

Supporting information for journal *Marine drugs*

Isolation, Structure-activity Relationship of Subergorgic Acid and Synthesis of Its Derivatives as Antifouling Agent

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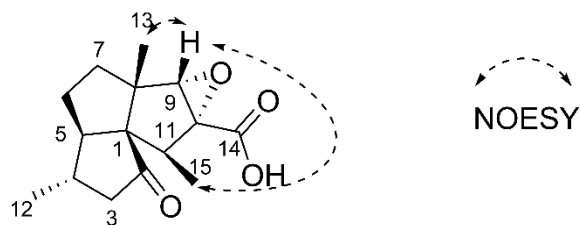


Figure S1. Key NOE correlations of **4**.

Figure S2. ^1H NMR (400 MHz, CDCl_3) of compound **SA**

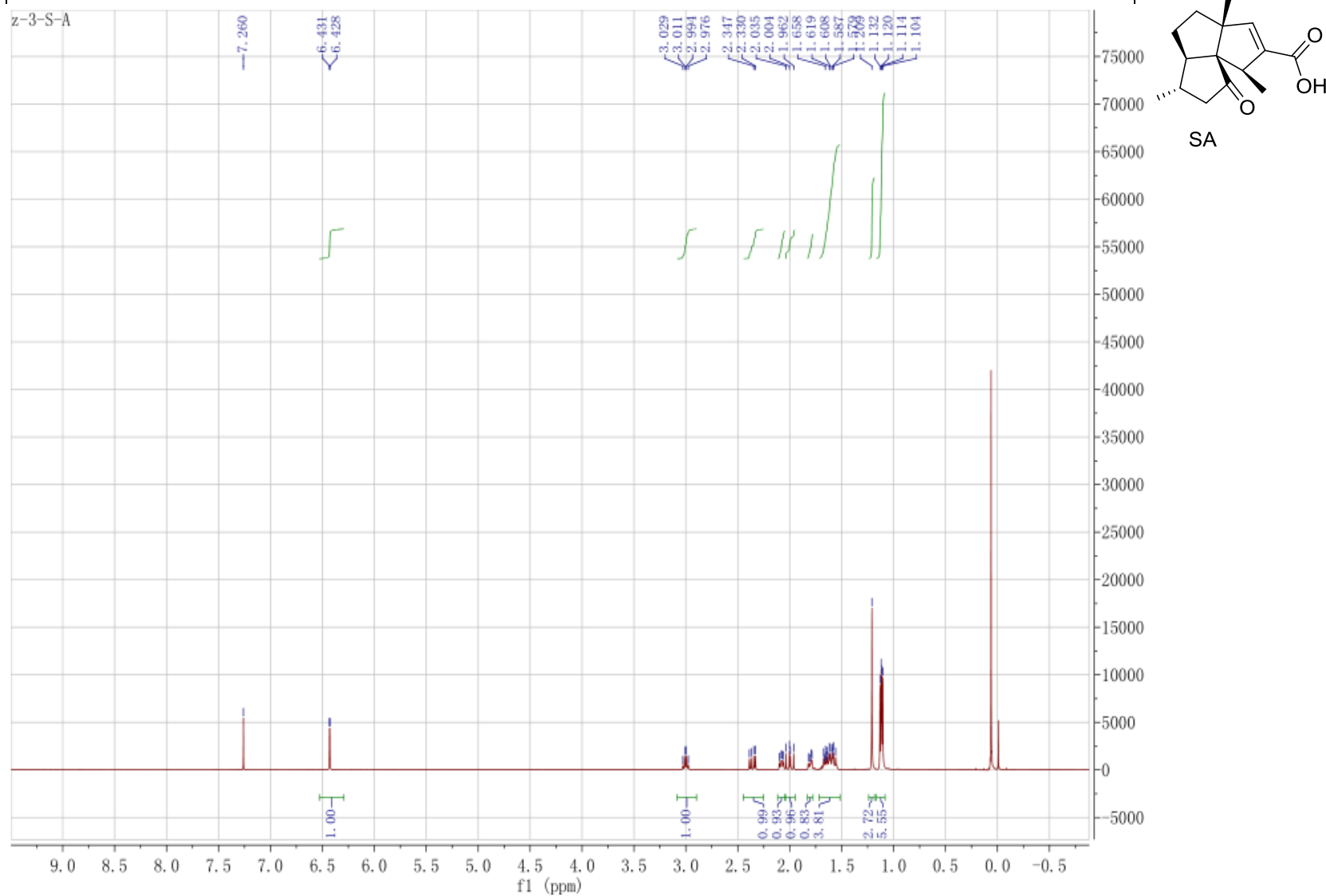


Figure S3. ^{13}C NMR (100 MHz, CDCl_3) of compound SA

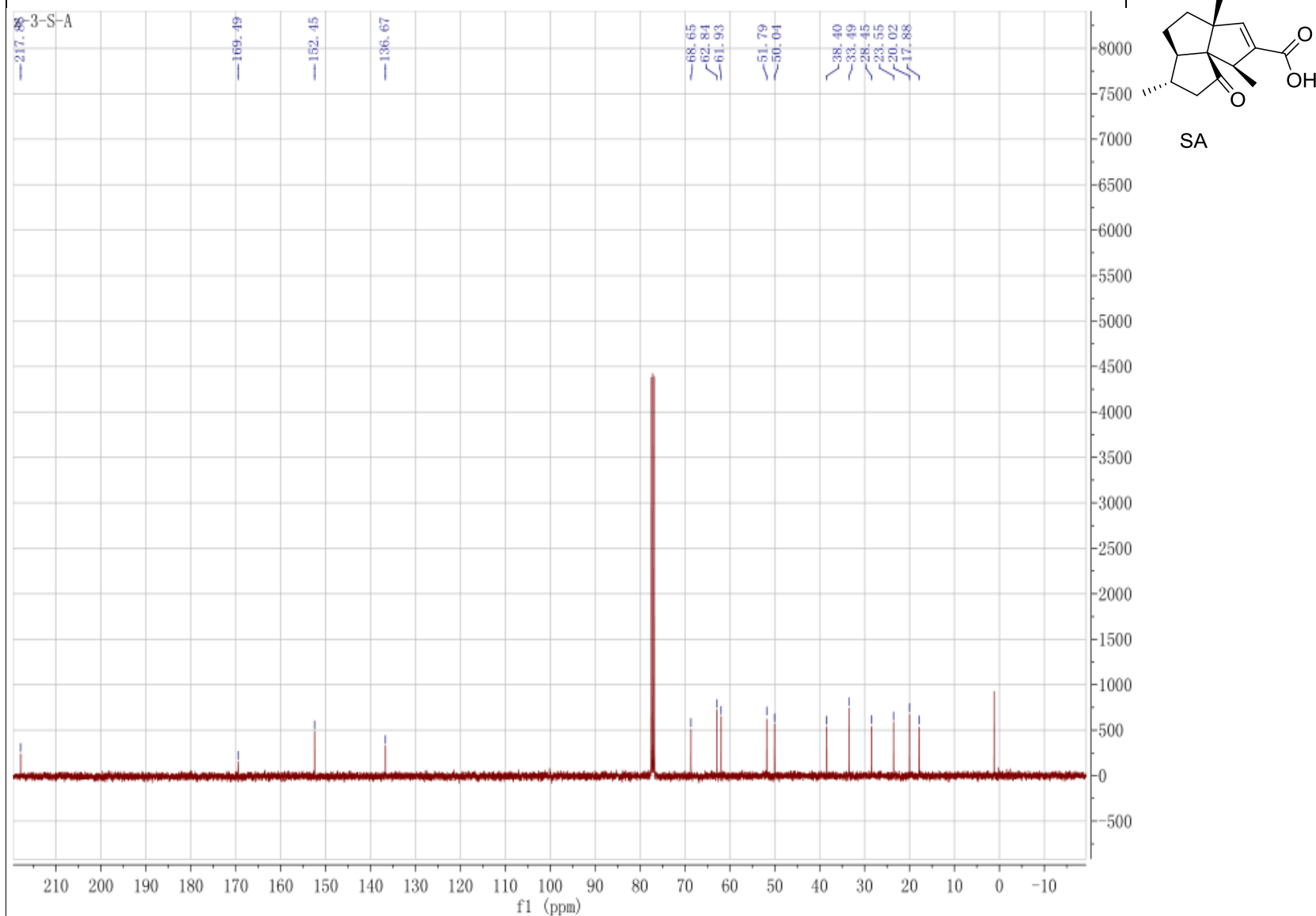


Figure S4. ^1H NMR (300 MHz, CDCl_3) of compound **1**

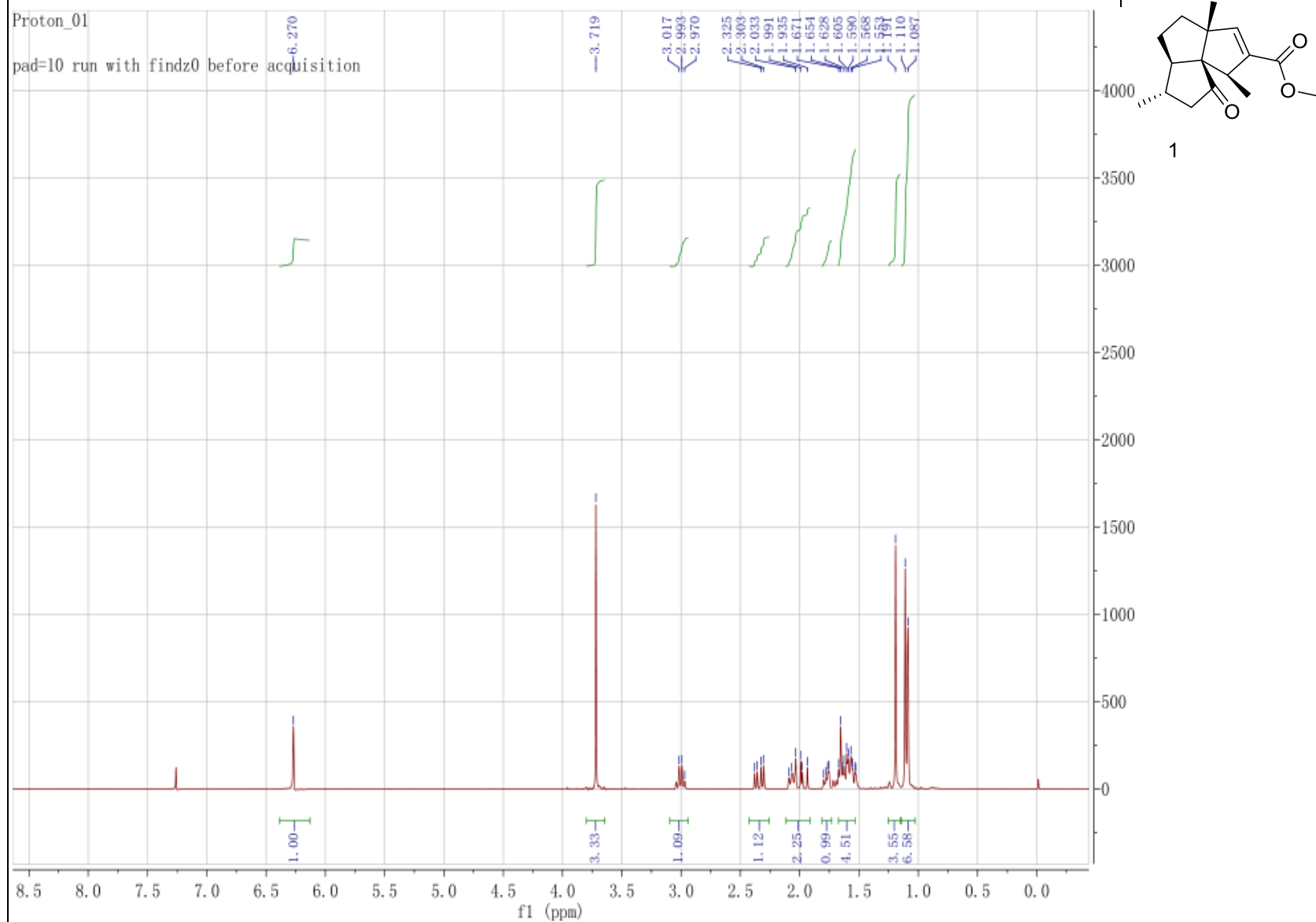


Figure S5. ^{13}C NMR (75 MHz, CDCl_3) of compound **1**

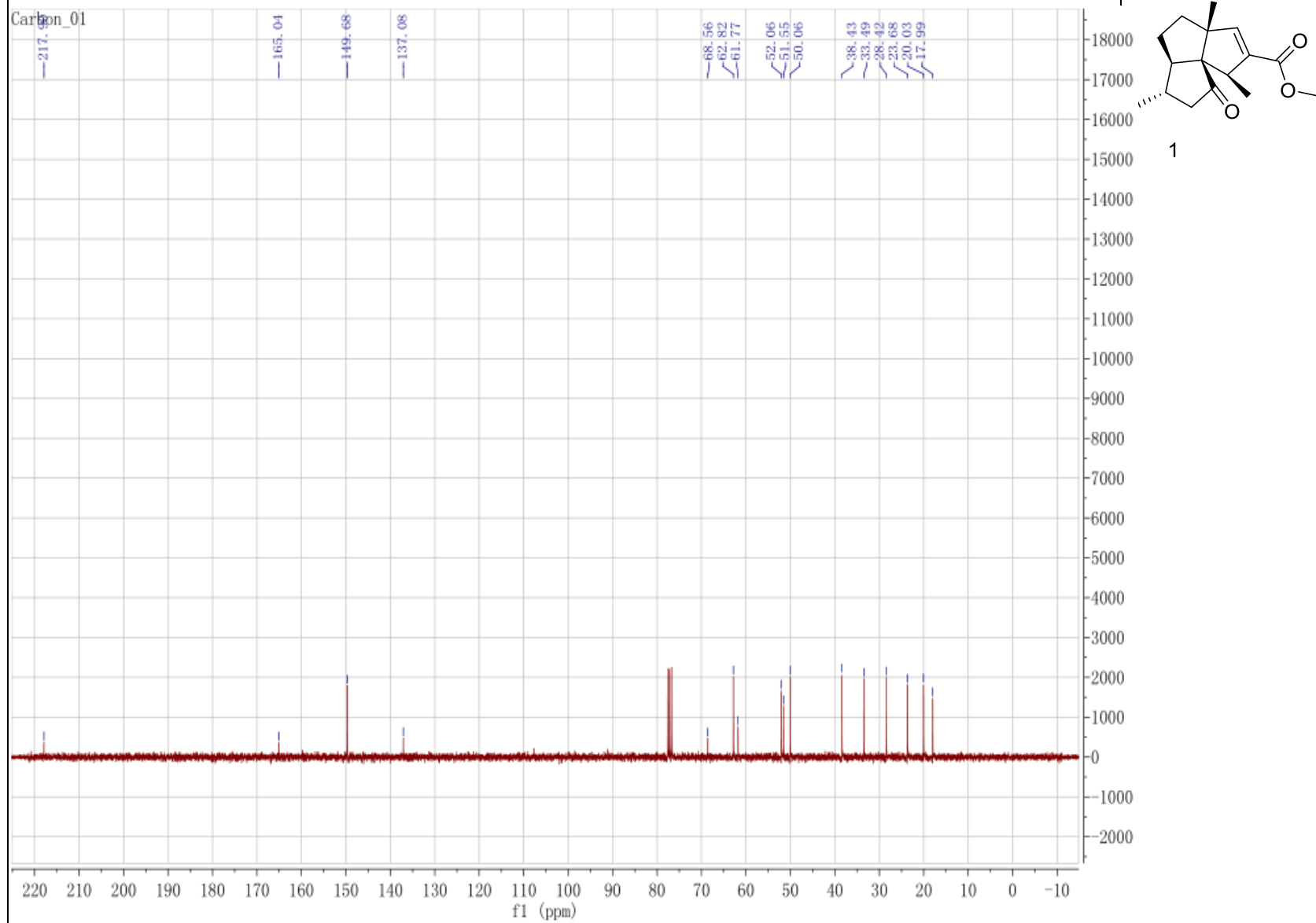


Figure S6. ^1H NMR (300 MHz, CDCl_3) of compound 2

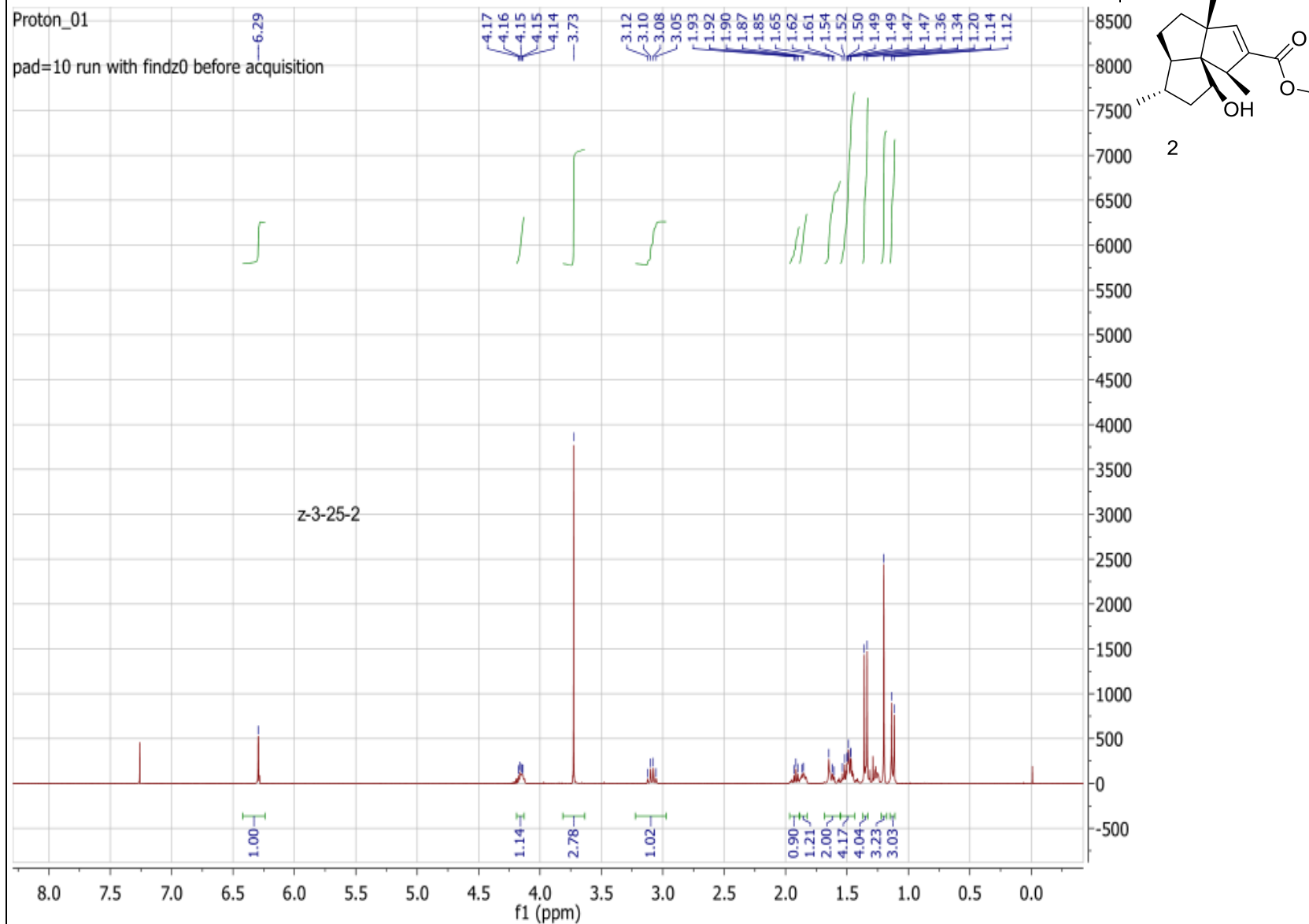


Figure S7. ^{13}C NMR (75 MHz, CDCl_3) of compound **2**

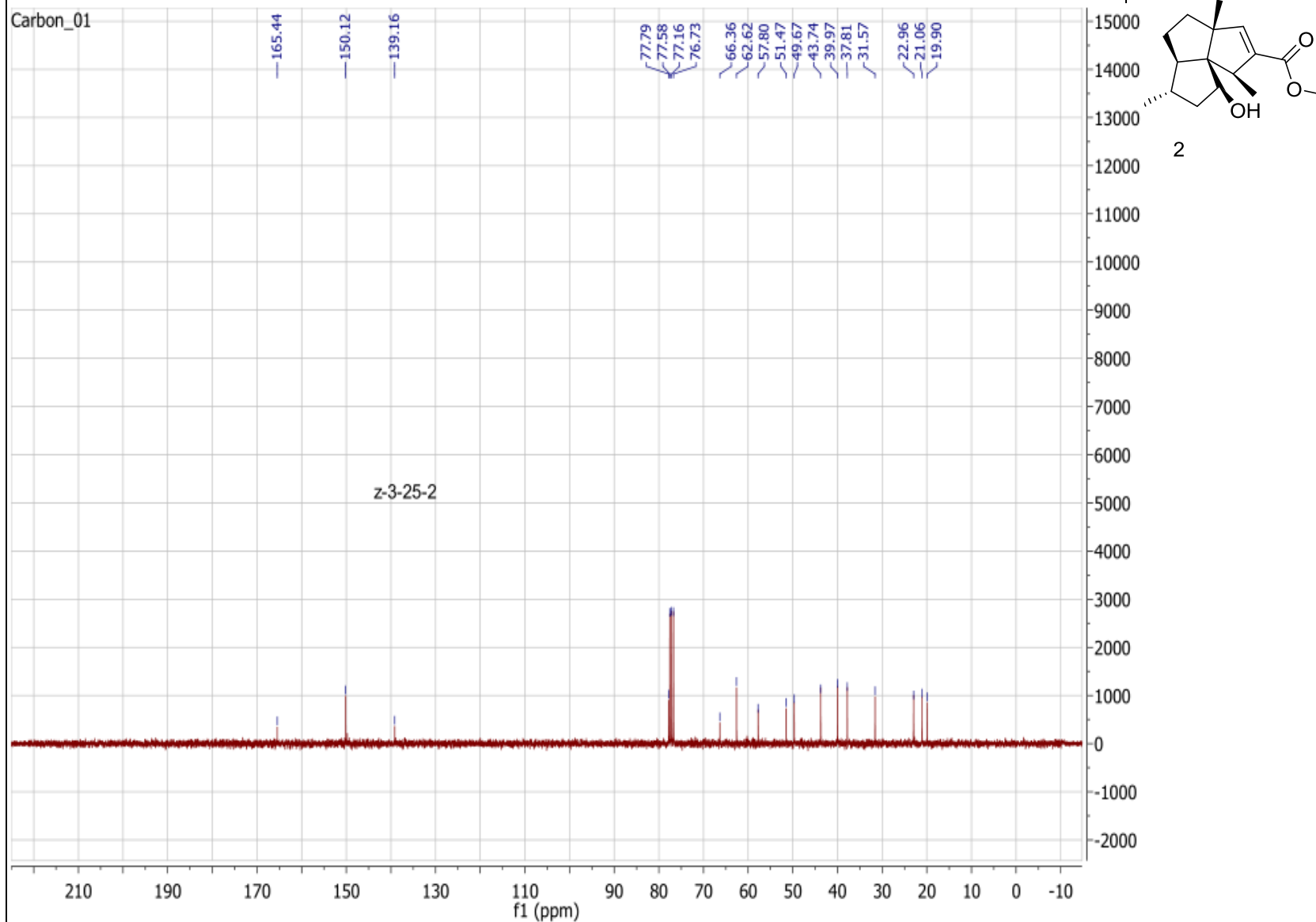


Figure S8. ^1H NMR (400 MHz, CDCl_3) of compound **3**

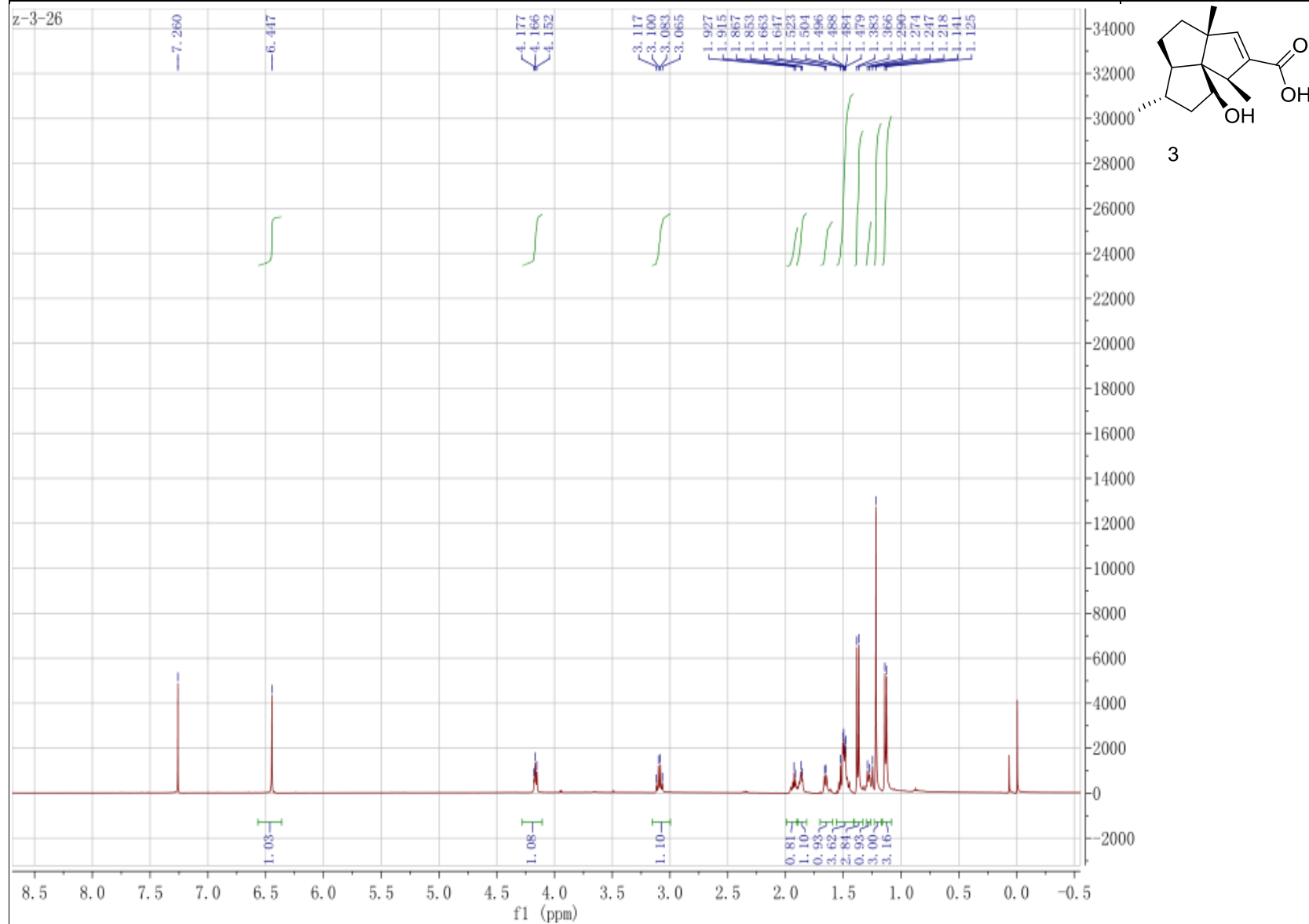


Figure S9. ^{13}C NMR (100 MHz, CDCl_3) of compound **3**

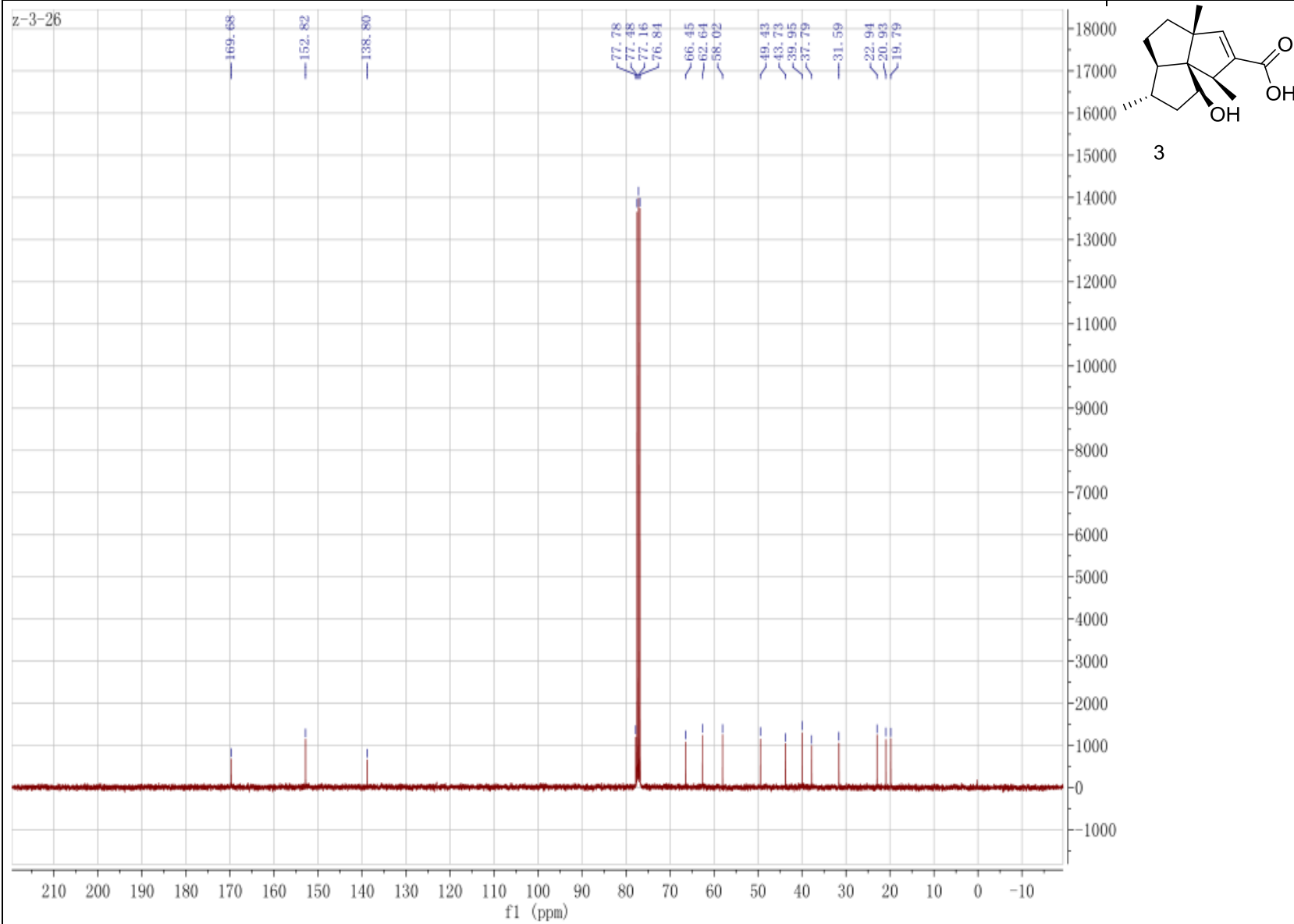


Figure S10. ^1H NMR (300 MHz, CDCl_3) of compound **4**

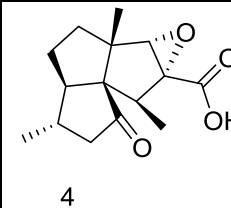
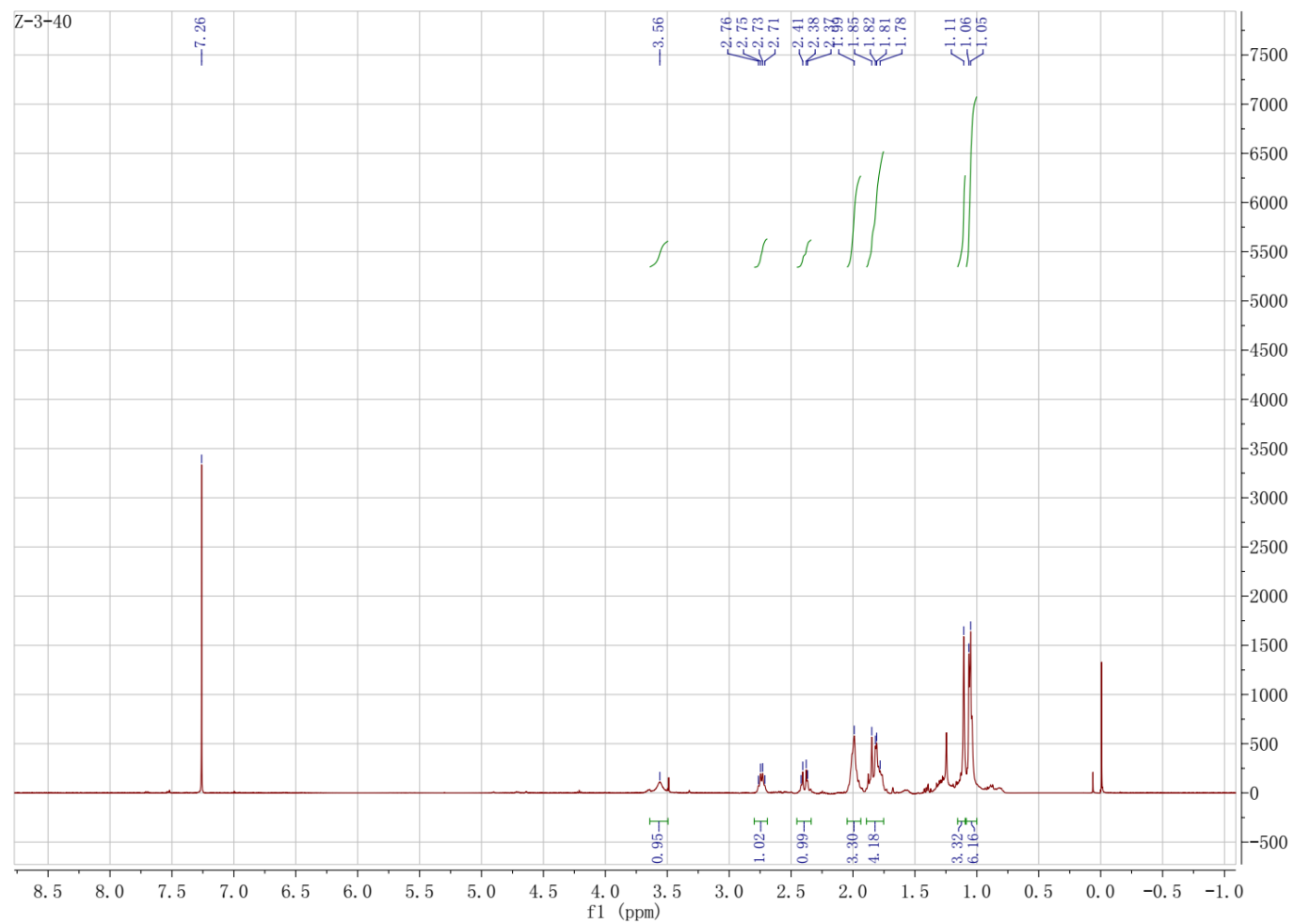


Figure S11. ^{13}C NMR (75 MHz, CDCl_3) of compound **4**

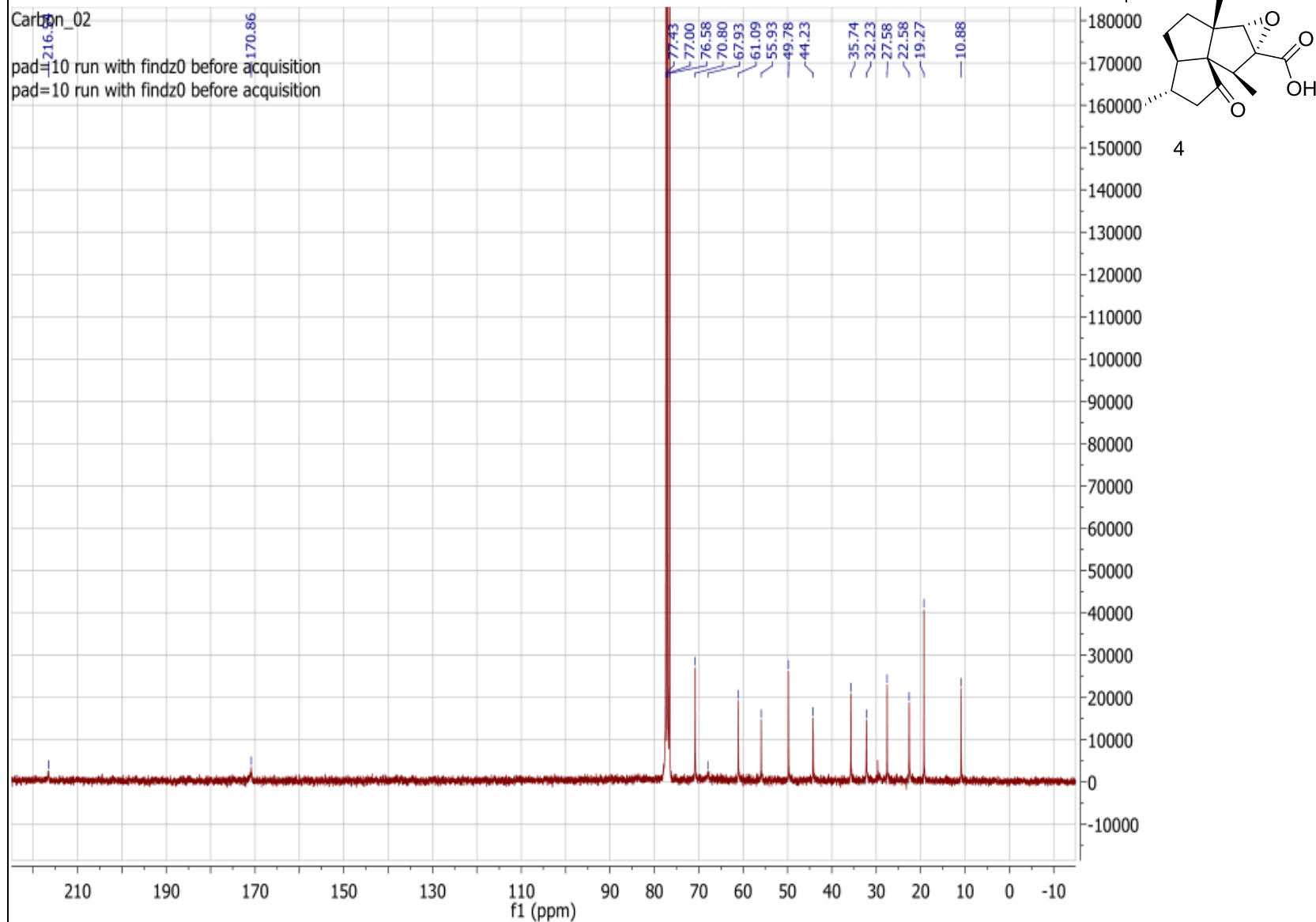


Figure S12. HSQC spectrum of compound 4

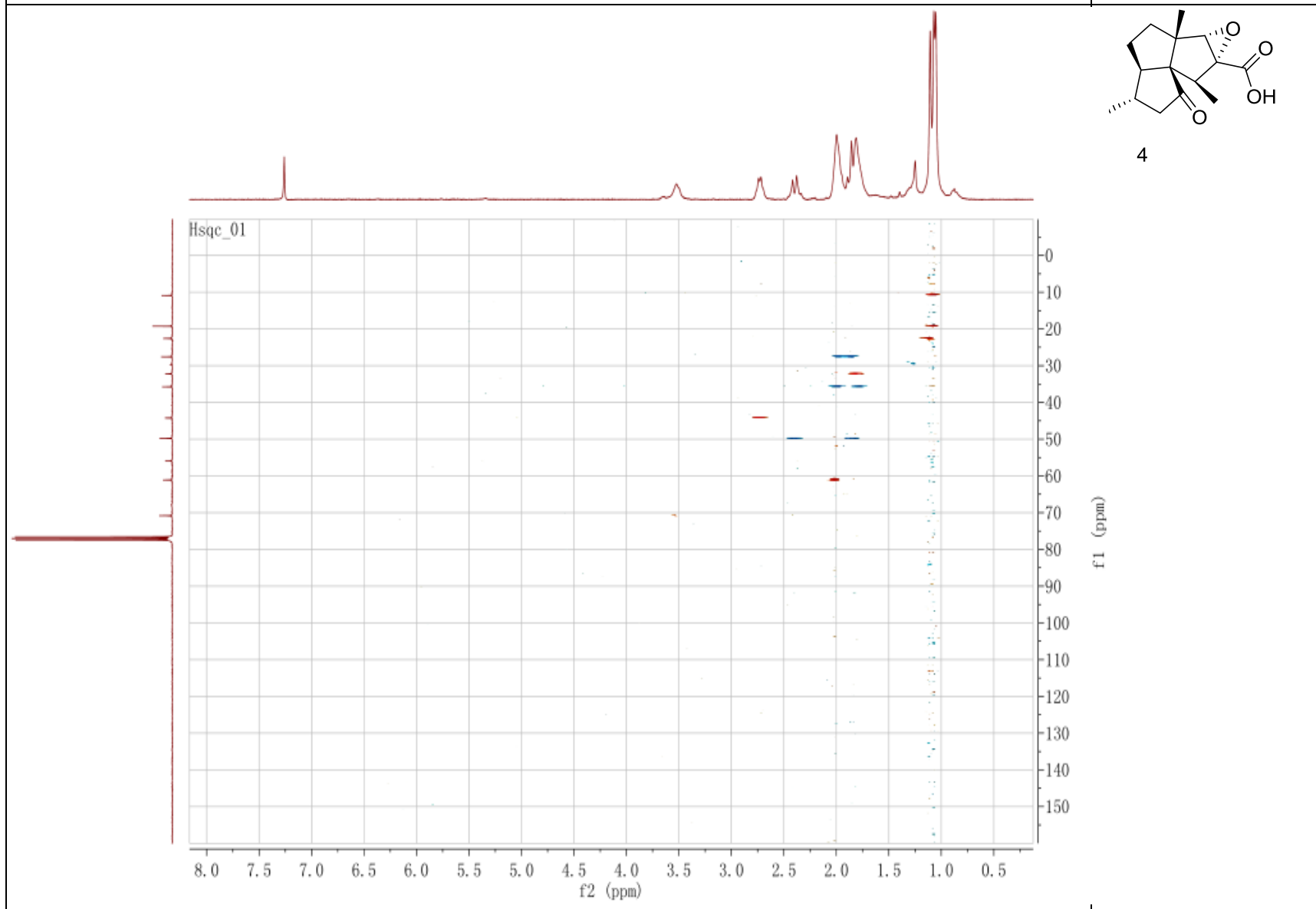
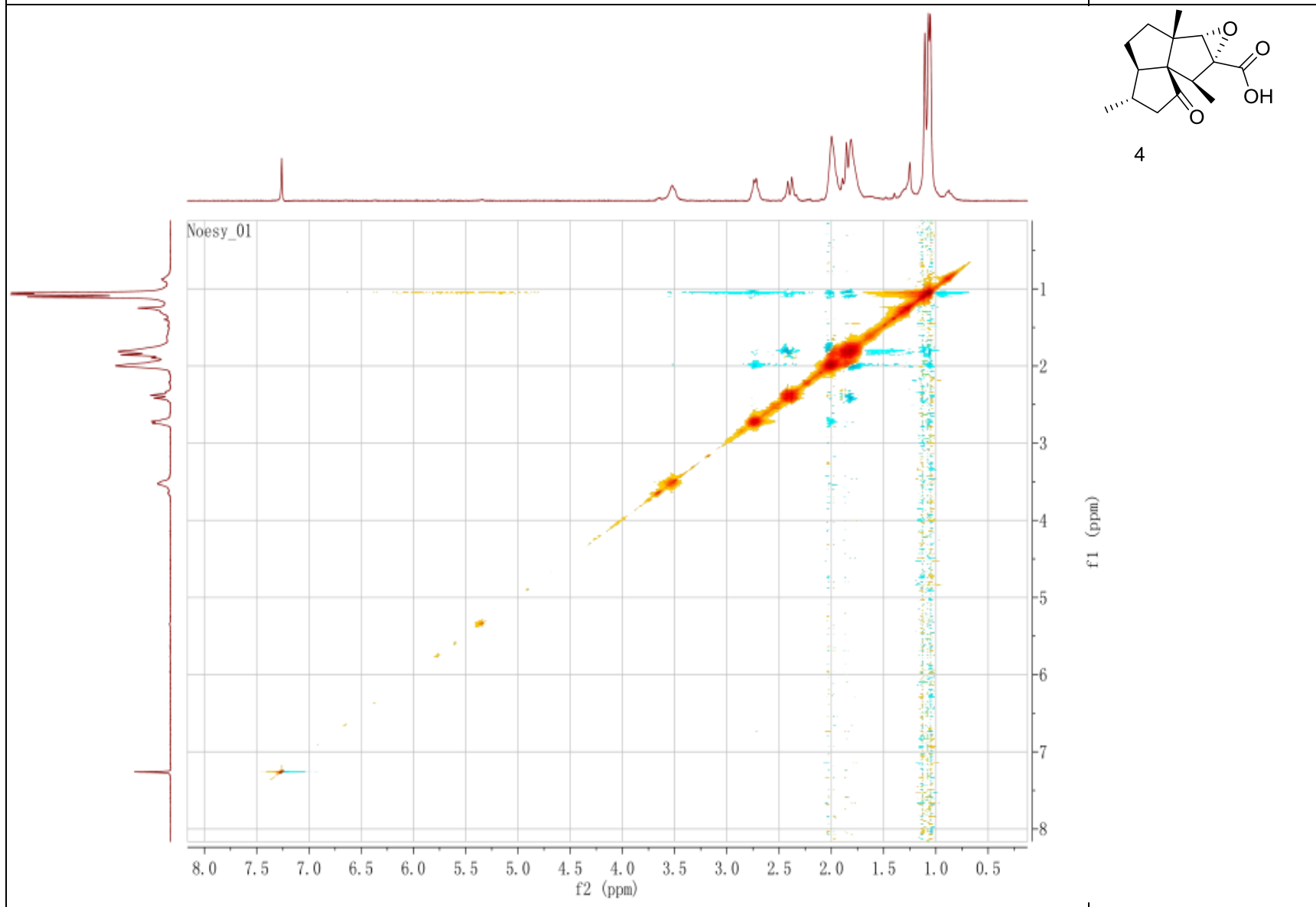


Figure S13. NOESY spectrum of compound **4**



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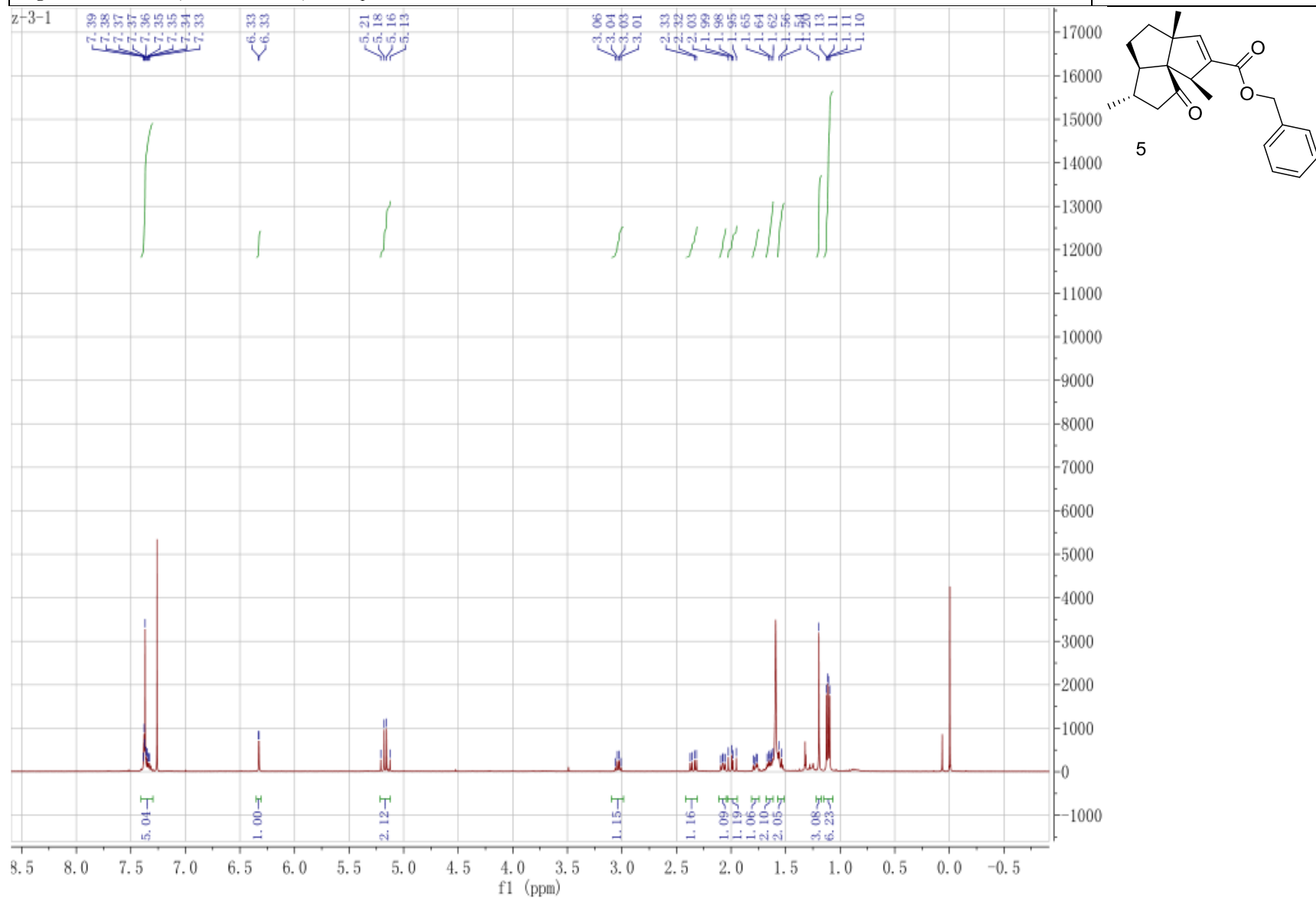


Figure S15. ^{13}C NMR (100 MHz, CDCl_3) of compound **5**

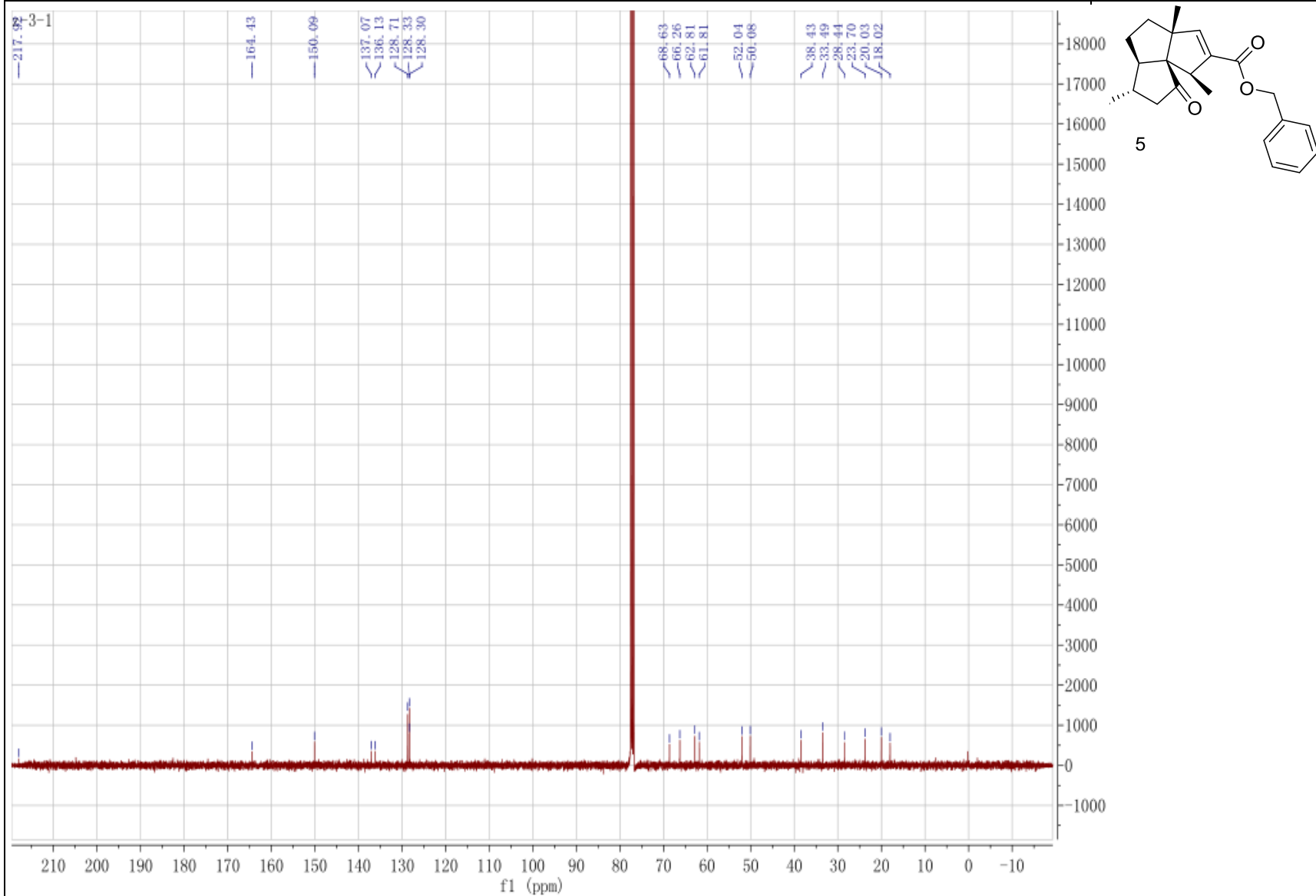


Figure S16. ^1H NMR (300 MHz, CDCl_3) of compound **6**

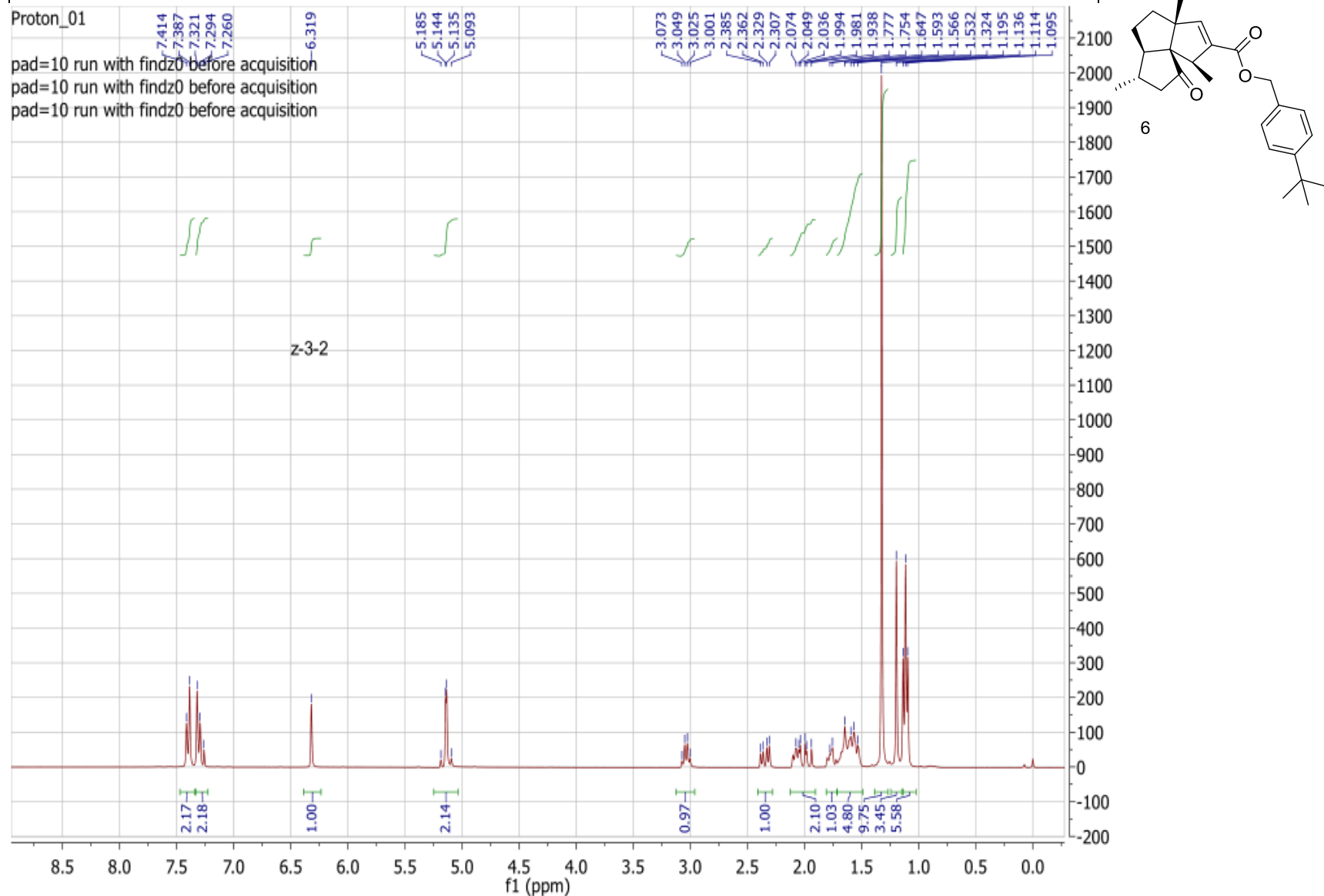


Figure S17. ^{13}C NMR (75 MHz, CDCl_3) of compound **6**

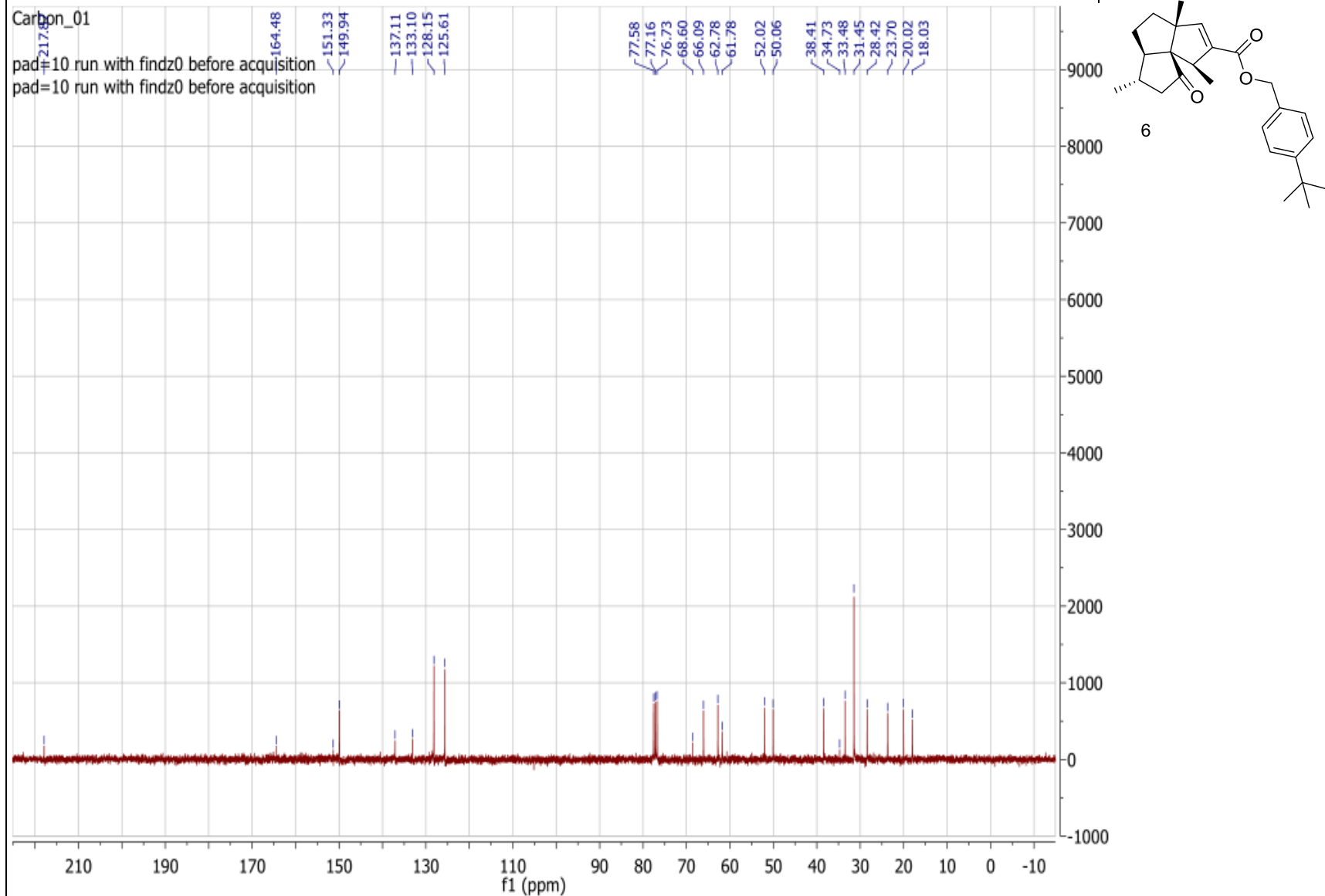


Figure S18. ^1H NMR (300 MHz, CDCl_3) of compound 7

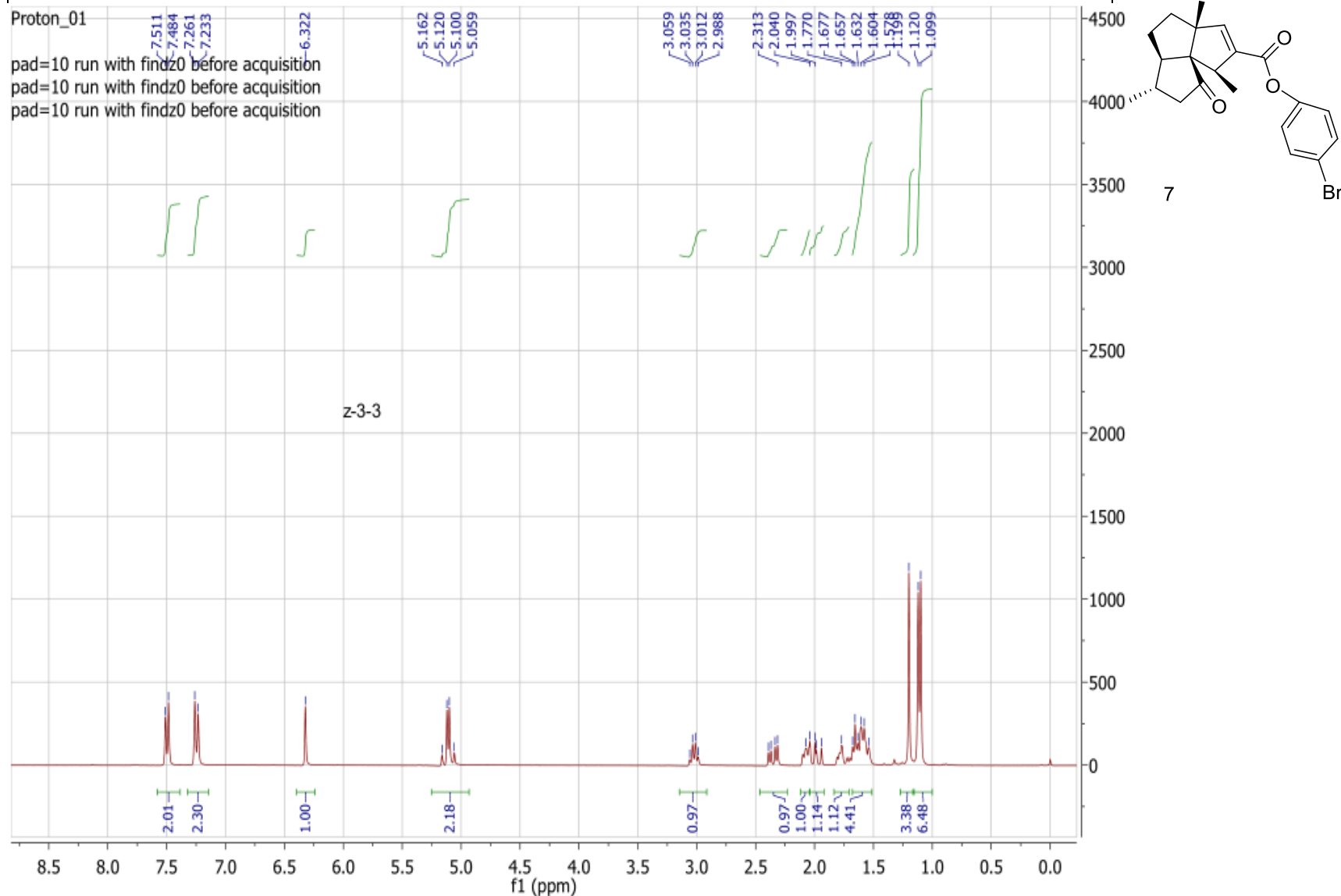


Figure S19. ^{13}C NMR (75 MHz, CDCl_3) of compound 7

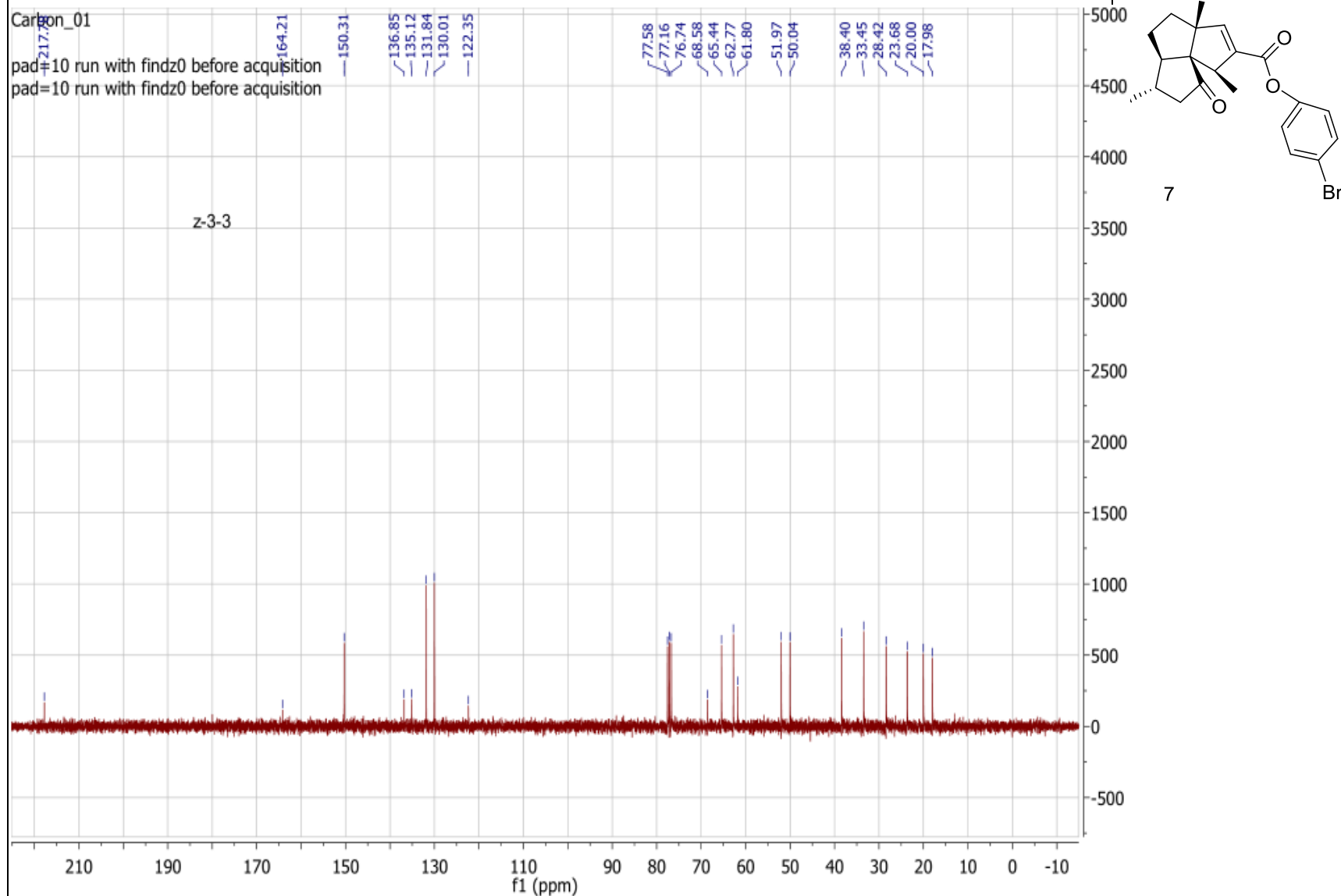


Figure S20. ^1H NMR (300 MHz, CDCl_3) of compound **8**

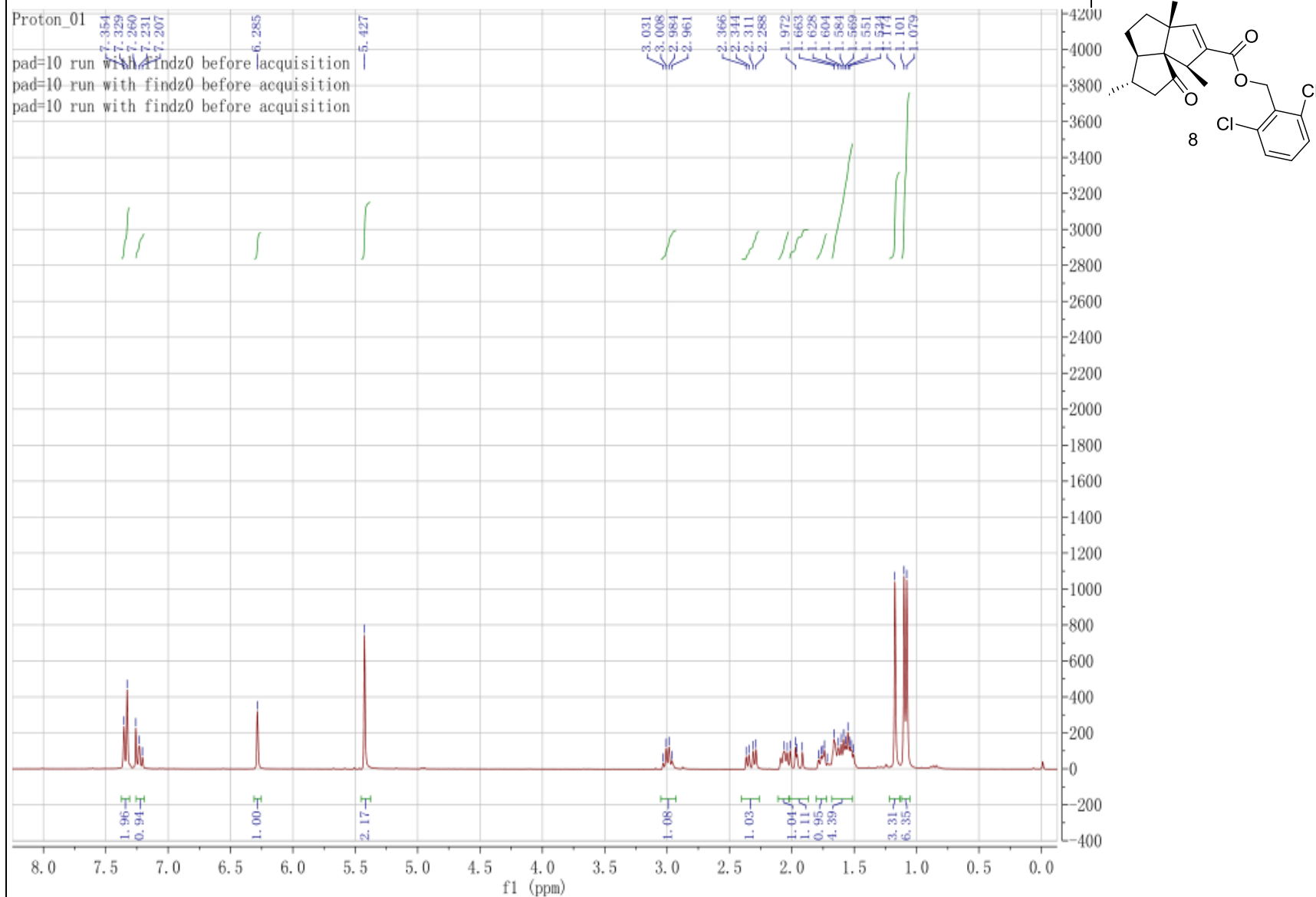


Figure S21. ^{13}C NMR (75 MHz, CDCl_3) of compound **8**

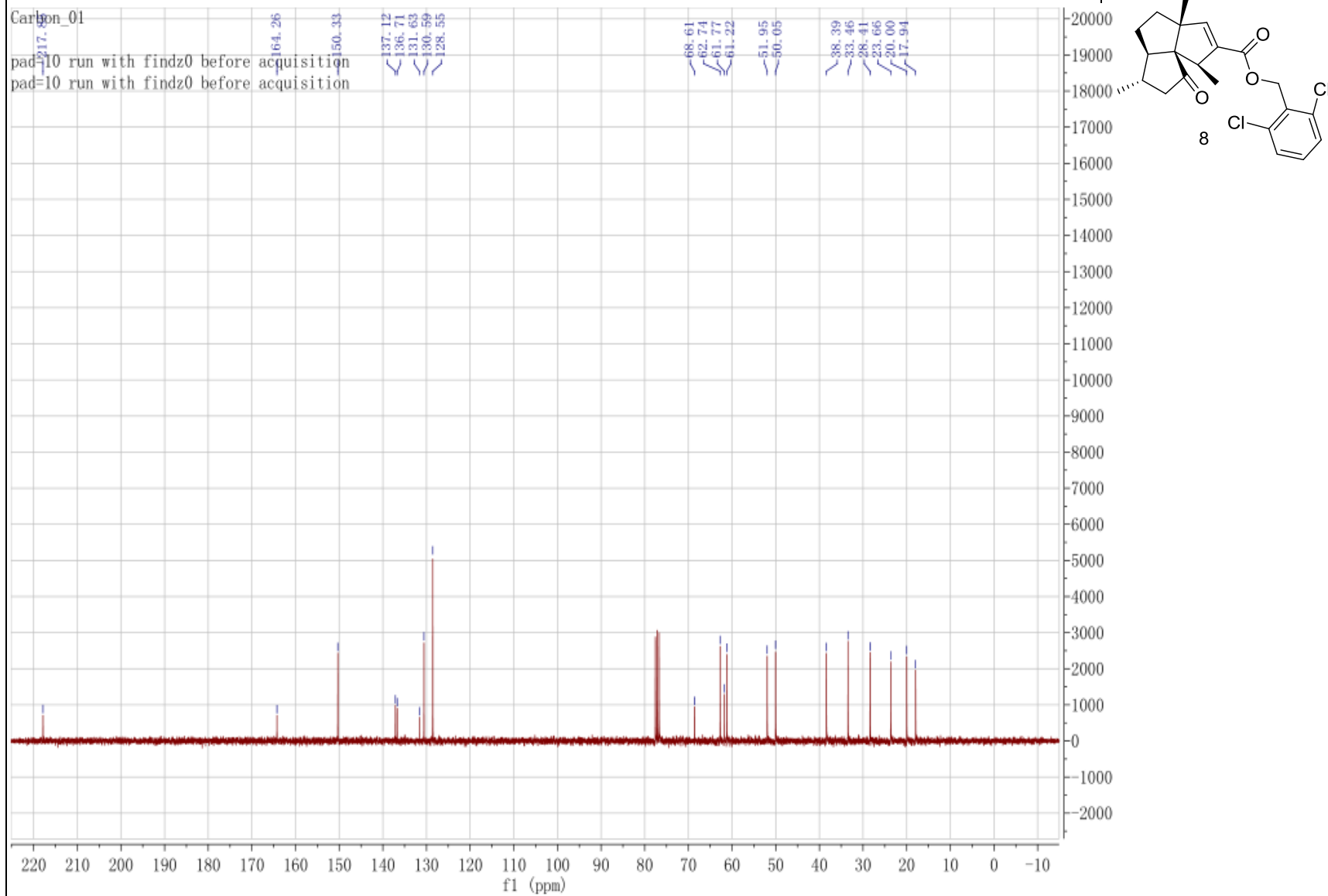


Figure S22. ^1H NMR (300 MHz, CDCl_3) of compound **9**

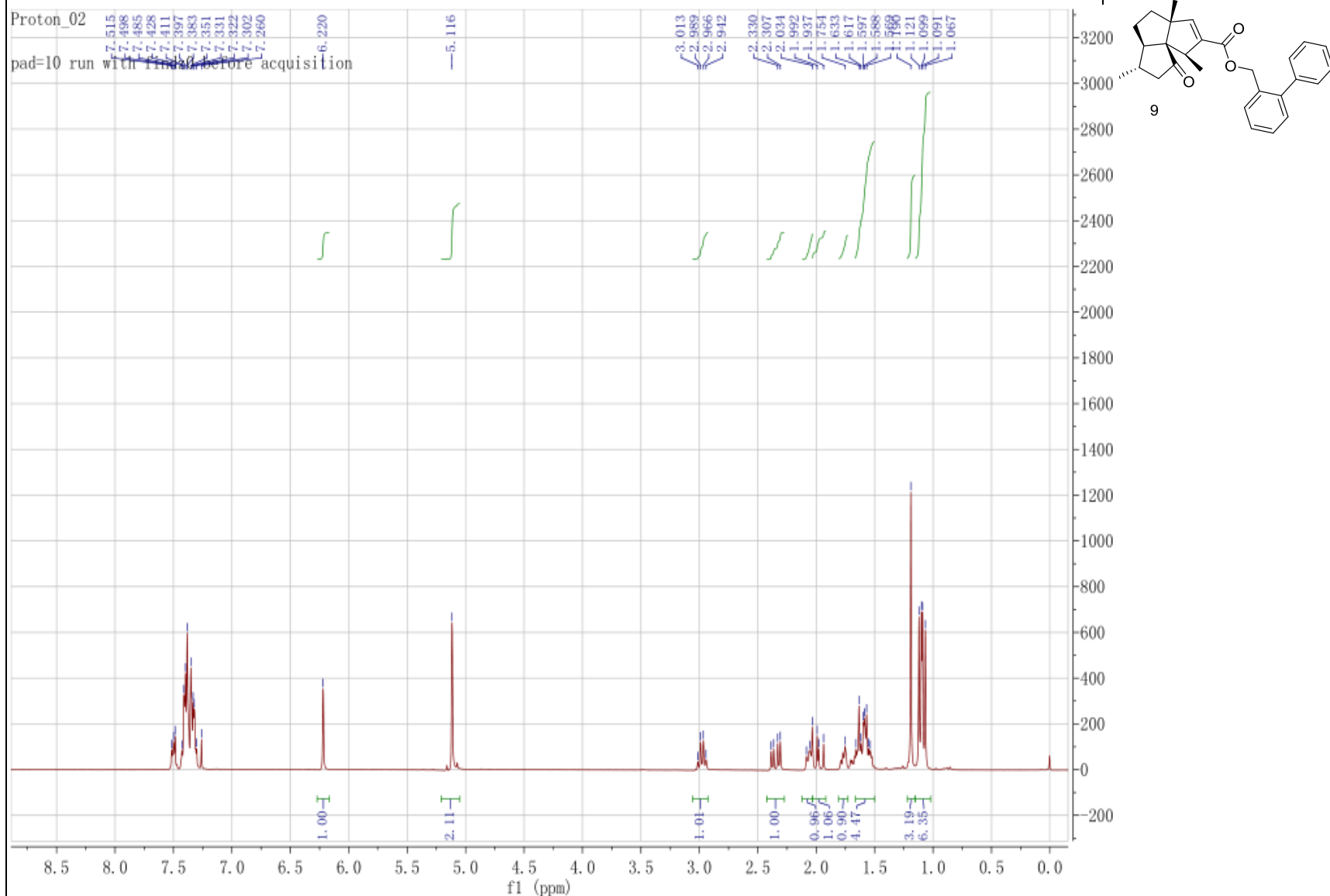


Figure S23. ^{13}C NMR (75 MHz, CDCl_3) of compound **9**

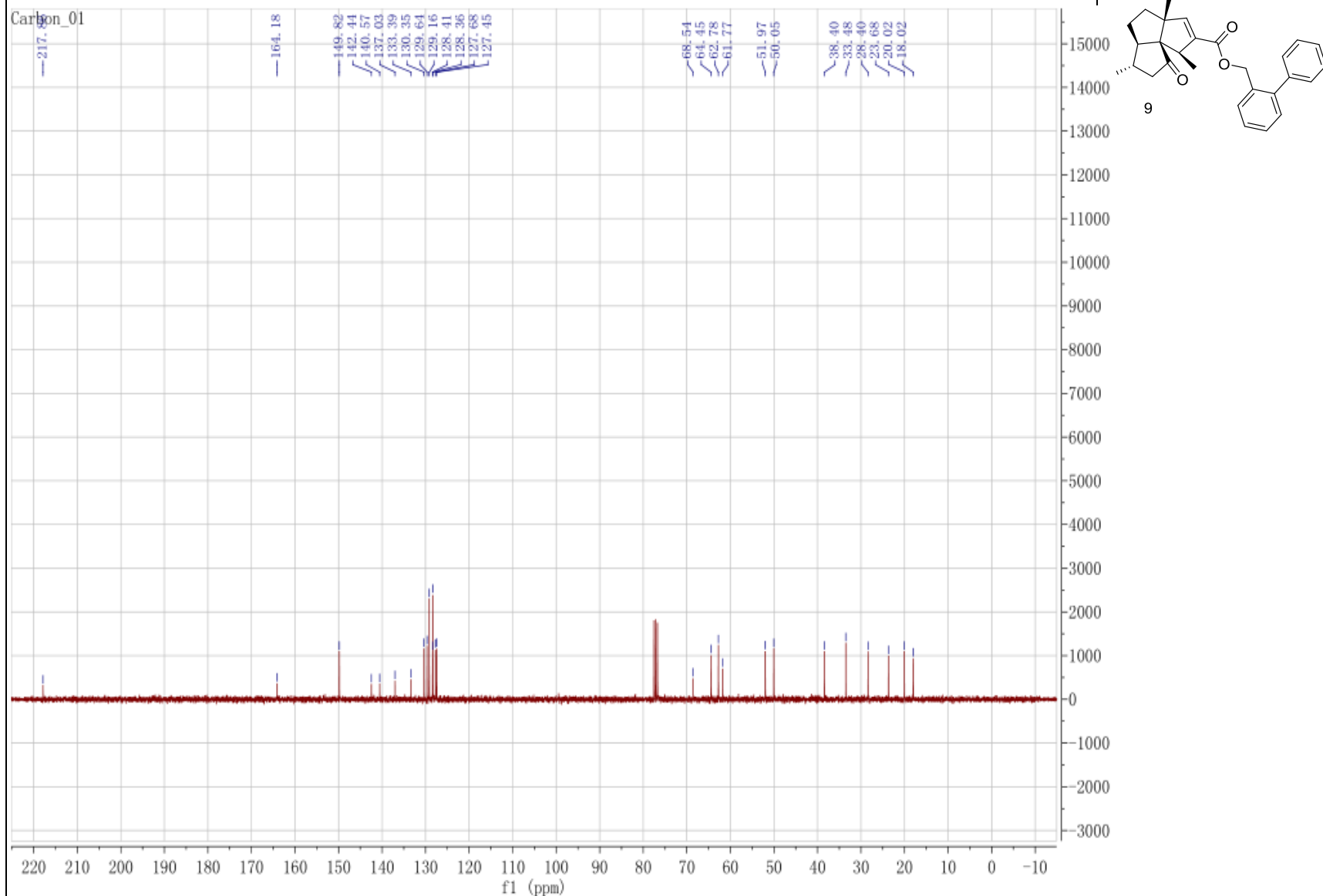


Figure S24. ^1H NMR (300 MHz, CDCl_3) of compound **10**

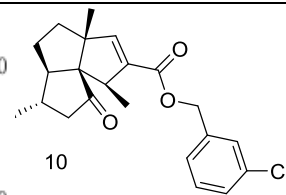
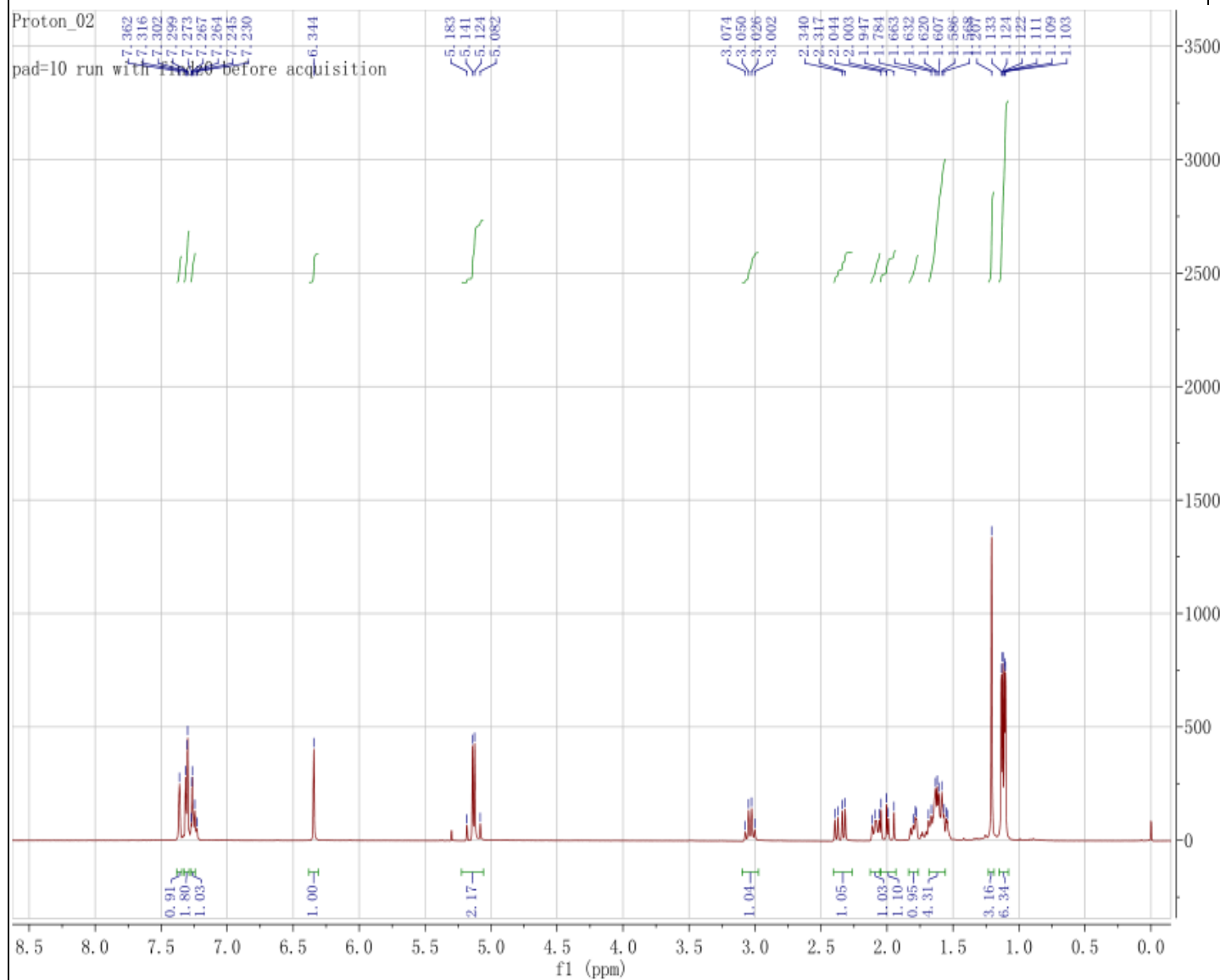


Figure S25. ^{13}C NMR (75 MHz, CDCl_3) of compound **10**

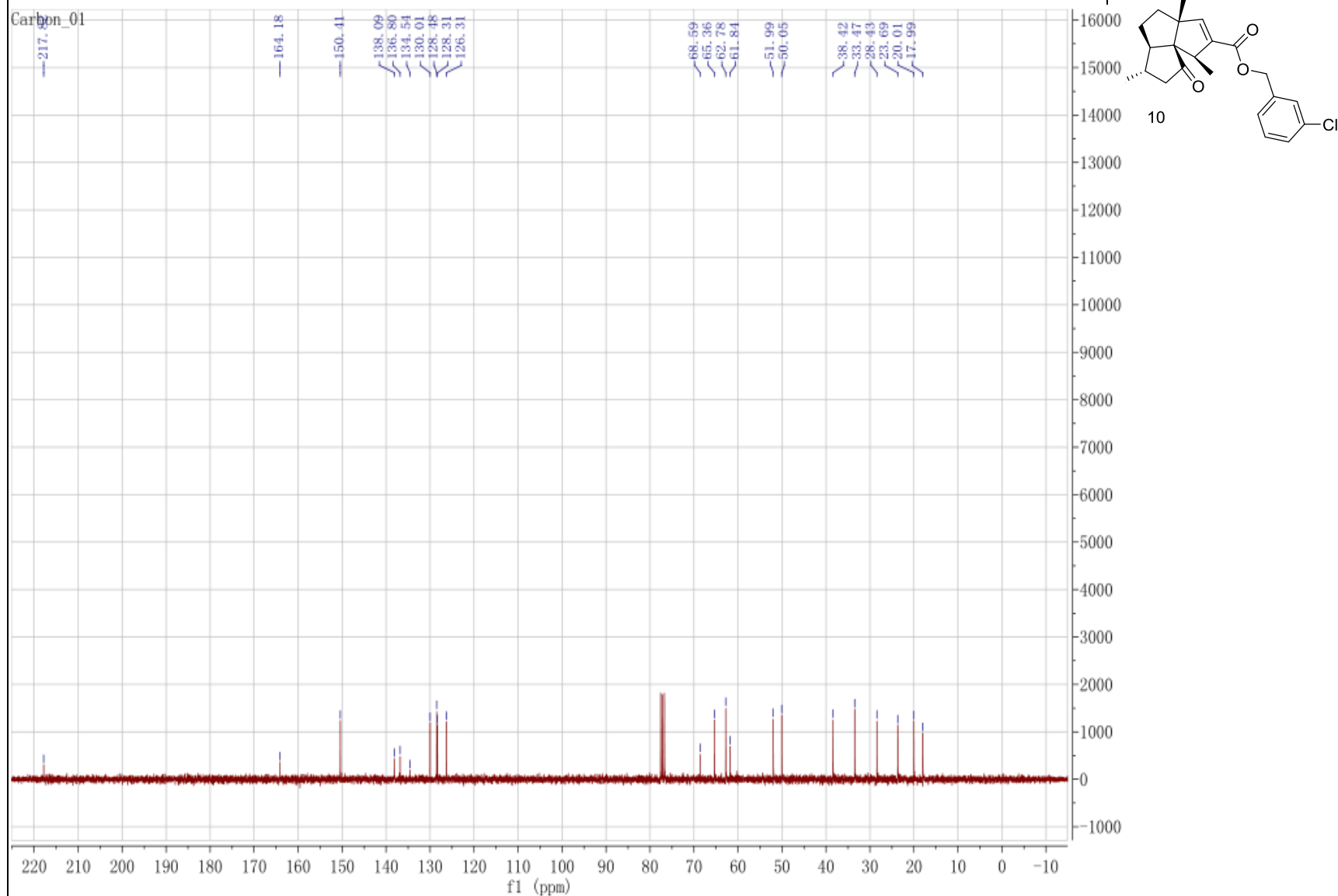


Figure S26. ^1H NMR (300 MHz, CDCl_3) of compound **11**

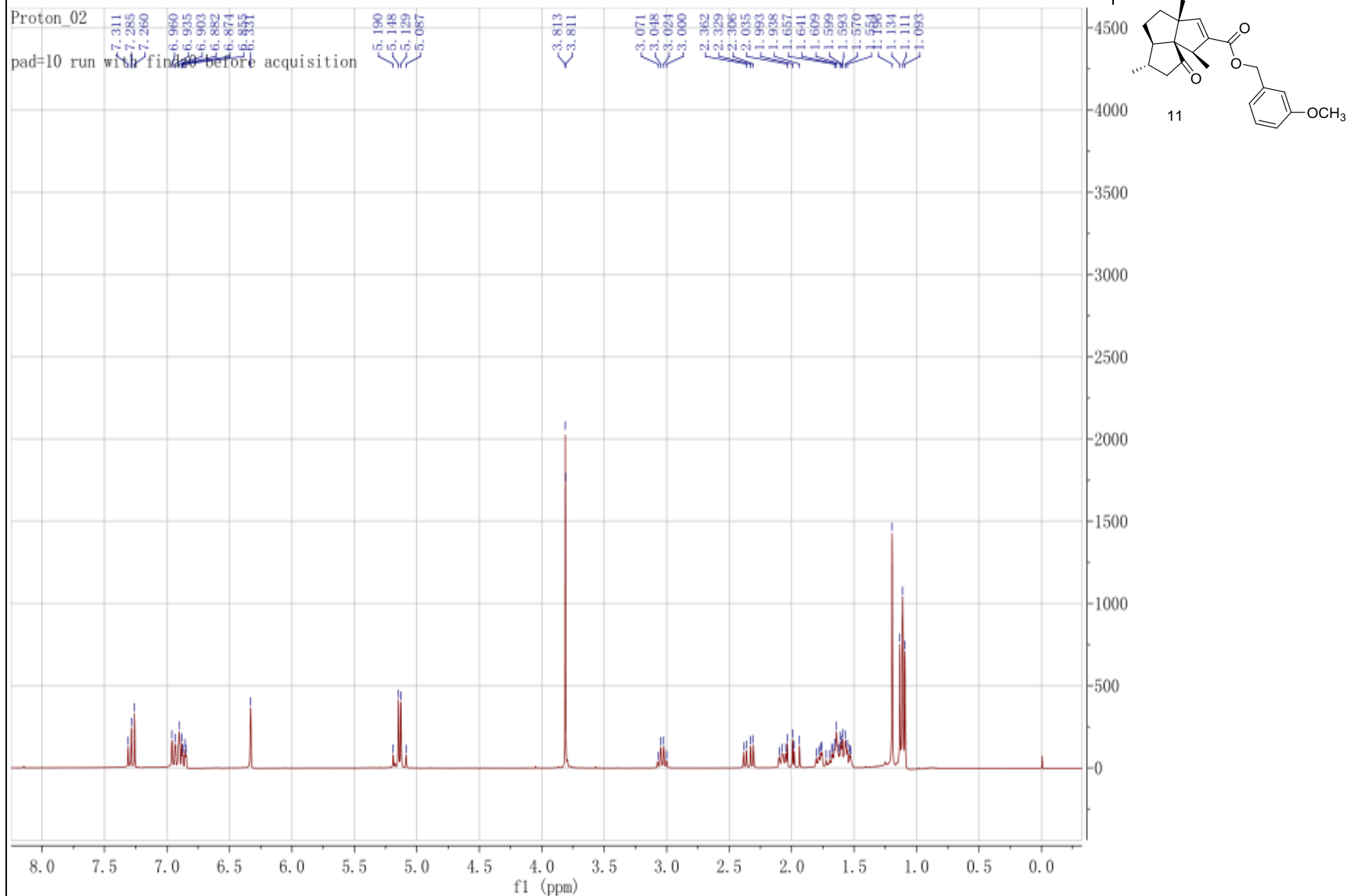


Figure S27. ^{13}C NMR (75 MHz, CDCl_3) of compound **11**

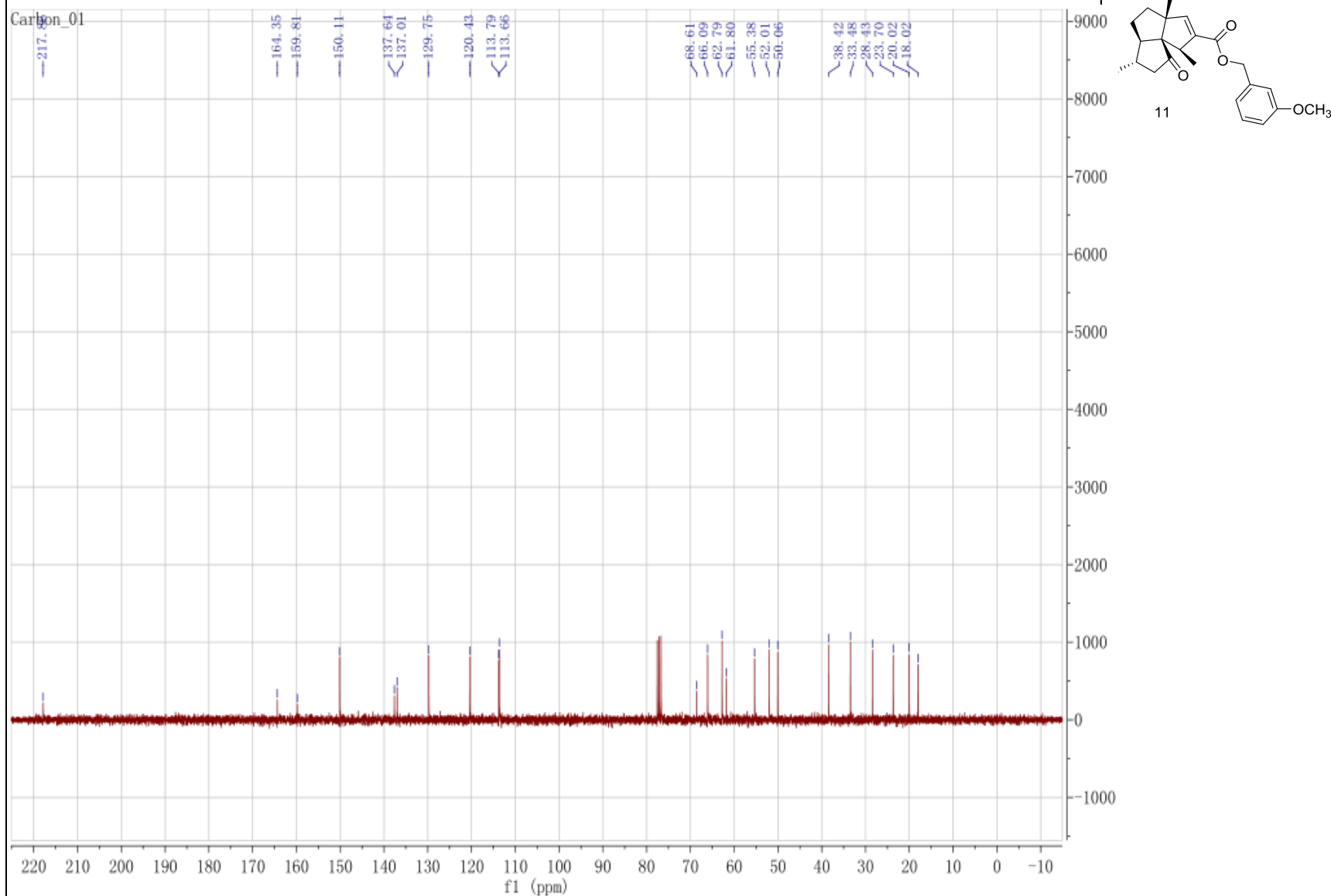


Figure S28. ^1H NMR (300 MHz, CDCl_3) of compound **12**

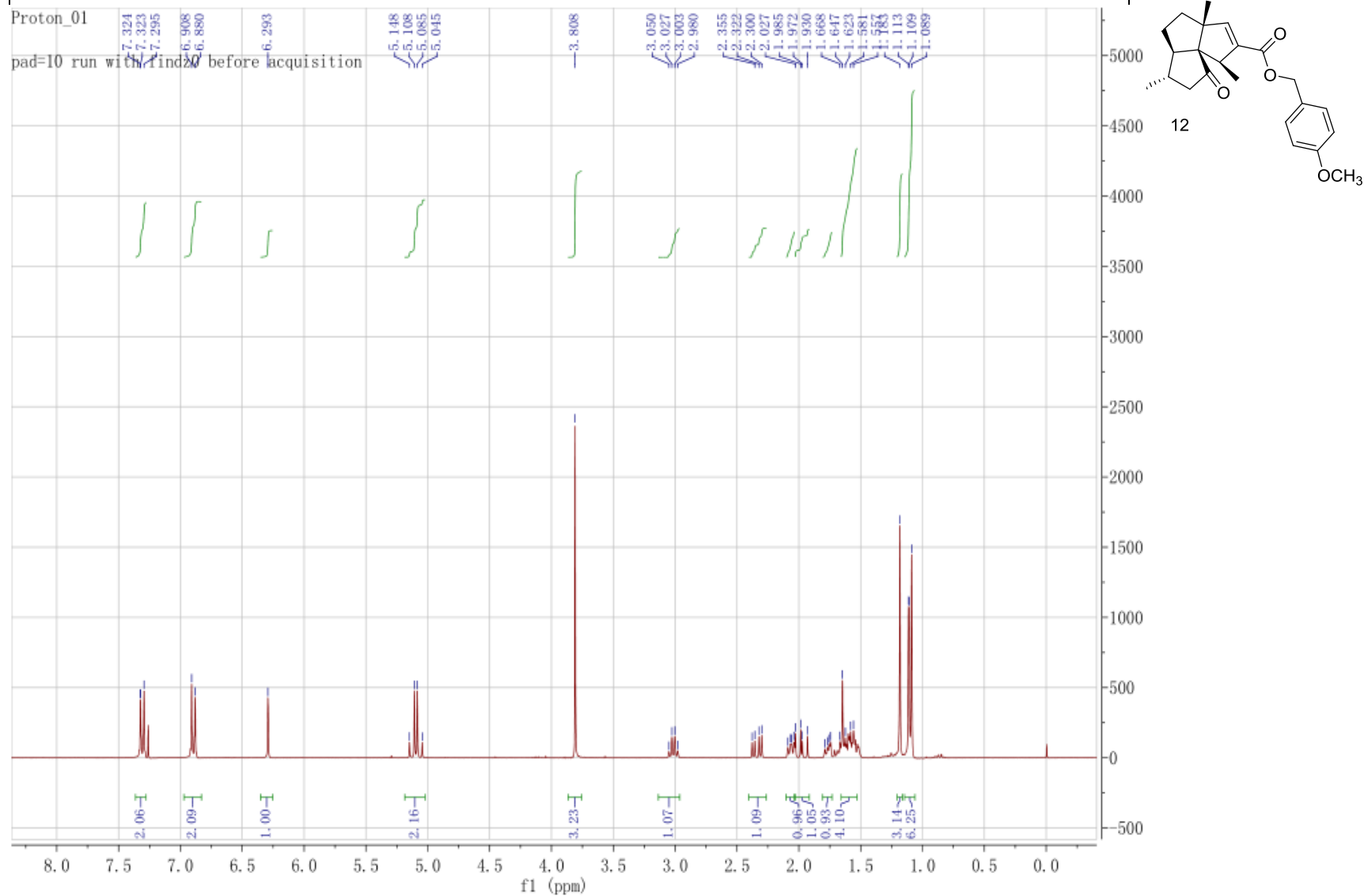


Figure S29. ^{13}C NMR (75 MHz, CDCl_3) of compound **12**

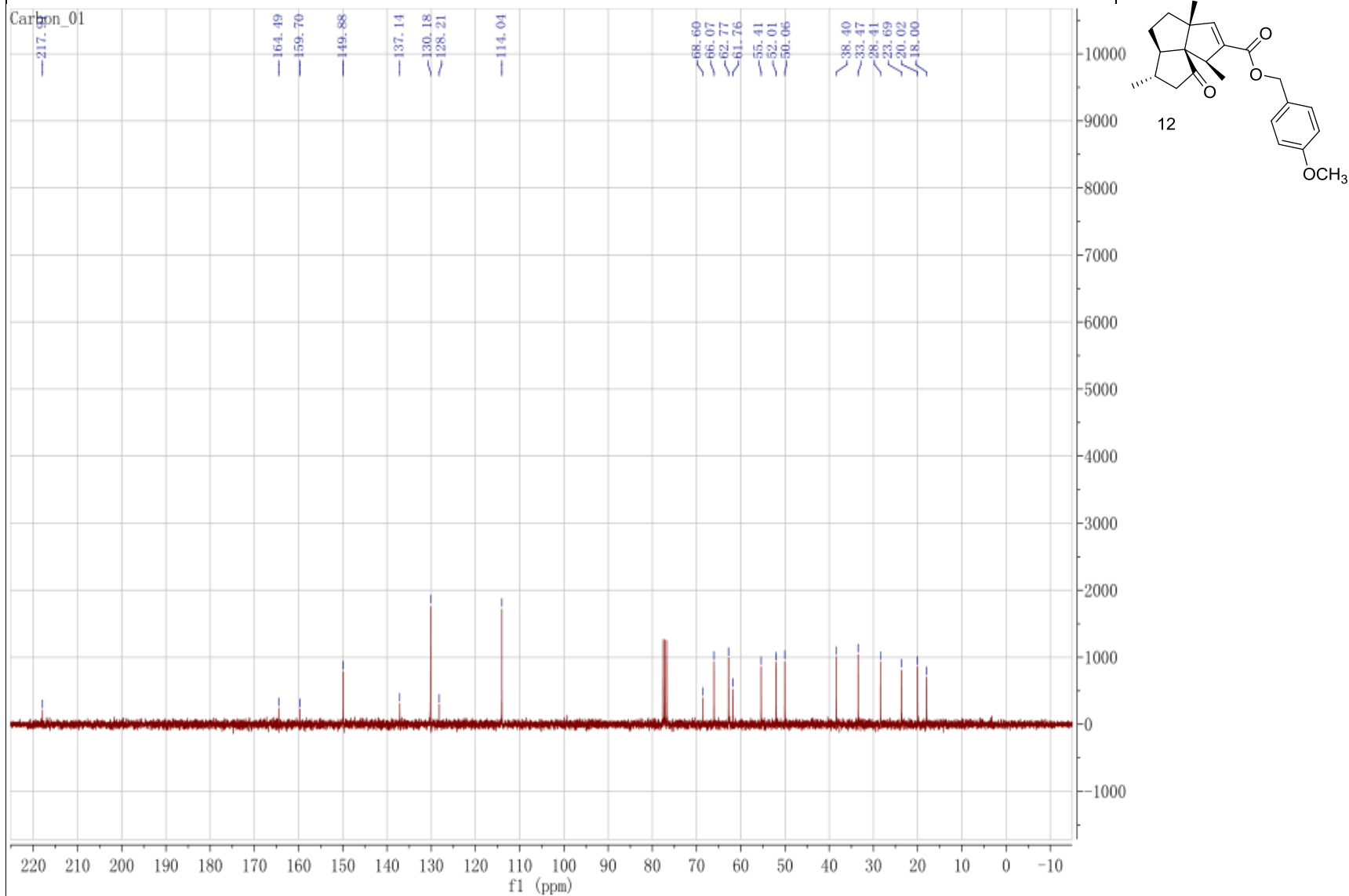


Figure S30. ^1H NMR (300 MHz, CDCl_3) of compound **13**

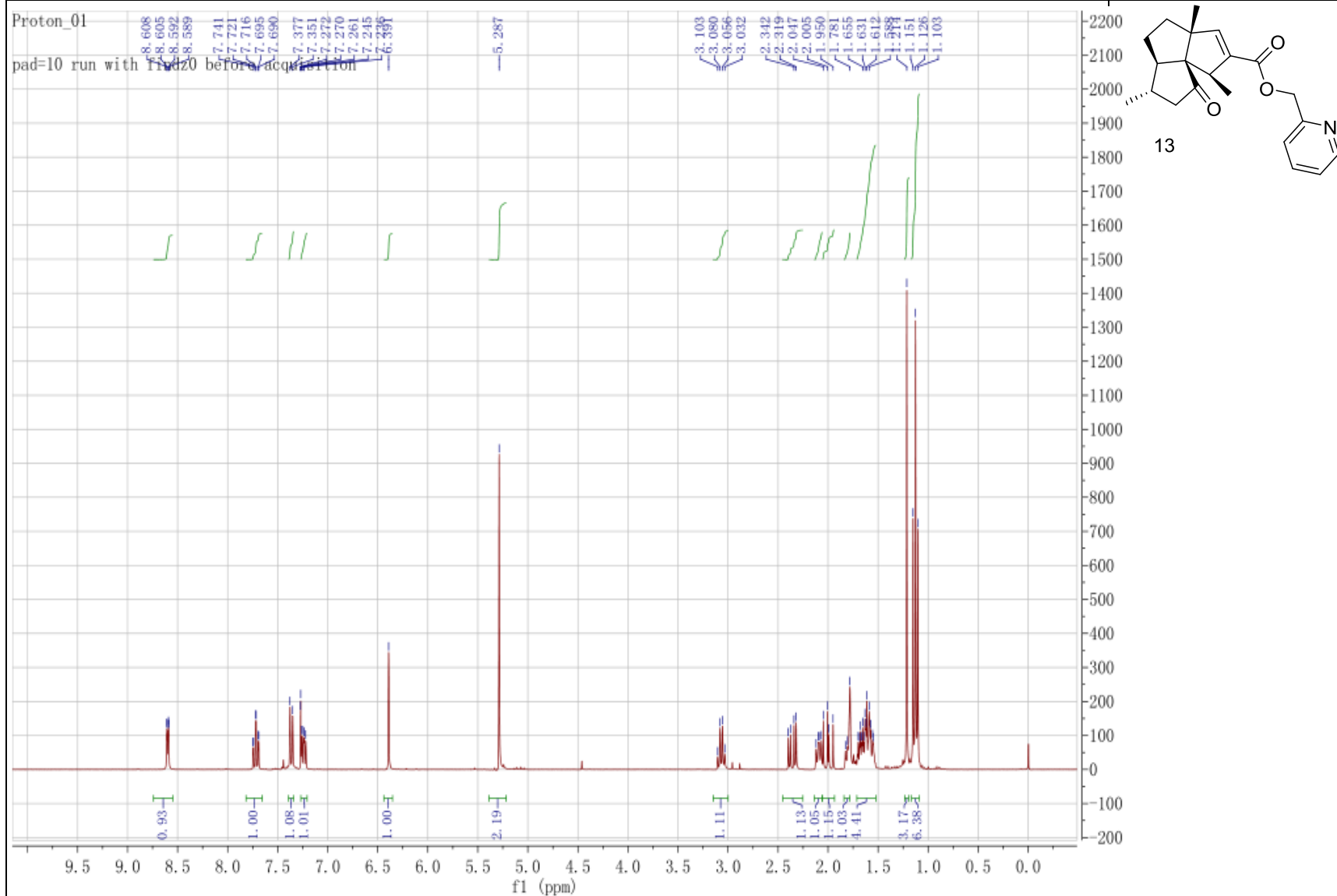


Figure S31. ^{13}C NMR (75 MHz, CDCl_3) of compound **13**

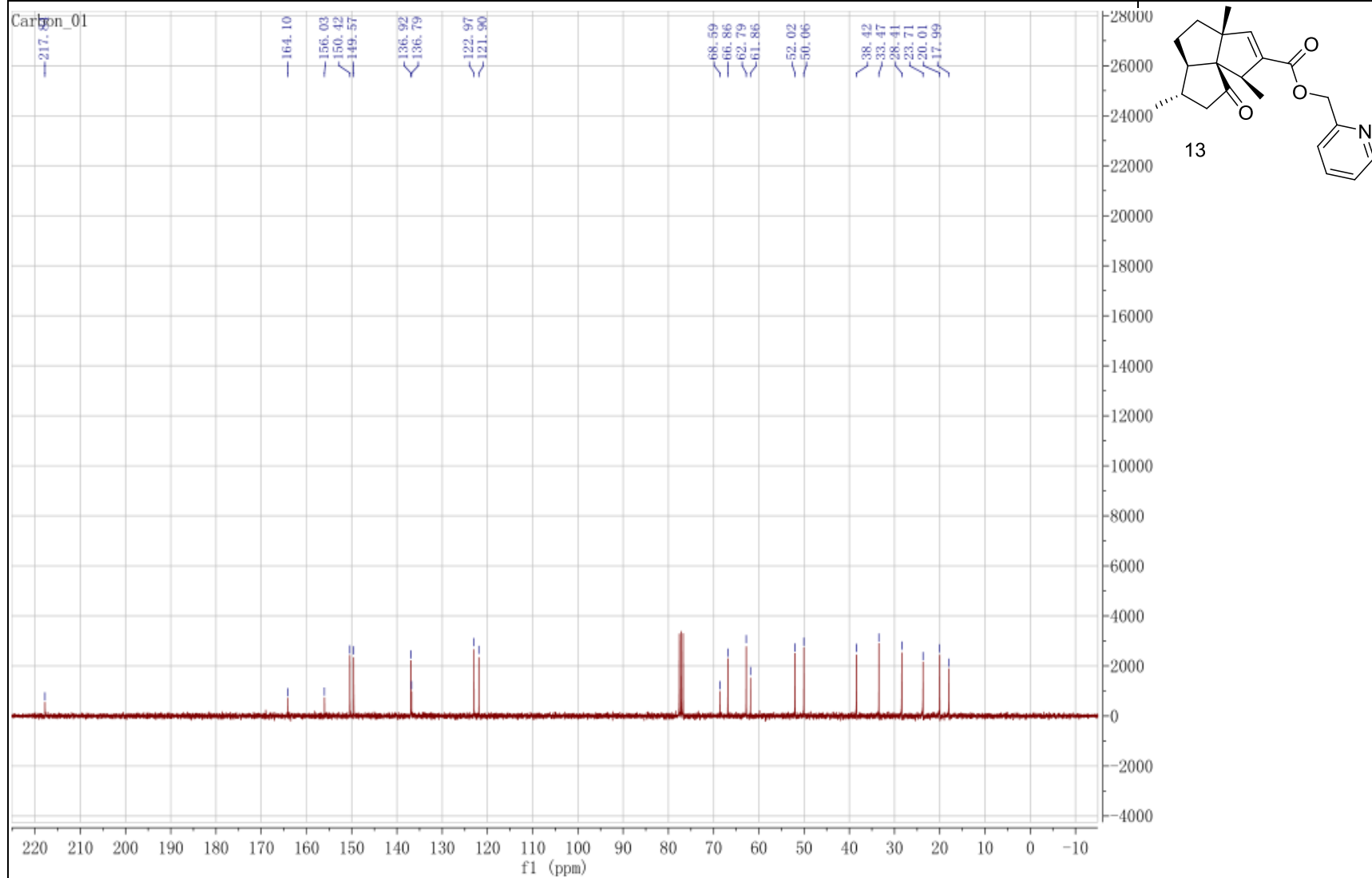


Figure S32. ^1H NMR (300 MHz, CDCl_3) of compound **14**

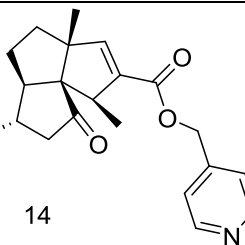
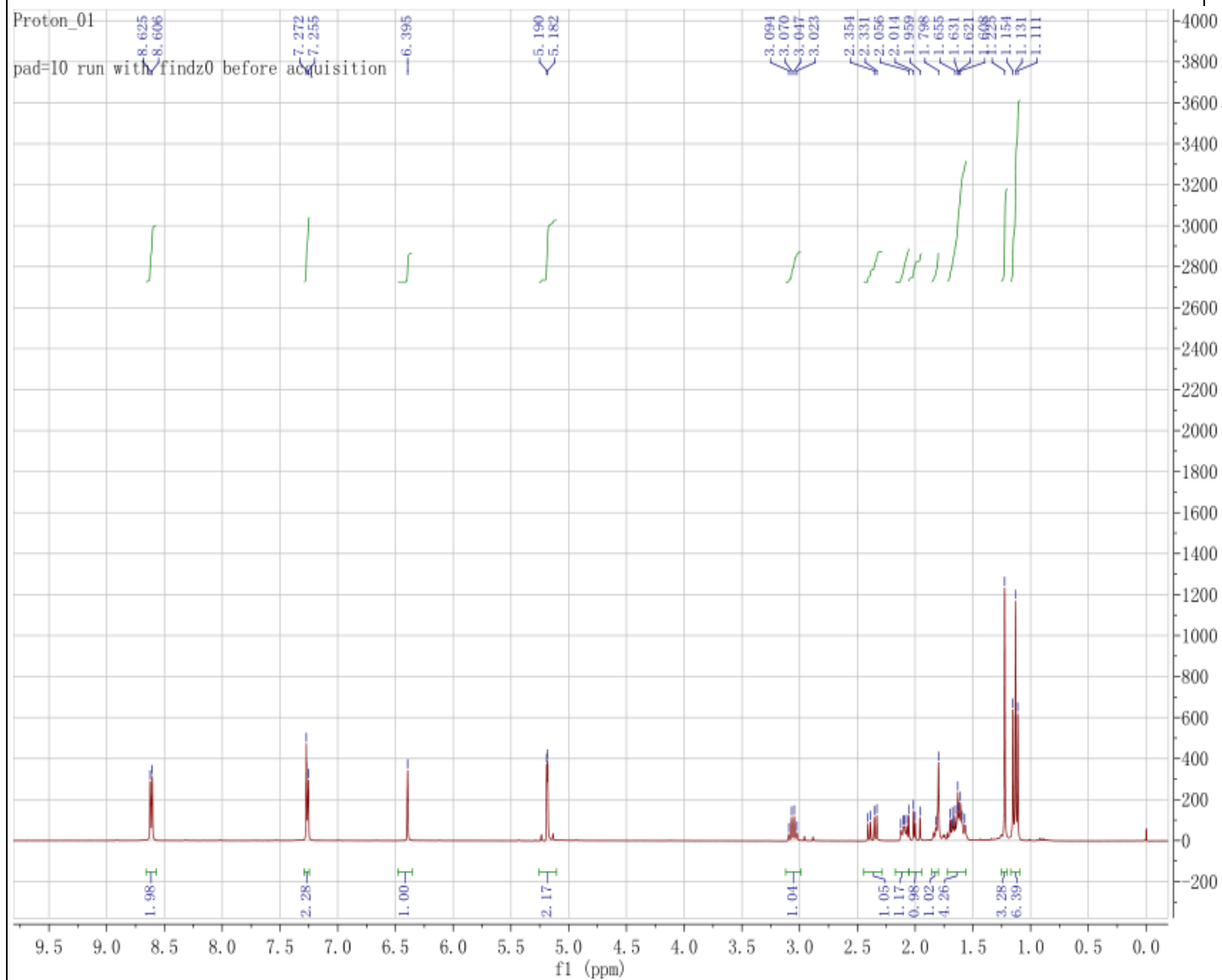


Figure S33. ^{13}C NMR (75 MHz, CDCl_3) of compound **14**

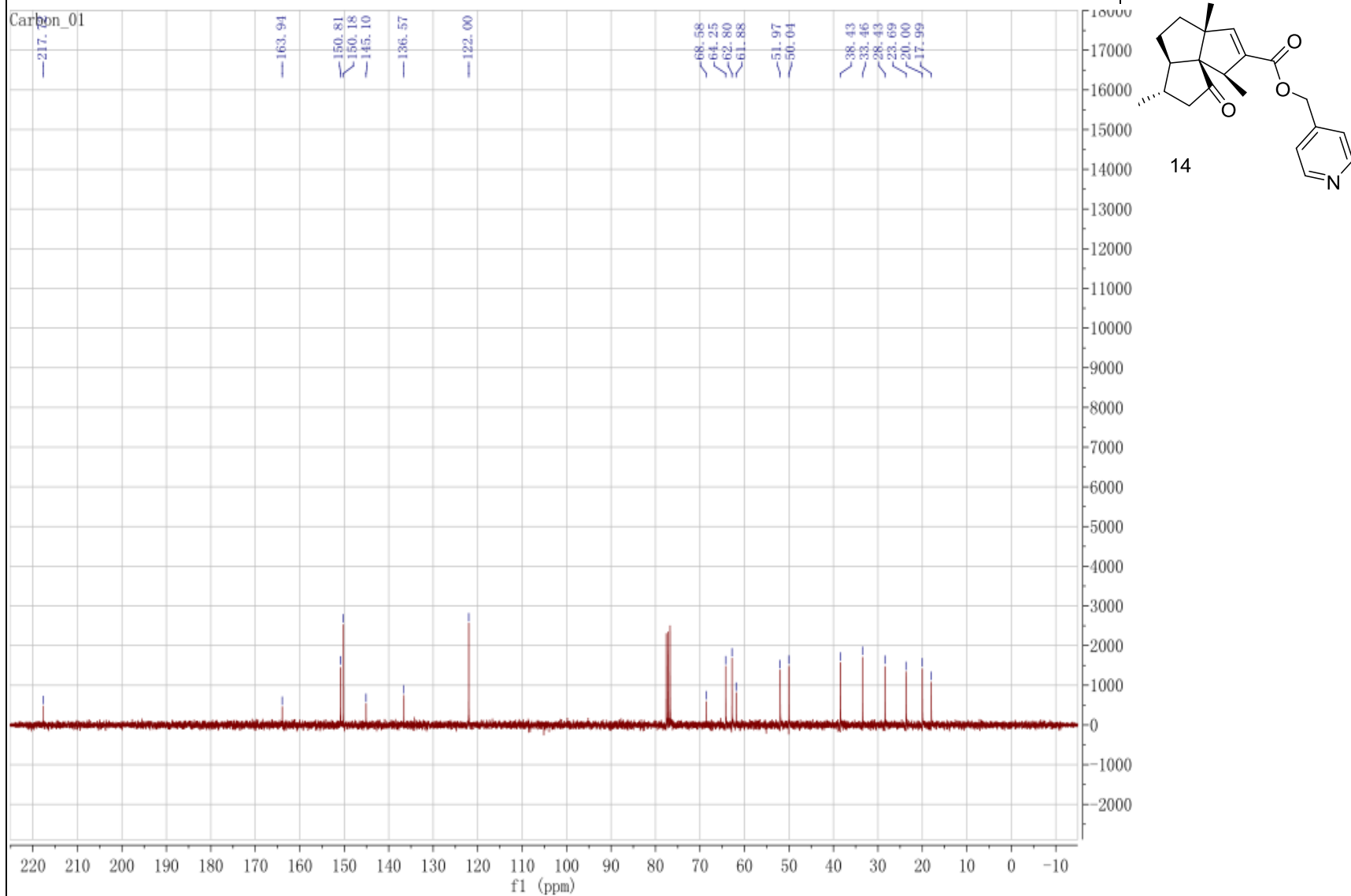


Figure S34. ^1H NMR (300 MHz, CDCl_3) of compound **15**

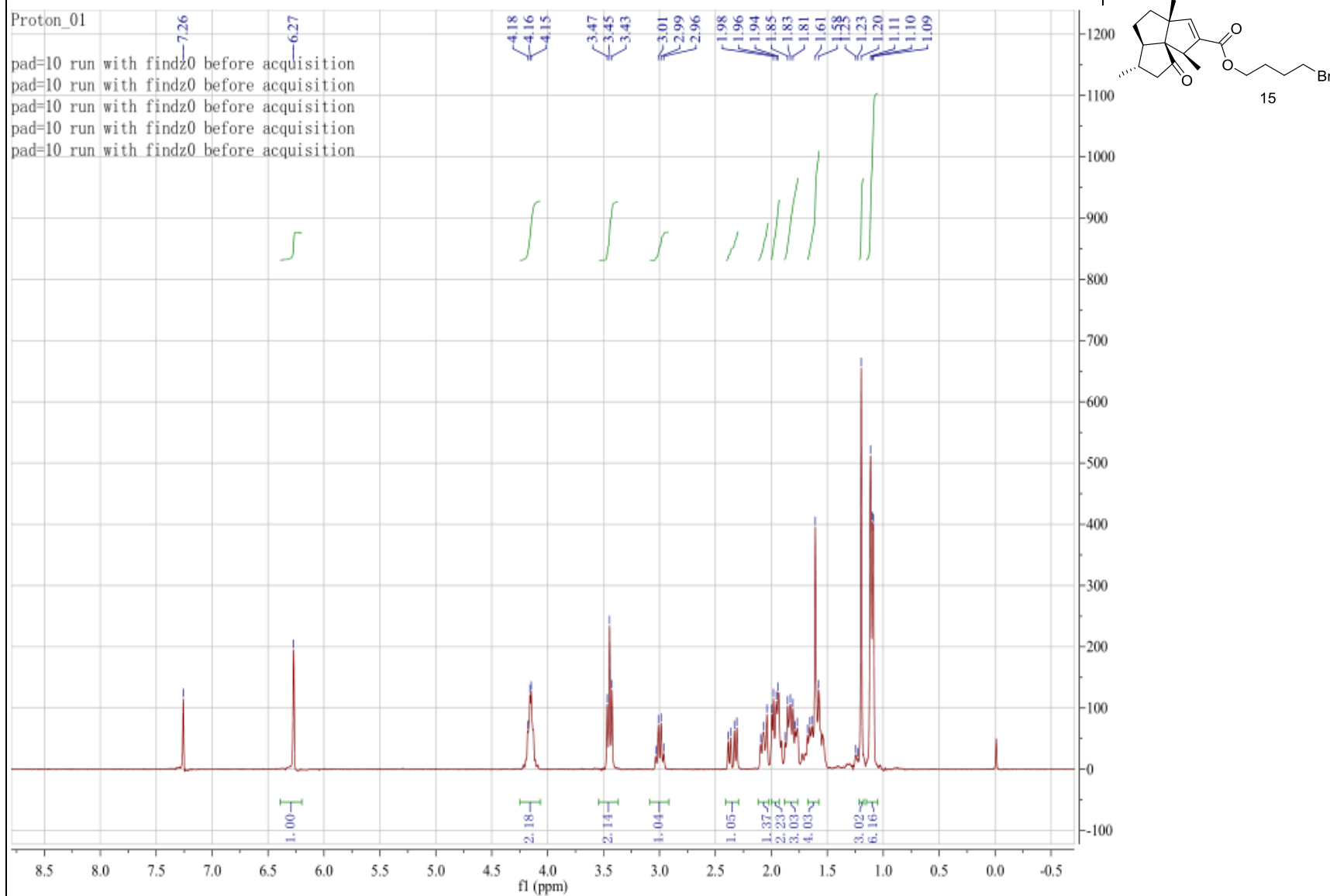


Figure S35. ^{13}C NMR (75 MHz, CDCl_3) of compound **15**

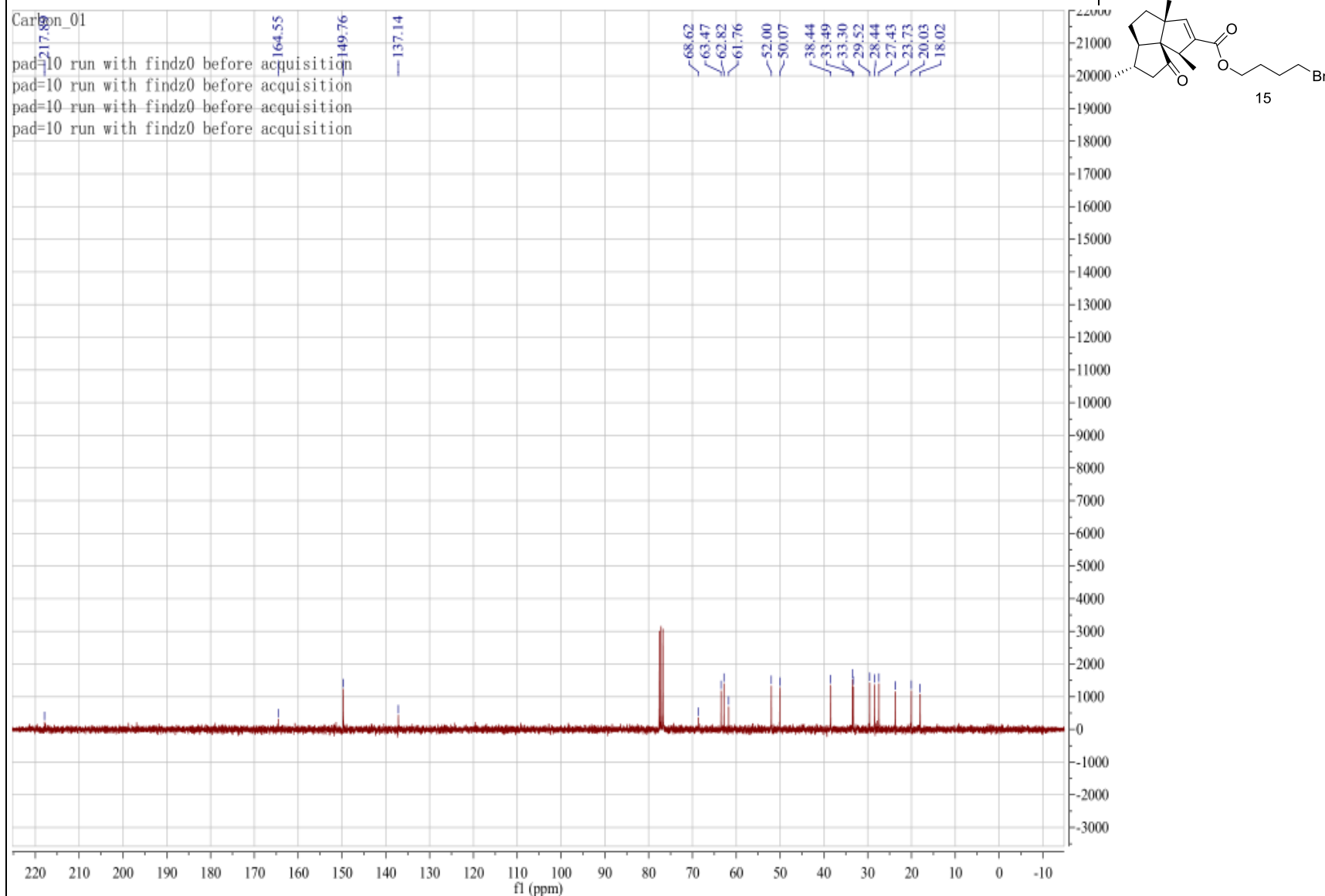


Figure S36. ^1H NMR (400 MHz, CDCl_3) of compound **16**

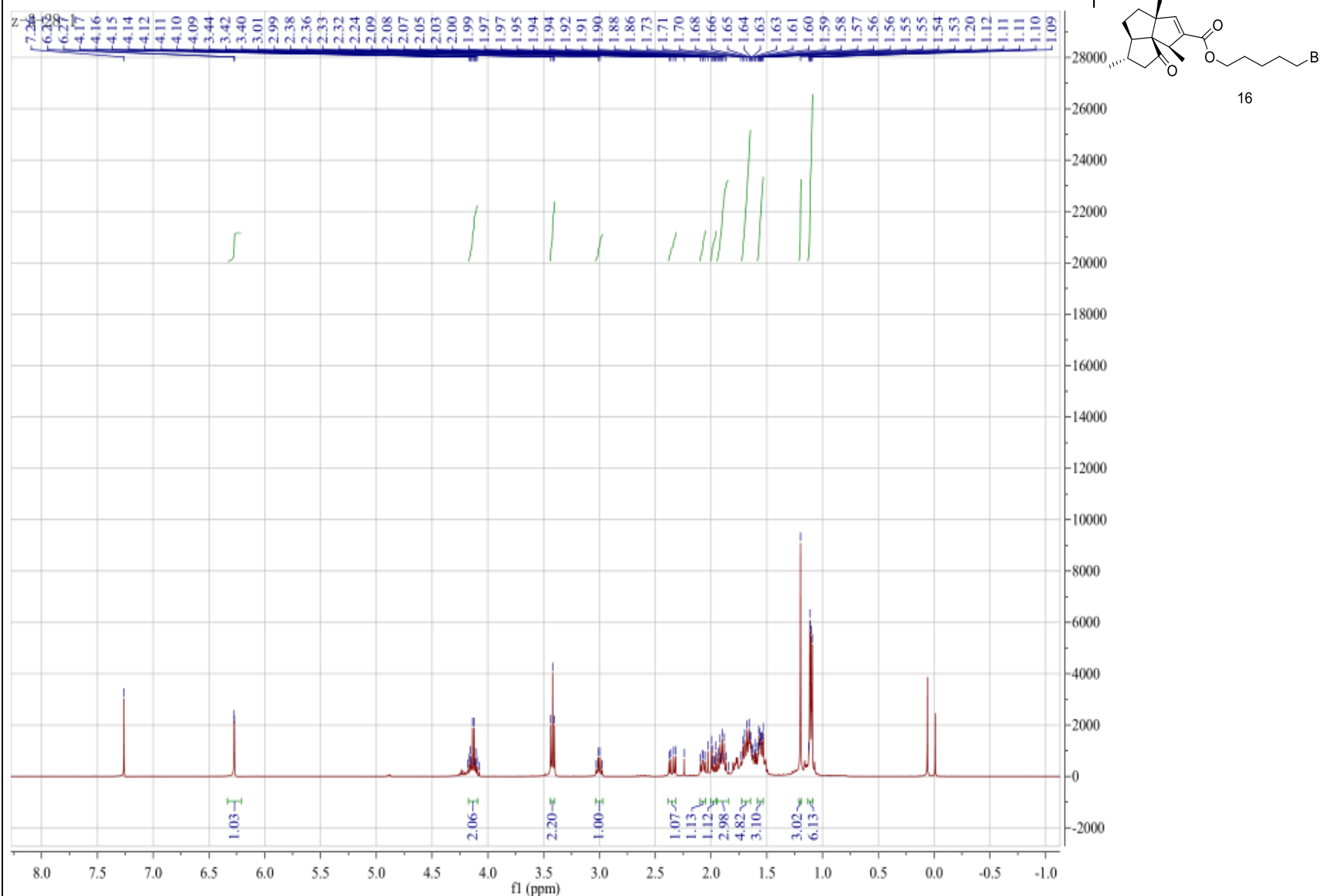


Figure S37. ^{13}C NMR (100 MHz, CDCl_3) of compound **16**

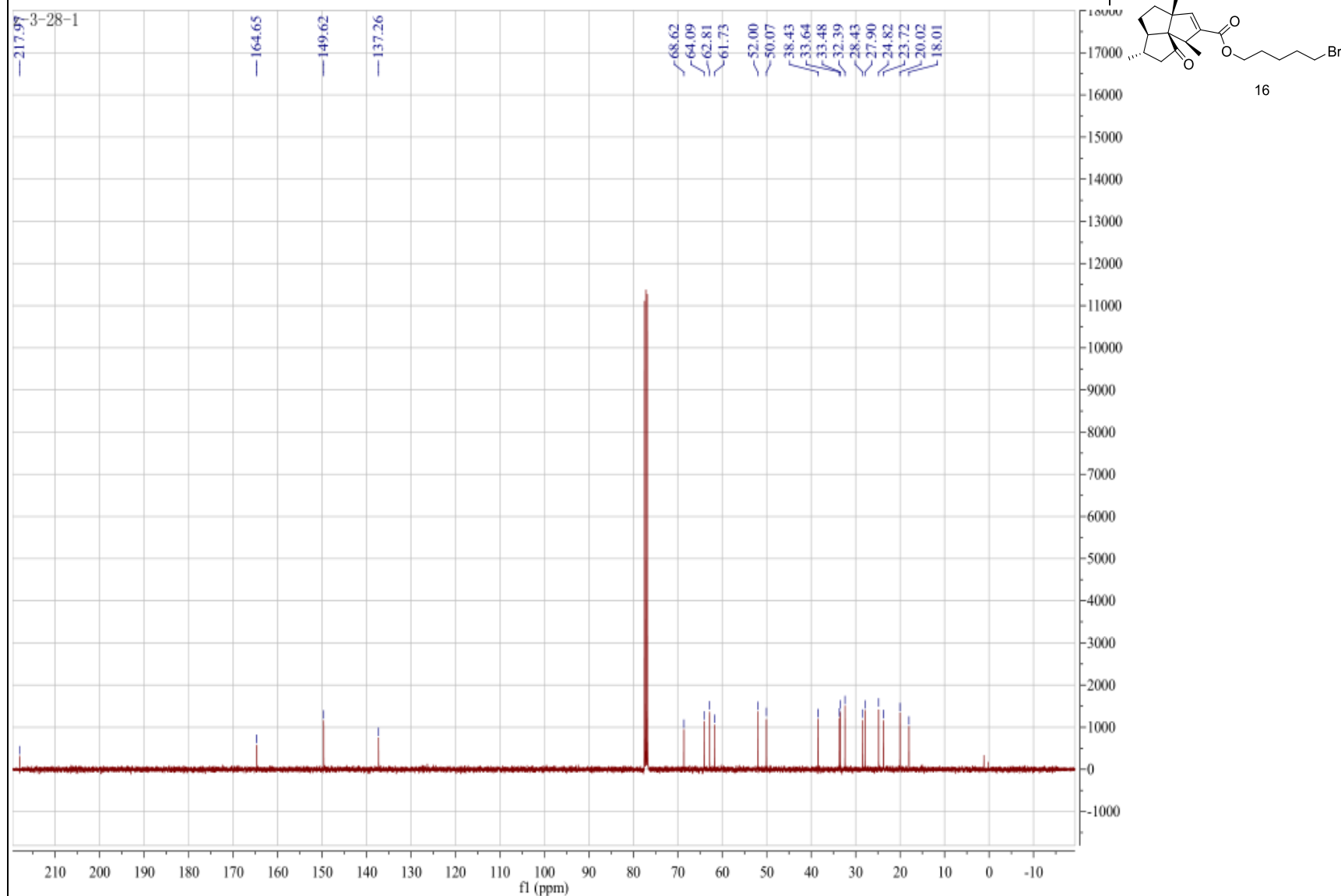


Figure S38. ^1H NMR (400 MHz, CDCl_3) of compound 17

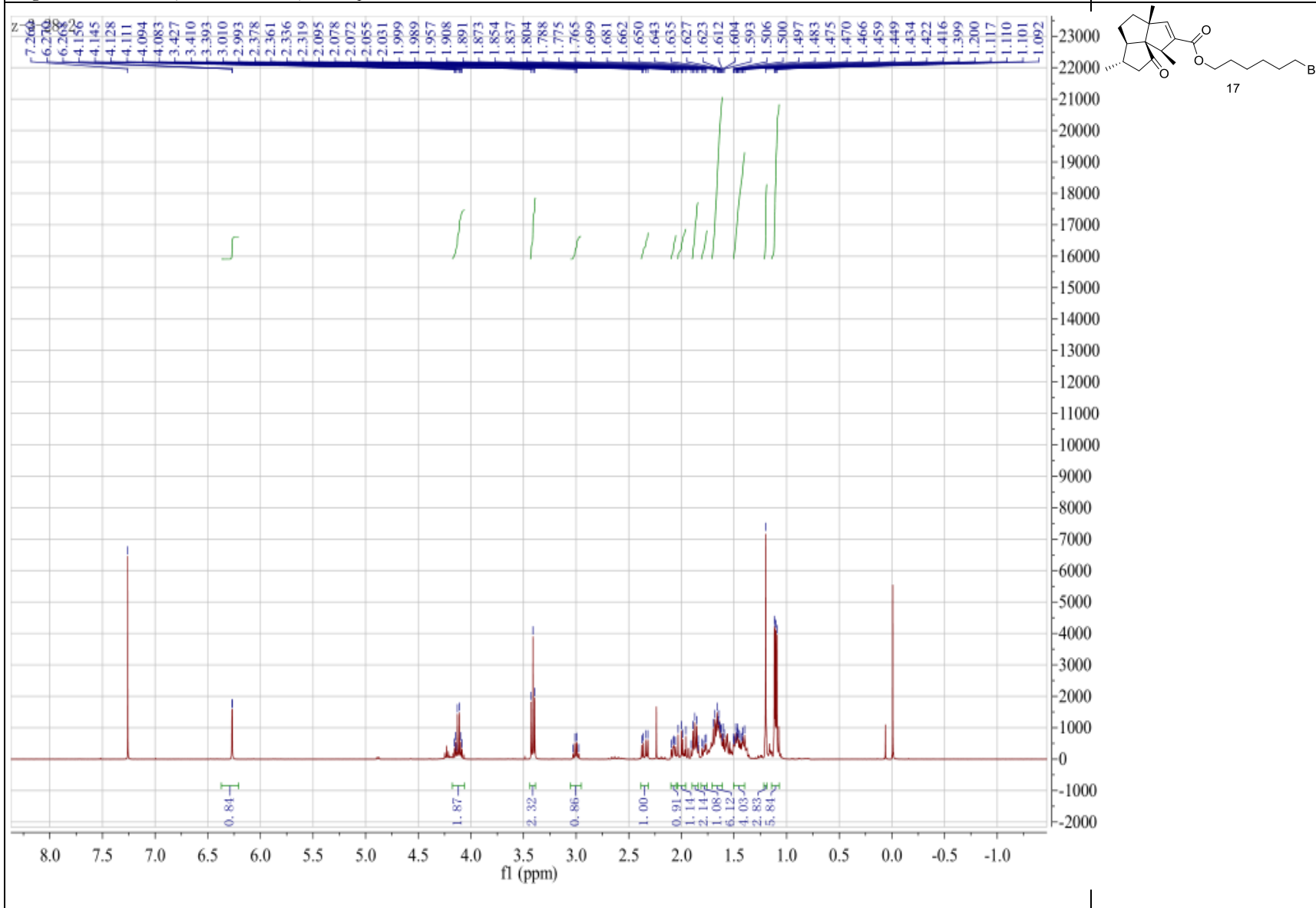


Figure S39. ^{13}C NMR (100 MHz, CDCl_3) of compound **17**

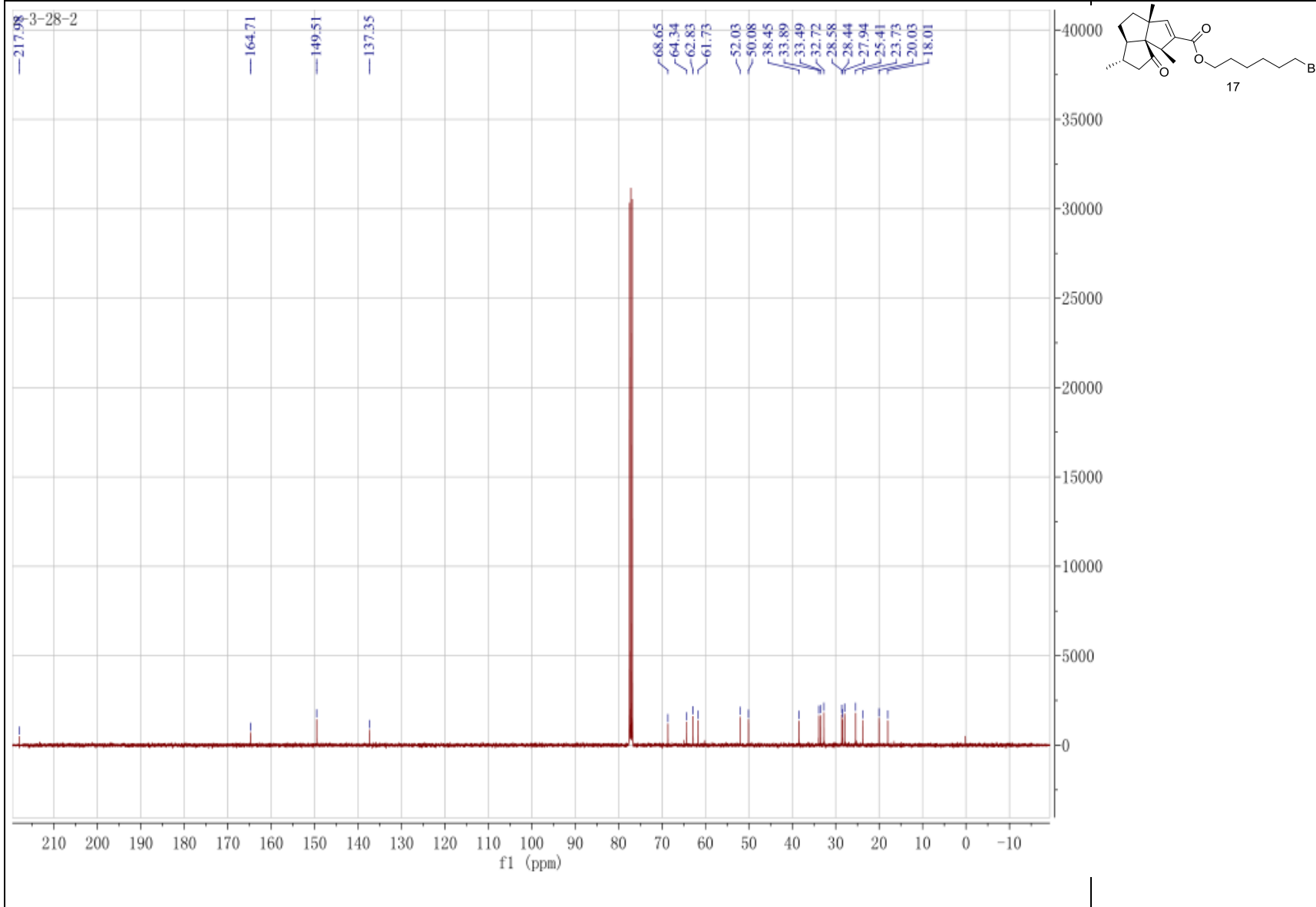


Figure S40. ^1H NMR (400 MHz, CDCl_3) of compound **18**

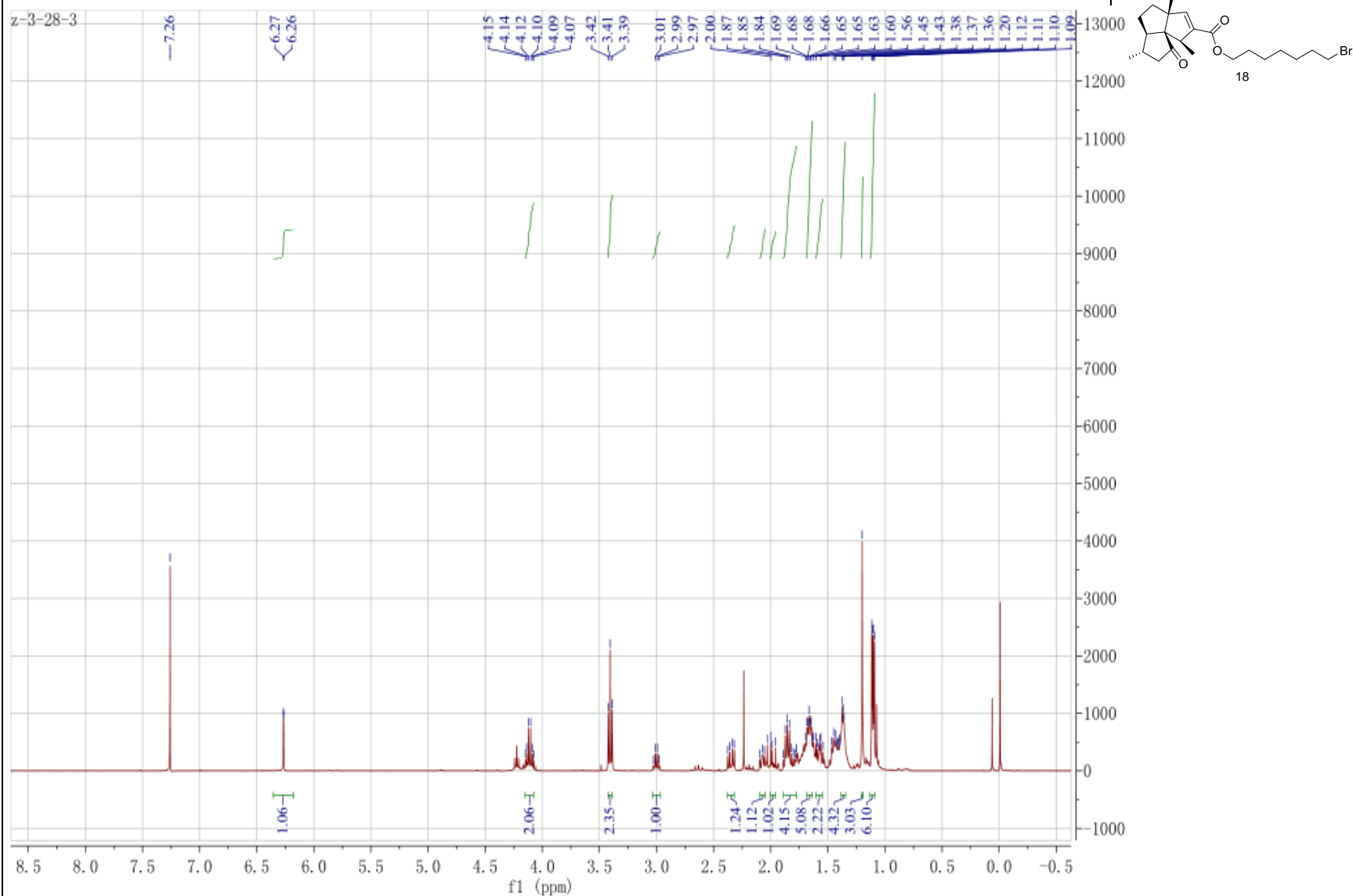


Figure S41. ^{13}C NMR (100 MHz, CDCl_3) of compound **18**

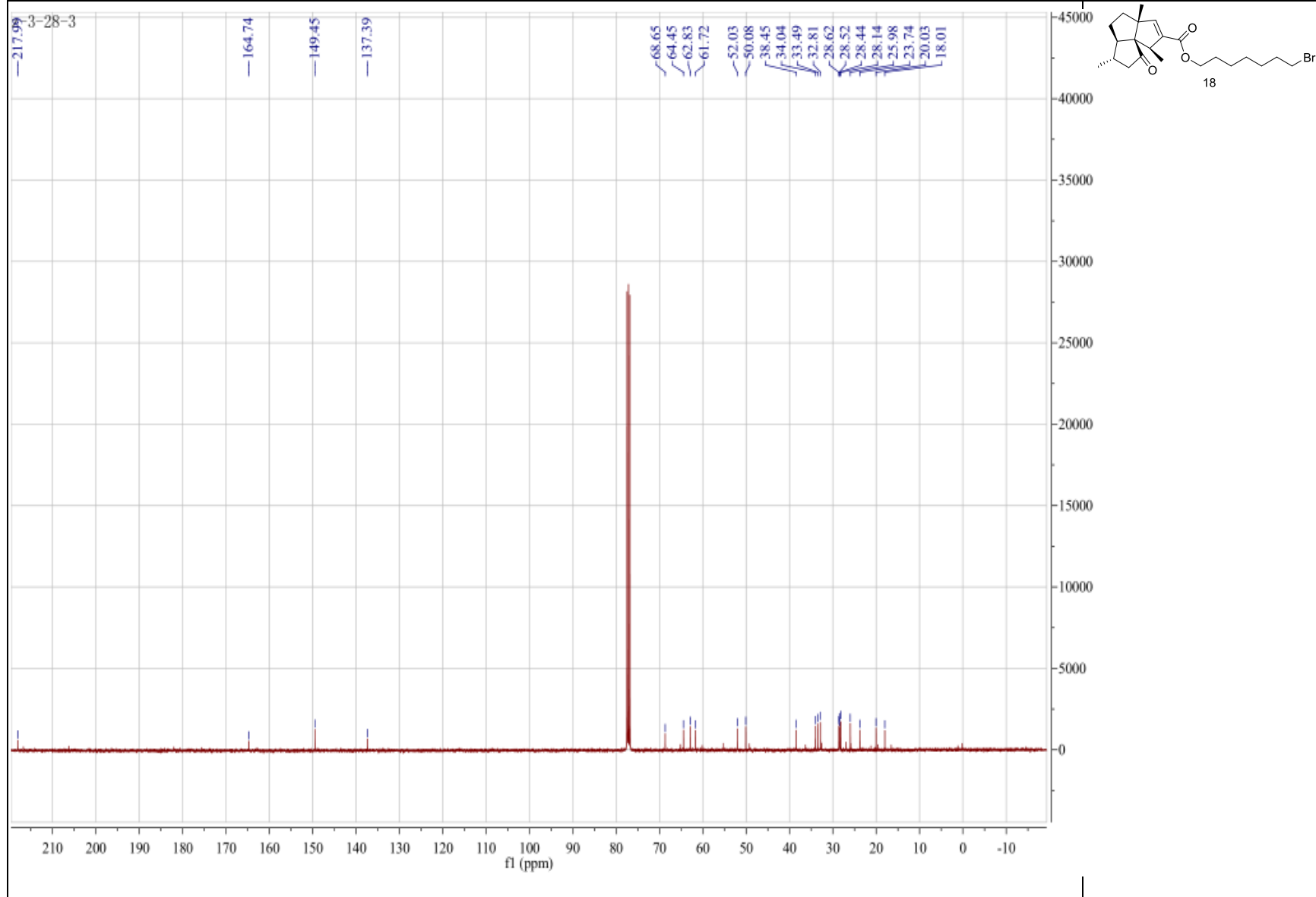


Figure S42. ^1H NMR (400 MHz, CDCl_3) of compound **19**

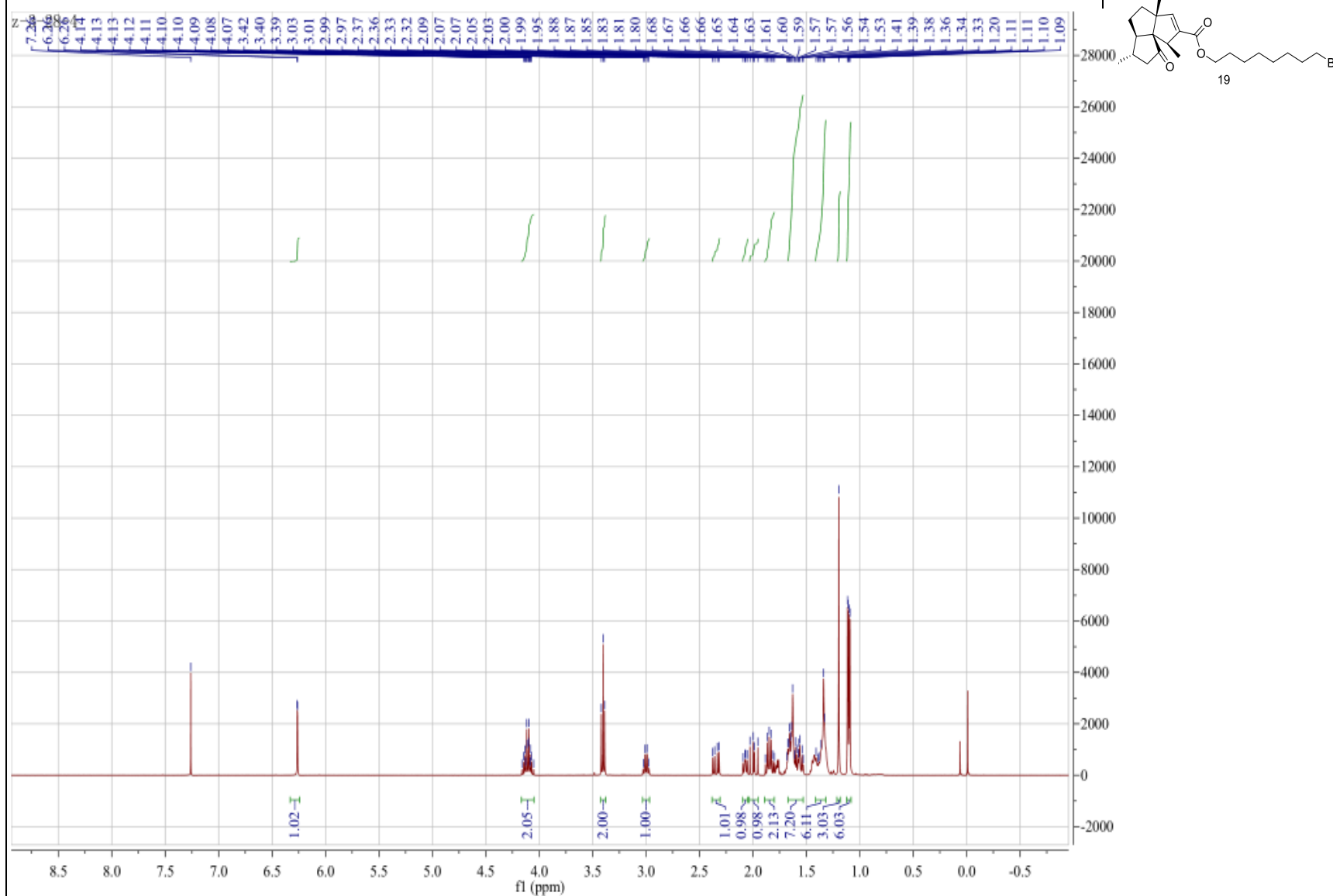


Figure S43. ^{13}C NMR (100 MHz, CDCl_3) of compound **19**

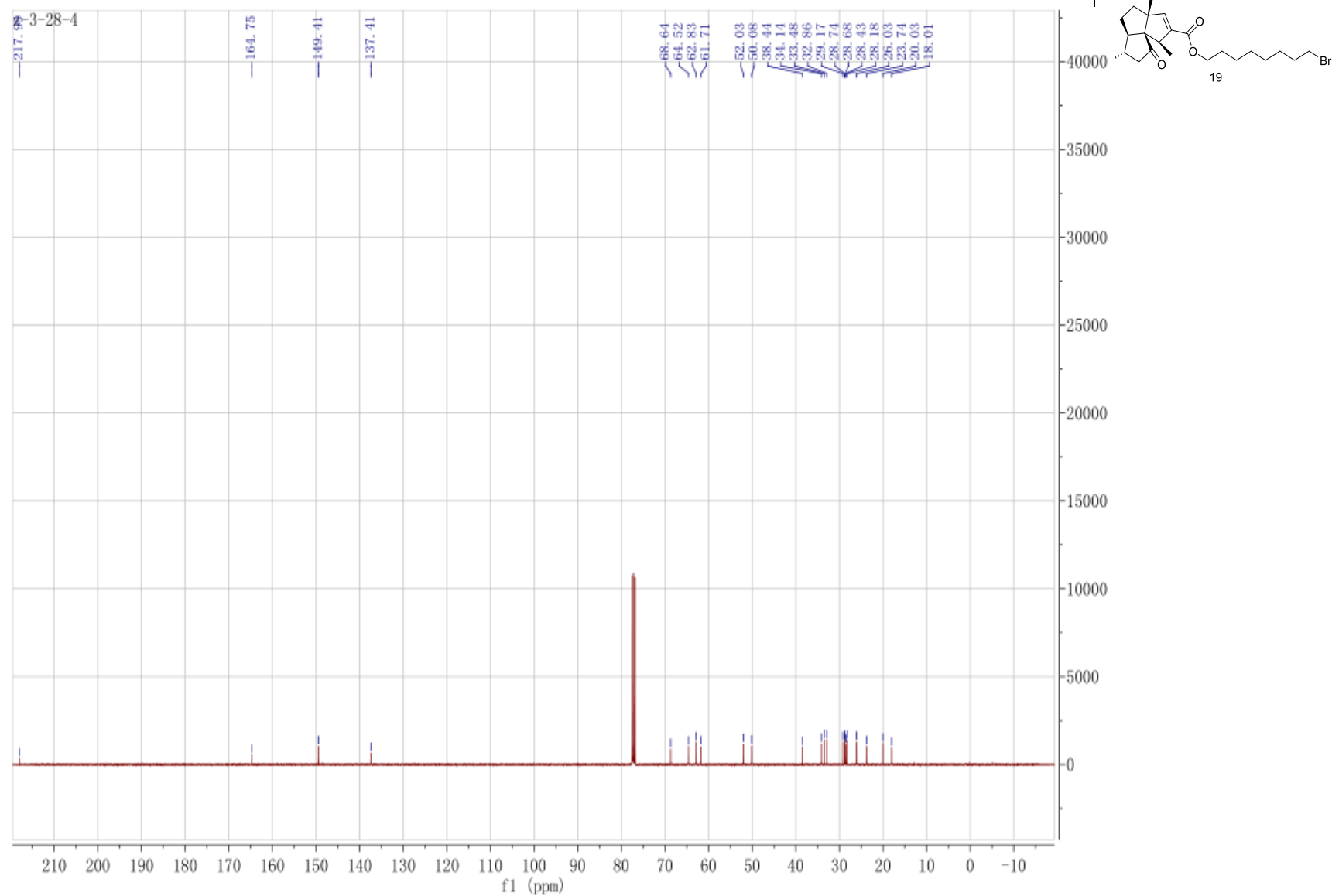


Figure S44. ^1H NMR (400 MHz, CDCl_3) of compound **20**

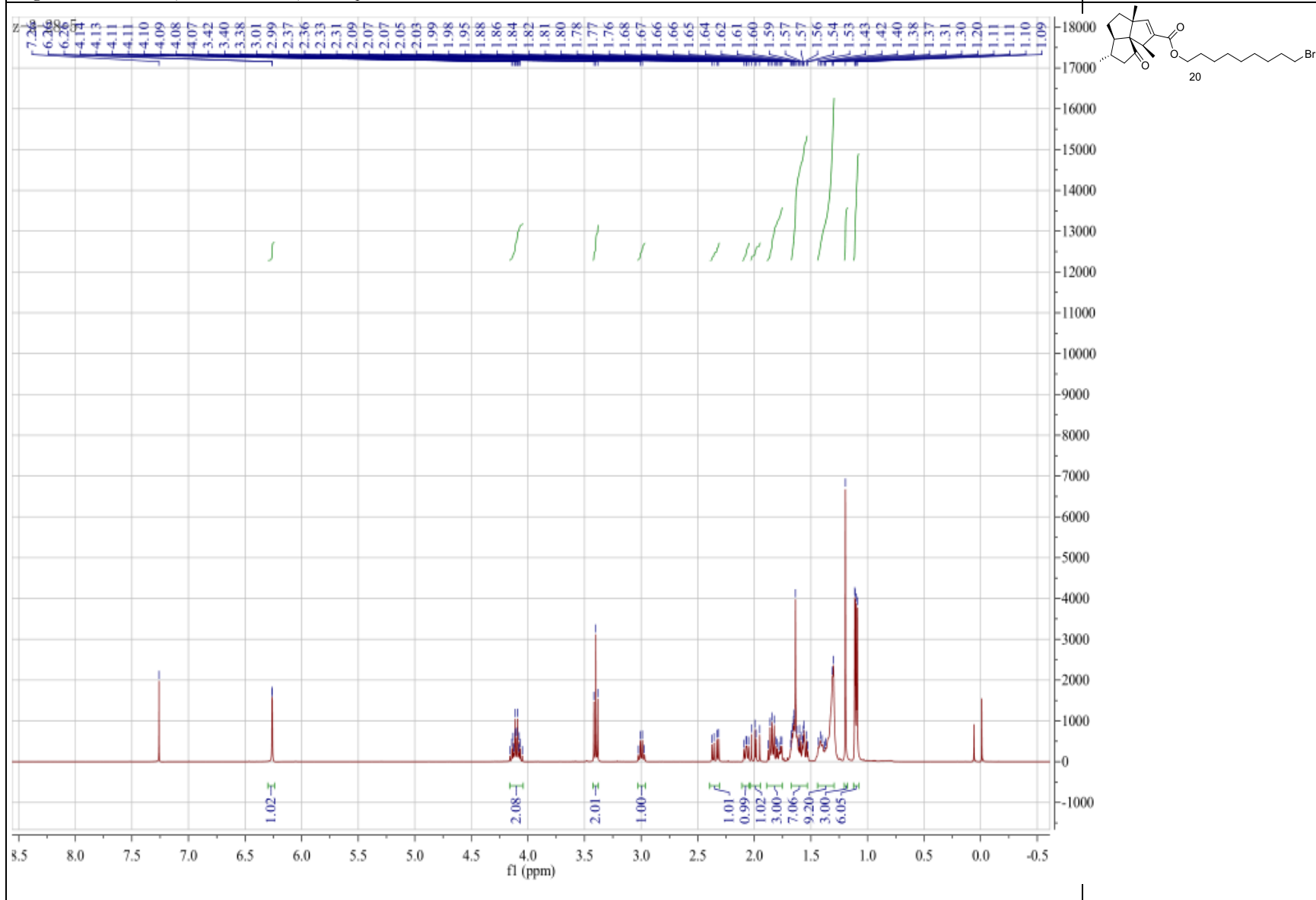


Figure S45. ^{13}C NMR (100 MHz, CDCl_3) of compound **20**

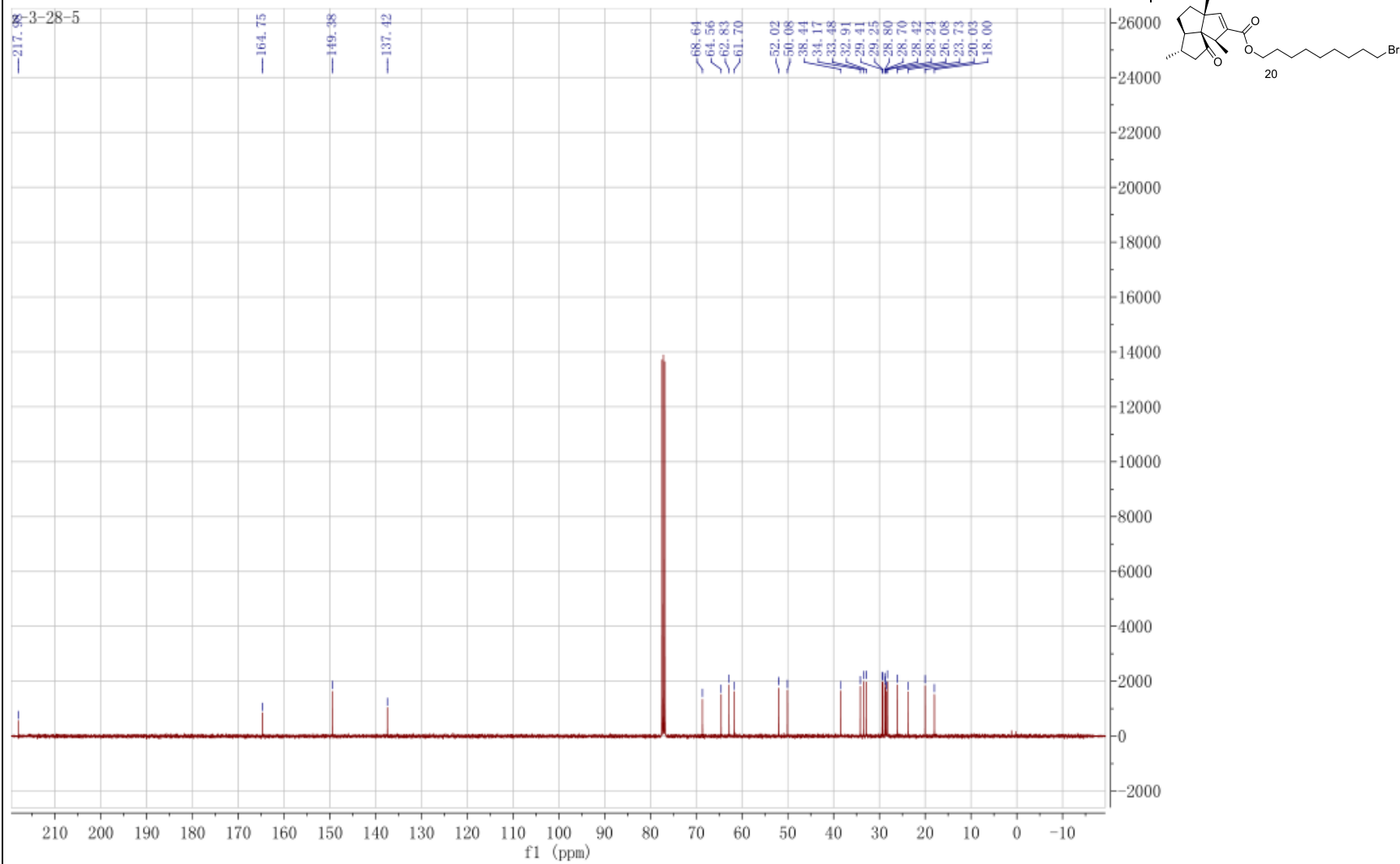


Figure S46. ^1H NMR (300 MHz, CDCl_3) of compound **21**

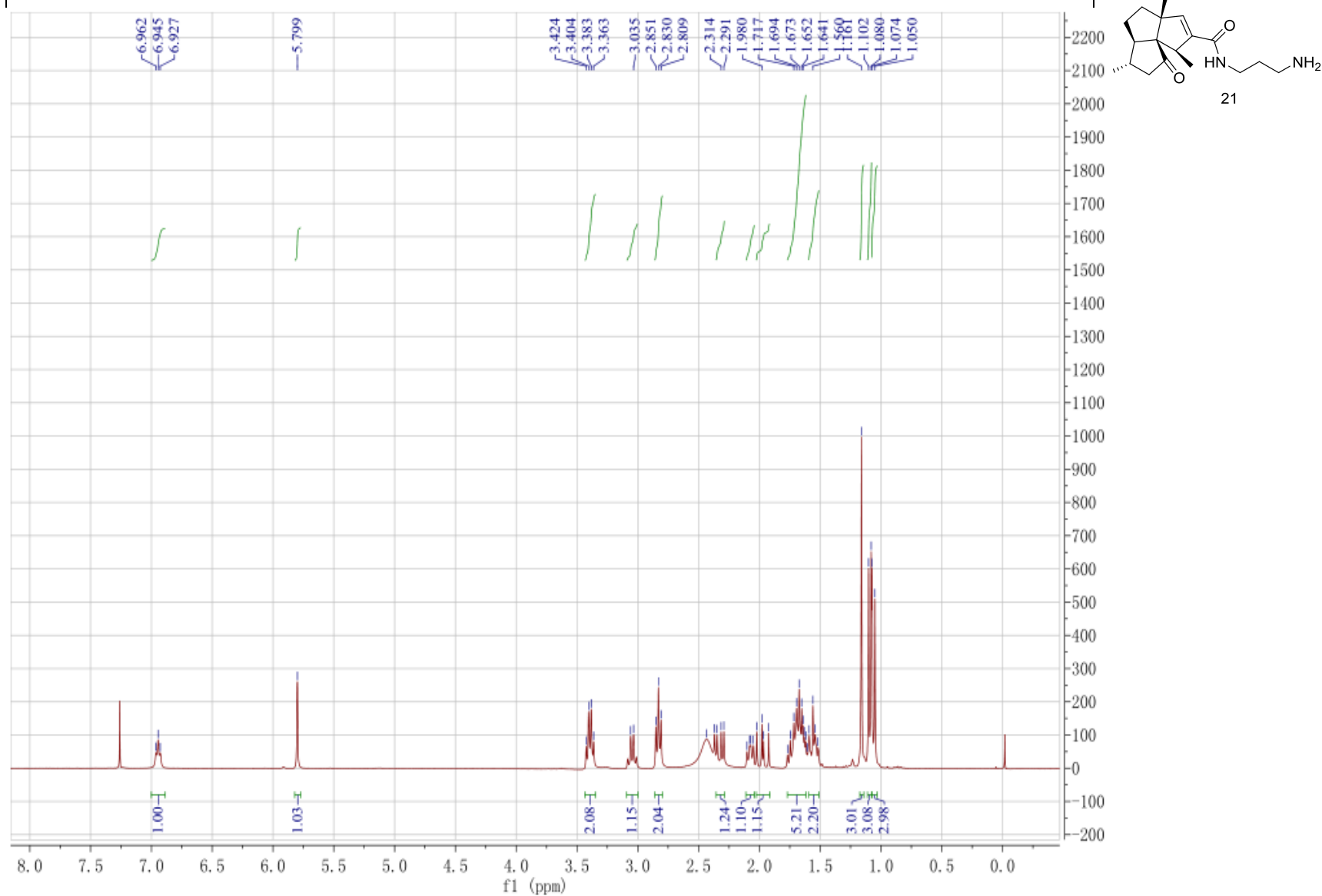


Figure S47. ^{13}C NMR (75 MHz, CDCl_3) of compound **21**

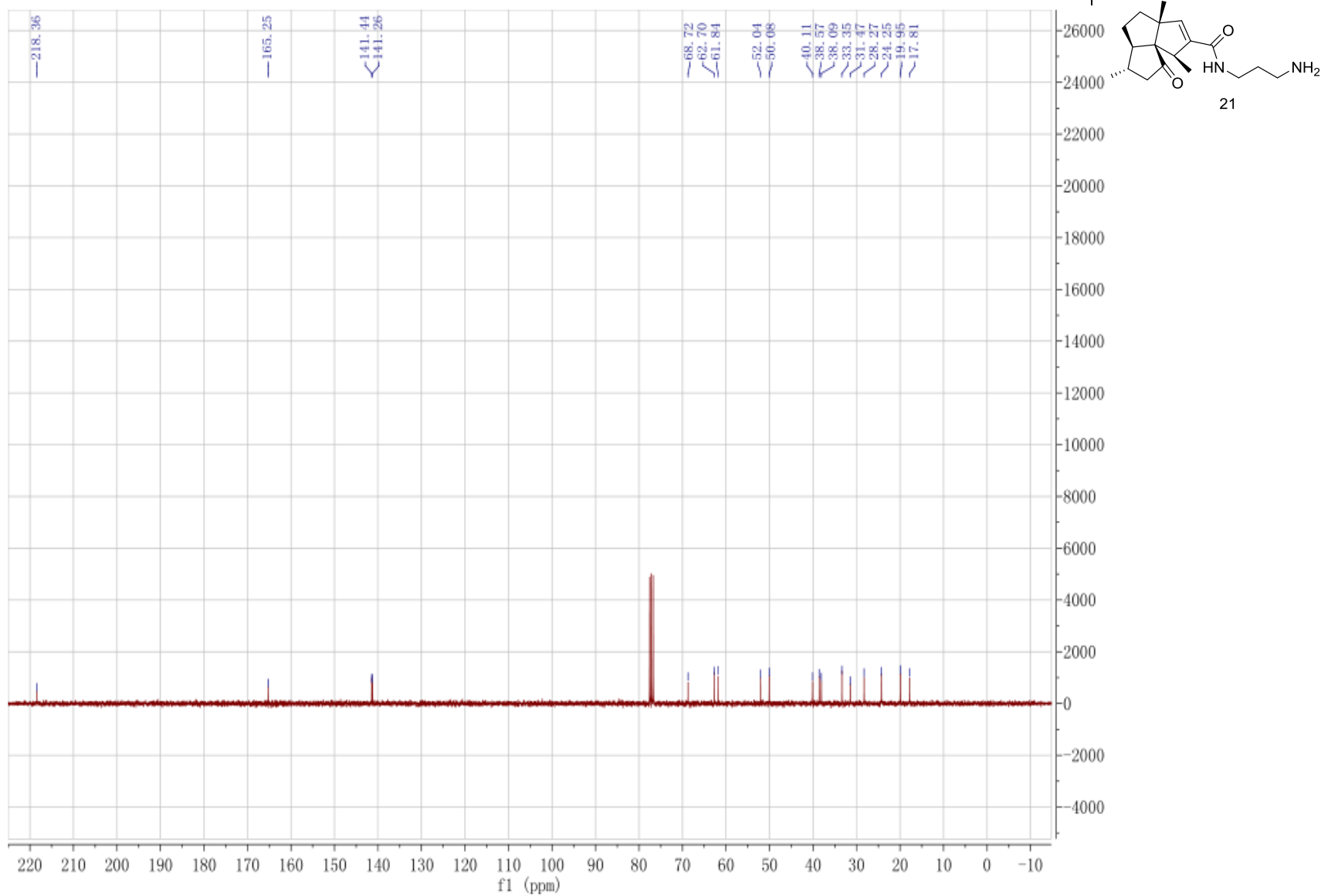


Figure S48. ^1H NMR (300 MHz, CDCl_3) of compound **22**

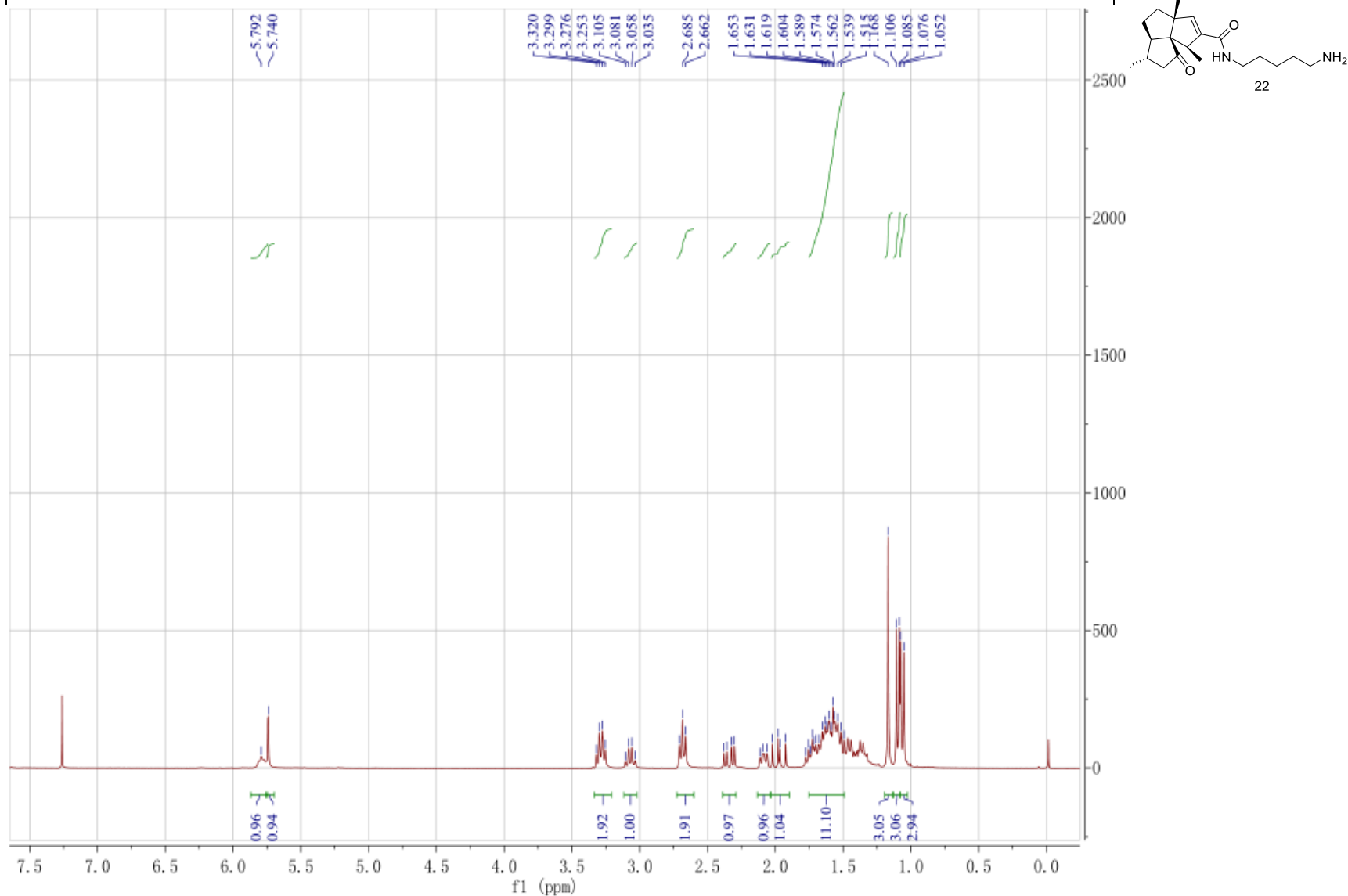


Figure S49. ^{13}C NMR (75 MHz, CDCl_3) of compound 22

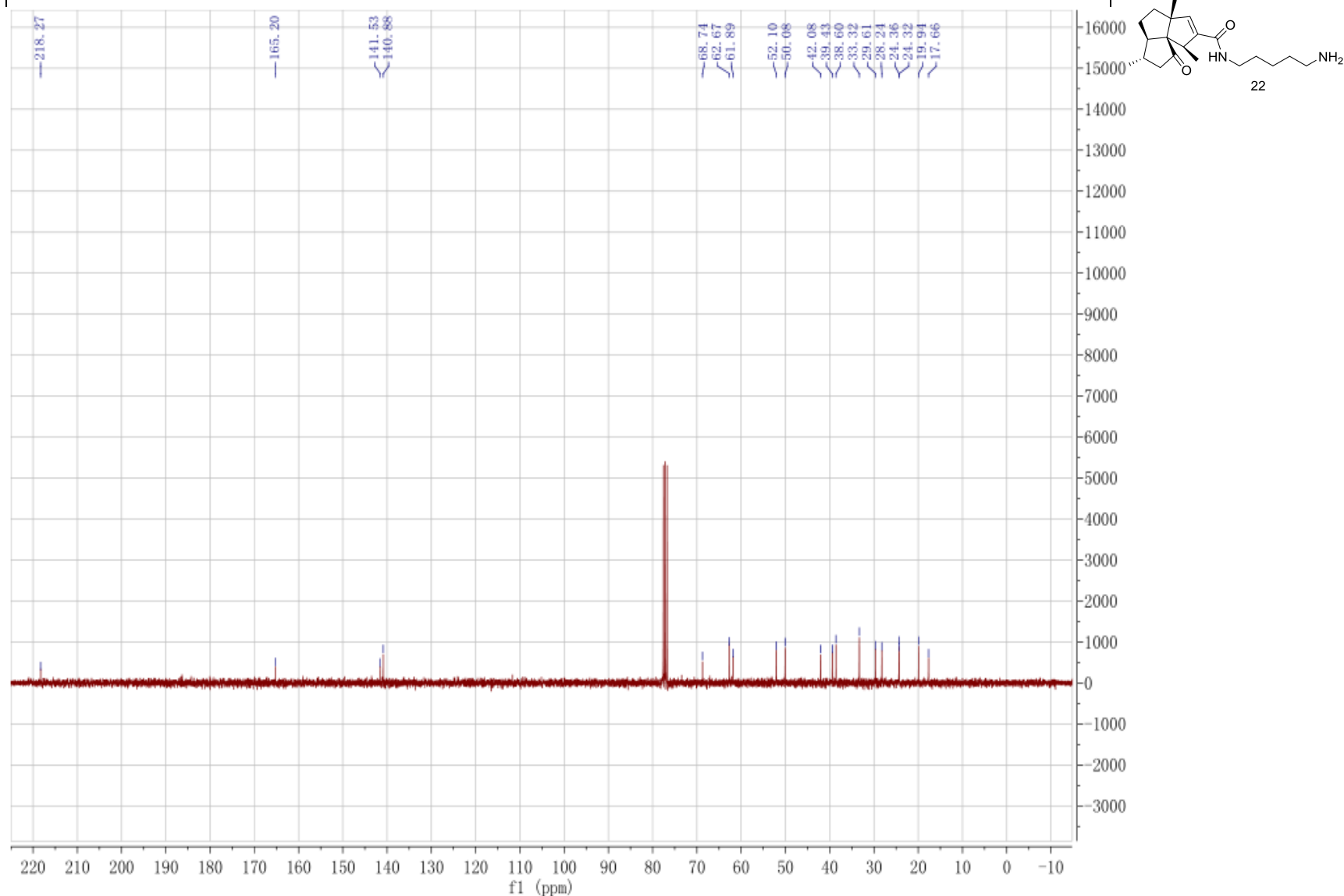


Figure S50. ^1H NMR (300 MHz, CDCl_3) of compound **23**

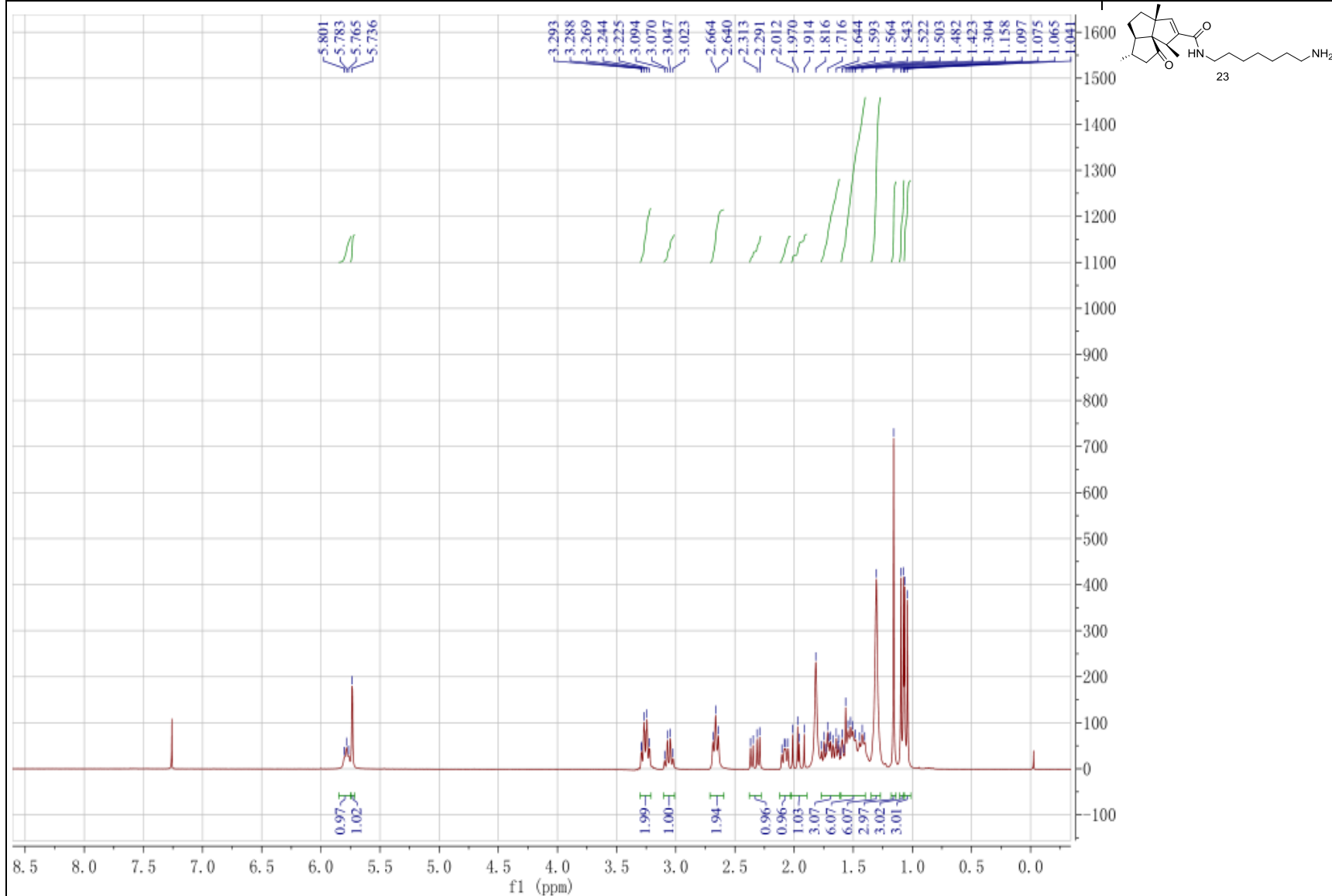


Figure S51. ^{13}C NMR (75 MHz, CDCl_3) of compound **23**

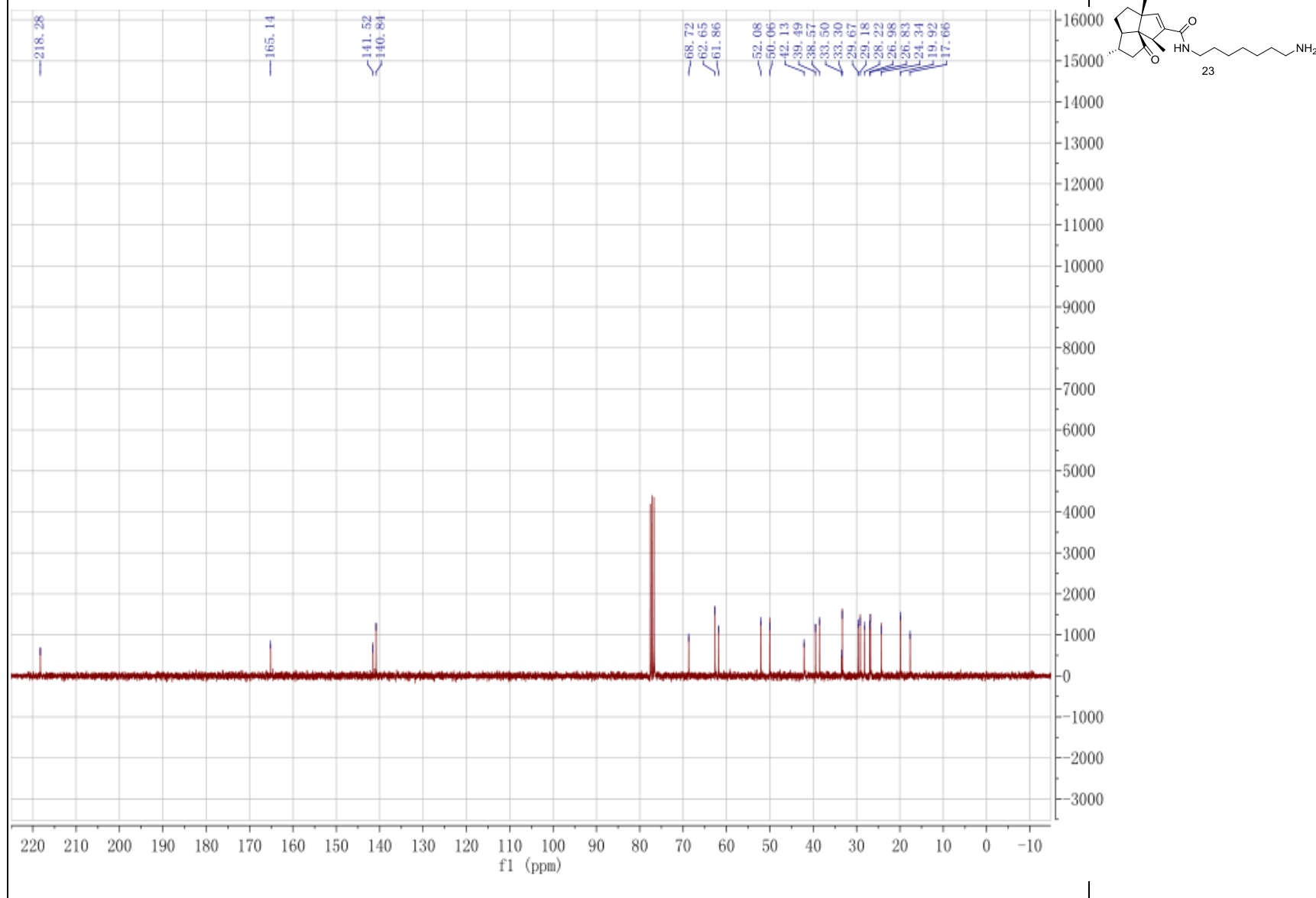


Figure S52. ^1H NMR (300 MHz, CDCl_3) of compound **24**

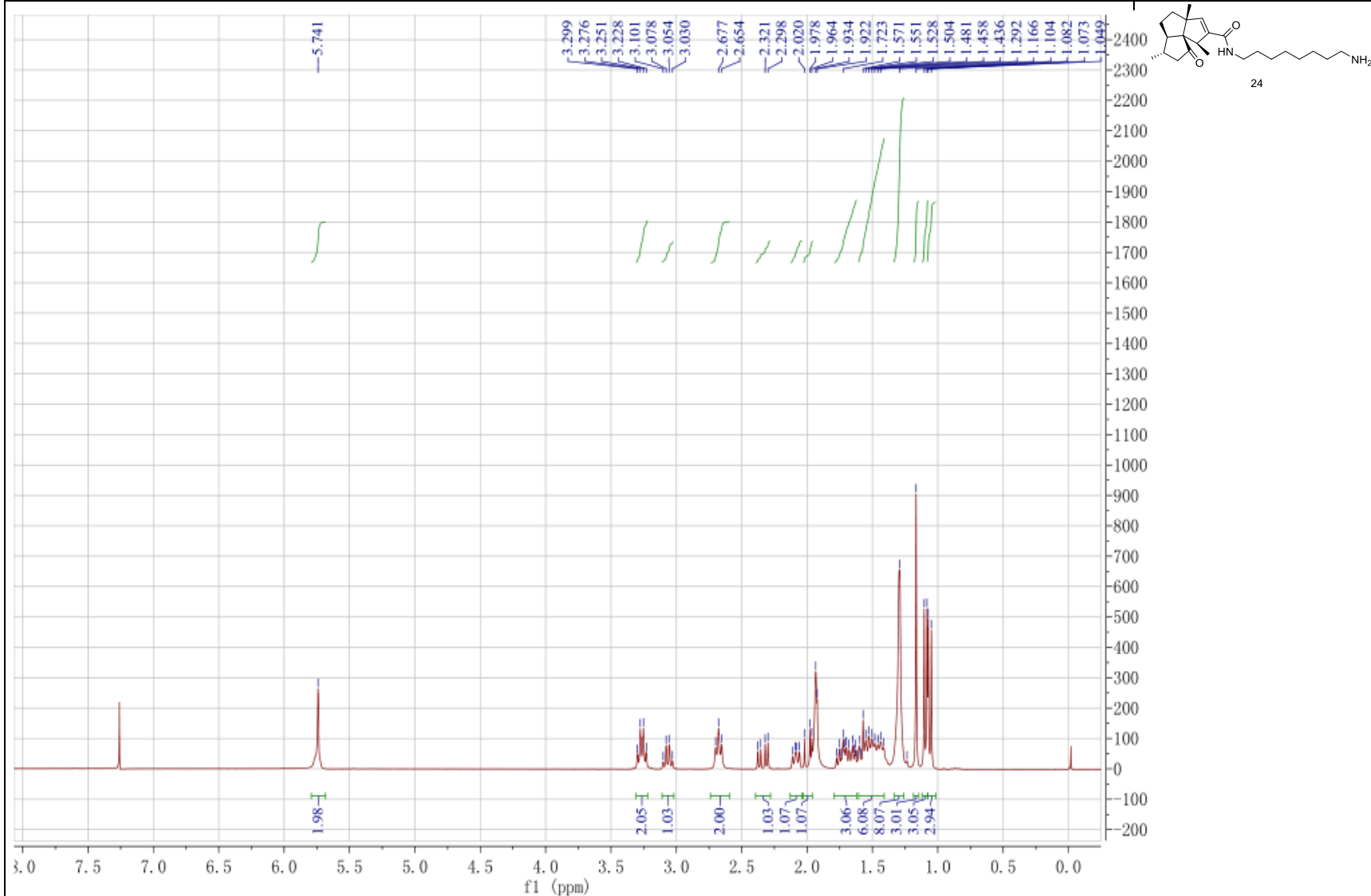


Figure S53. ^{13}C NMR (75 MHz, CDCl_3) of compound **24**

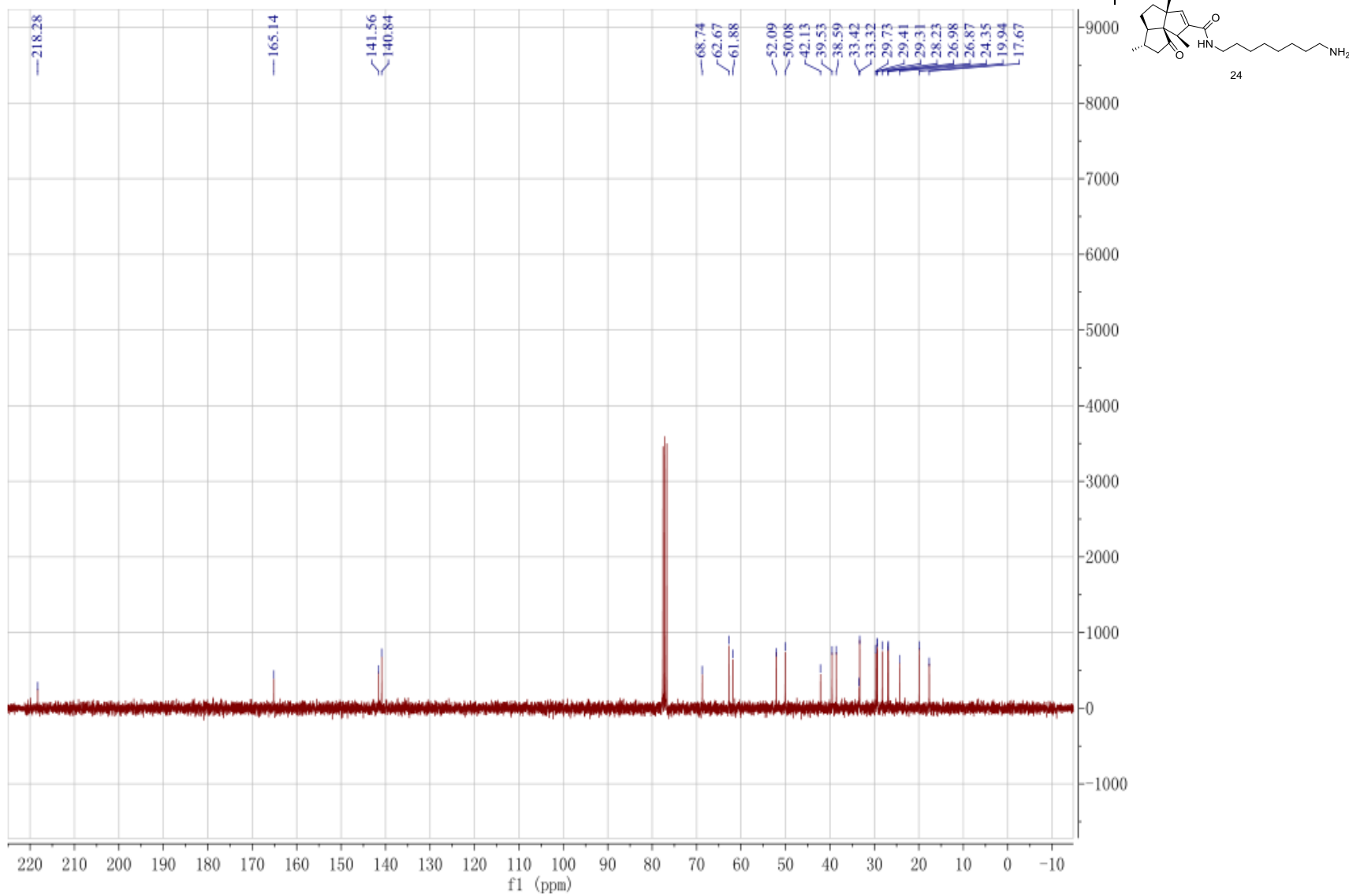


Figure S54. ^1H NMR (300 MHz, CDCl_3) of compound **25**

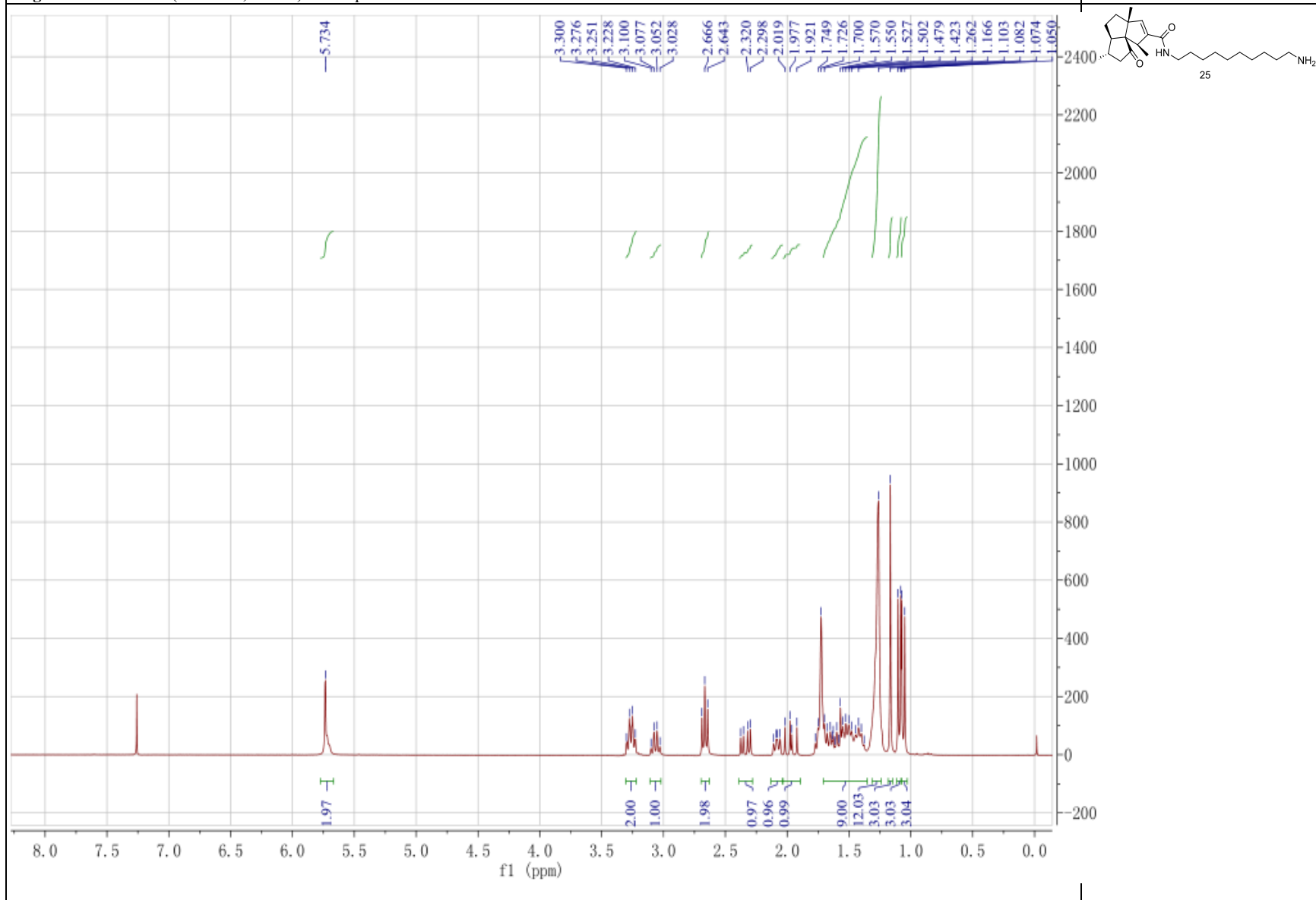


Figure S55. ^{13}C NMR (75 MHz, CDCl_3) of compound **25**

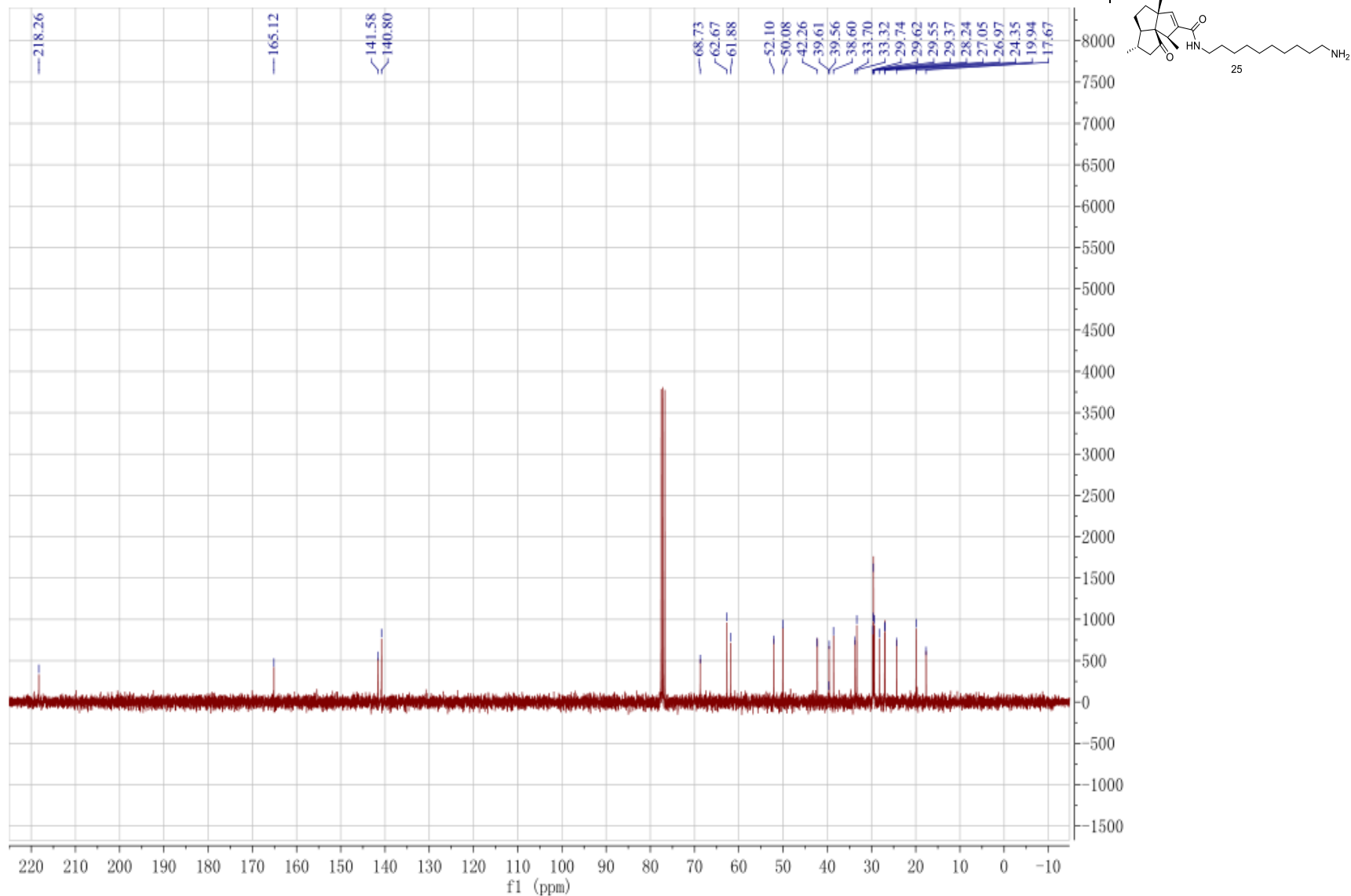


Figure S56. ^1H NMR (300 MHz, CDCl_3) of compound **26**

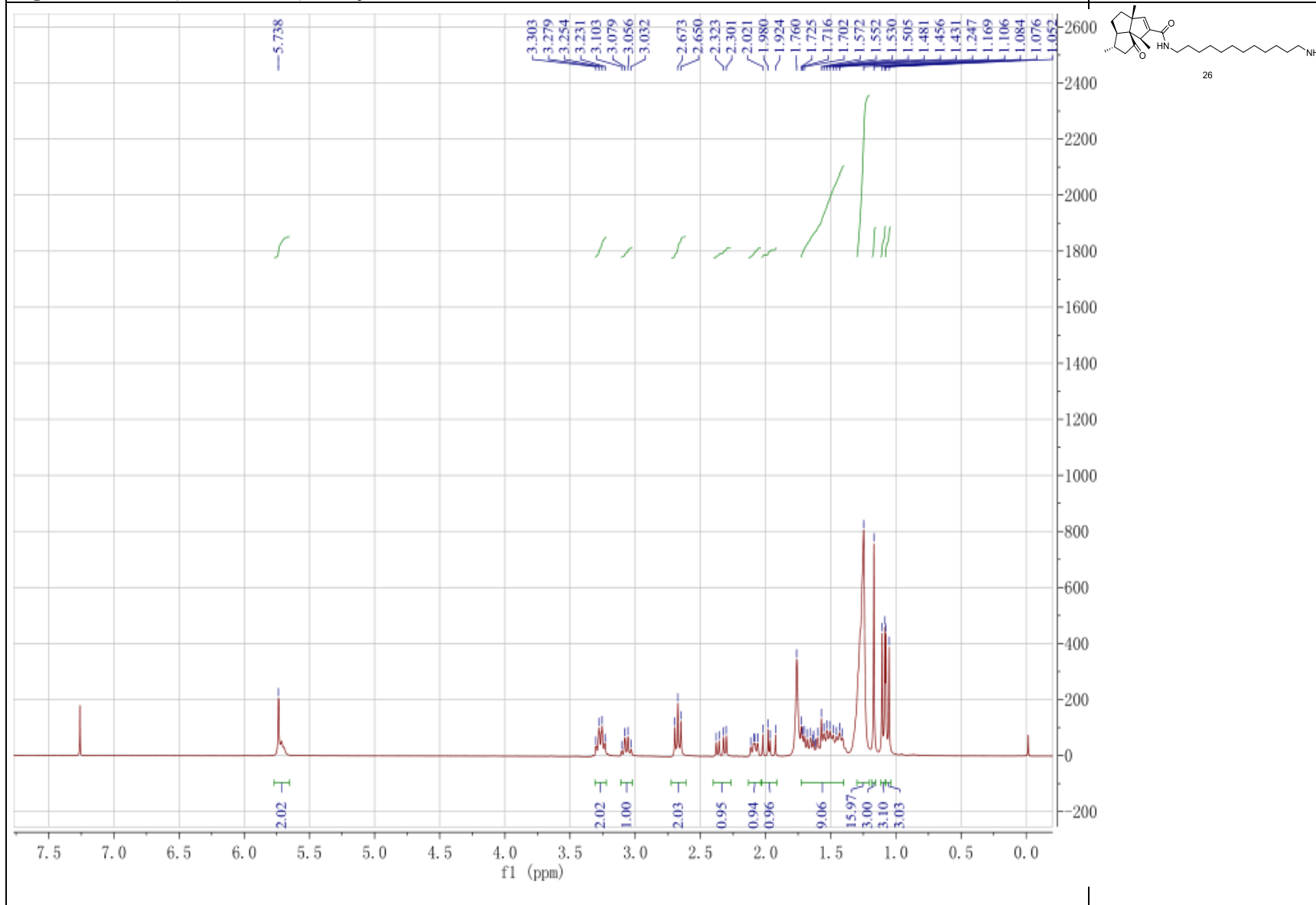


Figure S57. ^{13}C NMR (75 MHz, CDCl_3) of compound **26**

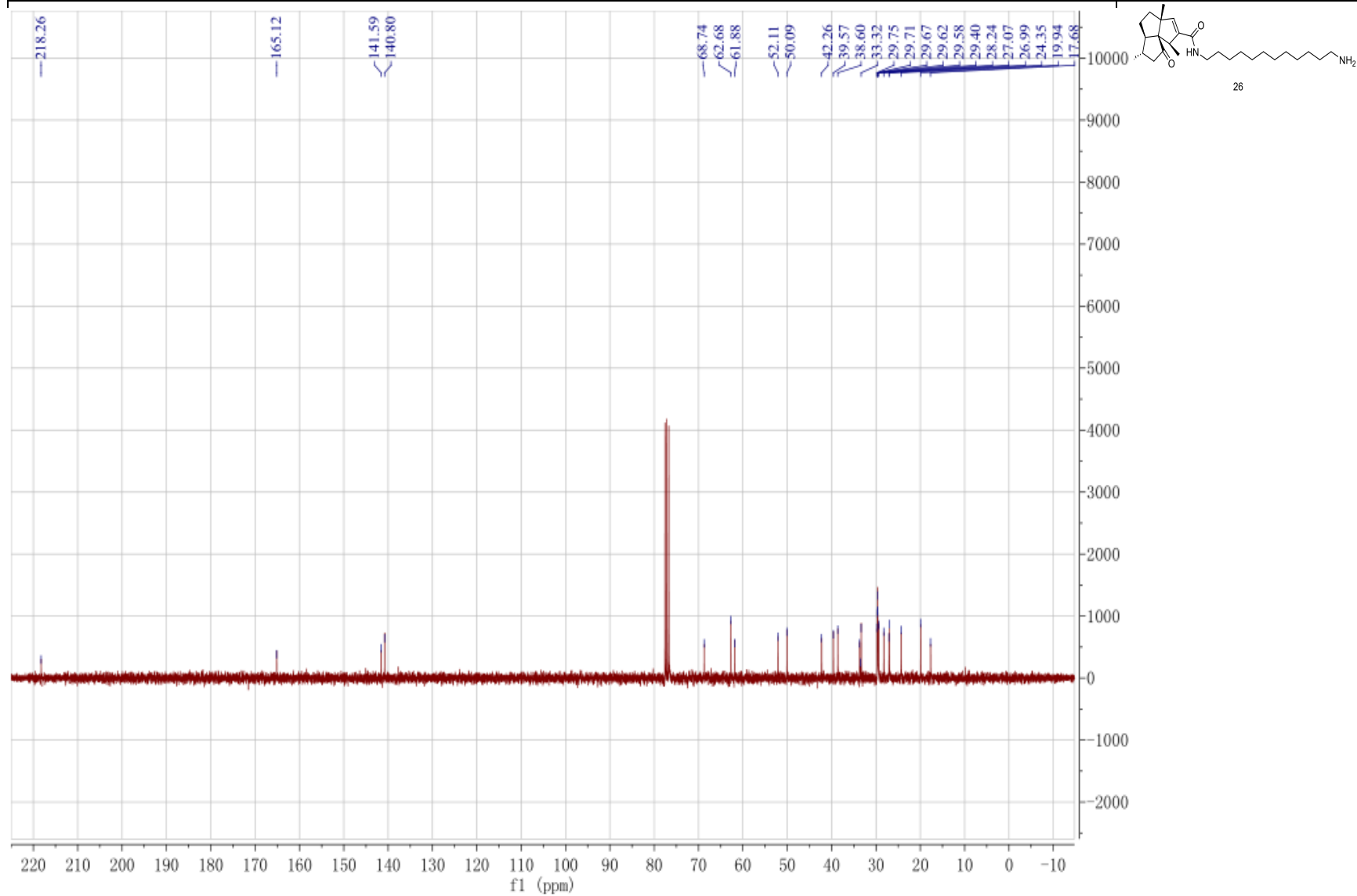


Figure S58. HRMS of compound 4

zi-10, MW=264, NH3; neg. ion
bri140808_10 184 (3.067) Cm (187:189-1:74)

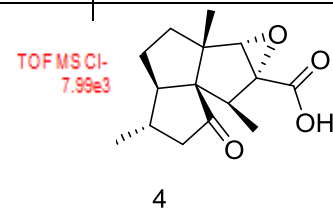
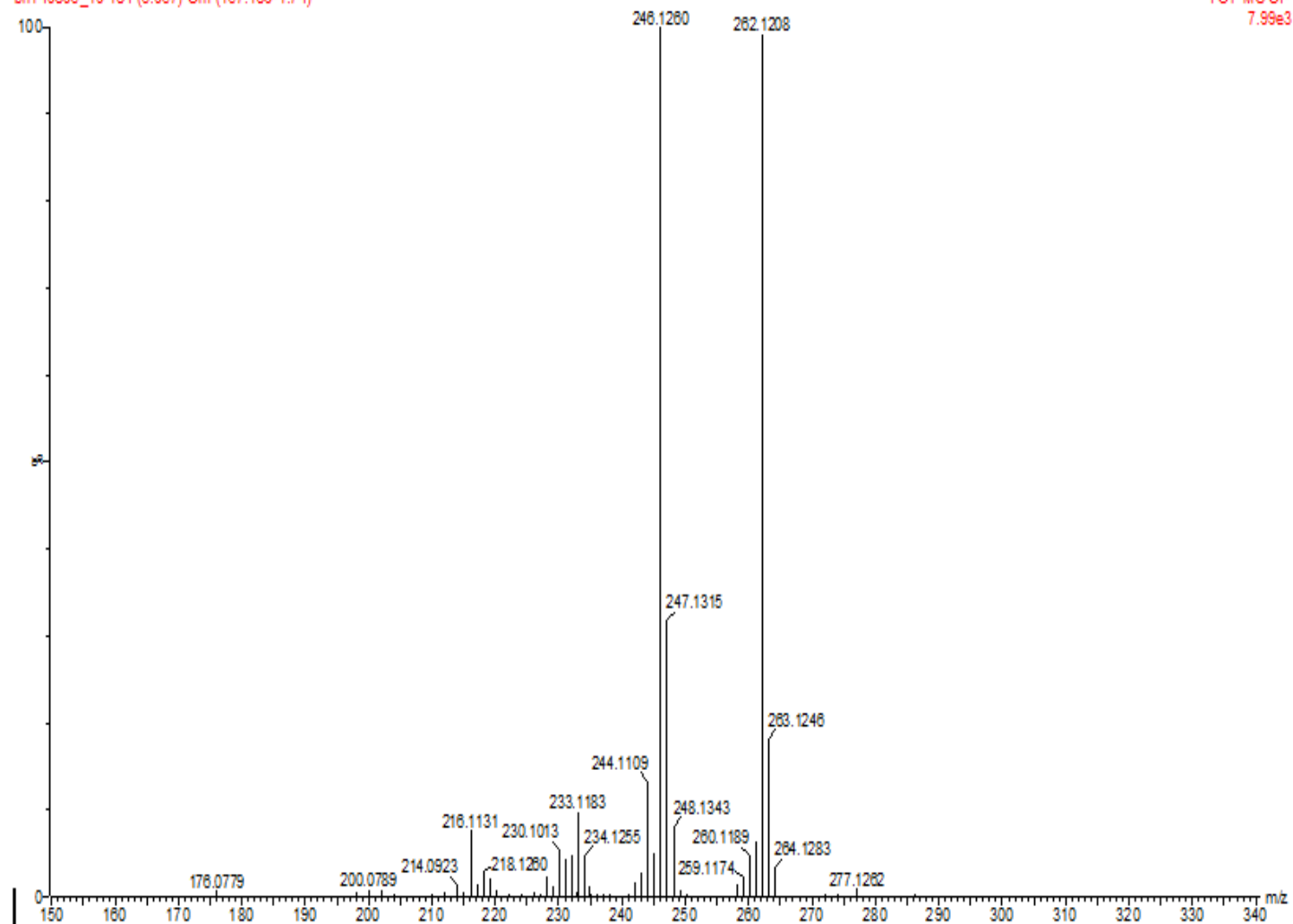


Figure S59. HRMS of compound **5**

z-**5**, MW=338, NH3; neg. ion
bri140808_5 89 (1.484) Cm (89.92-1.64)

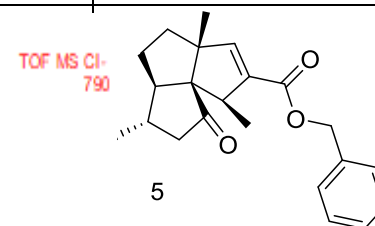
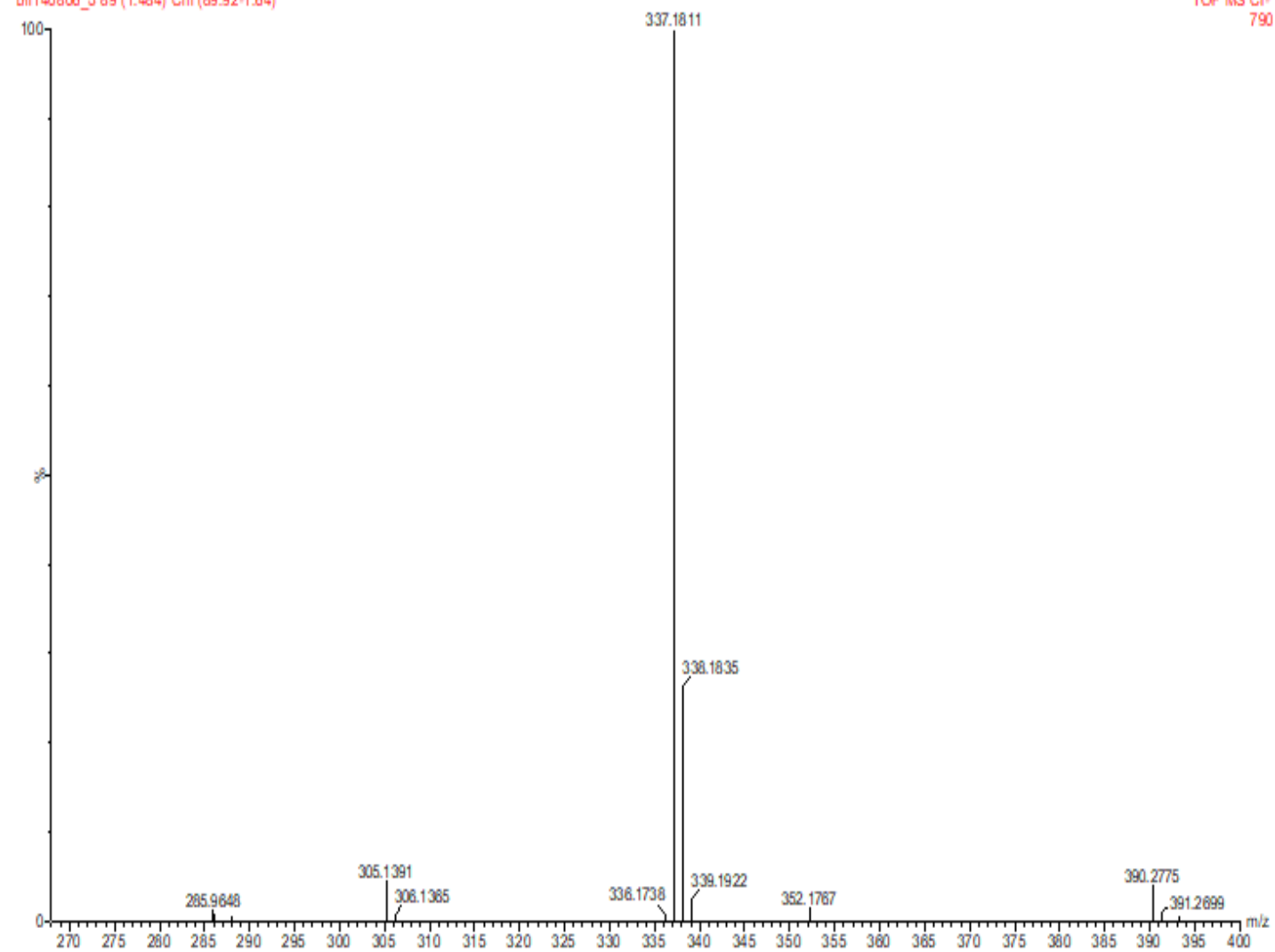


Figure S60. HRMS of compound 8

z-6, MW=406, NH3; neg. ion
bn140806_8 148 (2.467) Cm (145.160-1:105)

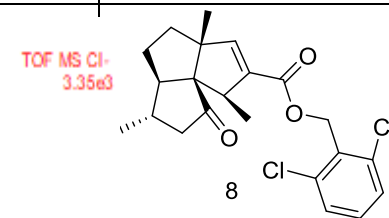
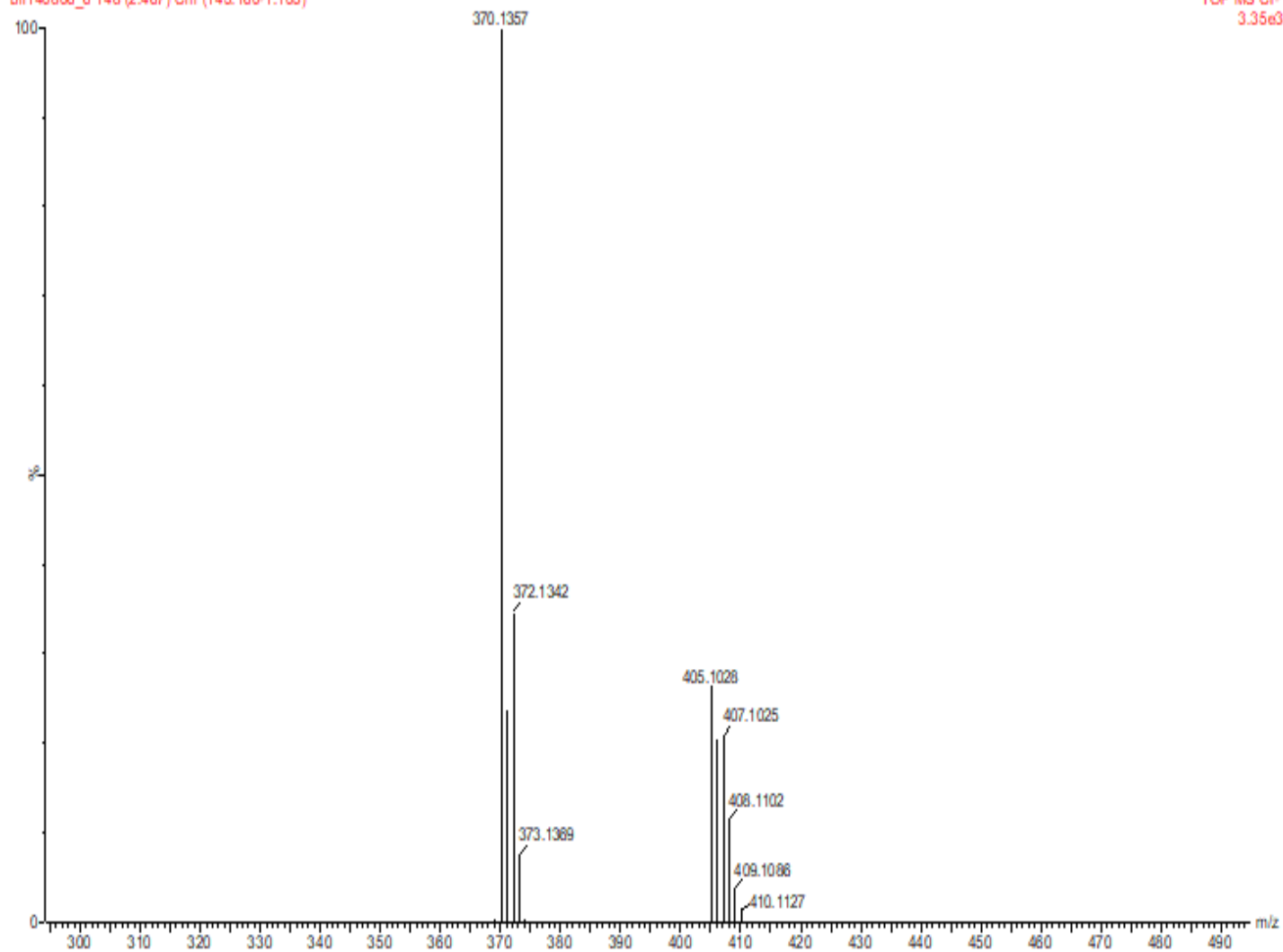


Figure S61. HRMS of compound **10**

z: 9, MW=372, NH3; neg. ion
bri140806_9 90 (1.500) Cm (90.96-1.67)

TOF MS Cl-
551

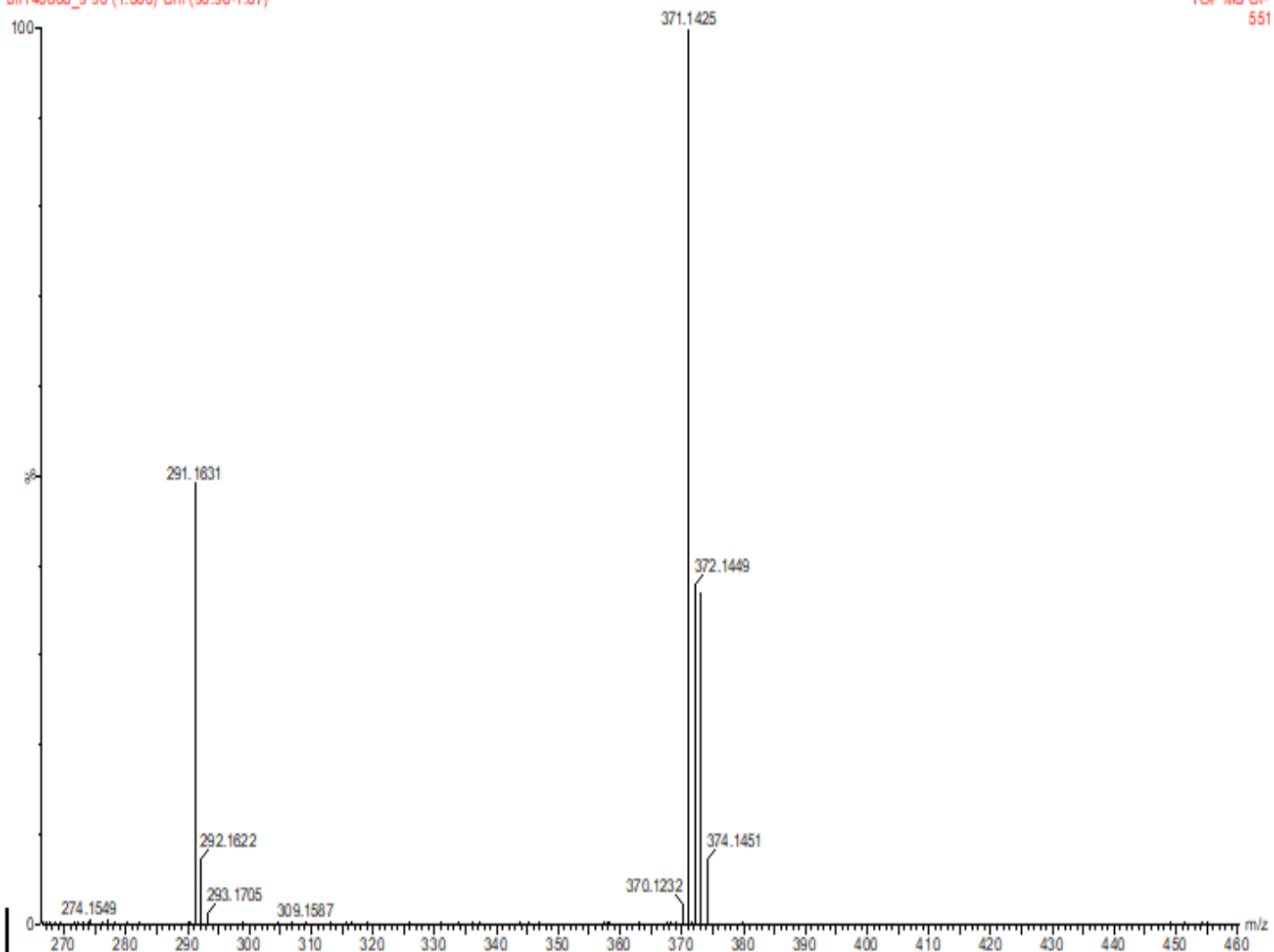
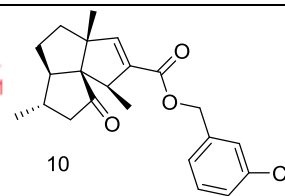
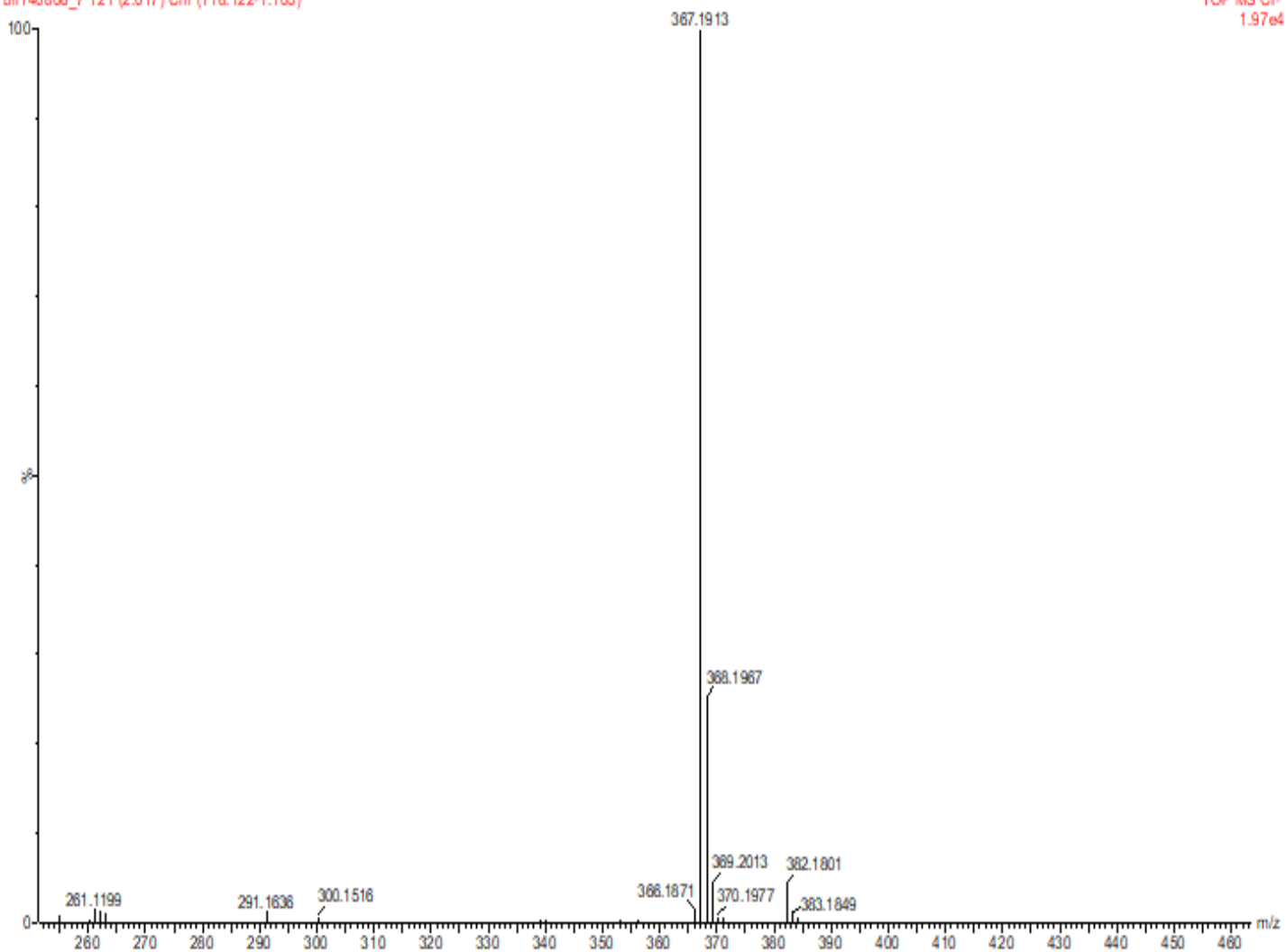


Figure S62. HRMS of compound **11**

$z+7$, MW=368, NH3; neg. ion
bri140808_7 121 (2.017) Cm (118:122-1:105)



TOF MS CI-
1.97e4

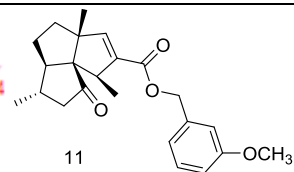


Figure S63. HRMS of compound **13**

z⁻-4, MW=339, NH3; neg. ion

br140806_4 251 (4.184) Cm (248:257-1:193)

TOF MS Cl-
1.06e4

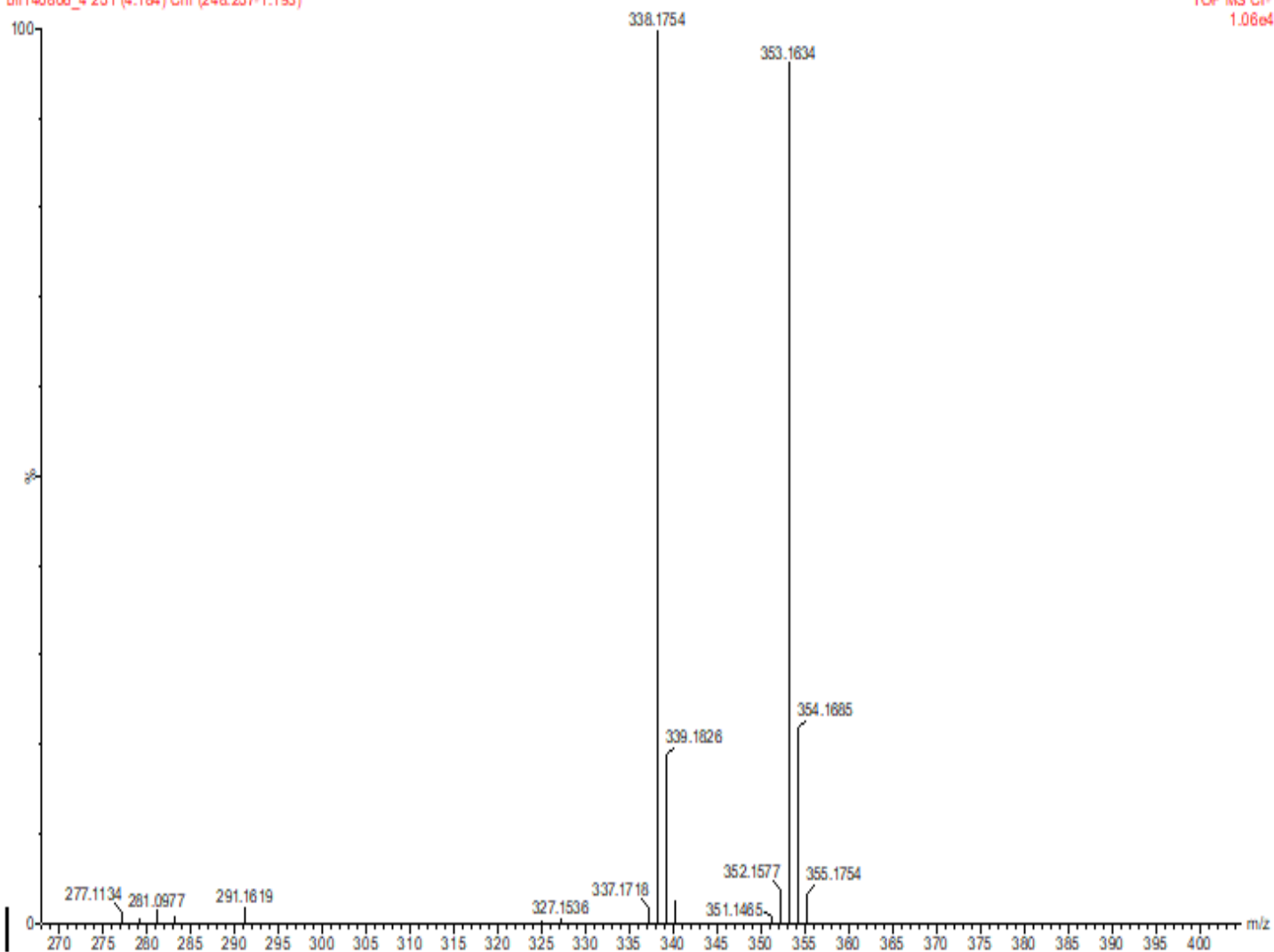
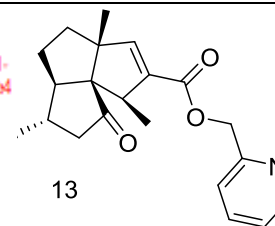


Figure S64. HRMS of compound **14**

z1-8, MW=339, NH3; neg. ion
bn140806_8 102 (1.700) Cm (98:102-1.88)

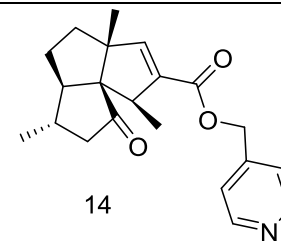
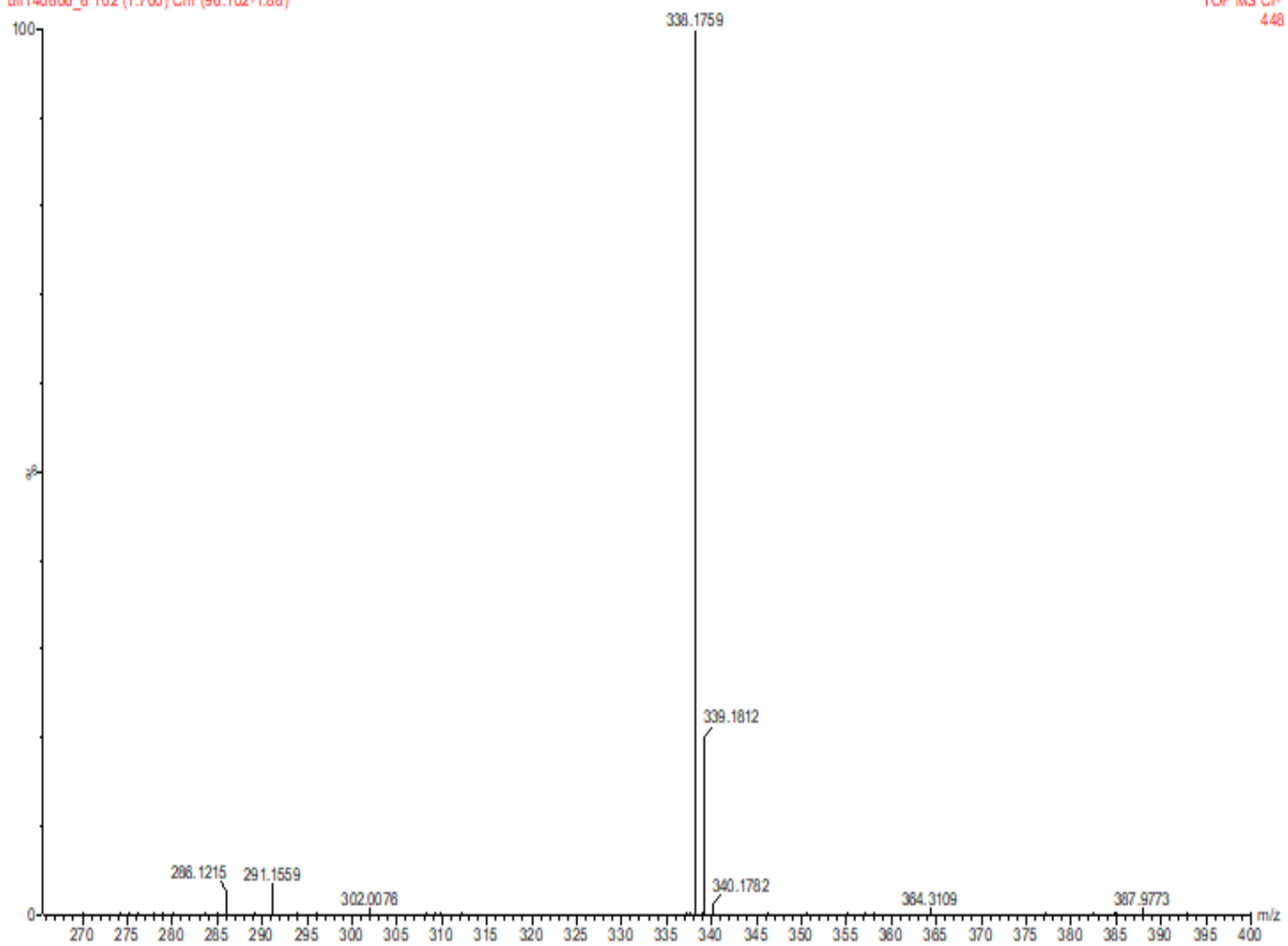
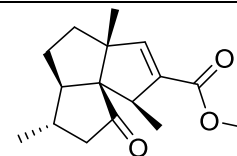


Figure S65. HRMS of compound **1**



Spectrum from Data20190113-Z-3-15.wiff (sample 1) - Sample020, +TOF MS (100 - 1000) from 0.100 to 0.150 min

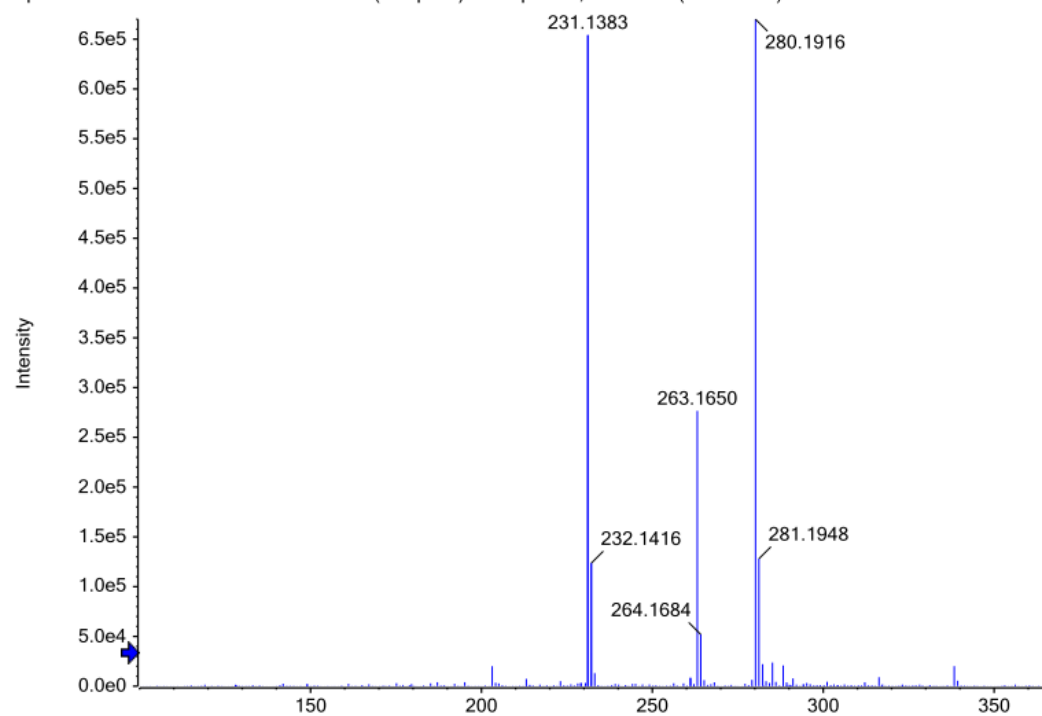


Figure S66. HRMS of compound 2

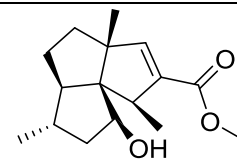
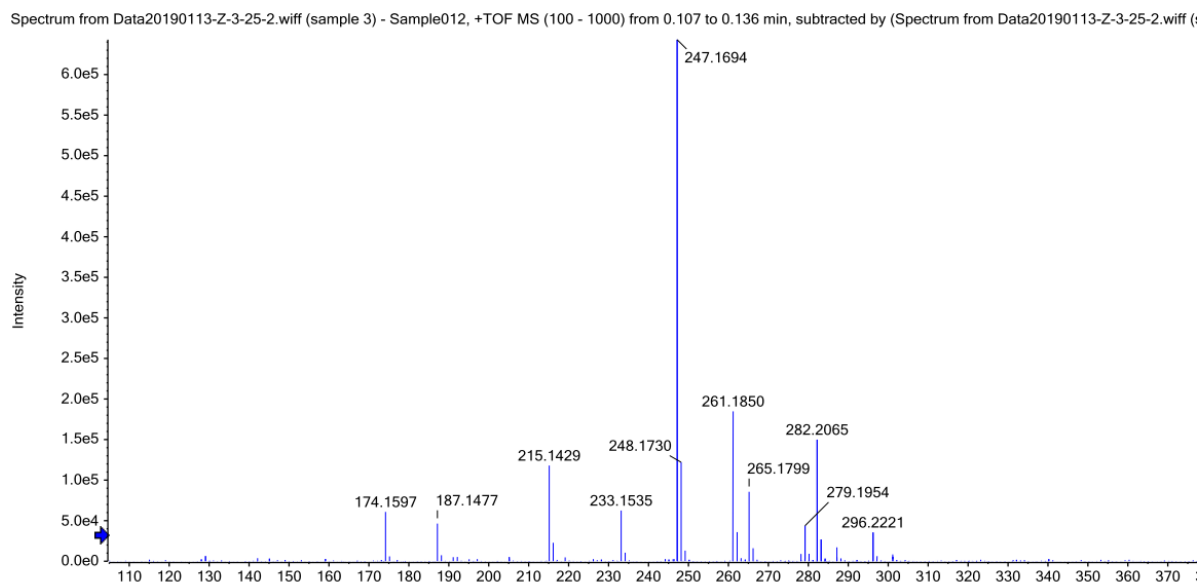


Figure S67. HRMS of compound **3**

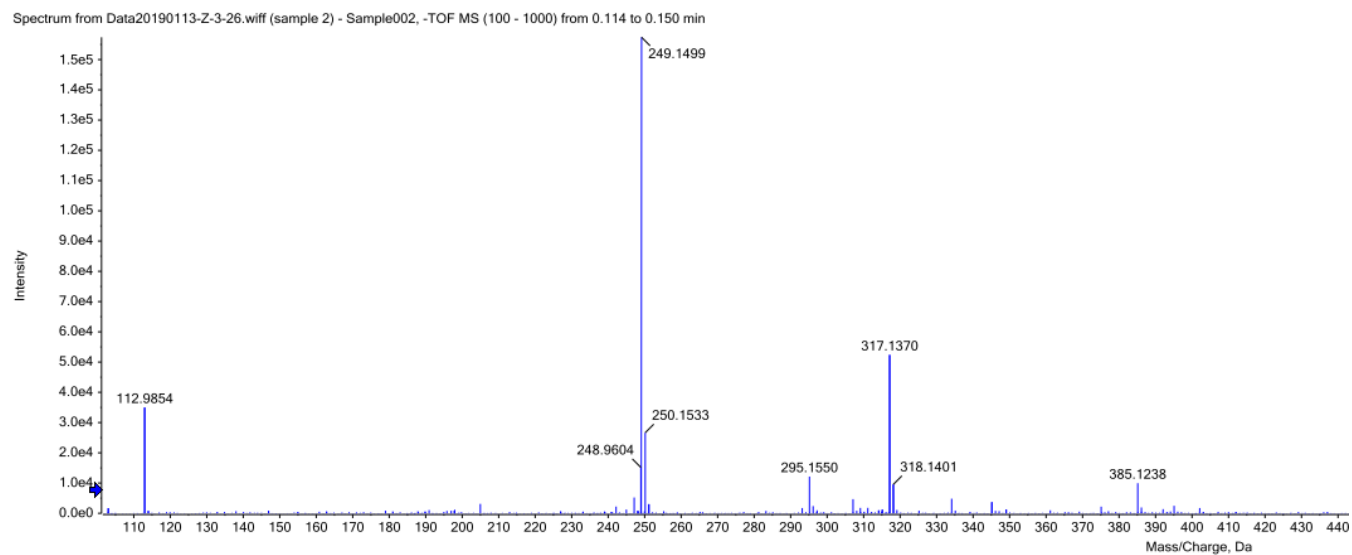
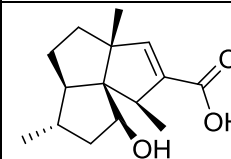


Figure S68. HRMS of compound **6**

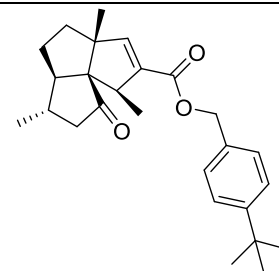
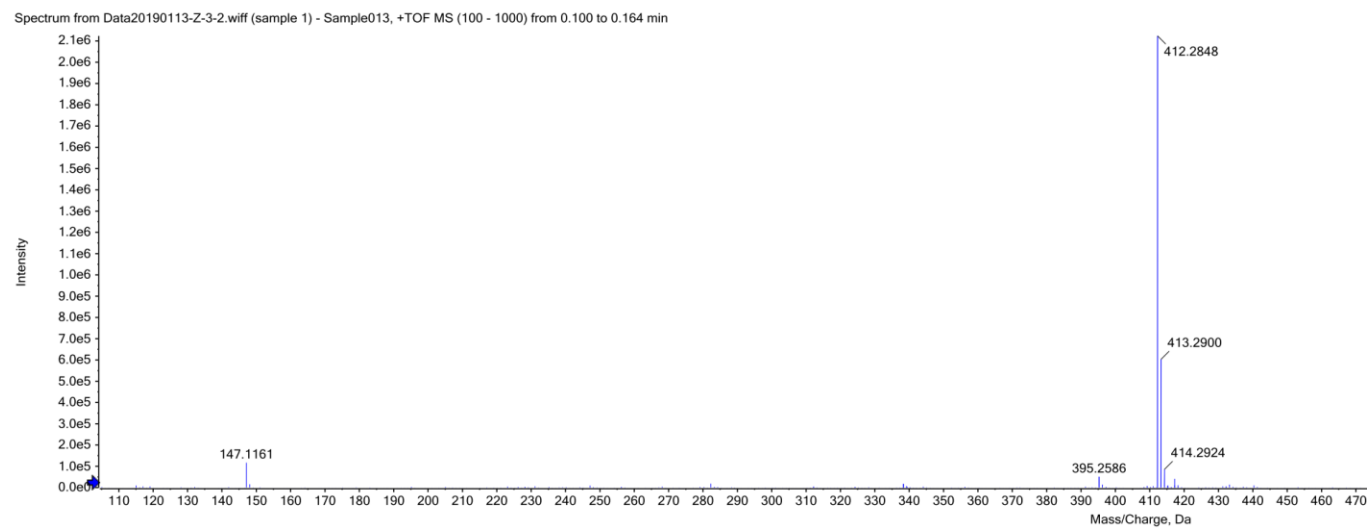


Figure S69. HRMS of compound **7**

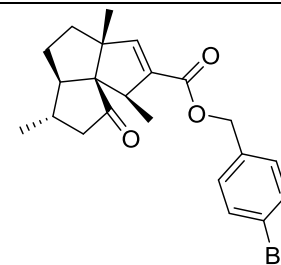
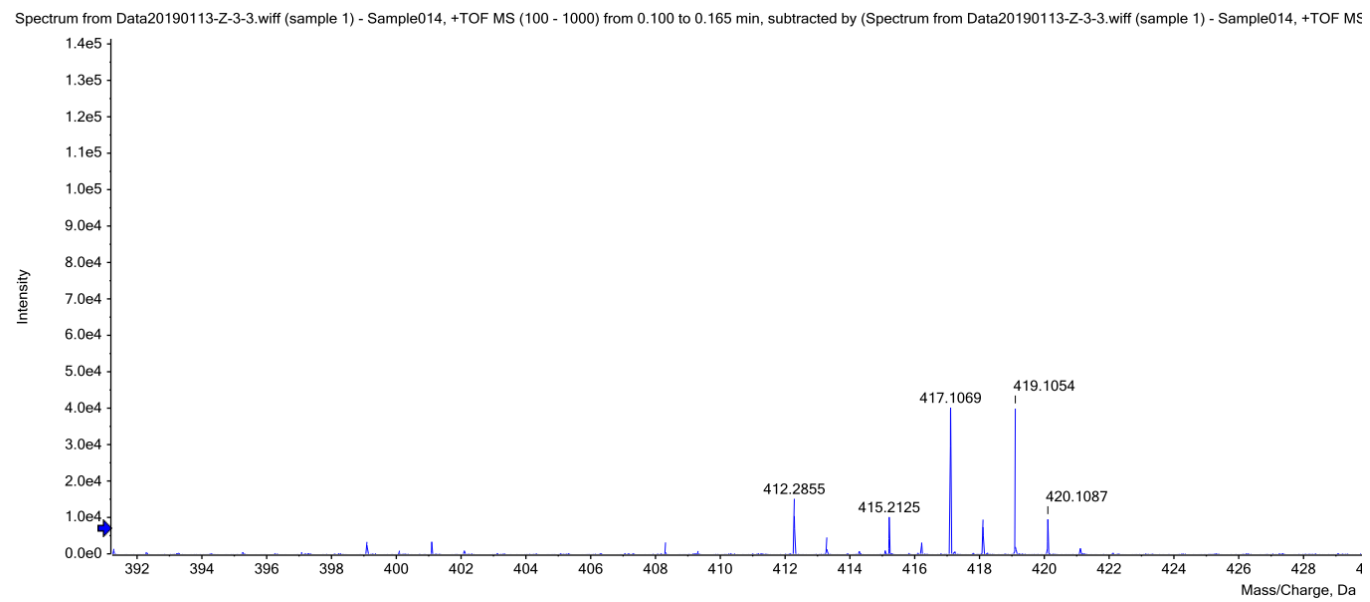


Figure S70. HRMS of compound **9**

Spectrum from Data20190113-Z-3-7.wiff (sample 1) - Sample016, +TOF MS (100 - 1000) from 0.100 to 0.157 min

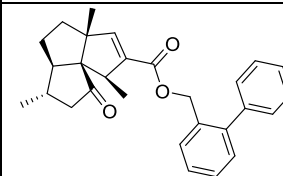
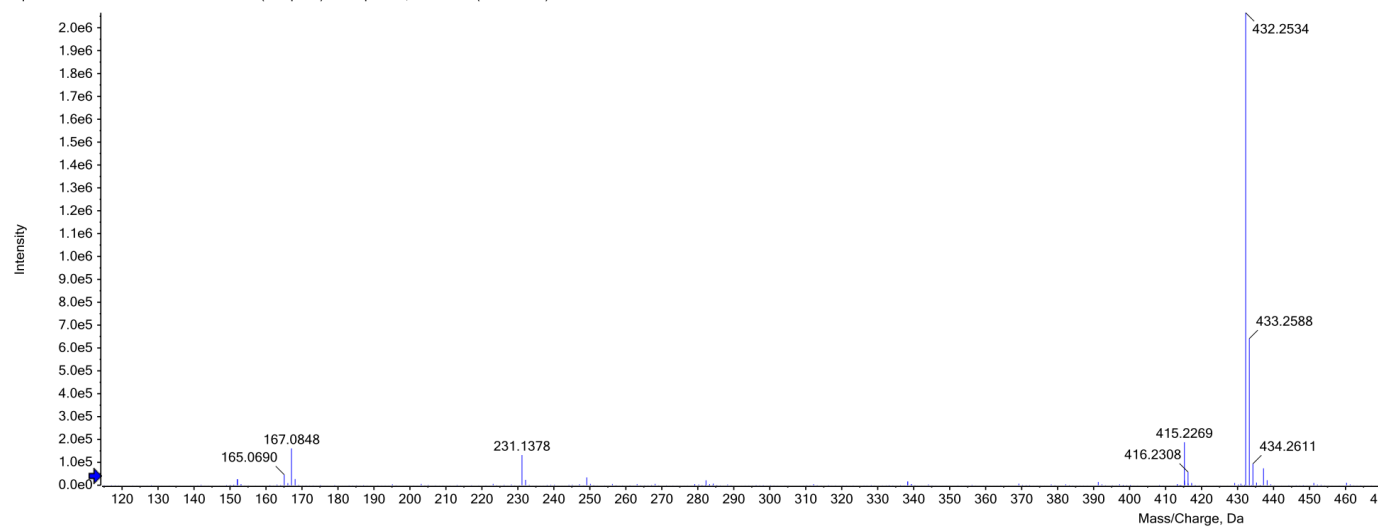


Figure S71. HRMS of compound **12**

Spectrum from Data20190113-Z-3-13.wiff (sample 1) - Sample015, +TOF MS (100 - 1000) from 0.093 to 0.164 min

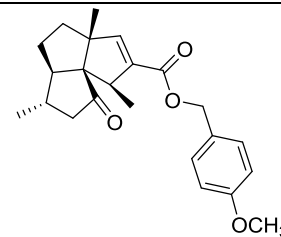
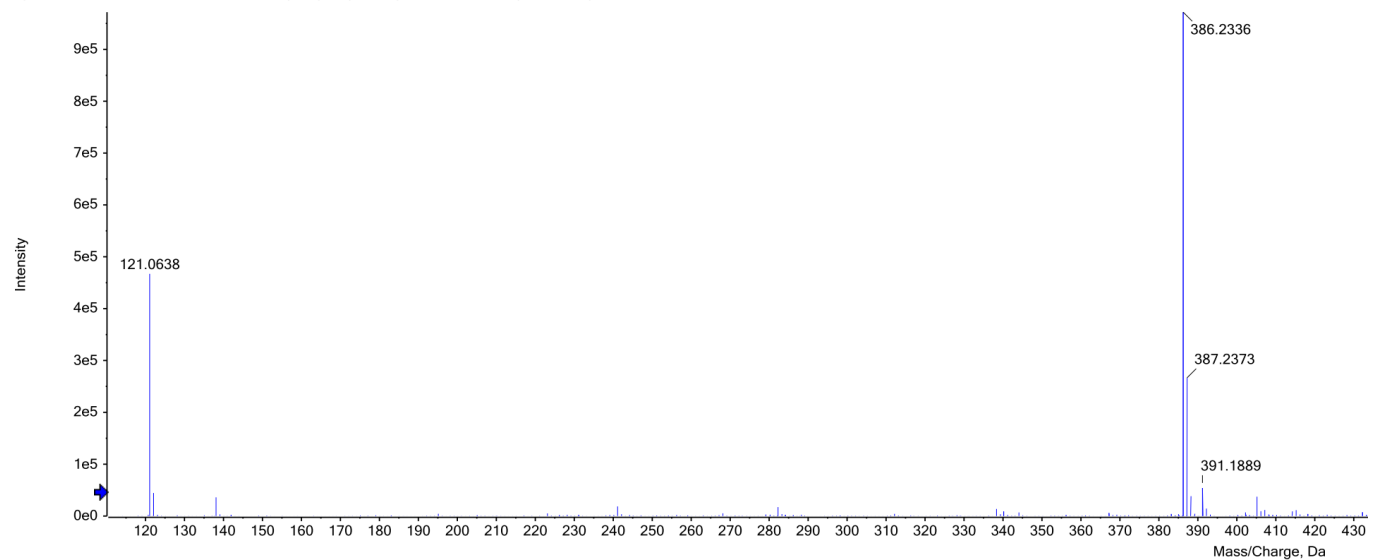
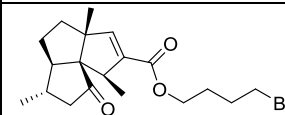


Figure S72. HRMS of compound **15**



Spectrum from Data20190113-Z-3-17.wiff (sample 1) - Sample019, +TOF MS (100 - 1000) from 0.107 to 0.150 min

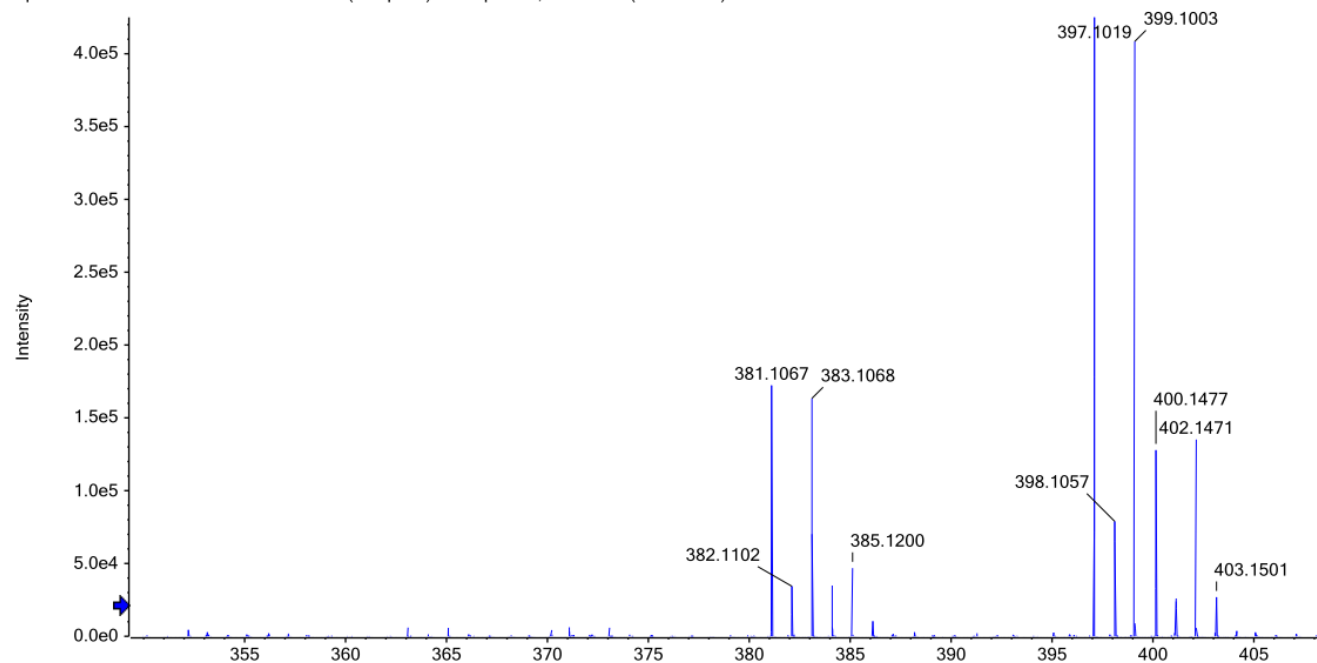


Figure S73. HRMS of compound **16**

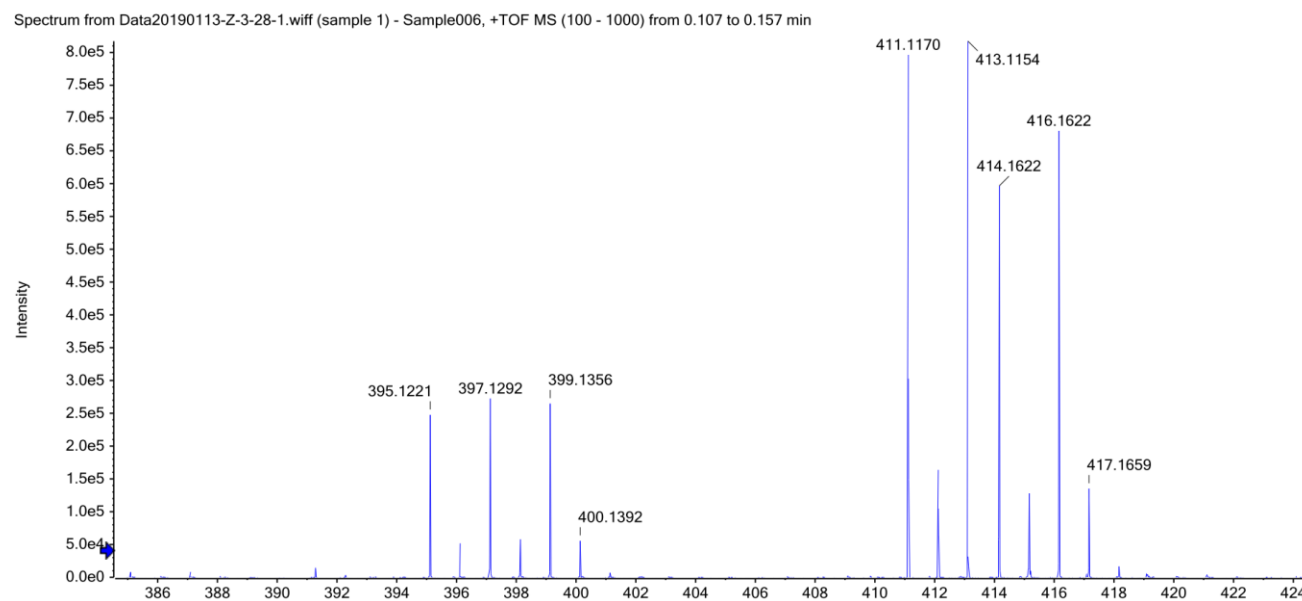
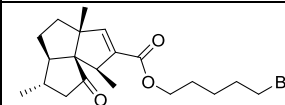


Figure S74. HRMS of compound **17**

Spectrum from Data20190113-Z-3-28-2.wiff (sample 1) - Sample010, +TOF MS (100 - 1000) from 0.107 to 0.150 min

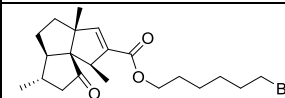
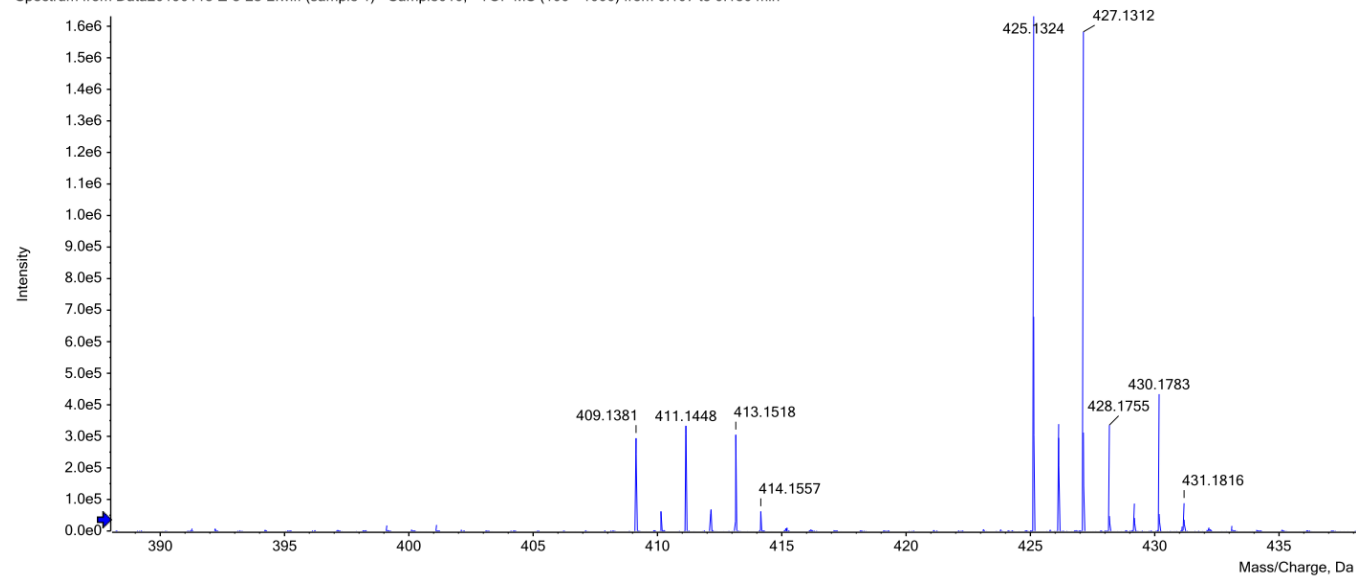


Figure S75. HRMS of compound **18**

Spectrum from Data20190113-Z-3-28-3.wiff (sample 1) - Sample003, +TOF MS (100 - 1000) from 0.114 to 0.164 min

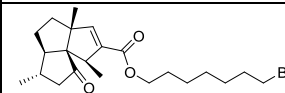
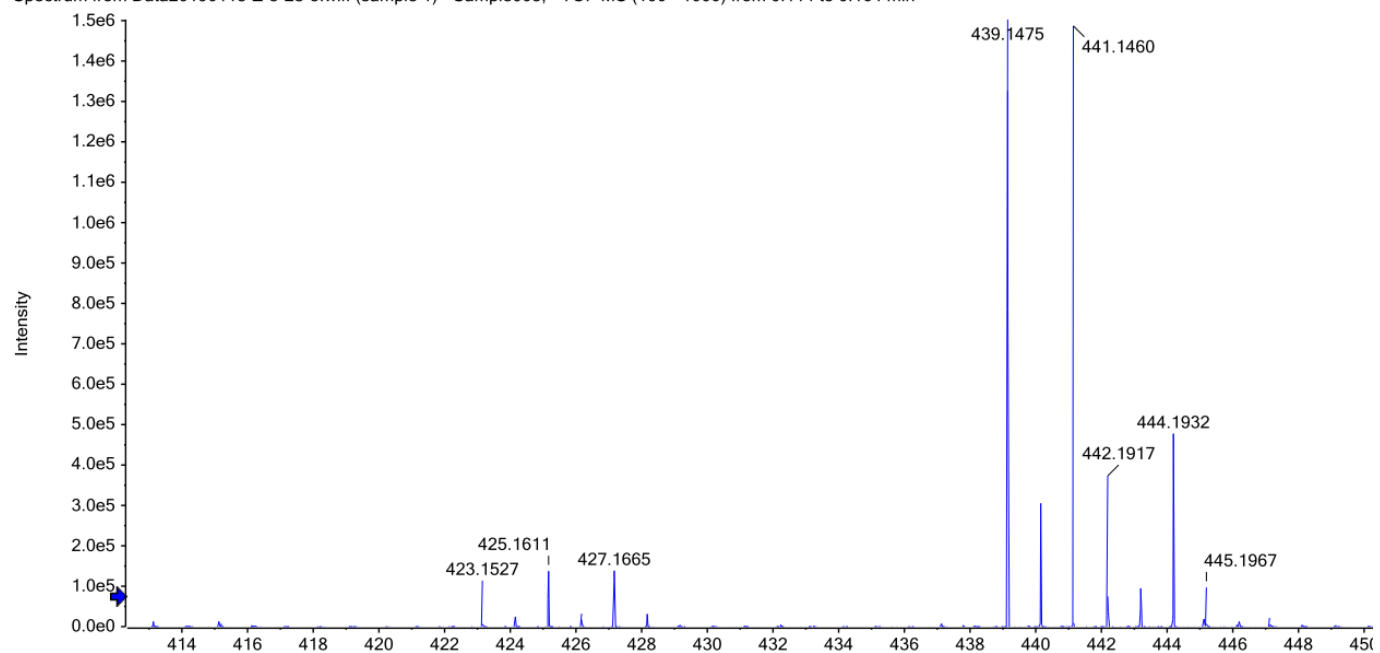


Figure S76. HRMS of compound **19**

Spectrum from Data20190113-Z-3-28-4.wiff (sample 1) - Sample011, +TOF MS (100 - 1000) from 0.100 to 0.172 min

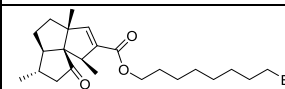
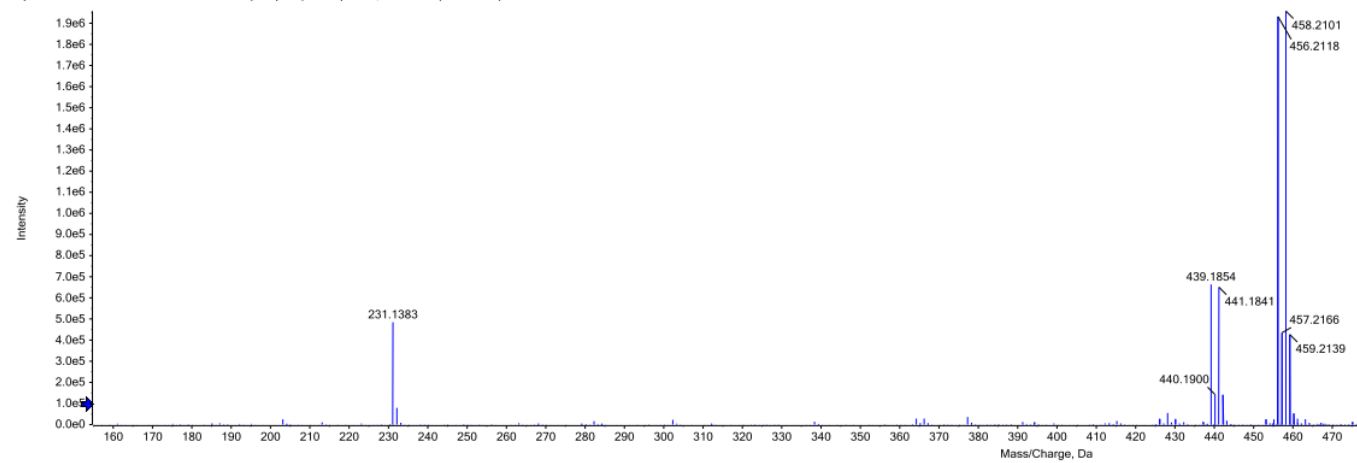


Figure S77. HRMS of compound **20**

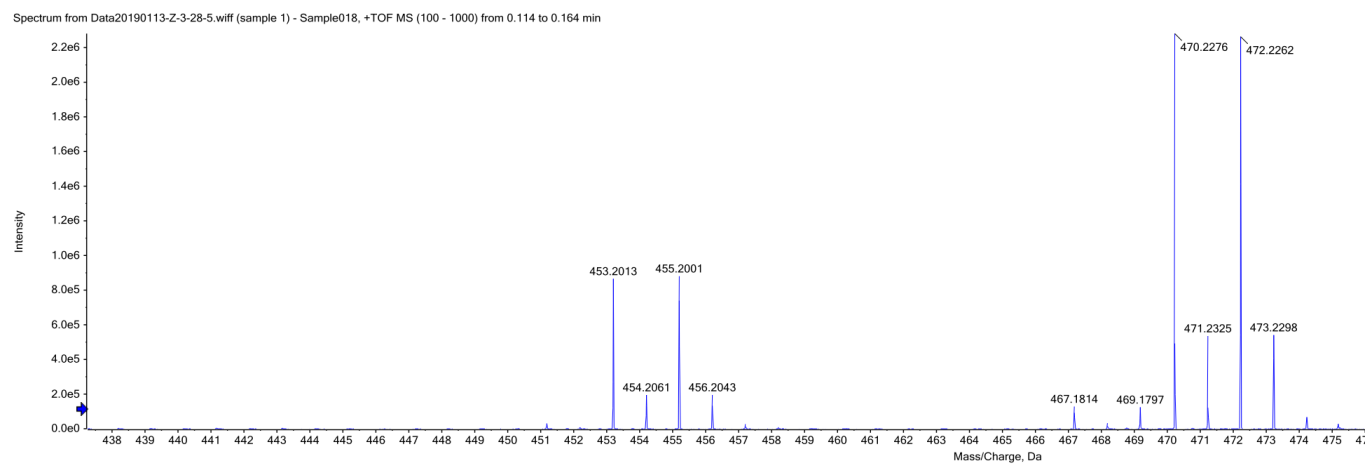
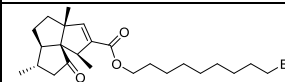


Figure S78. HRMS of compound **21**

Spectrum from Data20190113-Z-3-21-1.wiff (sample 1) - Sample017, +TOF MS (100 - 1000) from 0.114 to 0.164 min

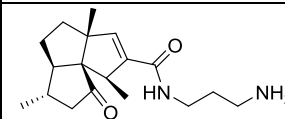
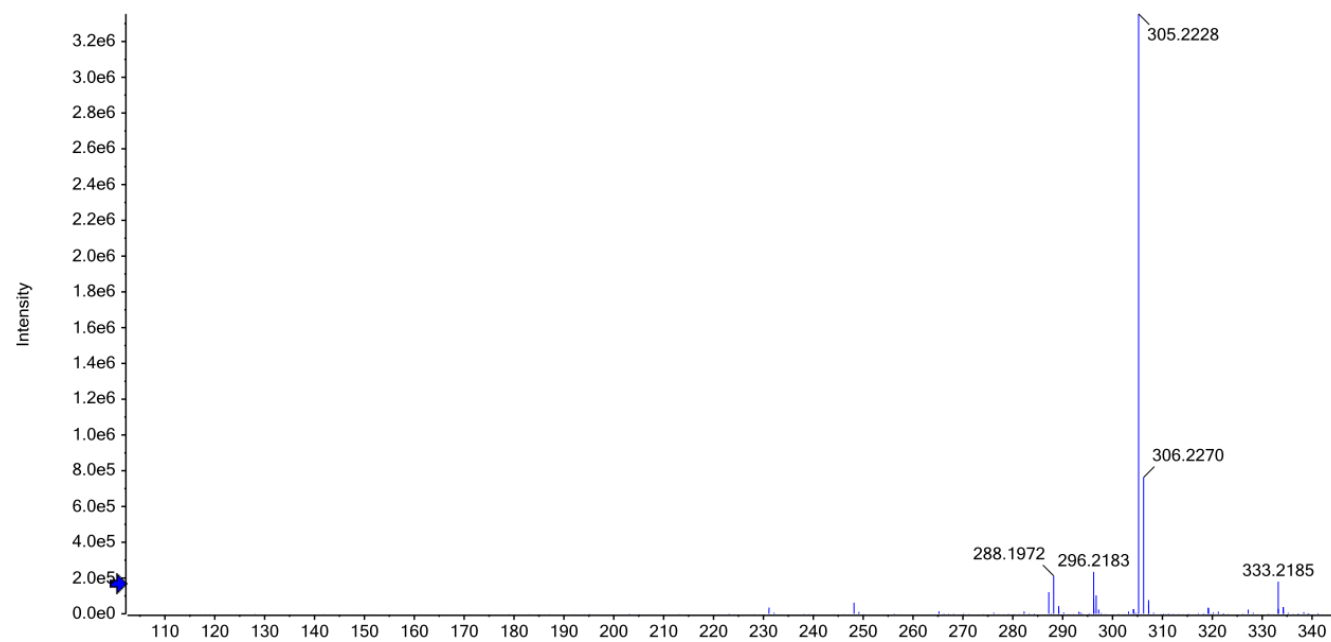


Figure S79. HRMS of compound **22**

Spectrum from Data20190113-Z-3-21-2.wiff (sample 1) - Sample004, +TOF MS (100 - 1000) from 0.107 to 0.150 min

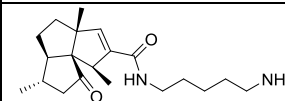
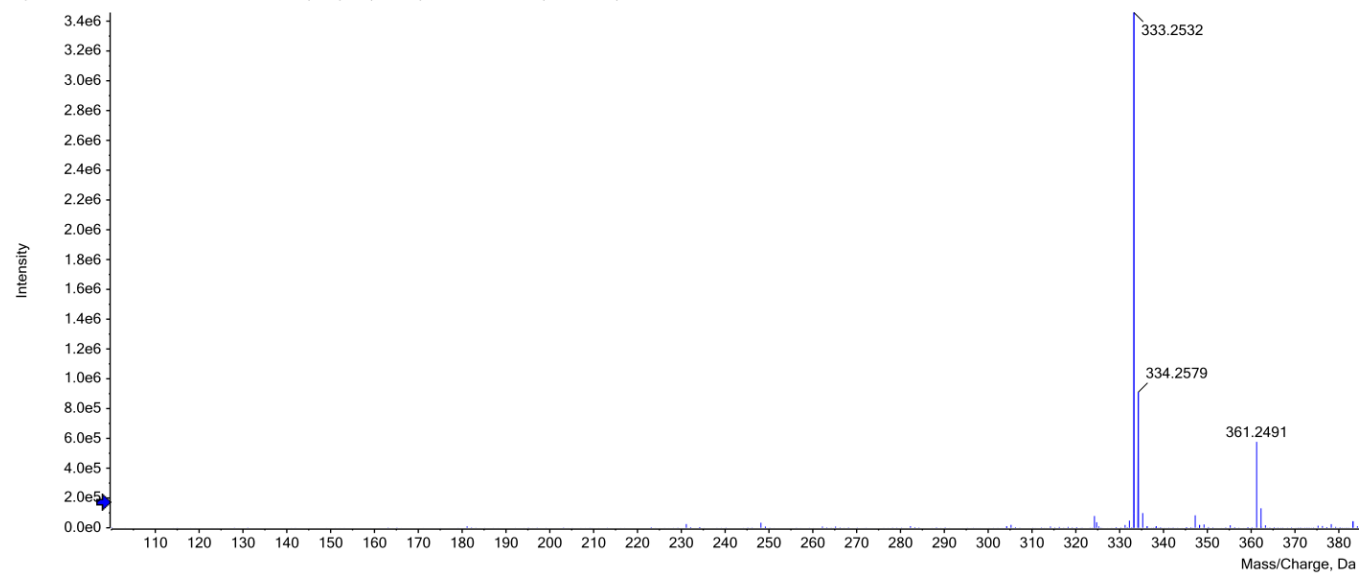


Figure S80. HRMS of compound **23**

Spectrum from Data20190113-Z-3-21-3.wiff (sample 1) - Sample009, +TOF MS (100 - 1000) from 0.093 to 0.172 min

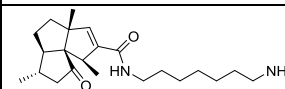
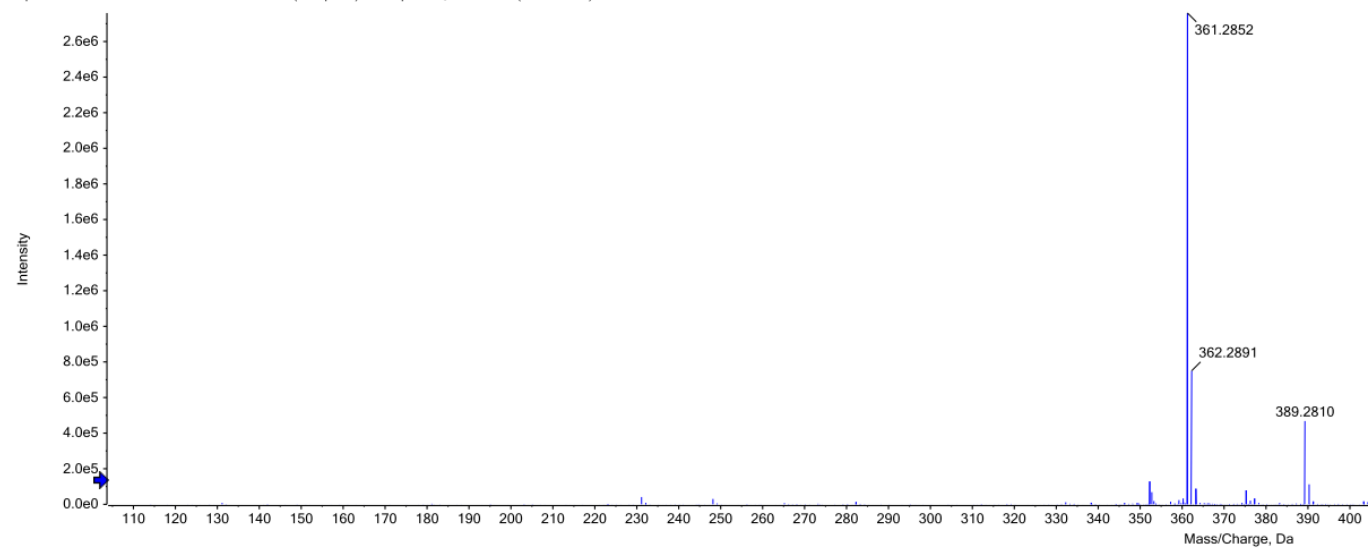


Figure S81. HRMS of compound **24**

Spectrum from Data20190113-Z-3-21-4.wiff (sample 1) - Sample007, +TOF MS (100 - 1000) from 0.100 to 0.172 min

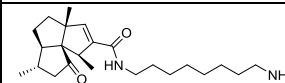
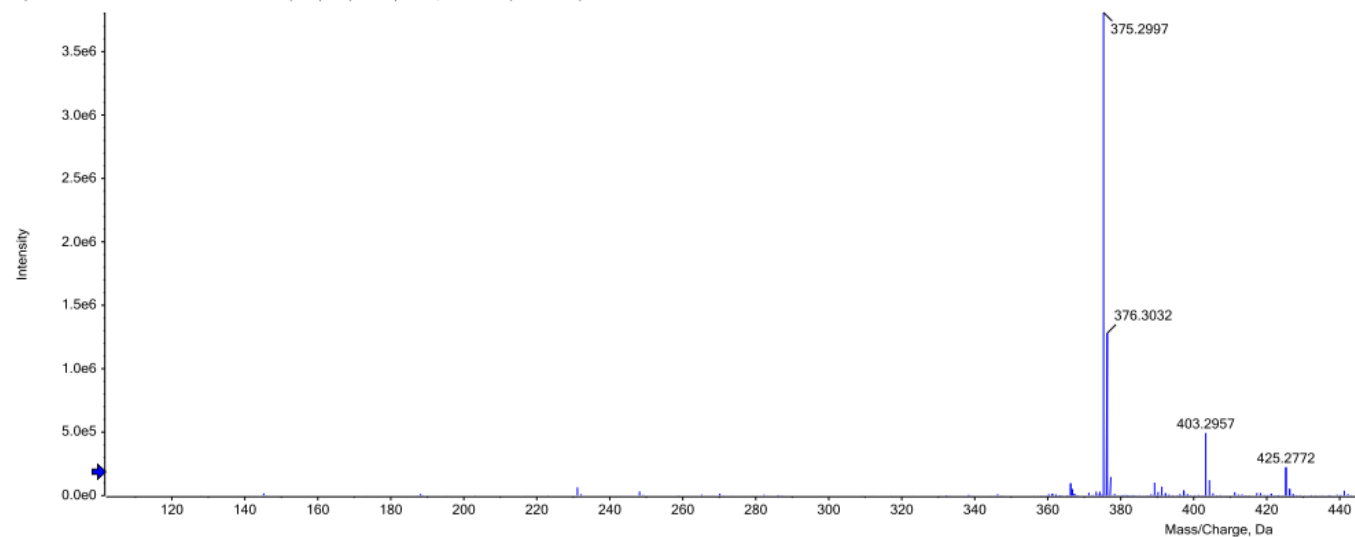


Figure S82. HRMS of compound **25**

Spectrum from Data20190113-Z-3-21-5.wiff (sample 1) - Sample008, +TOF MS (100 - 1000) from 0.107 to 0.164 min

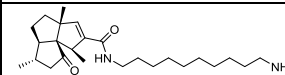
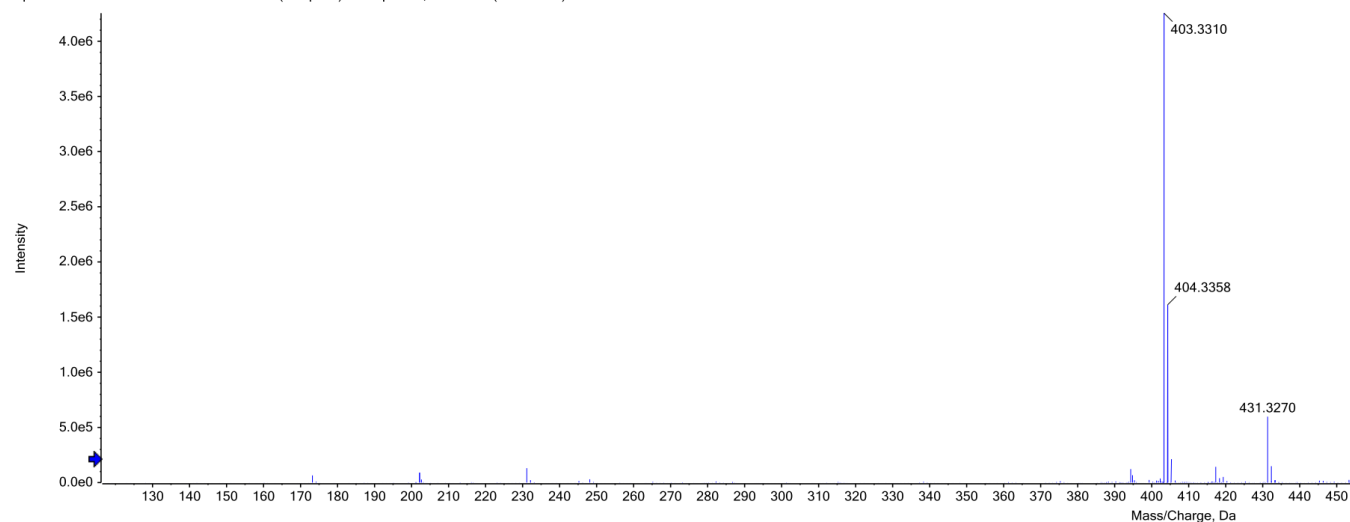


Figure S83. HRMS of compound **26**

