Supporting Information

A base-mediated aerobic oxidative synthesis of cyclopent-2-enols derivatives from doubly activated cyclopropanes and substituted acetonitriles

Xiao-Dan Han[1], Gao-Liang Peng[2], Wei Xiong[1], Ran Gan[3], Jian-Ping Fu[1], Lei Wu[1], Zhong-Sheng Tang[1], Ju-Wu Hu[1], Hui-Bin Wang[1*]*

1) Department of Applied Chemistry, Jiang Xi Academy of Sciences, Nanchang, 330096, China

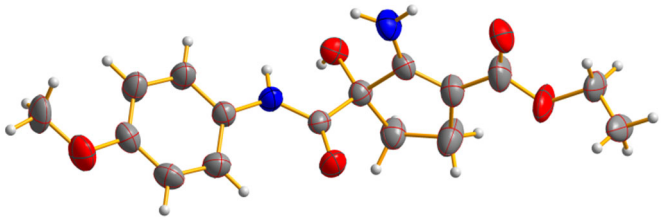
2) Jiangxi university of Applied Science, Nanchang, 330100, China

3) Jiangxi Academy of Forestry, Nanchang, 330096, China

email: hjw19771985@163.com; wanghb19801985@sina.com

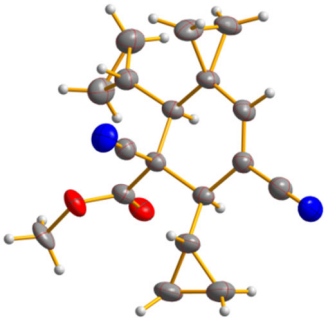
I. Crystal data and ORTEP drawing of compounds **3c**, **6b** and **8f**

Crystal data for **3c:** $C_{16}H_{20}N_2O_5$, H_2O: 338.35, colorless crystal, monoclinic, P 21/n, a = 12.2878(18)Å, b = 7.4046(10)Å, c = 19.762(3)Å, α= 90.0 º, β = 102.091 (2) º, γ = 90.0 º, V = 1758.2(4)Å^3, Z = 4, T = 296K, F_{000} = 720.0, R_1 = 0.0778(2351), wR_2 = 0.2531(3996). CCDC 2044495.



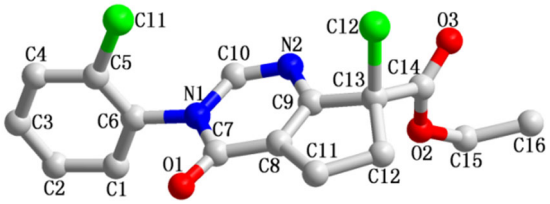
Compound **3c**

Crystal data for **6b**: $C_{18}H_{20}N_2O_2$, clorless crystal, M = 296.36,monoclinic, C 2/c, a = 18.7762(7) Å, b = 8.0291(2)Å, c = 23.0370 (8)Å, α= 90.0 º, β = 112.850 º, γ = 90.0 º, V = 3200.4(2)Å^3, Z = 8, T = 240K, F_{000} = 1264, R_1 = 0.0372(2476), wR_2 = 0.1067(2806). CCDC 2044497.



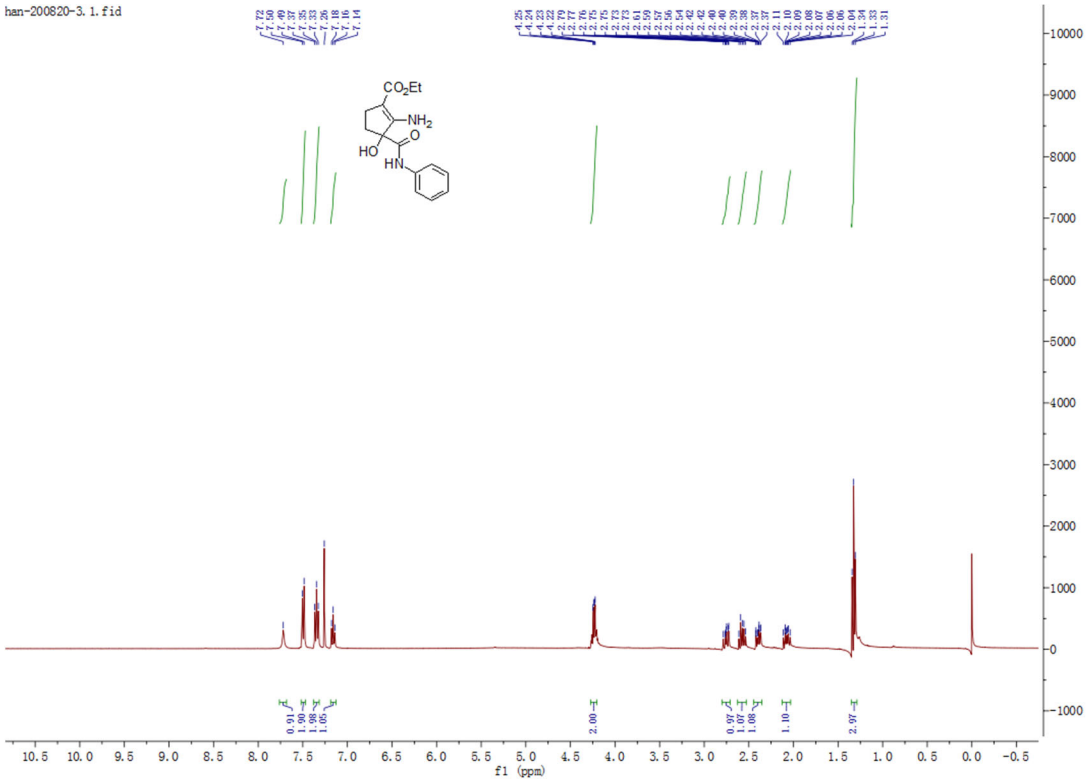
Compound **6b**

Crystal data for **8f**: $C_{16}H_{14}Cl_2N_2O_3$, colorless crystal, M =353.19, monoclinic, C 2/c, a = 33.761(16) Å, b = 6.7432(19)Å, c = 14.595(5) Å, α= 90.0 º, β = 101.90(3) º, γ = 90.0 º, V = 3251(2) Å^3, Z = 8, T = 250K, F_{000} = 1456, R_1 = 0.1106 (3245), wR_2 =0.2298(3832). CCDC 2092194.



Compound **8f**

II. Copies of ^{1}HNMR and ^{13}CNMR spectra of compounds **3, 4a, 6a-b , 7a , 8 (8') and 9**



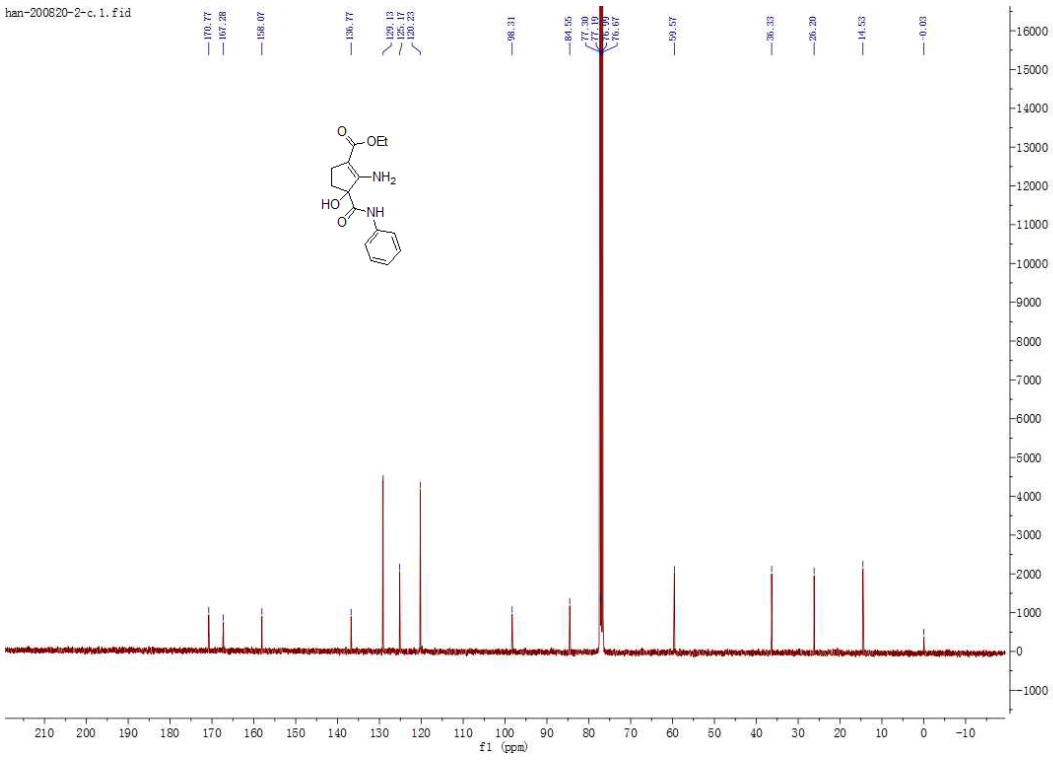
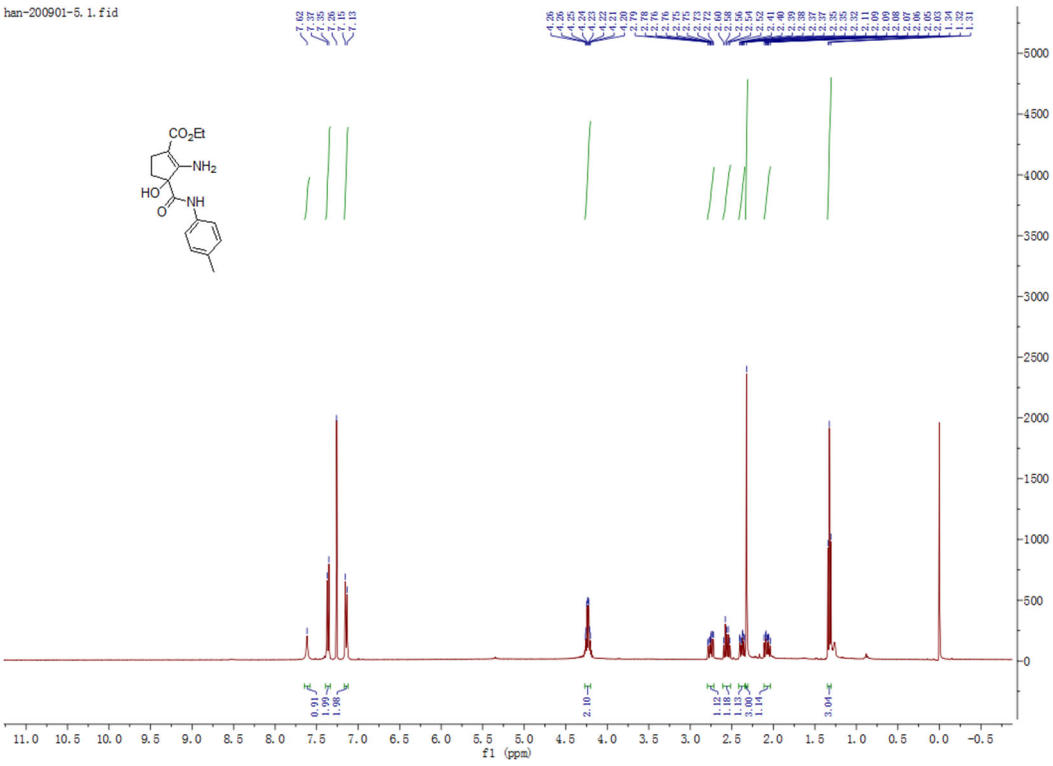


Figure 1. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3a**.



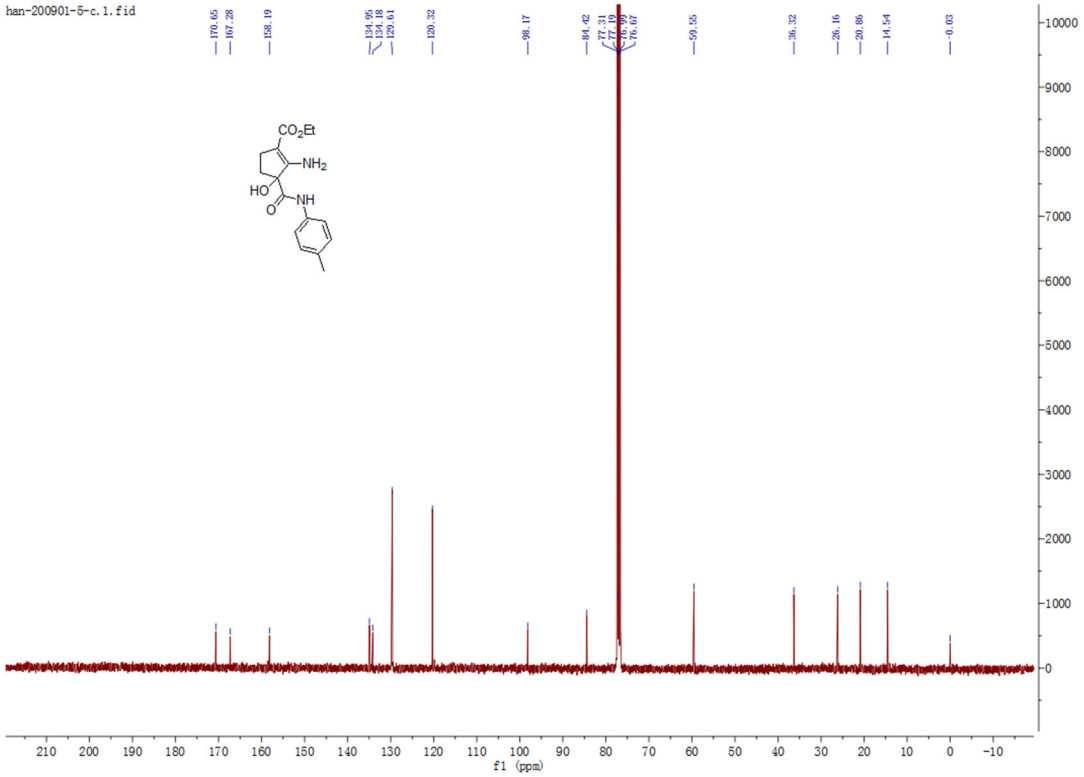
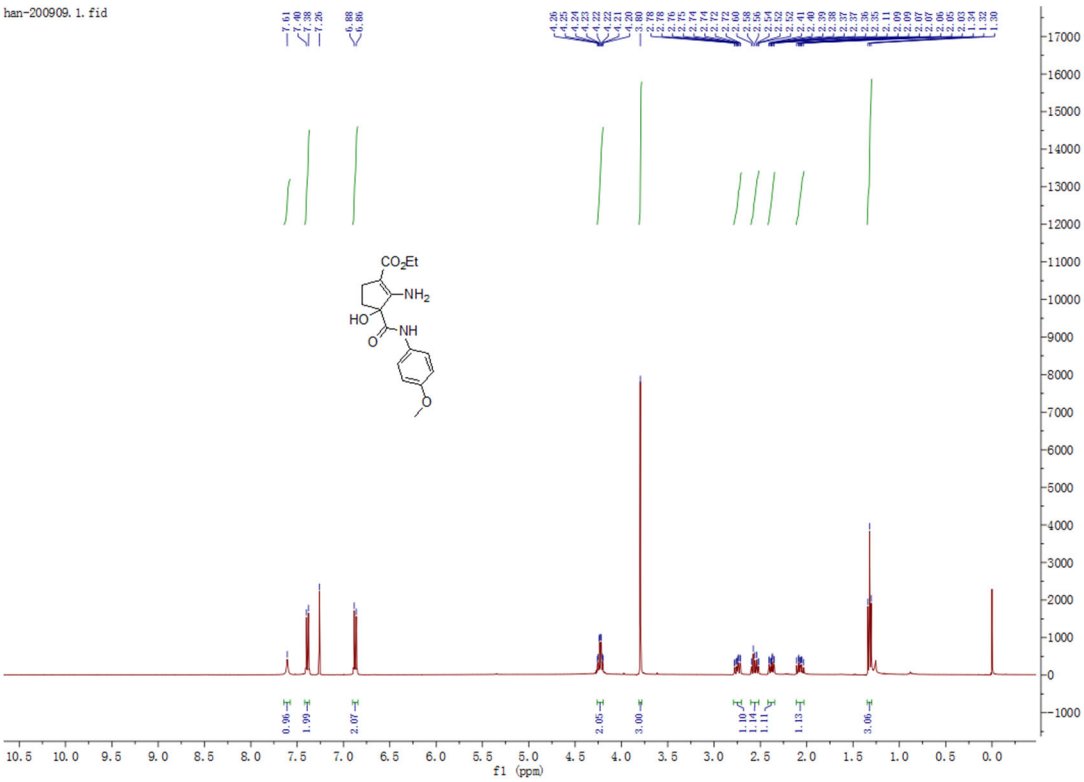


Figure 2. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3b**.



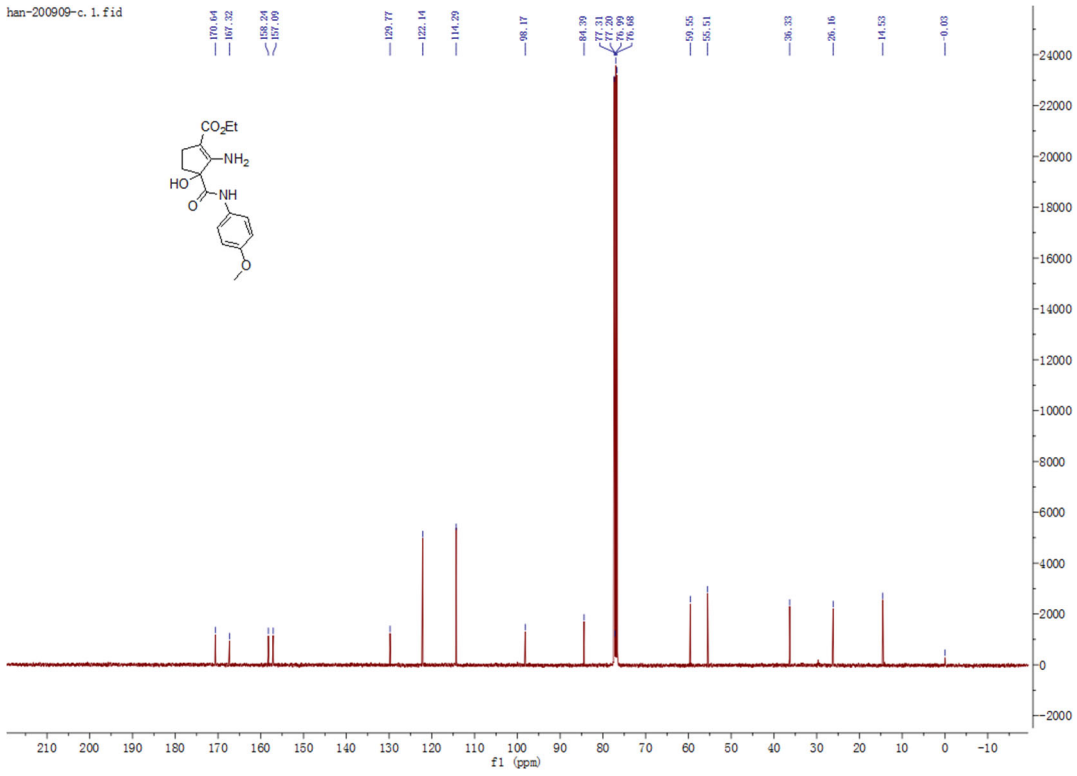
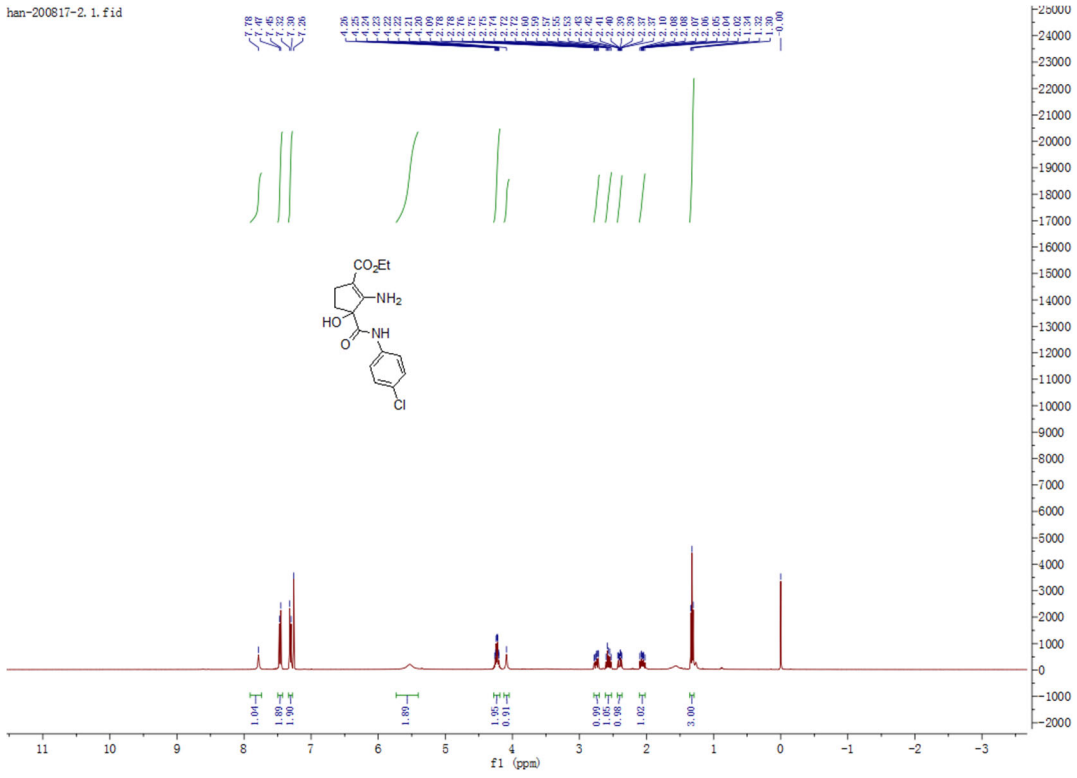


Figure 3. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound 3**c**.



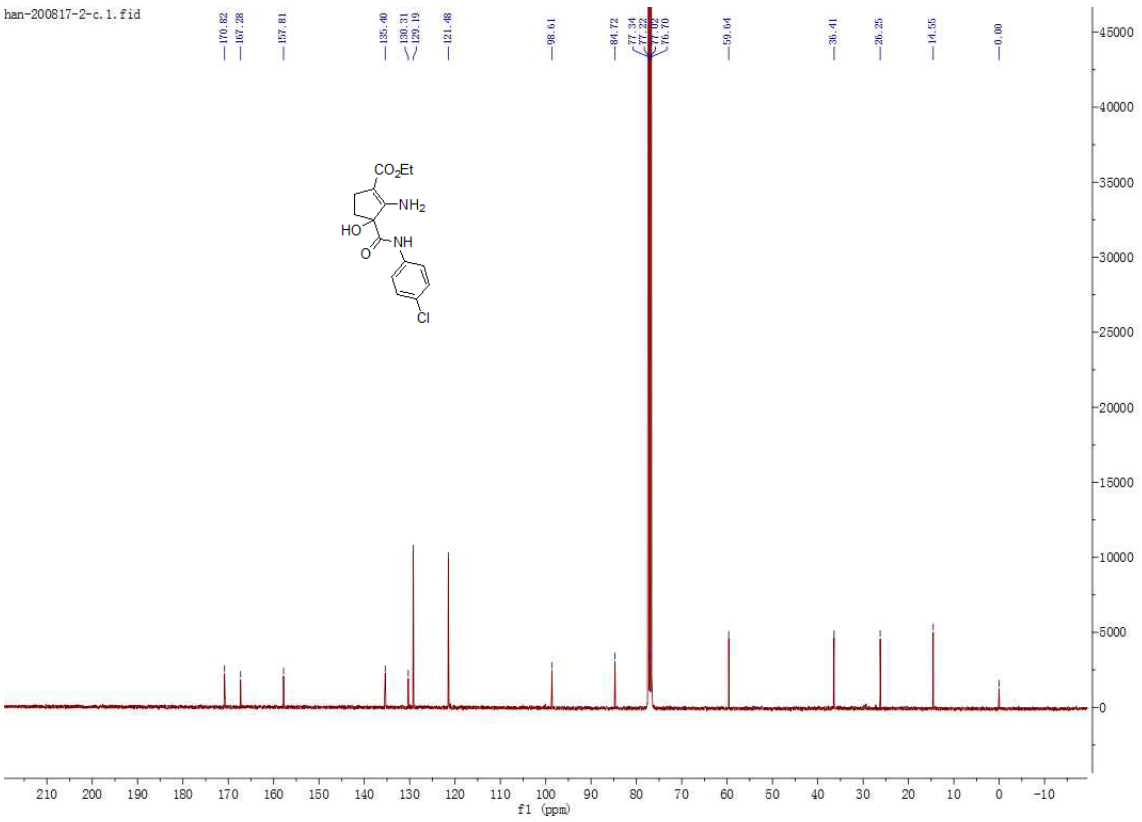
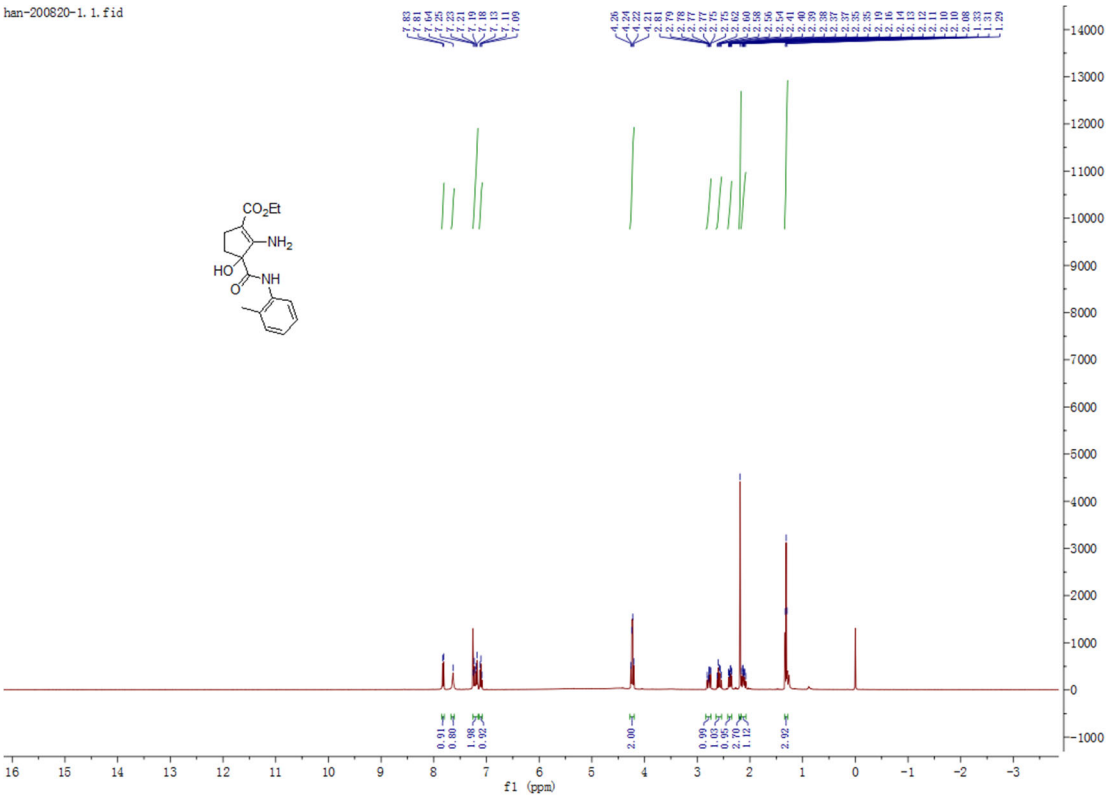


Figure 4. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound 3**d**.



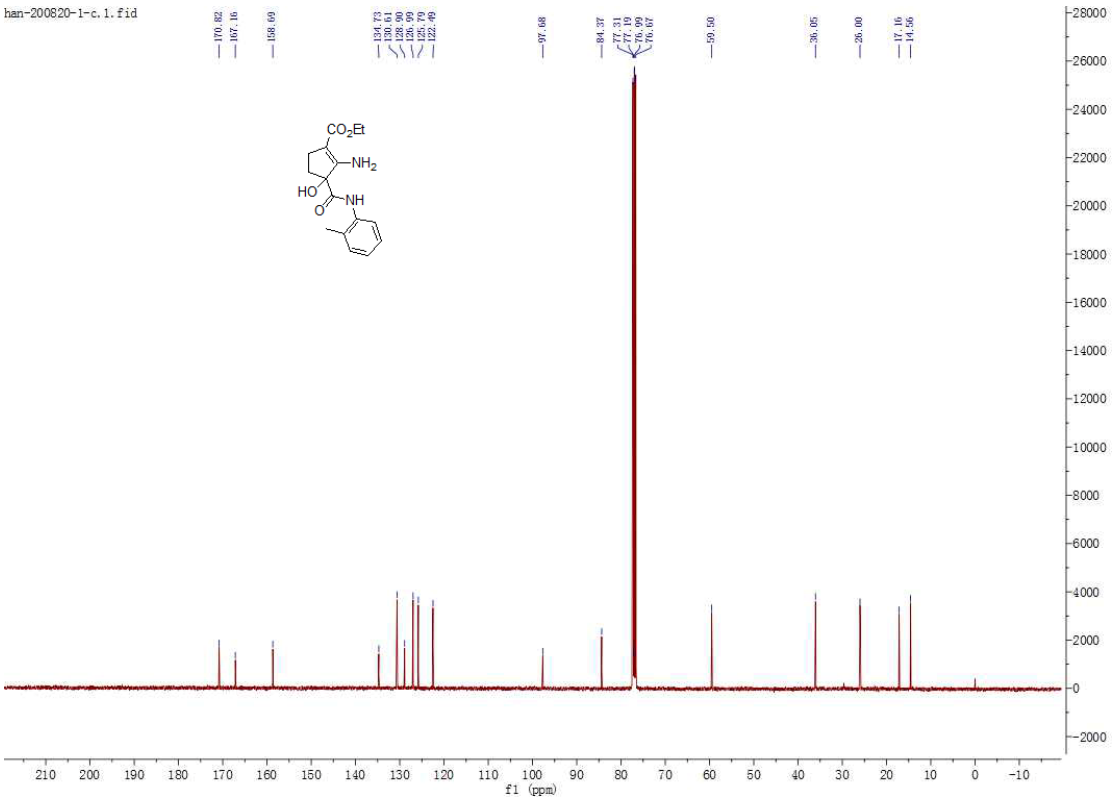
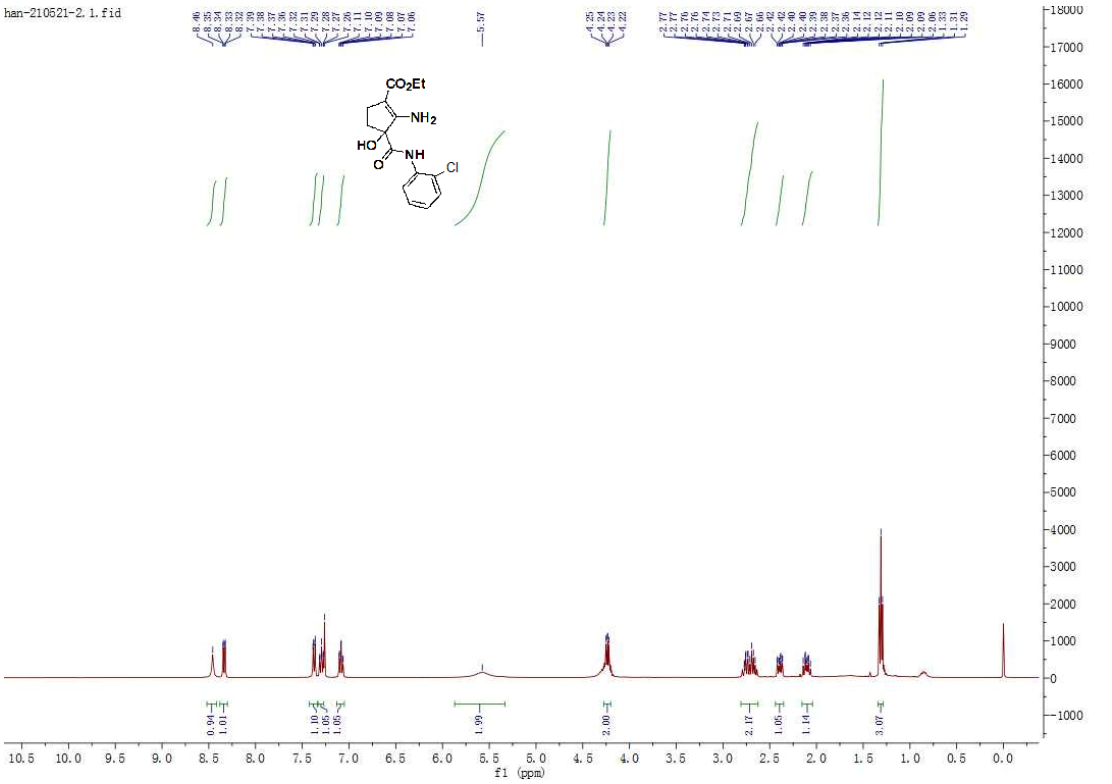


Figure 5. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3e**.



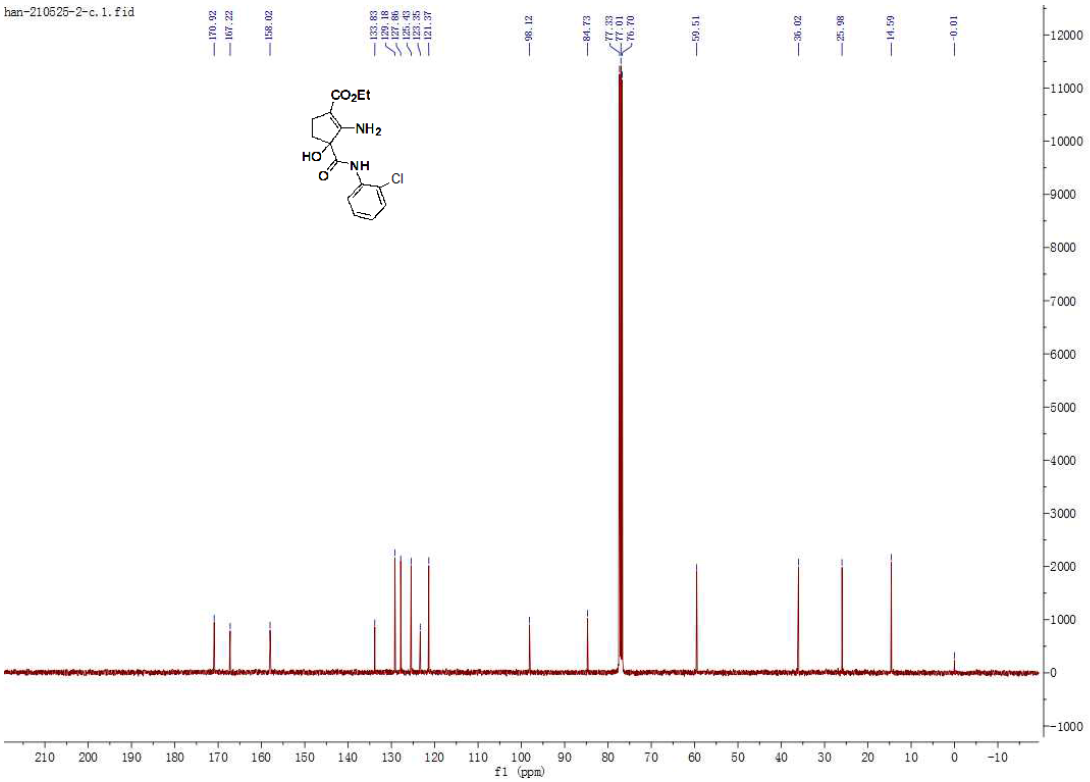
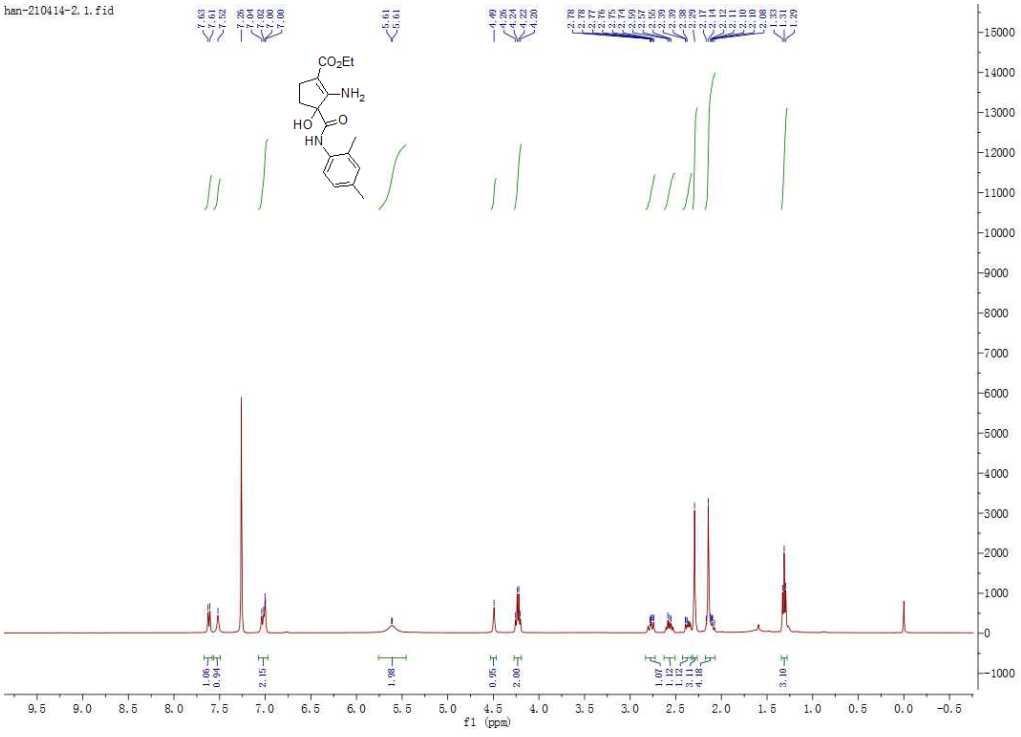


Figure 6. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3f**.



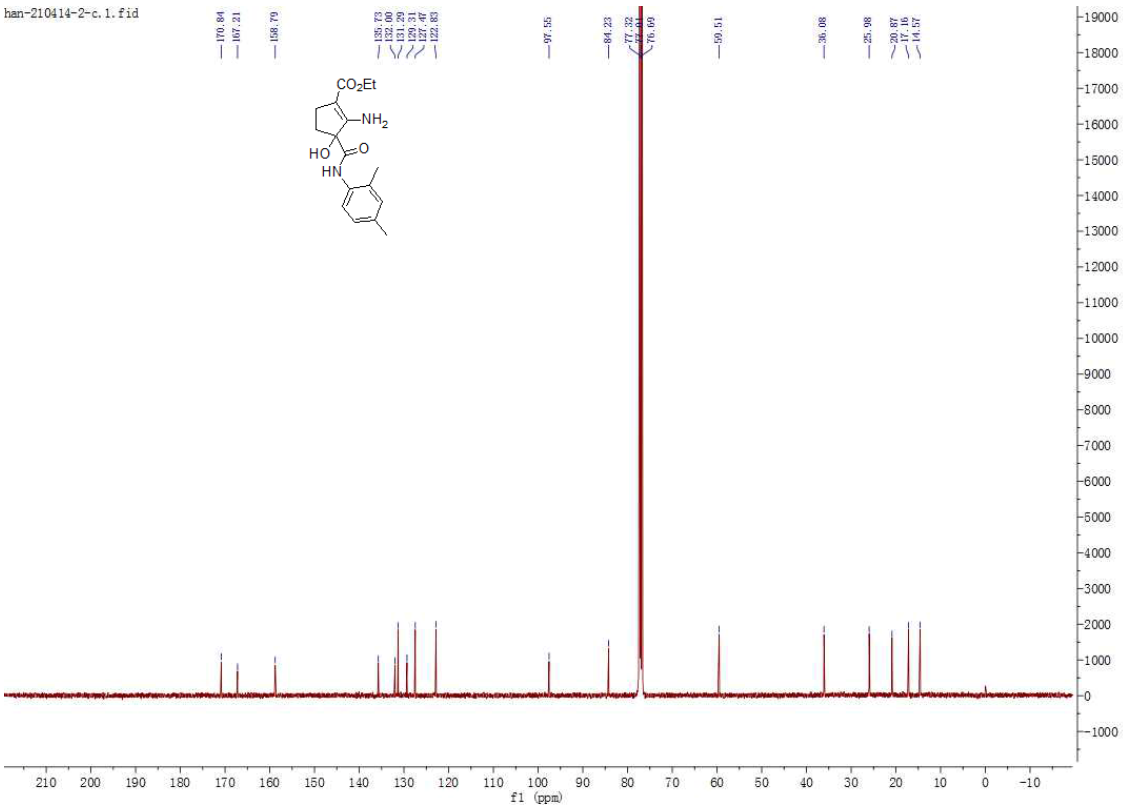
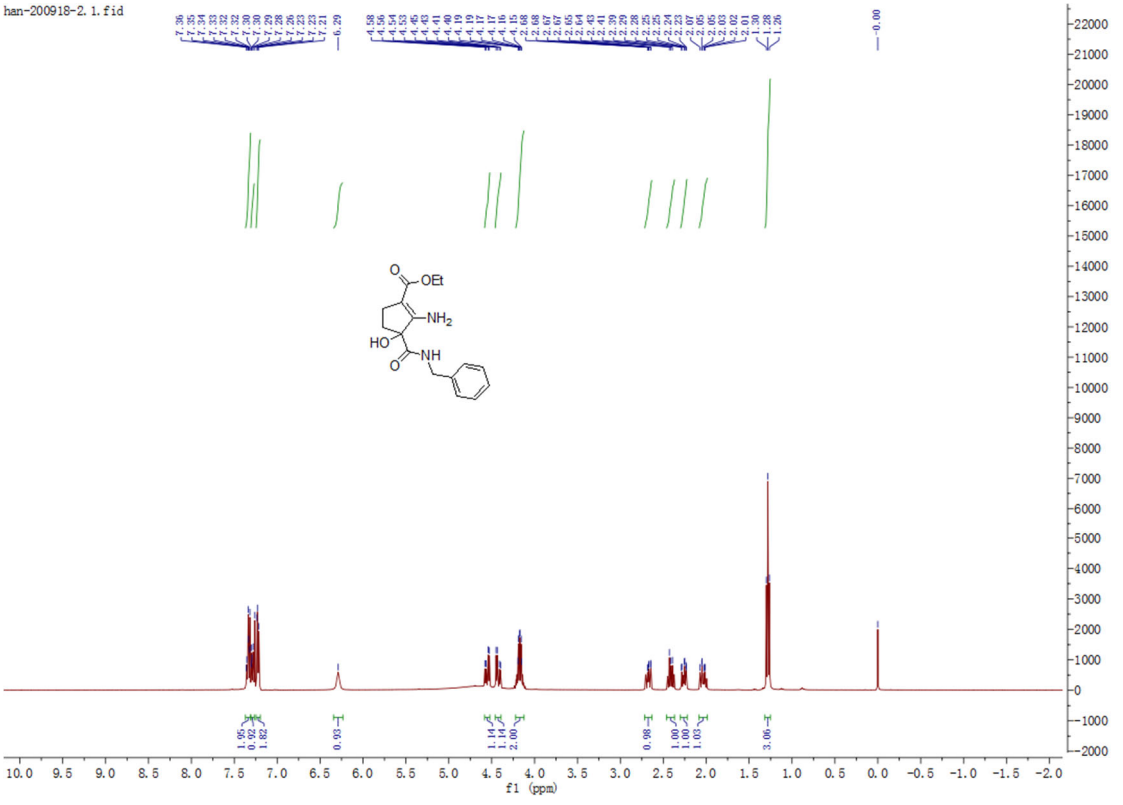


Figure 7. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3g**.



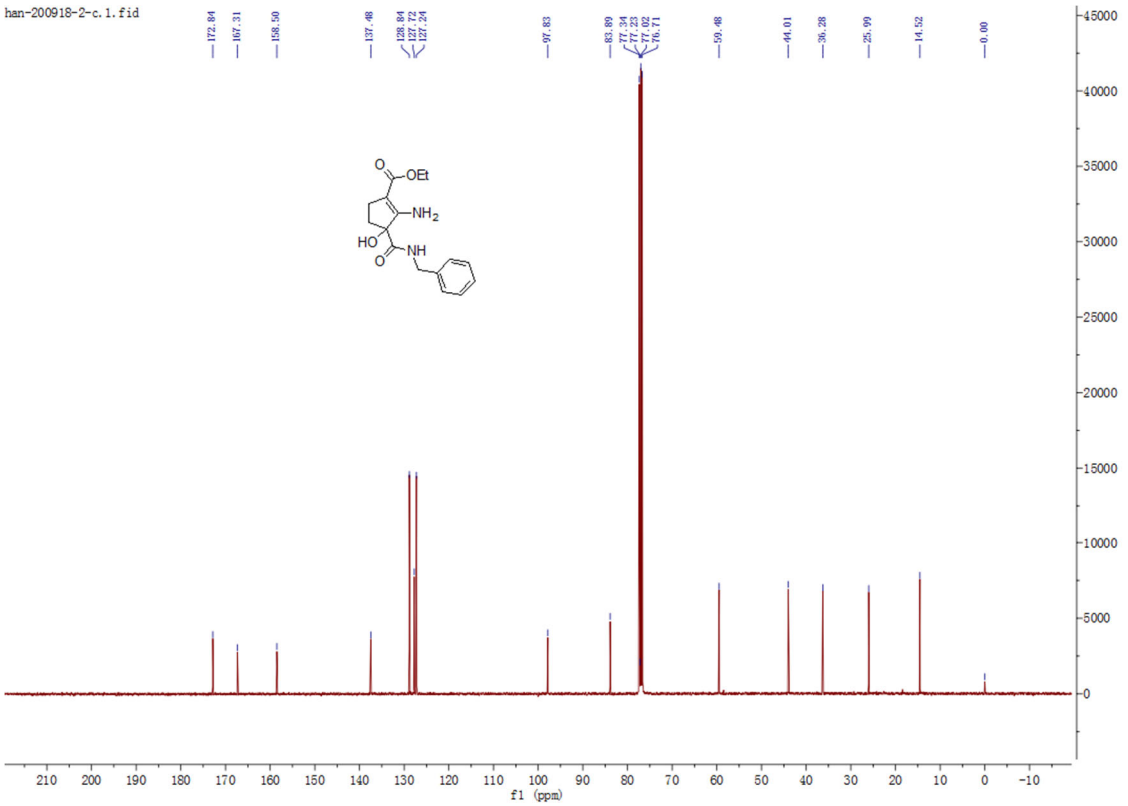
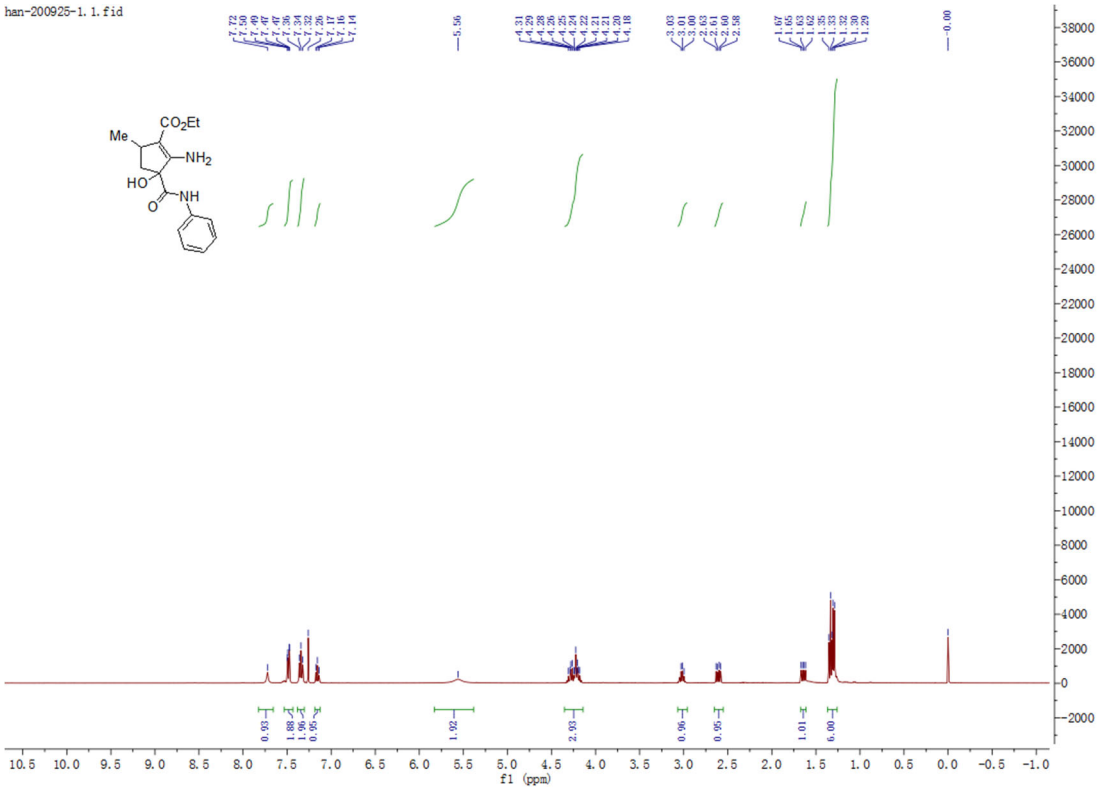


Figure 8. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3i**.



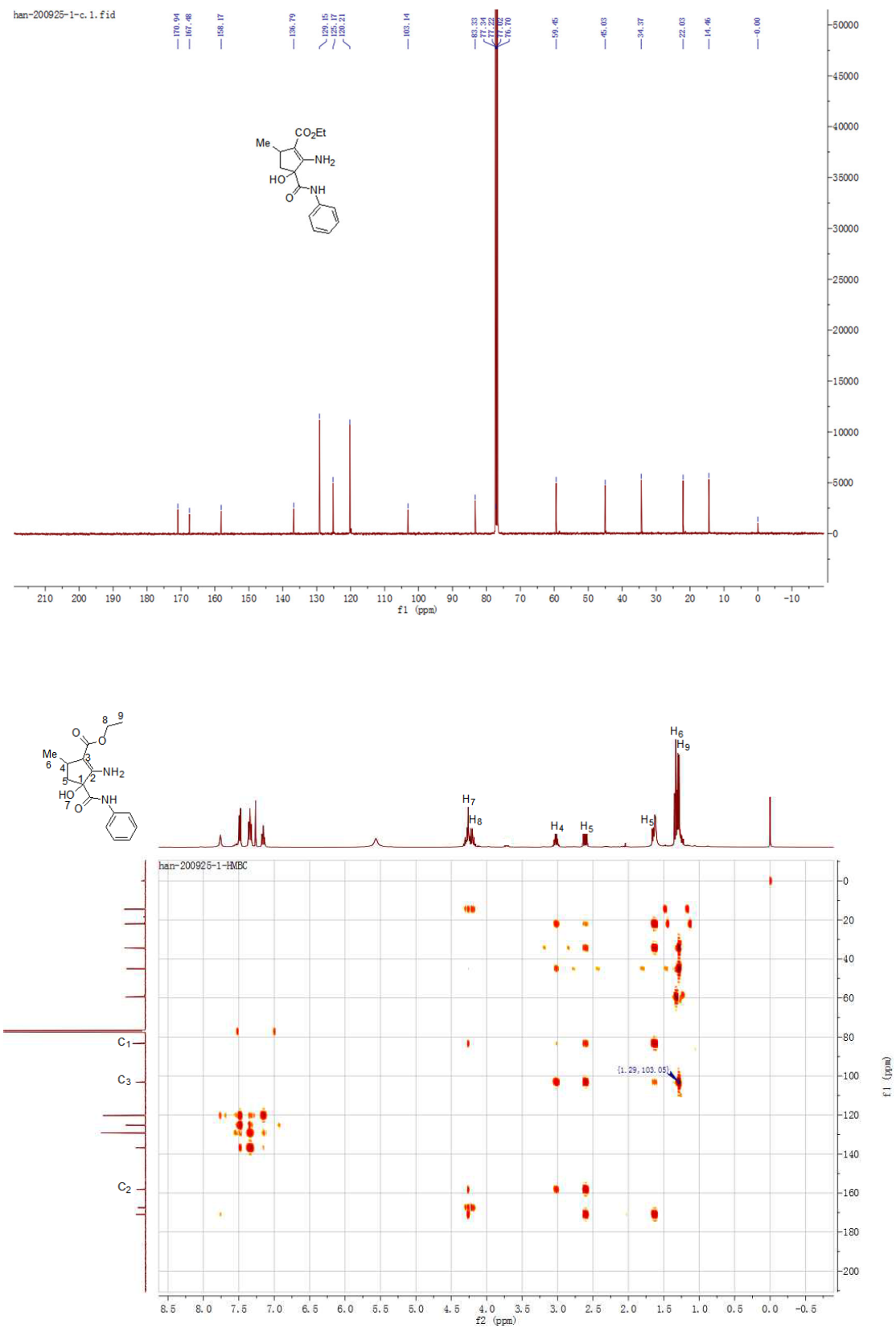


Figure 9. ^{1}H-(upper),^{13}C-NMR (middle) and HMBC (lower) spectra of **3j**.

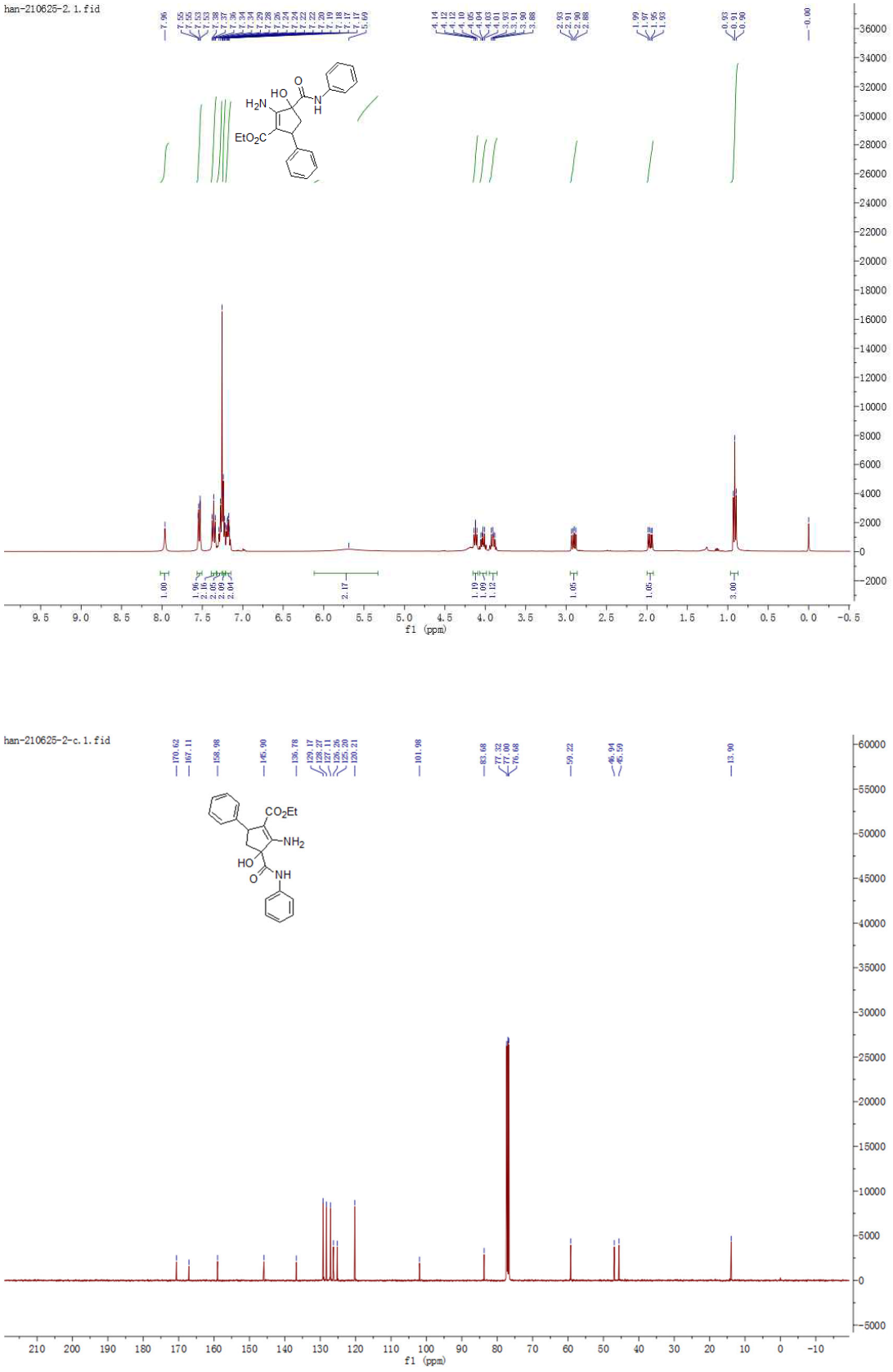


Figure 10. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3k**.

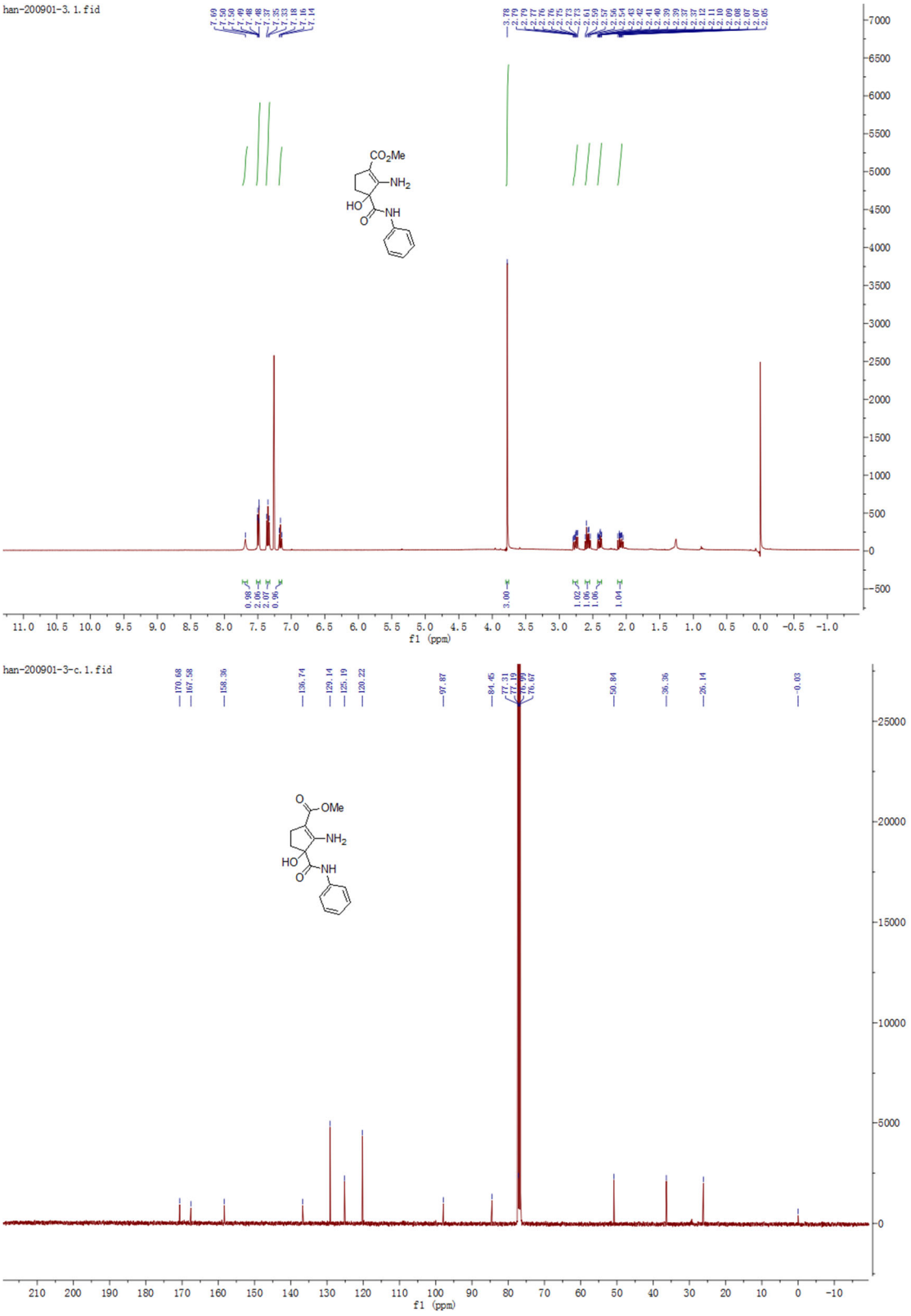


Figure 11. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3ab**.

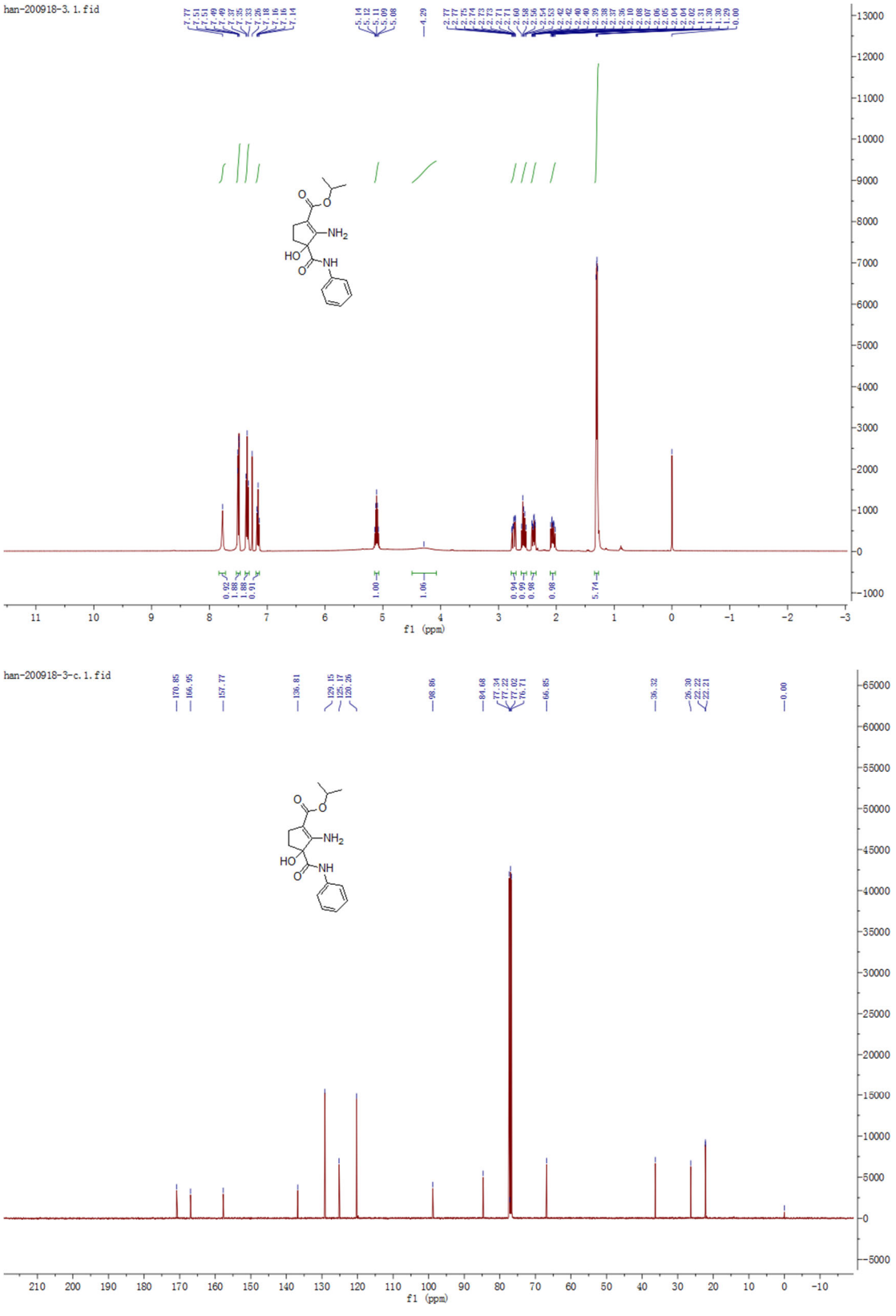


Figure 12. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3ac**.

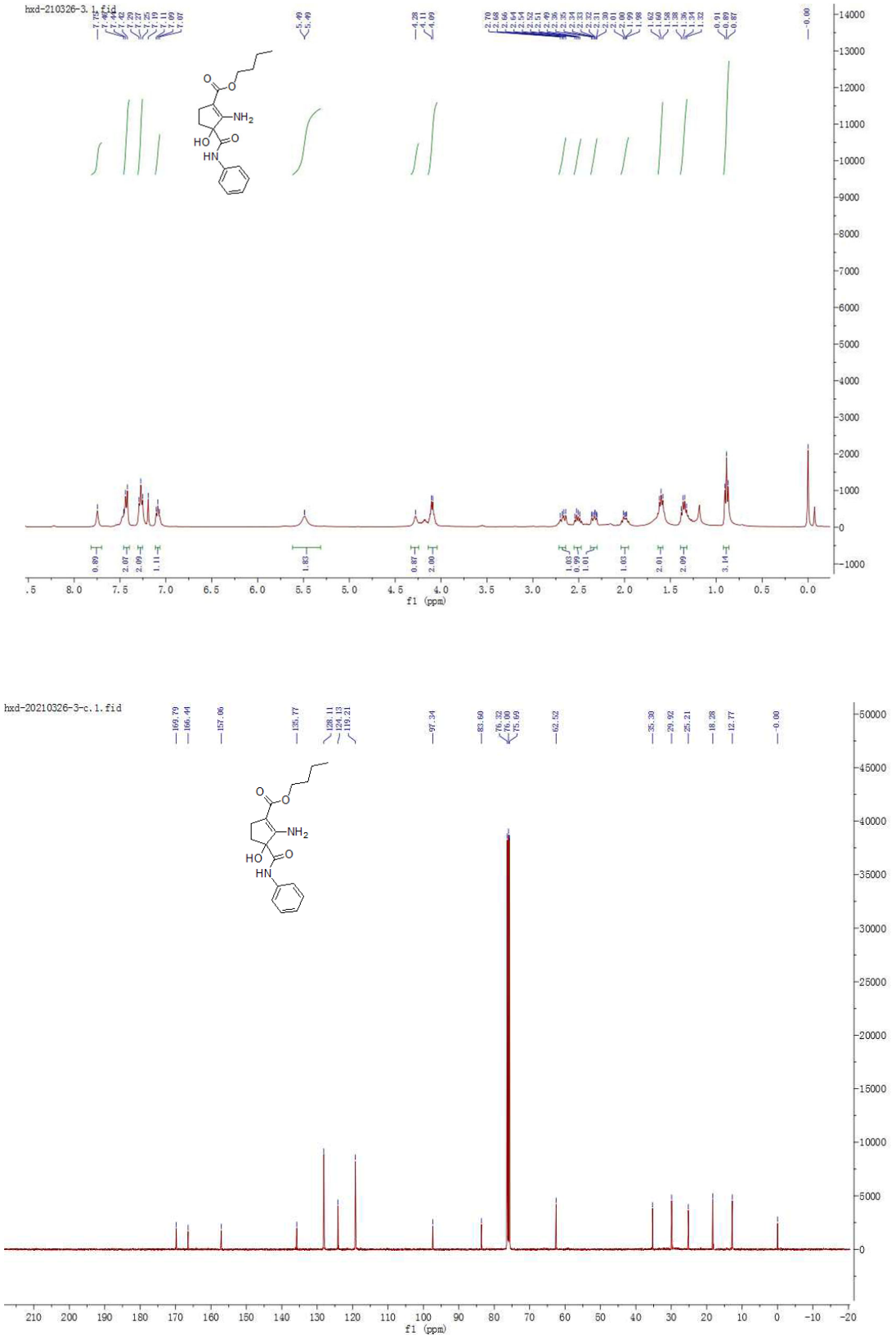


Figure 13. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3ad.**

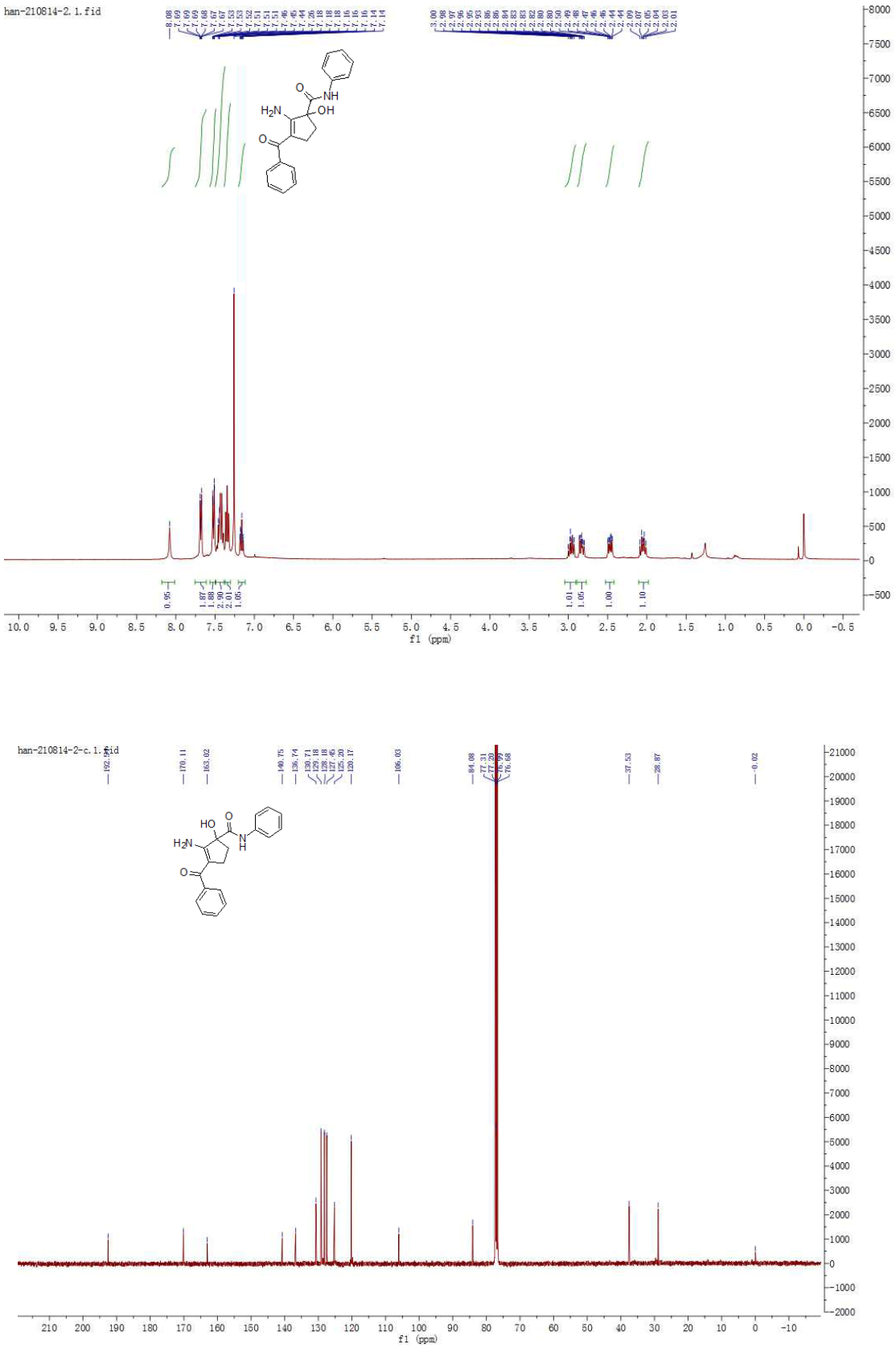


Figure 14. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3ae.**

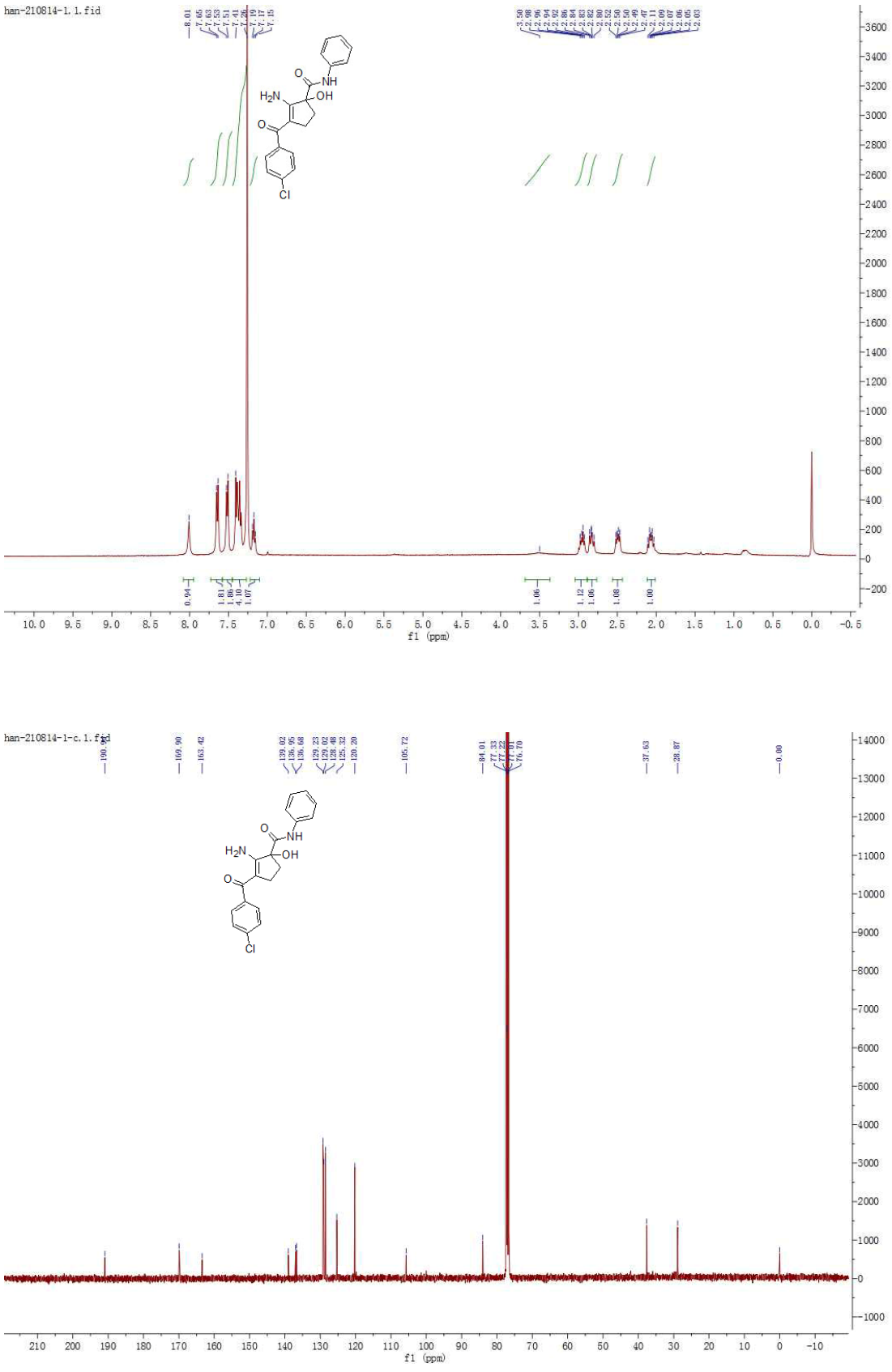


Figure 15. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3af.**

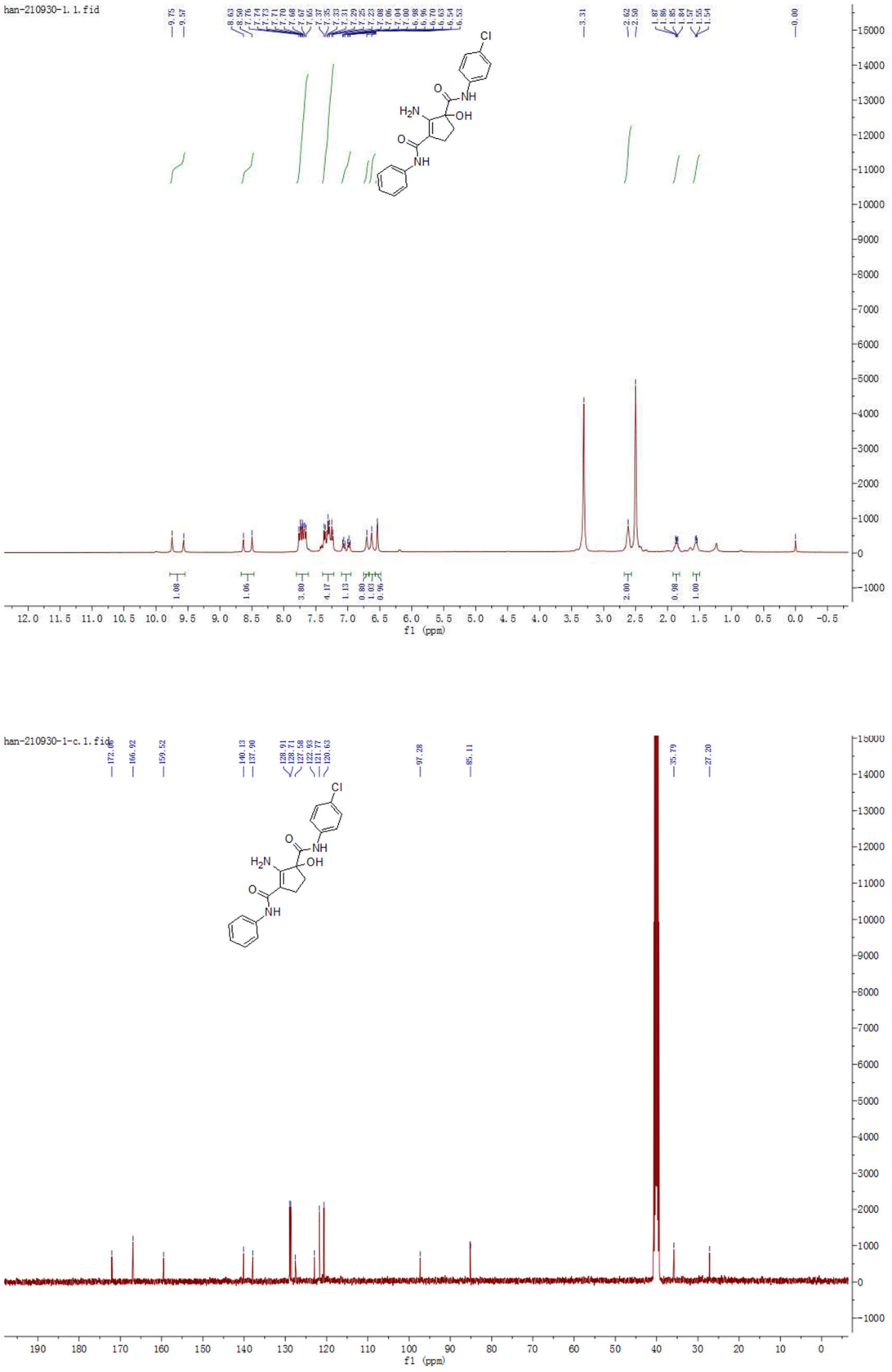


Figure 16. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3ag.**

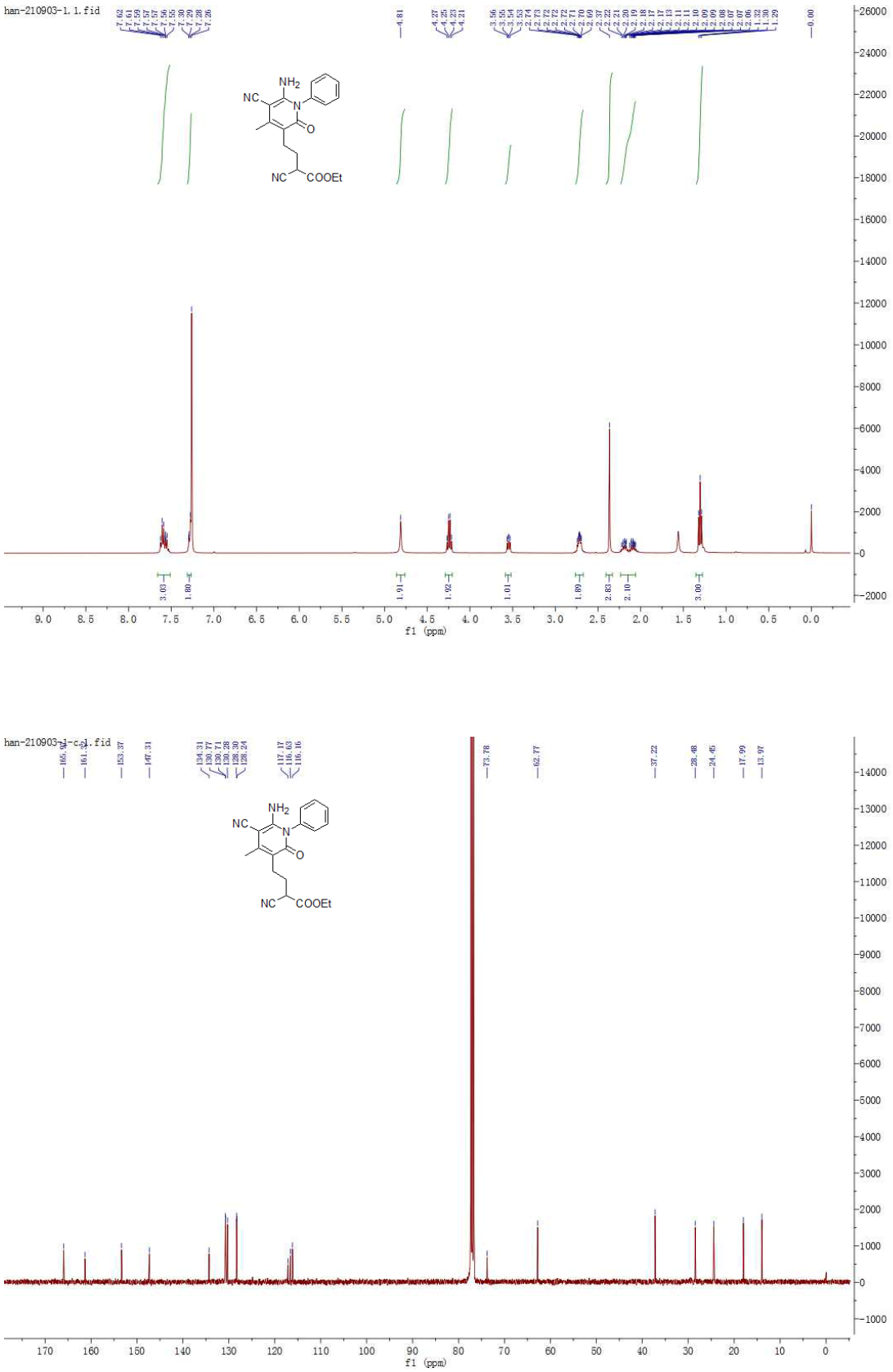


Figure 17. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3ah.**

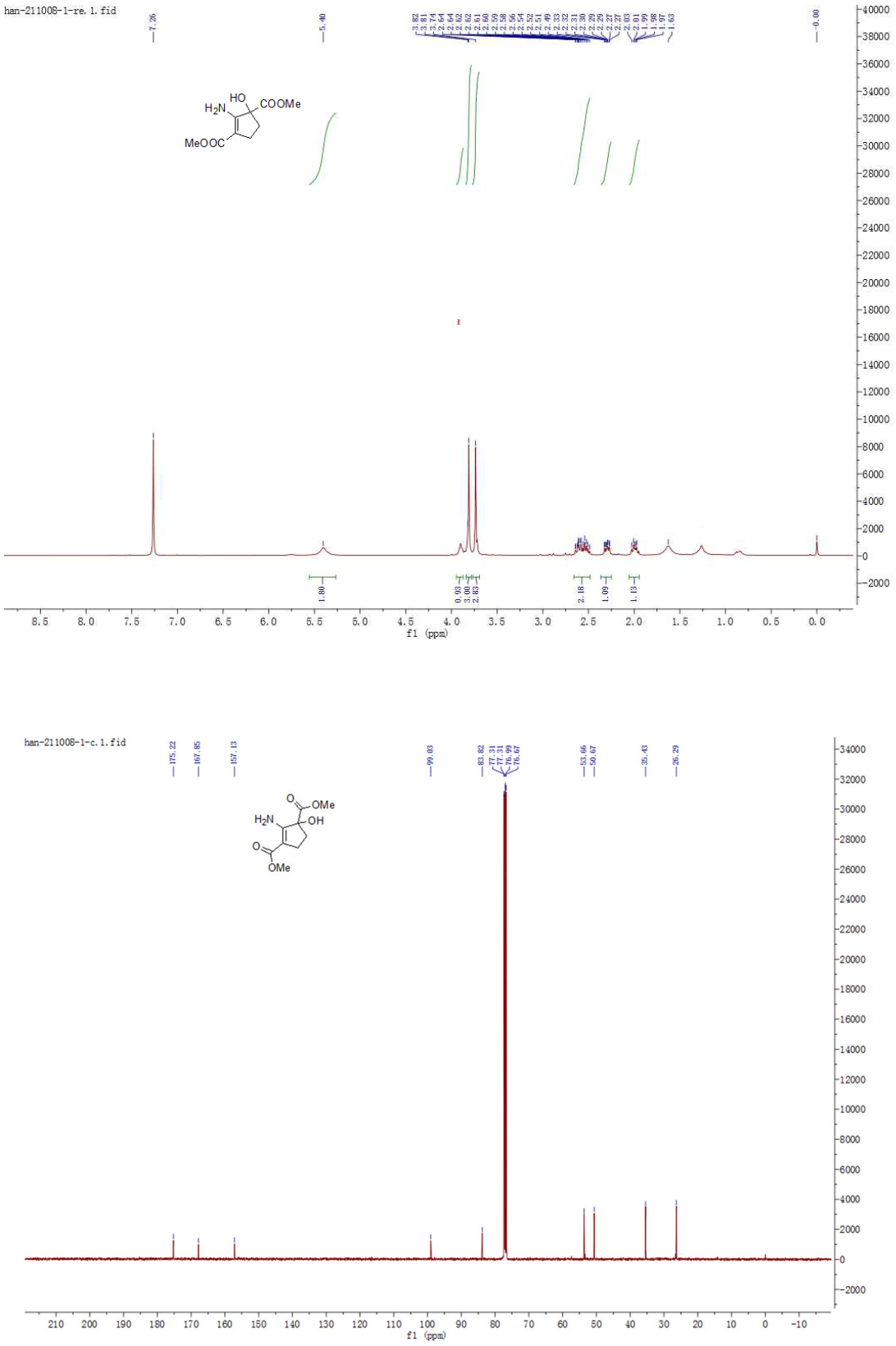


Figure 18. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3lb.**

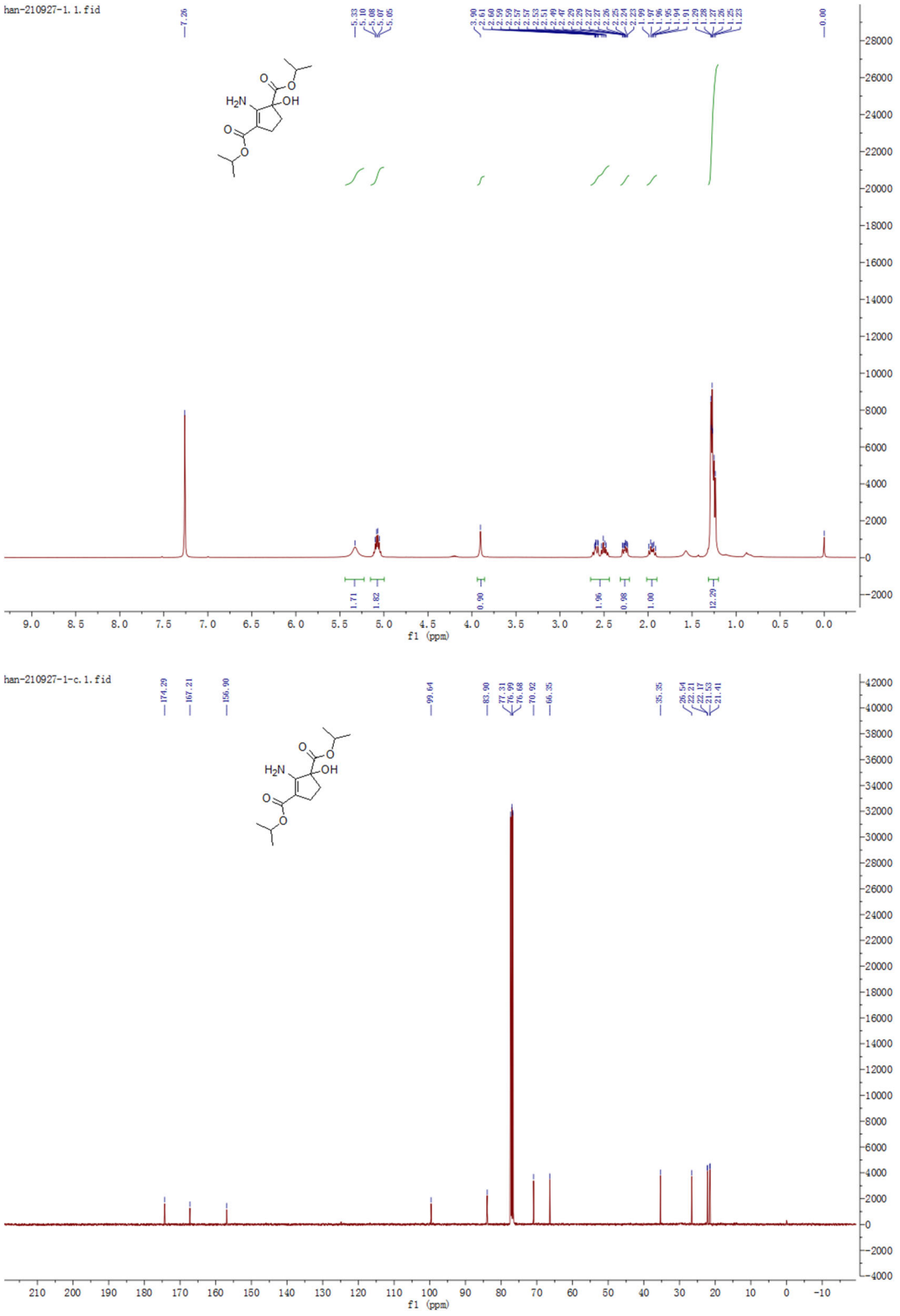
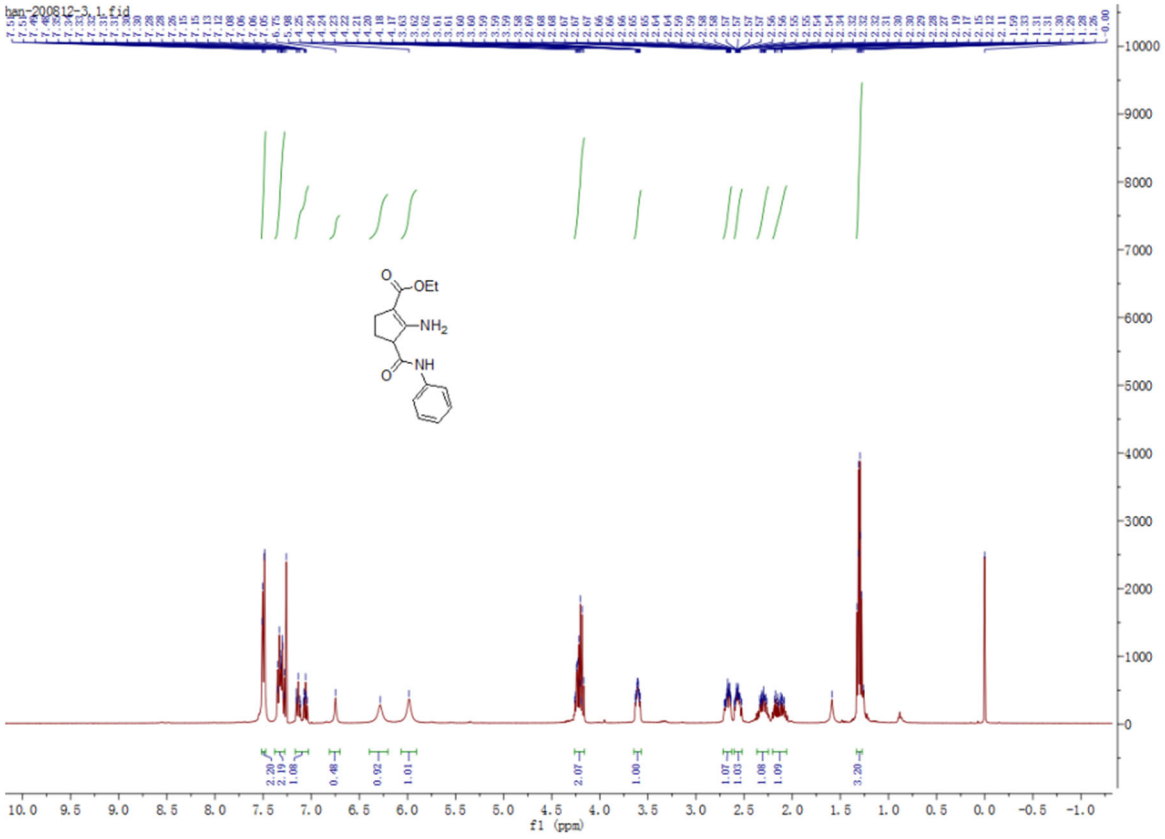


Figure 19. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **3lc.**



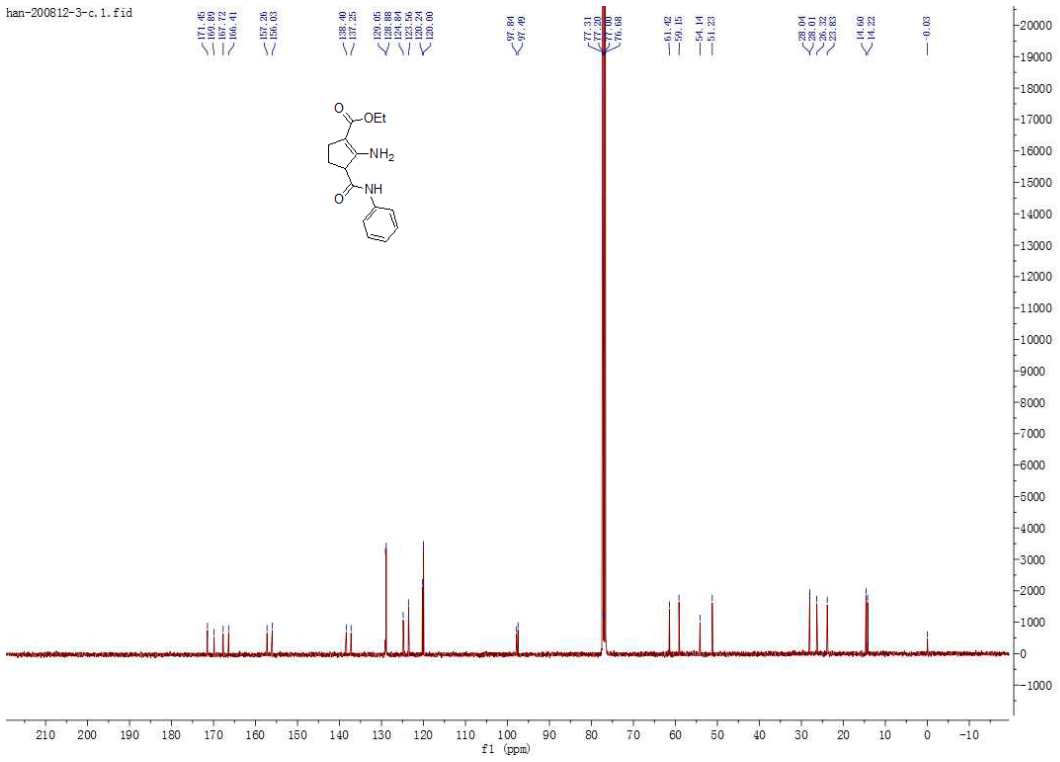


Figure 20. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **4a**.

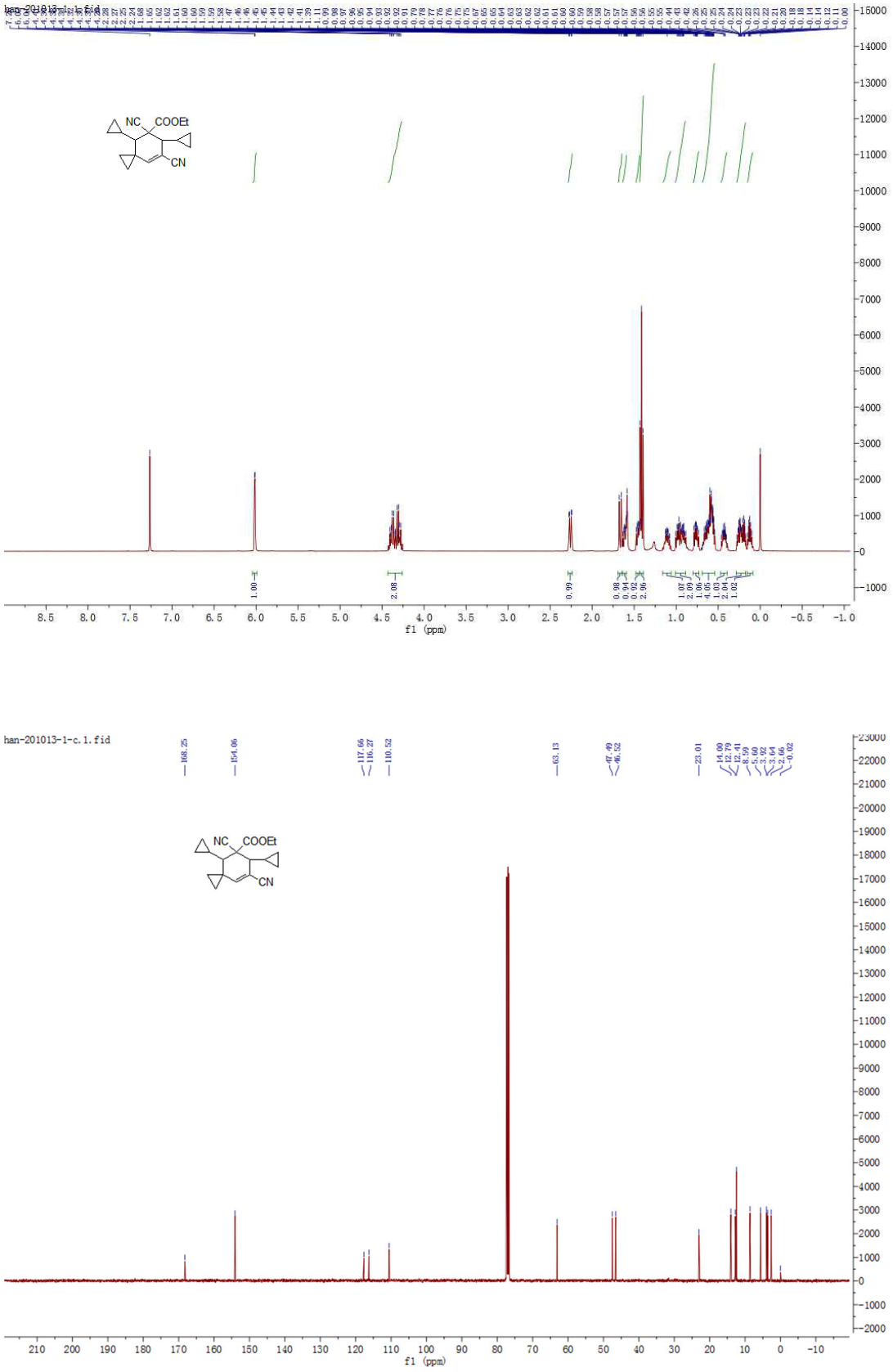


Figure 21. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **6a**.

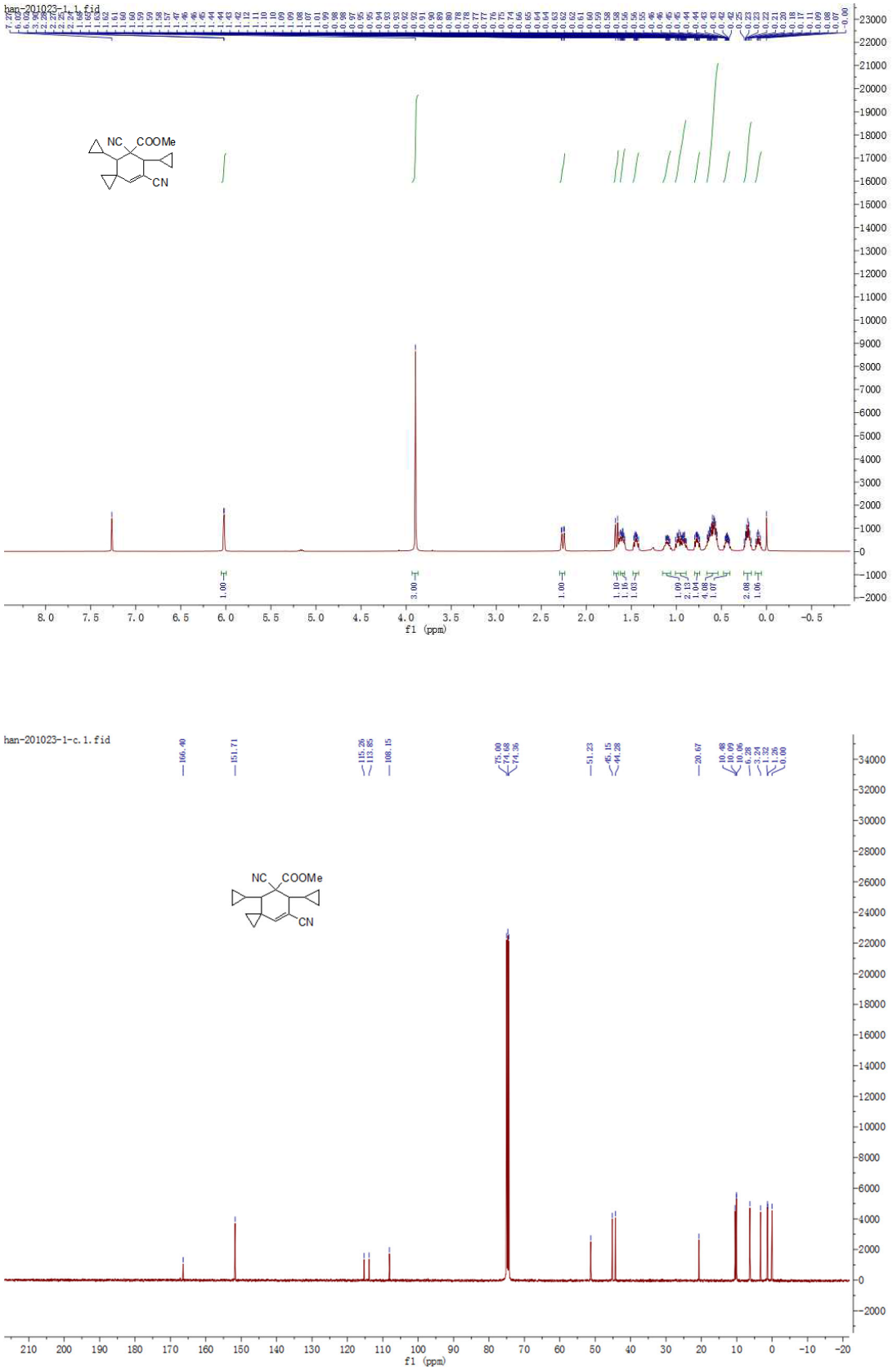


Figure 22. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **6b**.

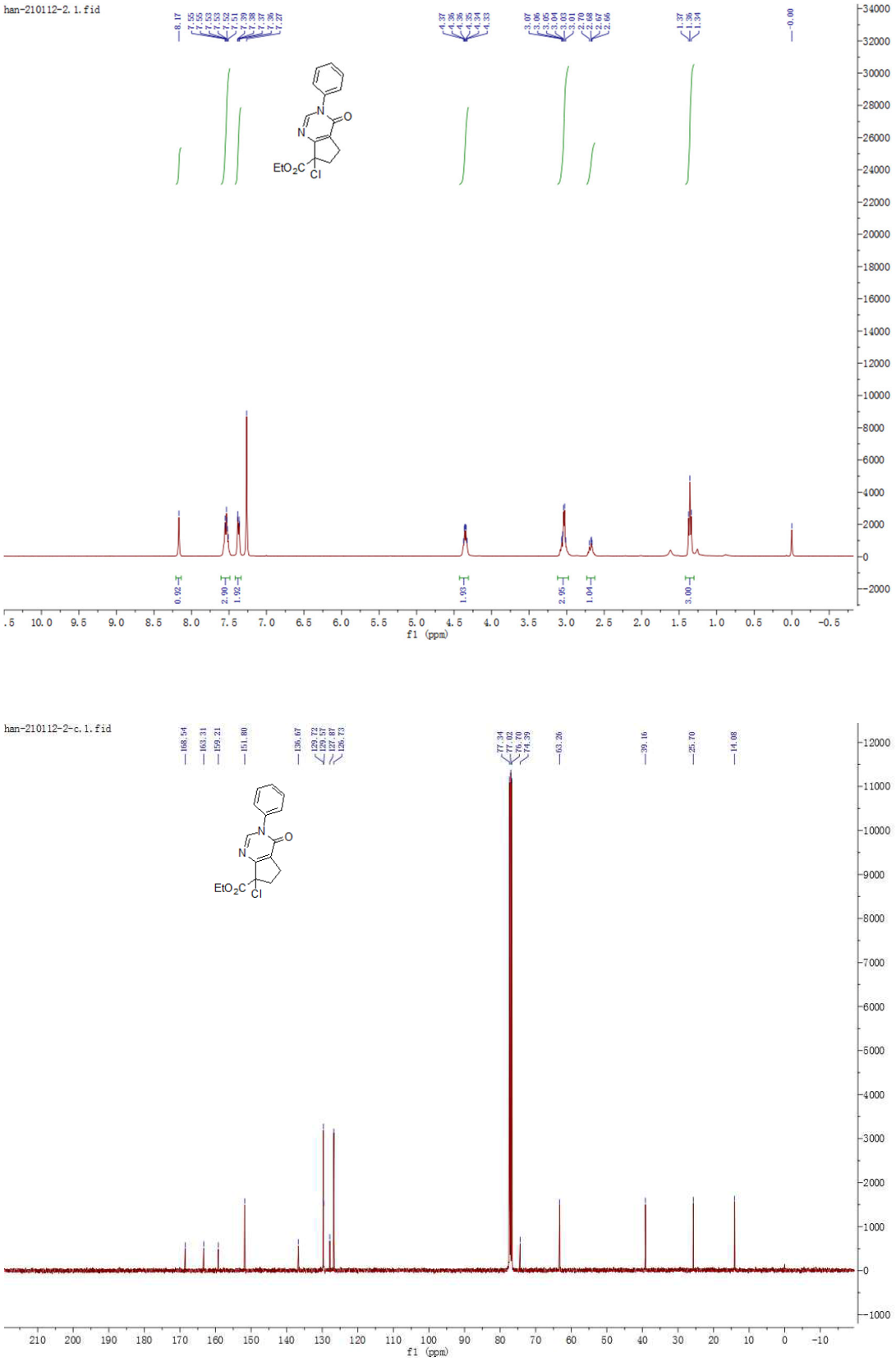


Figure 23. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **8a**.

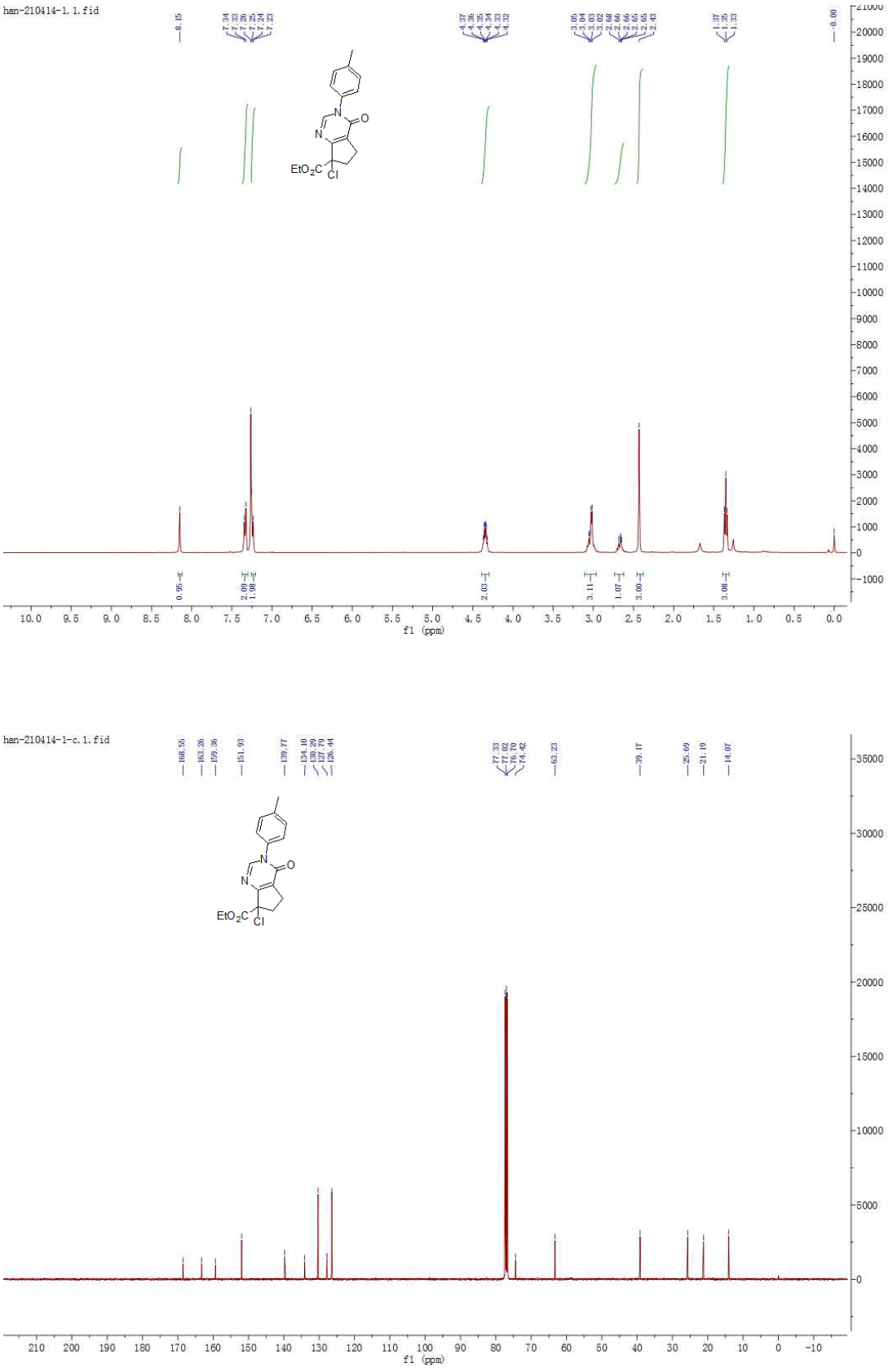


Figure 24. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **8b**.

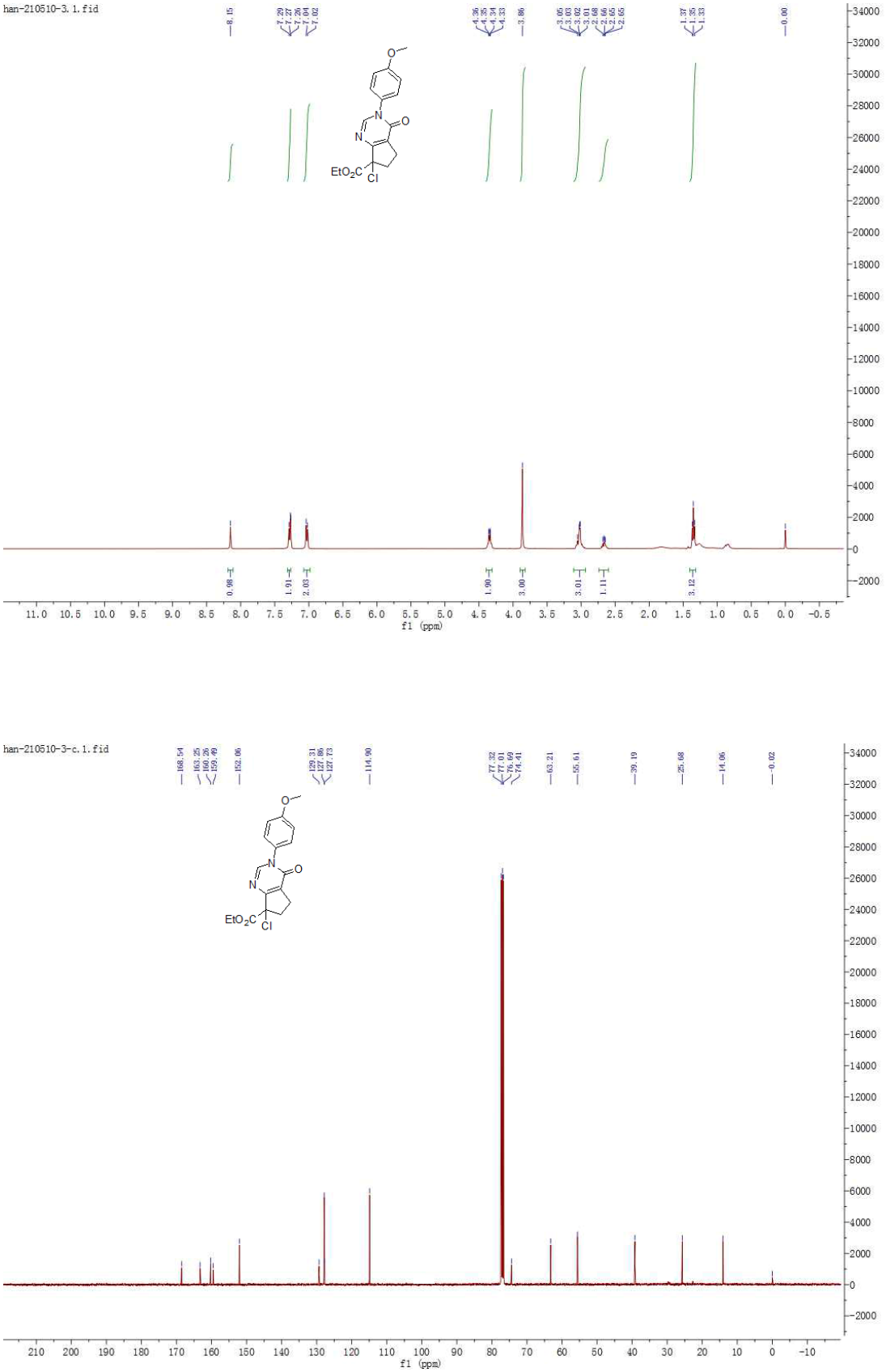


Figure 25. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **8c**.

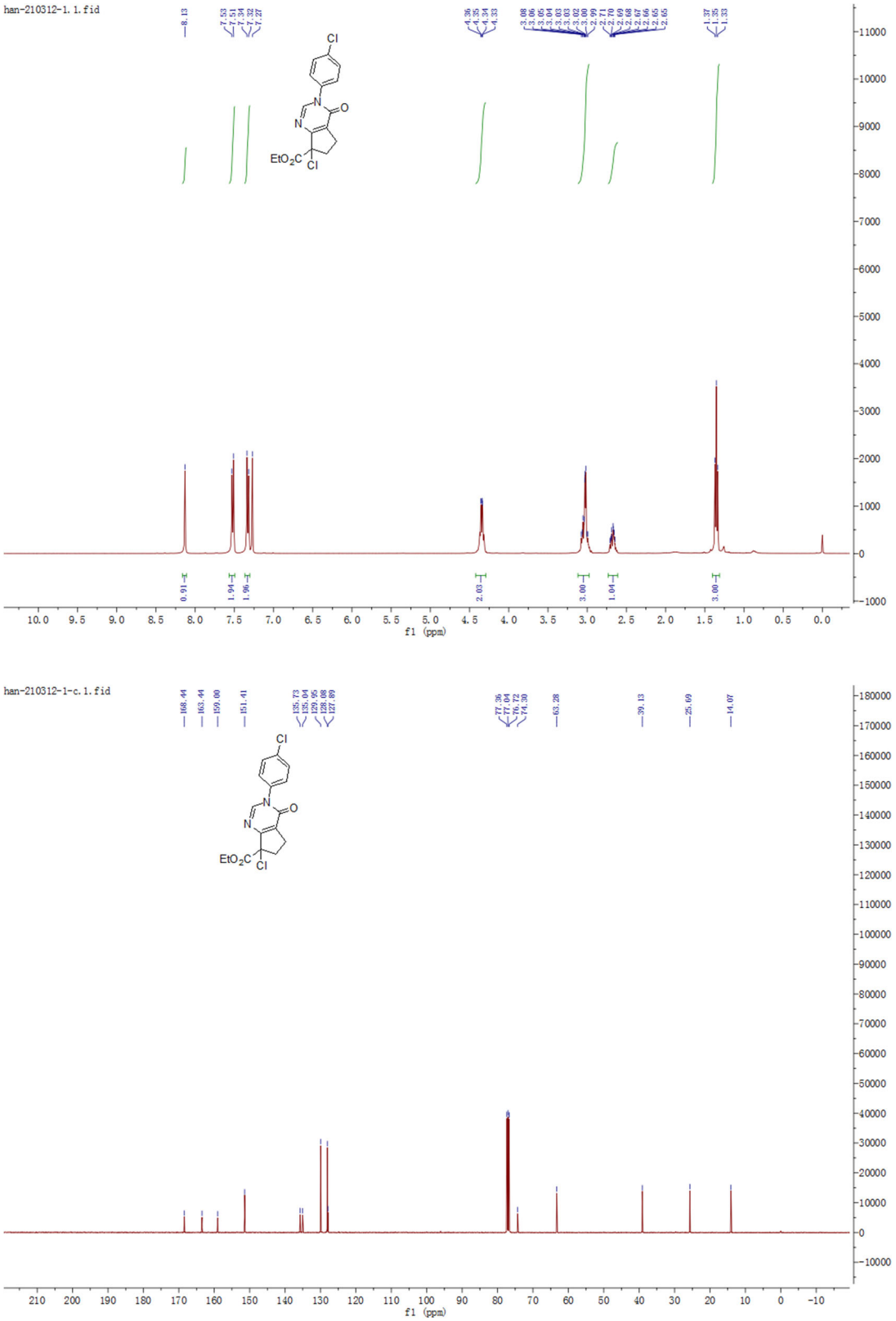


Figure 26. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **8d**.

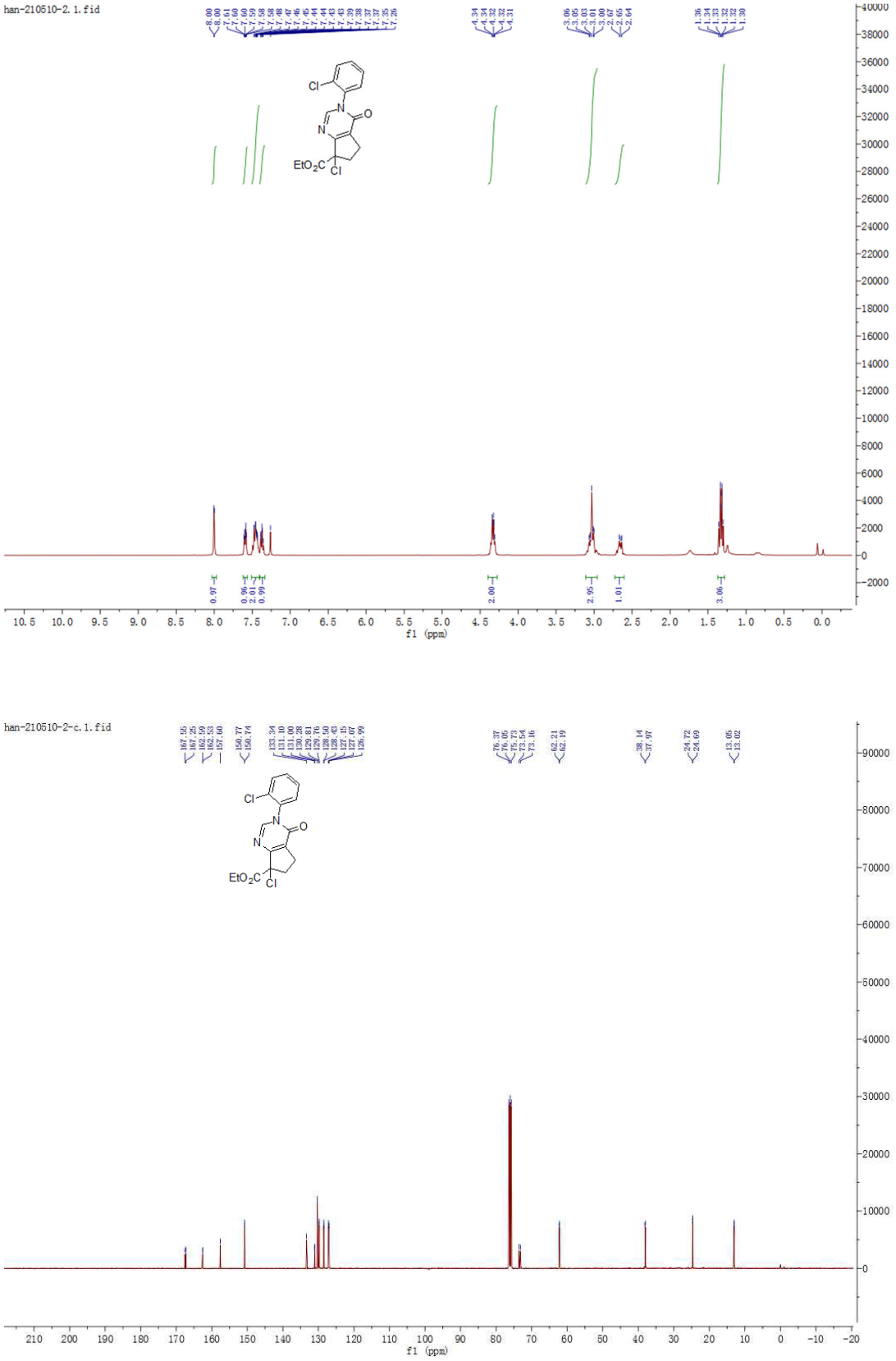


Figure 27. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **8f**.

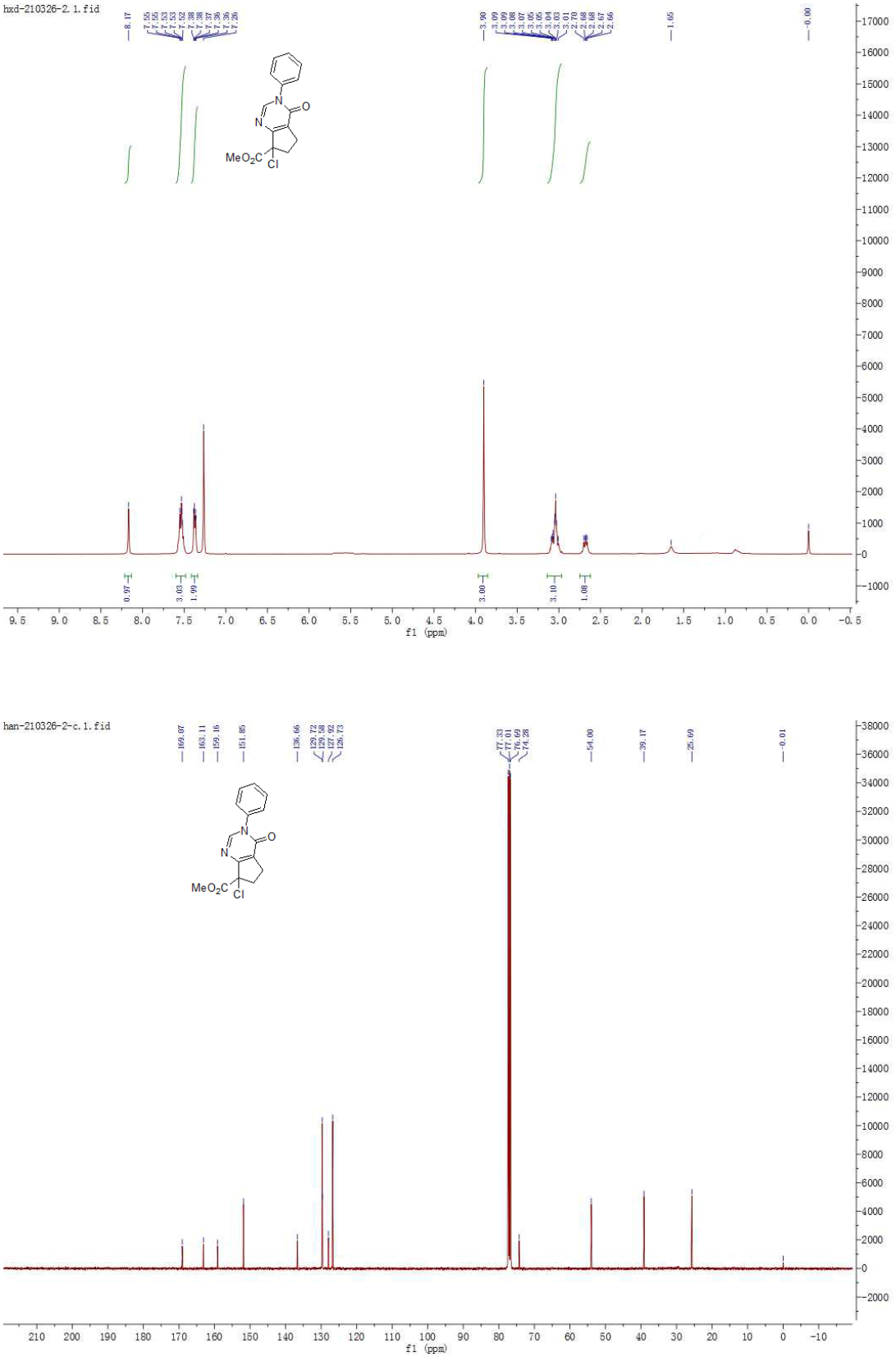


Figure 28. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **8ab**.

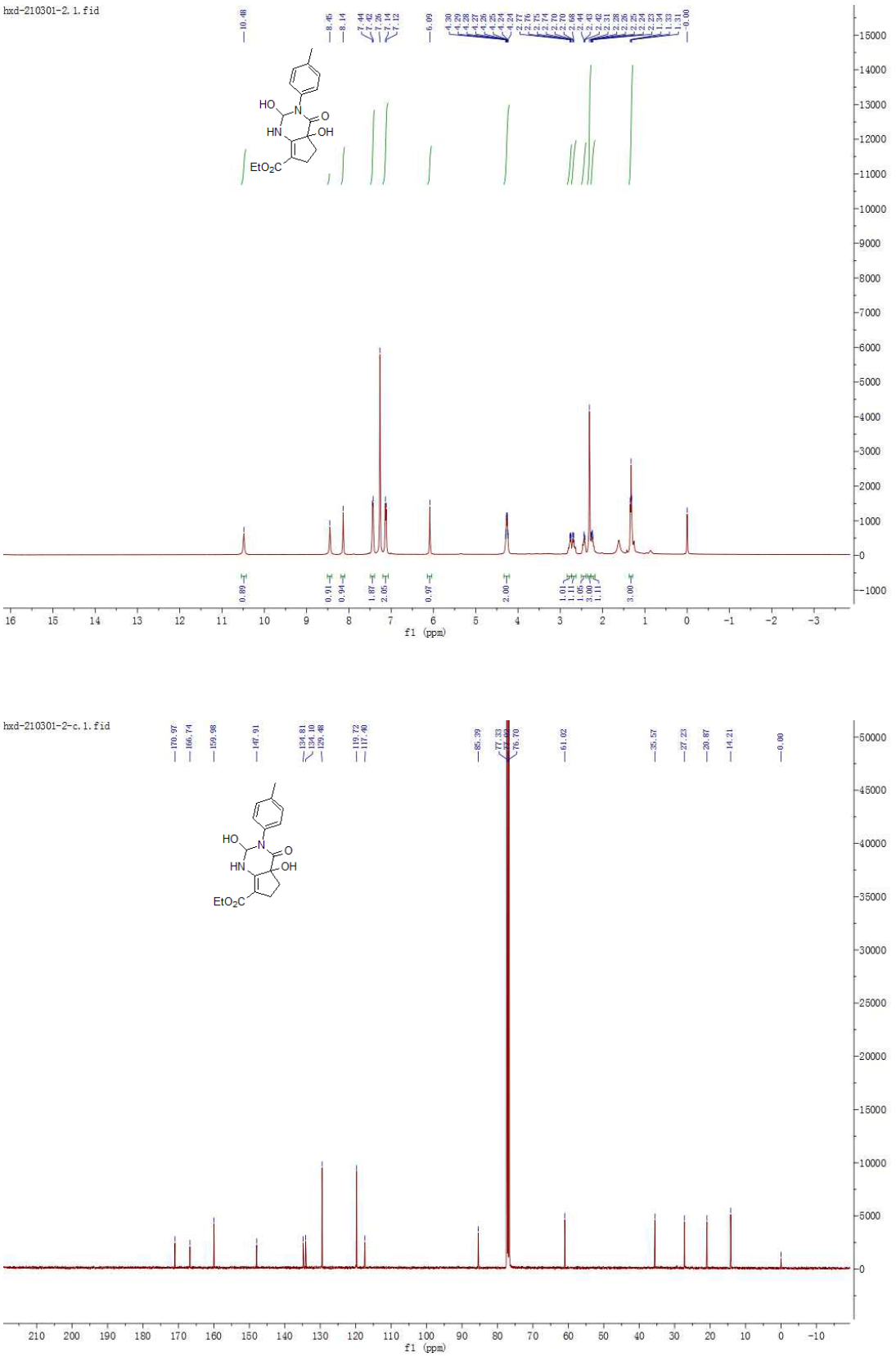


Figure 29. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **8'**.

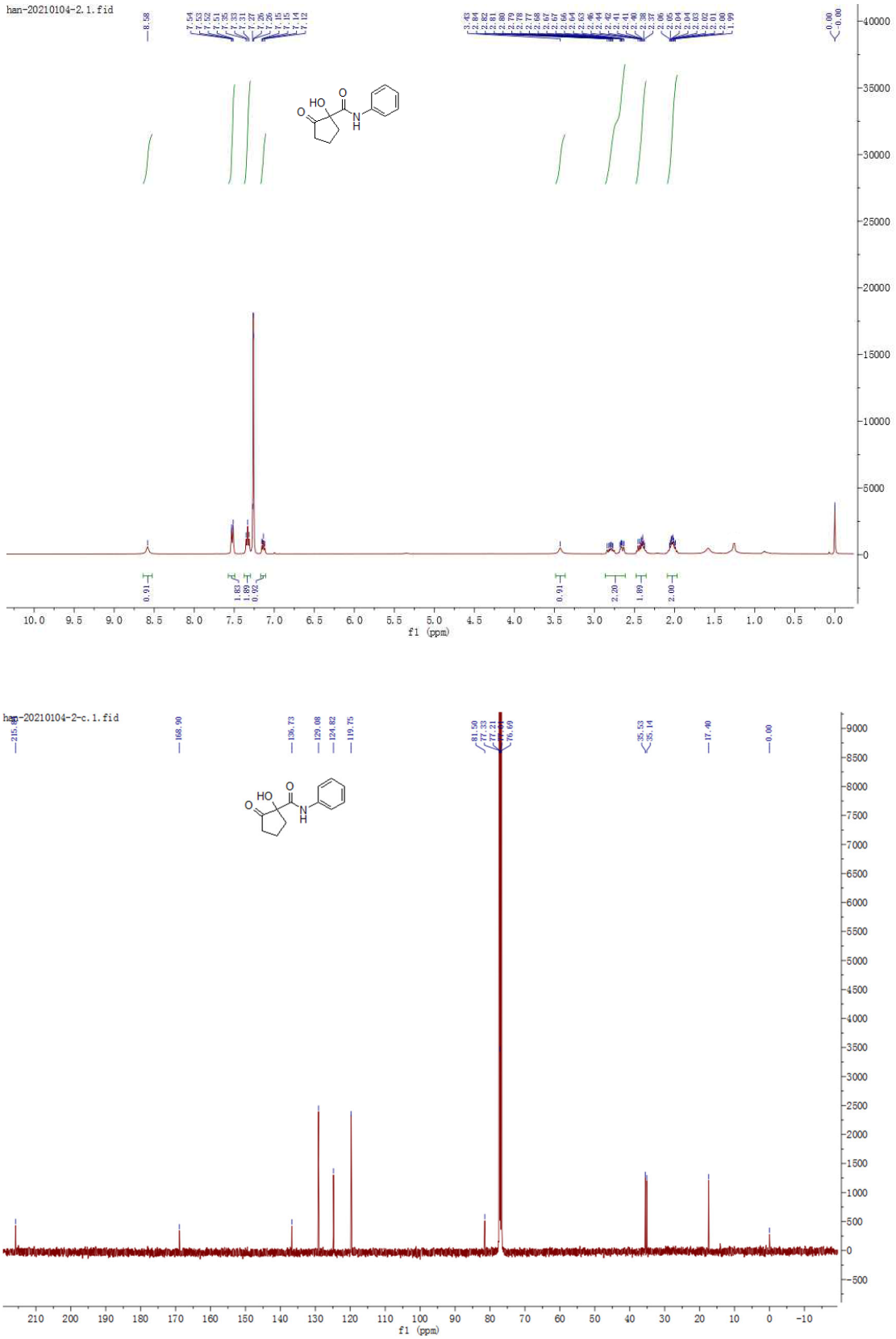


Figure 30. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **9a**.

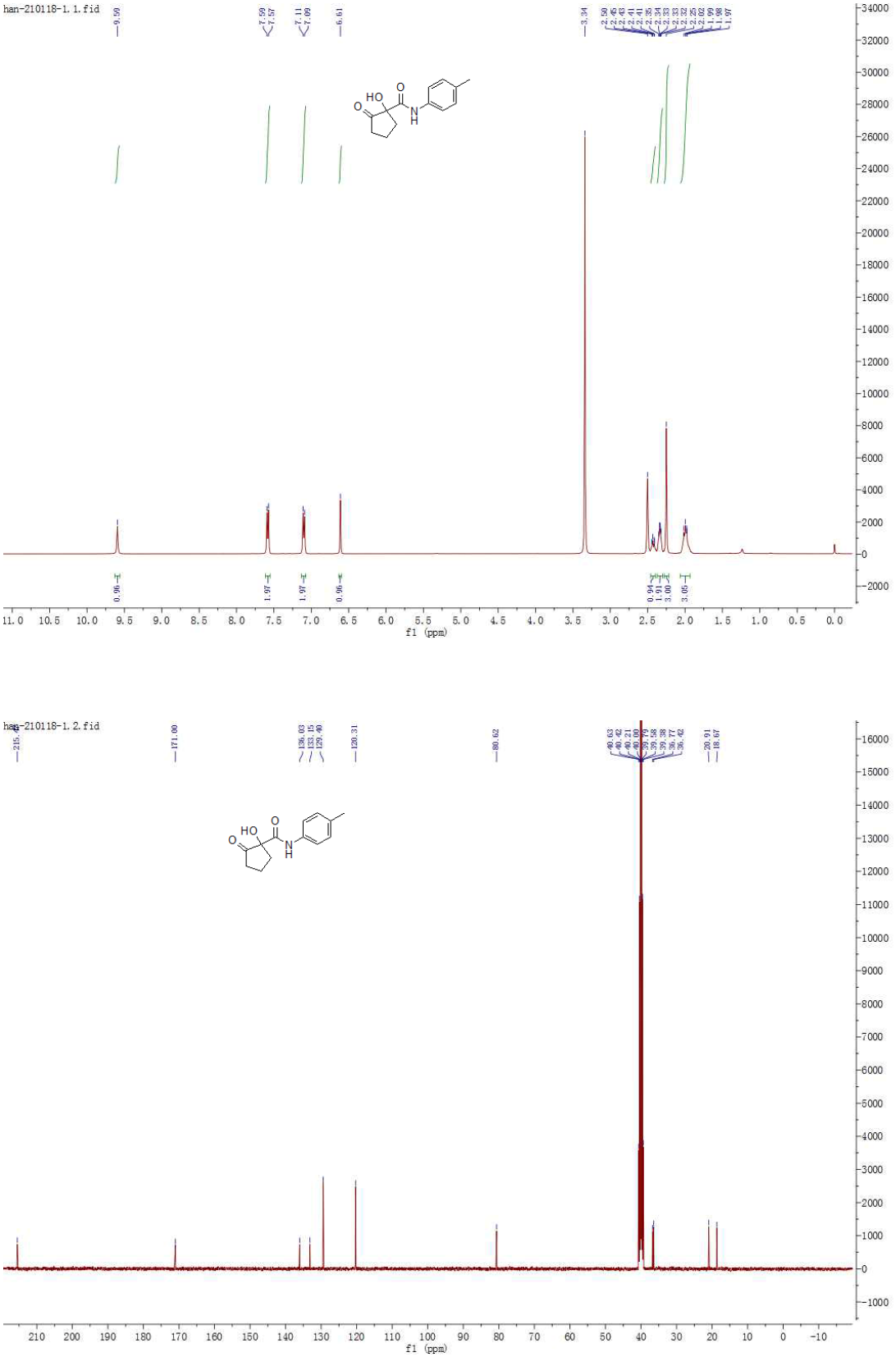


Figure 31. ^{1}H-(upper) and ^{13}C-NMR (lower) spectra of compound **9b**.