Electronic Supplementary Material (ESI) for RSC Advances.

WCl_6/DMF as a new reagent system for the phosphine-free Pd(0)-catalyzed aminocarbonylation of aryl halides

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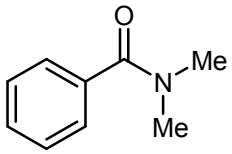
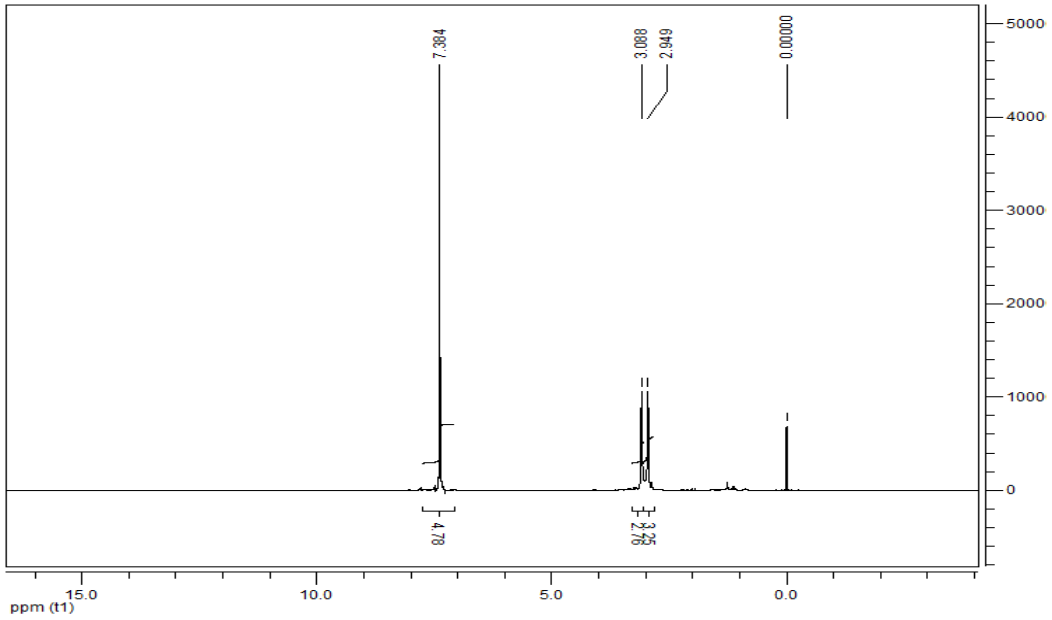
Spectral data and copy of ^{1}HNMR and ^{13}CNMR spectra for the synthesized compounds

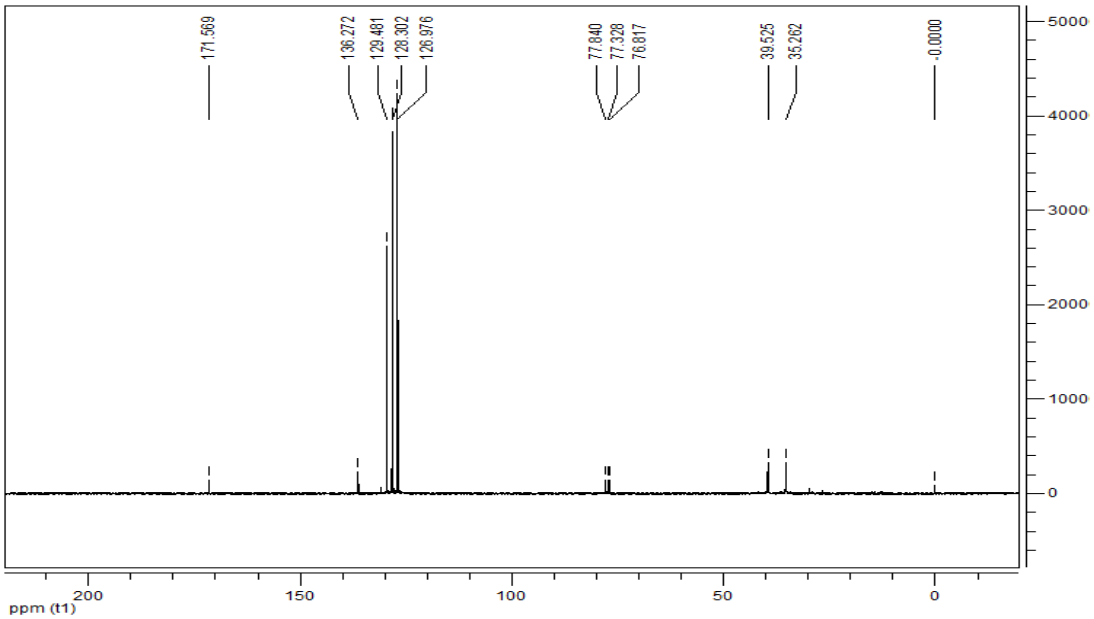
1. *N,N*-Dimethylbenzamide



^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 2.94 (3H, s), 3.08 (3H, s), 7.38 (5H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 35.3($\underline{C}H_3$), 39.5($\underline{C}H_3$), 126.9(Ar), 128.3(Ar), 129.5(Ar), 136.3(Ar), 171.6 ($\underline{C}$=O).

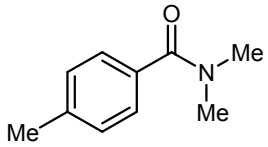


^{1}H-NMR

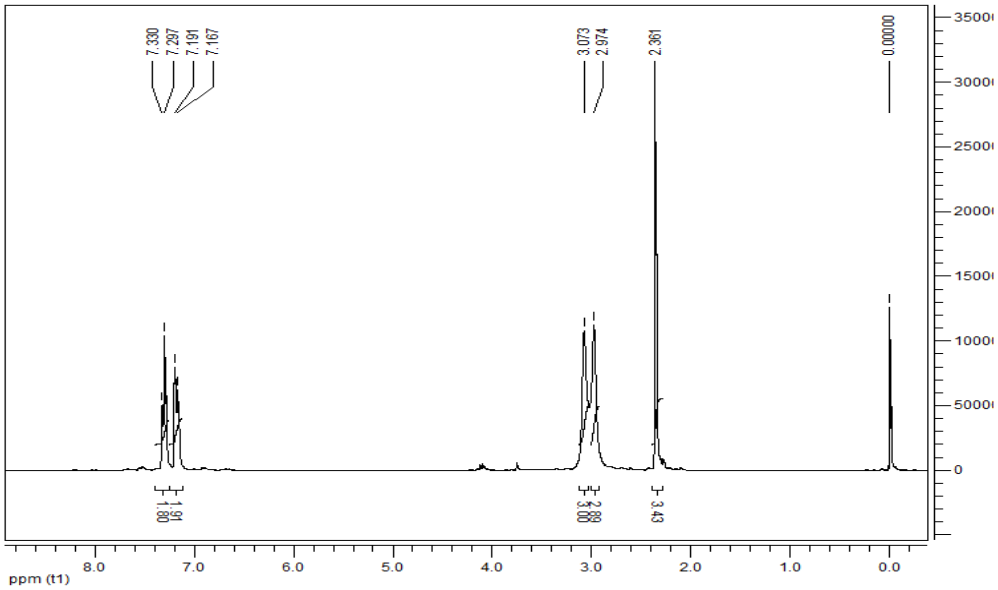


^{13}C-NMR

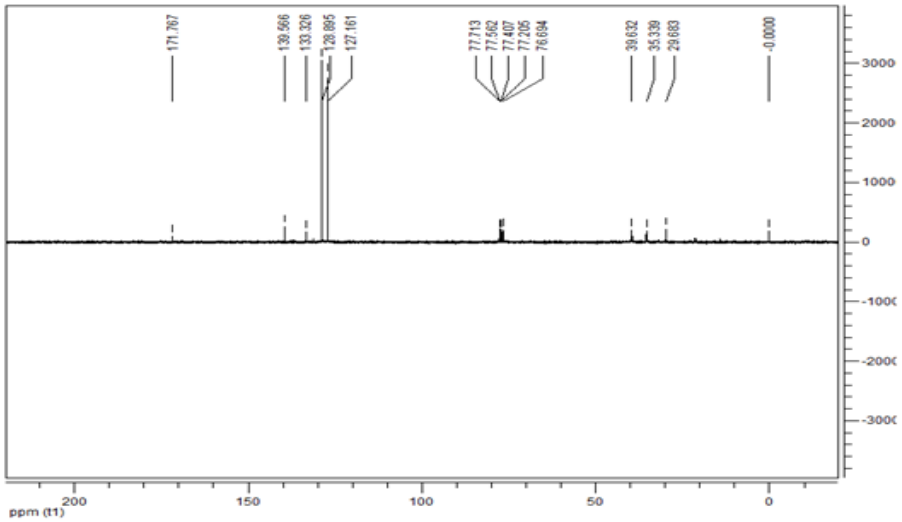
2. *N,N,4*-Timethylbenzamide



^{1}H-NMR (250 MHz CDC1$_3$) δ (ppm): 2.36 (3H, S), 2.97 (3H, S), 3.07 (3H, S), 7.19-7.30 (2H, m), 7.29-7.33 (2H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 28.3(CH_3), 35.3(CH_3), 39.6(4-CH_3), 127.2(Ar), 128.9(Ar), 133.3(Ar), 139.6(Ar), 171.7(C=O).

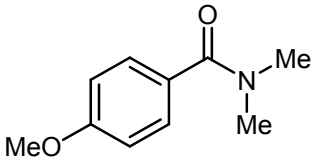


^{1}H-NMR

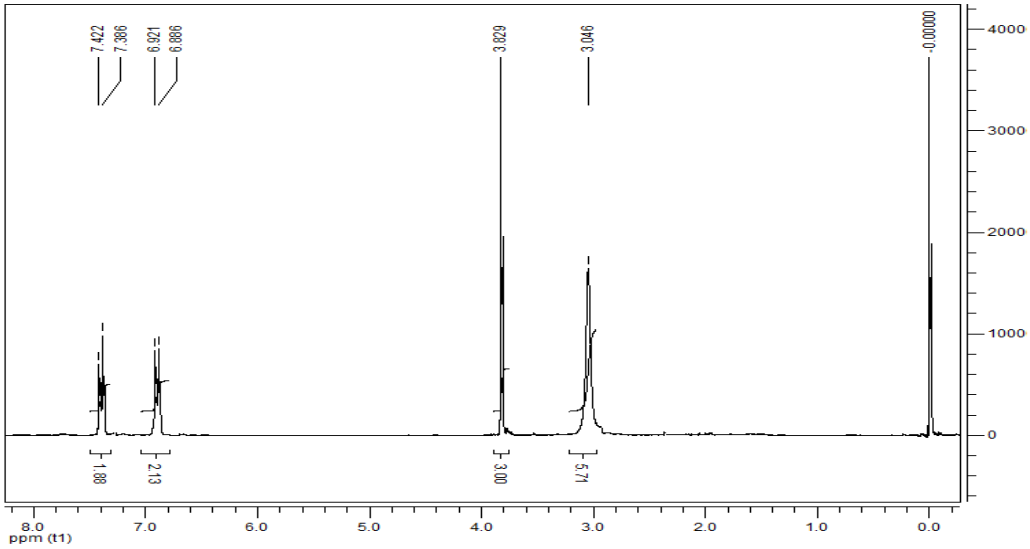


^{13}C-NMR

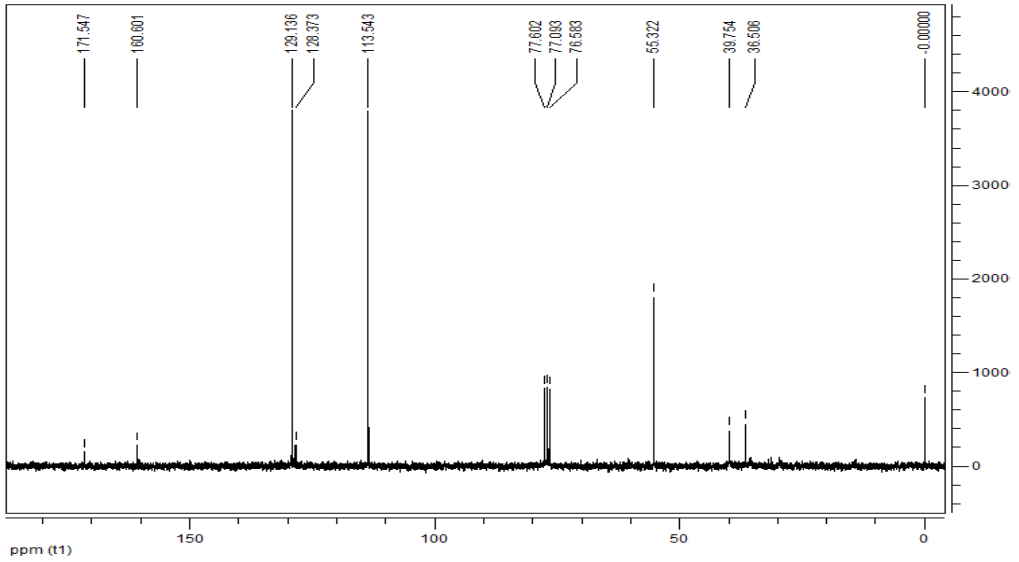
3. 4-Methoxy-*N*,*N*-dimethylbenzamide



^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 3.04 (6H, S), 3.82 (3H, S), 6.86-6.92 (2H, m), 7.36-7.42 (2H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 36.5($\underline{C}H_3$), 39.7($\underline{C}H_3$), 55.3(4-$\underline{C}H_3O$), 113.5(Ar), 128.4(Ar), 129.1(Ar), 160.6(Ar), 171.5($\underline{C}$=O)

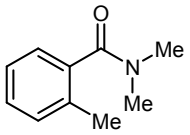


^{1}H-NMR

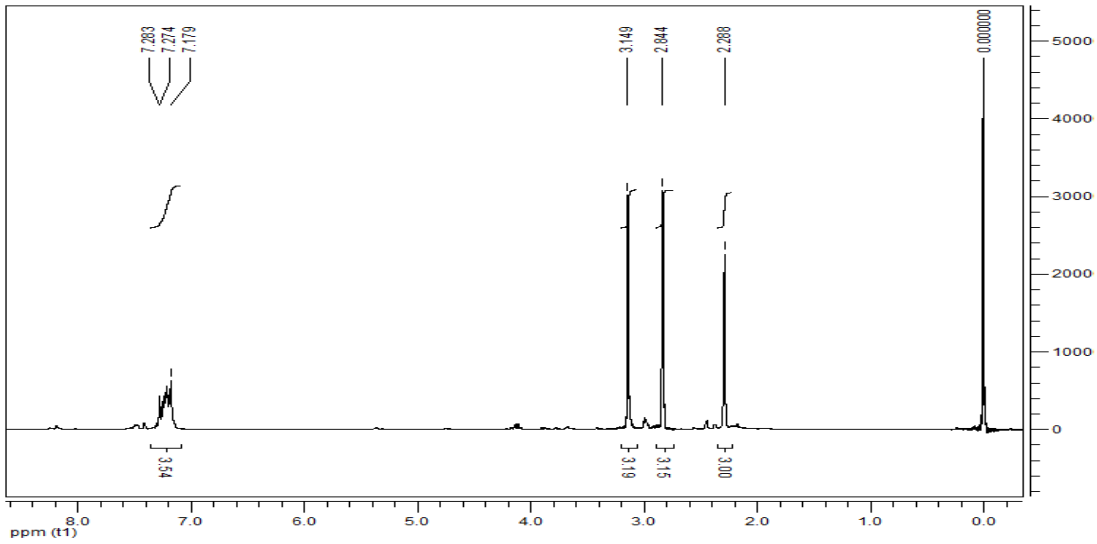


^{13}C-NMR

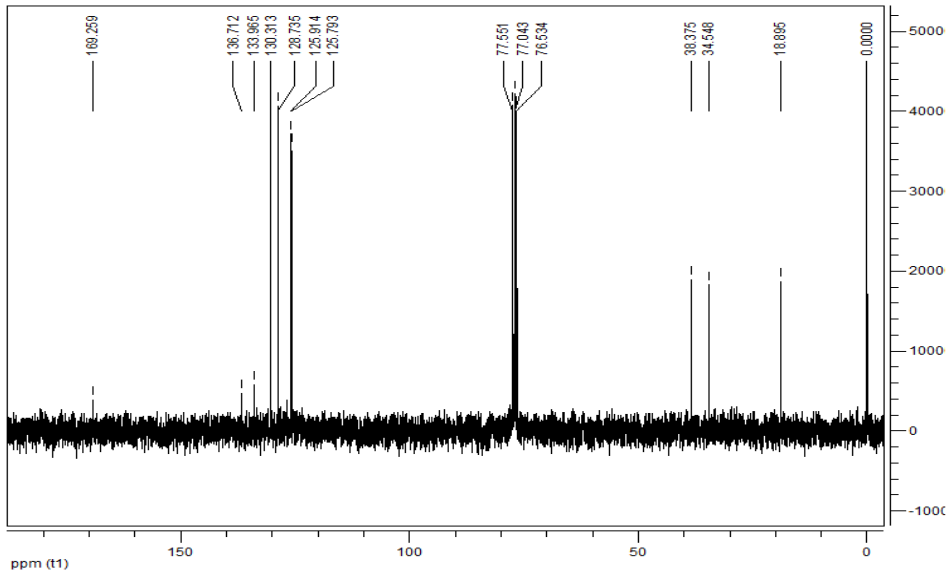
4. *N,N,2*-Trimethylbenzamide



^{1}H-NMR (250 MHz CDC1$_3$) δ (ppm): 2.29 (3H, S), 2.84 (3H, S), 3.14 (3H, S), 7.17-7.28 (4H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 18.8(CH_3), 34.5(CH_3), 38.3(2-CH_3), 125.7(Ar), 125.9(Ar), 128.7(Ar), 130.3(Ar), 133.9(Ar), 136.7(Ar), 169.2(C=O).

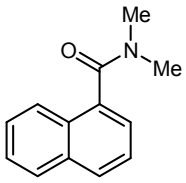


^{1}H-NMR

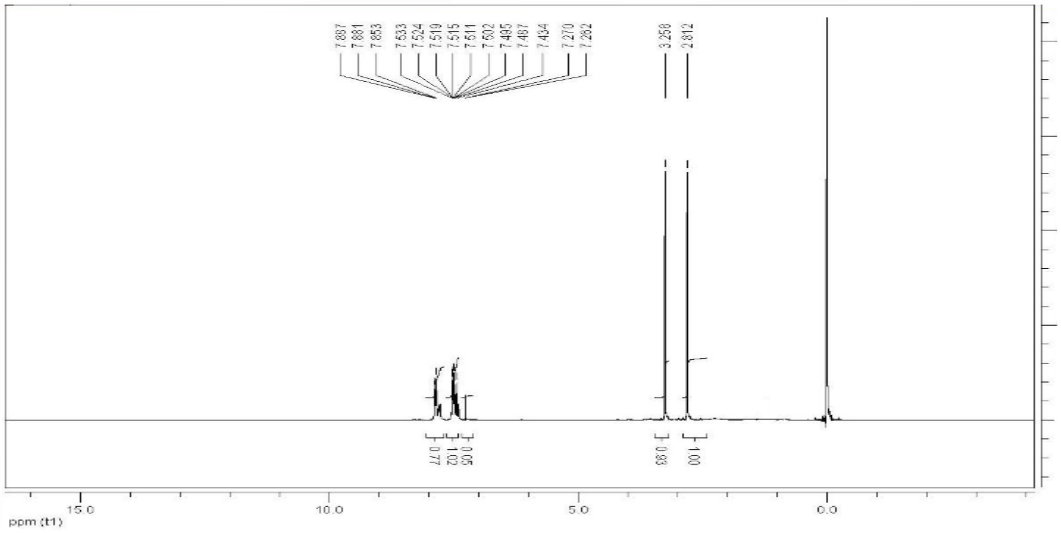


^{13}C-NMR

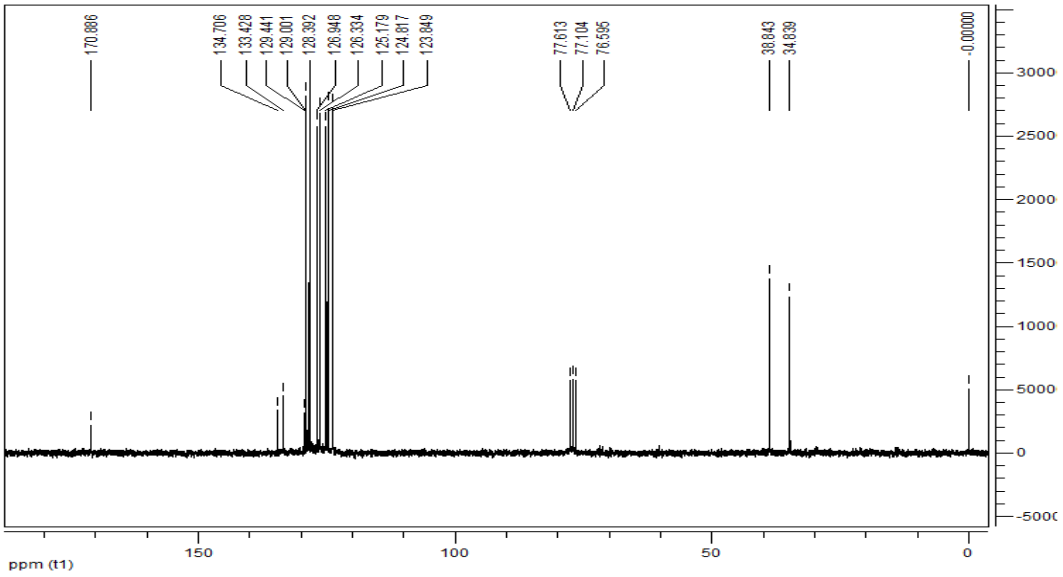
5. *N,N*-Dimethyl-1-naphthamide



^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 2.70 (3H, s), 3.15 (3H, s), 7.43-7.53 (4H, m), 7.85-7.89 (3H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 34.8($\underline{C}H_3$), 38.8($\underline{C}H_3$), 123.8(Ar), 124.8(Ar), 125.1(Ar), 126.3(Ar), 126.9(Ar), 128.3(Ar), 129.0(Ar), 129.4(Ar), 133.4(Ar), 134.7(Ar), 170.8($\underline{C}$=O).

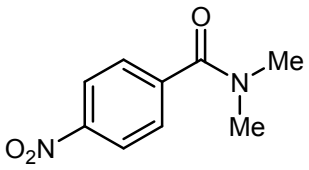


^{1}H-NMR

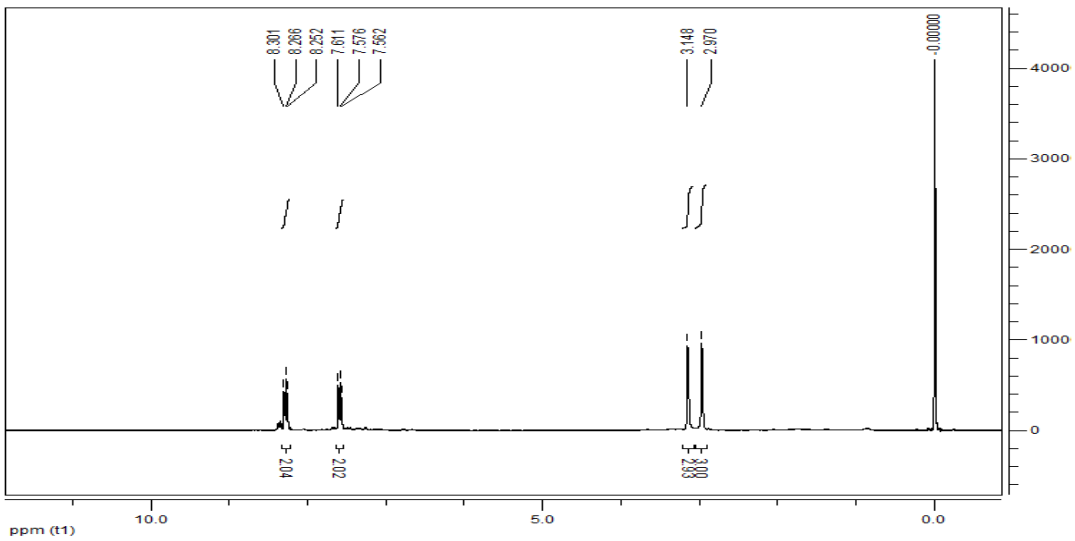


^{13}C-NMR

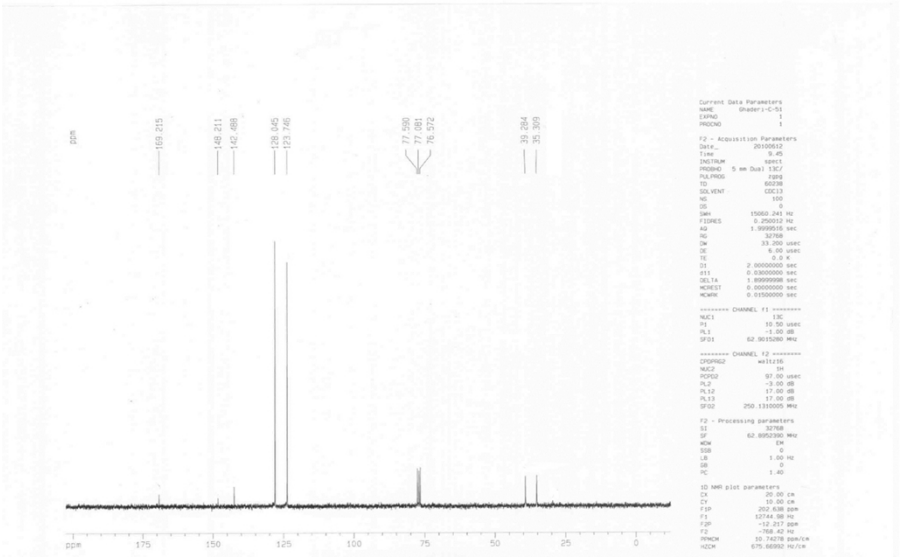
6. *N,N*-Dimethyl-4-nitrobenzamide



^{1}H-NMR (250 MHz CDC1$_3$) δ (ppm): 2.97 (3H,s), 3.14 (3H,s), 7.56-7.61 (2H, m), 8.25-8.30 (2H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 35.3(CH_3), 39.3(CH_3), 123.8(Ar), 128.0®, 142.4(Ar), 148.2(Ar), 169.2(C=O).

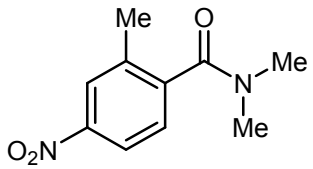


^{1}H-NMR

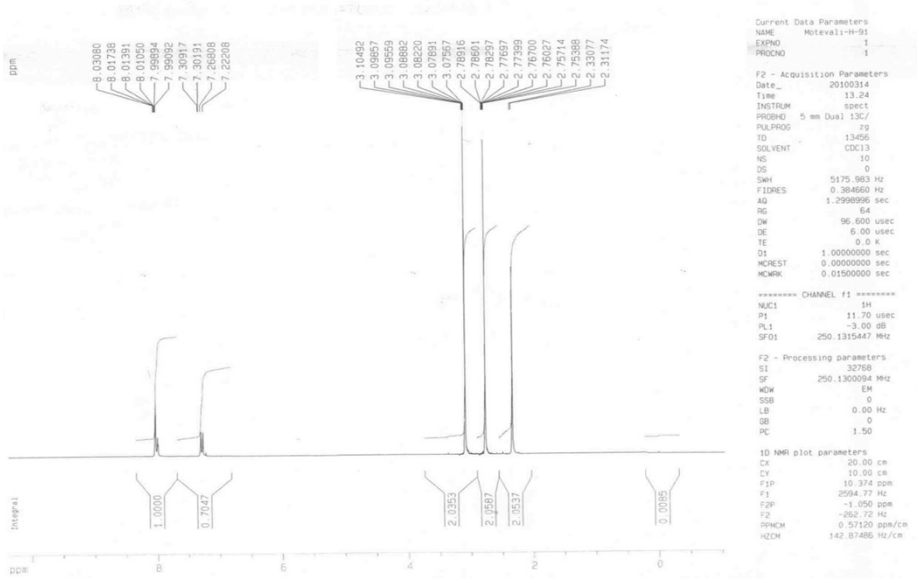


^{13}C-NMR

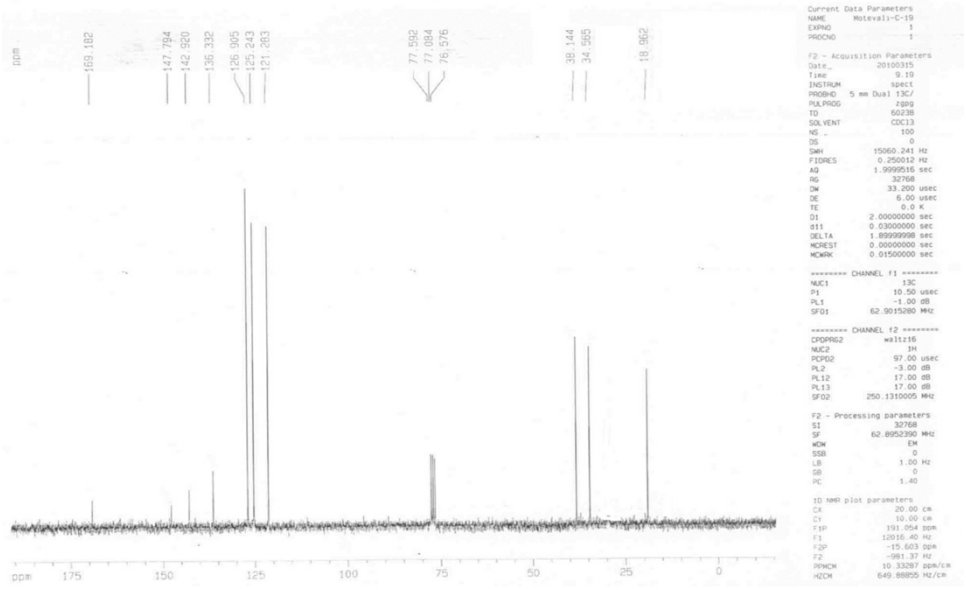
7. *N,N*,2-Trimethyl-4-nitrobenzamide



^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 2.33 (3H, s), 2.78 (3H, s), 3.07 (3H, s), 7.26 (1H, d, J = 10 Hz), 8.01 (2H, d, J = 8.4 Hz); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 18.9($\underline{C}H_3$), 34.5($\underline{C}H_3$), 38.1($\underline{C}H_3$), 121.2(Ar), 125.2(Ar), 126.9(Ar), 136.3(Ar), 142.9(Ar), 147.7(Ar), 169.1($\underline{C}$=O).

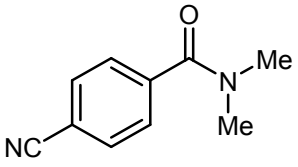


^{1}H-NMR

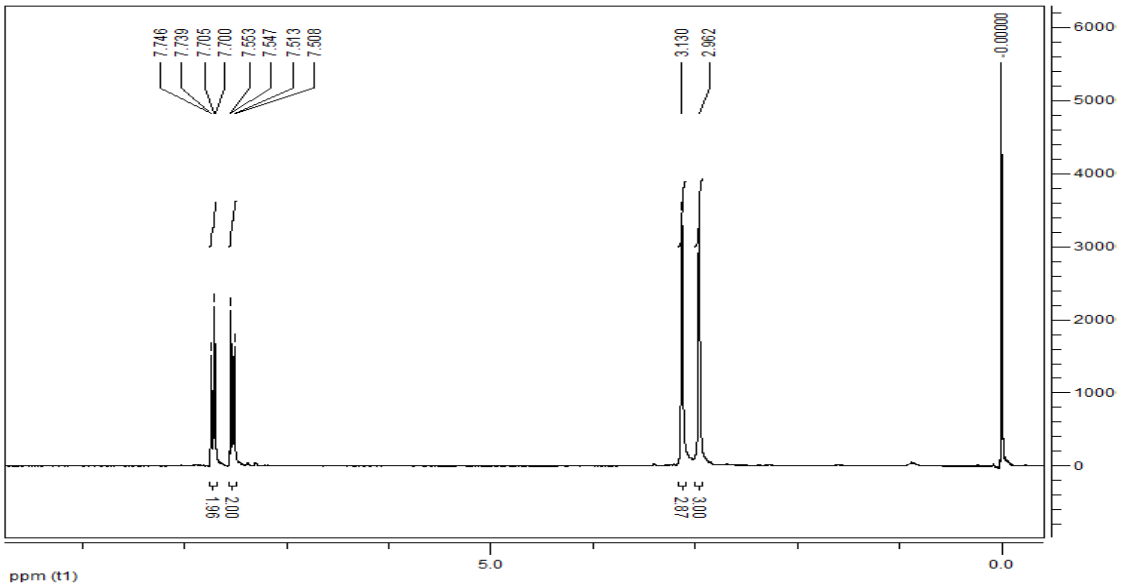


^{13}C-NMR

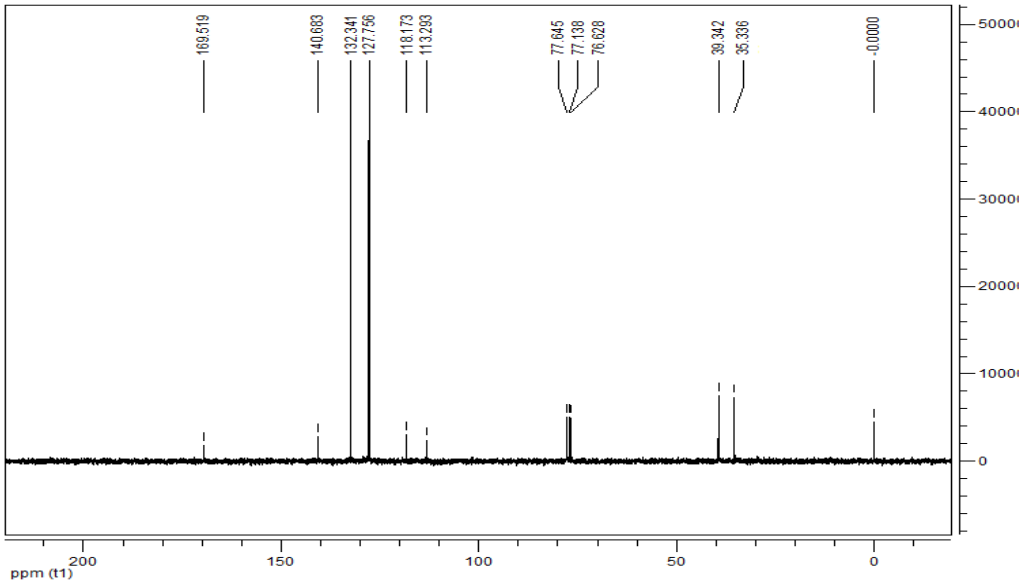
8. 4-Cyano-*N*,*N*-dimethylbenzamide



^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 2.96 (3H, s), 3.13 (3H, s), 7.50-7.55 (2H, m), 7.70-7.74 (2H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 35.3($\underline{C}H_3$), 39.3($\underline{C}H_3$), 113.2(Ar), 118.2(Ar), 127.7(Ar), 132.3(Ar), 140.7($\underline{C}N$), 169.5($\underline{C}$=O)

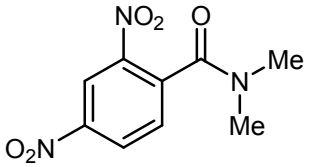


^{1}H-NMR



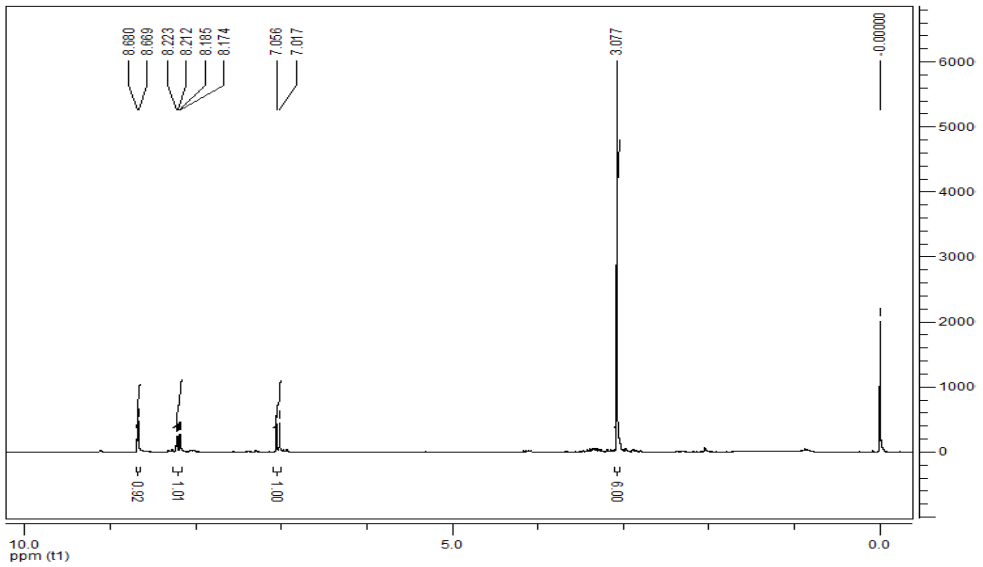
^{13}C-NMR

9. *N,N*-Dimethyl-2,4-dinitrobenzamide

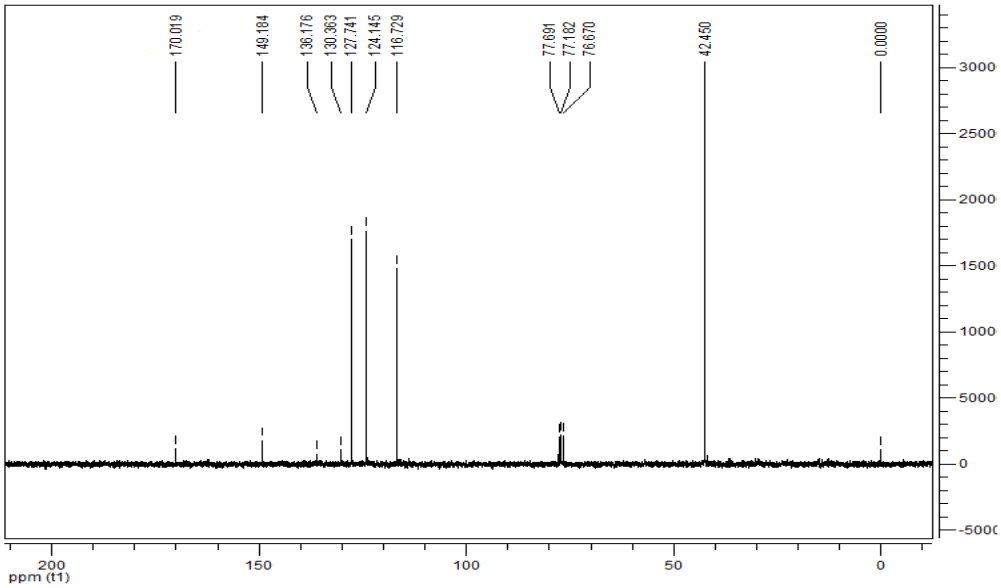


^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 3.07 (6H, s), 7.05 (1H, d, J = 9.7 Hz), 8.19 (1H, dd, J = 9.5 Hz, J′ = 2.7 Hz), 8.70 (1H, d, J = 2.7); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm):

42.4($\underline{C}H_3$), 116.7(Ar), 124.1(Ar), 127.7(Ar), 130.4(Ar), 136.2(Ar), 149.2(Ar), 170.0(C=O).

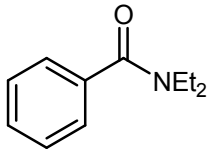


^{1}H-NMR



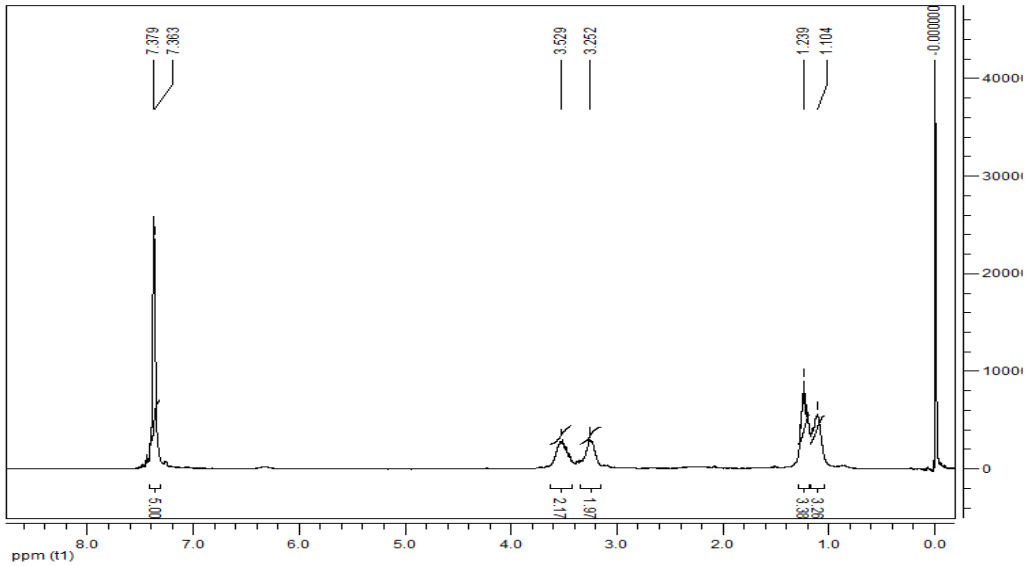
^{13}C-NMR

10. *N,N*-Diethylbenzamide

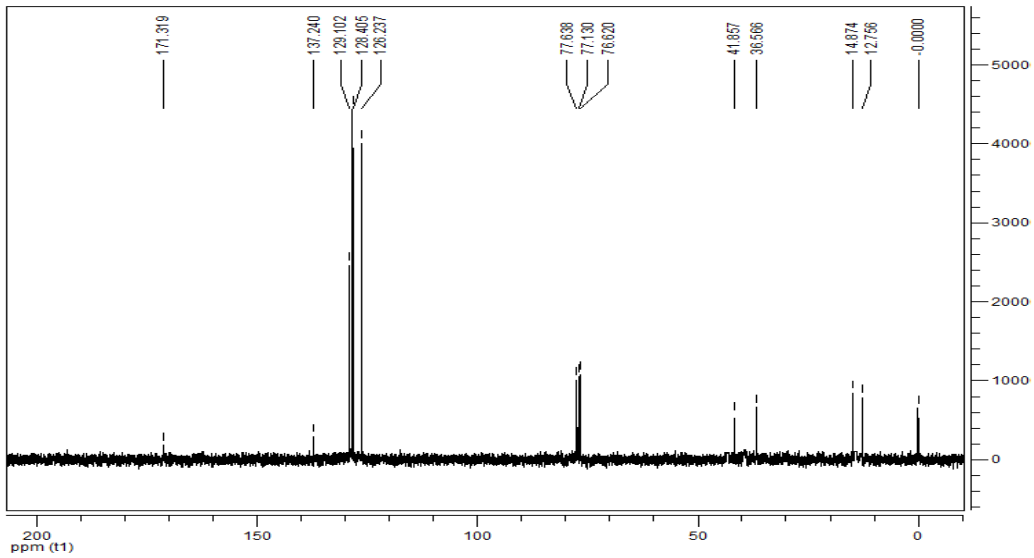


Yellow oil, ^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 1.10 (3H, unresolved triplet), 1.23 (3H, unresolved triplet), 3.25 (2H, unresolved broad band), 3.53 (2H, unresolved broad band),

7.36-7.38 (5H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 12.7($\underline{C}H_3$), 14.8($\underline{C}H_3$), 36.6($\underline{C}H_2$) 41.8($\underline{C}H_2$), 126.2(Ar), 128.4(Ar), 129.1(Ar), 137.2(Ar), 171.3($\underline{C}$=O).

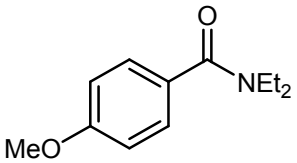


^{1}H-NMR



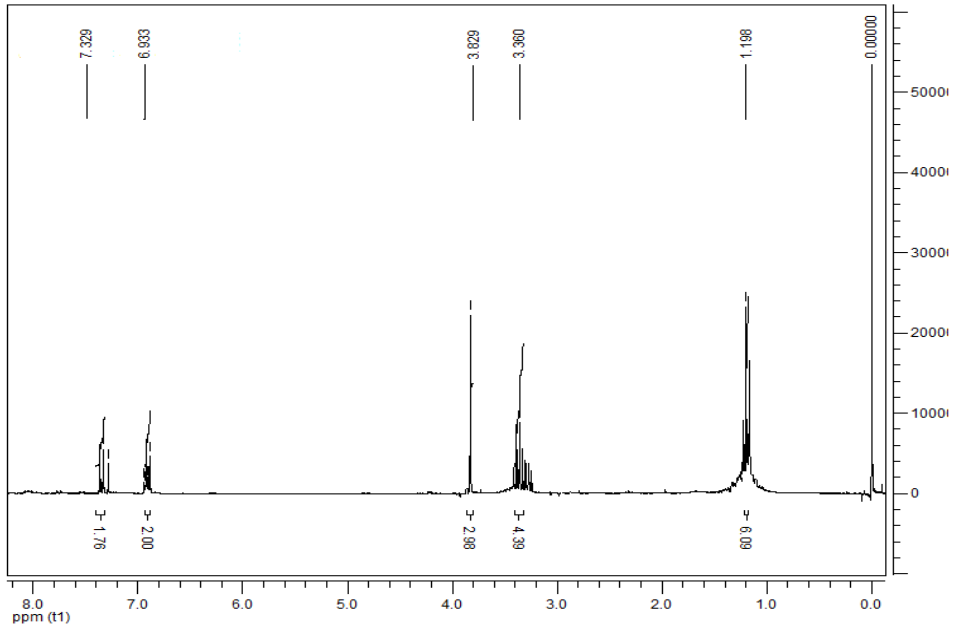
^{13}C-NMR

11. *N,N*-Diethyl-4-methoxybenzamide

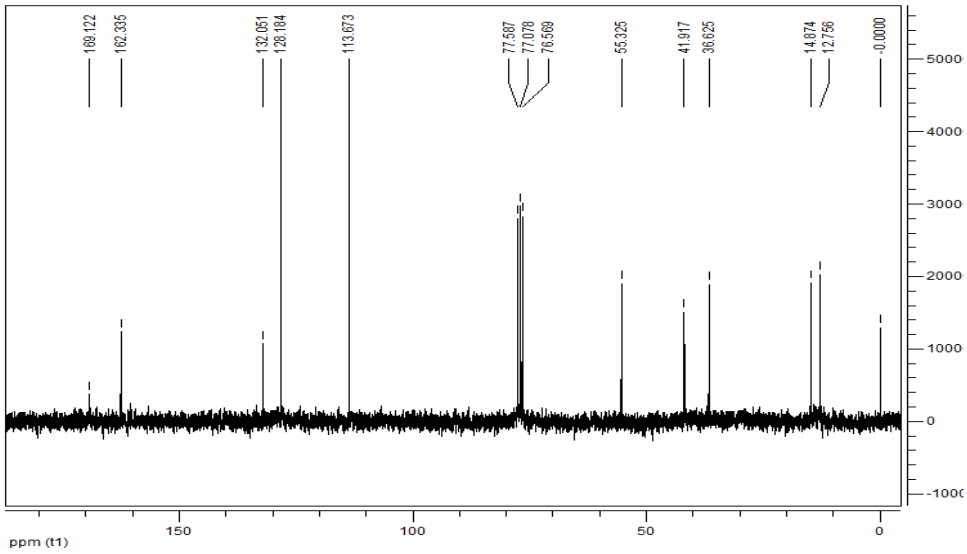


^{1}H-NMR (250 MHz $CDC1_3$) δ (ppm): 1.12 (6H, unresolved triplet), 3.36 (4H, unresolved broad band), 3.83 (3H, s), 6.93 (2H, m), 7.32 (2H, m); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm):

12.7($\underline{C}H_3$), 14.8($\underline{C}H_3$), 36.6($\underline{C}H_2$), 41.9($\underline{C}H_2$), 55.3($\underline{C}H_3O$), 113.7(Ar), 128.1(Ar), 132.0(Ar), 162.3(Ar), 169.1(Ar).



^{1}H-NMR



^{13}C-NMR