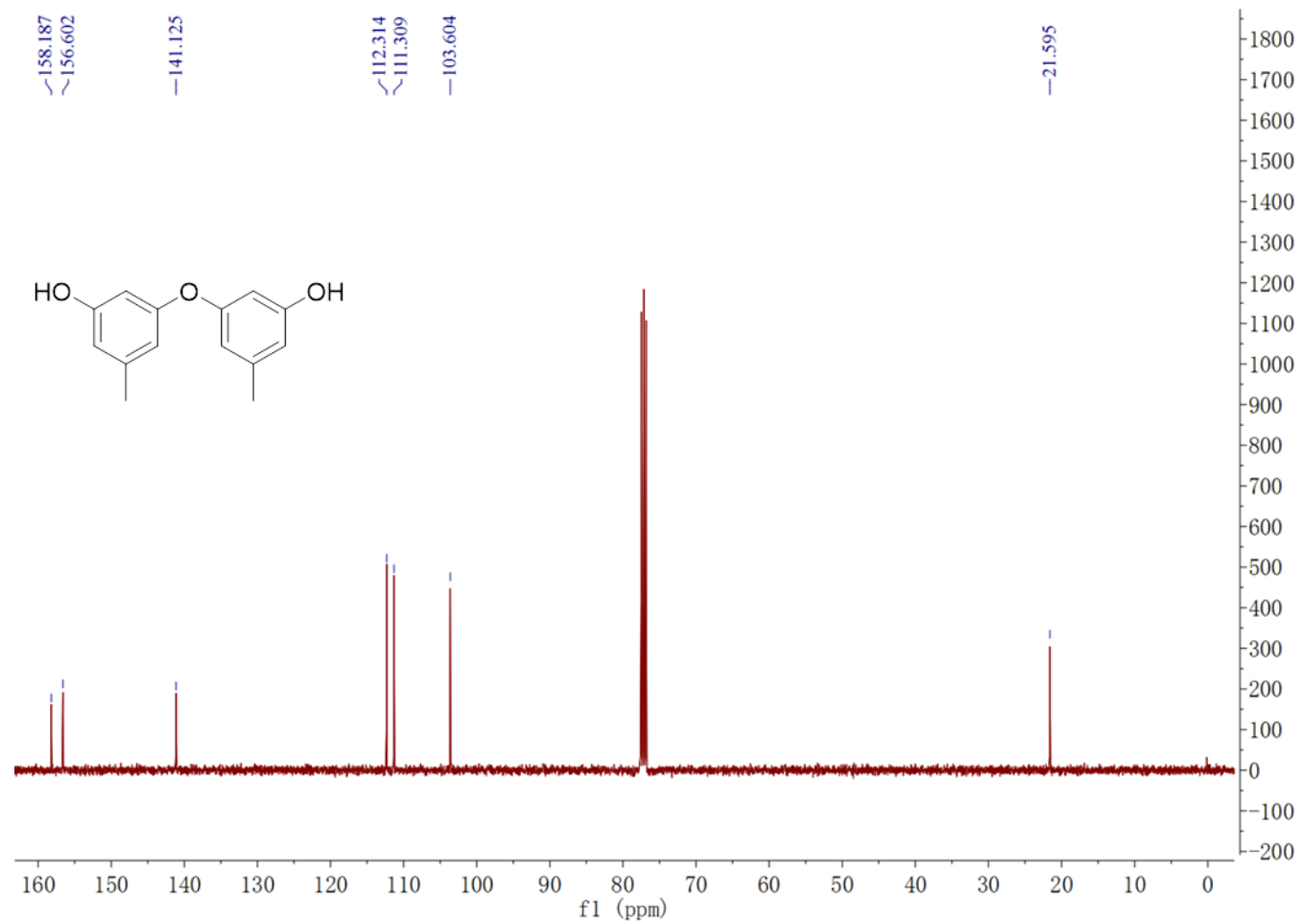


Figure S45. ¹H NMR spectrum of 3-O-methyldiorcinol (**8**) in CDCl₃ (400MHz)

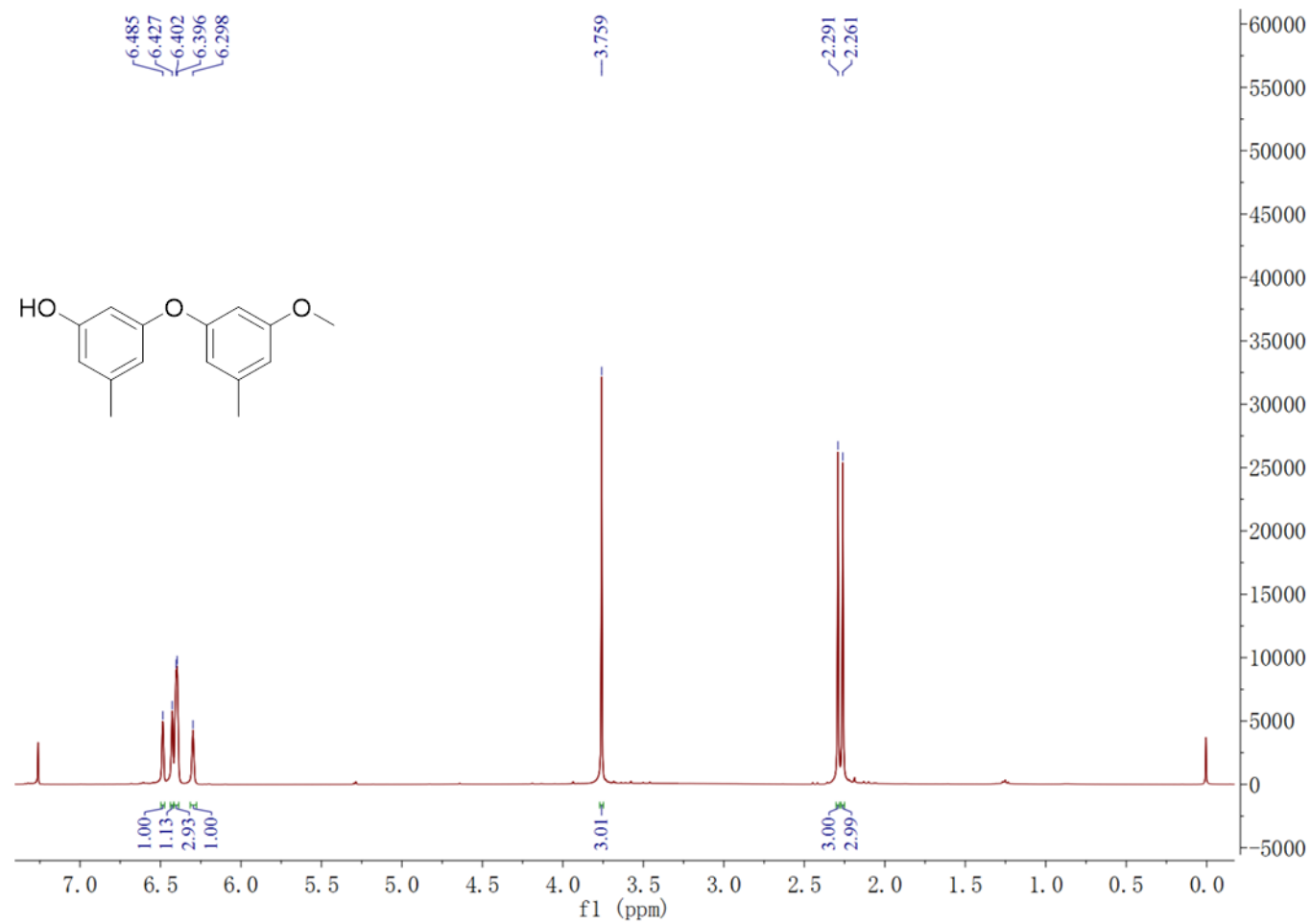


Figure S46. ^{13}C NMR spectrum of 3-O-methyldiorcinol (**8**) in CDCl_3 (100MHz)

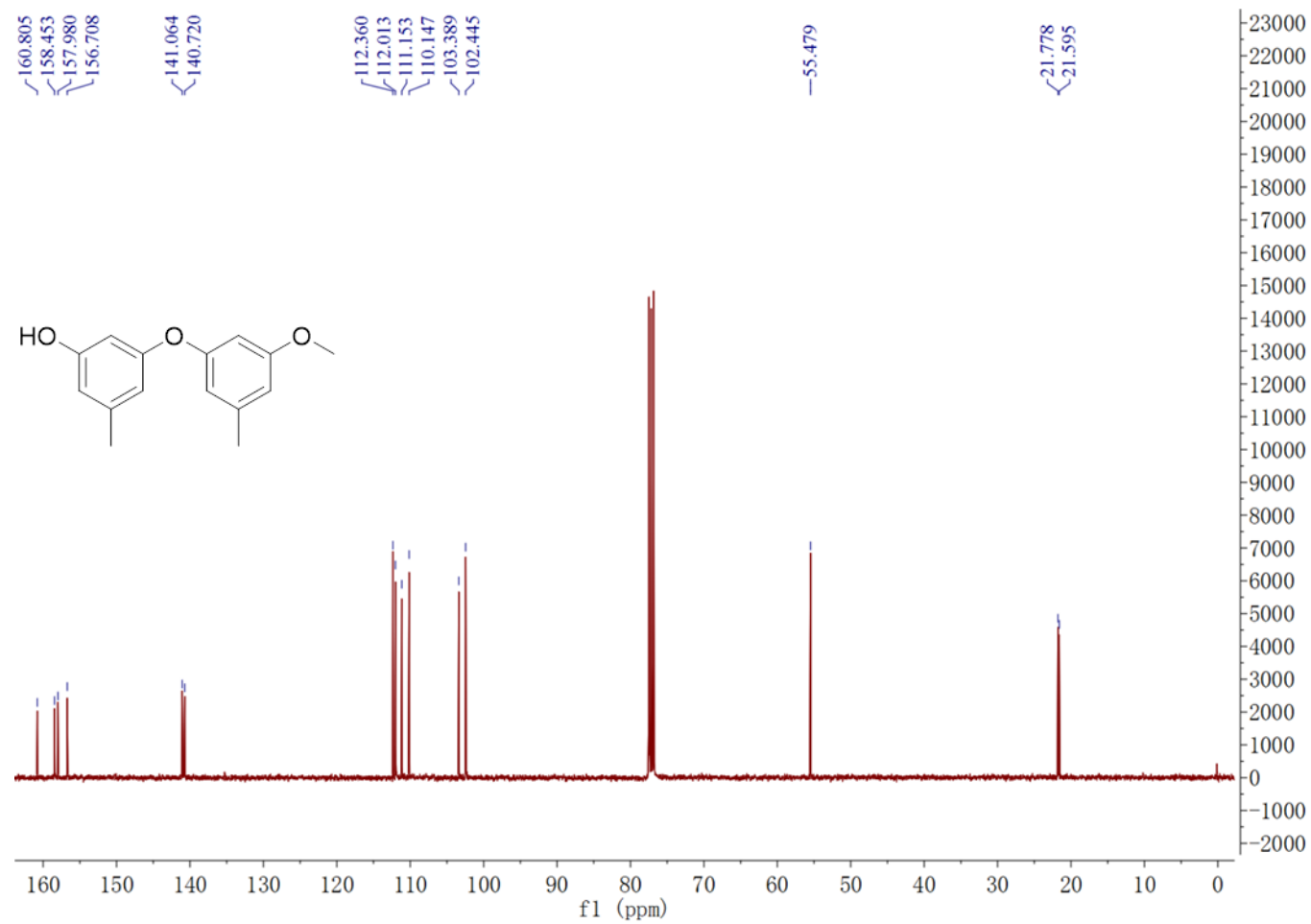


Figure.S47. ¹H NMR spectrum of 5,5'-oxybis(1-methoxy-3-methylbenzene) (**9**) in CDCl₃ (400MHz)

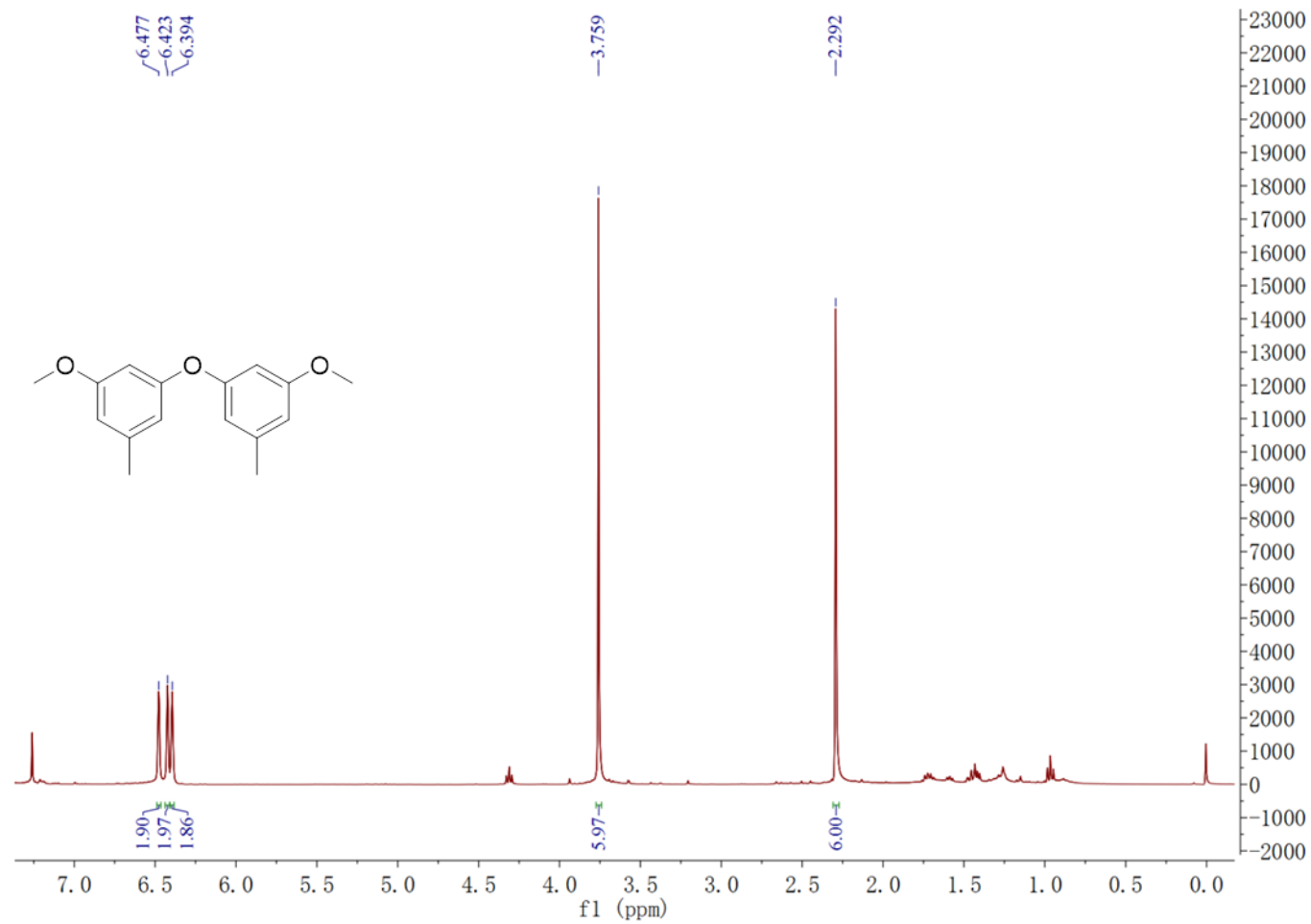


Figure S48. ^{13}C NMR spectrum of 5,5'-oxybis(1-methoxy-3-methylbenzene) (**9**) in CDCl_3 (100MHz)

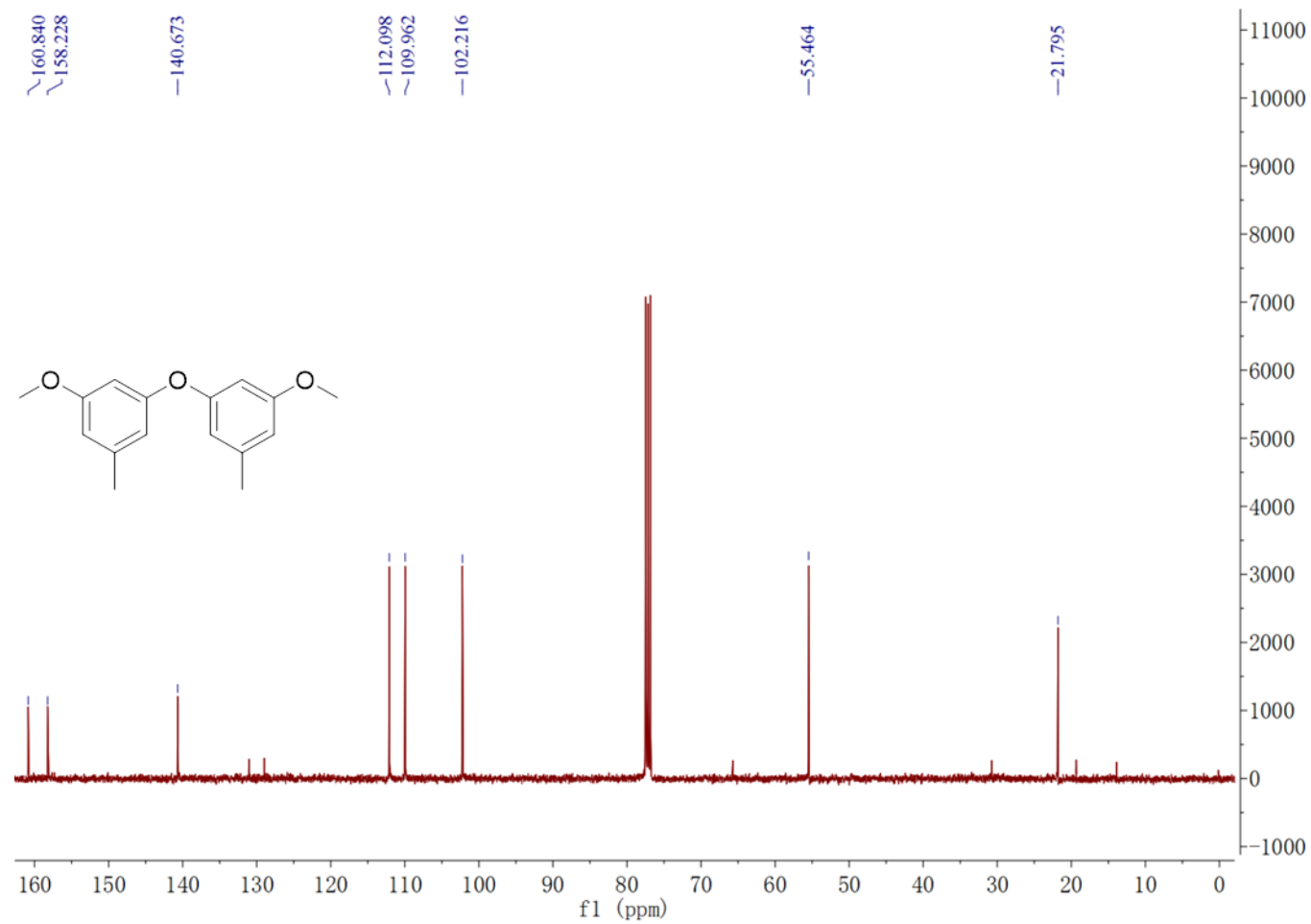


Figure S49. ^1H NMR spectrum of dibutyl phthalate (**10**) in CDCl_3 (400MHz)

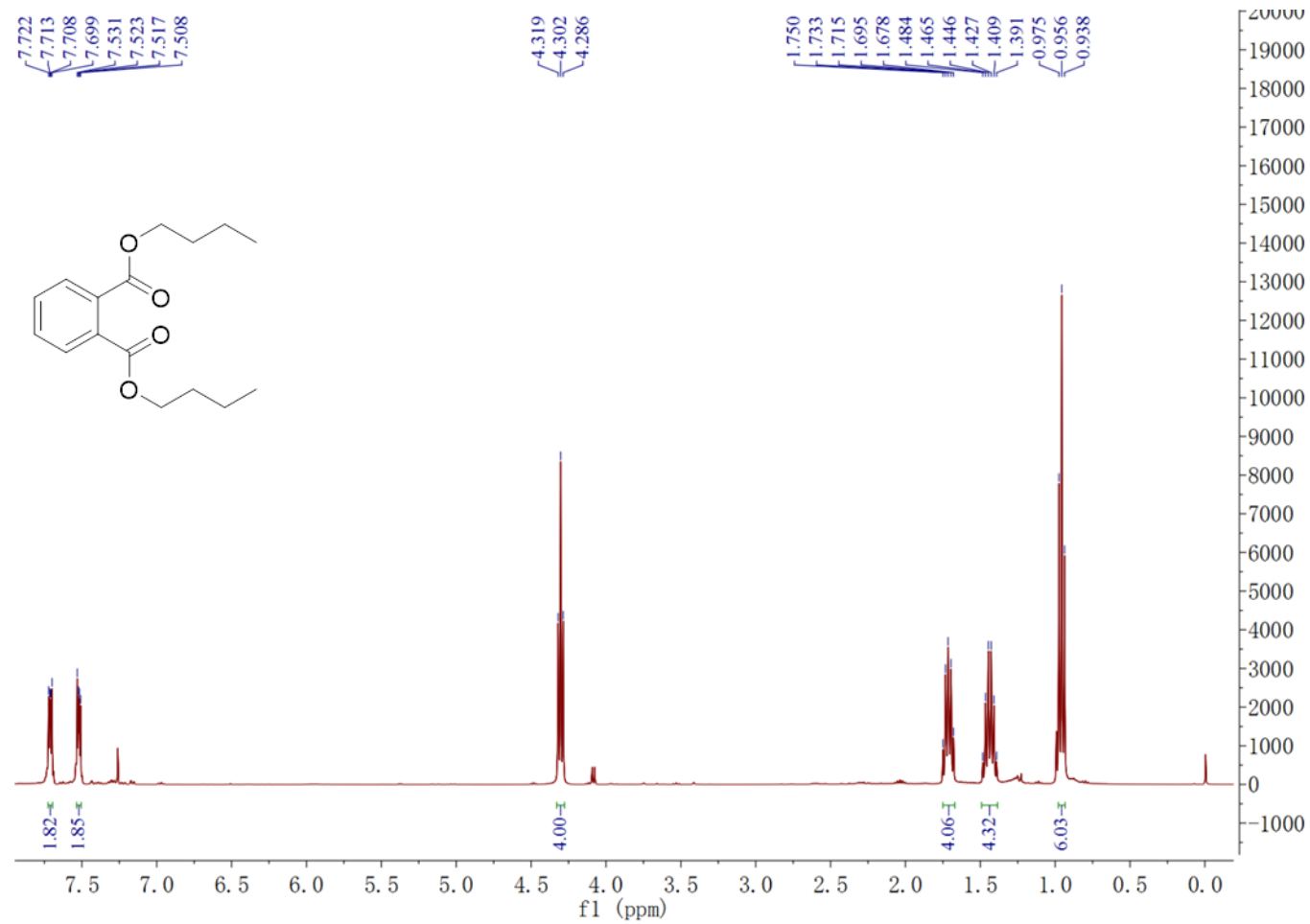


Figure S50. ^{13}C NMR spectrum of dibutyl phthalate (**10**) in CDCl_3 (100MHz)

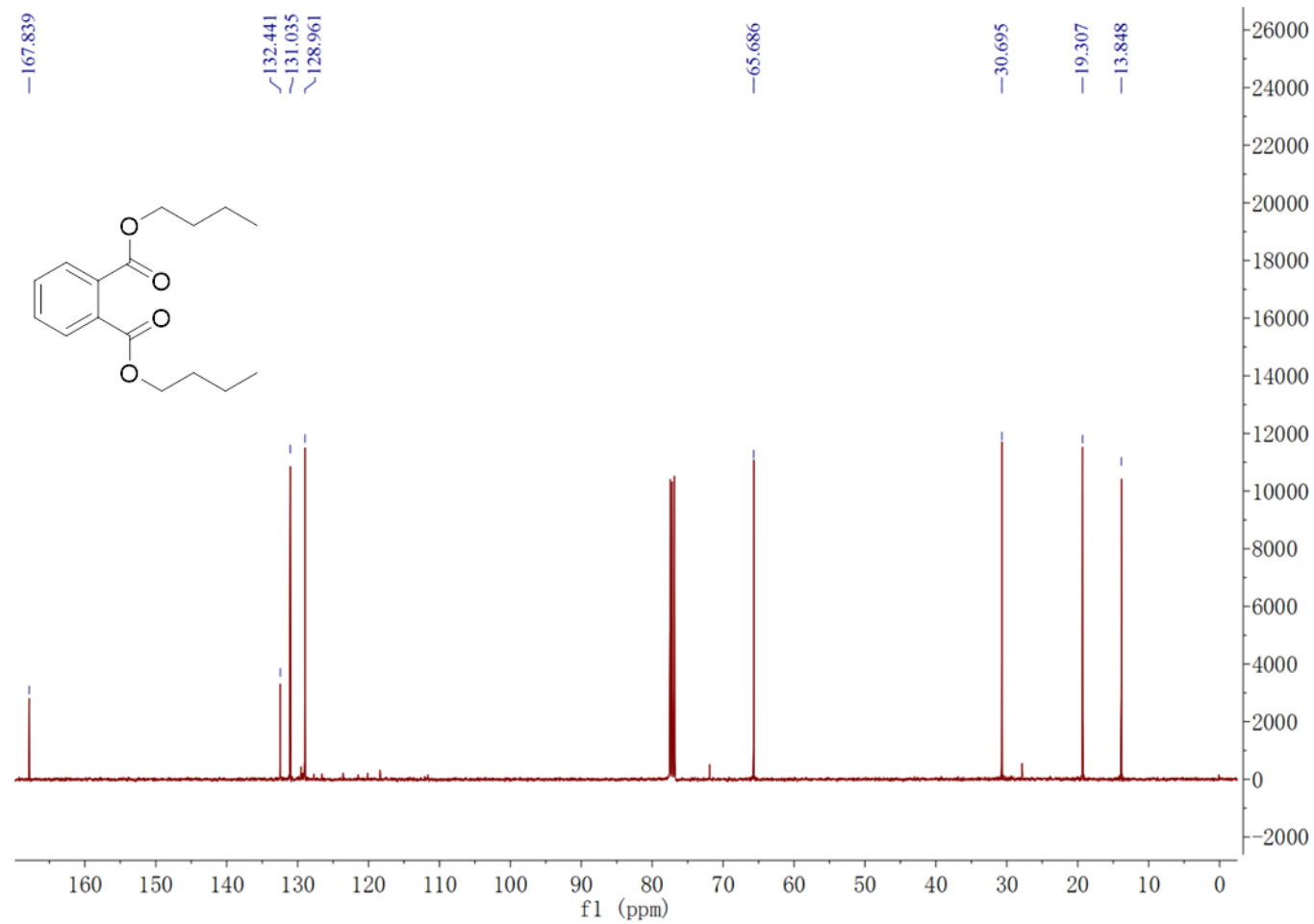


Figure S51. ^1H NMR spectrum of (2-ethylhexyl) phthalate (**11**) in CDCl_3 (400MHz)

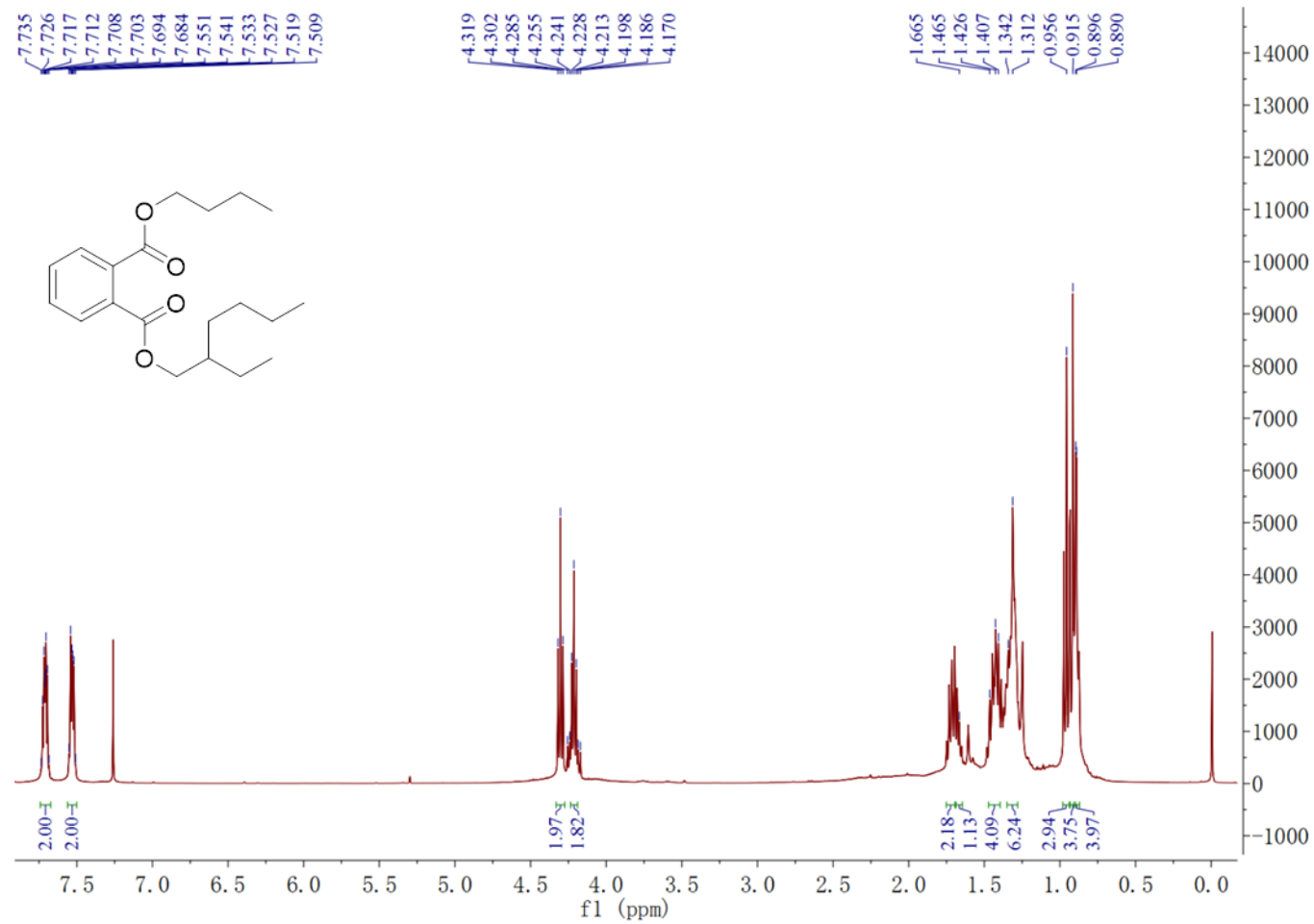


Figure S52. ^{13}C NMR spectrum of (2-ethylhexyl) phthalate (**11**) in CDCl_3 (100MHz)

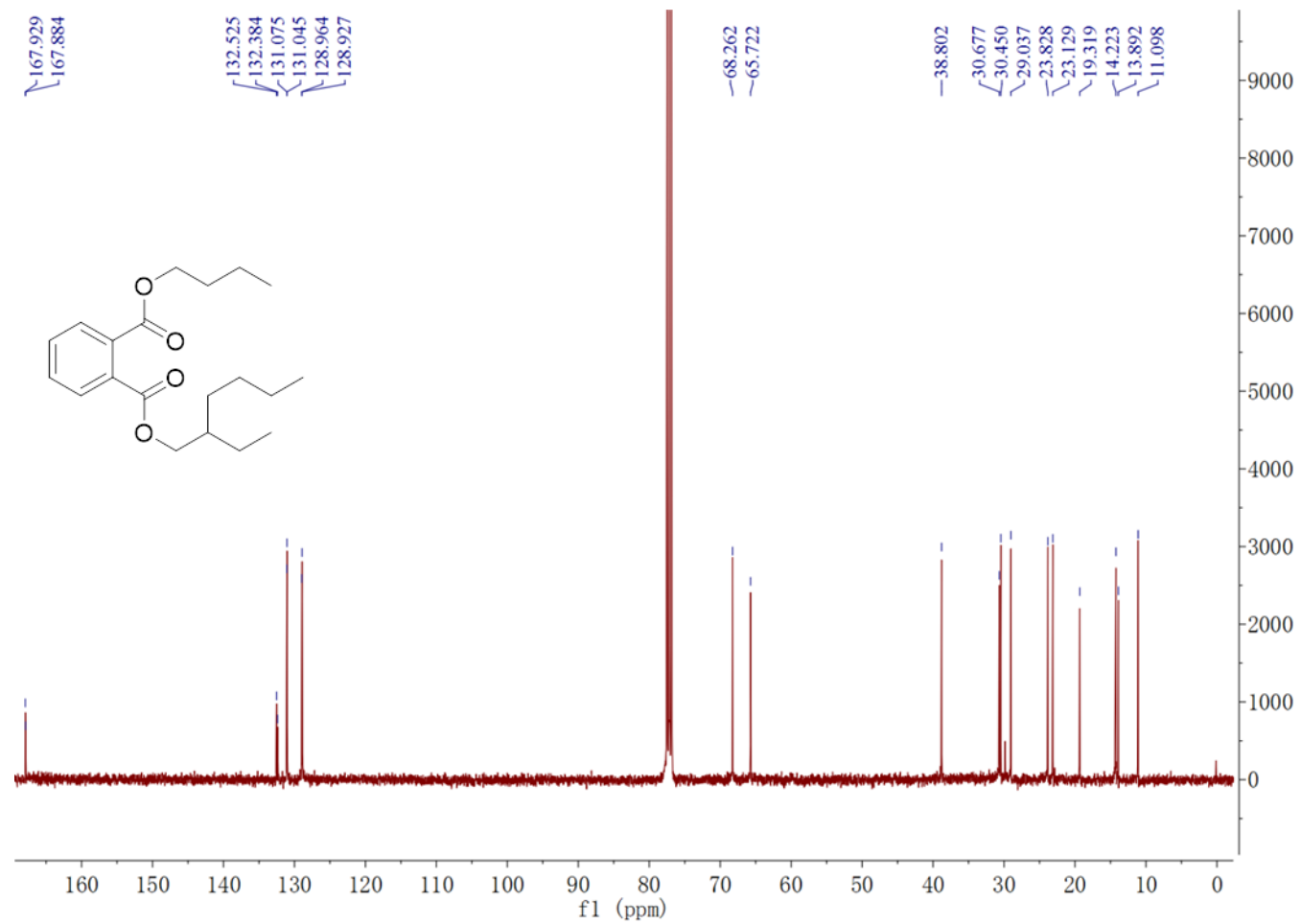


Figure S53. ^1H NMR spectrum of (2*aR*,5*R*,5*aR*,8*S*,8*aS*)-2,2,5,8-tetramethyldecahydro-2H-naphtho[1,8-*bc*]furan-5-ol (**12**) in CDCl_3 (400MHz)

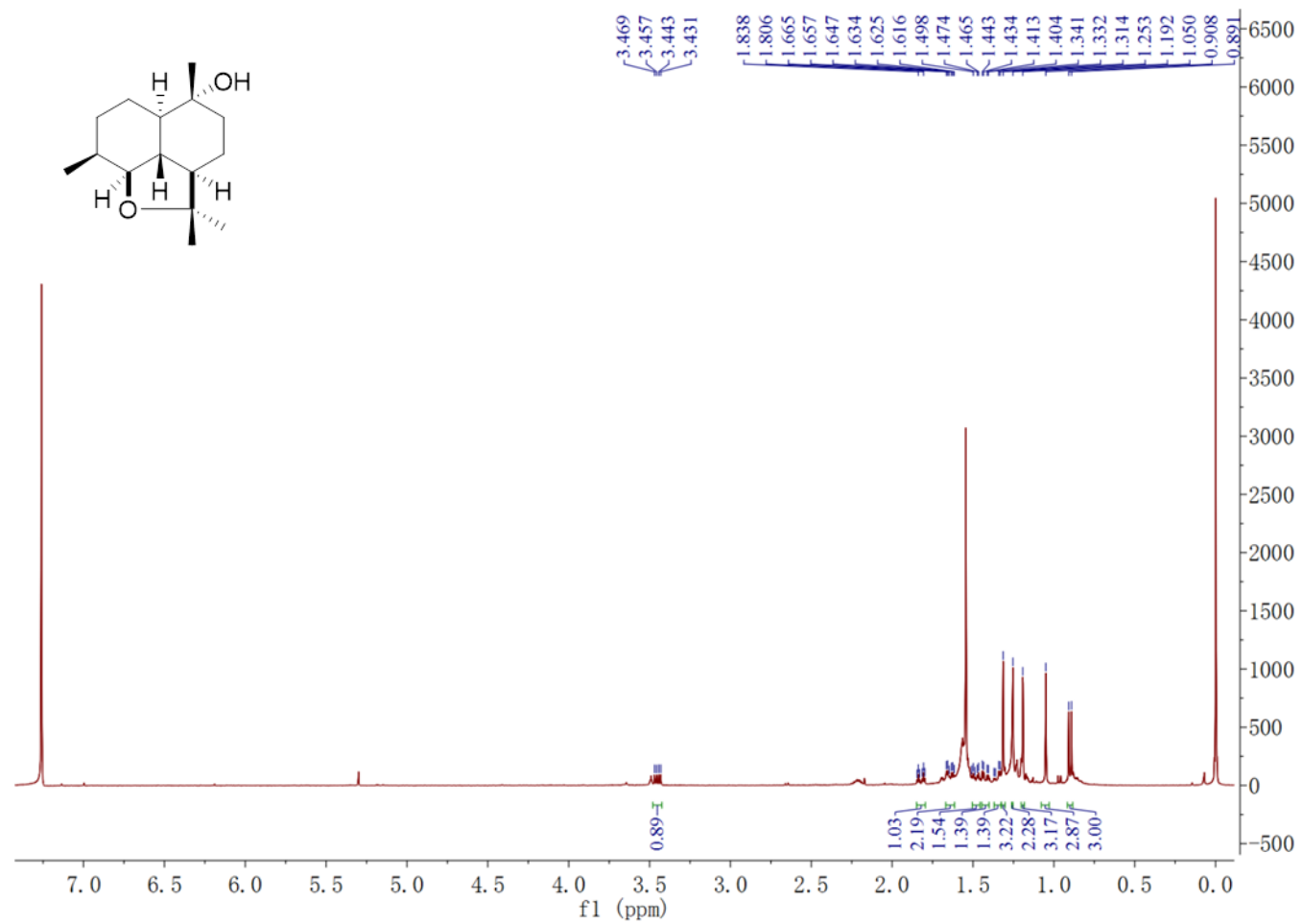


Figure S54. ^{13}C NMR spectrum of (2*aR*,5*R*,5*aR*,8*S*,8*aS*)-2,2,5,8-tetramethyldecahydro-2H-naphtho[1,8-*bc*]furan-5-ol (**12**) in CDCl_3 (100MHz)

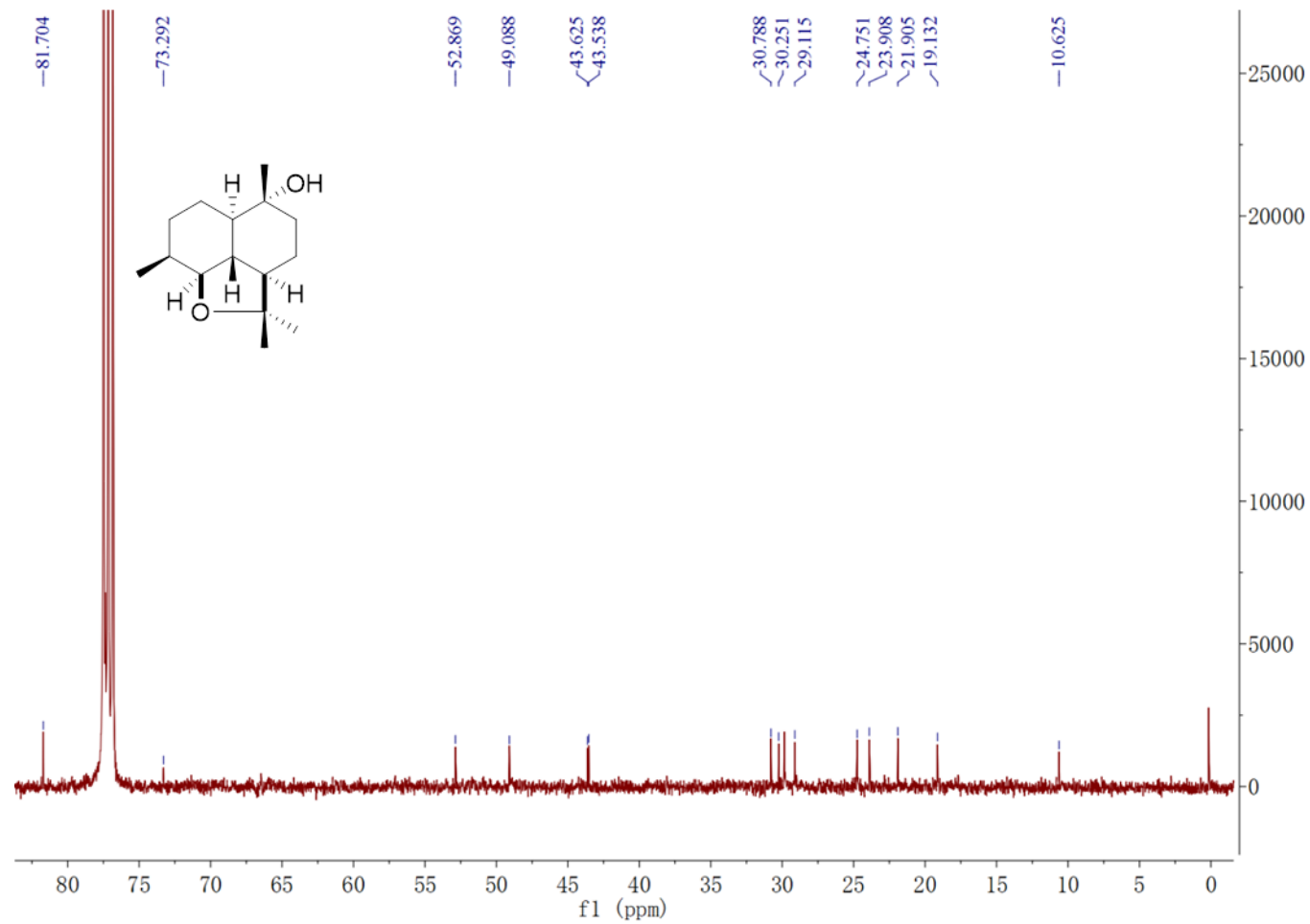


Figure S55 ^1H NMR spectrum of aspewentin A (**13**) in CDCl_3 (400MHz)

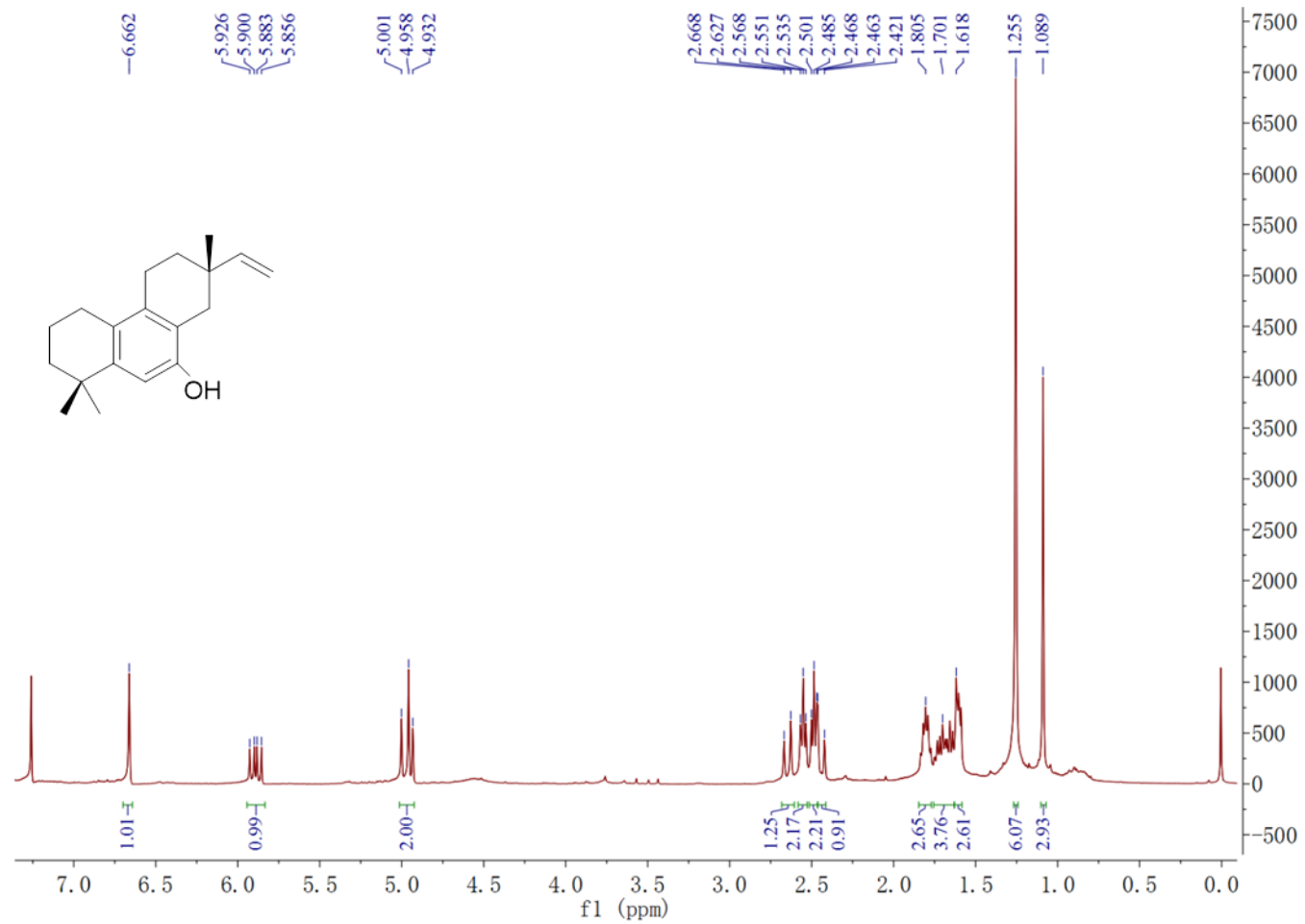


Figure S56. ^{13}C NMR spectrum of aspewentin A (**13**) in CDCl_3 (100MHz)

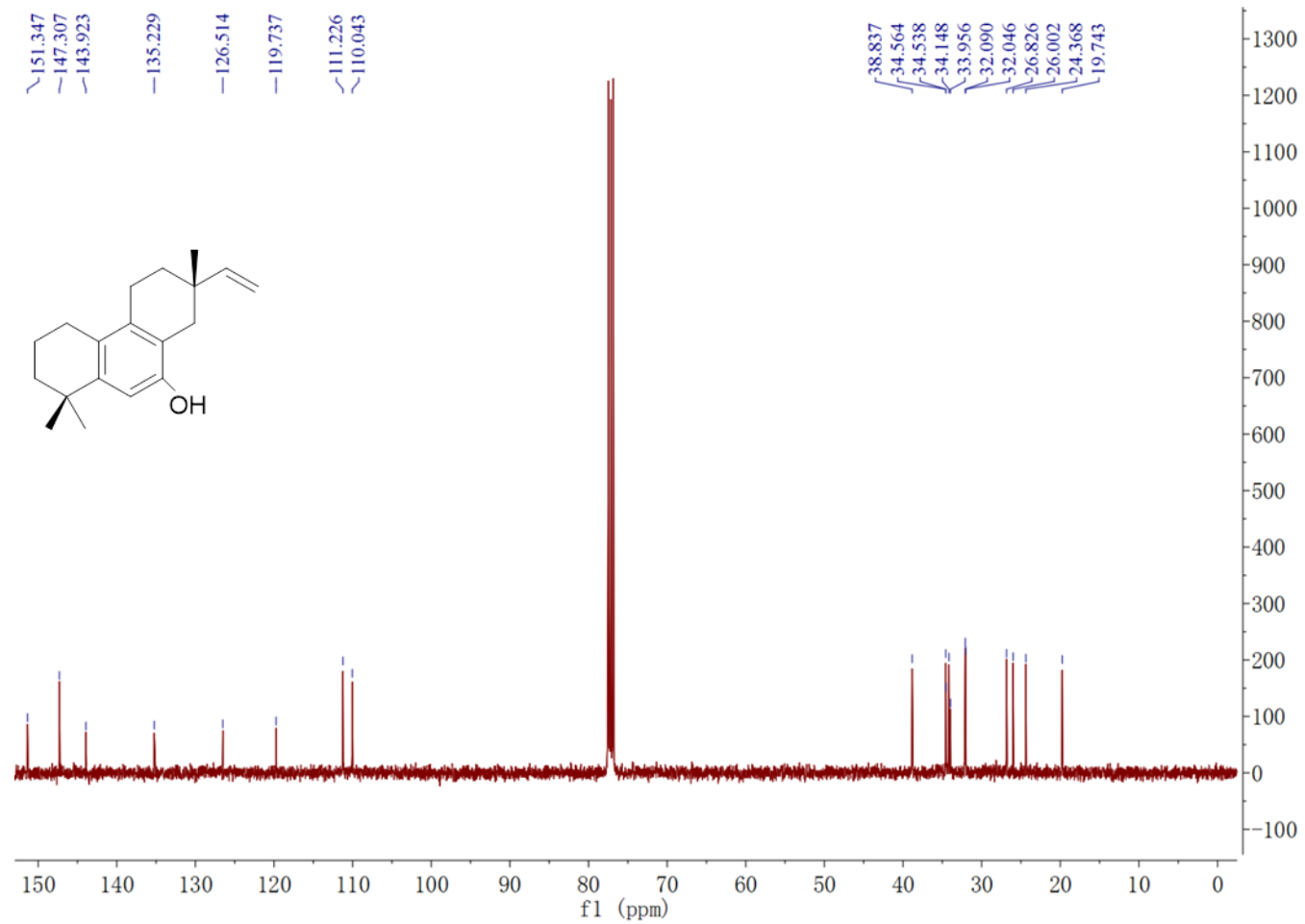


Figure S57. ¹H NMR spectrum of JBIR-03 (**14**) in CDCl₃ (400MHz)

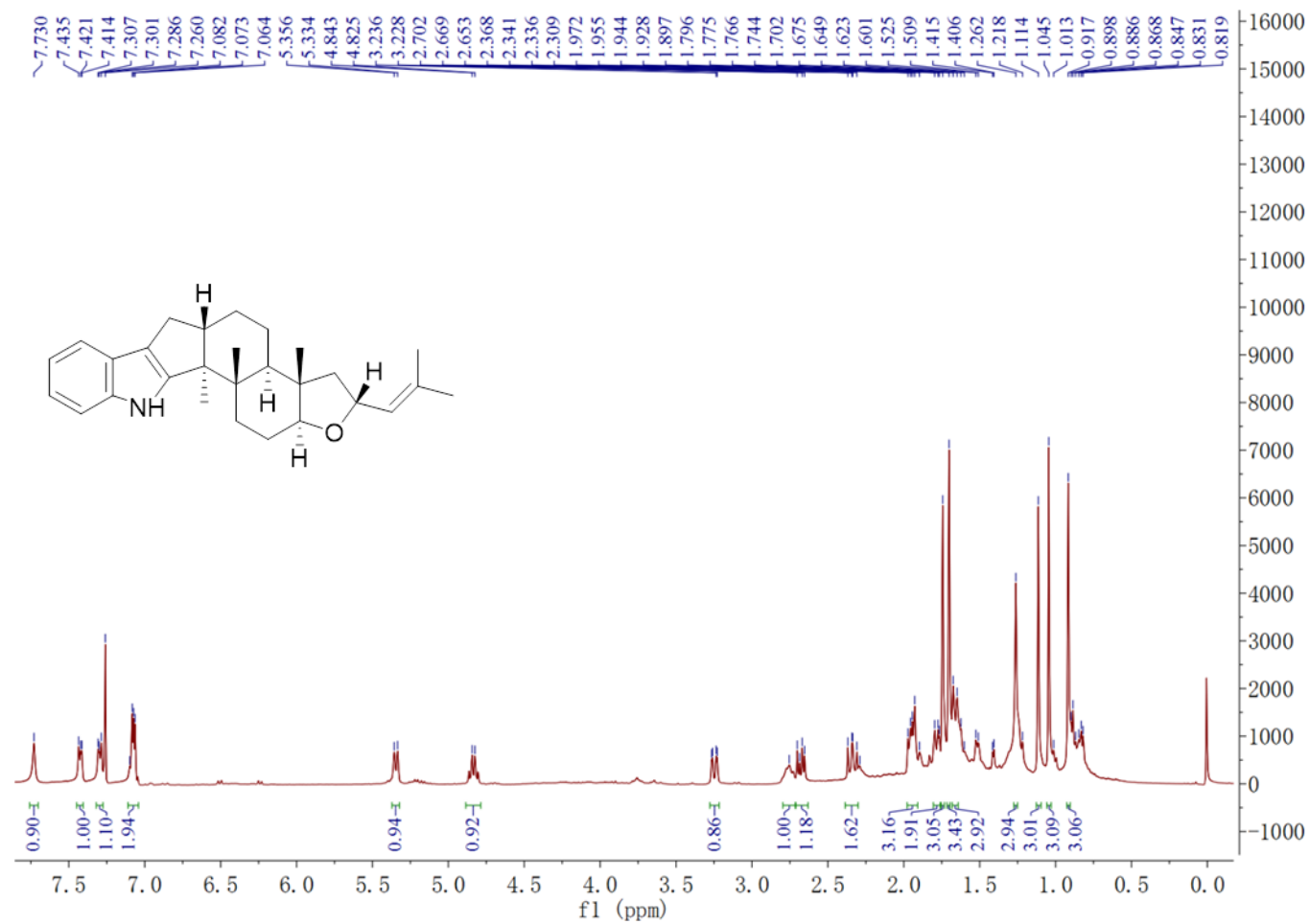


Figure S58. ^{13}C NMR spectrum of JBIR-03 (**14**) in CDCl_3 (100MHz)

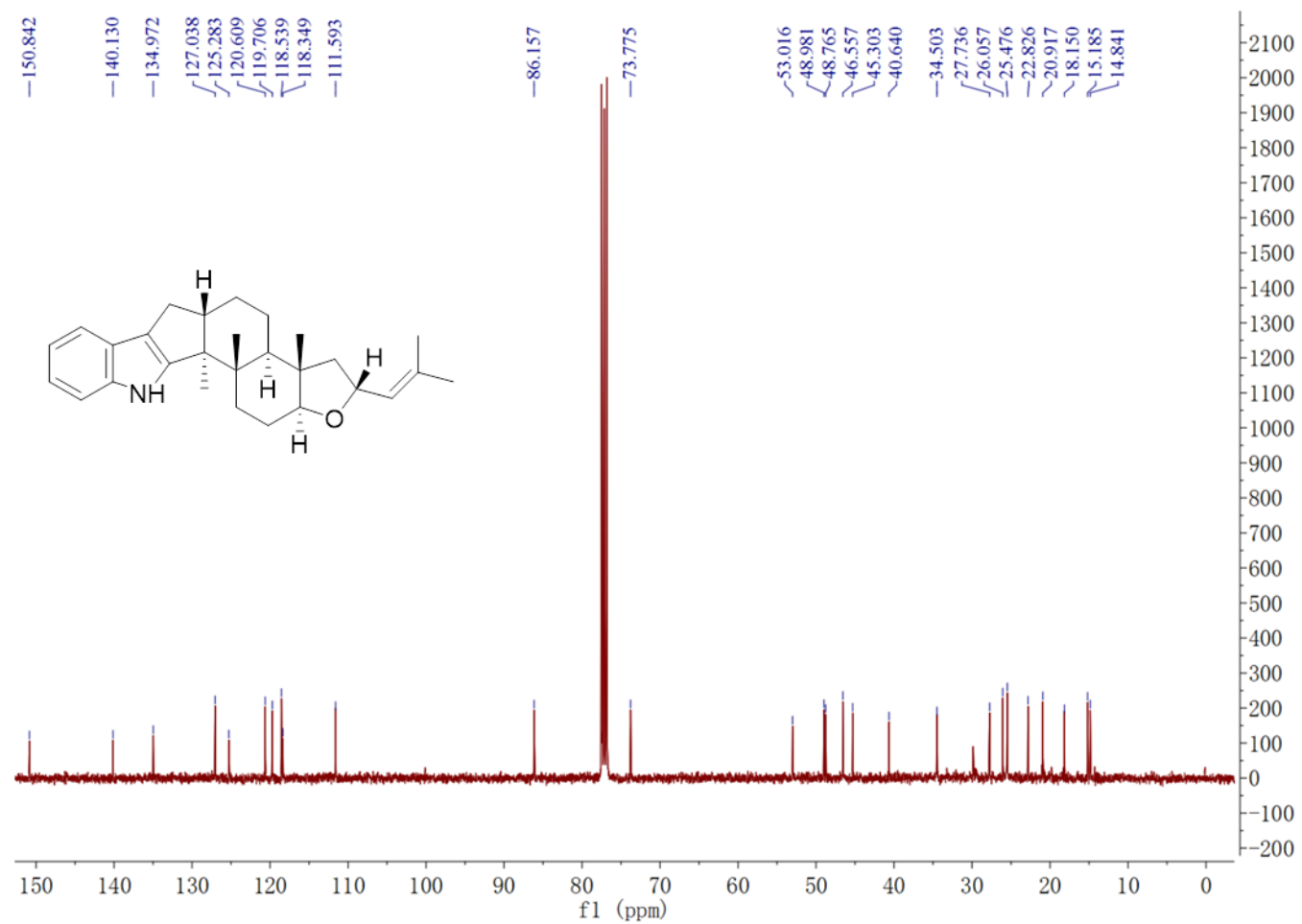


Figure S59. HR-ESI-MS spectrum of dichocerazine A (**15**)

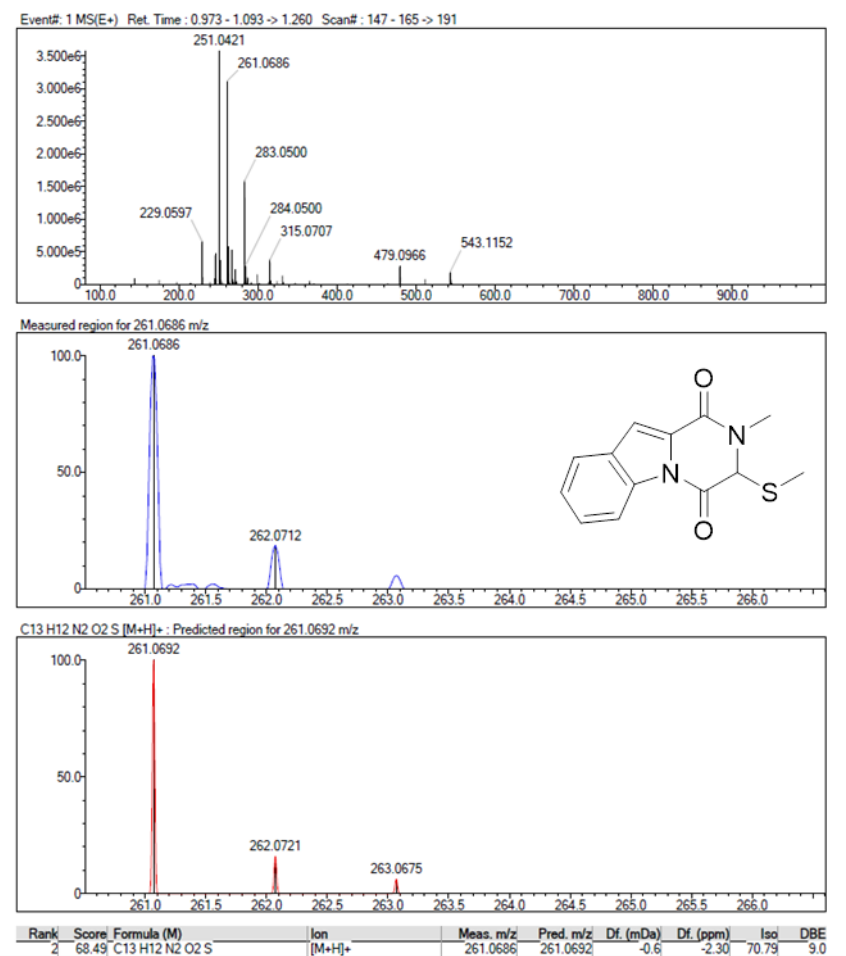


Figure S60. ^1H NMR spectrum of dichocerazine A (**15**) in CDCl_3 (400MHz)

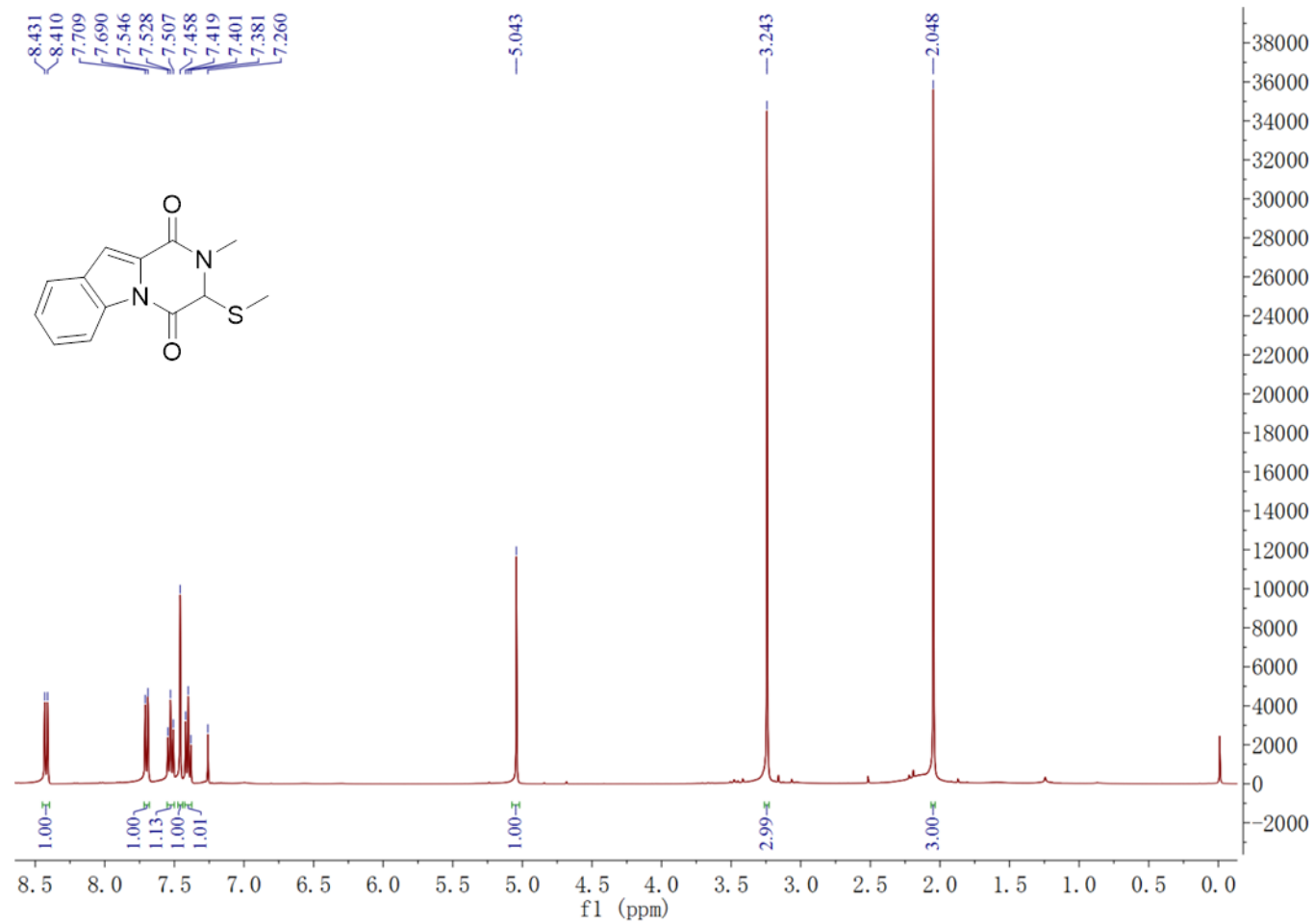


Figure S61. ^{13}C NMR spectrum of dichocerazine A (**15**) in CDCl_3 (100MHz)

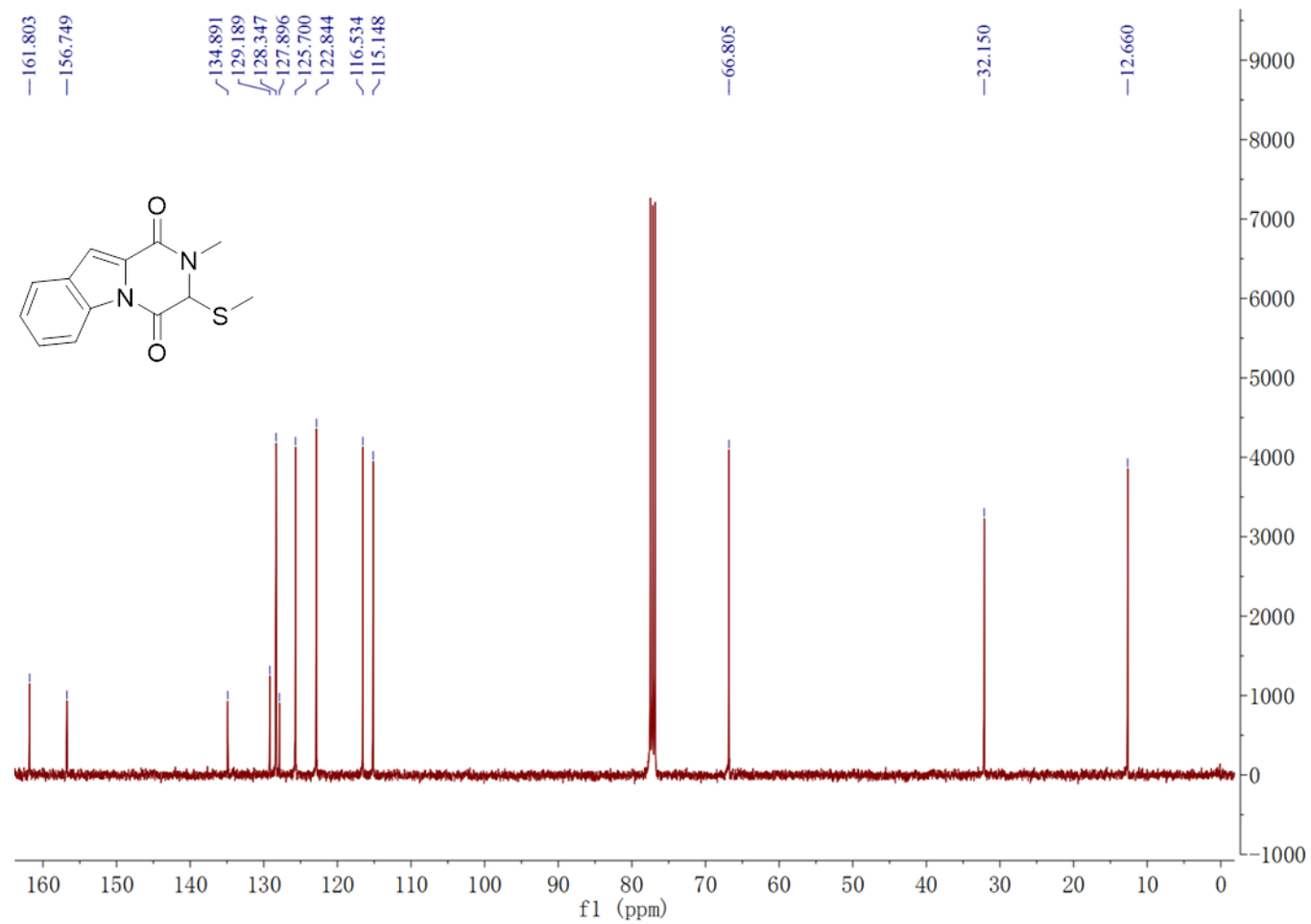


Figure S62. DEPT 135 spectrum of dichocerazine A (**15**) in CDCl₃ (100MHz)

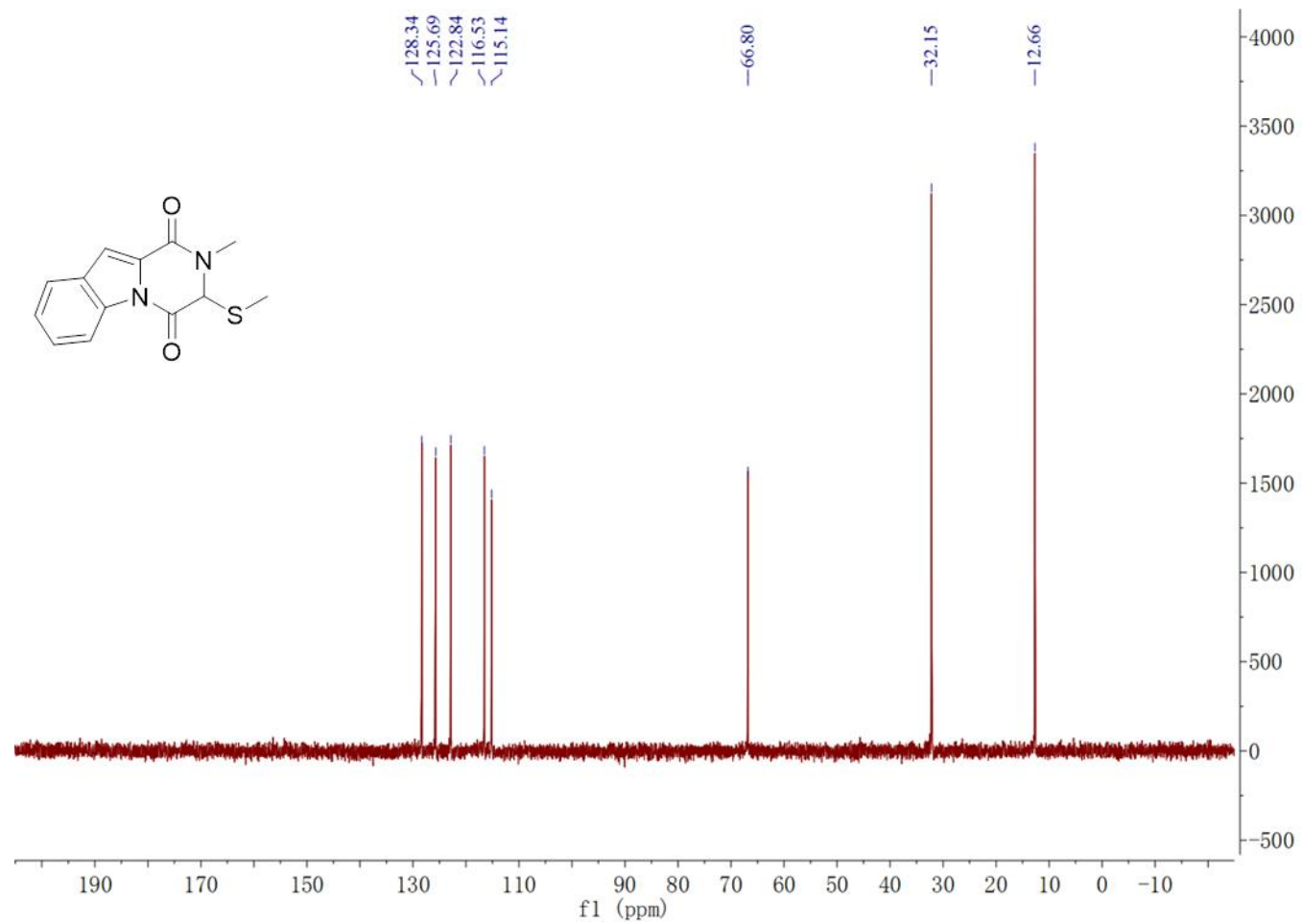


Figure S63. HMQC spectrum of dichocerazine A (**15**) in CDCl₃

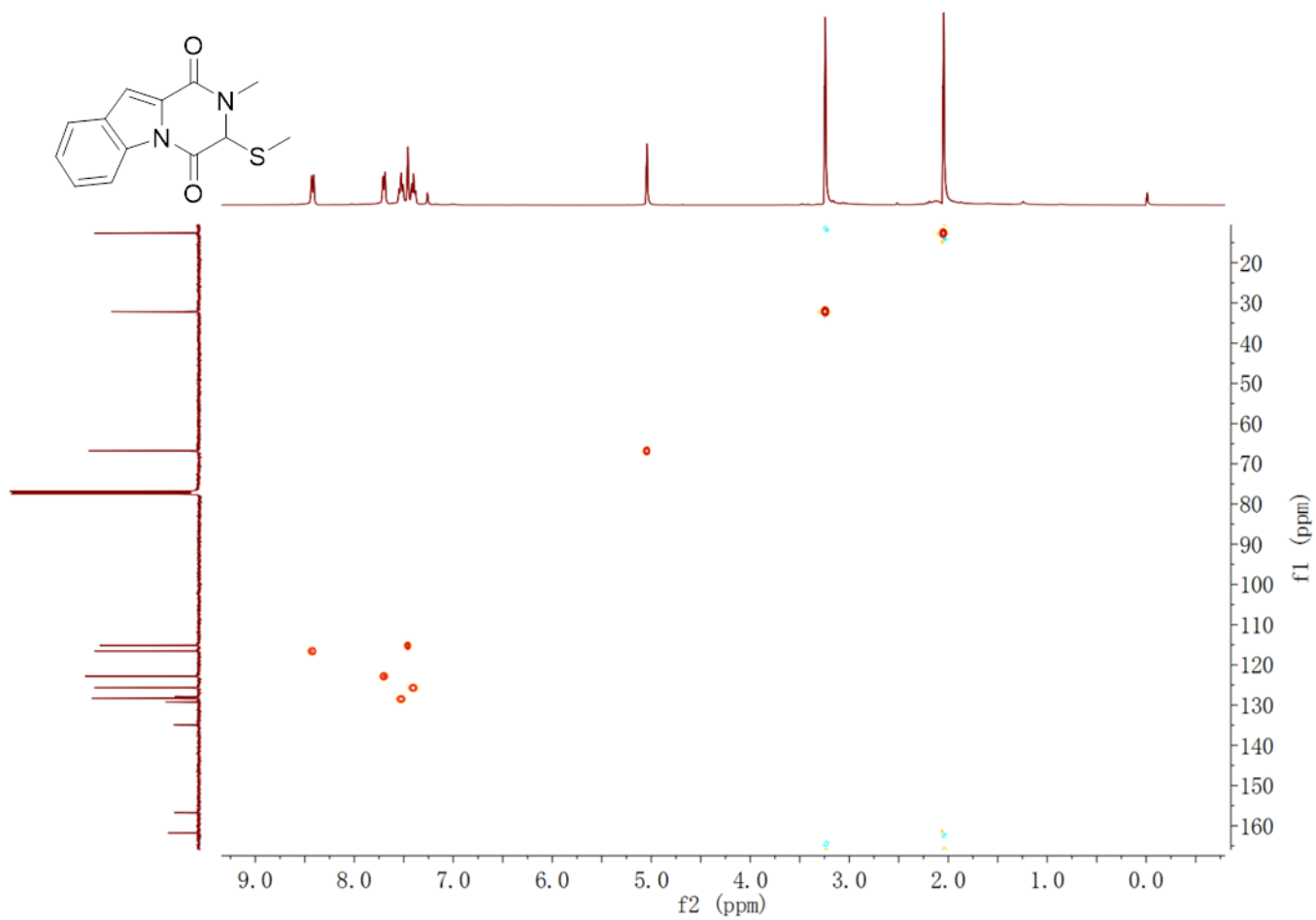


Figure S64. ^1H - ^1H COSY spectrum of dichocerazine A (**15**) in CDCl_3

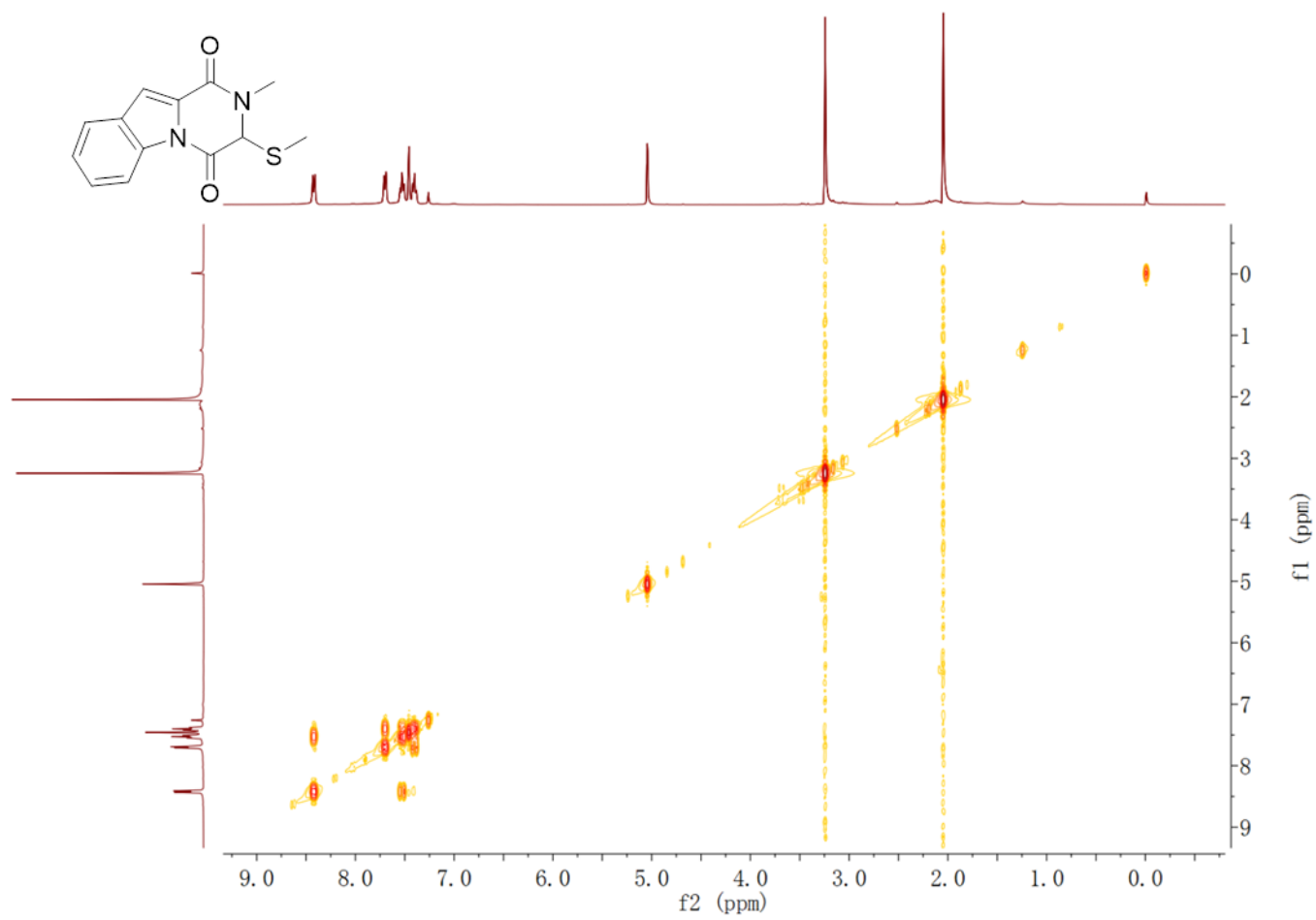


Figure S65. HMBC spectrum of dichocerazine A (**15**) in CDCl₃

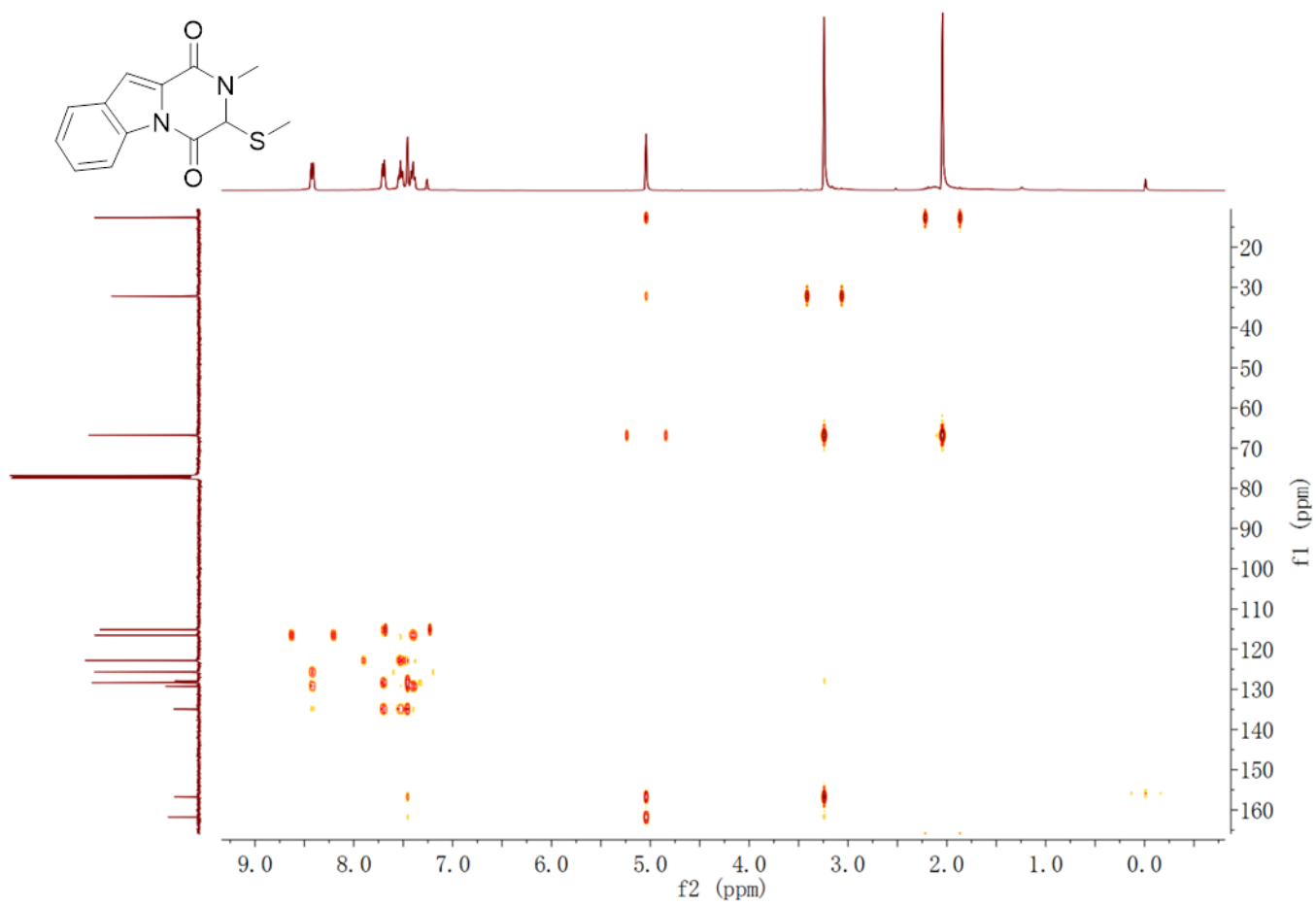


Figure S66. NOESY spectrum of dichocerazine A (**15**) in CDCl₃

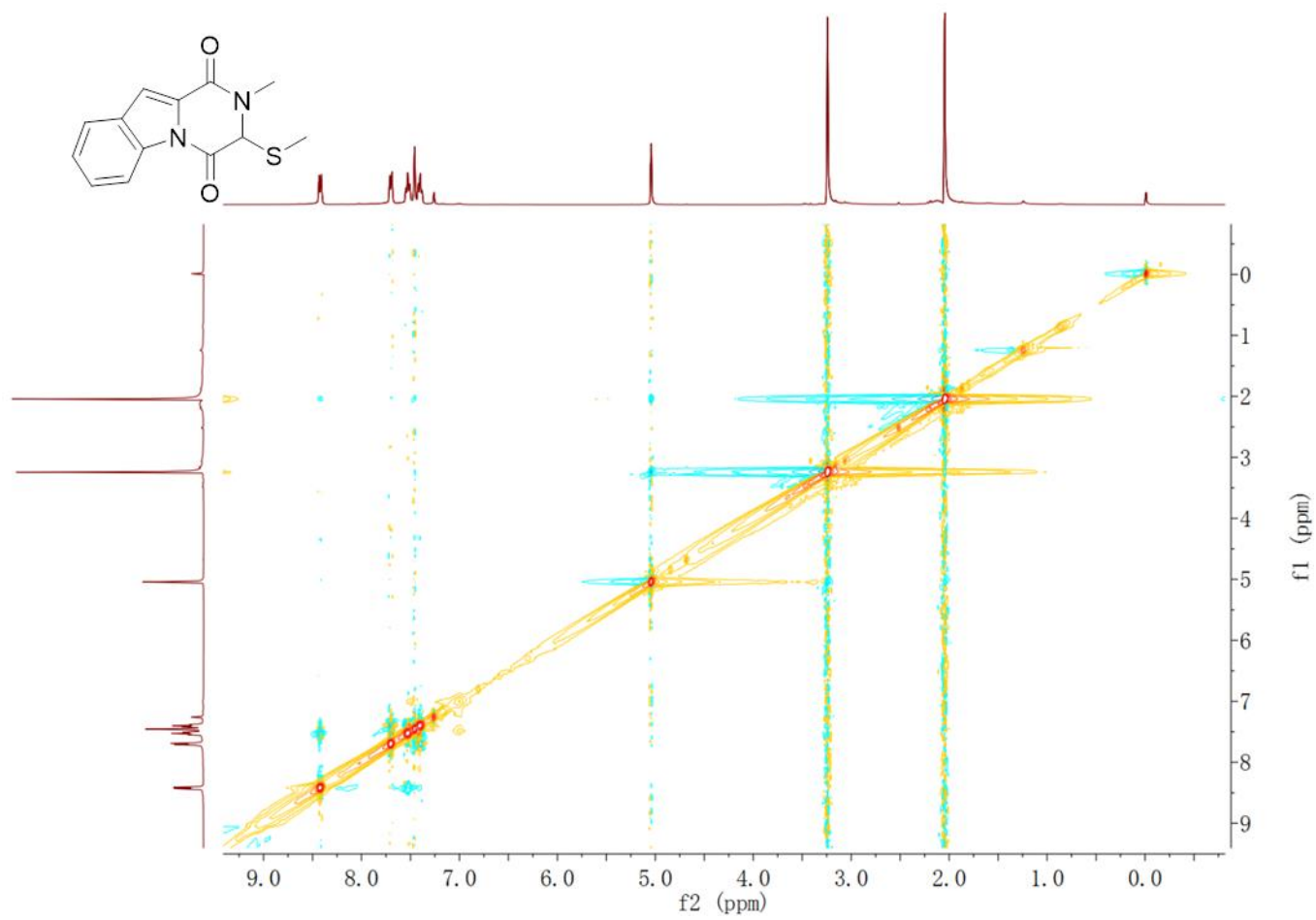


Figure S67. HR-ESI-MS spectrum of dichocerazine B (**16**)

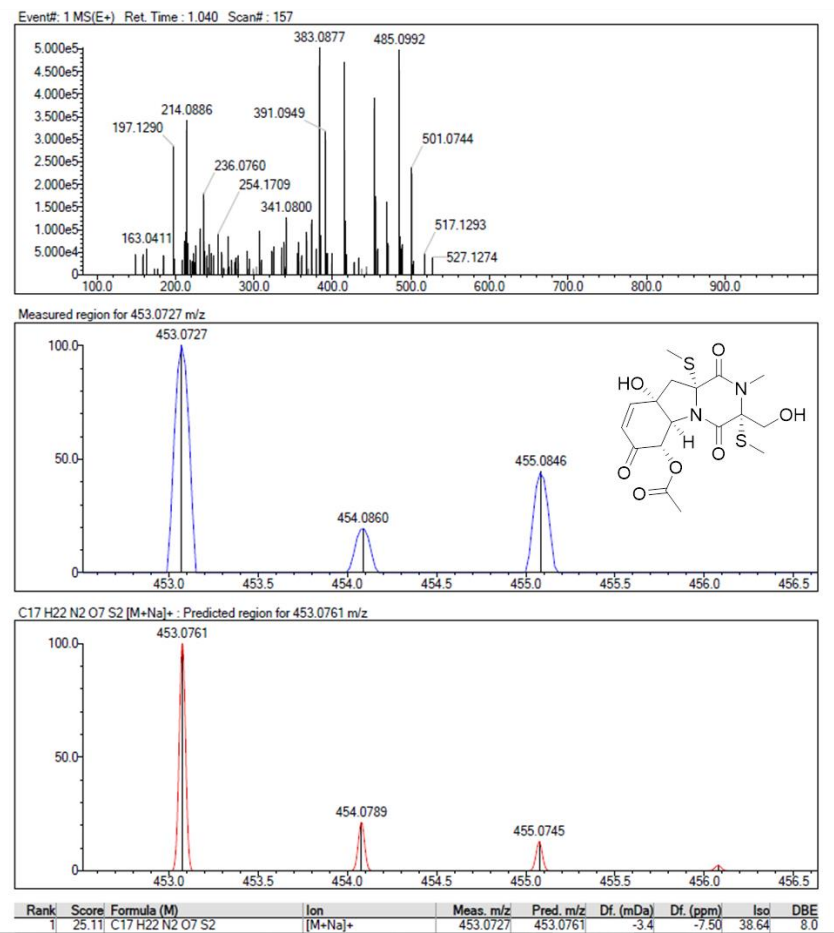


Figure S68. ^1H NMR spectrum of dichocerazine B (**16**) in CDCl_3 (400MHz)

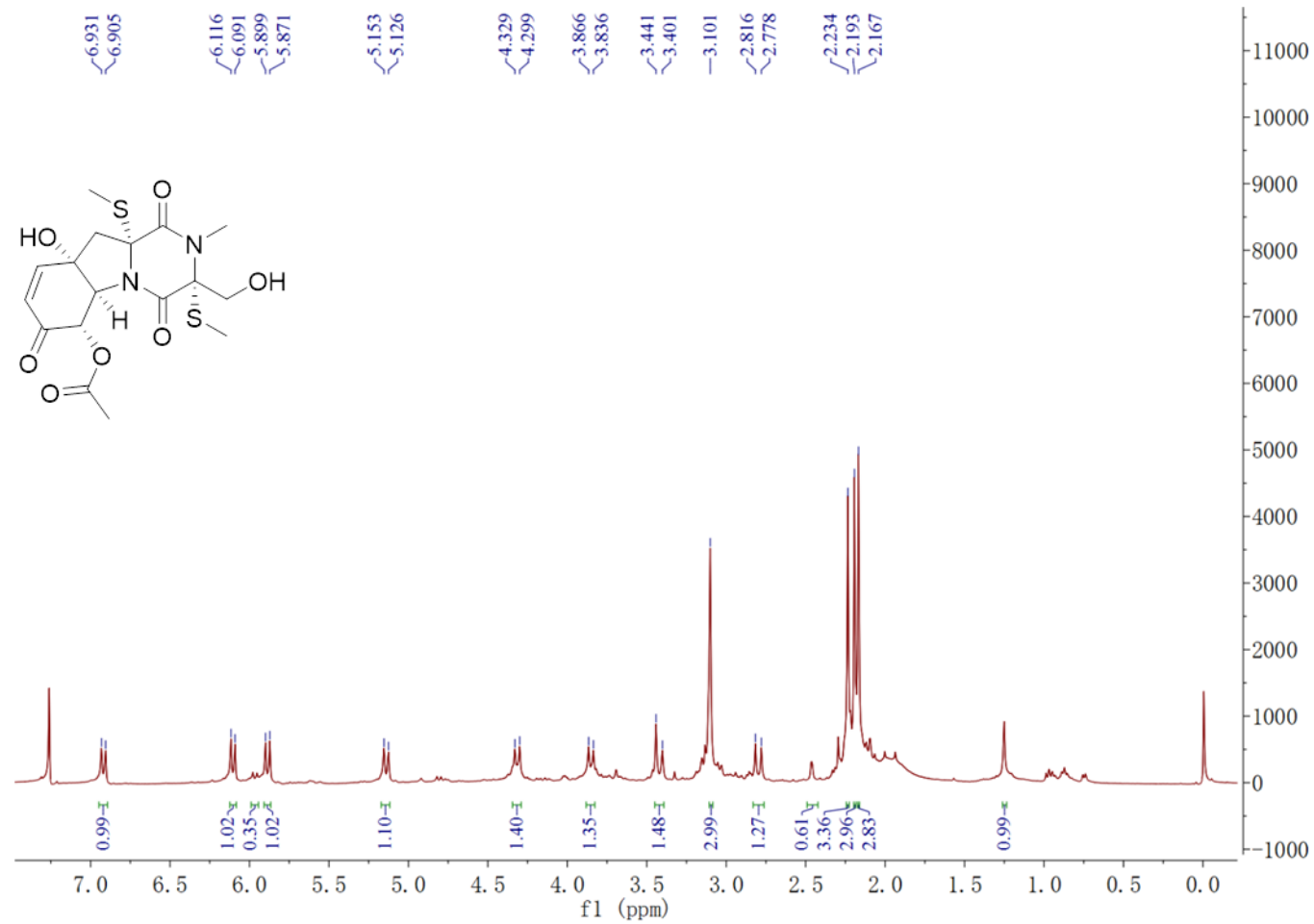


Figure S69 ^{13}C NMR spectrum of dichocerazine B (**16**) in CDCl_3 (100MHz)

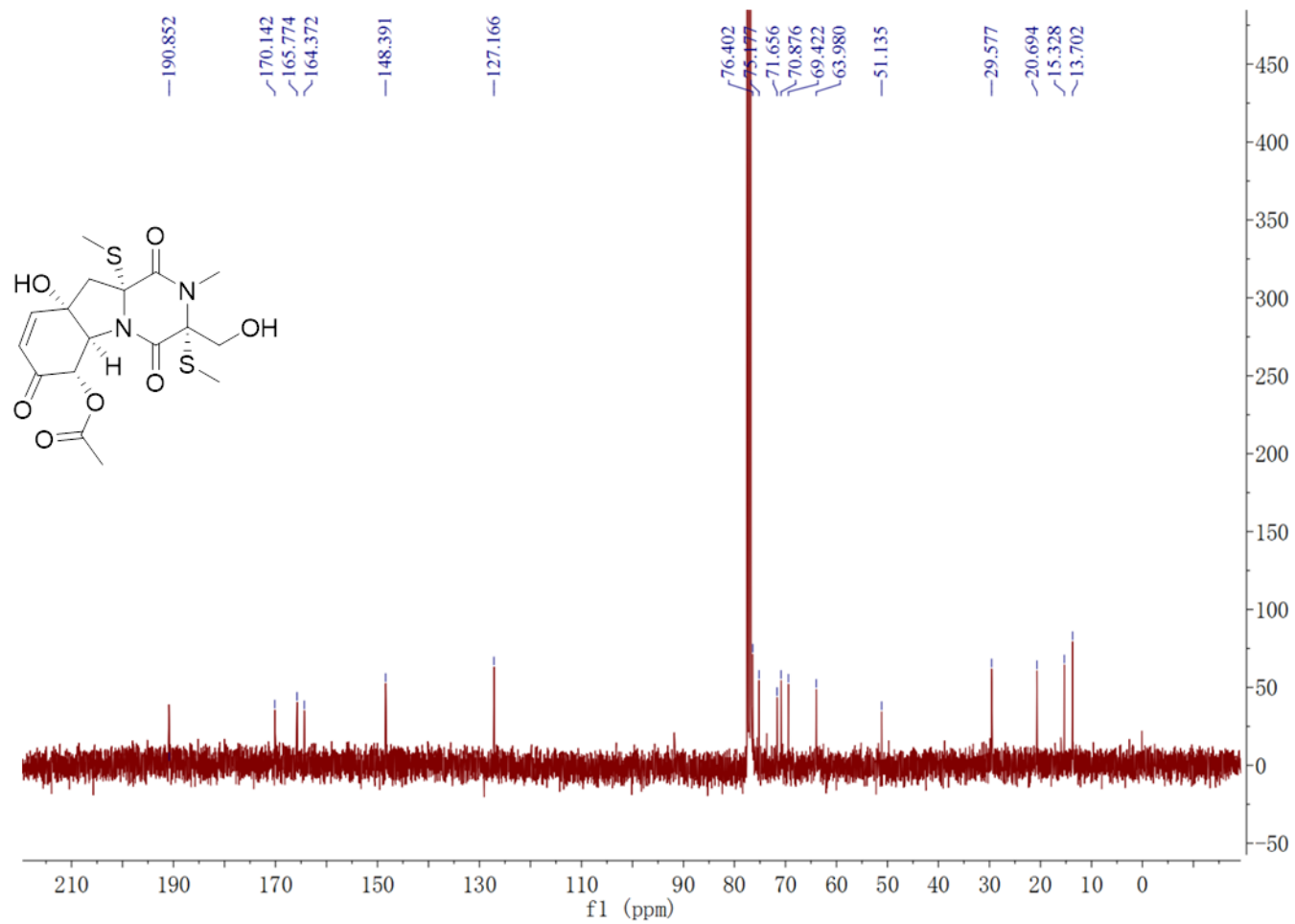


Figure S70. DEPT 135 spectrum of dichocerazine B (**16**) in CDCl₃ (100MHz)

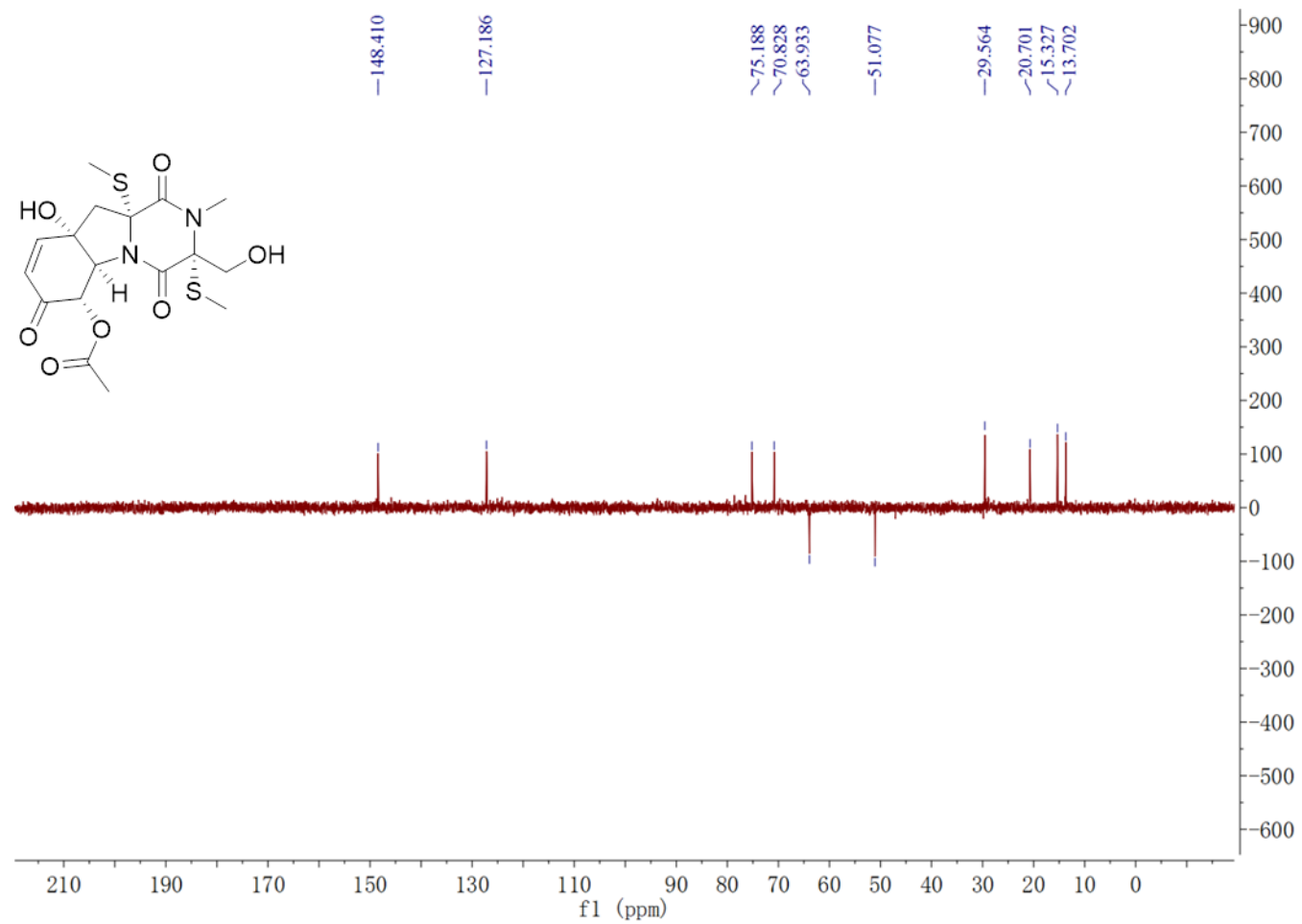


Figure S71. HMQC spectrum of dichocerazine B (**16**) in CDCl₃

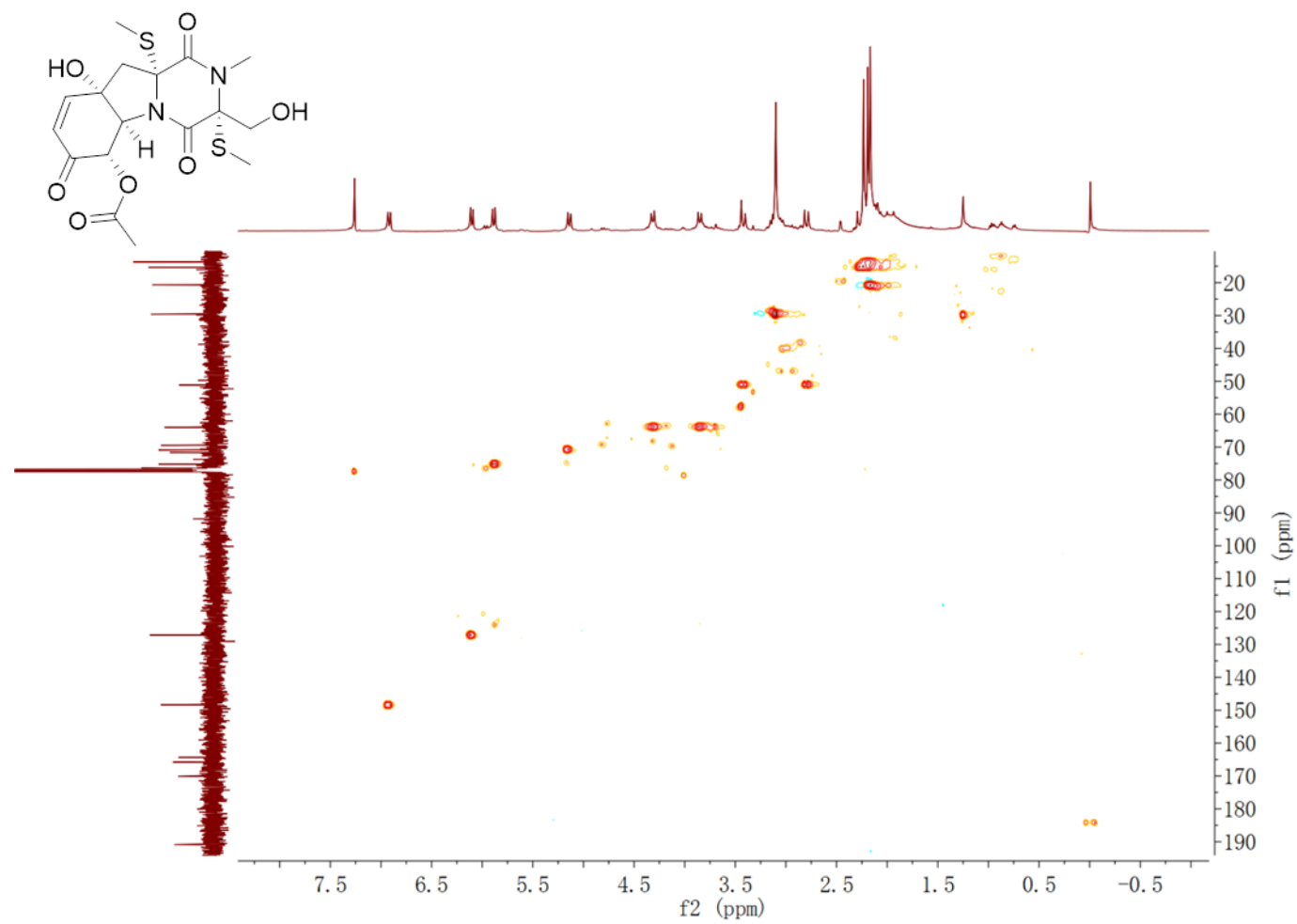


Figure S72. ^1H - ^1H COSY spectrum of dichocerazine B (**16**) in CDCl_3

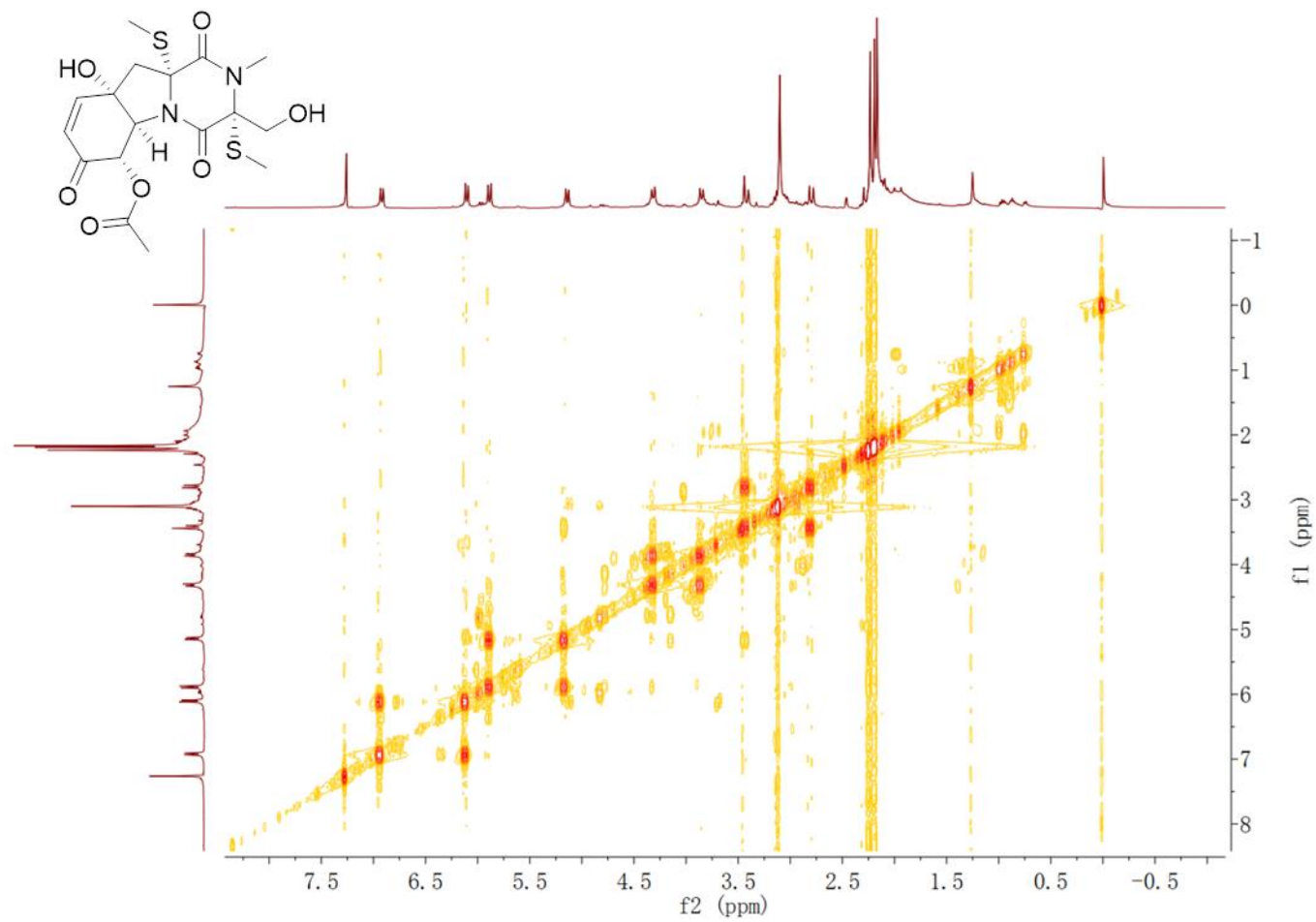


Figure S73. HMBC spectrum of dichocerazine B (**16**) in CDCl₃

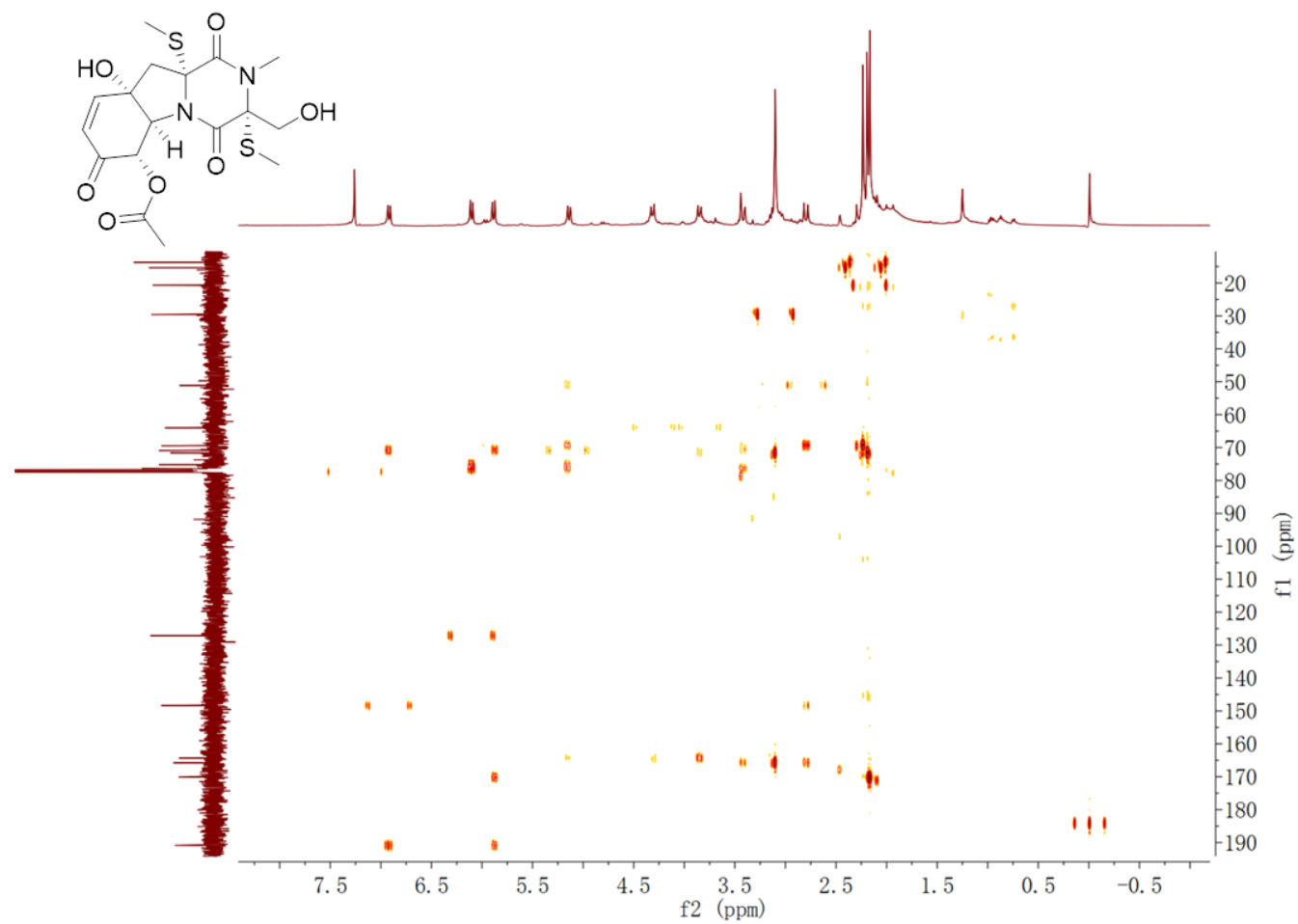


Figure S74. NOESY spectrum of dichocerazine B (**16**) in CDCl₃

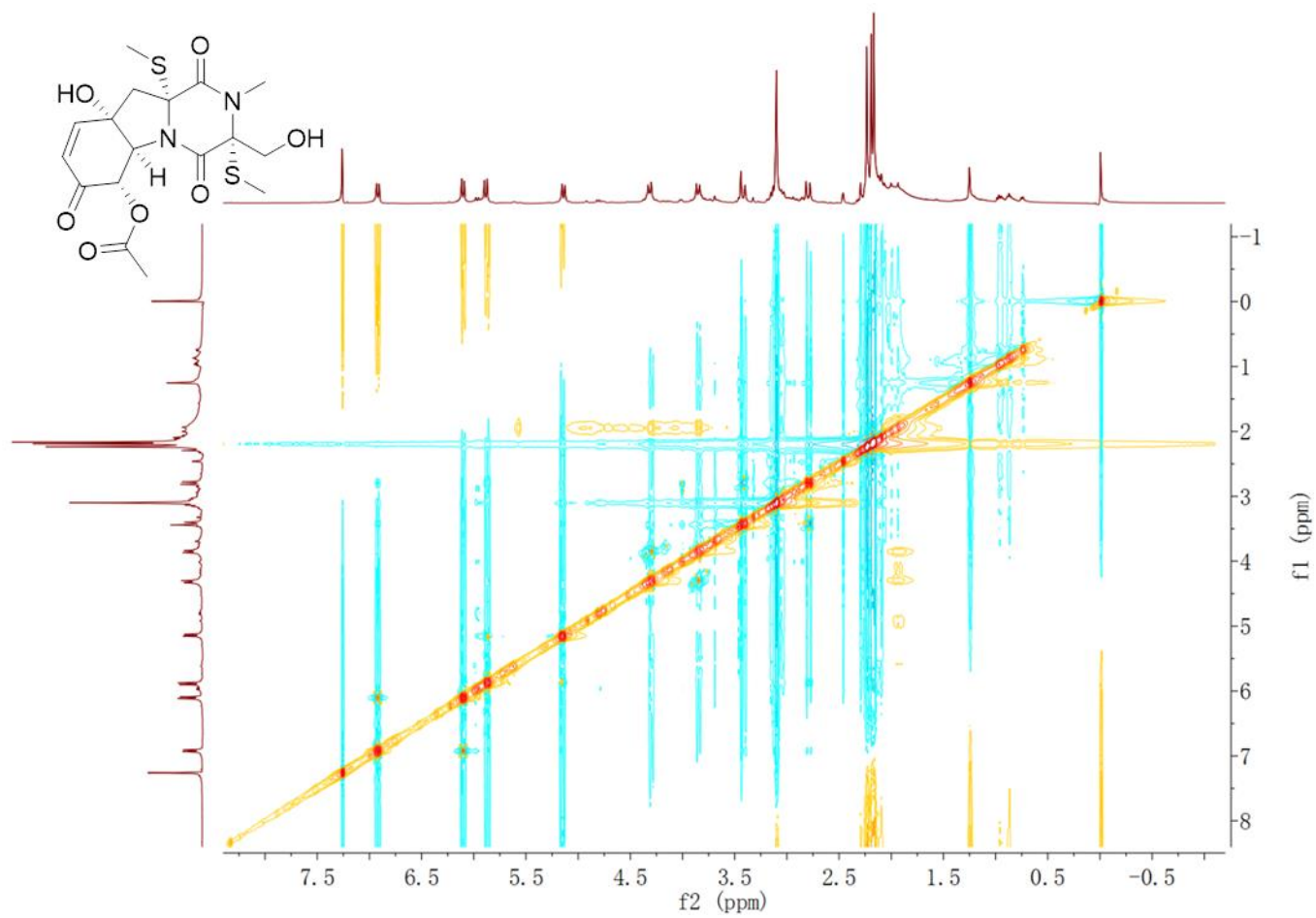


Figure S75. ^1H NMR spectrum of dichotocejpin A (**17**) in CDCl_3 (400MHz)

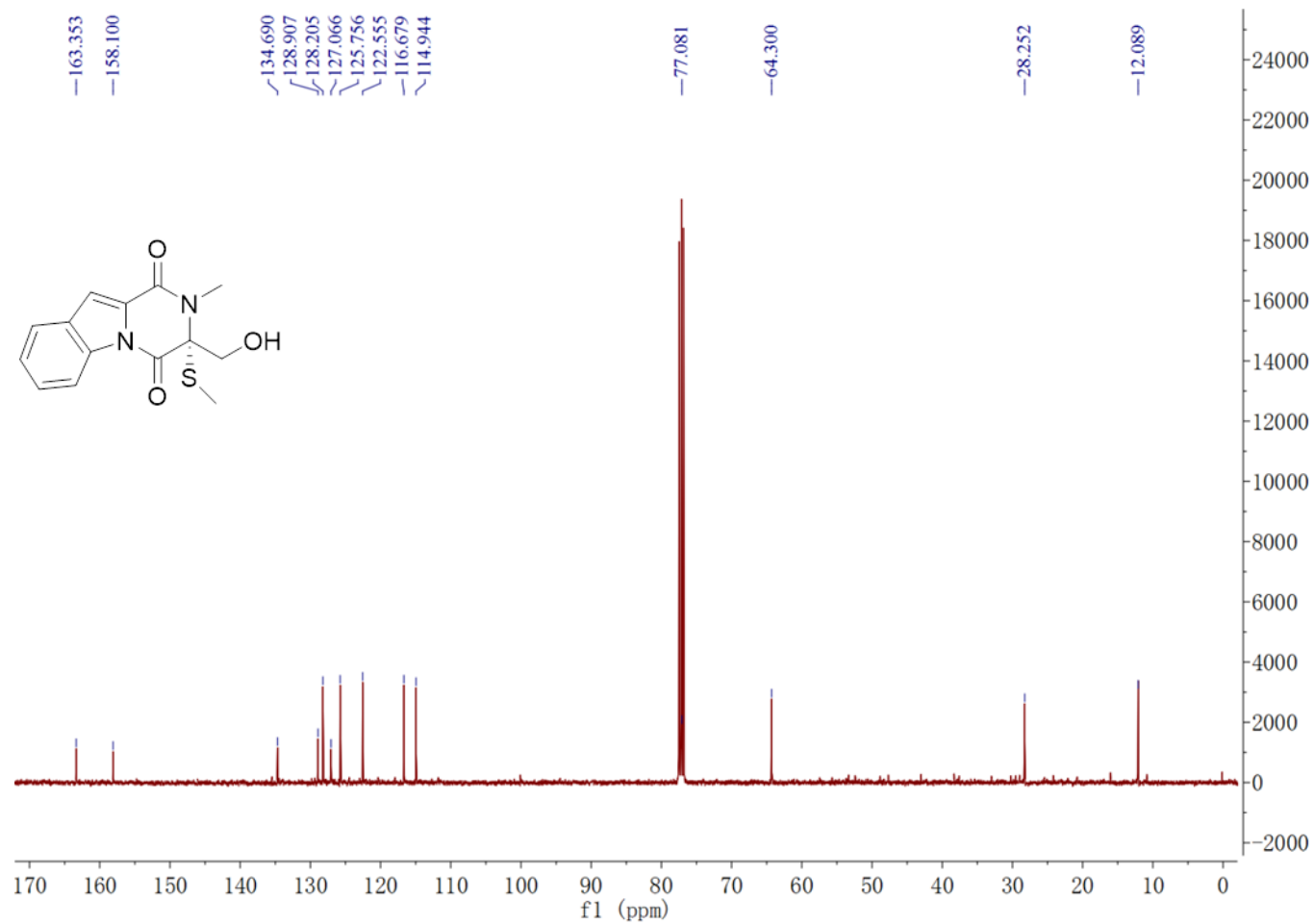


Figure S76. ^{13}C NMR spectrum of dichotocepin A (**17**) in CDCl_3 (100MHz)

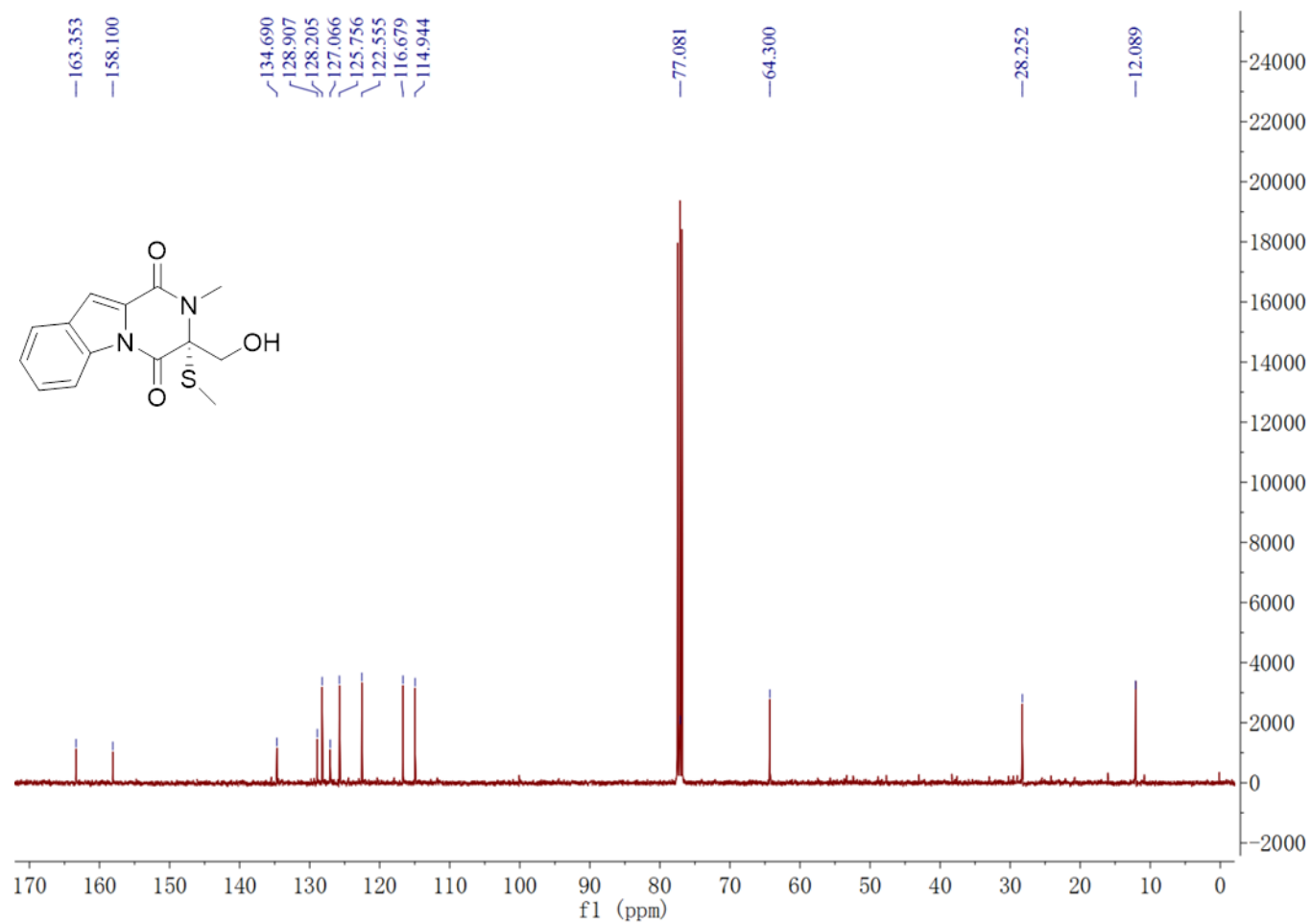


Figure S77. ¹H NMR spectrum of bisdethiobis (methylthio) gliotoxin (**18**) in CDCl₃ (400MHz)

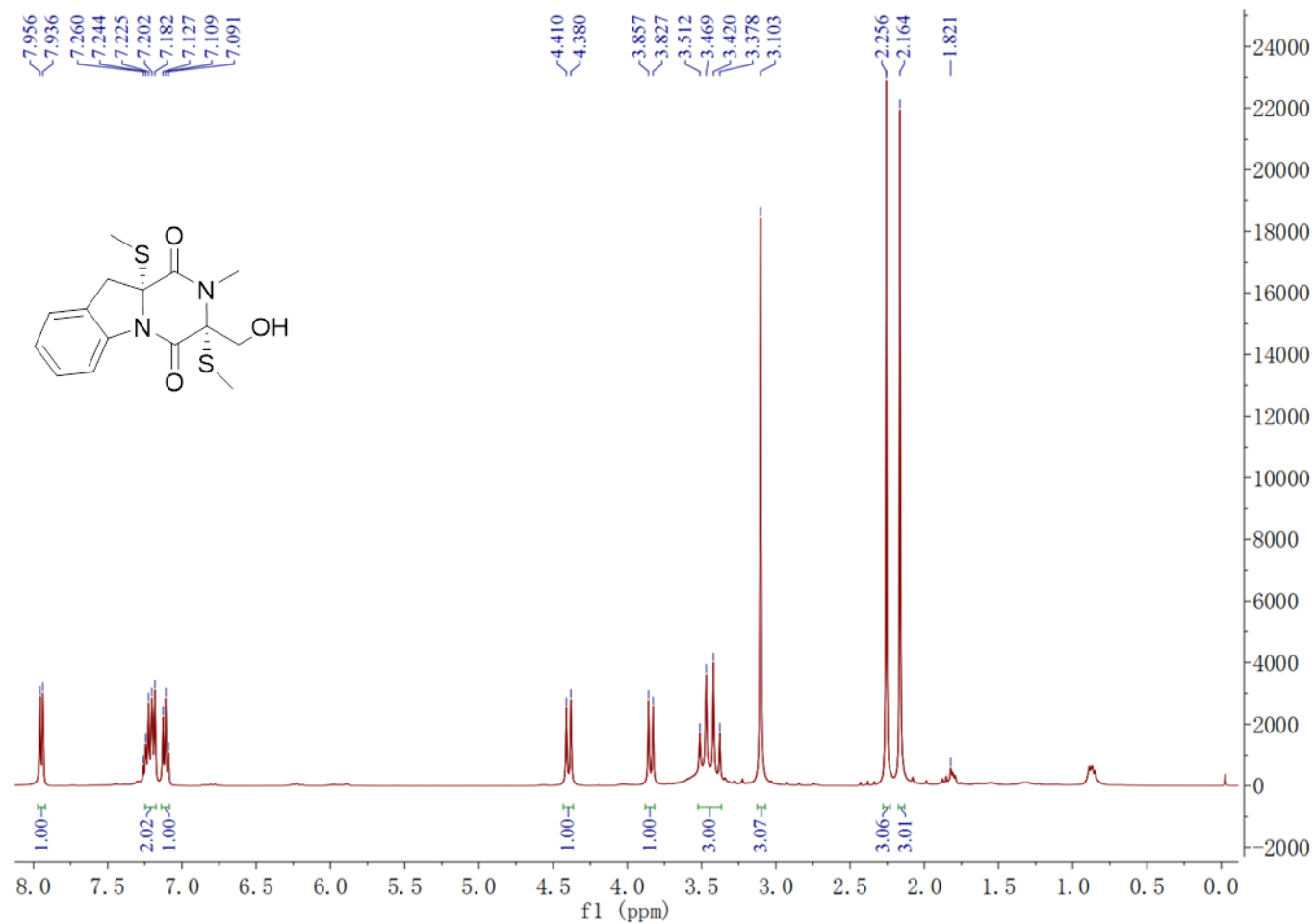


Figure S78. ^{13}C NMR spectrum of bisdethiobis (methylthio) gliotoxin (**18**) in CDCl_3 (100MHz)

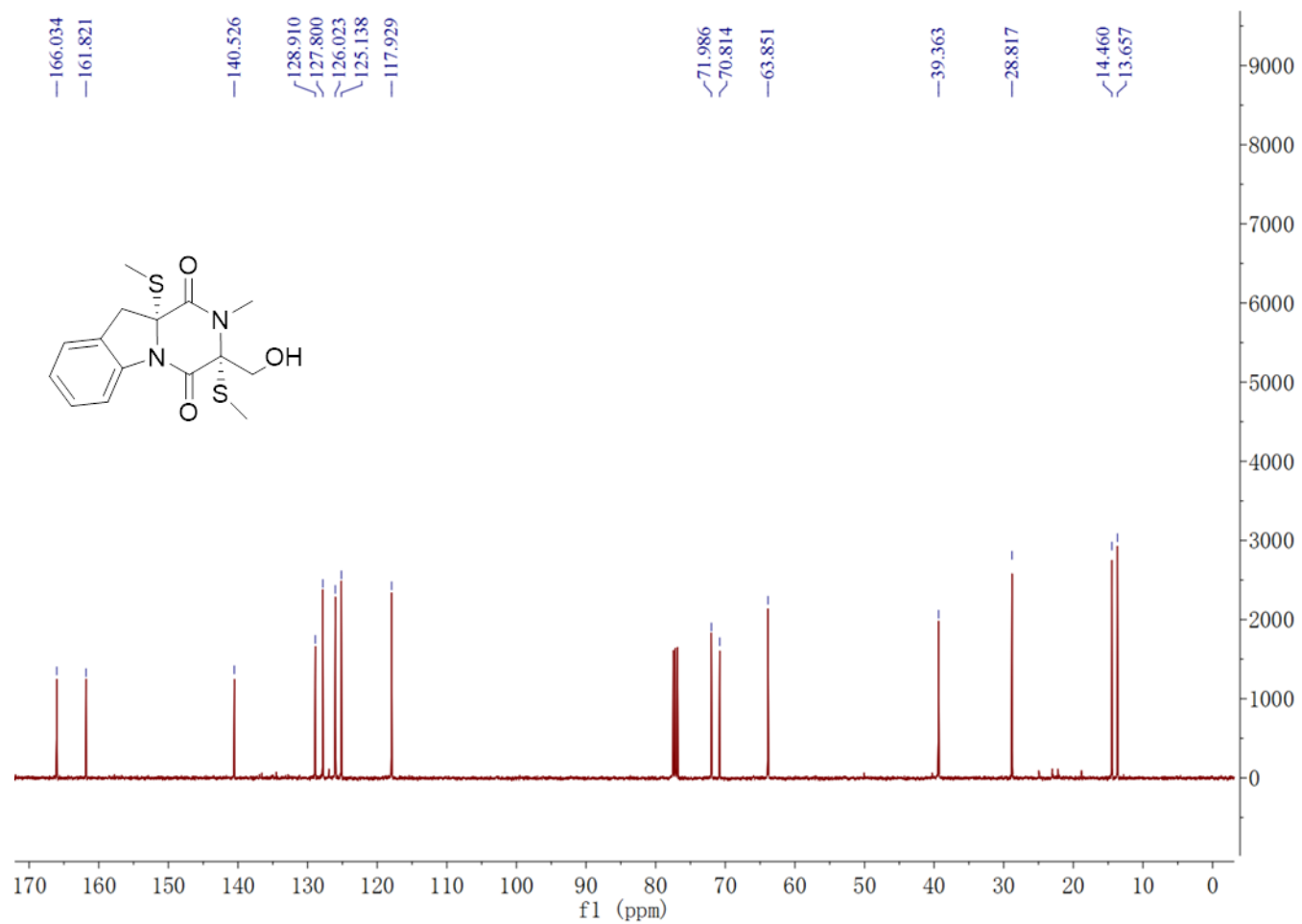


Figure S79. ^1H NMR spectrum of 6-acetylbis (methylthio) gliotoxin (**19**) in CDCl_3 (400MHz)

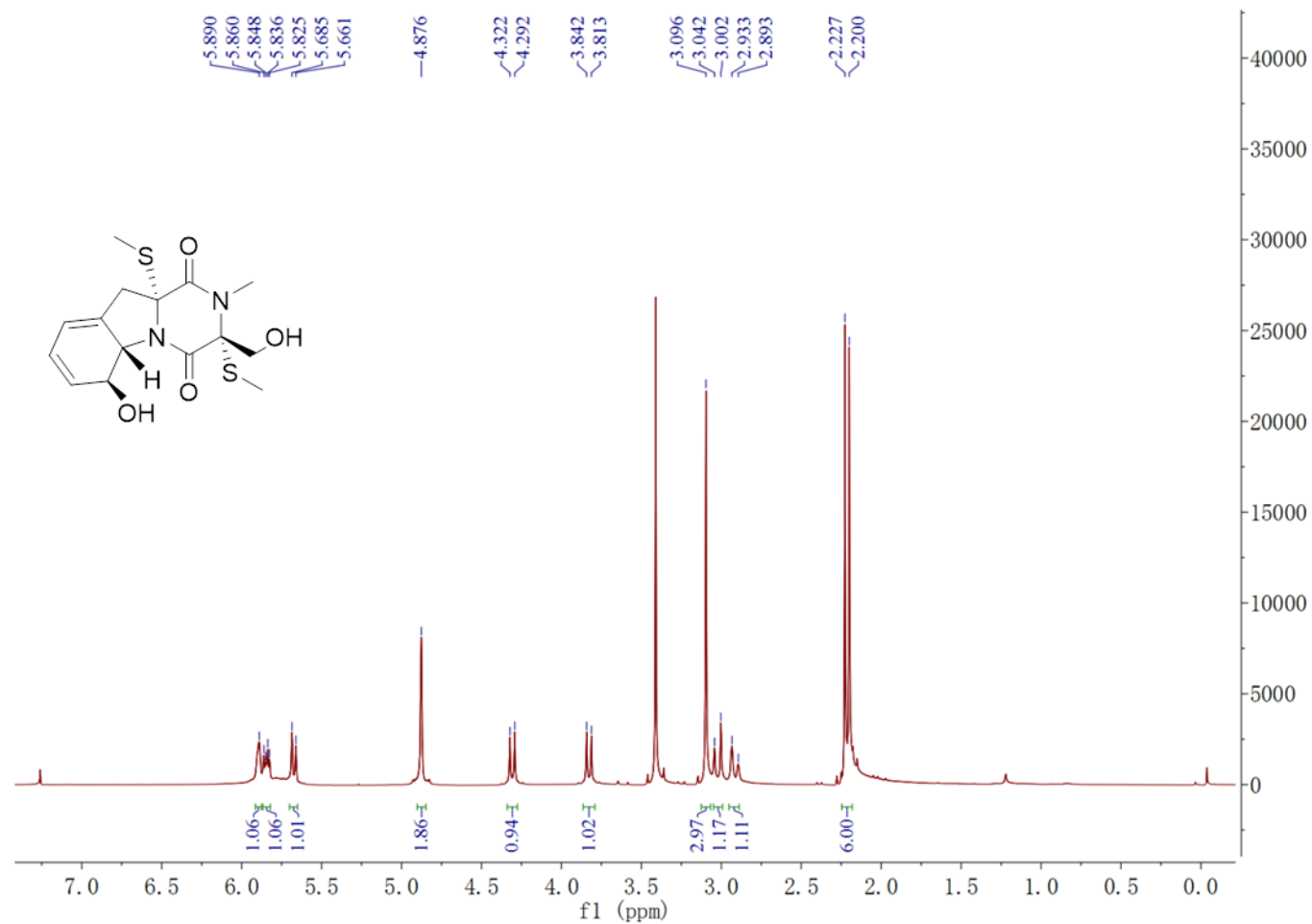


Figure S80. ^{13}C NMR spectrum of 6-acetylbis (methylthio) gliotoxin (**19**) in CDCl_3 (100MHz)

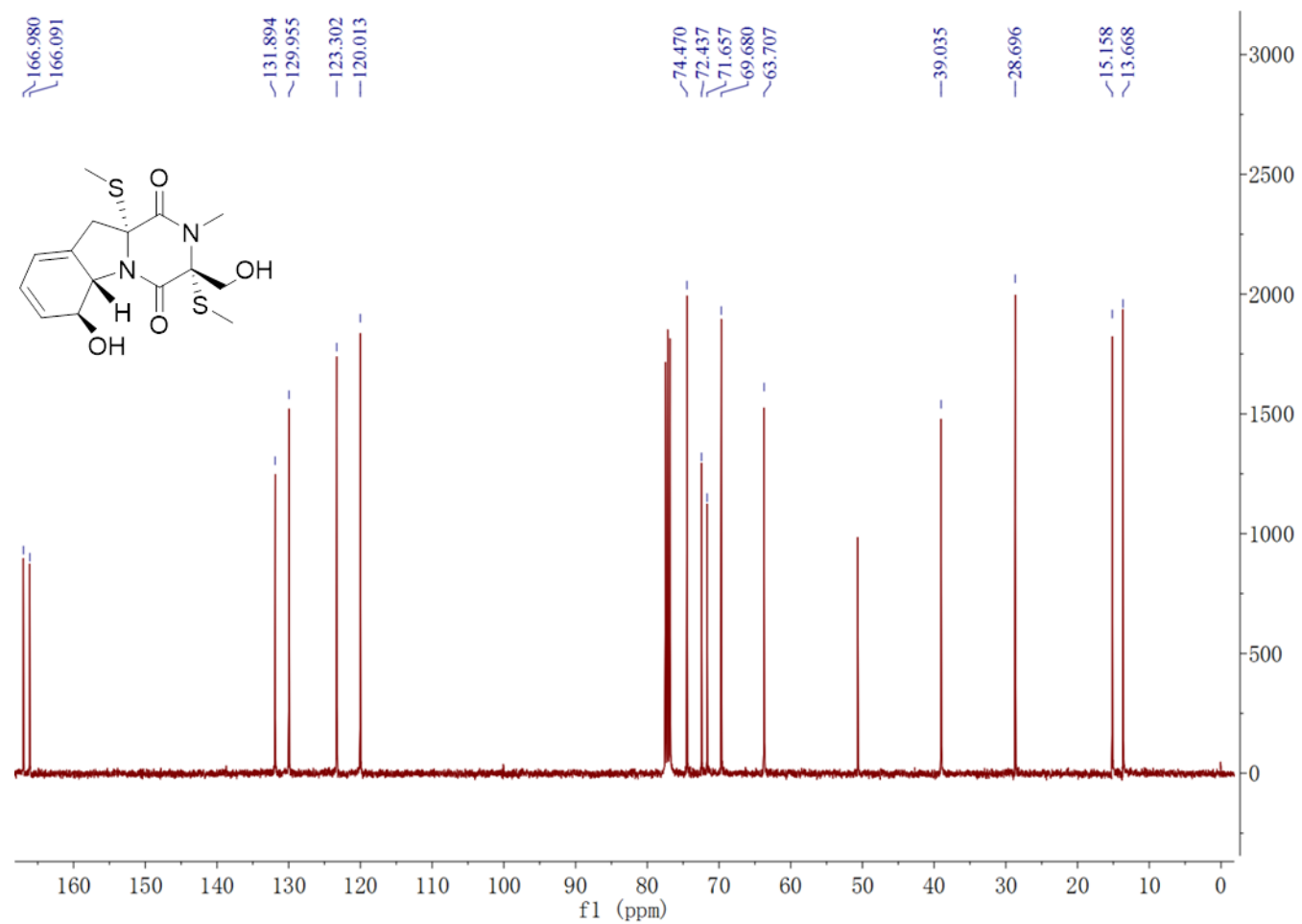


Figure S81. ^1H NMR spectrum of didehydrobisdethiobis (methylthio) gliotoxin (**20**) in CDCl_3 (400MHz)

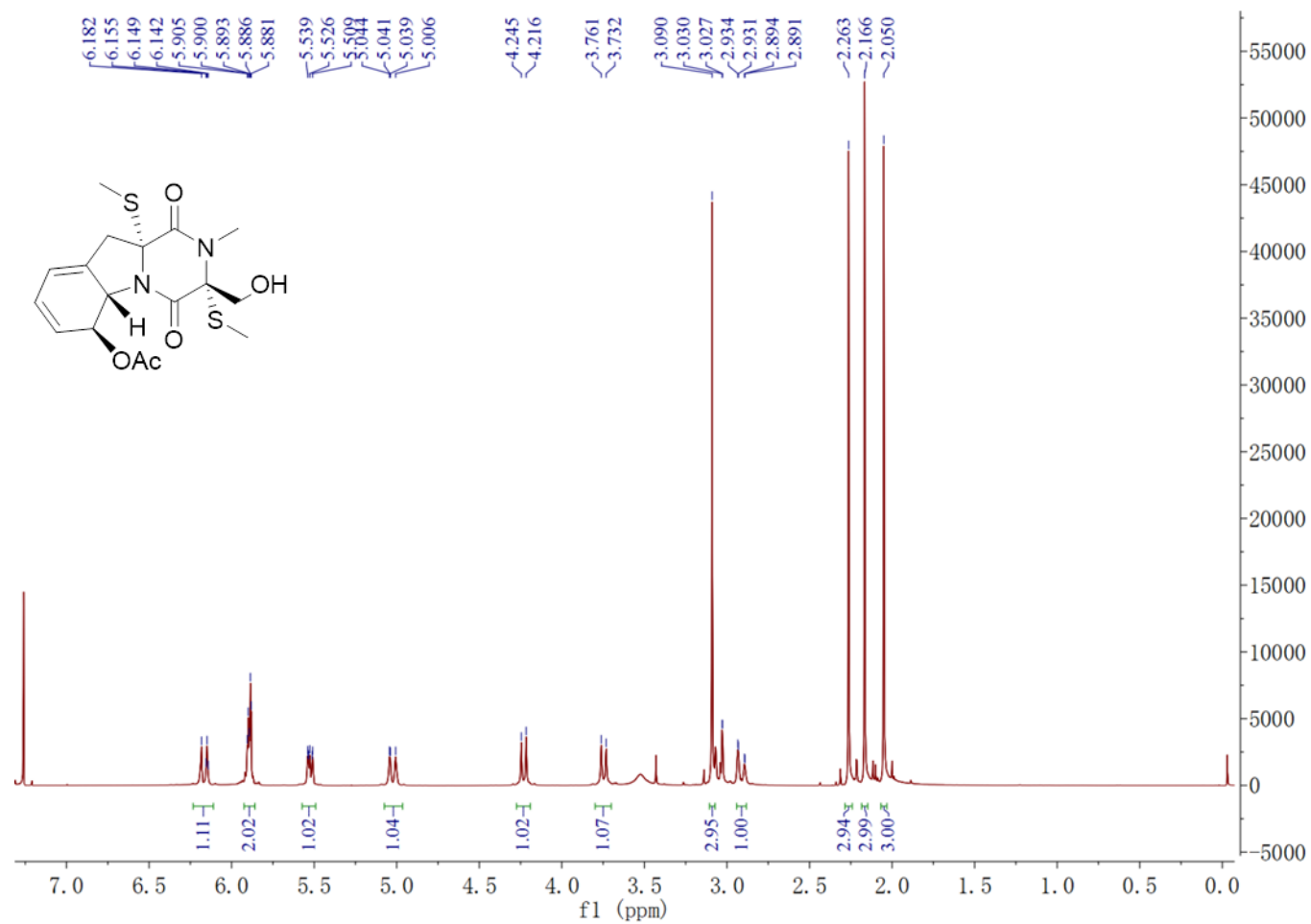


Figure S82. ^{13}C NMR spectrum of didehydrobisdethiobis (methylthio) gliotoxin (**20**) in CDCl_3 (100MHz)

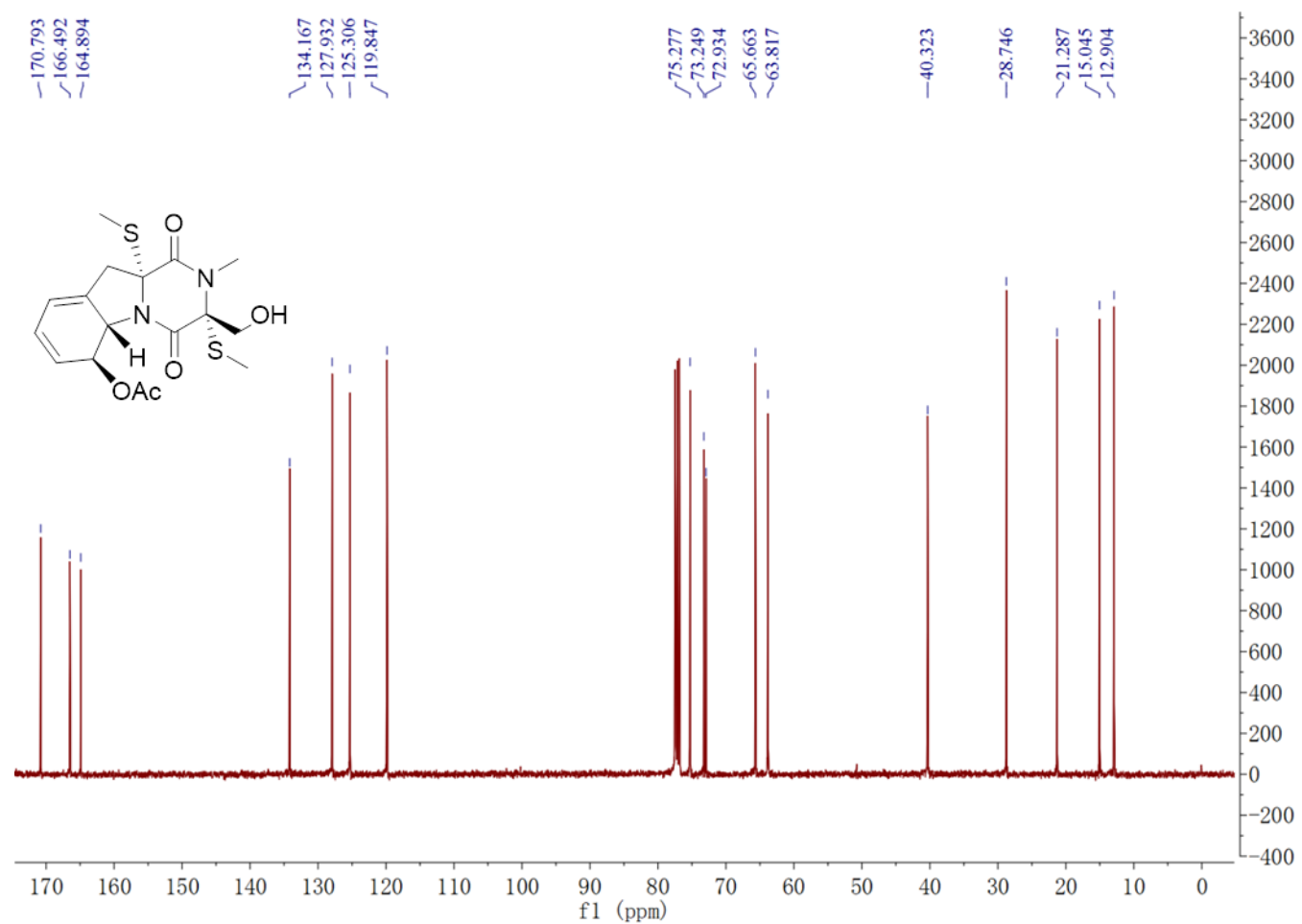


Figure S83. ^1H NMR spectrum of haematocin (**21**) in CDCl_3 (400MHz)

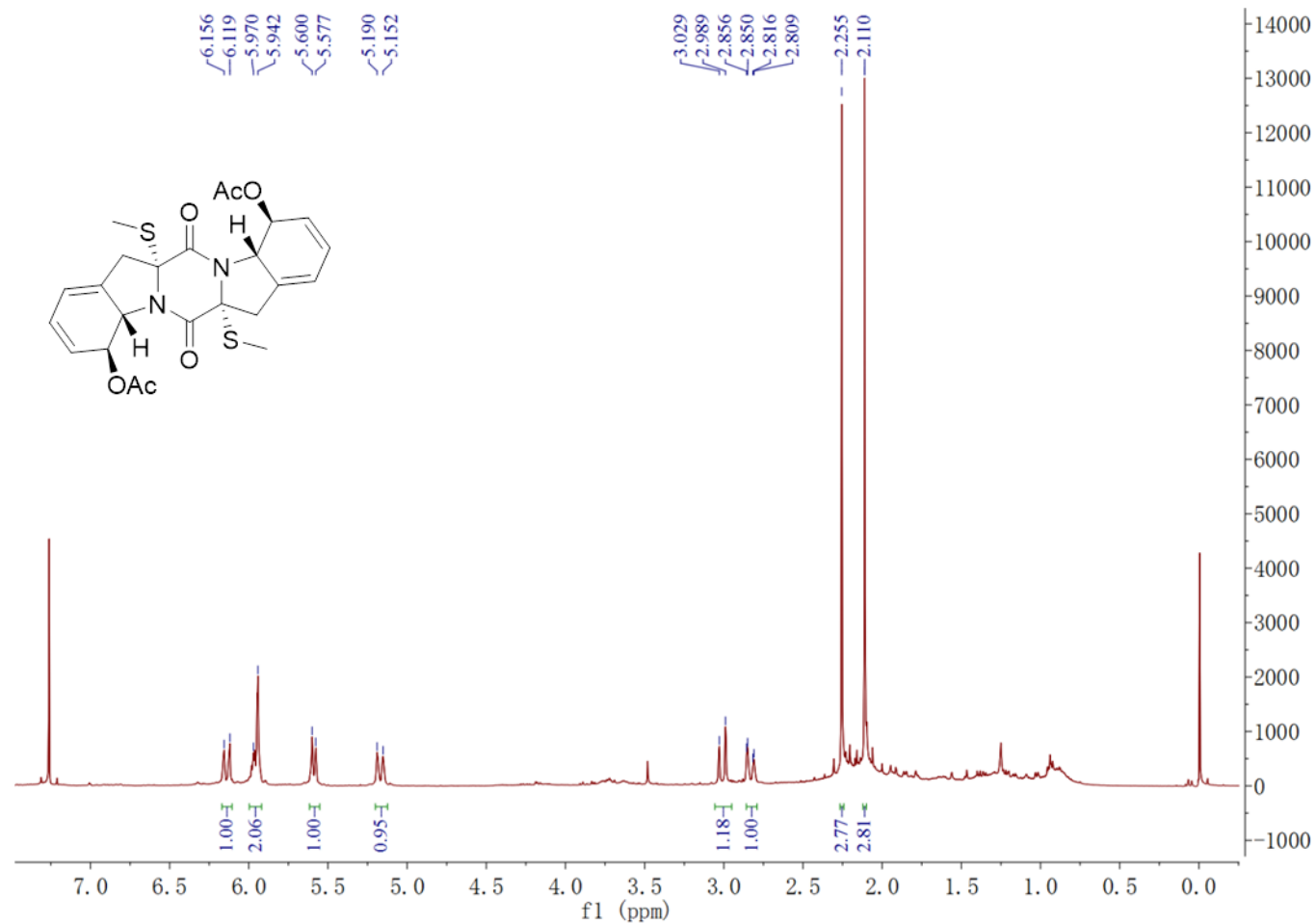


Figure S84. ^{13}C NMR spectrum of haematocin (**21**) in CDCl_3 (100MHz)

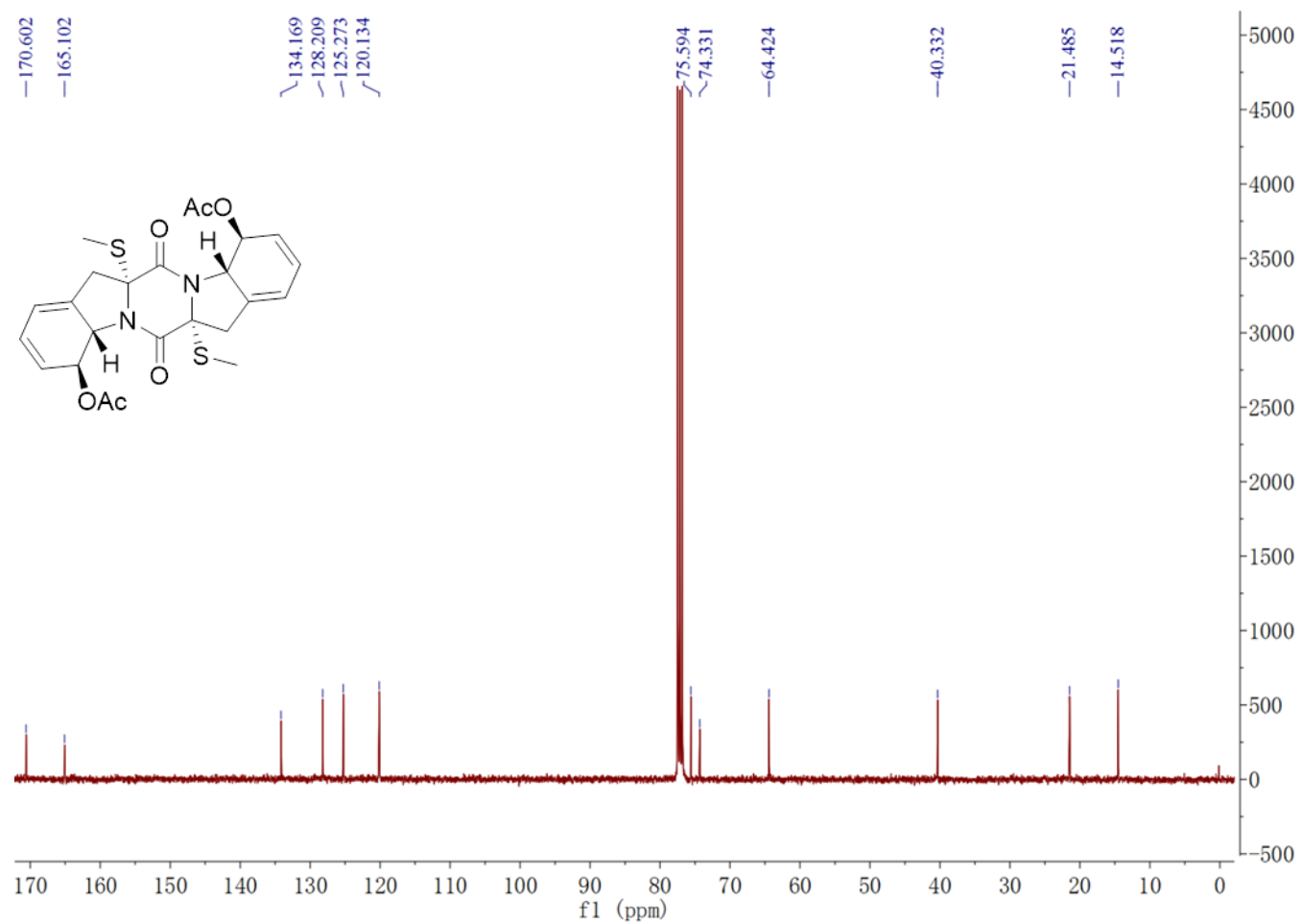


Figure S85. ^1H NMR spectrum of pityriacitrin (**22**) in Acetone- d_6 (400MHz)

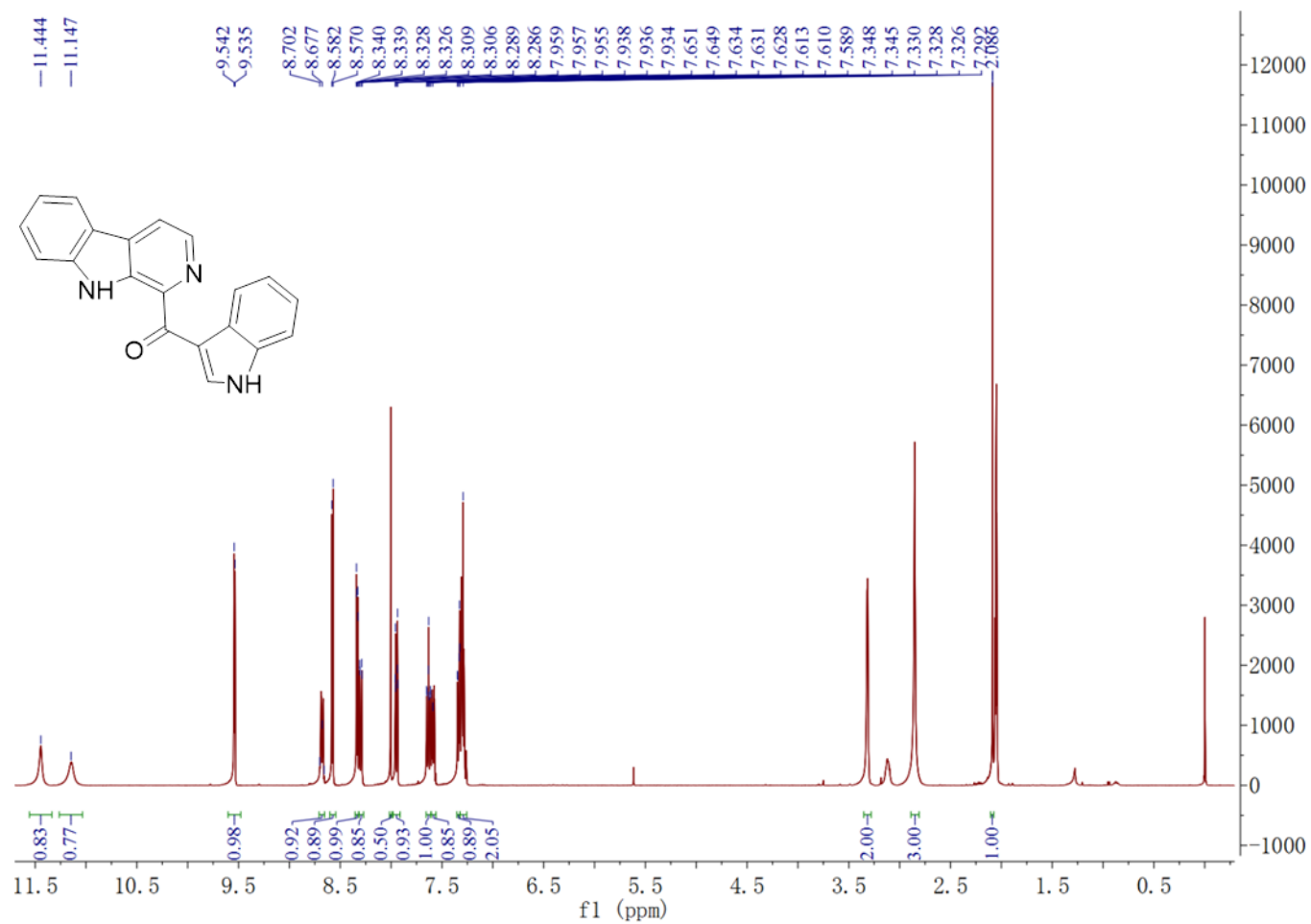


Figure S86. ^{13}C NMR spectrum of pityriacitrin (**22**) in Acetone- d_6 (100MHz)

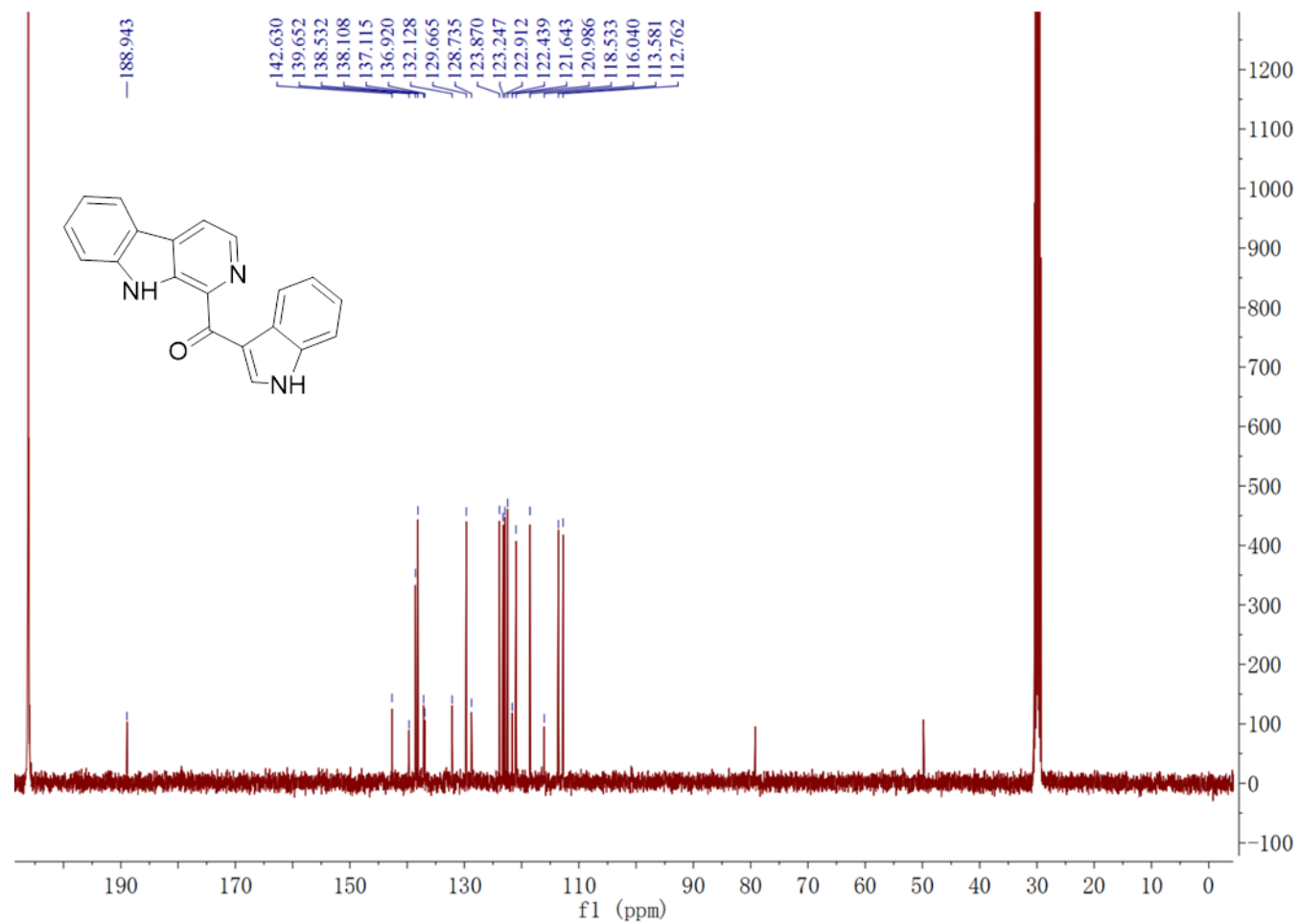


Figure S87. ^1H NMR spectrum of stellarine A (**23**) in $\text{DMSO-}d_6$ (400MHz)

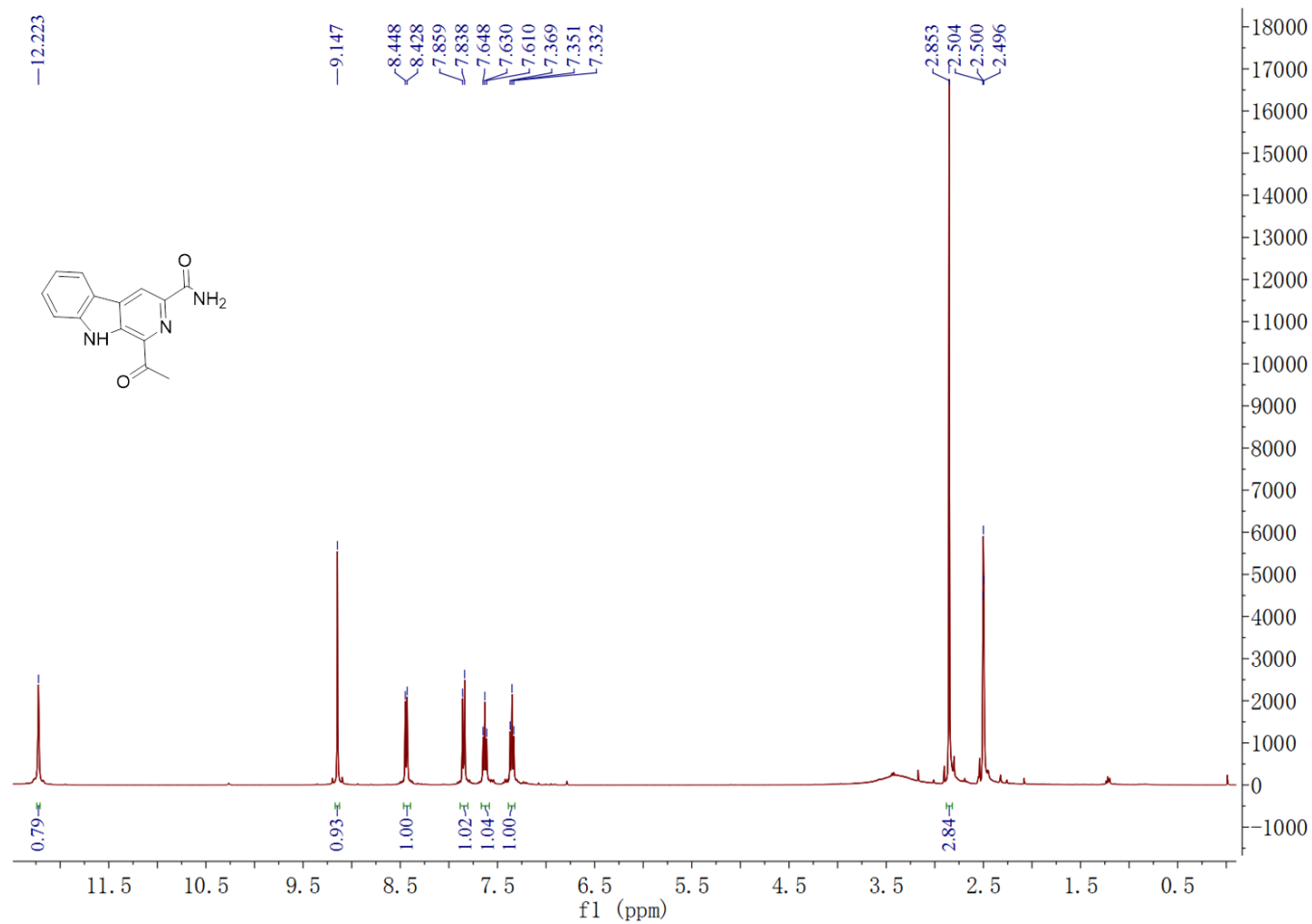


Figure S88. ^{13}C NMR spectrum of stellarine A (**23**) in $\text{DMSO-}d_6$ (100MHz)

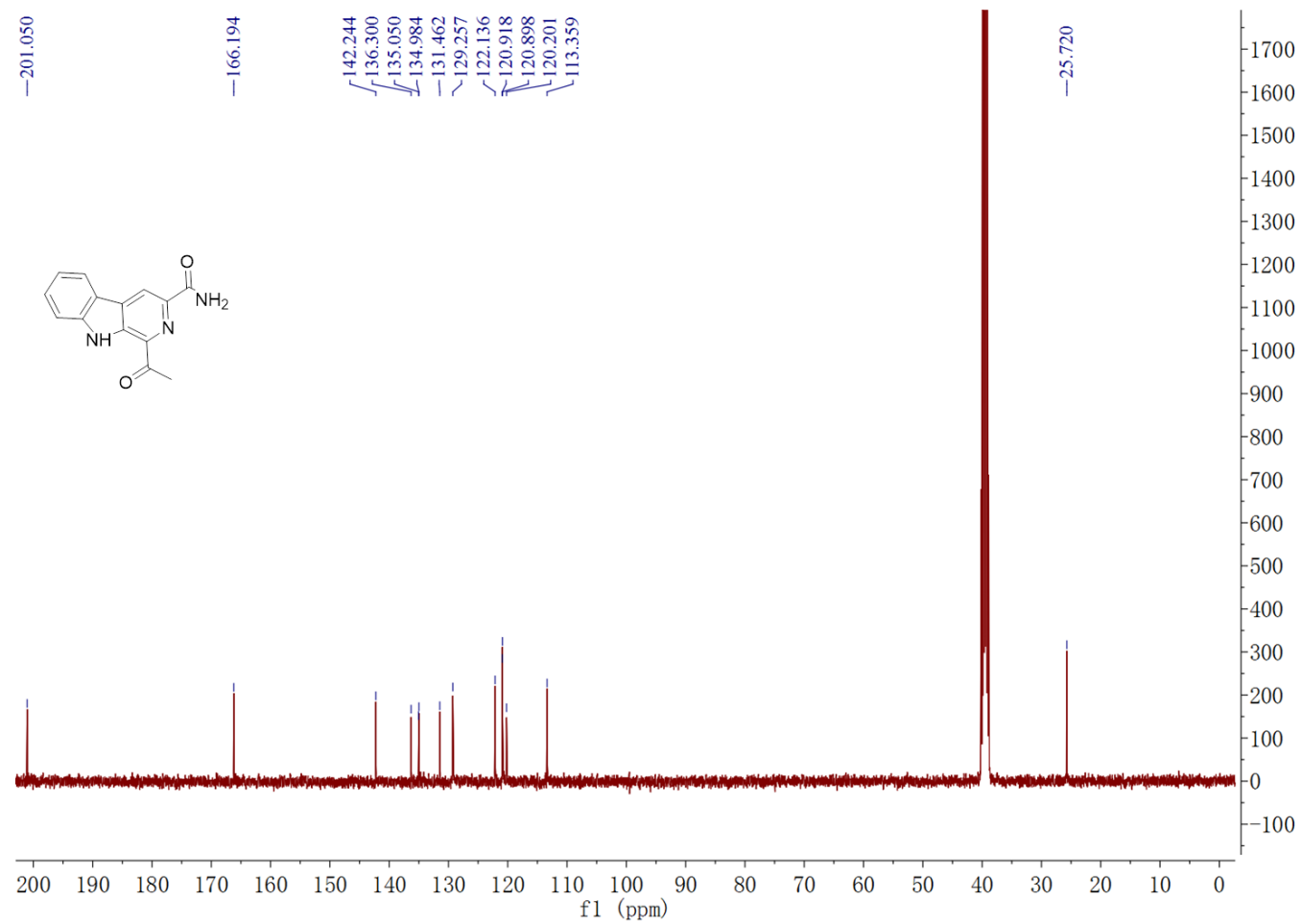


Figure S89. ^1H NMR spectrum of perlolyrine (**24**) in CDCl_3 (400MHz)

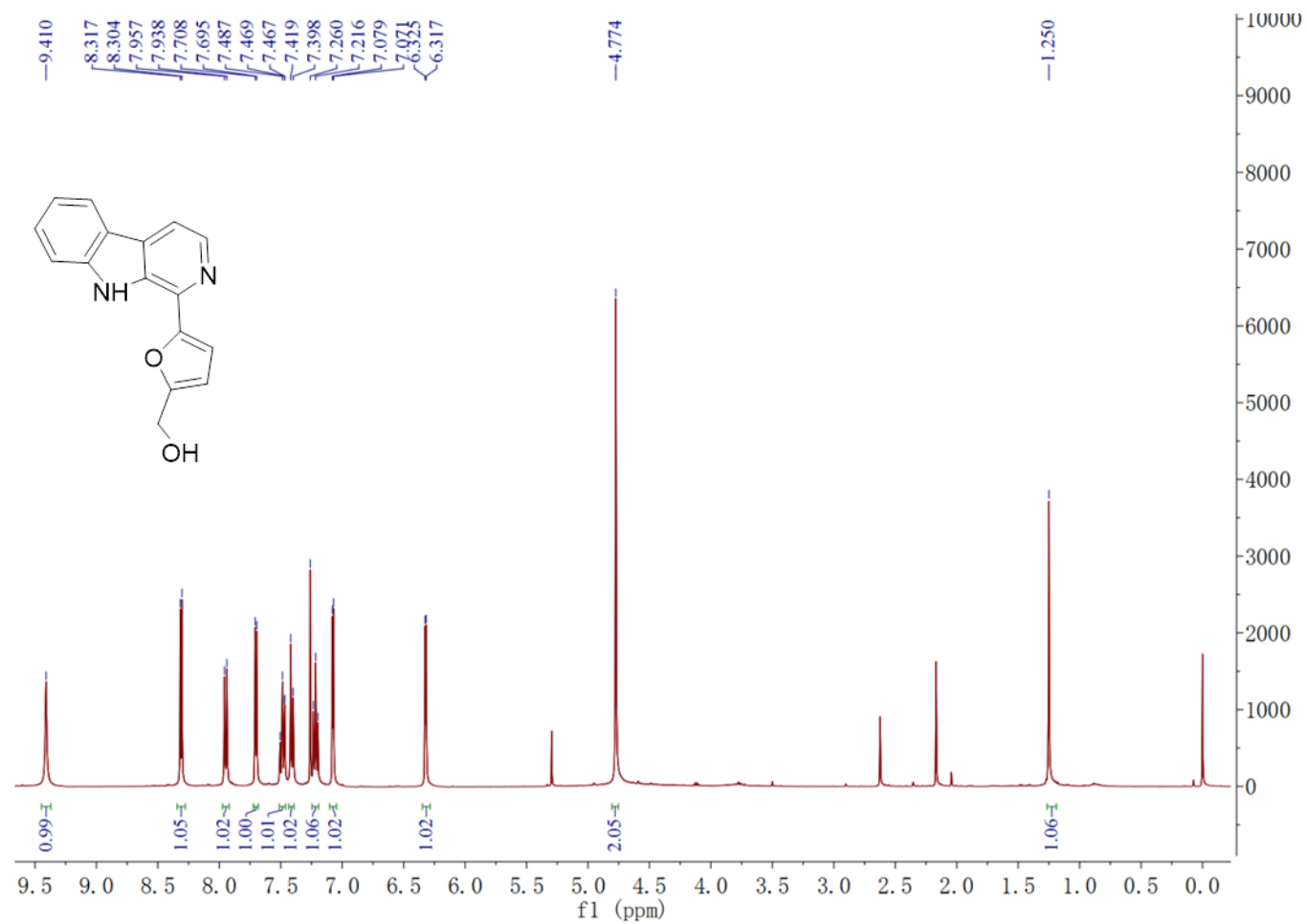


Figure S90. ^{13}C NMR spectrum of perlolyrine (**24**) in CDCl_3 (100MHz)

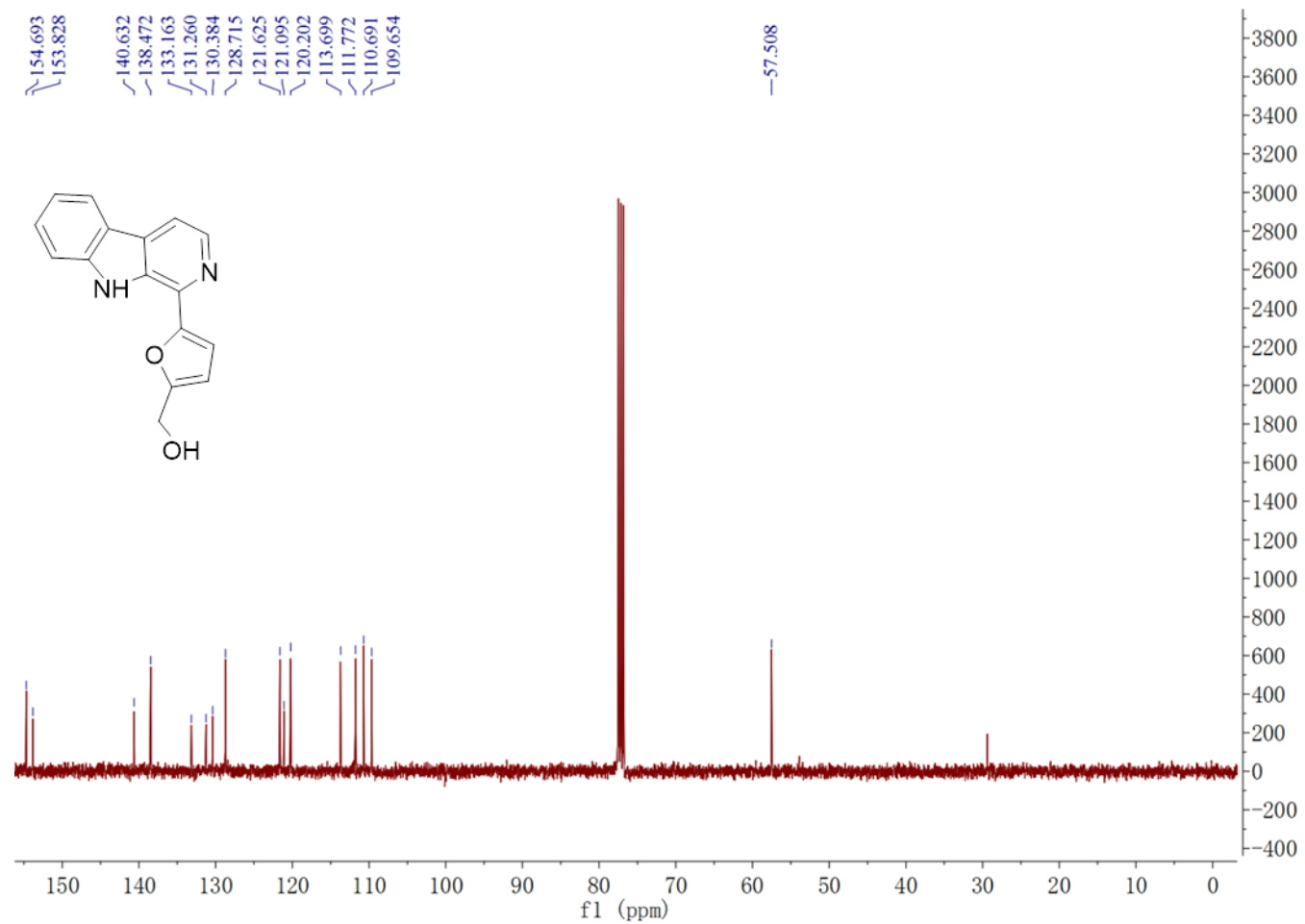


Figure S91. ¹H NMR spectrum of fiscalin C (**25**) in CDCl₃ (400MHz)

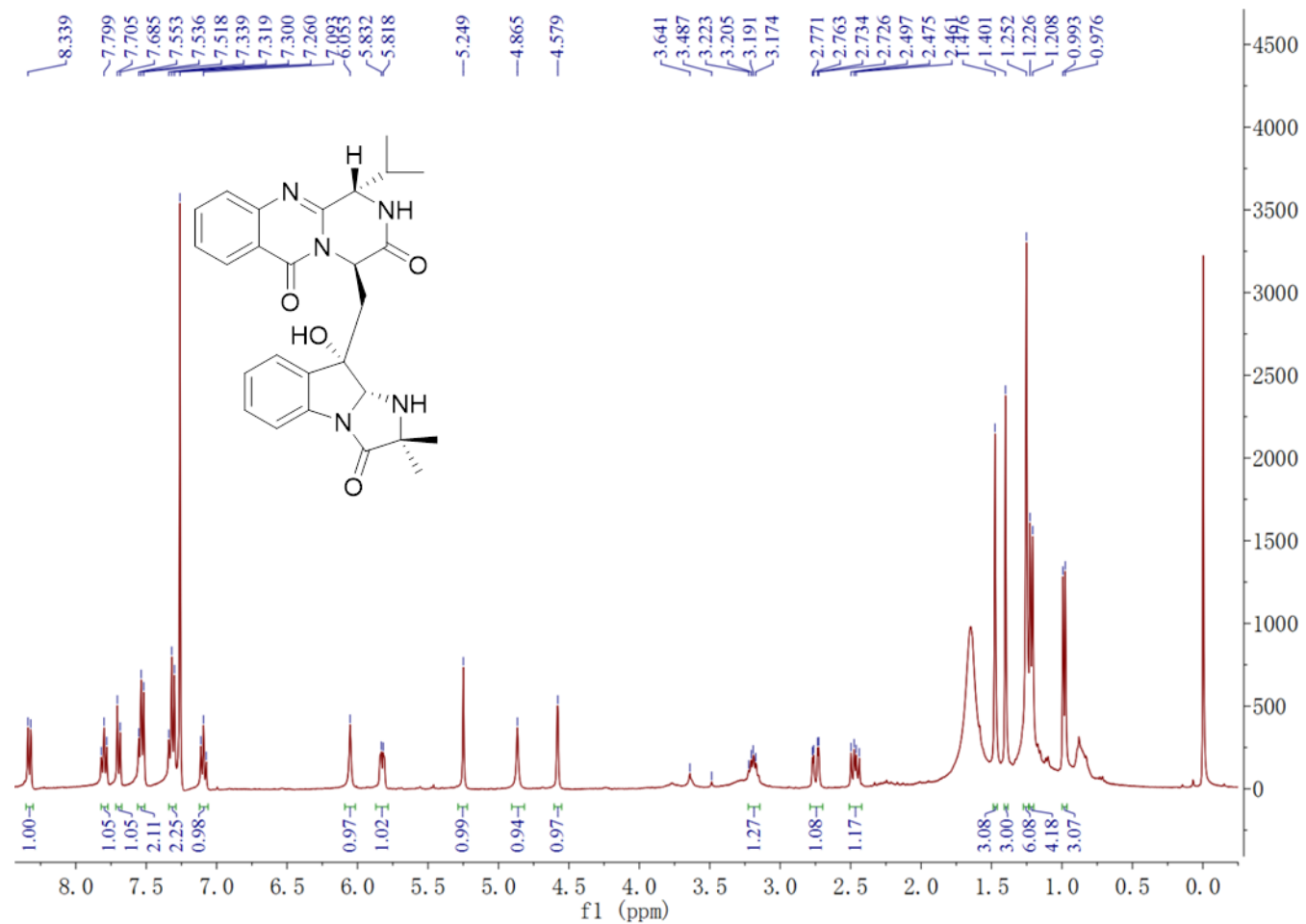


Figure S92. ^{13}C NMR spectrum of fiscalin C (25) in CDCl_3 (100MHz)

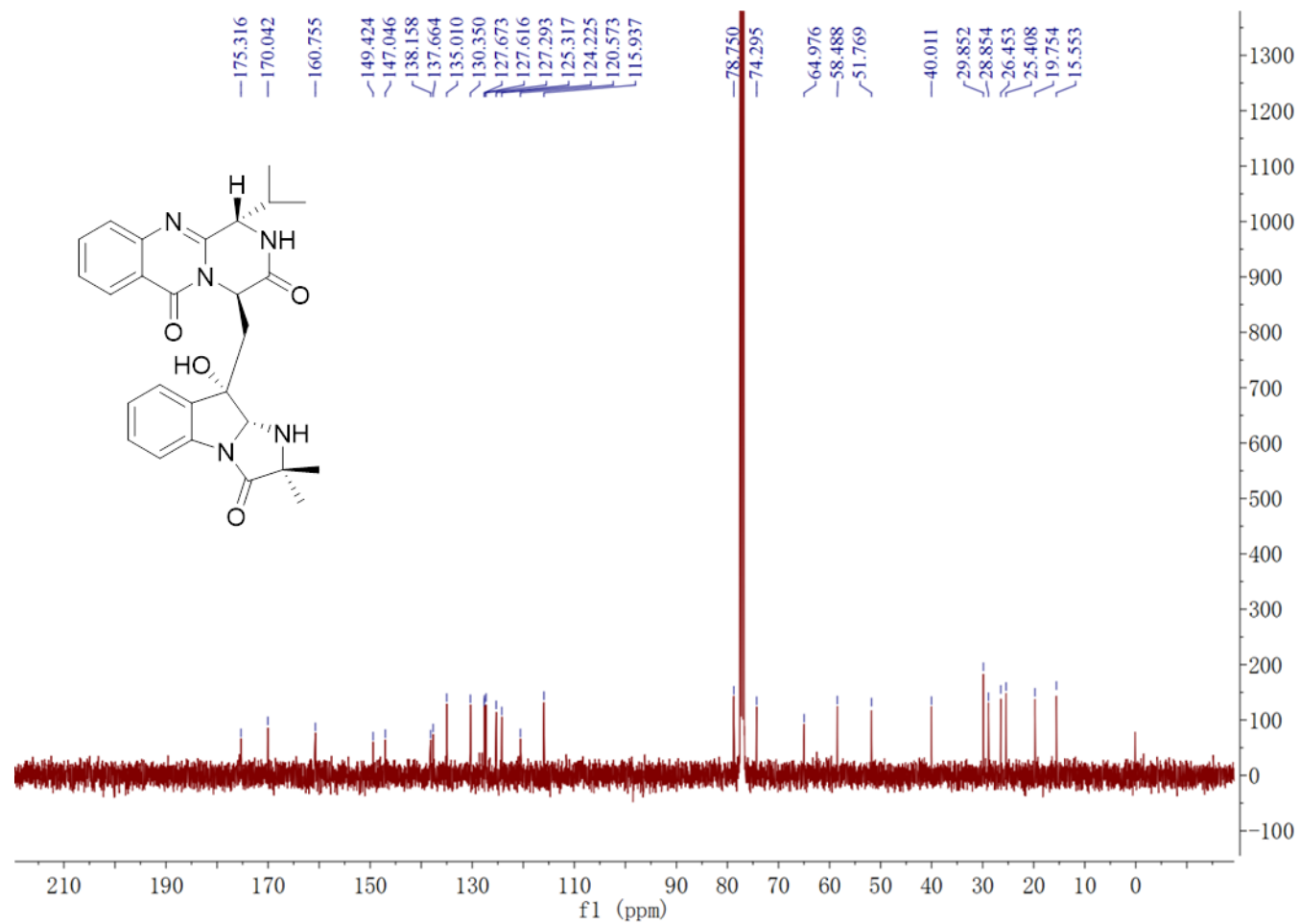


Figure S93. ¹H NMR spectrum of epi-fiscalin C (26) in CDCl₃ (400MHz)

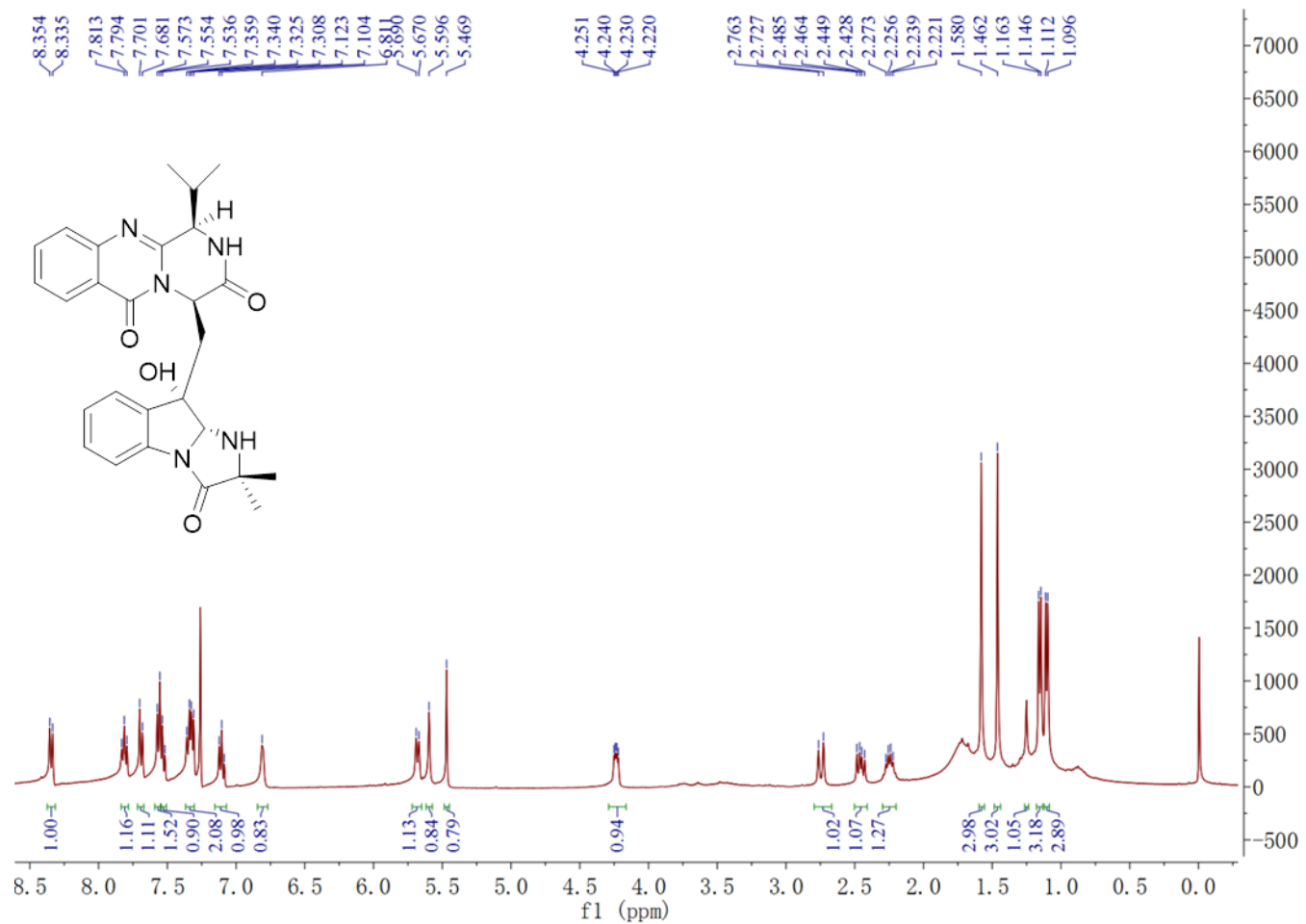


Figure S94. ^{13}C NMR spectrum of epi-fiscalin C (**26**) in CDCl_3 (100MHz)

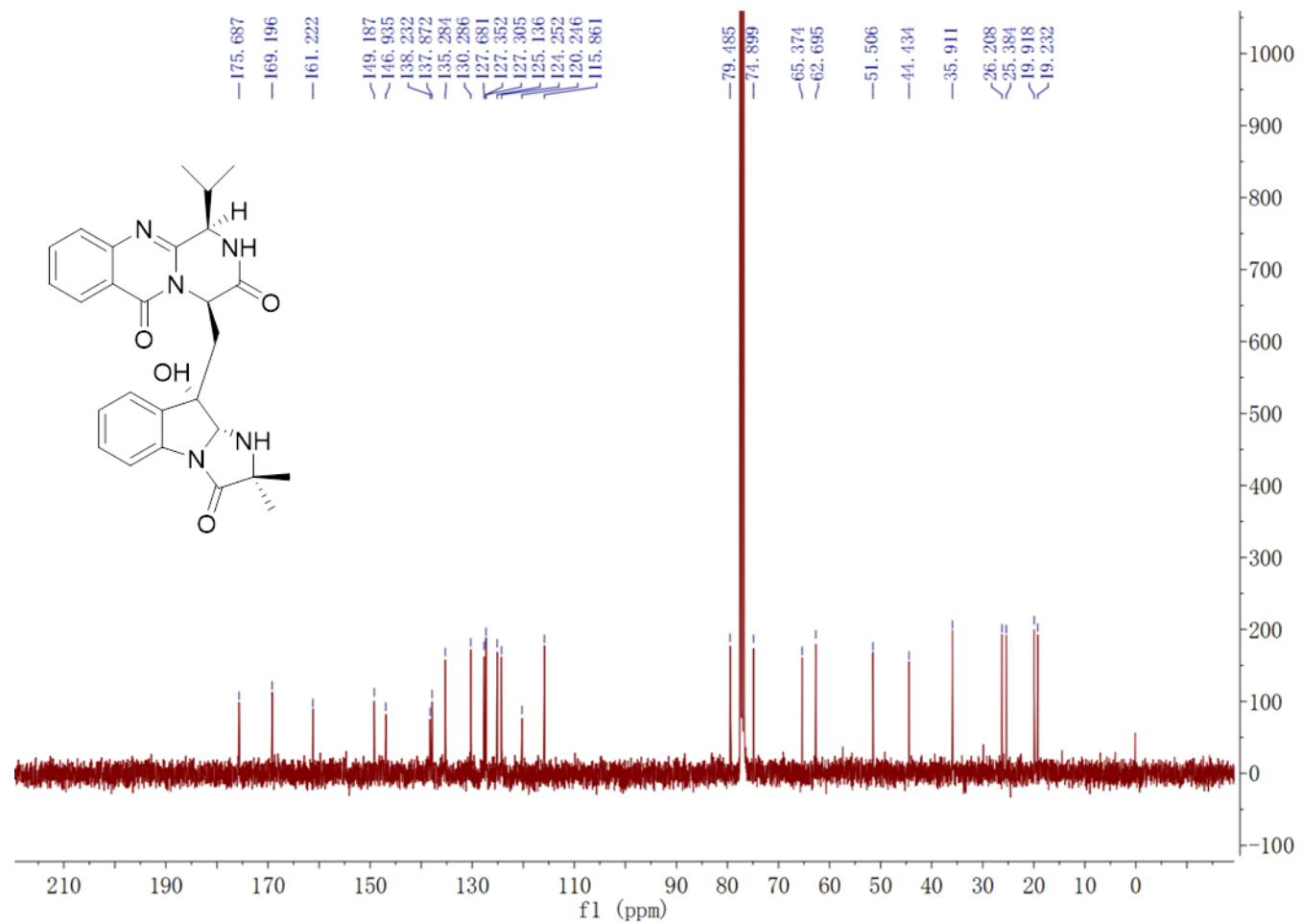


Figure S95. ^1H NMR spectrum of indolyl-3-acetic acid methyl ester (**27**) in CDCl_3 (400MHz)

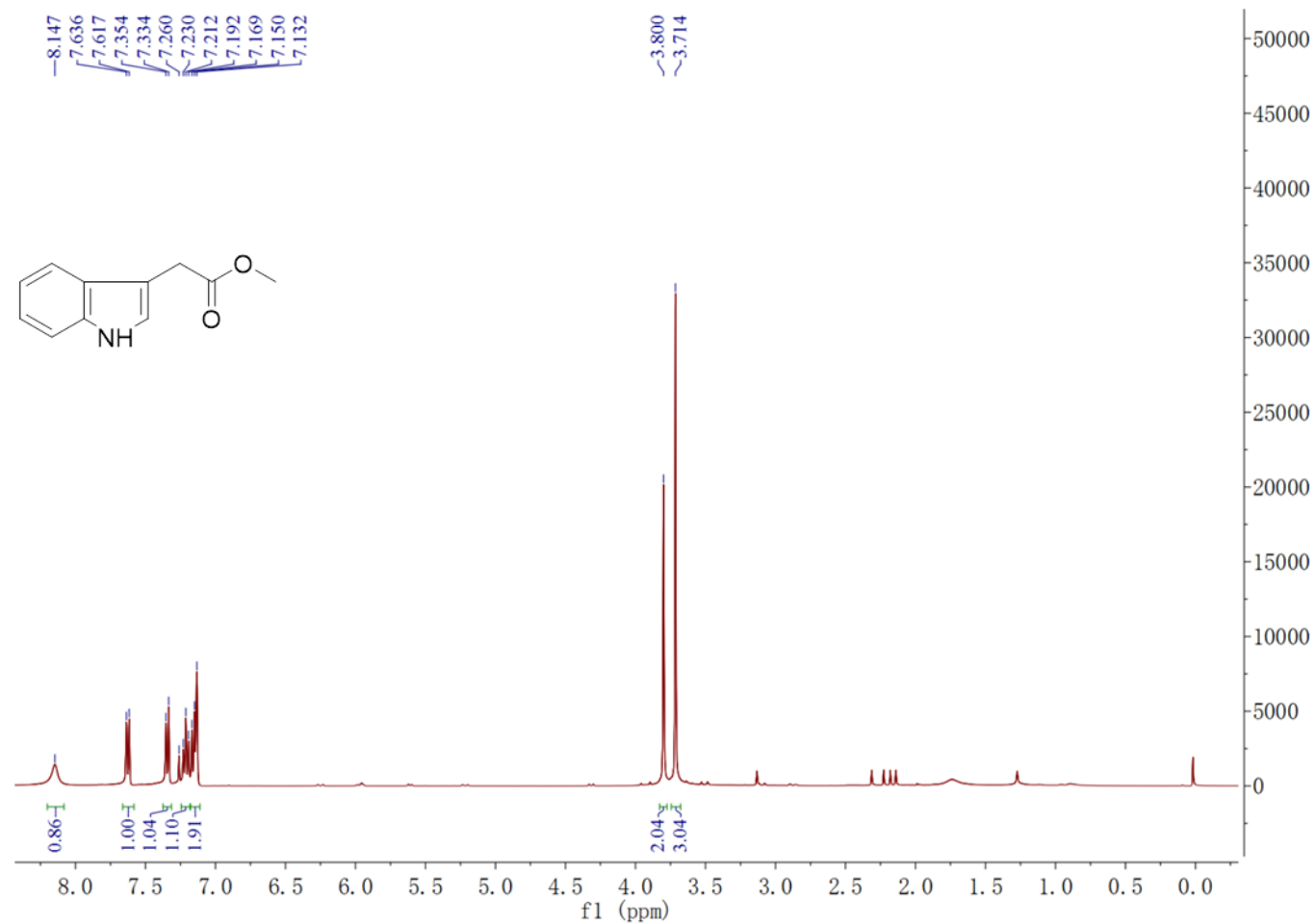


Figure S96. ^{13}C NMR spectrum of indolyl-3-acetic acid methyl ester (**27**) in CDCl_3 (100MHz)

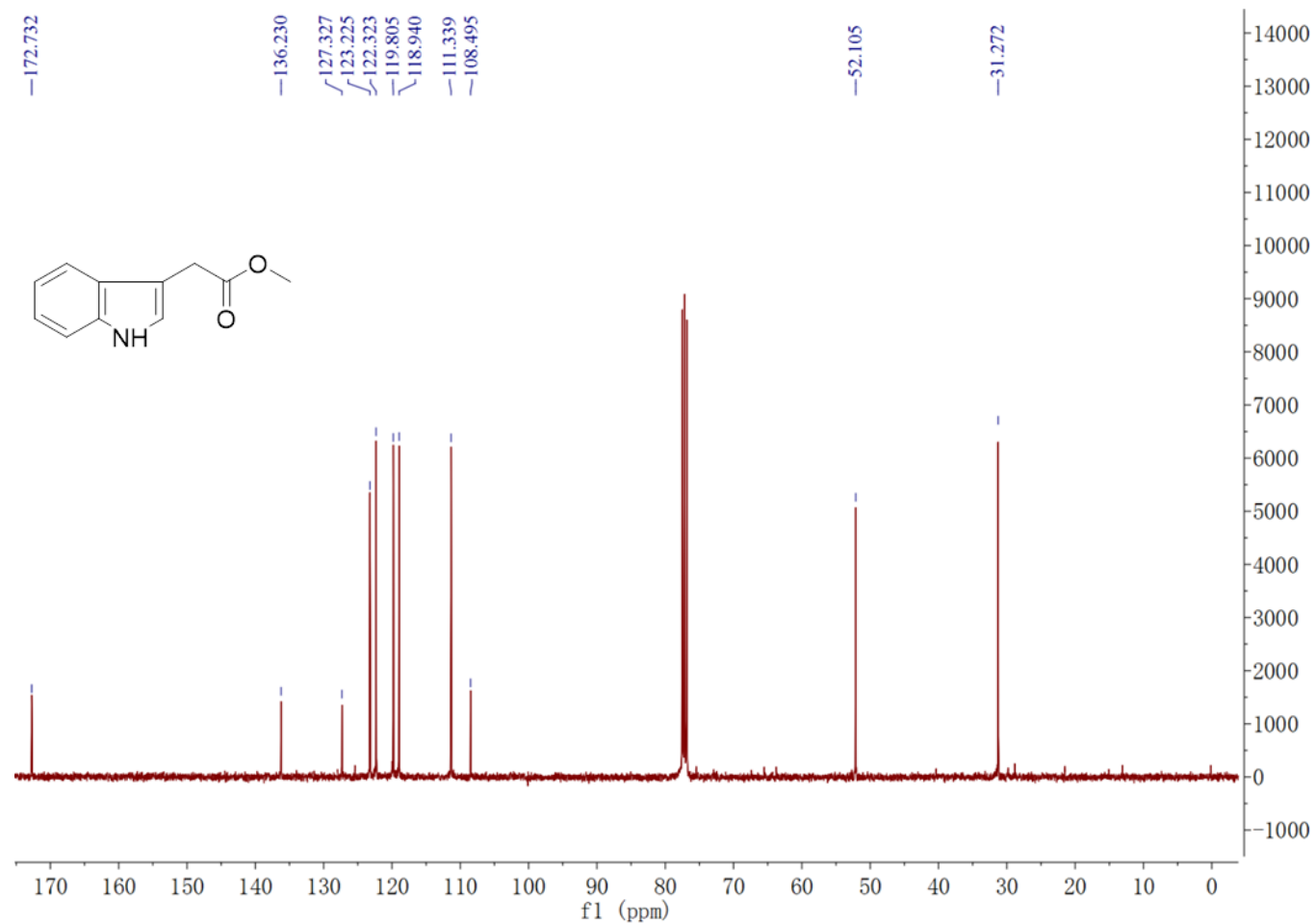


Figure S97. ^1H NMR spectrum of anthranilic acid (**28**) in Acetone- d_6 (400MHz)

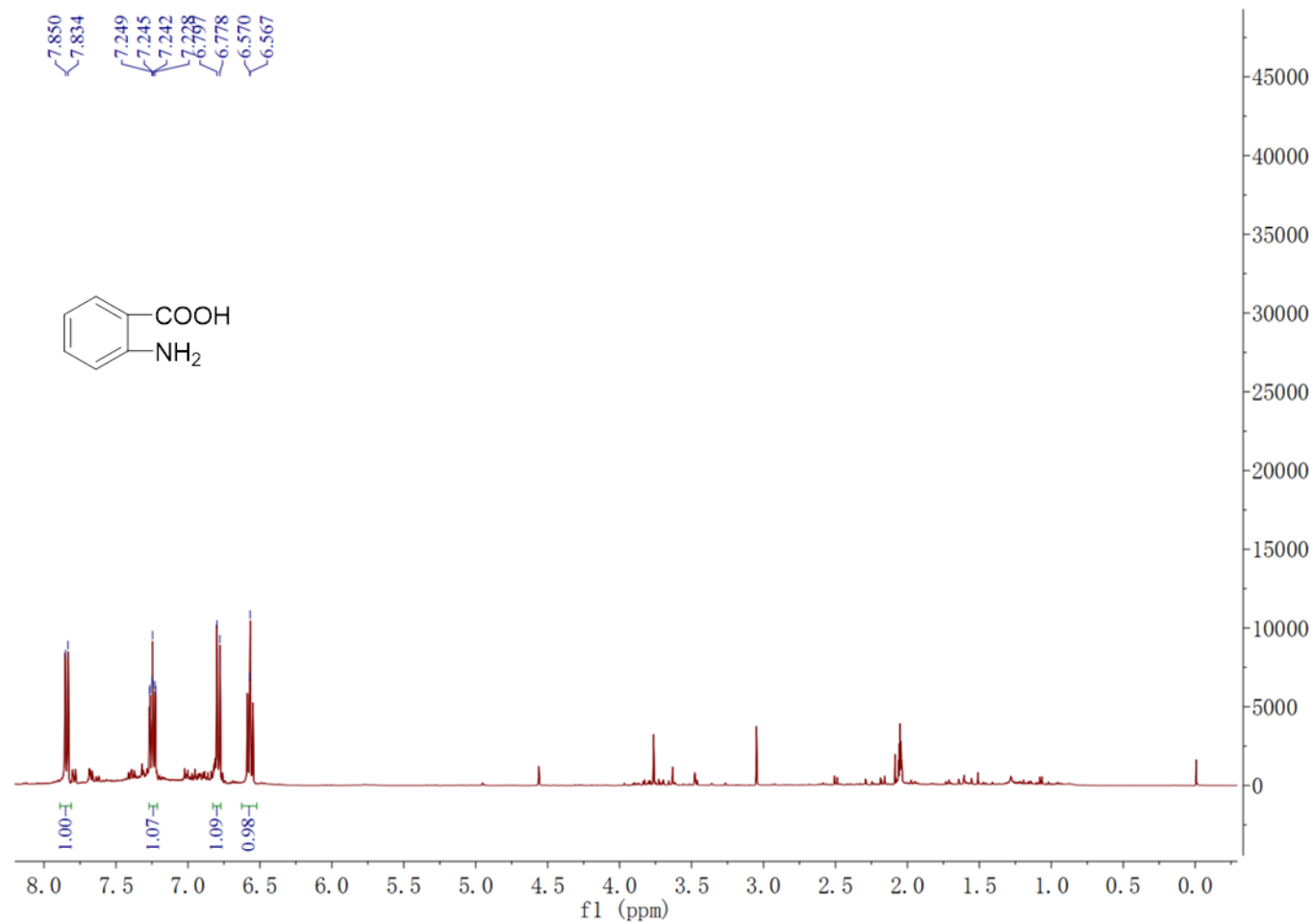


Figure S98. ^{13}C NMR spectrum of anthranilic acid (**28**) in Acetone- d_6 (100MHz)

