J. Braz. Chem. Soc., Vol. 22, No. 3, S1-S19, 2011.
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0103 - 5053 $6.00+0.00

Supplementary Information

Synthesis of a New Class of Triazole-Linked Benzoheterocycles via 1,3-Dipolar Cycloaddition

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*Synthesis of terminal alkynes (**1a**-**e**)*

1 mmol of benzoheterocyclic and 1 mmol of K_2CO_3 were suspended in anhydrous DMF (5 mL). Then, 1.5 equiv. of propargyl bromide (80% solution in toluene) was added. The reaction mixture was stirred for 20 h at room temperature. The mixture was then extracted with dichloromethane/water. The combined organic layers were dried over sodium sulfate anhydrous and concentrated under reduced pressure, and the residue was purified by chromatography on silica gel (hexane:EtOAc, 7:3) to afford the corresponding propargylic benzoheterocycles (**1a**-**e**).

*Synthesis of N-3-(azidopropyl)phthalimide (**2a**) or N-4-(azidobutyl)phthalimide (**2b**)*

N-(bromoalkyl)phthalimide (500 mg) in 2.5 mL of DMF was charged in a round-bottom flask. Then, 1.5 equiv. of sodium azide was introduced and the reaction mixture was allowed to stir at 60 °C for 24 h under argon atmosphere. The mixture was then cooled to room temperature and extraction with dichloromethane was done. The combined organic layers were dried over sodium sulfate anhydrous and concentrated under reduced pressure.

*N-3-(azidopropyl)phthalimide (**2a**)*

Yield 75%; white solid; IR ν_{max}/cm^{-1}: 2945, 2100 (N_3), 1711 (C=O), 1399, 1040, 723. ^{1}H NMR (300 MHz, CDCl3): δ 1.96 (q, 2H), 3.38 (t, 2H, *J* 6.9 Hz), 3.79 (t, 2H, *J* 6.9 Hz), 7.73 (dd, 2H, *J* 5.7 and 3.0 Hz), 7.86 (dd, 2H, *J* 5.7 and 3.0 Hz).

*N-4-(azidobutyl)phthalimide (**2b**)*

Yield 61%; white solid; IR ν_{max}/cm^{-1}: 2950, 2096 (N_3), 1709 (C=O), 1396, 719. ^{1}H NMR (300 MHz, CDCl3): δ 1.65 (m, 2H), 1.78 (m, 2H), 3.33 (t, 2H, *J* 6.6 Hz), 3.79 (t, 2H, *J* 6.9 Hz), 7.72 (dd, 2H, *J* 5.7 and 3.0 Hz), 7.85 (dd, 2H, *J* 5.7 and 3.0 Hz).

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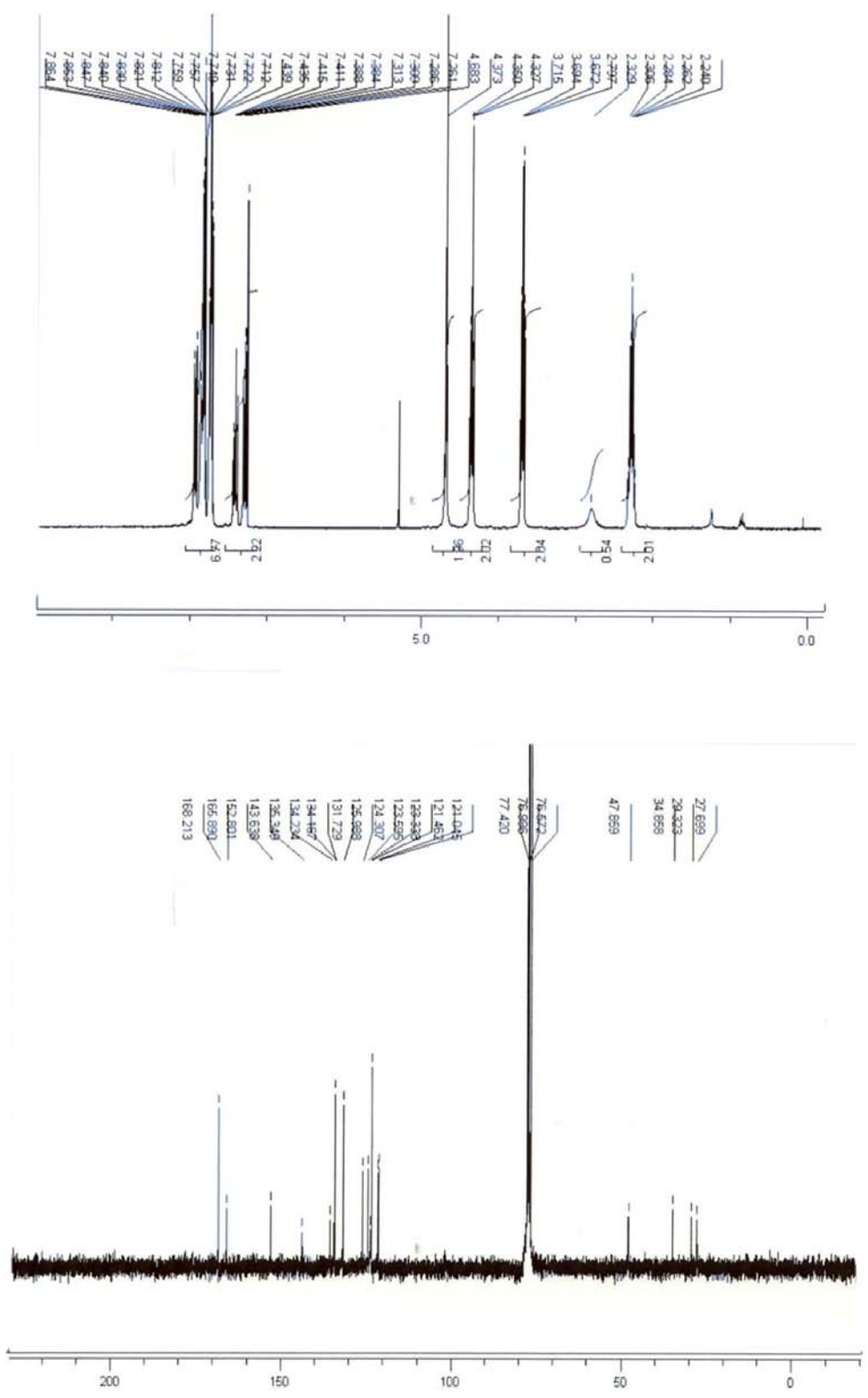

Figure S1. ^{1}H (300 MHz) and ^{13}C (75.5 MHz) NMR spectrum of compound **3a** in $CDCl_3$.

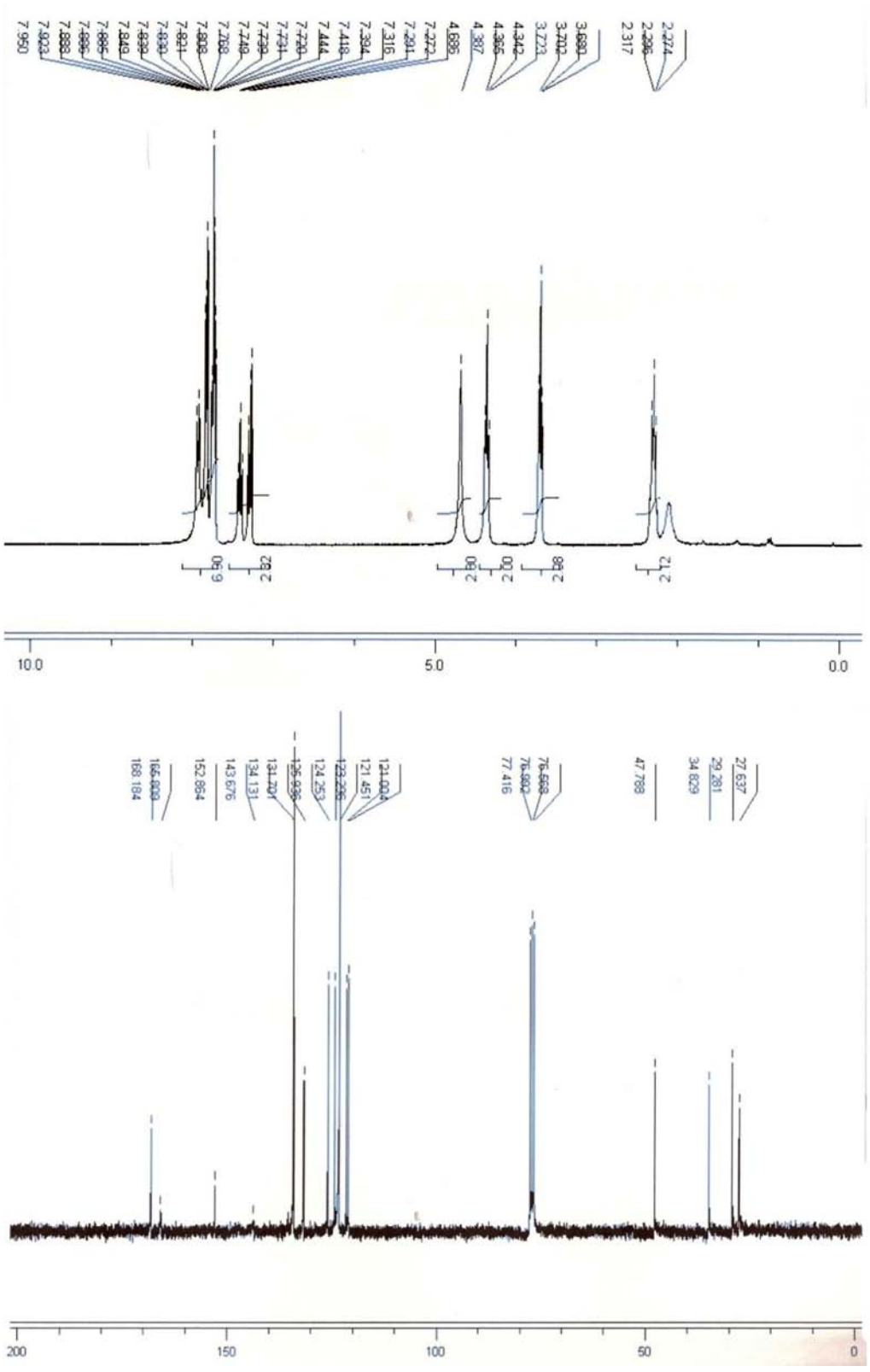

Figure S2. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectrum of compound **3b** in $CDCl_3$.

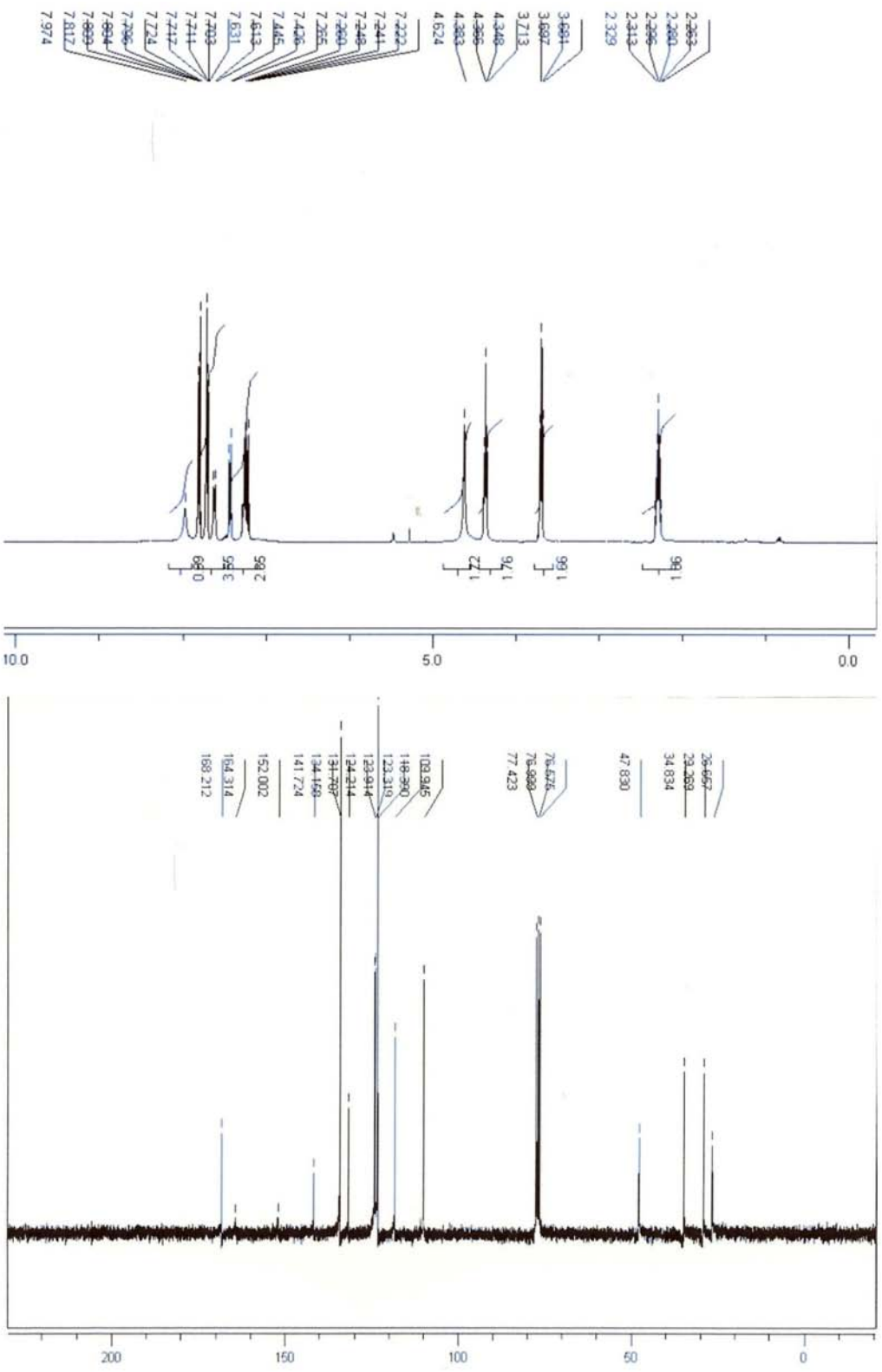

Figure S3. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectrum of compound **3c** in $CDCl_3$.

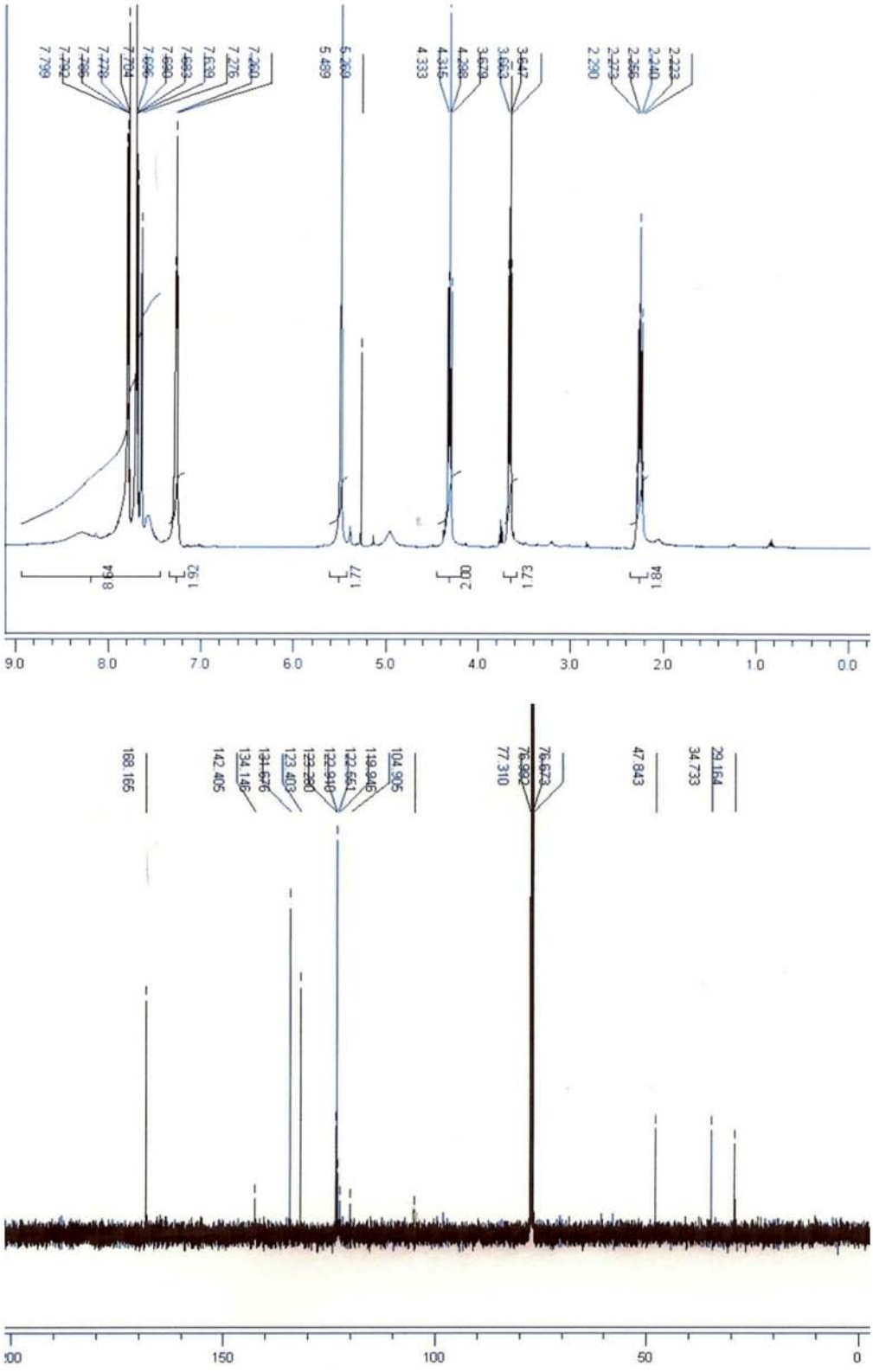

Figure S4. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectrum of compound **3d** in $CDCl_3$.

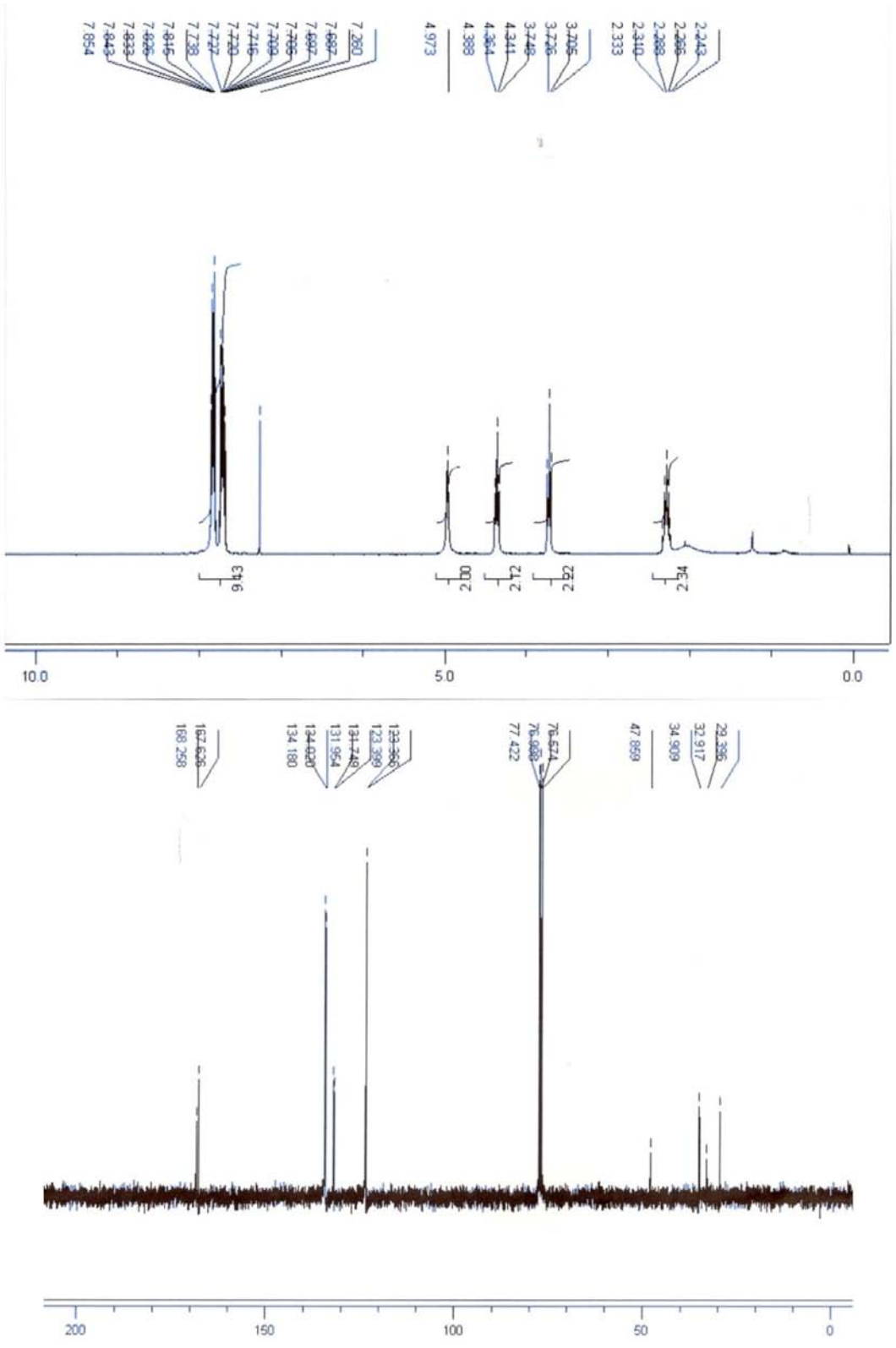

Figure S5. ^{1}H (300 MHz) and ^{13}C (75.5 MHz) NMR spectrum of compound **3e** in $CDCl_3$.

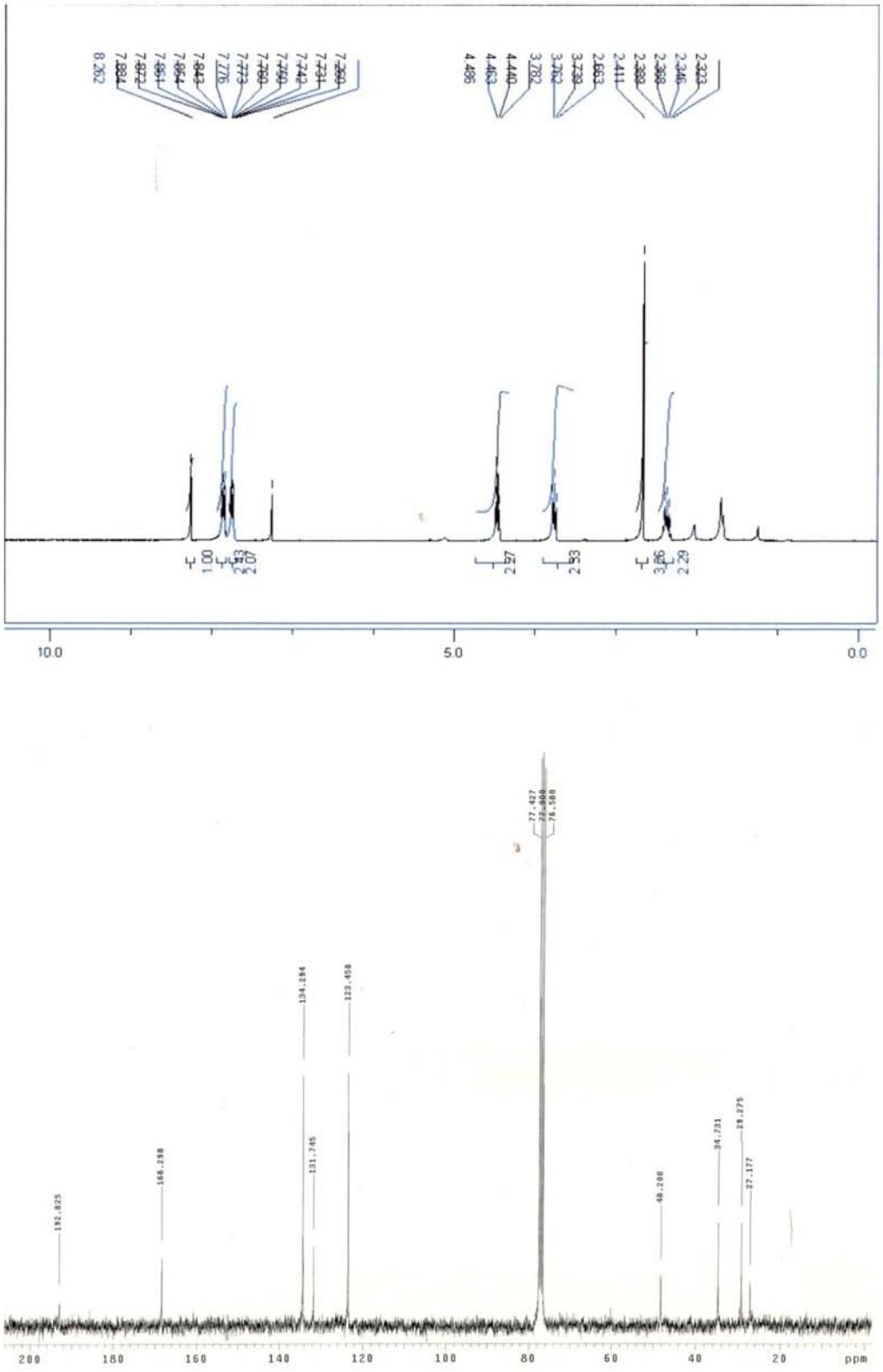

Figure S6. ^{1}H (300 MHz) and ^{13}C (75.5 M Hz) NMR spectrum of compound **3f** in $CDCl_3$.

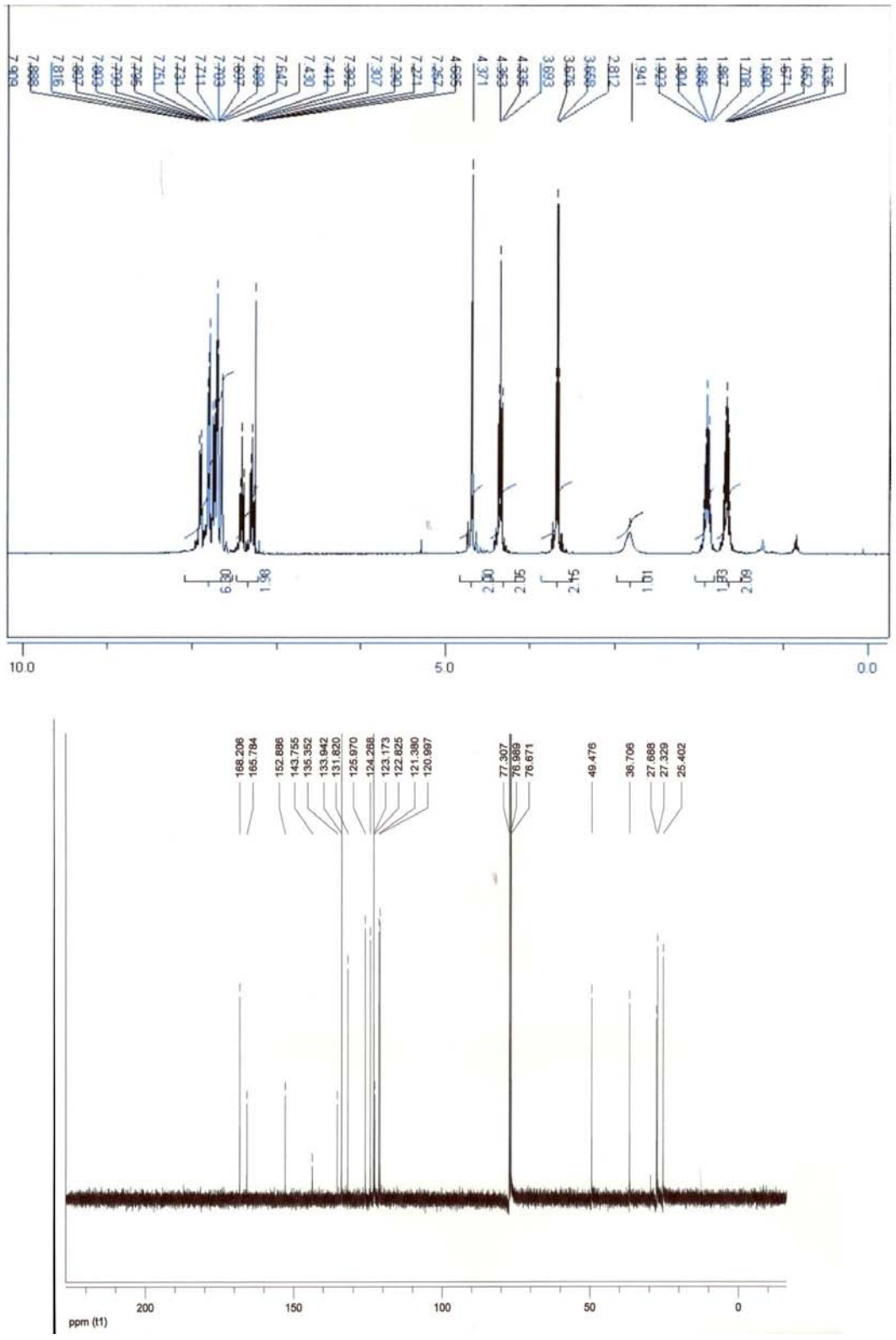

Figure S7. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectrum of compound **4a** in $CDCl_3$.

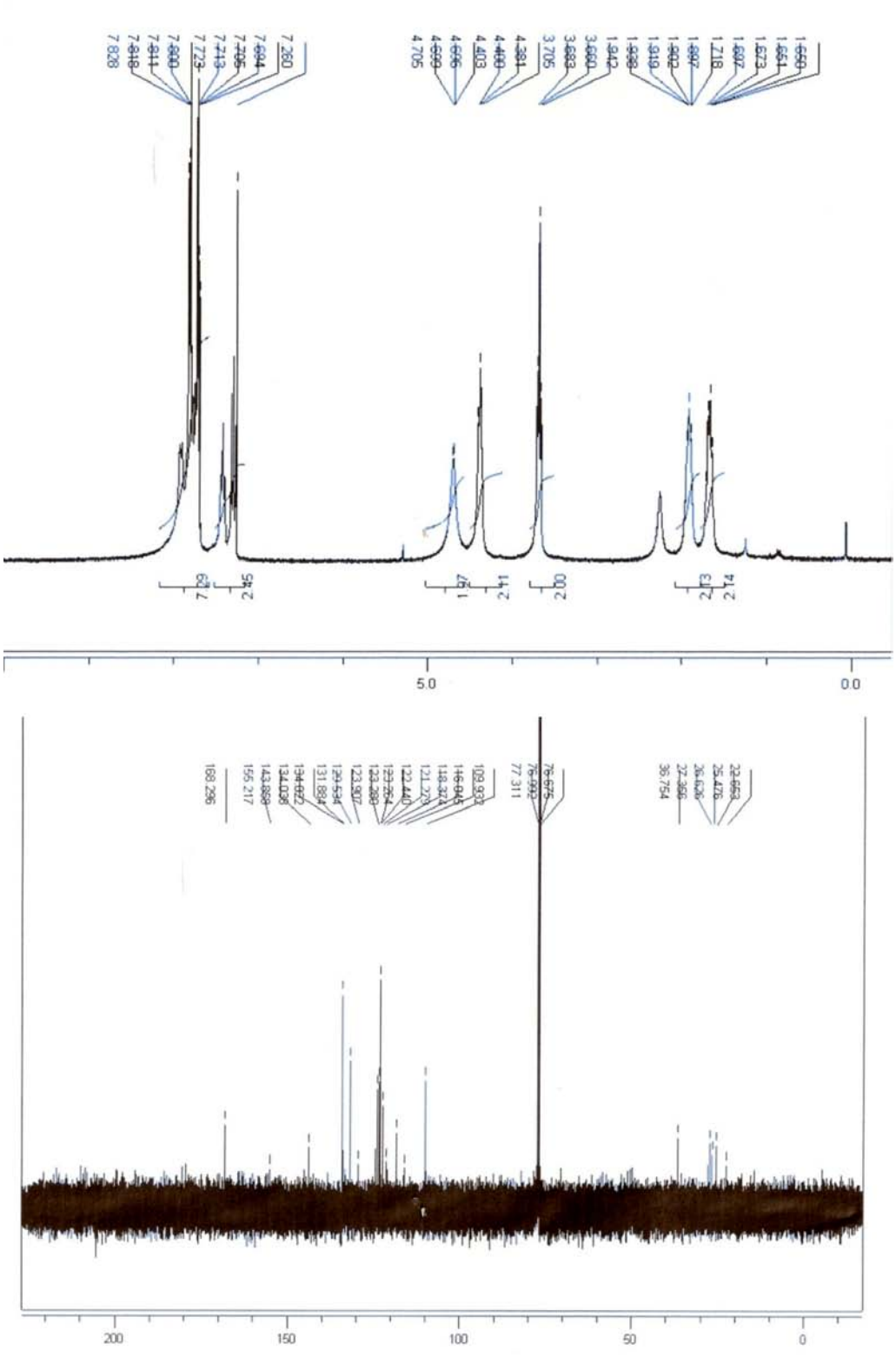

Figure S8. ^{1}H (300 MHz) and ^{13}C (75.5 MHz) NMR spectrum of compound **4b** in $CDCl_3$.

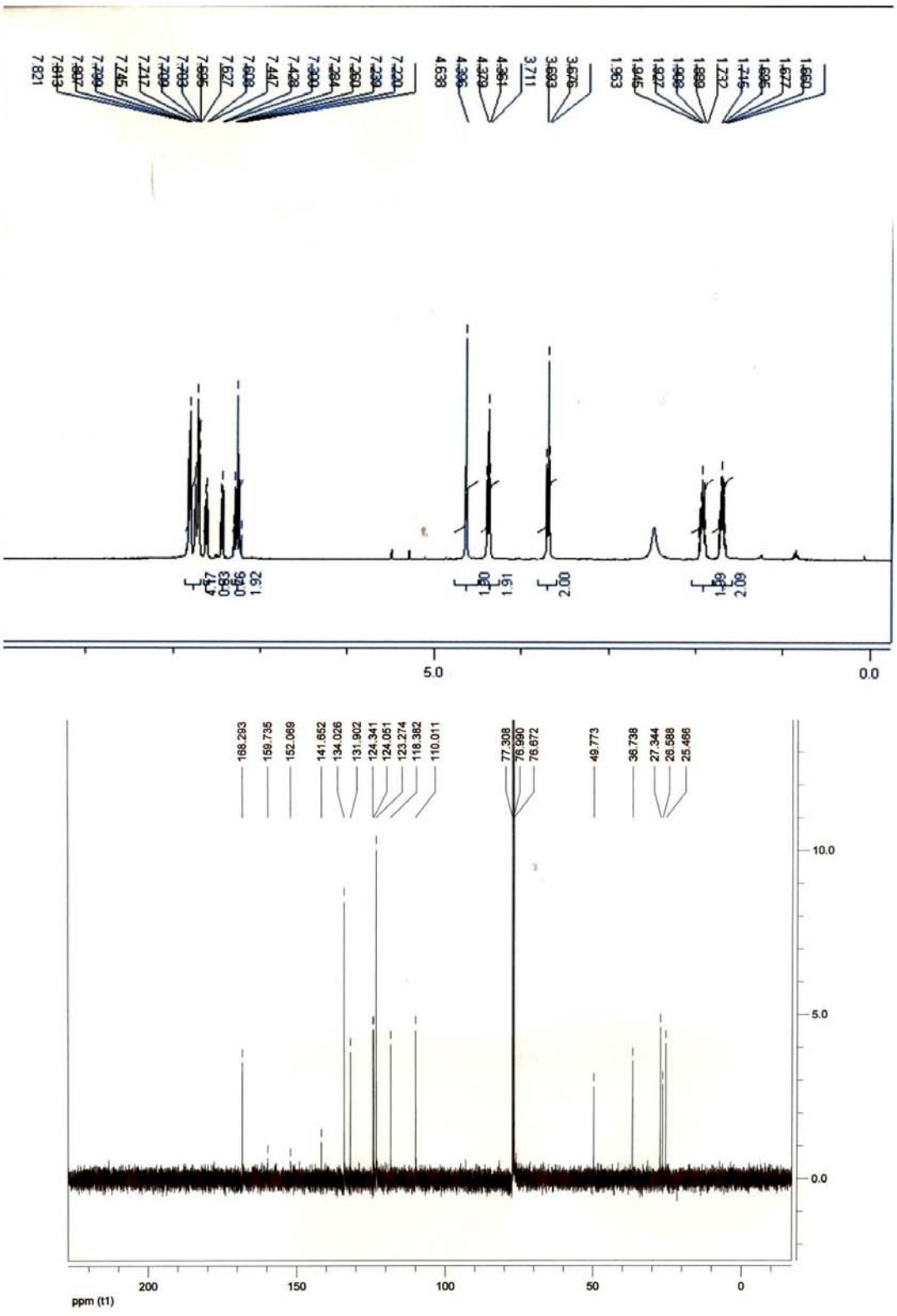

Figure S9. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectrum of compound **4c** in $CDCl_3$.

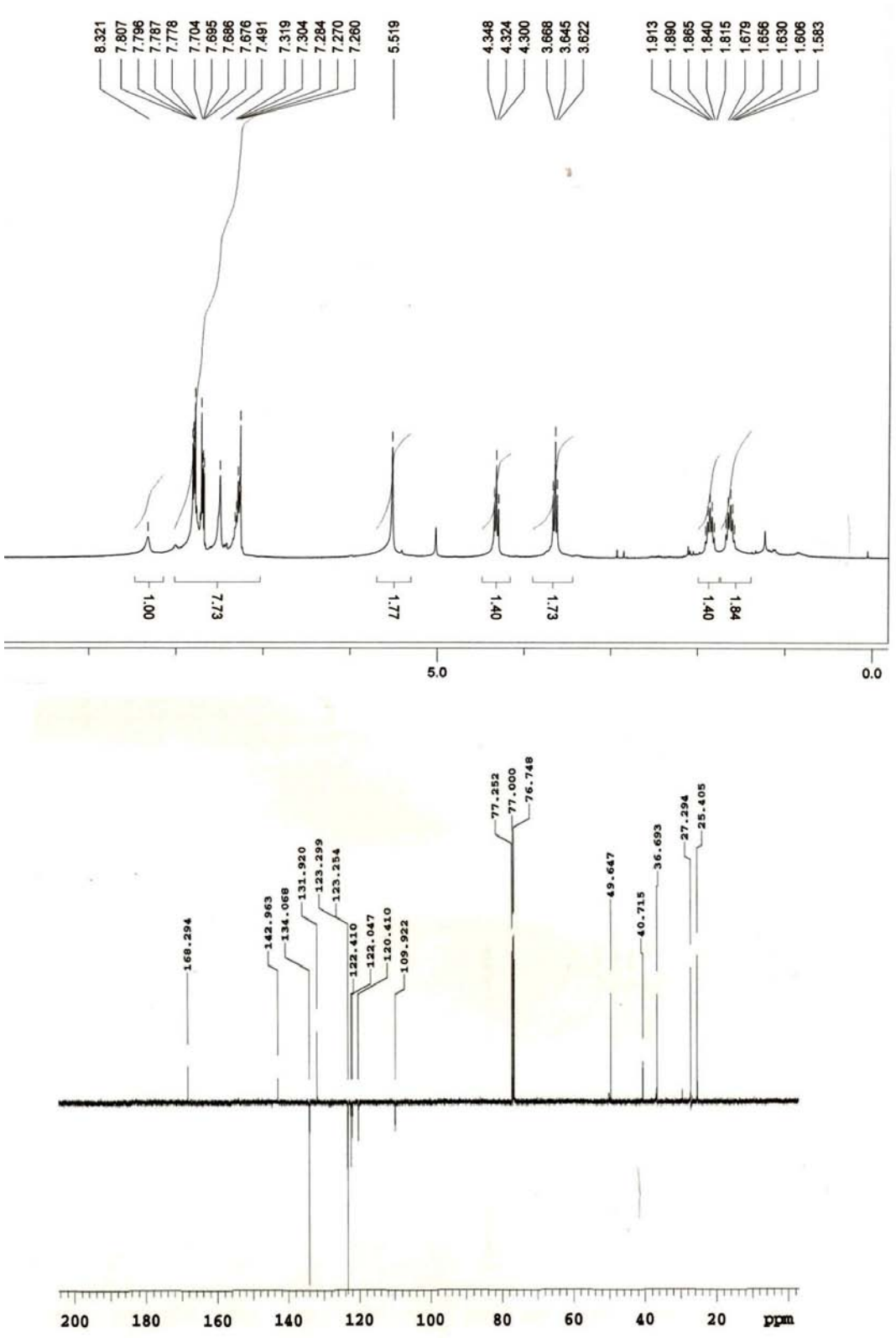

Figure S10. ^{1}H (300 MHz) and ^{13}C-APT (125 MHz) NMR spectrum of compound **4d** $CDCl_3$.

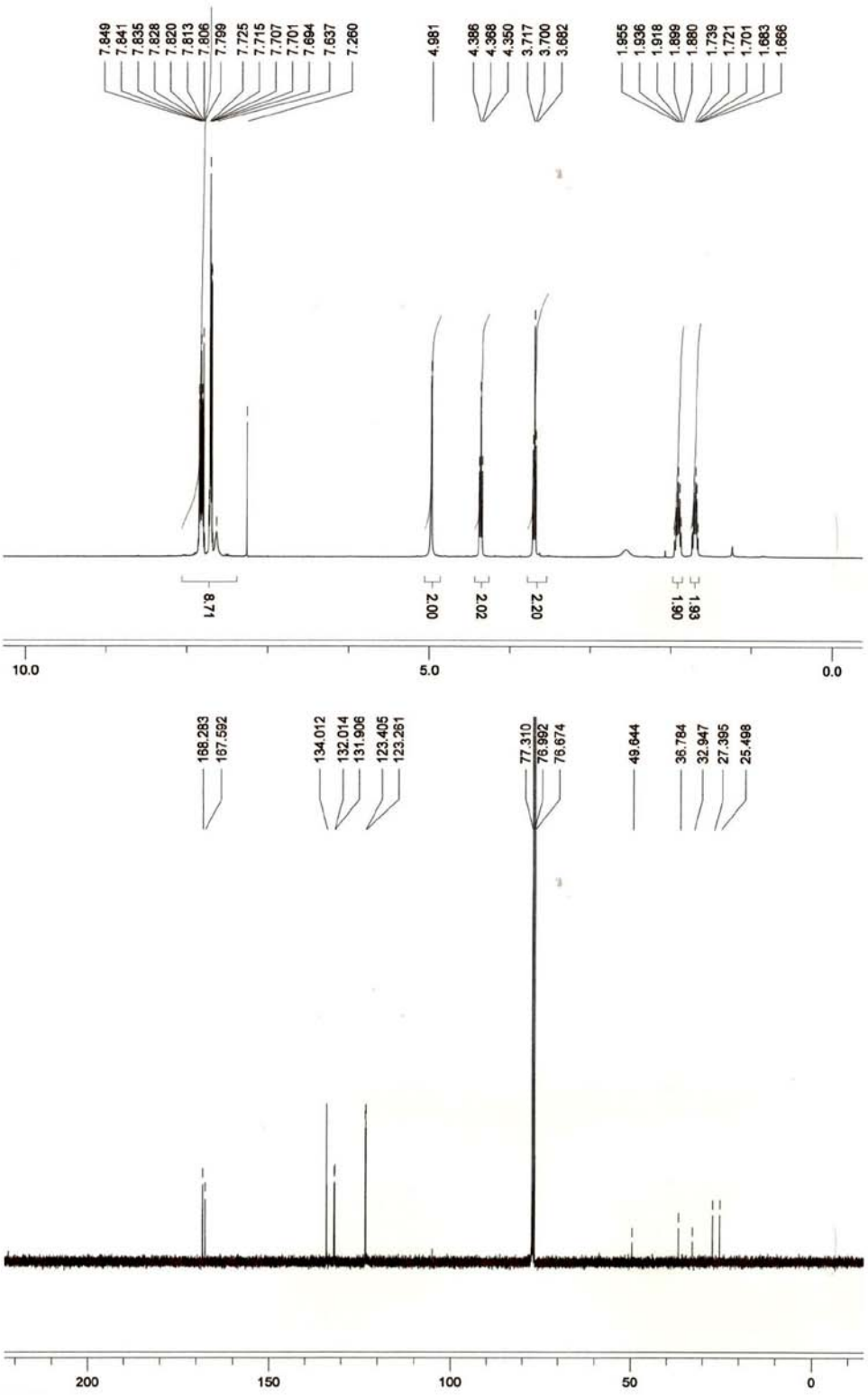

Figure S11. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectrum of compound **4e** $CDCl_3$.

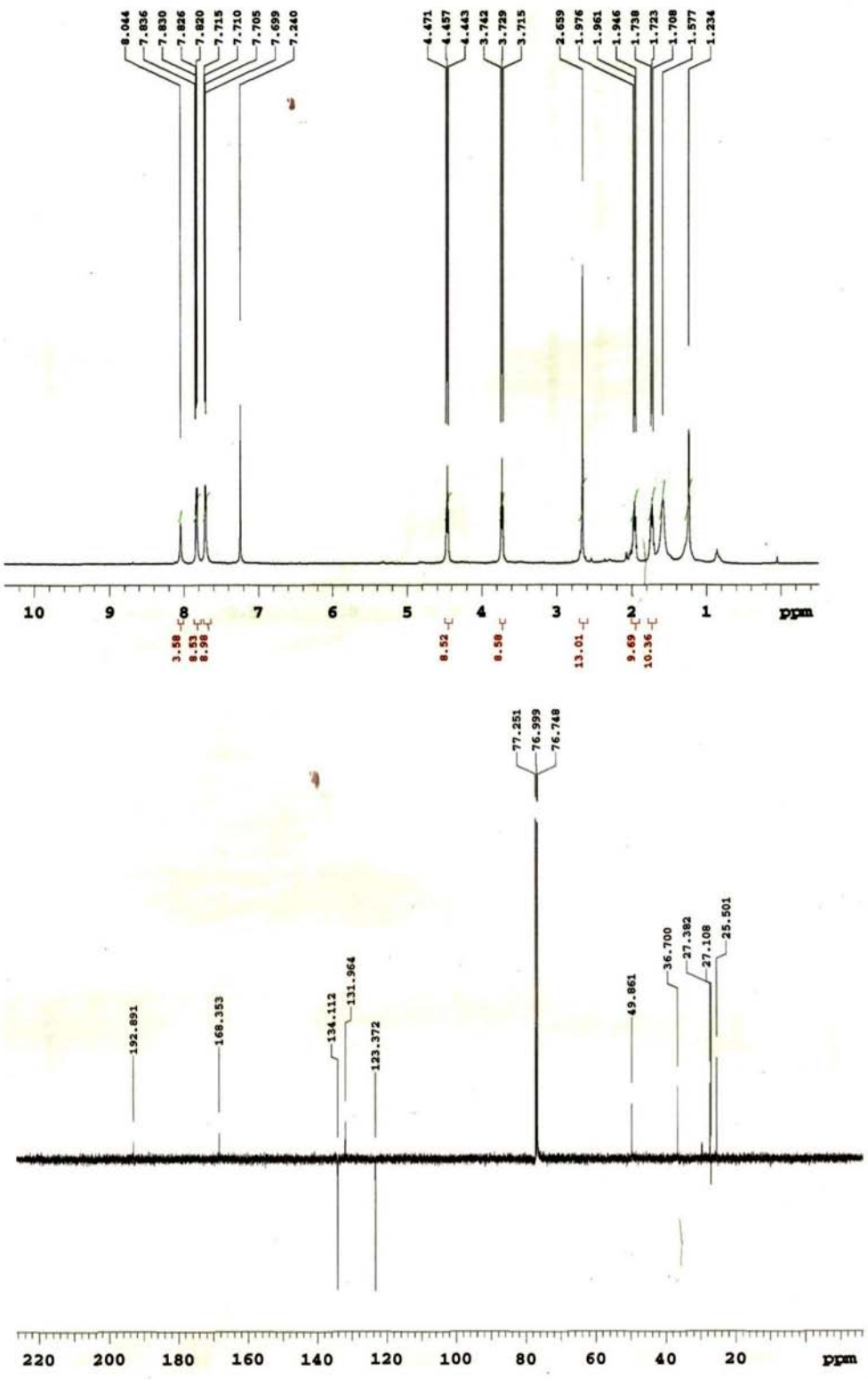

Figure S12. ^{1}H (500 MHz) and ^{13}C-APT (125 MHz) NMR spectrum of compound **4f** in $CDCl_3$.

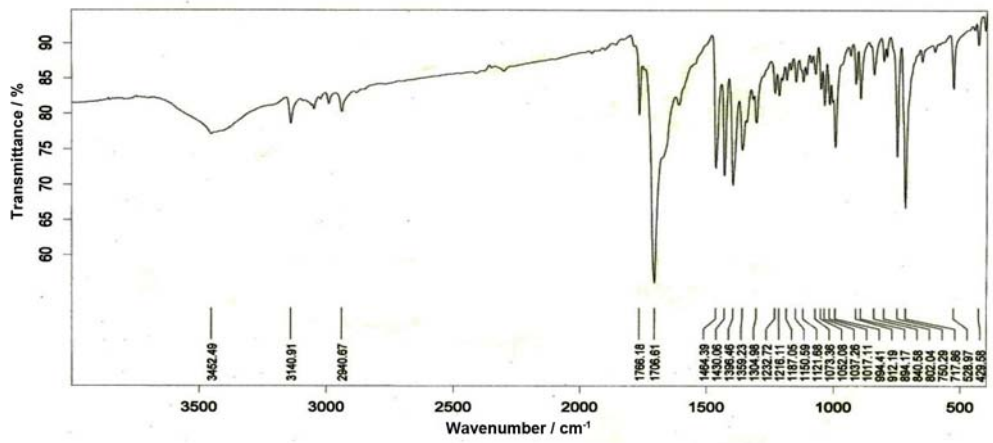

Figure S13. IR spectrum of compound **3a**.

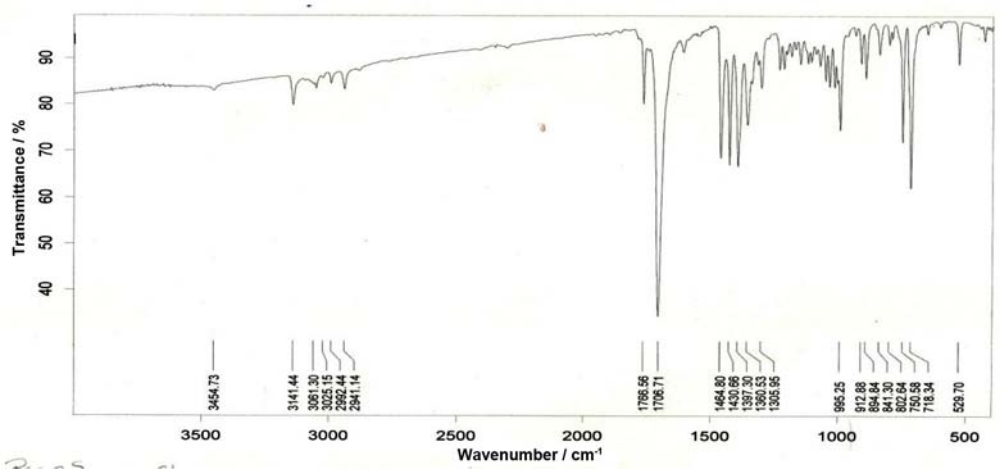

Figure S14. IR spectrum of compound **3b**.

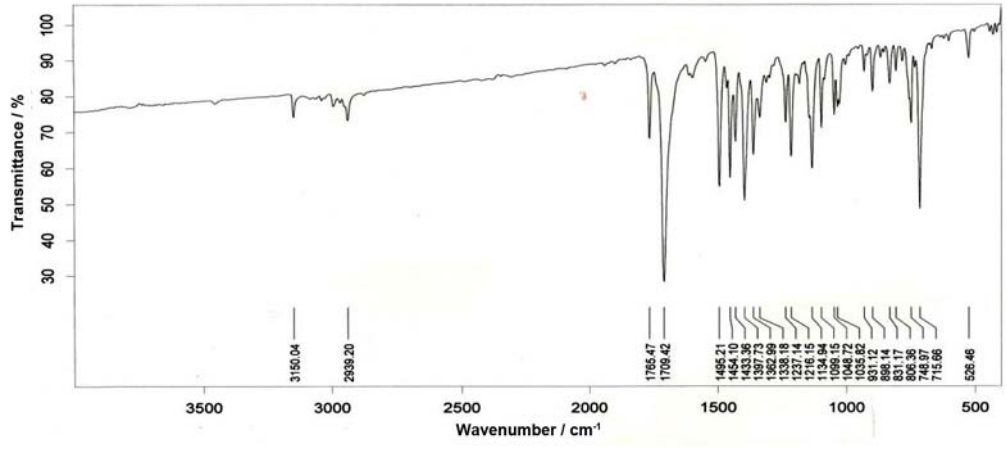

Figure S15. IR spectrum of compound **3c**.

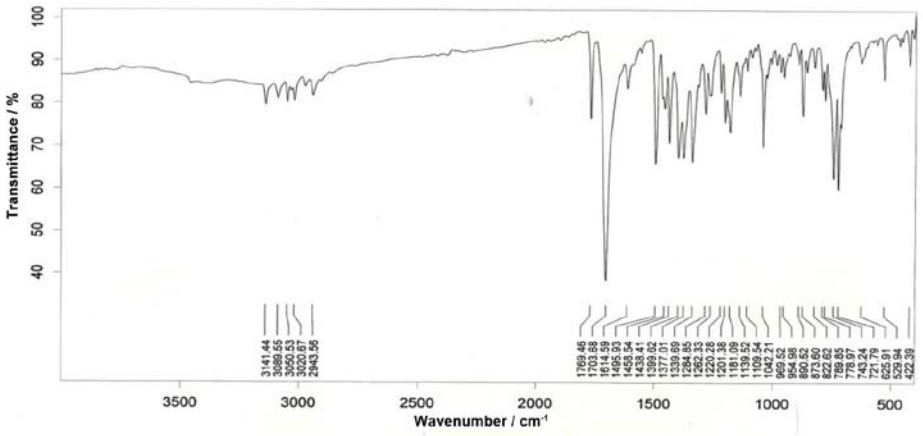

Figure S16. IR spectrum of compound **3d**.

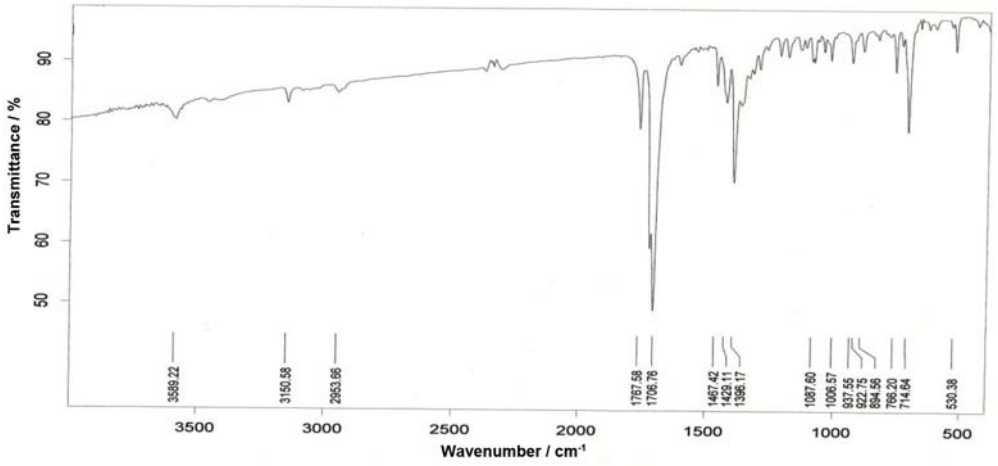

Figure S17. IR spectrum of compound **3e**.

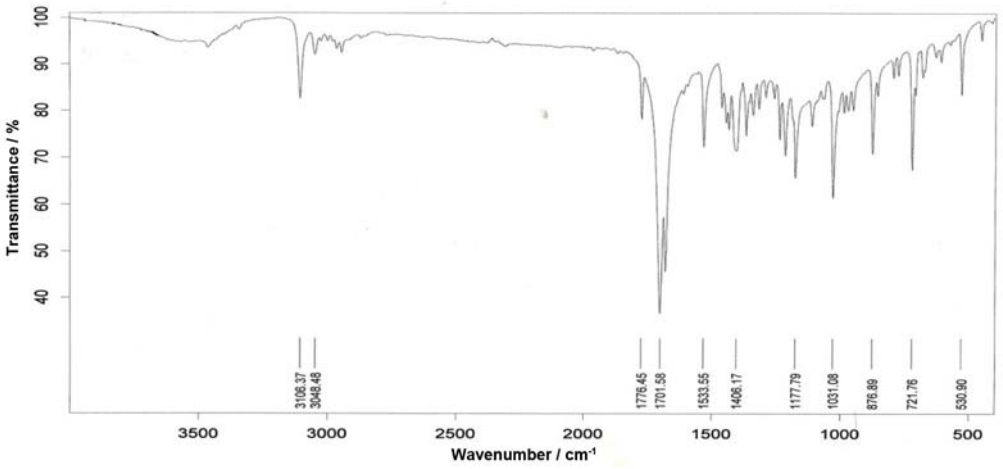

Figure S18. IR spectrum of compound **3f**.

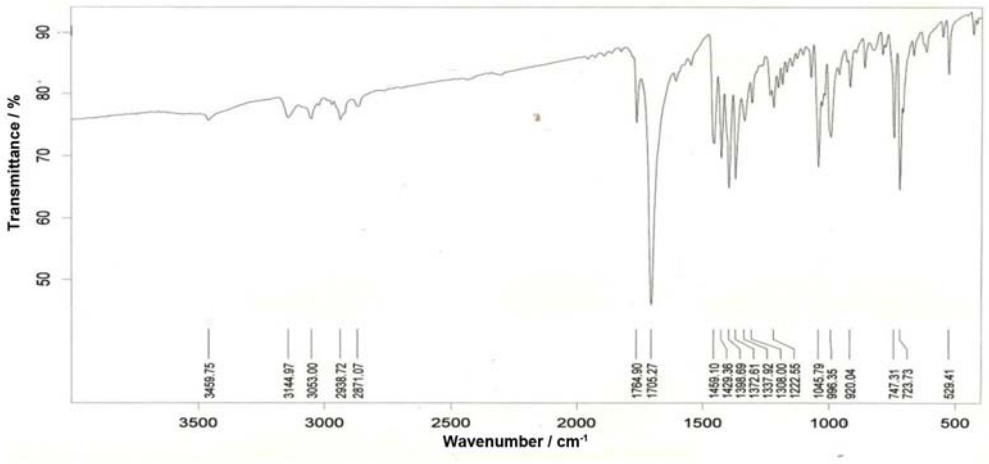

Figure S19. IR spectrum of compound **4a**.

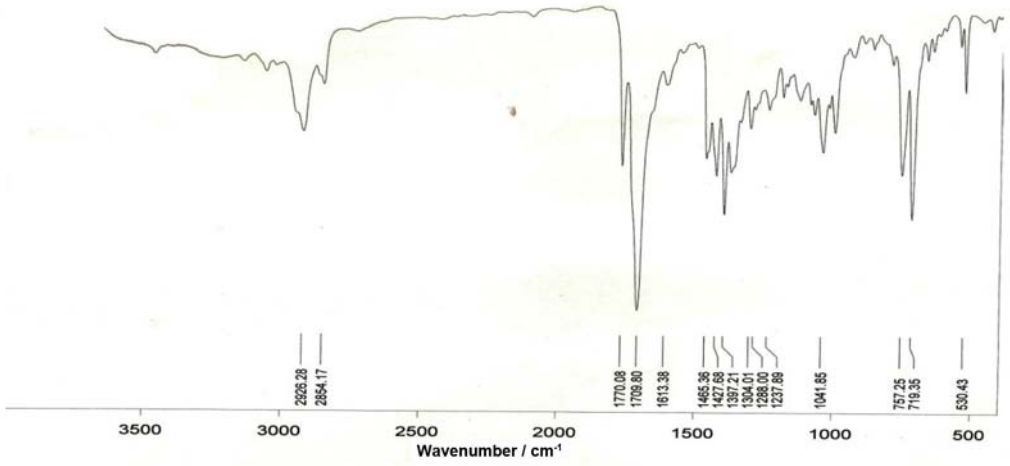

Figure S20. IR spectrum of compound **4b**.

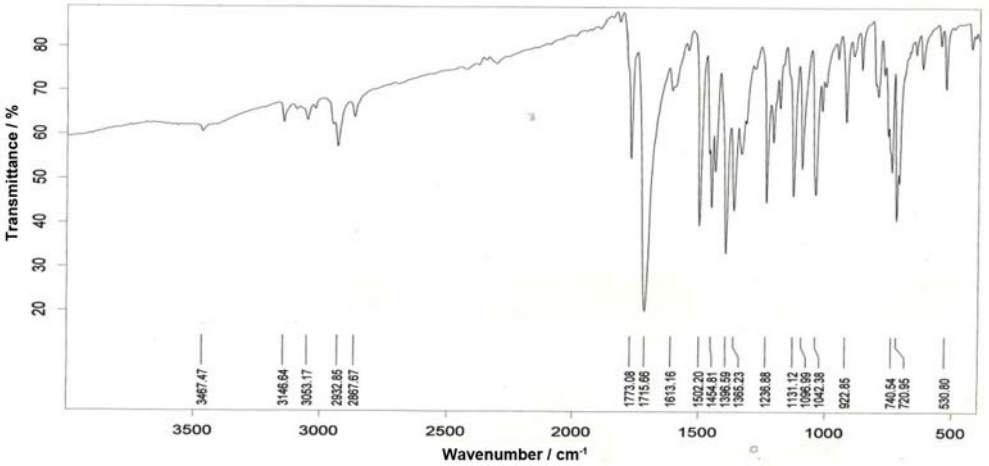

Figure S21. IR spectrum of compound **4c**.

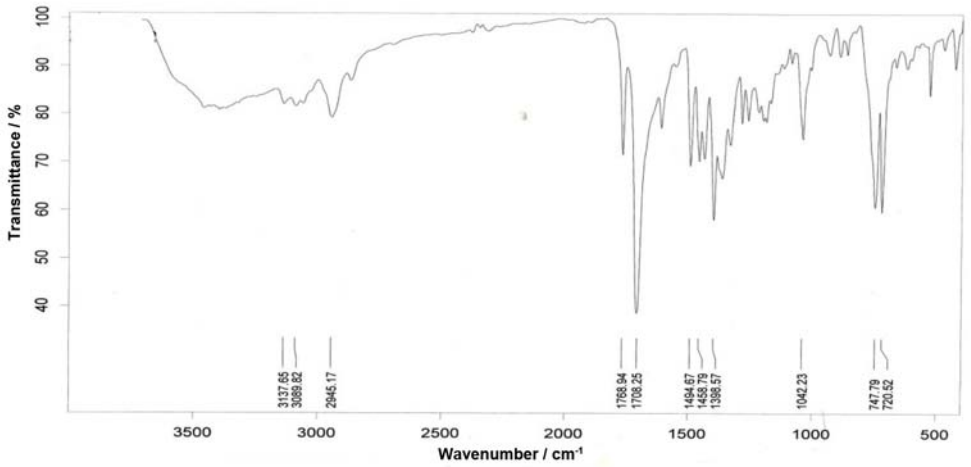

Figure S22. IR spectrum of compound **4d**.

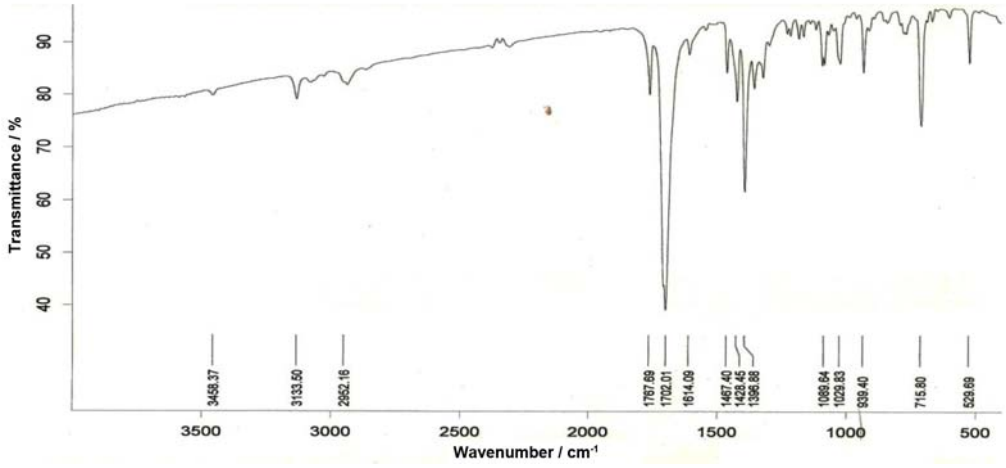

Figure S23. IR spectrum of compound **4e**.

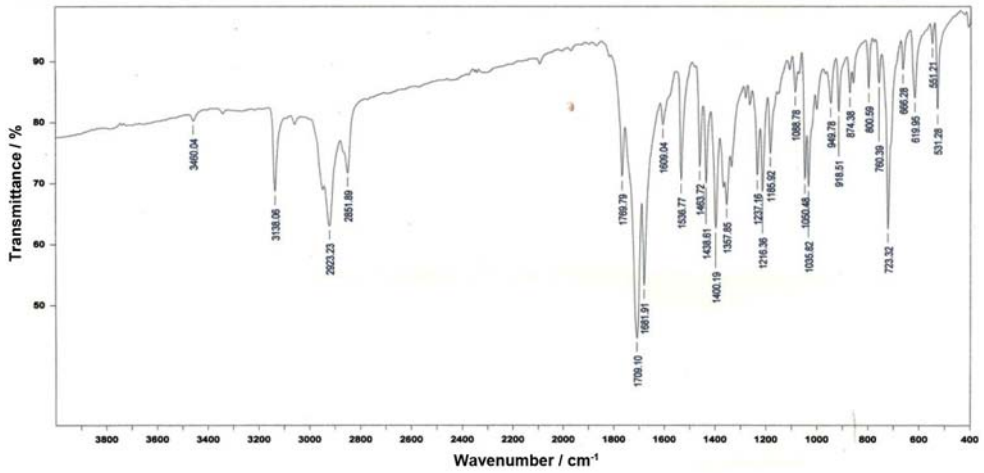

Figure S24. IR spectrum of compound **4f**.

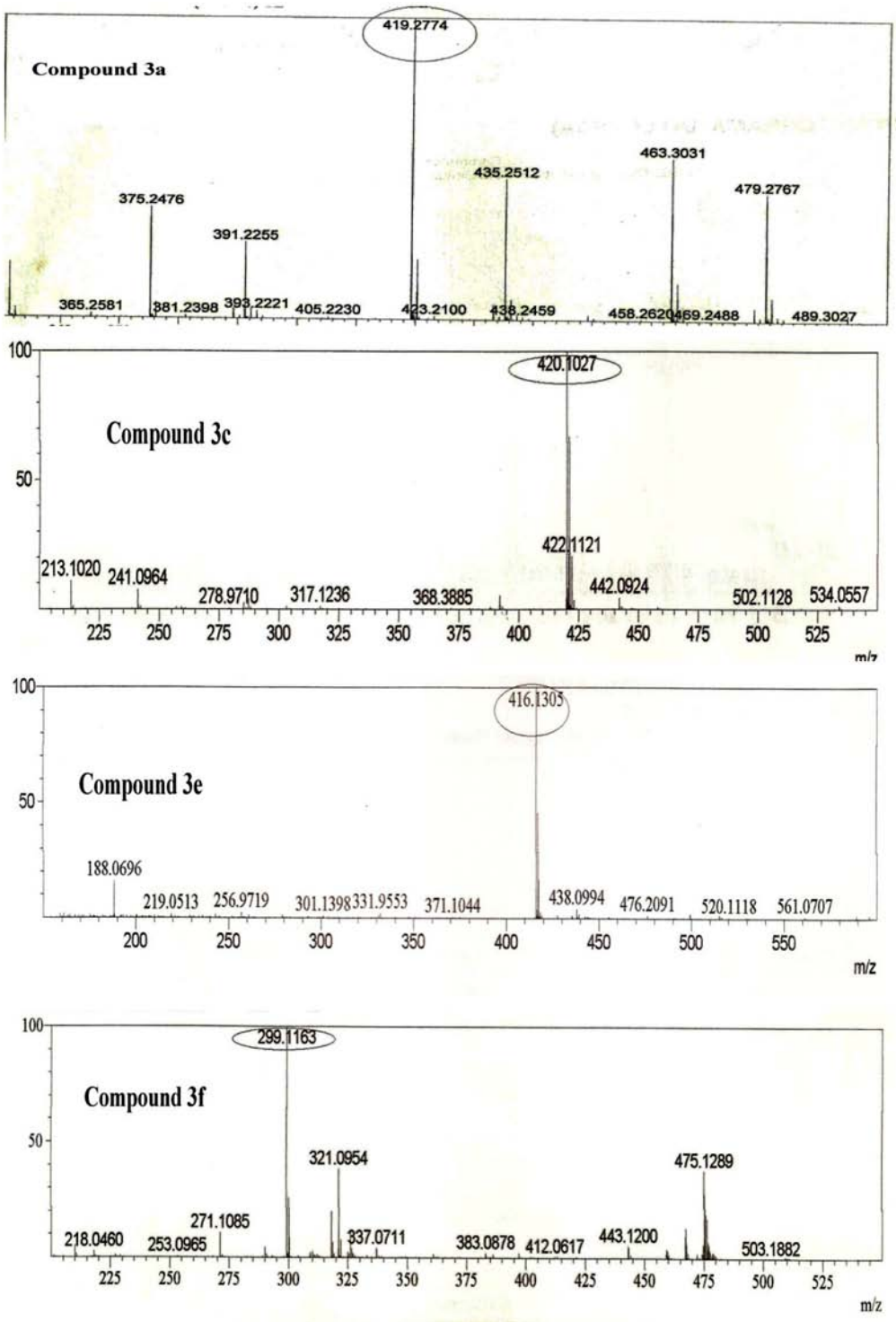

Figure S25. *m/z* LC-MS spectrum graph of the compounds **3a**, **3c**, **3e** and **3f**.

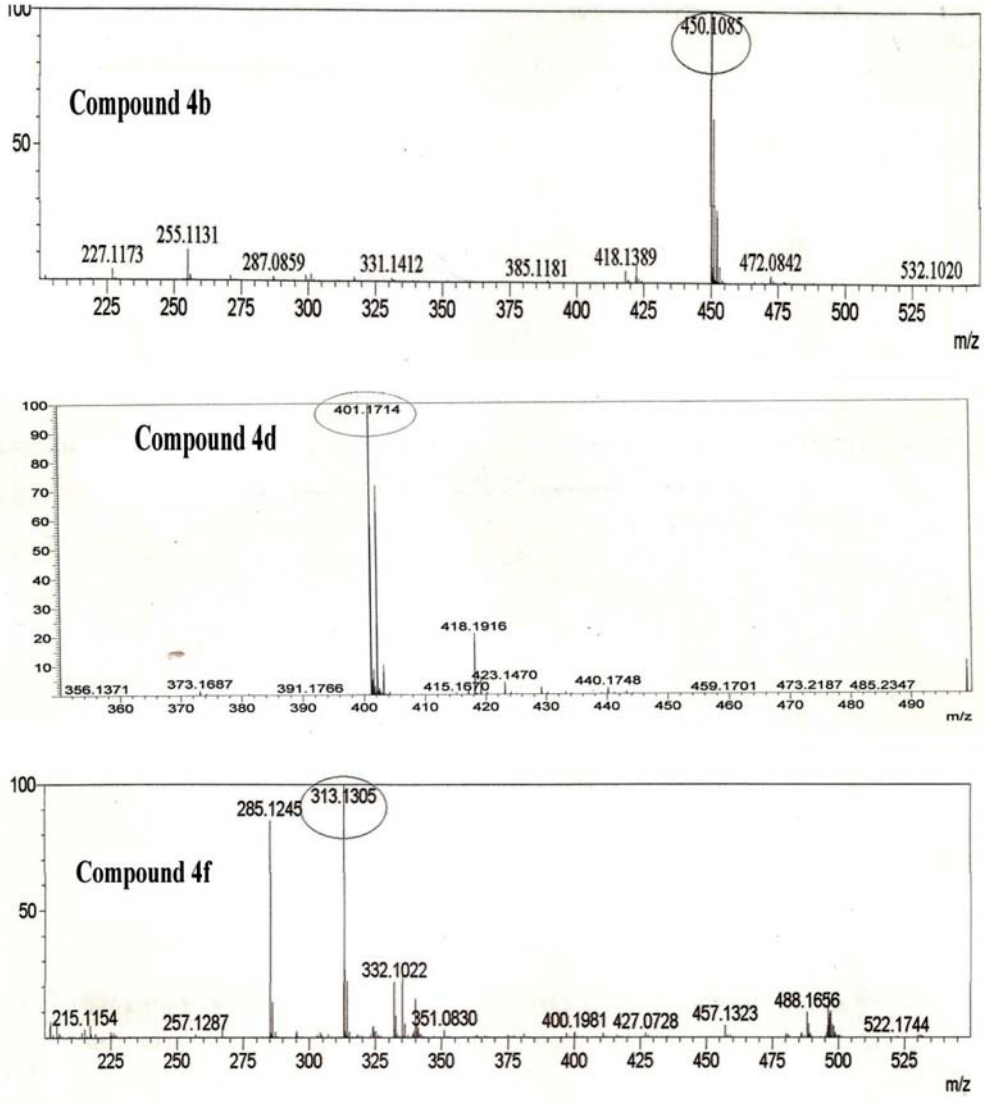

Figure S26. *m/z* LC-MS spectrum graph of the compounds **4b**, **4d** and **4f**.